EMA workbench Documentation

Release 3.0.0

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GETTING STARTED

CHAPTER

ONE

EXPLORATORY MODELLING AND ANALYSIS (EMA) WORKBENCH

Exploratory Modeling and Analysis (EMA) is a research methodology that uses computational experiments to analyze complex and uncertain systems (Bankes, 1993). That is, exploratory modeling aims at offering computational decision support for decision making under deep uncertainty and Robust Decision Making.

The EMA workbench aims at providing support for performing exploratory modeling with models developed in various modelling packages and environments. Currently, the workbench offers connectors to Vensim, Netlogo, and Excel.

The EMA workbench offers support for designing experiments, performing the experiments - including support for parallel processing on both a single machine as well as on clusters-, and analysing the results. To get started, take a look at the high level overview, the tutorial, or dive straight into the details of the API. For a comparison between the workbench and rhodium, see *this discusion*.

1.1 A High Level Overview

- *Exploratory modeling framework*
- *Connectors*
- *Analysis*

1.1.1 Exploratory modeling framework

The core package contains the core functionality for setting up, designing, and performing series of computational experiments on one or more models simultaneously.

- Model (`ema_workbench.em_framework.model`): an abstract base class for specifying the interface to the model on which you want to perform exploratory modeling.
- Samplers (`ema_workbench.em_framework.samplers`): the various sampling techniques that are readily available in the workbench.
- Uncertainties (`ema_workbench.em_framework.parameters`): various types of parameter classes that can be used to specify the uncertainties and/or levers on the model
- Outcomes (`ema_workbench.em_framework.outcomes`): various types of outcome classes
- Evaluators (`ema_workbench.em_framework.evaluators`): various evaluators for running experiments in sequence or in parallel.

1.1.2 Connectors

The connectors package contains connectors to some existing simulation modeling environments. For each of these, a standard ModelStructureInterface class is provided that users can use as a starting point for specifying the interface to their own model.

- Vensim connector (`ema_workbench.connectors.vensim`): This enables controlling (e.g. setting parameters, simulation setup, run, get output, etc .) a simulation model that is built in Vensim software, and conducting an EMA study based on this model.
- Excel connector (*ema_workbench.connectors.excel*): This enables controlling models build in Excel.
- NetLogo connector (`ema_workbench.connectors.netlogo`): This enables controlling (e.g. setting parameters, simulation setup, run, get output, etc .) a simulation model that is built in NetLogo software, and conducting an EMA study based on this model.
- Simio connector (`ema_workbench.connectors.simio_connector`): This enables controlling models built in Simio
- Pysd connector (`ema_workbench.connectors.pysd_connector`)

1.1.3 Analysis

The analysis package contains a variety of analysis and visualization techniques for analyzing the results from the exploratory modeling. The analysis scripts are tailored for use in combination with the workbench, but they can also be used on their own with data generated in some other manner.

- Patient Rule Induction Method (*ema_workbench.analysis.prim*)
- Classification Trees (*ema_workbench.analysis.cart*)
- Logistic Regression (*ema_workbench.analysis.logistic_regression*)
- Dimensional Stacking (*ema_workbench.analysis.dimensional_stacking*)
- Feature Scoring (*ema_workbench.analysis.feature_scoring*)
- Regional Sensitivity Analysis (*ema_workbench.analysis.regional_sa*)
- various plotting functions for time series data (*ema_workbench.analysis.plotting*)
- pair wise plots (*ema_workbench.analysis.pairs_plotting*)
- parallel coordinate plots (*ema_workbench.analysis.parcoords*)
- support for converting figures to black and white (`ema_workbench.analysis.b_an_w_plotting`)

1.2 Installing the workbench

From version 2.5.0 the workbench requires Python 3.9 or higher. Version 2.0.0 to 2.4.x support Python 3.8+.

1.2.1 Regular installations

A stable version of the workbench can be installed via pip.

```
pip install ema_workbench
```

This installs the EMAworkbench together with all the bare necessities to run Python models.

If you want to upgrade the workbench from a previous version, add `-U` (or `--upgrade`) to the pip command.

```
pip install -U ema_workbench
```

We have a few more install options available, which install optional dependencies not always necessary but either nice to have or for specific functions. These can be installed with so called "extras" using pip.

Therefore we recommended installing with:

```
pip install -U ema_workbench[recommended]
```

Which currently includes everything needed to use the workbench in Jupyter notebooks, with interactive graphs and to successfully complete the tests with pytest.

However, the EMAworkbench can connect to many other simulation software, such as Netlogo, Simio, Vensim (pysd) and Vadere. For these there are also extras available:

```
pip install -U ema_workbench[netlogo,simio,pysd]
```

Note that the Netlogo and Simio extras need Windows as OS.

These extras can be combined. If you're going to work with Netlogo for example, you can do:

```
pip install -U ema_workbench[recommended,netlogo]
```

You can use `all` to install all dependencies, except the connectors. Prepare for a large install.

```
pip install -U ema_workbench[all]
```

These are all the extras that are available:

- `jupyter` installs `["jupyter", "jupyter_client", "ipython", "ipykernel"]`
- `dev` installs `["pytest", "jupyter_client", "ipyparallel"]`
- `cov` installs `["pytest-cov", "coverage", "coveralls"]`
- `docs` installs `["sphinx", "nbsphinx", "myst", "pyscaffold"]`
- `graph` installs `["altair", "pydot", "graphviz"]`
- `parallel` installs `["ipyparallel", "traitlets"]`
- `netlogo` installs `["jpype-1", "pynetlogo"]`
- `pysd` installs `["pysd"]`
- `simio` installs `["pythonnet"]`

Then `recommended` is currently equivalent to `jupyter,dev,graph` and `all` installs everything, except the connectors. These are defined in the `pyproject.toml` file.

1.2.2 Developer installations

As a developer you will want an edible install, in which you can modify the installation itself. This can be done by adding `-e` (for edible) to the pip command.

```
pip install -e ema_workbench
```

The latest commit on the master branch can be installed with:

```
pip install -e git+https://github.com/quaquel/EMAworkbench#egg=ema-workbench
```

Or any other (development) branch on this repo or your own fork:

```
pip install -e git+https://github.com/YOUR_FORK/EMAworkbench@YOUR_BRANCH#egg=ema-
↪workbench
```

The code is also available from github.

1.2.3 Limitations

Some connectors have specific limitations, listed below.

- Vensim only works on Windows. If you have 64-bit Vensim, you need 64-bit Python. If you have 32-bit Vensim, you will need 32-bit Python.
- Excel also only works on Windows.

1.3 Alternative packages

So how does the workbench differ from other open source tools available for exploratory modeling? In Python there is rhodium, in R there is the open MORDM toolkit, and there is also OpenMole. Below we discuss the key differences with rhodium. Given a lack of familiarity with the other tools, we wont comment on those.

1.3.1 The workbench versus rhodium

For Python, the main alternative tool is rhodium, which is part of Project Platypus. Project Platypus is a collection of libraries for doing many objective optimization (platypus-opt), setting up and performing simulation experiments (rhodium), and scenario discovery using the Patient Rule Induction Method (prim). The relationship between the workbench and the tools that form project platypus is a bit messy. For example, the workbench too relies on platypus-opt for many objective optimization, the PRIM package is a, by now very dated, fork of the prim code in the workbench, and both rhodium and the workbench rely on SALib for global sensitivity analysis. Moreover, the API of rhodium was partly inspired by an older version of the workbench, while new ideas from the rhodium API have in turned resulting in profound changes in the API of the workbench.

Currently, the workbench is still actively being developed. It is also not just used in teaching but also for research, and in practice by various organization globally. Moreover, the workbench is quite a bit more developed when it comes to providing off the shelf connectors for some popular modeling and simulation tools. Basically, everything that can be done with project Platypus can be done with the workbench and then the workbench offers additional functionality, a more up to date code base, and active support.

1.4 Changelog

All notable changes to this project will be documented in this file.

The format is based on Keep a Changelog, and this project adheres to Semantic Versioning.

1.4.1 2.5.1

The 2.5.1 release is a small patch release with two bugfixes.

- The first PR (#346) corrects a dependency issue where the finalizer in `futures_util.py` incorrectly assumed the presence of `experiment_runner` in its module namespace, leading to failures in futures models like multiprocessing and mpi. This is resolved by adjusting the finalizer function to expect `experiment_runner` as an argument.
- The second PR (#349) addresses a redundancy problem in the MPI evaluator, where the pool was inadvertently created twice.

What's Changed

Bugs fixed

- Fix finalizer dependency on global experiment_runner by @quaquel in https://github.com/quaquel/EMAworkbench/pull/346
- bug fix in MPI evaluator by @quaquel in https://github.com/quaquel/EMAworkbench/pull/349

Full Changelog: https://github.com/quaquel/EMAworkbench/compare/2.5.0...2.5.1

1.4.2 2.5.0

Highlights

In the 2.5.0 release of the EMAworkbench we introduce a new experimental MPIevaluator to run on multi-node (HPC) systems (#299, #328). We would love feedback on it in #311.

Furthermore, the pair plots for scenario discovery now allow contour plots and bivariate histograms (#288). When doing Prim you can inspect multiple boxed and display them in a single figure (#317).

Breaking changes

From 3.0 onwards, the names of parameters, constants, constraints, and outcomes must be valid python identifiers. From this version onwards, a DeprecationWarning is raised if the name is not a valid Python identifier.

What's Changed

New features added

- Improved pair plots for scenario discovery by @steipatr in https://github.com/quaquel/EMAworkbench/pull/288
- Introducing MPIEvaluator: Run on multi-node HPC systems using mpi4py by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/299
- inspect multiple boxes and display them in a single figure by @quaquel in https://github.com/quaquel/EMAworkbench/pull/317

Enhancements made

- Enhancement for #271: raise exception by @quaquel in https://github.com/quaquel/EMAworkbench/pull/282
- em_framework/points: Add string representation to Experiment class by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/297
- Speed up of plot_discrete_cdfs by 2 orders of magnitude by @quaquel in https://github.com/quaquel/EMAworkbench/pull/306
- em_framework: Improve log messages, warning and errors by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/300
- analysis: Improve log messages, warning and errors by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/313
- change to log message and log level in feature scoring by @quaquel in https://github.com/quaquel/EMAworkbench/pull/318
- [WIP] MPI update by @quaquel in https://github.com/quaquel/EMAworkbench/pull/328

Bugs fixed

- Fix search in Readthedocs configuration with workaround by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/264
- bugfix introduced by #241 in general-introduction from docs by @quaquel in https://github.com/quaquel/EMAworkbench/pull/265
- prim: Replace deprecated Altair function by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/270
- bugfix to rebuild_platypus_population by @quaquel in https://github.com/quaquel/EMAworkbench/pull/276
- bugfix for #277 : load_results properly handles experiments dtypes by @quaquel in https://github.com/quaquel/EMAworkbench/pull/280
- fixes a bug where binomtest fails because of floating point math by @quaquel in https://github.com/quaquel/EMAworkbench/pull/315
- make workbench compatible with latest version of pysd by @quaquel in https://github.com/quaquel/EMAworkbench/pull/336
- bugfixes for string vs bytestring by @quaquel in https://github.com/quaquel/EMAworkbench/pull/339

Documentation improvements

- Drop Python 3.8 support, require 3.9+ by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/259
- readthedocs: Add search ranking and use latest Python version by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/242
- docs/examples: Always use n_processes=-1 in MultiprocessingEvaluator by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/278
- Docs: Add MPIEvaluator tutorial for multi-node HPC systems, including DelftBlue by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/308
- Add Mesa example by @steipatr in https://github.com/quaquel/EMAworkbench/pull/335
- Fix htmltheme of docs by @quaquel in https://github.com/quaquel/EMAworkbench/pull/342

Maintenance

- CI: Switch default jobs to Python 3.12 by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/314
- Reorganization of evaluator code and renaming of modules by @quaquel in https://github.com/quaquel/EMAworkbench/pull/320
- Replace deprecated zmq.eventloop.ioloop with Tornado's ioloop by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/334

Other changes

- examples: Speedup the lake_problem function by ~30x by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/301
- Create an GitHub issue chooser by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/331
- Depracation warning for parameter names not being valid python identifiers by @quaquel in https://github.com/quaquel/EMAworkbench/pull/337

Full Changelog: https://github.com/quaquel/EMAworkbench/compare/2.4.0...2.5.0

1.4.3 2.4.1

Highlights

2.4.1 is a small patch release of the EMAworkbench, primarily resolving issues #276 and #277 in the workbench itself, and a bug introduced by #241 in the docs. The EMAworkbench now also raise exception when sampling scenarios or policies while no uncertainties or levers are defined (#282).

What's Changed

Enhancements made

- Enhancement for #271: raise exception by @quaquel in https://github.com/quaquel/EMAworkbench/pull/282

Bugs fixed

- bugfix to `rebuild_platypus_population` by @quaquel in https://github.com/quaquel/EMAworkbench/pull/276
- Fixed dtype handling in `load_results` function. The dtype metadata is now correctly applied, resolving issue #277.
- Fixed the documentation bug introduced by #241 in the general introduction section, which now accurately reflects the handling of categorical uncertainties in the experiment dataframe.

Documentation improvements

- readthedocs: Add search ranking and use latest Python version by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/242
- docs/examples: Always use `n_processes=-1` in MultiprocessingEvaluator by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/278

1.4.4 2.4.0

Highlights

The latest release of the EMAworkbench introduces significant performance improvements and quality of life updates. The performance of `_store_outcomes` has been enhanced by approximately 35x in pull request #232, while the `combine` function has seen a 8x speedup in pull request #233. This results in the overhead of the EMAworkbench being reduced by over 70%. In a benchmark, a very simple Python model now performs approximately 40.000 iterations per second, compared to 15.000 in 2.3.0.

In addition to these performance upgrades, the examples have been added to the ReadTheDocs documentation, more documentation improvements have been made and many bugs and deprecations have been fixed.

The 2.4.x release series requires Python 3.8 and is tested on 3.8 to 3.11. It's the last release series supporting Python 3.8. It can be installed as usual via PyPI, with:

```
pip install --upgrade ema-workbench
```

What's Changed

New features added

- optional preallocation in callback based on outcome shape and type by @quaquel in https://github.com/quaquel/EMAworkbench/pull/229

Enhancements made

- util: Speed up `combine` by ~8x by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/233
- callbacks: Improve performance of _store_outcomes by ~35x by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/232

Bugs fixed

- fixes broken link to installation instructions by @quaquel in https://github.com/quaquel/EMAworkbench/pull/224
- Docs: Fix developer installation commands by removing a space by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/220
- fixes a bug where Prim modifies the experiments array by @quaquel in https://github.com/quaquel/EMAworkbench/pull/228
- bugfix for warning on number of processes and max_processes by @quaquel in https://github.com/quaquel/EMAworkbench/pull/234
- Fix deprecation warning and dtype issue in flu_example.py by @quaquel in https://github.com/quaquel/EMAworkbench/pull/235
- test for get_results and categorical fix by @quaquel in https://github.com/quaquel/EMAworkbench/pull/241
- Fix `pynetlogo` imports by decapitalizing `pyNetLogo` by @quaquel in https://github.com/quaquel/EMAworkbench/pull/248
- change default value of um_p to be consistent with Borg documentation by @irene-sophia in https://github.com/quaquel/EMAworkbench/pull/250
- Fix pretty print for RealParameter and IntegerParameter by @quaquel in https://github.com/quaquel/EMAworkbench/pull/255
- Fix bug in AutoadaptiveOutputSpaceExploration with wrong default probabilities by @quaquel in https://github.com/quaquel/EMAworkbench/pull/252

Documentation improvements

- Parallexaxis doc by @quaquel in https://github.com/quaquel/EMAworkbench/pull/249
- Examples added to the docs by @quaquel in https://github.com/quaquel/EMAworkbench/pull/244

Maintenance

- clusterer: Update AgglomerativeClustering keyword to fix deprecation by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/218
- Fix Matplotlib and SciPy deprecations by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/227
- CI: Add job that runs tests with pre-release dependencies by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/217
- Fix for stalling tests by @quaquel in https://github.com/quaquel/EMAworkbench/pull/247

Other changes

- add `metric` argument to allow for other linkages by @mikhailsirenko in https://github.com/quaquel/EMAworkbench/pull/222

New Contributors

- @mikhailsirenko made their first contribution in https://github.com/quaquel/EMAworkbench/pull/222
- @irene-sophia made their first contribution in https://github.com/quaquel/EMAworkbench/pull/250

Full Changelog: https://github.com/quaquel/EMAworkbench/compare/2.3.0...2.4.0

1.4.5 2.3.0

Highlights

This release adds a new algorithm for output space exploration. The way in which convergence tracking for optimization is supported has been overhauled completely, see the updated directed search user guide for full details. The documentation has moreover been expanded with a comparison to Rhodium.

With this new release, the installation process has been improved by reducing the number of required dependencies. Recommended packages and connectors can now be installed as *extras* using pip, for example `pip install -U ema-workbench[recommended,netlogo]`. See the updated installation instructions for all options and details.

The 2.3.x release series supports Python 3.8 to 3.11. It can be installed as usual via PyPI, with:

```
pip install --upgrade ema-workbench
```

What's Changed

New features added

- Output space exploration by @quaquel in https://github.com/quaquel/EMAworkbench/pull/170
- Convergence tracking by @quaquel in https://github.com/quaquel/EMAworkbench/pull/193

Enhancements made

- Switch to using format string in prim logging by @quaquel in https://github.com/quaquel/EMAworkbench/pull/161
- Replace setup.py with pyproject.toml and implement optional dependencies by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/166

Bugs fixed

- use masked arrays for storing outcomes by @quaquel in https://github.com/quaquel/EMAworkbench/pull/176
- Fix error for negative `n_processes` input in MultiprocessingEvaluator by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/189
- optimization.py: Fix "epsilons" keyword argument in `_optimize()` by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/150

Documentation improvements

- Create initial CONTRIBUTING.md documentation by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/162
- Create Read the Docs yaml configuration by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/173
- update to outcomes documentation by @quaquel in https://github.com/quaquel/EMAworkbench/pull/183
- Improved directed search tutorial by @quaquel in https://github.com/quaquel/EMAworkbench/pull/194
- Update Contributing.md with instructions how to merge PRs by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/200
- Update Readme with an introduction and documentation, installation and contribution sections by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/199
- Rhodium docs by @quaquel in https://github.com/quaquel/EMAworkbench/pull/184
- Fix spelling mistakes by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/195

Maintenance

- Replace depreciated `shade` keyword in Seaborn kdeplot with `fill` by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/169
- CI: Add pip depencency caching, don't run on doc changes, update setup-python to v4 by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/174
- Formatting: Format with Black, increase max line length to 100, combine multi-line blocks by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/178
- Add pre-commit configuration and auto update CI by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/181
- Fix Matplotlib, ipyparallel and dict deprecation warnings by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/202
- CI: Start testing on Python 3.11 by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/156
- Replace deprecated `saltelli` with `sobol` SALib 1.4.6+. by @quaquel in https://github.com/quaquel/EMAworkbench/pull/211

Other changes

- Adds CITATION.cff by @quaquel in https://github.com/quaquel/EMAworkbench/pull/209

Full Changelog: https://github.com/quaquel/EMAworkbench/compare/2.2.0...2.3

1.4.6 2.2.0

Highlights

With the 2.2 release, the EMAworkbench can now connect to Vadere models on pedestrian dynamics. When inspecting a Prim Box peeling trajectory, multiple points on the peeling trajectory can be inspected simultaneously by inputting a list of integers into `PrimBox.inspect()`.

When running experiments with multiprocessing using the `MultiprocessingEvaluator`, the number of processes can now be controlled using a negative integer as input for `n_processes` (for example, `-2` on a 12-thread CPU results in 10 threads used). Also, it will now default to max. 61 processes on windows machines due to limitations inherent in Windows in dealing with higher processor counts. Code quality, CI, and error reporting also have been improved. And finally, generating these release notes is now automated.

What's Changed

New features added

- Vadere model connector by @floristevito in https://github.com/quaquel/EMAworkbench/pull/145

Enhancements made

- Improve code quality with static analysis by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/119
- prim.py: Make `PrimBox.peeling_trajectory["id"]` int instead of float by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/121
- analysis: Allow optional annotation of plot_tradeoff graphs by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/123
- evaluators.py: Allow MultiprocessingEvaluator to initialize with cpu_count minus N processes by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/140
- `PrimBox.inspect()` now can also take a list of integers (aside from a single int) to inspect multiple points at once by @quaquel in https://github.com/quaquel/EMAworkbench/commit/6d83a6c33442ad4dce0974a384b03a225aaf830d (see also issue https://github.com/quaquel/EMAworkbench/issues/124)

Bugs fixed

- fixed typo in lake_model.py by @JeffreyDillonLyons in https://github.com/quaquel/EMAworkbench/pull/136

Documentation improvements

- Docs: Installation.rst: Add how to install master or custom branch by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/122
- Docs: Replace all http links with secure https URLs by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/134
- Maintain release notes at CHANGELOG.md and include them in Readthedocs by @quaquel in https://github.com/quaquel/EMAworkbench/commit/ebdbc9f5c77693fc75911ead472b420065dfe2aa
- Fix badge links in readme by @quaquel in https://github.com/quaquel/EMAworkbench/commit/28569bdcb149c070c32958996917

Maintenance

- feature_scoring: fix Regressor criterion depreciation by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/125
- feature_scoring.py: Change `max_features` in get_rf_feature_scores to `"sqrt"` by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/129
- CI: Use Pytest instead of Nose, update default build to Python 3.10 by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/131
- Release CI: Only upload packages if on main repo by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/132
- CI: Split off flake8 linting in a separate job by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/133
- CI: Add weekly scheduled jobs and manual trigger by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/137
- setup.py: Add `project_urls` for documentation and issue tracker links by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/142
- set scikit-learn requirement >= 1.0.0 by @rhysits in https://github.com/quaquel/EMAworkbench/pull/144
- Create release.yml file for automatic release notes generation by @EwoutH in https://github.com/quaquel/EMAworkbench/pull/152
- instantiating an Evaluator without one or more AbstractModel instances now raises a type error by @quaquel in https://github.com/quaquel/EMAworkbench/commit/a83533aa8166ca2414137cdfc3125a53ee3697ec
- removes depreciated DataFrame.append by replacing it with DataFrame.concat (see the conversation on issue https://github.com/quaquel/EMAworkbench/issues/126):
  - from feature scoring by @quaquel in https://github.com/quaquel/EMAworkbench/commit/8b8bfe41733e49b75c01e34b75563
  - from logistic_regression.py by @quaquel in https://github.com/quaquel/EMAworkbench/commit/255e3d6d9639dfe6fd4e797
- removes NumPy datatypes deprecated in 1.20 by @quaquel in https://github.com/quaquel/EMAworkbench/commit/e8fbf6fc64f14b
- replace deprecated scipy.stats.kde with scipy.stats by @quaquel in https://github.com/quaquel/EMAworkbench/commit/b5a9ca9677

New Contributors

- @JeffreyDillonLyons made their first contribution in https://github.com/quaquel/EMAworkbench/pull/136
- @rhysits made their first contribution in https://github.com/quaquel/EMAworkbench/pull/144
- @floristevito made their first contribution in https://github.com/quaquel/EMAworkbench/pull/145

Full Changelog: https://github.com/quaquel/EMAworkbench/compare/2.1.2...2.2.0

1.5 Tutorials

The code of these examples can be found in the examples package. The first three examples are meant to illustrate the basics of the EMA workbench. How to implement a model, specify its uncertainties and outcomes, and run it. The fourth example is a more extensive illustration based on Pruyt & Hamarat (2010). It shows some more advanced possibilities of the EMA workbench, including one way of handling policies.

- *A simple model in Python*
- *A simple model in Vensim*
- *A simple model in Excel*
- *A more elaborate example: Mexican Flu*

1.5.1 A simple model in Python

The simplest case is where we have a model available through a python function. For example, imagine we have the simple model.

```
def some_model(x1=None, x2=None, x3=None):
    return {'y':x1*x2+x3}
```

In order to control this model from the workbench, we can make use of the *Model*. We can instantiate a model object, by passing it a name, and the function.

```
model = Model('simpleModel', function=some_model) #instantiate the model
```

Next, we need to specify the uncertainties and the outcomes of the model. In this case, the uncertainties are x1, x2, and x3, while the outcome is y. Both uncertainties and outcomes are attributes of the model object, so we can say

```
#specify uncertainties
model.uncertainties = [RealParameter("x1", 0.1, 10),
                       RealParameter("x2", -0.01,0.01),
                       RealParameter("x3", -0.01,0.01)]
#specify outcomes
model.outcomes = [ScalarOutcome('y')]
```

Here, we specify that x1 is some value between 0.1, and 10, while both x2 and x3 are somewhere between -0.01 and 0.01. Having implemented this model, we can now investigate the model behavior over the set of uncertainties by simply calling

```
results = perform_experiments(model, 100)
```

The function `perform_experiments()` takes the model we just specified and will execute 100 experiments. By default, these experiments are generated using a Latin Hypercube sampling, but Monte Carlo sampling and Full factorial sampling are also readily available. Read the documentation for `perform_experiments()` for more details.

The complete code:

```
"""
Created on 20 dec. 2010

This file illustrated the use the EMA classes for a contrived example
It's main purpose has been to test the parallel processing functionality

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
"""

from ema_workbench import Model, RealParameter, ScalarOutcome, ema_logging, perform_
↪experiments


def some_model(x1=None, x2=None, x3=None):
    return {"y": x1 * x2 + x3}


if __name__ == "__main__":
    ema_logging.LOG_FORMAT = "[%(name)s/%(levelname)s/%(processName)s] %(message)s"
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = Model("simpleModel", function=some_model)  # instantiate the model

    # specify uncertainties
    model.uncertainties = [
        RealParameter("x1", 0.1, 10),
        RealParameter("x2", -0.01, 0.01),
        RealParameter("x3", -0.01, 0.01),
    ]
    # specify outcomes
    model.outcomes = [ScalarOutcome("y")]

    results = perform_experiments(model, 100)
```

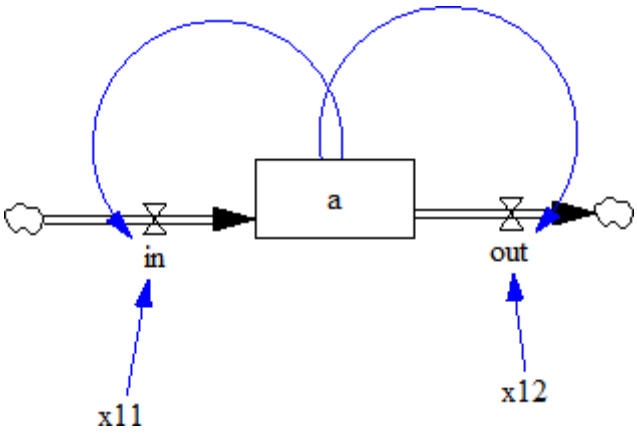
1.5.2 A simple model in Vensim

Imagine we have a very simple Vensim model:

For this example, we assume that 'x11' and 'x12' are uncertain. The state variable 'a' is the outcome of interest. Similar to the previous example, we have to first instantiate a vensim model object, in this case `VensimModel`. To this end, we need to specify the directory in which the vensim file resides, the name of the vensim file and the name of the model.

```
wd = r'./models/vensim example'
model = VensimModel("simpleModel", wd=wd, model_file=r'\model.vpm')
```

Next, we can specify the uncertainties and the outcomes.




```
model.uncertainties = [RealParameter("x11", 0, 2.5),
                       RealParameter("x12", -2.5, 2.5)]


model.outcomes = [TimeSeriesOutcome('a')]
```

Note that we are using a TimeSeriesOutcome, because vensim results are time series. We can now simply run this model by calling `perform_experiments()`.

```
with MultiprocessingEvaluator(model) as evaluator:
results = evaluator.perform_experiments(1000)
```

We now use a evaluator, which ensures that the code is executed in parallel.

Is it generally good practice to first run a model a small number of times sequentially prior to running in parallel. In this way, bugs etc. can be spotted more easily. To further help with keeping track of what is going on, it is also good practice to make use of the logging functionality provided by the workbench

```
ema_logging.log_to_stderr(ema_logging.INFO)
```

Typically, this line appears at the start of the script. When executing the code, messages on progress or on errors will be shown.

The complete code

```
"""
Created on 3 Jan. 2011

This file illustrated the use the EMA classes for a contrived vensim
example


.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                chamarat <c.hamarat (at) tudelft (dot) nl>
"""

from ema_workbench import TimeSeriesOutcome, perform_experiments, RealParameter, ema_
↪logging
```

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```

from ema_workbench.connectors.vensim import VensimModel

if __name__ == "__main__":
    # turn on logging
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate a model
    wd = "./models/vensim example"
    vensimModel = VensimModel("simpleModel", wd=wd, model_file="model.vpm")
    vensimModel.uncertainties = [RealParameter("x11", 0, 2.5), RealParameter("x12", -2.5,
↪ 2.5)]

    vensimModel.outcomes = [TimeSeriesOutcome("a")]

    results = perform_experiments(vensimModel, 1000)
```

1.5.3 A simple model in Excel

In order to perform EMA on an Excel model, one can use the `ExcelModel`. This base class makes uses of naming cells in Excel to refer to them directly. That is, we can assume that the names of the uncertainties correspond to named cells in Excel, and similarly, that the names of the outcomes correspond to named cells or ranges of cells in Excel. When using this class, make sure that the decimal separator and thousands separator are set correctly in Excel. This can be checked via file > options > advanced. These separators should follow the anglo saxon convention.

```
"""
Created on 27 Jul. 2011

This file illustrated the use the EMA classes for a model in Excel.

It used the excel file provided by
`A. Sharov <https://home.comcast.net/~sharov/PopEcol/lec10/fullmod.html>`_

This excel file implements a simple predator prey model.

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
"""

from ema_workbench import RealParameter, TimeSeriesOutcome, ema_logging, perform_
↪experiments

from ema_workbench.connectors.excel import ExcelModel
from ema_workbench.em_framework.evaluators import MultiprocessingEvaluator

if __name__ == "__main__":
    ema_logging.log_to_stderr(level=ema_logging.INFO)

    model = ExcelModel("predatorPrey", wd="./models/excelModel", model_file="excel␣
↪example.xlsx")
    model.uncertainties = [
        RealParameter("K2", 0.01, 0.2),
```

(continues on next page)

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```
        # we can refer to a cell in the normal way
        # we can also use named cells
        RealParameter("KKK", 450, 550),
        RealParameter("rP", 0.05, 0.15),
        RealParameter("aaa", 0.00001, 0.25),
        RealParameter("tH", 0.45, 0.55),
        RealParameter("kk", 0.1, 0.3),
    ]

    # specification of the outcomes
    model.outcomes = [
        TimeSeriesOutcome("B4:B1076"),
        # we can refer to a range in the normal way
        TimeSeriesOutcome("P_t"),
    ]  # we can also use named range

    # name of the sheet
    model.default_sheet = "Sheet1"

    with MultiprocessingEvaluator(model) as evaluator:
        results = perform_experiments(model, 100, reporting_interval=1,␣
↪evaluator=evaluator)
```

The example is relatively straight forward. We instantiate an excel model, we specify the uncertainties and the outcomes. We also need to specify the sheet in excel on which the model resides. Next we can call `perform_experiments()`.

Warning: when using named cells. Make sure that the names are defined at the sheet level and not at the workbook level

1.5.4 A more elaborate example: Mexican Flu

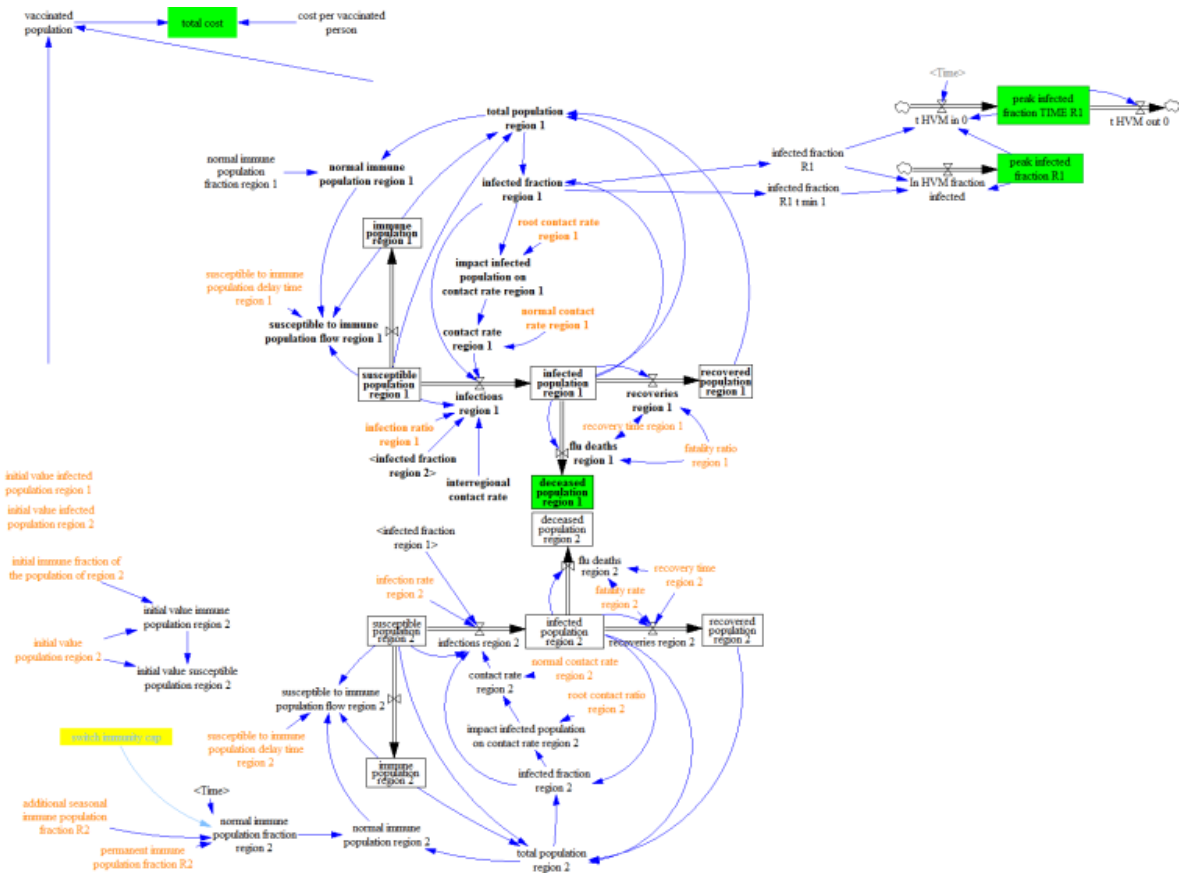
This example is derived from Pruyt & Hamarat (2010). This paper presents a small exploratory System Dynamics model related to the dynamics of the 2009 flu pandemic, also known as the Mexican flu, swine flu, or A(H1N1)v. The model was developed in May 2009 in order to quickly foster understanding about the possible dynamics of this new flu variant and to perform rough-cut policy explorations. Later, the model was also used to further develop and illustrate Exploratory Modelling and Analysis.

Mexican Flu: the basic model

In the first days, weeks and months after the first reports about the outbreak of a new flu variant in Mexico and the USA, much remained unknown about the possible dynamics and consequences of the at the time plausible/imminent epidemic/pandemic of the new flu variant, first known as Swine or Mexican flu and known today as Influenza A(H1N1)v.

The exploratory model presented here is small, simple, high-level, data-poor (no complex/special structures nor detailed data beyond crude guestimates), and history-poor.

The modelled world is divided in three regions: the Western World, the densely populated Developing World, and the scarcely populated Developing World. Only the two first regions are included in the model because it is assumed that the scarcely populated regions are causally less important for dynamics of flu pandemics. Below, the figure shows the basic stock-and-flow structure. For a more elaborate description of the model, see Pruyt & Hamarat (2010).


vaccinated population
total cost
cost per vaccinated person
total population region 1
normal immune population fraction region 1
normal immune population region 1
infected fraction region 1
immune population region 1
root contact rate region 1
impact infected population on contact rate region 1
susceptible to immune population delay time region 1
susceptible to immune population flow region 1
normal contact rate region 1
contact rate region 1
susceptible population region 1
infectious region 1
infected population region 1
recoveries region 1
recovered population region 1
infection ratio region 1
<infected fraction region 2>
recovery rate region 1
flu deaths region 1
fatality ratio region 1
interregional contact rate
deceased population region 1
deceased population region 2
initial value infected population region 1
initial value infected population region 2
initial immune fraction of the population of region 2
initial value immune population region 2
initial value population region 2
initial value susceptible population region 2
<infected fraction region 1>
infection rate region 2
flu deaths region 2
recovery time region 2
fatality rate region 2
susceptible population region 2
infections region 2
infected population region 2
recoveries region 2
recovered population region 2
normal contact rate region 2
contact rate region 2
root contact ratio region 2
susceptible to immune population flow region 2
impact infected population on contact rate region 2
susceptible to immune population delay time region 2
switch immunity cap
immune population region 2
infected fraction region 2
<Time>
additional seasonal immune population fraction R2
normal immune population fraction region 2
permanent immune population fraction R2
normal immune population region 2
total population region 2
<Time>
t HVM in 0
peak infected fraction TIME R1
t HVM out 0
infected fraction R1
infected fraction R1 t min 1
ln HVM fraction infected
peak infected fraction R1

Given the various uncertainties about the exact characteristics of the flu, including its fatality rate, the contact rate, the susceptibility of the population, etc. the flu case is an ideal candidate for EMA. One can use EMA to explore the kinds of dynamics that can occur, identify undesirable dynamic, and develop policies targeted at the undesirable dynamics.

In the original paper, Pruyt & Hamarat (2010). recoded the model in Python and performed the analysis in that way. Here we show how the EMA workbench can be connected to Vensim directly.

The flu model was build in Vensim. We can thus use `VensimModelS` as a base class.

We are interested in two outcomes:

- **deceased population region 1**: the total number of deaths over the duration of the simulation.
- **peak infected fraction**: the fraction of the population that is infected.

These are added to `self.outcomes`, using the TimeSeriesOutcome class.

The table below is adapted from Pruyt & Hamarat (2010). It shows the uncertainties, and their bounds. These are added to `self.uncertainties` as `ParameterUncertainty` instances.

Parameter	Lower Limit	Upper Limit
additional seasonal immune population fraction region 1	0.0	0.5
additional seasonal immune population fraction region 2	0.0	0.5
fatality ratio region 1	0.0001	0.1
fatality ratio region 2	0.0001	0.1
initial immune fraction of the population of region 1	0.0	0.5
initial immune fraction of the population of region 2	0.0	0.5
normal interregional contact rate	0.0	0.9
permanent immune population fraction region 1	0.0	0.5
permanent immune population fraction region 2	0.0	0.5
recovery time region 1	0.2	0.8
recovery time region 2	0.2	0.8
root contact rate region 1	1.0	10.0
root contact rate region 2	1.0	10.0
infection ratio region 1	0.0	0.1
infection ratio region 2	0.0	0.1
normal contact rate region 1	10	200
normal contact rate region 2	10	200

Together, this results in the following code:

```
"""
Created on 20 May, 2011

This module shows how you can use vensim models directly
instead of coding the model in Python. The underlying case
is the same as used in fluExample

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                epruyt <e.pruyt (at) tudelft (dot) nl>
"""

from ema_workbench import (
    RealParameter,
    TimeSeriesOutcome,
```

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```
    ema_logging,
    perform_experiments,
    MultiprocessingEvaluator,
    save_results,
)

from ema_workbench.connectors.vensim import VensimModel

if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = VensimModel("fluCase", wd=r"./models/flu", model_file=r"FLUvensimV1basecase.
↪vpm")

    # outcomes
    model.outcomes = [
        TimeSeriesOutcome(
            "deceased_population_region_1", variable_name="deceased population region 1"
        ),
        TimeSeriesOutcome("infected_fraction_R1", variable_name="infected fraction R1"),
    ]

    # Plain Parametric Uncertainties
    model.uncertainties = [
        RealParameter(
            "additional_seasonal_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R1",
        ),
        RealParameter(
            "additional_seasonal_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R2",
        ),
        RealParameter(
            "fatality_ratio_region_1", 0.0001, 0.1, variable_name="fatality ratio region␣
↪1"
        ),
        RealParameter(
            "fatality_rate_region_2", 0.0001, 0.1, variable_name="fatality rate region 2"
        ),
        RealParameter(
            "initial_immune_fraction_of_the_population_of_region_1",
            0,
            0.5,
            variable_name="initial immune fraction of the population of region 1",
        ),
        RealParameter(
            "initial_immune_fraction_of_the_population_of_region_2",
            0,
```

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```
            0.5,
            variable_name="initial immune fraction of the population of region 2",
        ),
        RealParameter(
            "normal_interregional_contact_rate",
            0,
            0.9,
            variable_name="normal interregional contact rate",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="permanent immune population fraction R1",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="permanent immune population fraction R2",
        ),
        RealParameter("recovery_time_region_1", 0.1, 0.75, variable_name="recovery time region 1"),
        RealParameter("recovery_time_region_2", 0.1, 0.75, variable_name="recovery time region 2"),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_1",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 1",
        ),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_2",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 2",
        ),
        RealParameter(
            "root_contact_rate_region_1", 0.01, 5, variable_name="root contact rate region 1"
        ),
        RealParameter(
            "root_contact_ratio_region_2", 0.01, 5, variable_name="root contact ratio region 2"
        ),
        RealParameter(
            "infection_ratio_region_1", 0, 0.15, variable_name="infection ratio region 1"
        ),
        RealParameter("infection_rate_region_2", 0, 0.15, variable_name="infection rate region 2"),
        RealParameter(
            "normal_contact_rate_region_1", 10, 100, variable_name="normal contact rate
```

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```
↪region 1"
        ),
        RealParameter(
            "normal_contact_rate_region_2", 10, 200, variable_name="normal contact rate␣
↪region 2"
        ),
    ]

    nr_experiments = 1000
    with MultiprocessingEvaluator(model) as evaluator:
        results = perform_experiments(model, nr_experiments, evaluator=evaluator)

    save_results(results, "./data/1000 flu cases no policy.tar.gz")
```

We have now instantiated the model, specified the uncertain factors and outcomes and run the model. We now have generated a dataset of results and can proceed to analyse the results using various analysis scripts. As a first step, one can look at the individual runs using a line plot using `lines()`. See `plotting` for some more visualizations using results from performing EMA on `FluModel`.

```
import matplotlib.pyplot as plt
from ema_workbench.analysis.plotting import lines

figure = lines(results, density=True) #show lines, and end state density
plt.show() #show figure
```

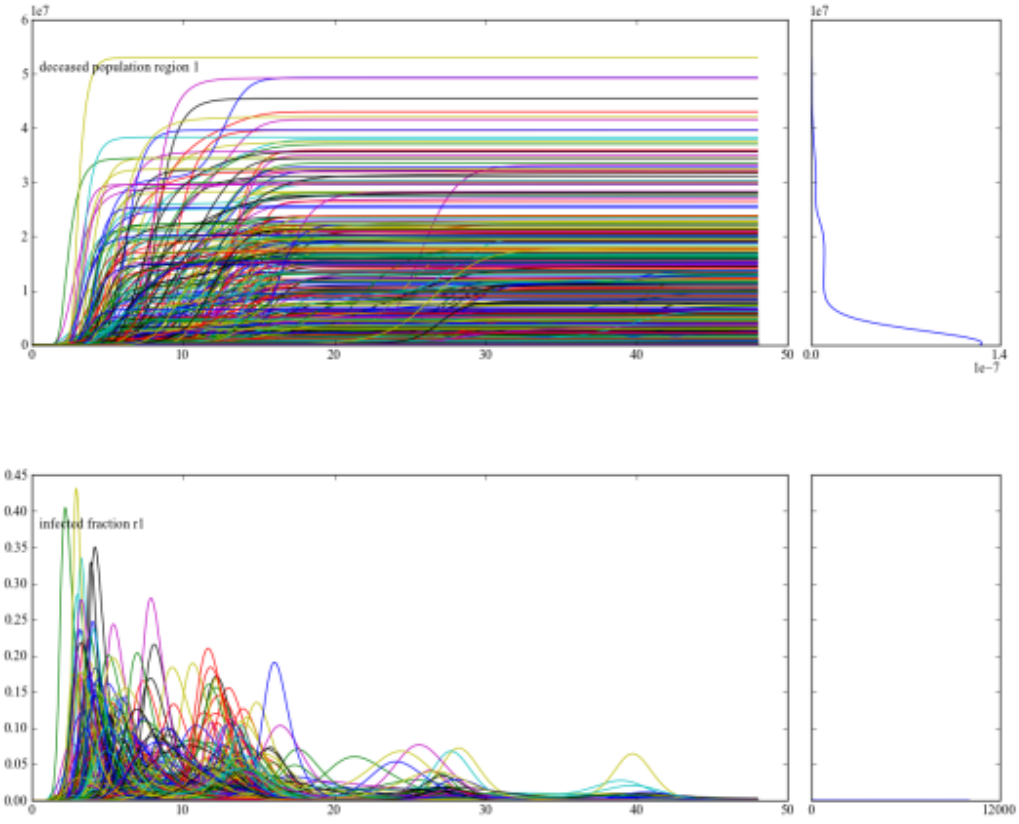
generates the following figure:

From this figure, one can deduce that across the ensemble of possible futures, there is a subset of runs with a substantial amount of deaths. We can zoom in on those cases, identify their conditions for occurring, and use this insight for policy design.

For further analysis, it is generally convenient, to generate the results for a series of experiments and save these results. One can then use these saved results in various analysis scripts.

```
from ema_workbench import save_results
save_results(results, './1000 runs.tar.gz')
```

The above code snippet shows how we can use `save_results()` for saving the results of our experiments. `save_results()` stores the as csv files in a tarball.


1e7
deceased population region 1
1e7
1e−7
infected fraction r1

Mexican Flu: policies

For this paper, policies were developed by using the system understanding of the analysts.

static policy

adaptive policy

running the policies

In order to be able to run the models with the policies and to compare their results with the no policy case, we need to specify the policies

```
#add policies
policies = [Policy('no policy',
                   model_file=r'/FLUvensimV1basecase.vpm'),
            Policy('static policy',
                   model_file=r'/FLUvensimV1static.vpm'),
            Policy('adaptive policy',
                   model_file=r'/FLUvensimV1dynamic.vpm')
            ]
```

In this case, we have chosen to have the policies implemented in separate vensim files. Policies require a name, and can take any other keyword arguments you like. If the keyword matches an attribute on the model object, it will be updated, so model_file is an attribute on the vensim model. When executing the policies, we update this attribute for each policy. We can pass these policies to `perform_experiment()` as an additional keyword argument

```
results = perform_experiments(model, 1000, policies=policies)
```

We can now proceed in the same way as before, and perform a series of experiments. Together, this results in the following code:

```
"""
Created on 20 May, 2011

This module shows how you can use vensim models directly
instead of coding the model in Python. The underlying case
is the same as used in fluExample

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                epruyt <e.pruyt (at) tudelft (dot) nl>
"""

import numpy as np

from ema_workbench import (
    RealParameter,
    TimeSeriesOutcome,
    ema_logging,
    ScalarOutcome,
    perform_experiments,
    Policy,
```

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```
    save_results,
)
from ema_workbench.connectors.vensim import VensimModel

if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = VensimModel("fluCase", wd=r"./models/flu", model_file=r"FLUvensimV1basecase.vpm")

    # outcomes
    model.outcomes = [
        TimeSeriesOutcome(
            "deceased_population_region_1", variable_name="deceased population region 1"
        ),
        TimeSeriesOutcome("infected_fraction_R1", variable_name="infected fraction R1"),
        ScalarOutcome(
            "max_infection_fraction", variable_name="infected fraction R1", function=np.max
        ),
    ]

    # Plain Parametric Uncertainties
    model.uncertainties = [
        RealParameter(
            "additional_seasonal_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R1",
        ),
        RealParameter(
            "additional_seasonal_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R2",
        ),
        RealParameter(
            "fatality_ratio_region_1", 0.0001, 0.1, variable_name="fatality ratio region 1"
        ),
        RealParameter(
            "fatality_rate_region_2", 0.0001, 0.1, variable_name="fatality rate region 2"
        ),
        RealParameter(
            "initial_immune_fraction_of_the_population_of_region_1",
            0,
            0.5,
            variable_name="initial immune fraction of the population of region 1",
        ),
        RealParameter(
            "initial_immune_fraction_of_the_population_of_region_2",
            0,
```

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```
            0.5,
            variable_name="initial immune fraction of the population of region 2",
        ),
        RealParameter(
            "normal_interregional_contact_rate",
            0,
            0.9,
            variable_name="normal interregional contact rate",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="permanent immune population fraction R1",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="permanent immune population fraction R2",
        ),
        RealParameter("recovery_time_region_1", 0.1, 0.75, variable_name="recovery time␣
↪region 1"),
        RealParameter("recovery_time_region_2", 0.1, 0.75, variable_name="recovery time␣
↪region 2"),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_1",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 1",
        ),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_2",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 2",
        ),
        RealParameter(
            "root_contact_rate_region_1", 0.01, 5, variable_name="root contact rate␣
↪region 1"
        ),
        RealParameter(
            "root_contact_ratio_region_2", 0.01, 5, variable_name="root contact ratio␣
↪region 2"
        ),
        RealParameter(
            "infection_ratio_region_1", 0, 0.15, variable_name="infection ratio region 1"
        ),
        RealParameter("infection_rate_region_2", 0, 0.15, variable_name="infection rate␣
↪region 2"),
        RealParameter(
            "normal_contact_rate_region_1", 10, 100, variable_name="normal contact rate␣
```

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```
↪region 1"
        ),
        RealParameter(
            "normal_contact_rate_region_2", 10, 200, variable_name="normal contact rate␣
↪region 2"
        ),
    ]

    # add policies
    policies = [
        Policy("no policy", model_file=r"FLUvensimV1basecase.vpm"),
        Policy("static policy", model_file=r"FLUvensimV1static.vpm"),
        Policy("adaptive policy", model_file=r"FLUvensimV1dynamic.vpm"),
    ]

    results = perform_experiments(model, 1000, policies=policies)
    save_results(results, "./data/1000 flu cases with policies.tar.gz")
```

comparison of results

Using the following script, we reproduce figures similar to the 3D figures in Pruyt & Hamarat (2010). But using `pairs_scatter()`. It shows for the three different policies their behavior on the total number of deaths, the height of the highest peak of the pandemic, and the point in time at which this peak was reached.

```
"""
Created on 20 sep. 2011

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
"""

import matplotlib.pyplot as plt
import numpy as np

from ema_workbench import load_results, ema_logging
from ema_workbench.analysis.pairs_plotting import pairs_lines, pairs_scatter, pairs_
↪density

ema_logging.log_to_stderr(level=ema_logging.DEFAULT_LEVEL)

# load the data
fh = "./data/1000 flu cases no policy.tar.gz"
experiments, outcomes = load_results(fh)

# transform the results to the required format
# that is, we want to know the max peak and the casualties at the end of the
# run
tr = {}

# get time and remove it from the dict
time = outcomes.pop("TIME")

```

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```
for key, value in outcomes.items():
    if key == "deceased_population_region_1":
        tr[key] = value[:, -1]  # we want the end value
    else:
        # we want the maximum value of the peak
        max_peak = np.max(value, axis=1)
        tr["max peak"] = max_peak

        # we want the time at which the maximum occurred
        # the code here is a bit obscure, I don't know why the transpose
        # of value is needed. This however does produce the appropriate results
        logical = value.T == np.max(value, axis=1)
        tr["time of max"] = time[logical.T]

pairs_scatter(experiments, tr, filter_scalar=False)
pairs_lines(experiments, outcomes)
pairs_density(experiments, tr, filter_scalar=False)
plt.show()
```

no policy

static policy

adaptive policy

1.6 General Introduction

Since 2010, I have been working on the development of an open source toolkit for supporting decision-making under deep uncertainty. This toolkit is known as the exploratory modeling workbench. The motivation for this name is that in my opinion all model-based deep uncertainty approaches are forms of exploratory modeling as first introduced by Bankes (1993). The design of the workbench has undergone various changes over time, but it has started to stabilize in the fall of 2016. In the summer 0f 2017, I published a paper detailing the workbench (Kwakkel, 2017). There is an in depth example in the paper, but for the documentation I want to provide a more tutorial style description of the functionality of the workbench.

As a starting point, I will use the Direct Policy Search example that is available for Rhodium (Quinn et al 2017). A quick note on terminology is in order here. I have a background in transport modeling. Here we often use discrete event simulation models. These are intrinsically stochastic models. It is standard practice to run these models several times and take descriptive statistics over the set of runs. In discrete event simulation, and also in the context of agent based modeling, this is known as running replications. The workbench adopts this terminology and draws a sharp distinction between designing experiments over a set of deeply uncertain factors, and performing replications of this experiment to cope with stochastic uncertainty.

[1]:
```
import math

# more or less default imports when using
# the workbench
import numpy as np
import pandas as pd
import seaborn as sns
```

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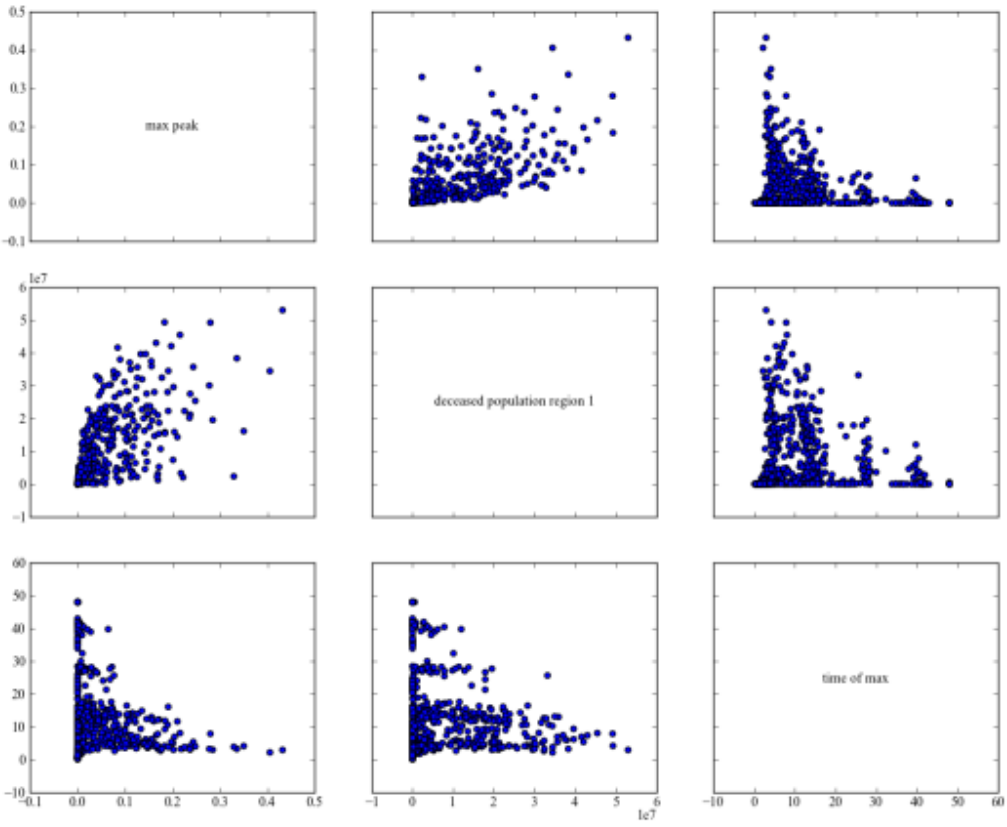
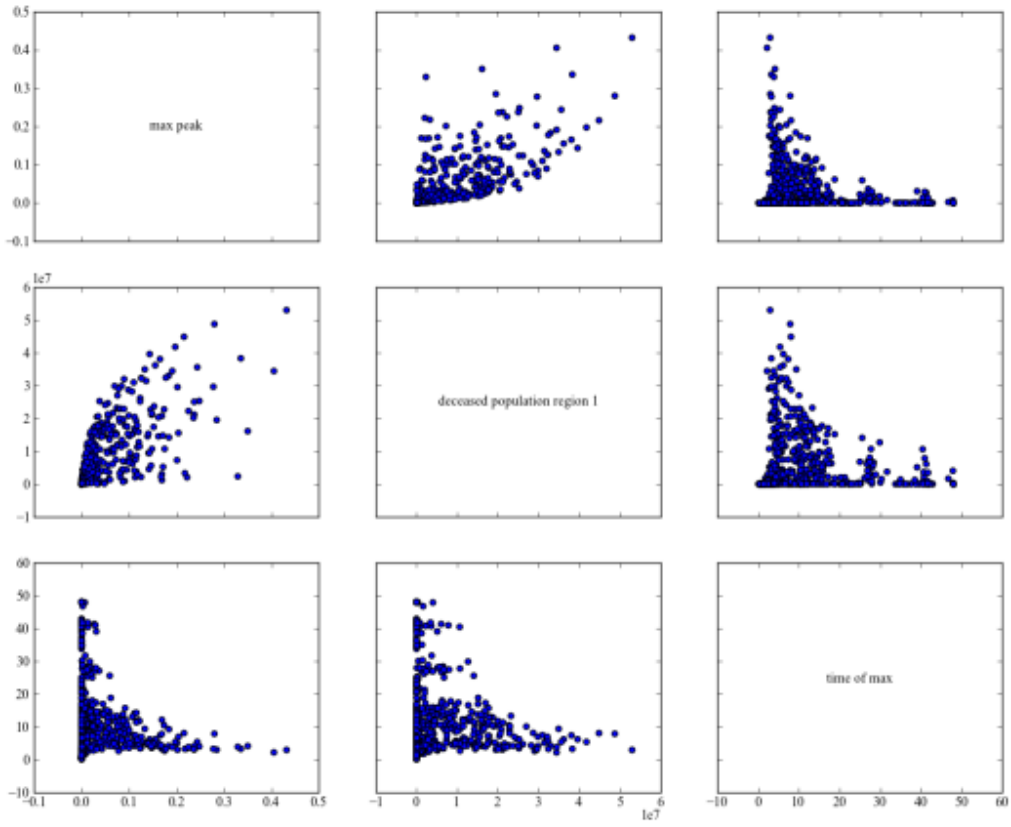
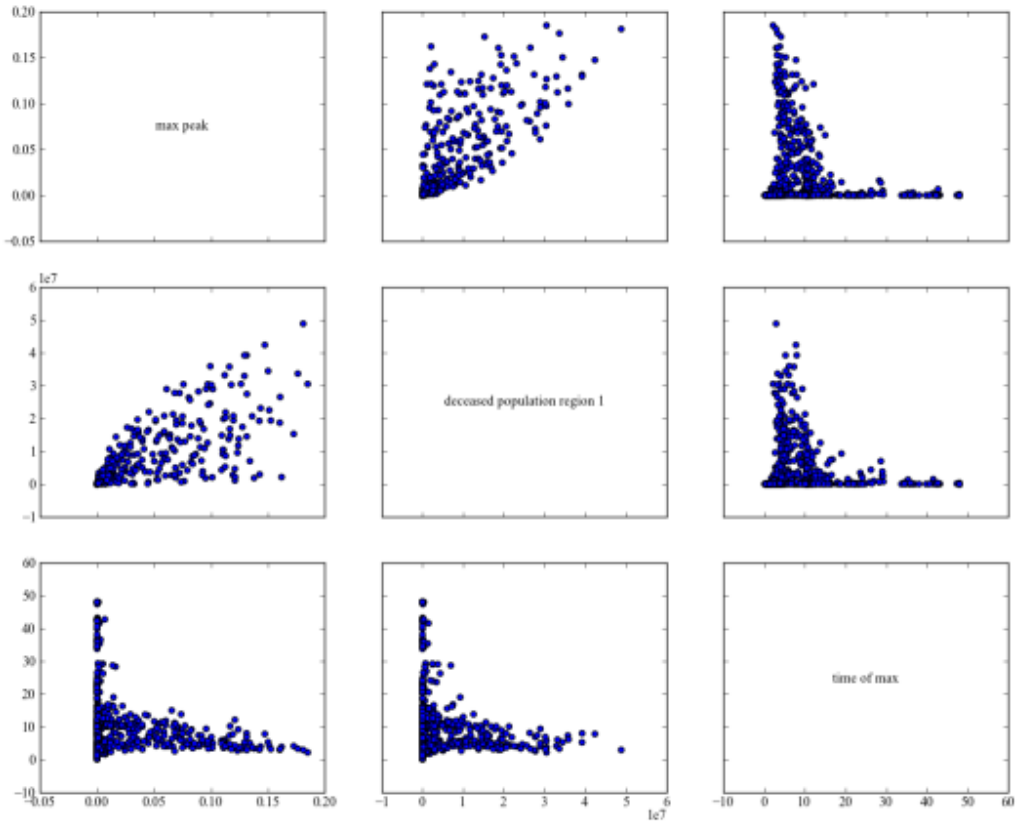

max peak
deceased population region 1
time of max
1e7
1e7


max peak
deceased population region 1
time of max
1e7
1e7


max peak
deceased population region 1
time of max
1e7
1e7

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```
import matplotlib.pyplot as plt

from scipy.optimize import brentq


def get_antropogenic_release(xt, c1, c2, r1, r2, w1):
    """

    Parameters
    ----------
    xt : float
         pollution in lake at time t
    c1 : float
         center rbf 1
    c2 : float
         center rbf 2
    r1 : float
         ratius rbf 1
    r2 : float
         ratius rbf 2
    w1 : float
         weight of rbf 1

    Returns
    -------
    float

    note:: w2 = 1 - w1

    """

    rule = w1 * (abs(xt - c1) / r1) ** 3 + (1 - w1) * (abs(xt - c2) / r2) ** 3
    at1 = max(rule, 0.01)
    at = min(at1, 0.1)

    return at


def lake_model(
    b=0.42,
    q=2.0,
    mean=0.02,
    stdev=0.001,
    delta=0.98,
    alpha=0.4,
    nsamples=100,
    myears=100,
    c1=0.25,
    c2=0.25,
    r1=0.5,
    r2=0.5,
    w1=0.5,
```

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```
    seed=None,
):
    """runs the lake model for nsamples stochastic realisation using
    specified random seed.

    Parameters
    ----------
    b : float
        decay rate for P in lake (0.42 = irreversible)
    q : float
        recycling exponent
    mean : float
           mean of natural inflows
    stdev : float
           standard deviation of natural inflows
    delta : float
           future utility discount rate
    alpha : float
           utility from pollution
    nsamples : int, optional
    myears : int, optional
    c1 : float
    c2 : float
    r1 : float
    r2 : float
    w1 : float
    seed : int, optional
          seed for the random number generator

    Returns
    -------
    tuple

    """
    np.random.seed(seed)
    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)

    X = np.zeros((myears,))
    average_daily_P = np.zeros((myears,))
    reliability = 0.0
    inertia = 0
    utility = 0

    for _ in range(nsamples):
        X[0] = 0.0
        decision = 0.1

        decisions = np.zeros(myears)
        decisions[0] = decision

        natural_inflows = np.random.lognormal(
            math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
```

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```
            math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
            size=myears,
        )

        for t in range(1, myears):
            # here we use the decision rule
            decision = get_antropogenic_release(X[t - 1], c1, c2, r1, r2, w1)
            decisions[t] = decision

            X[t] = (
                (1 - b) * X[t - 1]
                + X[t - 1] ** q / (1 + X[t - 1] ** q)
                + decision
                + natural_inflows[t - 1]
            )
            average_daily_P[t] += X[t] / nsamples

        reliability += np.sum(X < Pcrit) / (nsamples * myears)
        inertia += np.sum(np.absolute(np.diff(decisions) < 0.02)) / (nsamples * myears)
        utility += np.sum(alpha * decisions * np.power(delta, np.arange(myears))) /␣
↪nsamples
    max_P = np.max(average_daily_P)
    return max_P, utility, inertia, reliability
```

1.6.1 Connecting a python function to the workbench

Now we are ready to connect this model to the workbench. We have to specify the uncertainties, the outcomes, and the policy levers. For the uncertainties and the levers, we can use real valued parameters, integer valued parameters, and categorical parameters. For outcomes, we can use either scalar, single valued outcomes or time series outcomes. For convenience, we can also explicitly control constants in case we want to have them set to a value different from their default value.

[2]:
```
from ema_workbench import RealParameter, ScalarOutcome, Constant, Model
from dps_lake_model import lake_model

model = Model("lakeproblem", function=lake_model)

# specify uncertainties
model.uncertainties = [
    RealParameter("b", 0.1, 0.45),
    RealParameter("q", 2.0, 4.5),
    RealParameter("mean", 0.01, 0.05),
    RealParameter("stdev", 0.001, 0.005),
    RealParameter("delta", 0.93, 0.99),
]

# set levers
model.levers = [
    RealParameter("c1", -2, 2),
    RealParameter("c2", -2, 2),
    RealParameter("r1", 0, 2),
```

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```
    RealParameter("r2", 0, 2),
    RealParameter("w1", 0, 1),
]

# specify outcomes
model.outcomes = [
    ScalarOutcome("max_P"),
    ScalarOutcome("utility"),
    ScalarOutcome("inertia"),
    ScalarOutcome("reliability"),
]

# override some of the defaults of the model
model.constants = [
    Constant("alpha", 0.41),
    Constant("nsamples", 150),
    Constant("myears", 100),
]
```

1.6.2 Performing experiments

Now that we have specified the model with the workbench, we are ready to perform experiments on it. We can use evaluators to distribute these experiments either over multiple cores on a single machine, or over a cluster using `ipyparallel`. Using any parallelization is an advanced topic, in particular if you are on a windows machine. The code as presented here will run fine in parallel on a mac or Linux machine. If you are trying to run this in parallel using multiprocessing on a windows machine, from within a jupyter notebook, it won't work. The solution is to move the `lake_model` and `get_antropogenic_release` to a separate python module and import the lake model function into the notebook.

Another common practice when working with the exploratory modeling workbench is to turn on the logging functionality that it provides. This will report on the progress of the experiments, as well as provide more insight into what is happening in particular in case of errors.

If we want to perform experiments on the model we have just defined, we can use the perform_experiments method on the evaluator, or the stand alone perform_experiments function. We can perform experiments over the uncertainties and/or over the levers. Any given parameterization of the levers is known as a policy, while any given parametrization over the uncertainties is known as a scenario. Any policy is evaluated over each of the scenarios. So if we want to use 100 scenarios and 10 policies, this means that we will end up performing 100 * 10 = 1000 experiments. By default, the workbench uses Latin hypercube sampling for both sampling over levers and sampling over uncertainties. However, the workbench also offers support for full factorial, partial factorial, and Monte Carlo sampling, as well as wrappers for the various sampling schemes provided by SALib.

The ema_workbench offers support for parallelization of the execution of the experiments using either the multiprocessing or ipyparallel. There are various OS specific concerns you have to keep in mind when using either of these libraries. Please have a look at the documentation of these libraries, before using them.

[3]:
```
from ema_workbench import MultiprocessingEvaluator, ema_logging, perform_experiments

ema_logging.log_to_stderr(ema_logging.INFO)

with MultiprocessingEvaluator(model) as evaluator:
    results = evaluator.perform_experiments(scenarios=1000, policies=10)
```

```
[MainProcess/INFO] pool started with 10 workers
[MainProcess/INFO] performing 1000 scenarios * 10 policies * 1 model(s) = 10000␣
↪experiments
100%|| 10000/10000 [00:57<00:00, 173.34it/s]
[MainProcess/INFO] experiments finished
[MainProcess/INFO] terminating pool
```

1.6.3 Processing the results of the experiments

By default, the return of `perform_experiments` is a tuple of length 2. The first item in the tuple is the experiments. The second item is the outcomes. Experiments and outcomes are aligned by index. The experiments are stored in a Pandas DataFrame, while the outcomes are a dict with the name of the outcome as key, and the values are in a numpy array.

[4]:
```
experiments, outcomes = results
print(experiments.shape)
print(list(outcomes.keys()))
```

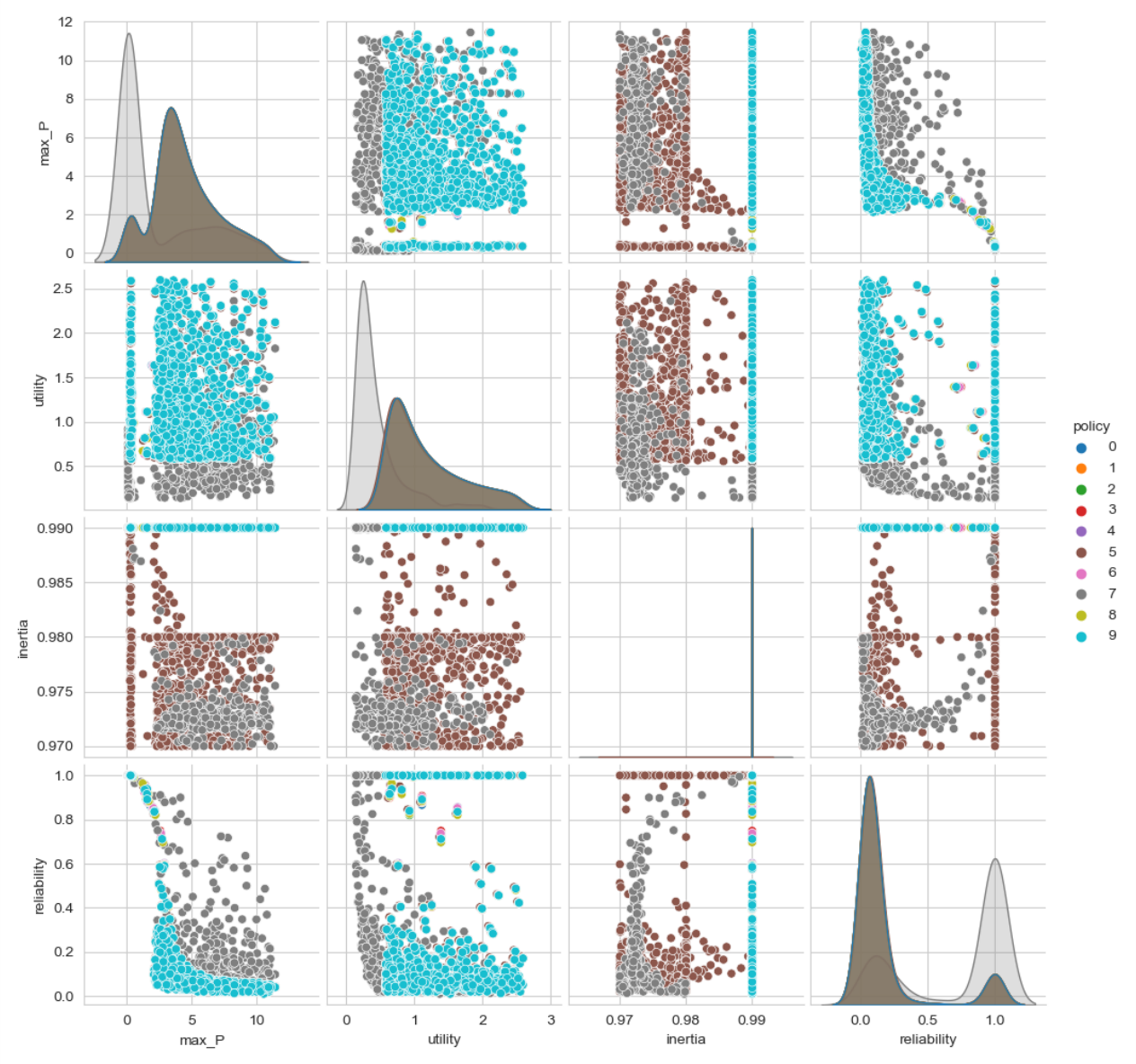
```
(10000, 13)
['max_P', 'utility', 'inertia', 'reliability']
```

We can easily visualize these results. The workbench comes with various convenience plotting functions built on top of matplotlib and seaborn. We can however also easily use seaborn or matplotlib directly. For example, we can create a pairplot using seaborn where we group our outcomes by policy. For this, we need to create a dataframe with the outcomes and a policy column. By default the name of a policy is a string representation of the dict with lever names and values. We can replace this easily with a number as shown below.

[5]:
```
data = pd.DataFrame(outcomes)
data["policy"] = experiments["policy"]
```

Next, all that is left is to use seaborn's pairplot function to visualize the data.

[6]:
```
sns.pairplot(data, hue="policy", vars=list(outcomes.keys()))
plt.show()
```



[ ]:

1.7 Open exploration

In this second tuturial, I will showcase how to use the ema_workbench for performing open exploration. This tuturial will continue with the same example as used in the previous tuturial.

1.7.1 some background

In exploratory modeling, we are interested in understanding how regions in the uncertainty space and/or the decision space map to the whole outcome space, or partitions thereof. There are two general approaches for investigating this mapping. The first one is through systematic sampling of the uncertainty or decision space. This is sometimes also known as open exploration. The second one is to search through the space in a directed manner using some type of optimization approach. This is sometimes also known as directed search.

The workbench support both open exploration and directed search. Both can be applied to investigate the mapping of the uncertainty space and/or the decision space to the outcome space. In most applications, search is used for finding promising mappings from the decision space to the outcome space, while exploration is used to stress test these mappings under a whole range of possible resolutions to the various uncertainties. This need not be the case however. Optimization can be used to discover the worst possible scenario, while sampling can be used to get insight into the sensitivity of outcomes to the various decision levers.

1.7.2 open exploration

To showcase the open exploration functionality, let's start with a basic example using the Direct Policy Search (DPS) version of the lake problem (Quinn et al 2017). This is the same model as we used in the general introduction. Note that for convenience, I have moved the code for the model to a module called dps_lake_model.py, which I import here for further use.

We are going to simultaneously sample over uncertainties and decision levers. We are going to generate 1000 scenarios and 5 policies, and see how they jointly affect the outcomes. A *scenario* is understood as a point in the uncertainty space, while a *policy* is a point in the decision space. The combination of a scenario and a policy is called *experiment*. The uncertainty space is spanned by uncertainties, while the decision space is spanned by levers.

Both uncertainties and levers are instances of *RealParameter* (a continuous range), *IntegerParameter* (a range of integers), or *CategoricalParameter* (an unorder set of things). By default, the workbench will use Latin Hypercube sampling for generating both the scenarios and the policies. Each policy will be always evaluated over all scenarios (i.e. a full factorial over scenarios and policies).

[1]:
```
from ema_workbench import RealParameter, ScalarOutcome, Constant, Model
from dps_lake_model import lake_model

import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt

model = Model("lakeproblem", function=lake_model)

# specify uncertainties
model.uncertainties = [
    RealParameter("b", 0.1, 0.45),
    RealParameter("q", 2.0, 4.5),
    RealParameter("mean", 0.01, 0.05),
    RealParameter("stdev", 0.001, 0.005),
    RealParameter("delta", 0.93, 0.99),
]

# set levers
model.levers = [
    RealParameter("c1", -2, 2),
```

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```
    RealParameter("c2", -2, 2),
    RealParameter("r1", 0, 2),
    RealParameter("r2", 0, 2),
    RealParameter("w1", 0, 1),
]

# specify outcomes
model.outcomes = [
    ScalarOutcome("max_P"),
    ScalarOutcome("utility"),
    ScalarOutcome("inertia"),
    ScalarOutcome("reliability"),
]

# override some of the defaults of the model
model.constants = [
    Constant("alpha", 0.41),
    Constant("nsamples", 150),
    Constant("myears", 100),
]
```

[2]:
```
from ema_workbench import MultiprocessingEvaluator, ema_logging, perform_experiments

ema_logging.log_to_stderr(ema_logging.INFO)

# The n_processes=-1 ensures that all cores except 1 are used, which is kept free to␣
↪keep using the computer
with MultiprocessingEvaluator(model, n_processes=-1) as evaluator:
    # Run 1000 scenarios for 5 policies
    experiments, outcomes = evaluator.perform_experiments(scenarios=1000, policies=5)
```

```
[MainProcess/INFO] pool started with 7 workers
[MainProcess/INFO] performing 1000 scenarios * 5 policies * 1 model(s) = 5000 experiments
100%|| 5000/5000 [01:02<00:00, 80.06it/s]
[MainProcess/INFO] experiments finished
[MainProcess/INFO] terminating pool
```

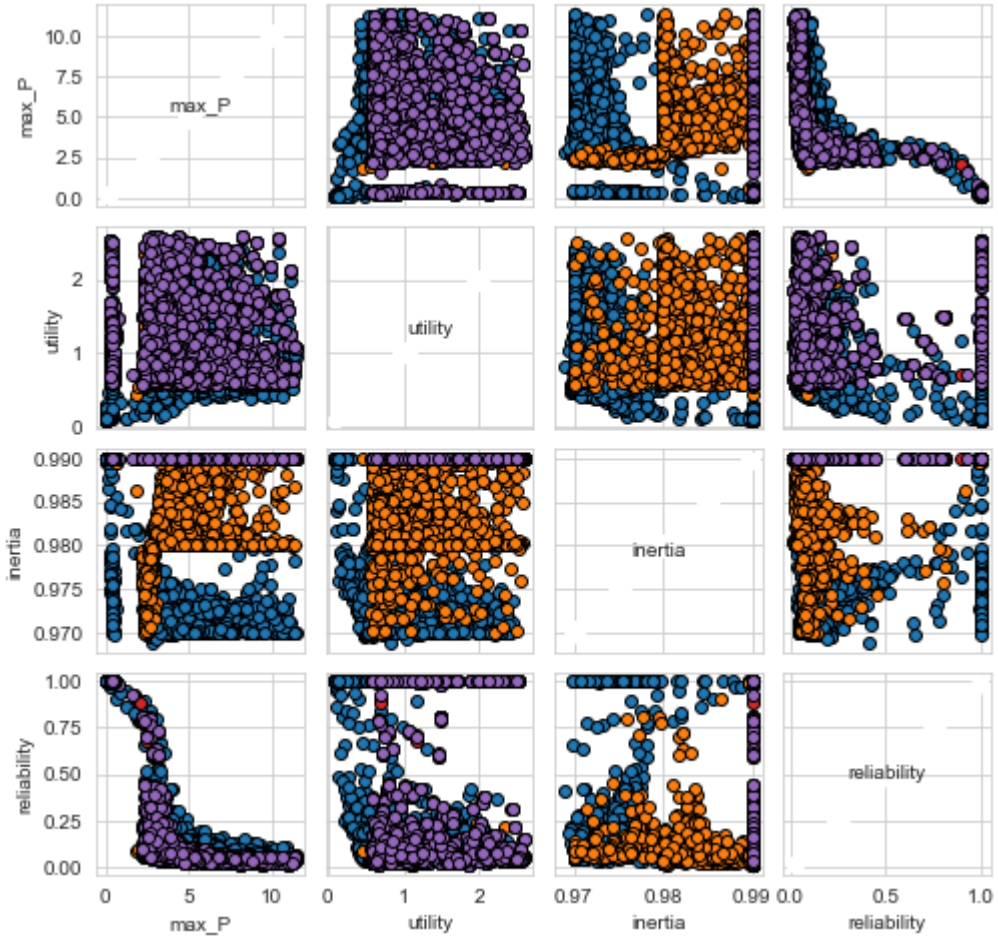
Visual analysis

Having generated these results, the next step is to analyze them and see what we can learn from the results. The workbench comes with a variety of techniques for this analysis. A simple first step is to make a few quick visualizations of the results. The workbench has convenience functions for this, but it also possible to create your own visualizations using the scientific Python stack.

[3]:
```
from ema_workbench.analysis import pairs_plotting

fig, axes = pairs_plotting.pairs_scatter(experiments, outcomes, group_by="policy",␣
↪legend=False)
fig.set_size_inches(8, 8)
plt.show()
```

```
[MainProcess/INFO] no time dimension found in results
```



Often, it is convenient to separate the process of performing the experiments from the analysis. To make this possible, the workbench offers convenience functions for storing results to disc and loading them from disc. The workbench will store the results in a tarbal with .csv files and separate metadata files. This is a convenient format that has proven sufficient over the years.

```
from ema_workbench import save_results
save_results(results, '1000 scenarios 5 policies.tar.gz')

from ema_workbench import load_results
results = load_results('1000 scenarios 5 policies.tar.gz')
```

1.7.3 advanced analysis

In addition to visual analysis, the workbench comes with a variety of techniques to perform a more in-depth analysis of the results. In addition, other analyses can simply be performed by utilizing the scientific python stack. The workbench comes with

- Scenario Discovery, a model driven approach to scenario development
- Feature Scoring, a poor man's alternative to global sensitivity analysis
- Dimensional stacking, a quick visual approach drawing on feature scoring to enable scenario discovery. This approach has received limited attention in the literature. The implementation in the workbench replaces the rule mining approach with a feature scoring approach.
- Regional sensitivity analysis

Scenario Discovery

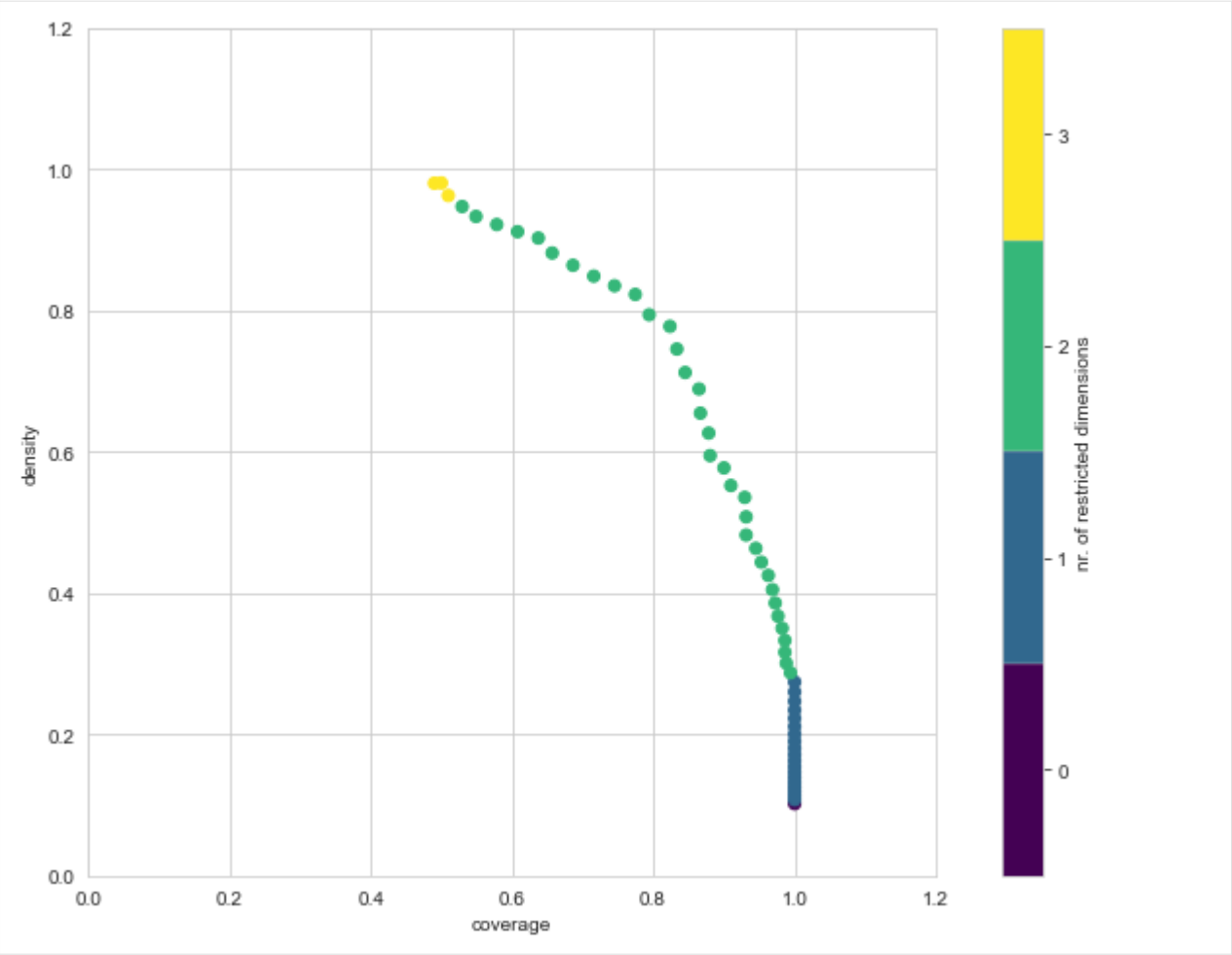
A detailed discussion on scenario discovery can be found in an earlier blogpost. For completeness, I provide a code snippet here. Compared to the previous blog post, there is one small change. The library mpld3 is currently not being maintained and broken on Python 3.5. and higher. To still utilize the interactive exploration of the trade offs within the notebook, one could use the interactive back-end (% matplotlib notebook).

[4]:
```
from ema_workbench.analysis import prim

x = experiments
y = outcomes["max_P"] < 0.8
prim_alg = prim.Prim(x, y, threshold=0.8)
box1 = prim_alg.find_box()
```

```
[MainProcess/INFO] model dropped from analysis because only a single category
[MainProcess/INFO] 5000 points remaining, containing 510 cases of interest
[MainProcess/INFO] mean: 0.9807692307692307, mass: 0.052, coverage: 0.5, density: 0.
↪9807692307692307 restricted_dimensions: 3
```

[5]:
```
box1.show_tradeoff()
plt.show()
```

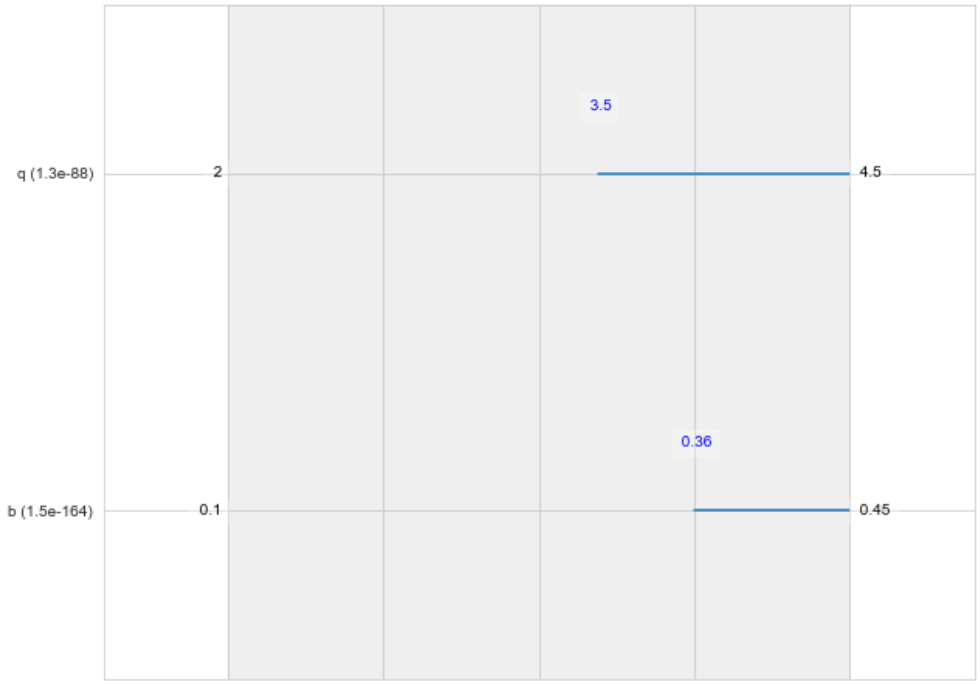


We can inspect any of the points on the trade off curve using the inspect method. As shown, we can show the results either in a table format or in a visual format.

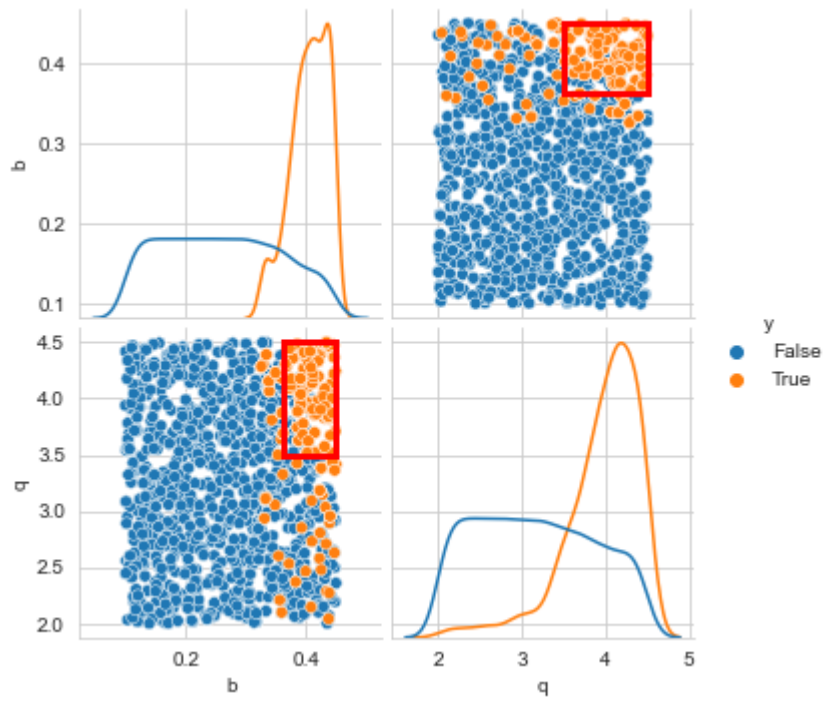
[6]:
```
box1.inspect(43)
box1.inspect(43, style="graph")
plt.show()
```

```
coverage    0.794118
density     0.794118
id                43
mass           0.102
mean        0.794118
res_dim            2
Name: 43, dtype: object

     box 43
        min       max                         qp values
b  0.362596  0.449742  [1.5372285485377317e-164, -1.0]
q  3.488834  4.498362   [1.3004137205191903e-88, -1.0]
```



[7]:
```
box1.show_pairs_scatter(43)
plt.show()
```



feature scoring

Feature scoring is a family of techniques often used in machine learning to identify the most relevant features to include in a model. This is similar to one of the use cases for global sensitivity analysis, namely factor prioritisation. The main advantage of feature scoring techniques is that they impose no specific constraints on the experimental design, while they can handle real valued, integer valued, and categorical valued parameters. The workbench supports multiple techniques, the most useful of which generally is extra trees (Geurts et al. 2006).

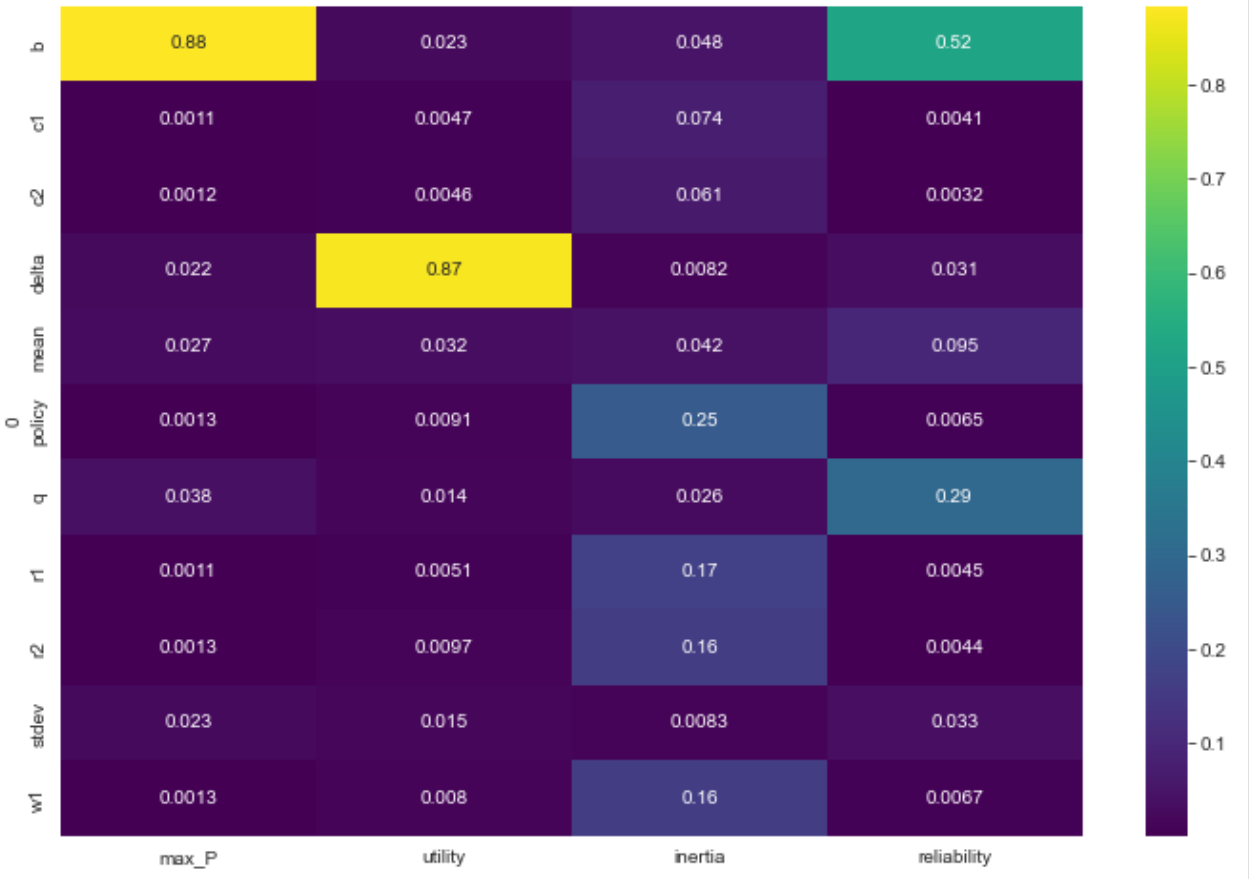
For this example, we run feature scoring for each outcome of interest. We can also run it for a specific outcome if desired. Similarly, we can choose if we want to run in regression mode or classification mode. The later is applicable if the outcome is a categorical variable and the results should be interpreted similar to regional sensitivity analysis results. For more details, see the documentation.

[8]:
```
from ema_workbench.analysis import feature_scoring

x = experiments
y = outcomes

fs = feature_scoring.get_feature_scores_all(x, y)
sns.heatmap(fs, cmap="viridis", annot=True)
plt.show()
```

```
[MainProcess/INFO] model dropped from analysis because only a single category
[MainProcess/INFO] model dropped from analysis because only a single category
[MainProcess/INFO] model dropped from analysis because only a single category
[MainProcess/INFO] model dropped from analysis because only a single category
```



From the results, we see that max_P is primarily influenced by b, while utility is driven by delta, for inertia and reliability the situation is a little bit less clear cut.

The foregoing feature scoring was using the raw values of the outcomes. However, in scenario discovery applications, we are typically dealing with a binary clasification. This might produce slightly different results as demonstrated below

[11]:
```
from ema_workbench.analysis import RuleInductionType

x = experiments
y = outcomes["max_P"] < 0.8

fs, alg = feature_scoring.get_ex_feature_scores(x, y, mode=RuleInductionType.
↪CLASSIFICATION)
fs.sort_values(ascending=False, by=1)
```

```
[MainProcess/INFO] model dropped from analysis because only a single category
```

[11]:

	1
0	
b	0.458094
q	0.310989
mean	0.107732
delta	0.051212
stdev	0.047653
policy	0.005475
w1	0.004815
r2	0.003658
r1	0.003607
c1	0.003467
c2	0.003299

Here we ran extra trees feature scoring on a binary vector for *max_P*. the *b* parameter is still important, similar to in the previous case, but the introduction of the binary classifiaction now also highlights some addtional parameters as being potentially relevant.

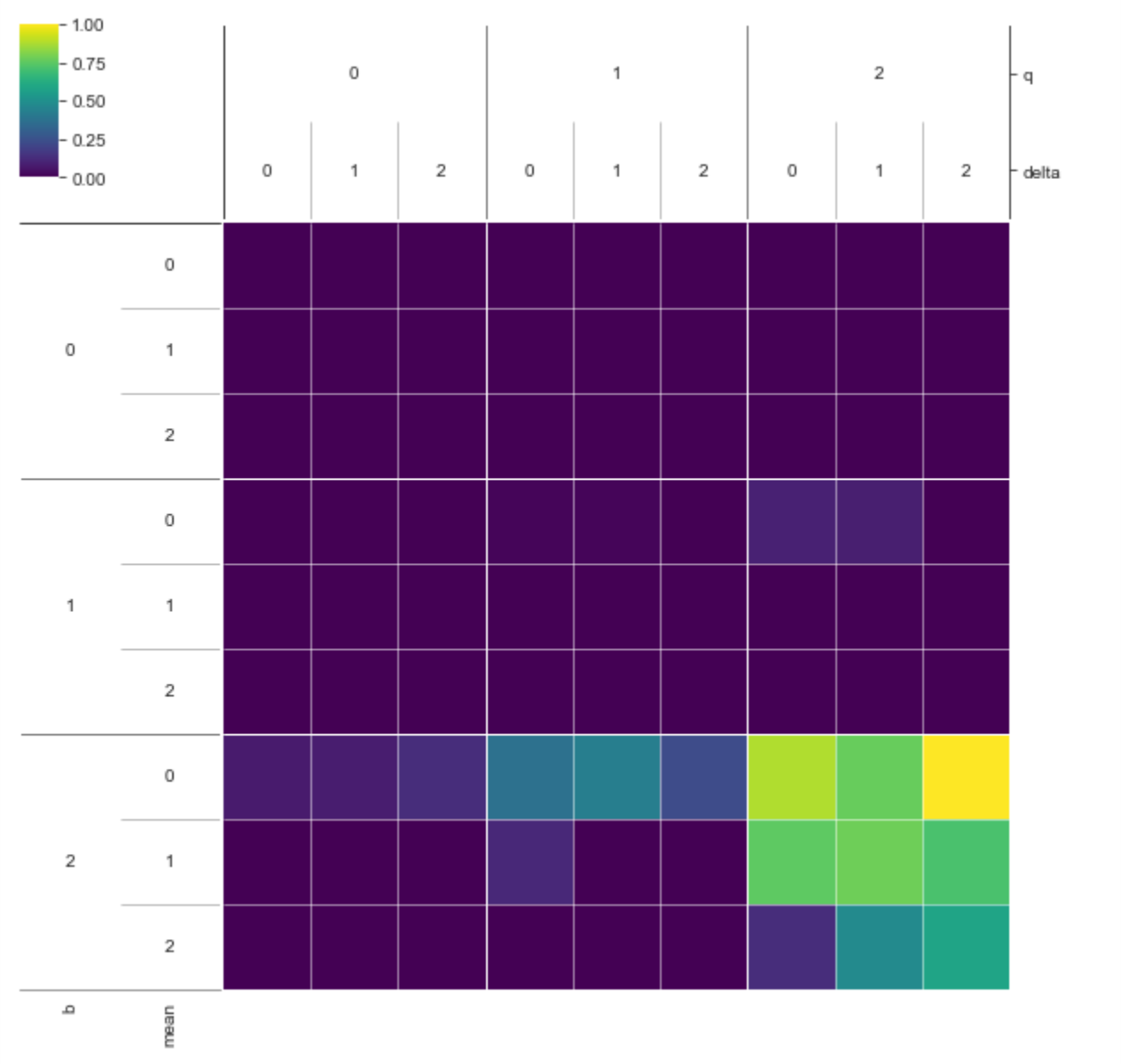
dimensional stacking

Dimensional stacking was suggested as a more visual approach to scenario discovery. It involves two steps: identifying the most important uncertainties that affect system behavior, and creating a pivot table using the most influential uncertainties. In order to do this, we first need, as in scenario discovery, specify the outcomes that are of interest. The creating of the pivot table involves binning the uncertainties. More details can be found in Suzuki et al. (2015) or by looking through the code in the workbench. Compared to Suzuki et al, the workbench uses feature scoring for determining the most influential uncertainties. The code is set up in a modular way so other approaches to global sensitivity analysis can easily be used as well if so desired.

[12]:
```
from ema_workbench.analysis import dimensional_stacking

x = experiments
y = outcomes["max_P"] < 0.8
dimensional_stacking.create_pivot_plot(x, y, 2, nbins=3)
plt.show()
```

```
[MainProcess/INFO] model dropped from analysis because only a single category
```



We can see from this visual that if B is high, while Q is high, we have a high concentration of cases where pollution stays below 0.8. The mean and stdev have some limited additional influence. By playing around with an alternative number of bins, or different number of layers, patterns can be coarsened or refined.

regional sensitivity analysis

A fourth approach for supporting scenario discovery is to perform a regional sensitivity analysis. The workbench implements a visual approach based on plotting the empirical CDF given a classification vector. Please look at section 3.4 in Pianosi et al (2016) for more details.

[13]:
```
from ema_workbench.analysis import regional_sa
from numpy.lib import recfunctions as rf

sns.set_style("white")
```

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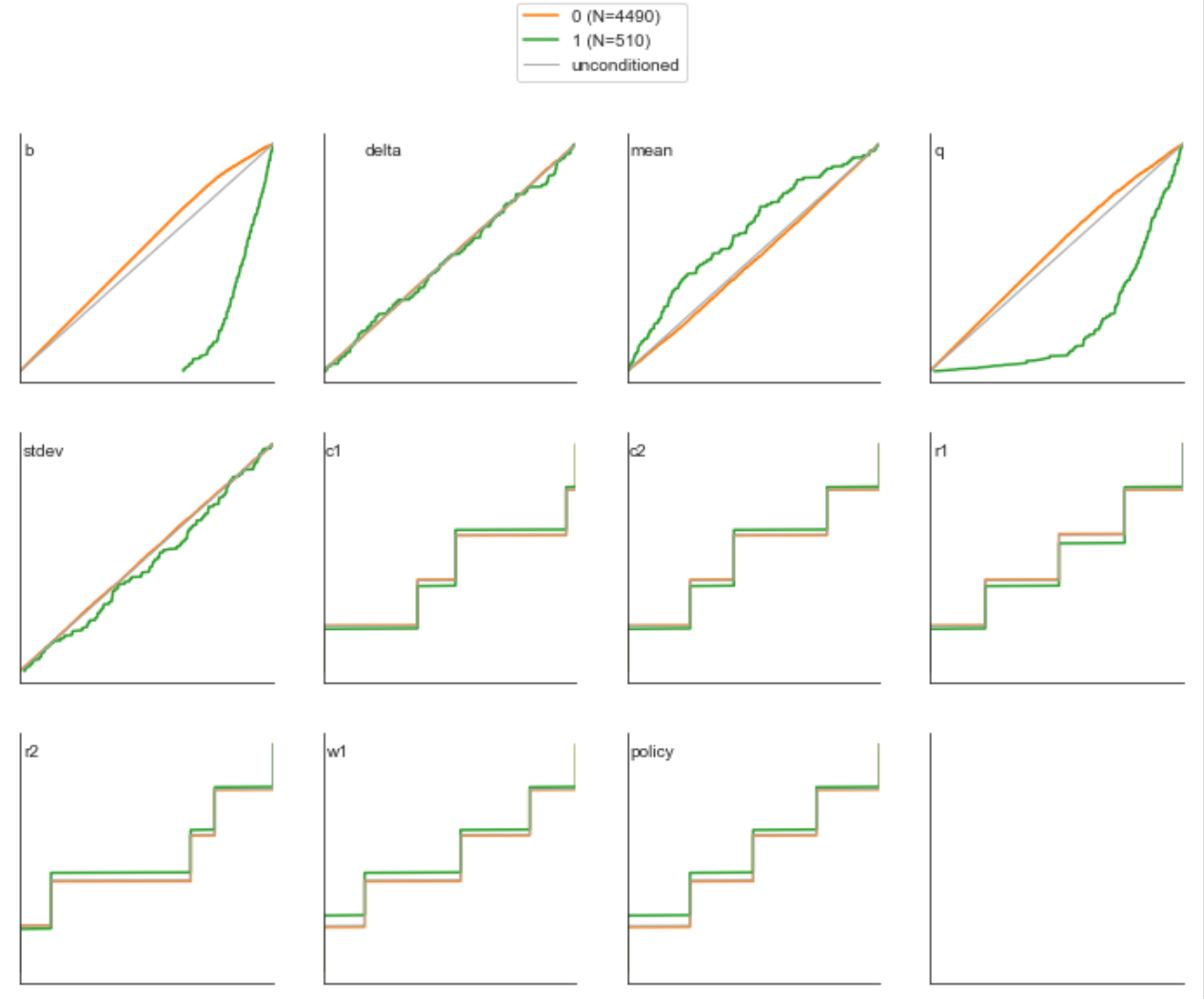
```
# model is the same across experiments
x = experiments.copy()
x = x.drop("model", axis=1)
y = outcomes["max_P"] < 0.8
fig = regional_sa.plot_cdfs(x, y)
sns.despine()
plt.show()
```



The above results clearly show that both B and Q are important. to a lesser extend, the mean also is relevant.

1.7.4 More advanced sampling techniques

The workbench can also be used for more advanced sampling techniques. To achieve this, it relies on SALib. On the workbench side, the only change is to specify the sampler we want to use. Next, we can use SALib directly to perform the analysis. To help with this, the workbench provides a convenience function for generating the problem dict which SALib provides. The example below focusses on performing SOBOL on the uncertainties, but we could do the exact same thing with the levers instead. The only changes required would be to set `lever_sampling` instead of `uncertainty_sampling`, and get the SALib problem dict based on the levers.

[17]:
```
from SALib.analyze import sobol
from ema_workbench import Samplers
from ema_workbench.em_framework.salib_samplers import get_SALib_problem

with MultiprocessingEvaluator(model) as evaluator:
    sa_results = evaluator.perform_experiments(scenarios=1000, uncertainty_
↪sampling=Samplers.SOBOL)

experiments, outcomes = sa_results

problem = get_SALib_problem(model.uncertainties)
Si = sobol.analyze(problem, outcomes["max_P"], calc_second_order=True, print_to_
↪console=False)
```

```
[MainProcess/INFO] pool started with 12 workers
/Users/jhkwakkel/opt/anaconda3/lib/python3.9/site-packages/SALib/sample/saltelli.py:94:␣
↪UserWarning:
        Convergence properties of the Sobol' sequence is only valid if
        `N` (1000) is equal to `2^n`.

  warnings.warn(msg)
[MainProcess/INFO] performing 12000 scenarios * 1 policies * 1 model(s) = 12000␣
↪experiments
100%|| 12000/12000 [02:37<00:00, 76.17it/s]
[MainProcess/INFO] experiments finished
[MainProcess/INFO] terminating pool
```

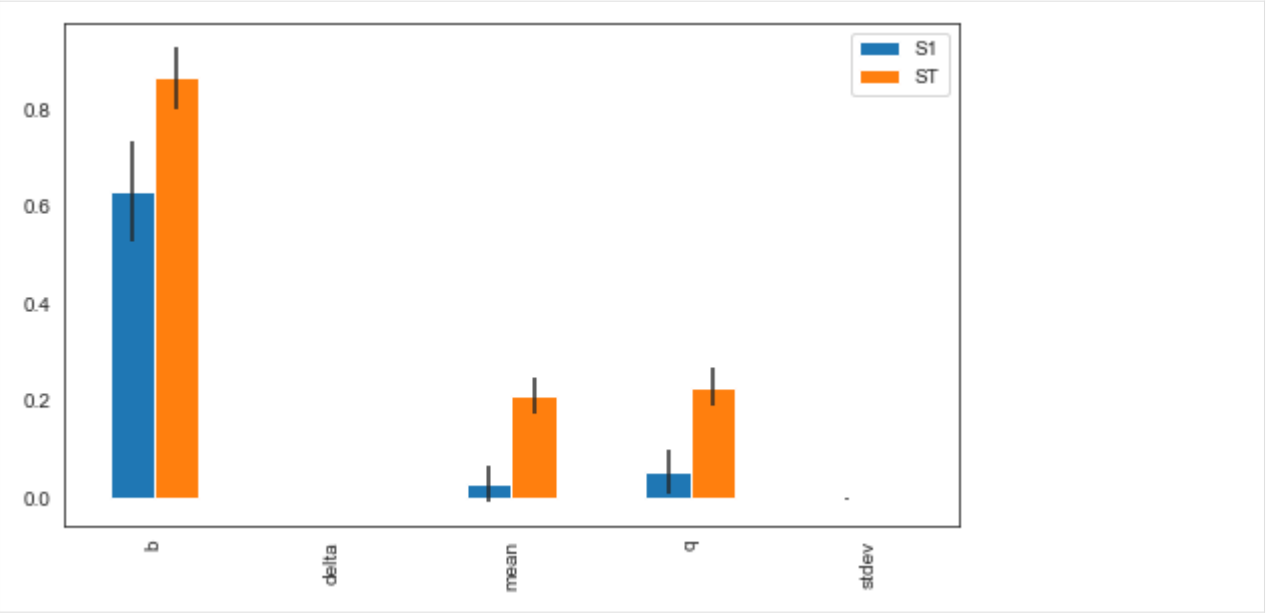
We have now completed the sobol analysis and have calculated the metrics. What remains is to visualize the metrics. Which can be done as shown below, focussing on St and S1. The error bars indicate the confidence intervals.

[18]:
```
scores_filtered = {k: Si[k] for k in ["ST", "ST_conf", "S1", "S1_conf"]}
Si_df = pd.DataFrame(scores_filtered, index=problem["names"])

sns.set_style("white")
fig, ax = plt.subplots(1)

indices = Si_df[["S1", "ST"]]
err = Si_df[["S1_conf", "ST_conf"]]

indices.plot.bar(yerr=err.values.T, ax=ax)
fig.set_size_inches(8, 6)
fig.subplots_adjust(bottom=0.3)
plt.show()
```



[ ]:

1.8 Directed search

This is the third turial in a series showcasing the functionality of the Exploratory Modeling workbench. Exploratory modeling entails investigating the way in which uncertainty and/or policy levers map to outcomes. To investigate these mappings, we can either use sampling based strategies (open exploration) or optimization based strategies (directed search).

In this tutorial, I will demonstrate in more detail how to use the workbench for directed search. We are using the same example as in the previous tutorials. When using optimization, it is critical that you specify for each Scalar Outcome the direction in which it should move. There are three possibilities: info which is ignored, maximize, and minimize. If the `kind` keyword argument is not specified, it defaults to info.

[1]:
```
from ema_workbench import RealParameter, ScalarOutcome, Constant, Model
from dps_lake_model import lake_model

model = Model("lakeproblem", function=lake_model)

# specify uncertainties
model.uncertainties = [
    RealParameter("b", 0.1, 0.45),
    RealParameter("q", 2.0, 4.5),
    RealParameter("mean", 0.01, 0.05),
    RealParameter("stdev", 0.001, 0.005),
    RealParameter("delta", 0.93, 0.99),
]

# set levers
model.levers = [
    RealParameter("c1", -2, 2),
```

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```
    RealParameter("c2", -2, 2),
    RealParameter("r1", 0, 2),
    RealParameter("r2", 0, 2),
    RealParameter("w1", 0, 1),
]

# specify outcomes
model.outcomes = [
    ScalarOutcome("max_P", ScalarOutcome.MINIMIZE),
    ScalarOutcome("utility", ScalarOutcome.MAXIMIZE),
    ScalarOutcome("inertia", ScalarOutcome.MAXIMIZE),
    ScalarOutcome("reliability", ScalarOutcome.MAXIMIZE),
]

# override some of the defaults of the model
model.constants = [
    Constant("alpha", 0.41),
    Constant("nsamples", 150),
    Constant("myears", 100),
]
```

Using directed search with the ema_workbench requires platypus-opt. Please check the installation suggestions provided in the readme of the github repository. I personally either install from github directly

```
pip git+https://github.com/Project-Platypus/Platypus.git
```

or through pip

```
pip install platypus-opt
```

One note of caution: don't install platypus, but platypus-opt. There exists a python package on pip called platypus, but that is quite a different kind of library.

There are three ways in which we can use optimization in the workbench: 1. Search over the decision levers, conditional on a reference scenario 2. Search over the uncertain factors, conditional on a reference policy 3. Search over the decision levers given a set of scenarios

1.8.1 Search over levers

Directed search is most often used to search over the decision levers in order to find good candidate strategies. This is for example the first step in the Many Objective Robust Decision Making process. This is straightforward to do with the workbench using the optimize method.

Note that I have kept the number of functional evaluations (nfe) very low. In real applications this should be substantially higher and be based on convergence considerations which are demonstrated below.

[2]:
```
from ema_workbench import MultiprocessingEvaluator, ema_logging

ema_logging.log_to_stderr(ema_logging.INFO)

with MultiprocessingEvaluator(model) as evaluator:
    results = evaluator.optimize(nfe=250, searchover="levers", epsilons=[0.1] *␣
↪len(model.outcomes))
```

```
[MainProcess/INFO] pool started with 10 workers
298it [00:03, 75.48it/s]
[MainProcess/INFO] optimization completed, found 5 solutions
[MainProcess/INFO] terminating pool
```

The results from optimize is a DataFrame with the decision variables and outcomes of interest. This dataframe contains both the decision variables (c1-w1) and the outcomes (max_P-reliability). Each row is thus a single unique solution.

Note also that there might be a difference between the specified number of nfe (250 in this case) and the actual number of nfe. The default algorithm is population based and the nfe-based stopping condition is only checked after evaluating an entire generation.

[3]:
```
results
```

[3]:
```
         c1        c2        r1        r2        w1     max_P   utility  \
0 -0.682559  0.026569  1.738125  1.035683  0.514804  2.283760  1.655153
1 -1.667796 -0.624652  0.914360  0.582130  0.243352  2.283627  1.778130
2  1.869933  1.822573  0.798277  0.886831  0.686324  1.961235  0.615122
3  0.442190  1.680330  0.989541  1.958483  0.979940  0.190612  0.523998
4  0.096997  0.329009  0.500270  0.946994  0.344109  0.092322  0.233183

   inertia  reliability
0     0.99     0.100133
1     0.99     0.070000
2     0.99     0.070000
3     0.99     1.000000
4     0.99     1.000000
```

Specifying constraints

It is possible to specify a constrained optimization problem. A model can have one or more constraints. A constraint can be applied to the model input parameters (both uncertainties and levers), and/or outcomes. A constraint is essentially a function that should return the distance from the feasibility threshold. The distance should be 0 if the constraint is met.

In the example below, we add a constrait saying that the value of the outcome `max_P` should be below 1. Given that this is a very simple constrain, I chose to use a lambda function to implement it. For more complicated constraints, you can also define your own function and pass that instead.

[4]:
```
from ema_workbench import Constraint

constraints = [Constraint("max pollution", outcome_names="max_P", function=lambda x:␣
↪max(0, x - 1))]
```

[5]:
```
from ema_workbench import MultiprocessingEvaluator
from ema_workbench import ema_logging

ema_logging.log_to_stderr(ema_logging.INFO)

with MultiprocessingEvaluator(model) as evaluator:
    results = evaluator.optimize(
        nfe=250, searchover="levers", epsilons=[0.1] * len(model.outcomes),␣
↪constraints=constraints
    )
```

```
[MainProcess/INFO] pool started with 10 workers
298it [00:03, 76.22it/s]
[MainProcess/INFO] optimization completed, found 2 solutions
[MainProcess/INFO] terminating pool
```

[6]:
```
results
```

[6]:
```
         c1        c2        r1        r2        w1     max_P   utility  \
0  0.517330  0.130095  1.648766  1.005694  0.616171  0.093374  0.232173
1  0.034839  0.763078  1.654288  1.185964  0.783527  0.190797  0.510802

   inertia  reliability
0     0.99          1.0
1     0.99          1.0
```

The new results with this simple constraint contains only a few solutions. This suggests that it is difficult to find solutions that are able to meet this constraint.

Seed analysis

Genetic algorithms rely on randomness in the search process. This implies that a single run of the algorithm does not tell you that much because the results might be due to randomness. It is thus best practice to allways repeat the optimization for several different seeds and next merge the results across the different optimizations. This is supported by the workbench. We first need to run multiple optimization like this:

[7]:
```
results = []
with MultiprocessingEvaluator(model) as evaluator:
    # we run 5 seperate optimizations
    for _ in range(5):
        result = evaluator.optimize(
            nfe=5000, searchover="levers", epsilons=[0.05] * len(model.outcomes)
        )
        results.append(result)
```

```
[MainProcess/INFO] pool started with 10 workers
5036it [00:37, 133.58it/s]
[MainProcess/INFO] optimization completed, found 25 solutions
5058it [00:36, 140.03it/s]
[MainProcess/INFO] optimization completed, found 41 solutions
5049it [00:35, 140.43it/s]
[MainProcess/INFO] optimization completed, found 26 solutions
5054it [00:35, 140.87it/s]
[MainProcess/INFO] optimization completed, found 16 solutions
5052it [00:36, 140.17it/s]
[MainProcess/INFO] optimization completed, found 30 solutions
[MainProcess/INFO] terminating pool
```

We now have the results for each of the five different runs of the optimization. The next step is to combine these into a singe comprehensive set. Since by default the workbench uses -NSGAII, it makes sense to also merge the results across the seeds using an -nondominated sort.

[11]:
```
from ema_workbench.em_framework.optimization import epsilon_nondominated, to_problem
```

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```
problem = to_problem(model, searchover="levers")
epsilons = [0.05] * len(model.outcomes)
merged_archives = epsilon_nondominated(results, epsilons, problem)
```

[9]:
```
merged_archives.shape
```

[9]:
```
(34, 9)
```

As can be seen, the new merged archive contains 34 solutions. Which is is quite a bit smaller than the sum of solutions across the 5 seeds. This implies that many of the solutions found in each seed land in the same -gridcell.

Tracking convergence

An important part of using many-objective evolutionary algorithms is to carefully monitor whether they have converged to the best possible solutions. Various different metrics can be used for this. Some of these metrics must be collected at runtime, such as -progress. Others, like hypervolume, are better calculated after the optimization has been completed. The metrics that are better calculated after the optimization require, however, storing the state of the archive over the course of the optimization. Both types of metrics are supported by the workbench.

[23]:
```
from ema_workbench.em_framework.optimization import ArchiveLogger, EpsilonProgress

# we need to store our results for each seed
results = []
convergences = []

with MultiprocessingEvaluator(model) as evaluator:
    # we run again for 5 seeds
    for i in range(5):
        # we create 2 covergence tracker metrics
        # the archive logger writes the archive to disk for every x nfe
        # the epsilon progress tracks during runtime
        convergence_metrics = [
            ArchiveLogger(
                "./archives",
                [l.name for l in model.levers],
                [o.name for o in model.outcomes],
                base_filename=f"{i}.tar.gz",
            ),
            EpsilonProgress(),
        ]

        result, convergence = evaluator.optimize(
            nfe=50000,
            searchover="levers",
            epsilons=[0.05] * len(model.outcomes),
            convergence=convergence_metrics,
        )

        results.append(result)
        convergences.append(convergence)
```

```
[MainProcess/INFO] pool started with 10 workers
50061it [06:17, 132.46it/s]
[MainProcess/INFO] optimization completed, found 39 solutions
50117it [06:23, 130.56it/s]
[MainProcess/INFO] optimization completed, found 31 solutions
50081it [06:11, 134.92it/s]
[MainProcess/INFO] optimization completed, found 32 solutions
50085it [05:57, 139.98it/s]
[MainProcess/INFO] optimization completed, found 37 solutions
50062it [1:12:08, 11.57it/s]
[MainProcess/INFO] optimization completed, found 33 solutions
[MainProcess/INFO] terminating pool
```

Varous metrics are provied by platypus. For details on these metrics see *e.g.*, Zatarain-Salazar et al (2016) and Gupta et al (2020) for hypervolume, generational distance and additive ϵ-indicator; Hadka and Reed (2012) for spacing; and Hadka and Reed (2013) for ϵ-pgrogress. To use these metrics, we first need to load the archives into memory. Next, these metrics need a set of platypus solutions, instead of the dataframes that the workbench has stored. Moreover, most of these metrics need a reference set. The reference set, typically, is the union of best solutions found across the seeds and next filtered using an -nondominated sort. All these steps are supported by the workbench as shown below.

[24]:
```
all_archives = []

for i in range(5):
    archives = ArchiveLogger.load_archives(f"./archives/{i}.tar.gz")
    all_archives.append(archives)
```

[25]:
```
from ema_workbench import (
    HypervolumeMetric,
    GenerationalDistanceMetric,
    EpsilonIndicatorMetric,
    InvertedGenerationalDistanceMetric,
    SpacingMetric,
)
from ema_workbench.em_framework.optimization import to_problem

problem = to_problem(model, searchover="levers")

reference_set = epsilon_nondominated(results, [0.05] * len(model.outcomes), problem)

hv = HypervolumeMetric(reference_set, problem)
gd = GenerationalDistanceMetric(reference_set, problem, d=1)
ei = EpsilonIndicatorMetric(reference_set, problem)
ig = InvertedGenerationalDistanceMetric(reference_set, problem, d=1)
sm = SpacingMetric(problem)


metrics_by_seed = []
for archives in all_archives:
    metrics = []
    for nfe, archive in archives.items():
        scores = {
            "generational_distance": gd.calculate(archive),
            "hypervolume": hv.calculate(archive),
```

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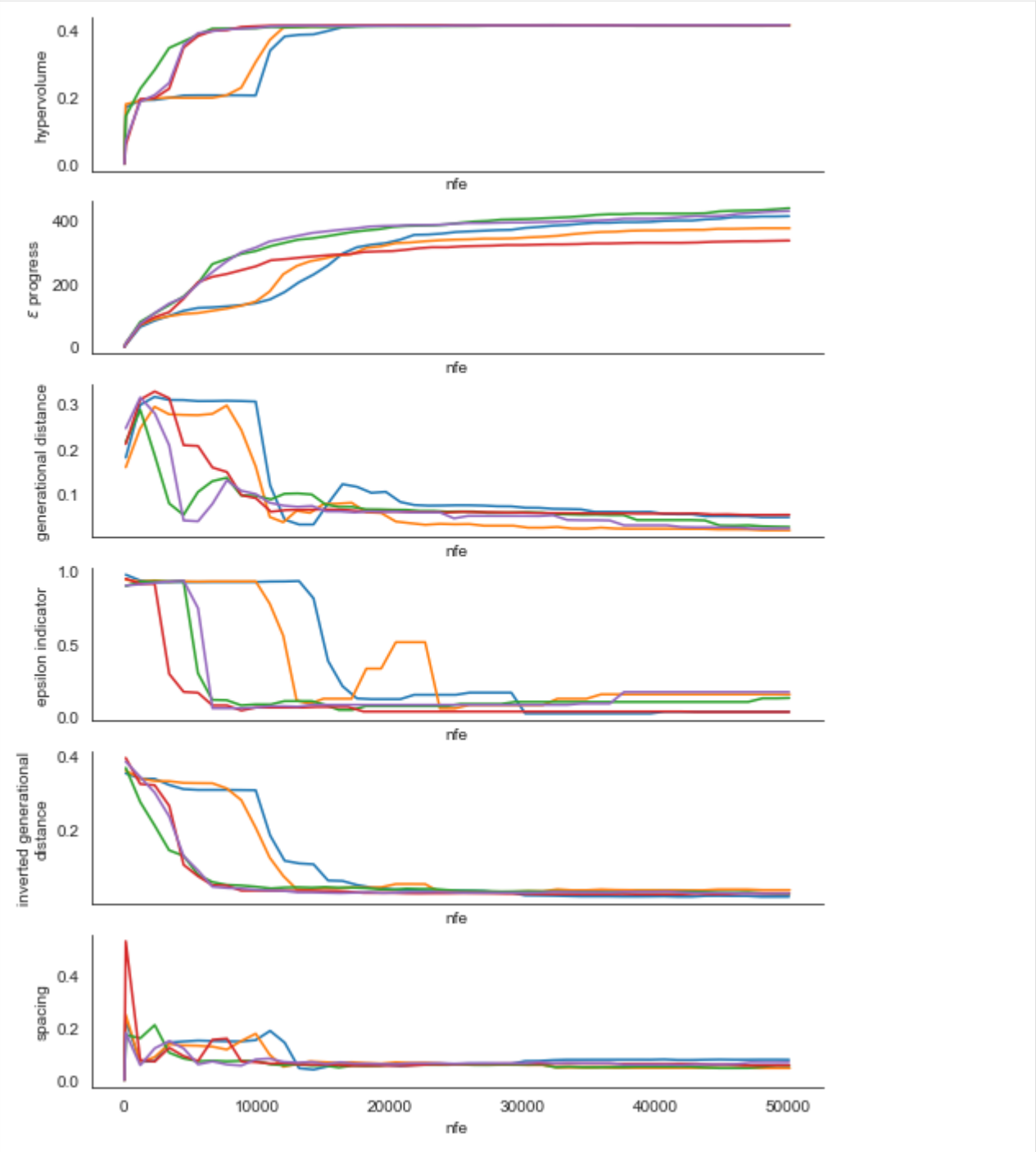
```
            "epsilon_indicator": ei.calculate(archive),
            "inverted_gd": ig.calculate(archive),
            "spacing": sm.calculate(archive),
            "nfe": int(nfe),
        }
        metrics.append(scores)
    metrics = pd.DataFrame.from_dict(metrics)

    # sort metrics by number of function evaluations
    metrics.sort_values(by="nfe", inplace=True)
    metrics_by_seed.append(metrics)
```

Now that we have calculated all our metrics, we can visualize them using matplotlib.

[26]:
```
sns.set_style("white")
fig, axes = plt.subplots(nrows=6, figsize=(8, 12), sharex=True)

ax1, ax2, ax3, ax4, ax5, ax6 = axes

for metrics, convergence in zip(metrics_by_seed, convergences):
    ax1.plot(metrics.nfe, metrics.hypervolume)
    ax1.set_ylabel("hypervolume")

    ax2.plot(convergence.nfe, convergence.epsilon_progress)
    ax2.set_ylabel("$\epsilon$ progress")

    ax3.plot(metrics.nfe, metrics.generational_distance)
    ax3.set_ylabel("generational distance")

    ax4.plot(metrics.nfe, metrics.epsilon_indicator)
    ax4.set_ylabel("epsilon indicator")

    ax5.plot(metrics.nfe, metrics.inverted_gd)
    ax5.set_ylabel("inverted generational\ndistance")

    ax6.plot(metrics.nfe, metrics.spacing)
    ax6.set_ylabel("spacing")

ax6.set_xlabel("nfe")


sns.despine(fig)

plt.show()
```



As we can see, for this problem across all the metrics and for each of the seeds we see that the line stabilizes which is indicative of convergence. The fact that the lines for each of the seeds stabilizes at roughly the same value moreover suggests that the seeds are converging to similar sets of solutions.

Changing the reference scenario

The workbench offers control over the reference scenario or policy under which you are performing the optimization. This makes it easy to apply multi-scenario MORDM (Watson & Kasprzyk, 2017;Eker & Kwakkel, 2018;Bartholomew & Kwakkel, 2020). Alternatively, you can also use it to change the policy for which you are applying worst case scenario discovery (see below).

```
reference = Scenario('reference', b=0.4, q=2, mean=0.02, stdev=0.01)

with MultiprocessingEvaluator(lake_model) as evaluator:
    results = evaluator.optimize(searchover='levers', nfe=1000,
                         epsilons=[0.1, ]*len(lake_model.outcomes),
                         reference=reference)
```

1.8.2 Search over uncertainties: worst case discovery

Up till now, the focus has been on applying search to find promising candidate strategies. That is, we search through the lever space. However, there might also be good reasons to search through the uncertainty space. For example to search for worst case scenarios (Halim et al, 2015). This is easily achieved as shown below. We change the kind attribute on each outcome so that we search for the worst outcome and specify that we would like to search over the uncertainties instead of the levers.

Any of the foregoing additions such as constraints or convergence works as shown above. Note that if you would like to to change the reference policy, reference should be a Policy object rather than a Scenario object.

[7]:
```
# change outcomes so direction is undesirable
minimize = ScalarOutcome.MINIMIZE
maximize = ScalarOutcome.MAXIMIZE

for outcome in model.outcomes:
    if outcome.kind == minimize:
        outcome.kind = maximize
    else:
        outcome.kind = minimize

with MultiprocessingEvaluator(model) as evaluator:
    results = evaluator.optimize(
        nfe=1000, searchover="uncertainties", epsilons=[0.1] * len(model.outcomes)
    )
```

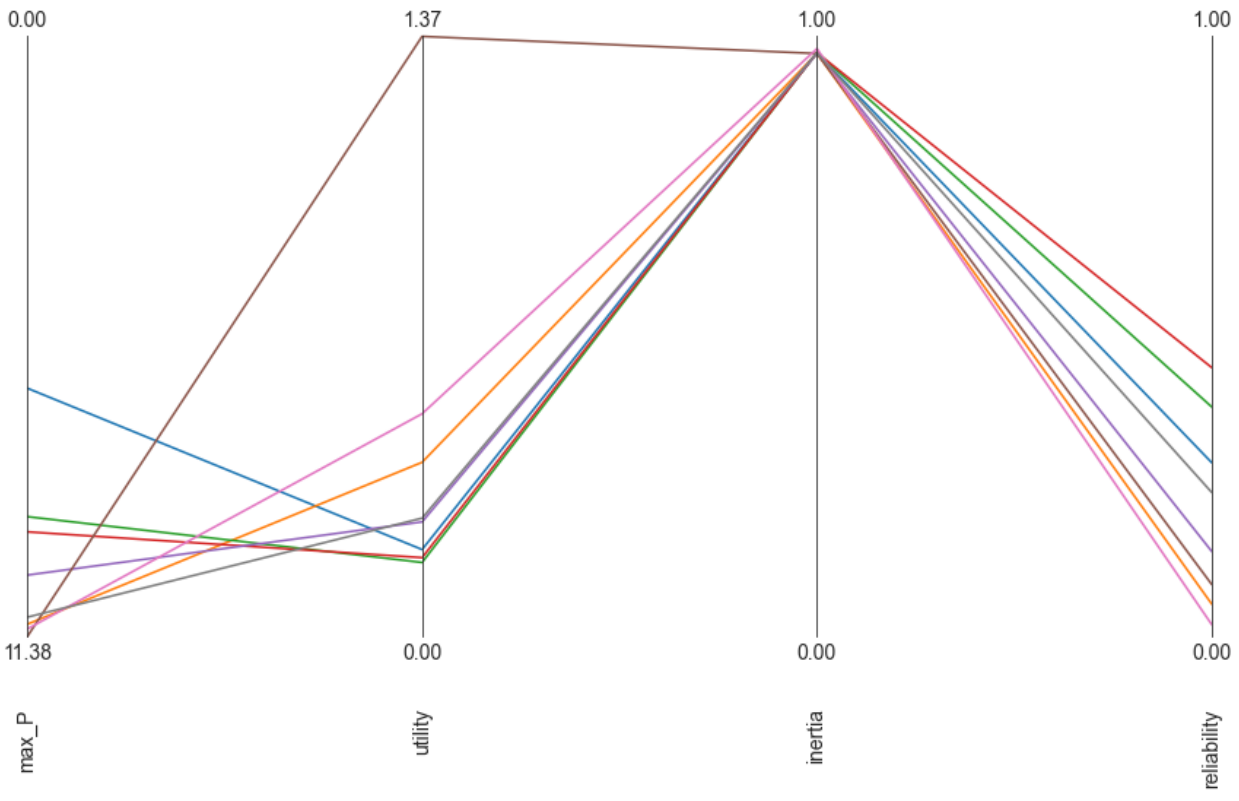
```
[MainProcess/INFO] pool started with 10 workers
1090it [00:09, 116.02it/s]
[MainProcess/INFO] optimization completed, found 8 solutions
[MainProcess/INFO] terminating pool
```

1.8.3 Parallel coordinate plots

The workbench comes with support for making parallel axis plots through the parcoords module. This module offers a parallel axes object on which we can plot data.

The typical workflow is to first instantiate this parallel axes object given a pandas dataframe with the upper and lower limits for each axes. Next, one or more datasets can be plotted on this axes. Any dataframe passed to the plot method will be normalized using the limits passed first. We can also invert any of the axes to ensure that the desirable direction is the same for all axes.

[9]:
```
from ema_workbench.analysis import parcoords

data = results.loc[:, [o.name for o in model.outcomes]]

# get the minimum and maximum values as present in the dataframe
limits = parcoords.get_limits(data)

# we know that the lowest possible value for all objectives is 0
limits.loc[0, ["utility", "inertia", "reliability", "max_P"]] = 0
# inertia and reliability are defined on unit interval, so their theoretical maximum is 1
limits.loc[1, ["inertia", "reliability"]] = 1

paraxes = parcoords.ParallelAxes(limits)
paraxes.plot(data)
paraxes.invert_axis("max_P")
plt.show()
```



The above parallel coordinate plot shows the results from the worst case discovery. The worst possible solution would

be a straight line at the bottom. A key insight from this result is that there seems to be a trade-off between max_P and utility. This can be inferred from the crossing lines between these two axes.

1.8.4 Robust Search

In the foregoing, we have been using optimization over levers or uncertainties, while assuming a reference scenario or policy. However, we can also formulate a robust many objective optimization problem (Kwakkel et al. 2015; Bartholomew et al. 2020), where we are going to search over the levers for solutions that have robust performance over a set of scenarios. To do this with the workbench, there are several steps that one has to take.

First, we need to specify our robustness metrics. A robustness metric takes as input the performance of a candidate policy over a set of scenarios and returns a single robustness score. For a more in depth overview, see McPhail et al. (2018). In case of the workbench, we can use the ScalarOutcome class for this. We need to specify the name of the robustness metric a function that takes as input a numpy array and returns a single number, and the model outcome to which this function should be applied.

Below, we use a percentile based robustness metric, which we apply to each model outcome.

[20]:
```
import functools

# our robustness functions
percentile10 = functools.partial(np.percentile, q=10)
percentile90 = functools.partial(np.percentile, q=90)

# convenient short hands
MAXIMIZE = ScalarOutcome.MAXIMIZE
MINIMIZE = ScalarOutcome.MINIMIZE

robustnes_functions = [
    ScalarOutcome(
        "90th percentile max_p", kind=MINIMIZE, variable_name="max_P",␣
↪function=percentile90
    ),
    ScalarOutcome(
        "10th percentile reliability",
        kind=MAXIMIZE,
        variable_name="reliability",
        function=percentile10,
    ),
    ScalarOutcome(
        "10th percentile inertia", kind=MAXIMIZE, variable_name="inertia",␣
↪function=percentile10
    ),
    ScalarOutcome(
        "10th percentile utility", kind=MAXIMIZE, variable_name="utility",␣
↪function=percentile10
    ),
]
```

Next, we have to generate the scenarios we want to use. Below we generate 10 scenarios, which we will keep fixed over the optimization. The exact number of scenarios to use is to be established through trial and error. Typically it involves balancing computational costs of more scenarios, with the stability of the robustness metric over the number of scenarios

[23]:
```
from ema_workbench.em_framework import sample_uncertainties

n_scenarios = 10
scenarios = sample_uncertainties(model, n_scenarios)
```

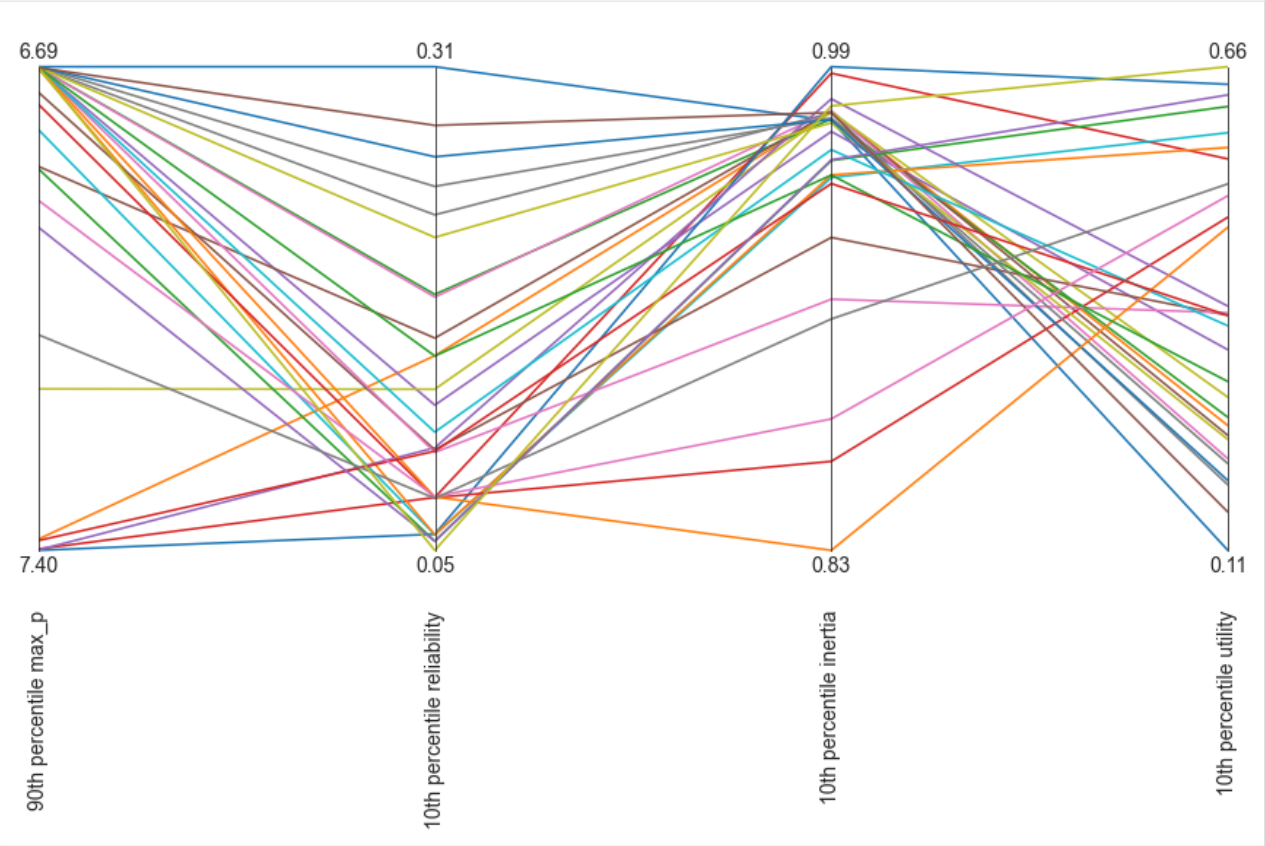
With the robustness metrics specified, and the scenarios, sampled, we can now perform robust many-objective optimization. Below is the code that one would run. Note that this is computationally very expensive since each candidate solution is going to be run for ten scenarios before we can calculate the robustness for each outcome of interest.

[24]:
```
from ema_workbench.em_framework import ArchiveLogger

nfe = int(5e4)
with MultiprocessingEvaluator(model) as evaluator:
    robust_results = evaluator.robust_optimize(
        robustnes_functions,
        scenarios,
        nfe=nfe,
        epsilons=[
            0.025,
        ]
        * len(robustnes_functions),
    )
```

```
[MainProcess/INFO] pool started with 10 workers
50039it [2:10:57,  6.37it/s]
[MainProcess/INFO] optimization completed, found 29 solutions
[MainProcess/INFO] terminating pool
```

We can now again visualize the results using a parallel coordinate plot. Note that we are visualizing the robustness scores rather than the outcomes of interest as specified in the underlying model.

[29]:
```
from ema_workbench.analysis import parcoords


data = robust_results.loc[:, [o.name for o in robustnes_functions]]
limits = parcoords.get_limits(data)

paraxes = parcoords.ParallelAxes(limits)
paraxes.plot(data)
paraxes.invert_axis("90th percentile max_p")
plt.show()
```



What we can see in this parallel axis plot is that there is a clear tradeoff between robust high reliability and robsut low maximum polution. Likewise with inertia and utility. This can be seen from the crossing lines between these respective axes.

[ ]:

1.9 MPIEvaluator: Run on multi-node HPC systems

The `MPIEvaluator` is a new addition to the EMAworkbench that allows experiment execution on multi-node systems, including high-performance computers (HPCs). This capability is particularly useful if you want to conduct large-scale experiments that require distributed processing. Under the hood, the evaluator leverages the `MPIPoolExecutor` from `` `mpi4py.futures <https://mpi4py.readthedocs.io/en/stable/mpi4py.futures.html>`__ ``.

1.9.1 Limiations

- Currently, the MPIEvaluator is only tested on Linux and macOS, while it might work on other operating systems.
- Currently, the MPIEvaluator only works with Python-based models, and won't work with file-based model types (like NetLogo or Vensim).
- The MPIEvaluator is most useful for large-scale experiments, where the time spent on distributing the experiments over the cluster is negligible compared to the time spent on running the experiments. For smaller experiments, the overhead of distributing the experiments over the cluster might be significant, and it might be more efficient to run the experiments locally.

The MPIEvaluator is experimental and its interface and functionality might change in future releases. We appreciate feedback on the MPIEvaluator, share any thoughts about it at https://github.com/quaquel/EMAworkbench/discussions/311.

1.9.2 Contents

This tutorial will first show how to set up the environment, and then how to use the MPIEvaluator to run a model on a cluster. Finally, we'll use the DelftBlue supercomputer as an example, to show how to run on a system which uses a SLURM scheduler.

1. Setting up the environment

To use the MPIEvaluator, MPI and mpi4py must be installed.

Installing MPI on Linux typically involves the installation of a popular MPI implementation such as OpenMPI or MPICH. Below are the instructions for installing OpenMPI:

1a. Installing OpenMPI

If you use conda, it might install MPI automatically along when installing mpi4py (see 1b).

You can install OpenMPI using you package manager. First, update your package repositories, and then install OpenMPI:

For **Debian/Ubuntu**: `bash sudo apt update sudo apt install openmpi-bin libopenmpi-dev`

For **Fedora**: `bash sudo dnf check-update sudo dnf install openmpi openmpi-devel`

For **CentOS/RHEL**: `bash sudo yum update sudo yum install openmpi openmpi-devel`

Many times, the necessary environment variables are automatically set up. You can check if this is the case by running the following command:

```
mpiexec --version
```

If not, add OpenMPI's `bin` directory to your `PATH`:

```
export PATH=$PATH:/usr/lib/openmpi/bin
```

1b. Installing mpi4py

The python package mpi4py needs to installed as well. This is most easily done from PyPI, by running the following command:

```
pip install -U mpi4py
```

2. Creating a model

First, let's set up a minimal model to test with. This can be any Python-based model, we're using the `example_python.py <https://emaworkbench.readthedocs.io/en/latest/examples/example_python.html>`__ model from the EMA Workbench documentation as example.

We recommend crafting and testing your model in a separate Python file, and then importing it into your main script. This way, you can test your model without having to run it through the MPIEvaluator, and you can easily switch between running it locally and on a cluster.

2a. Define the model

First, we define a Python model function.

```
[ ]: def some_model(x1=None, x2=None, x3=None):
         return {"y": x1 * x2 + x3}
```

Now, create the EMAworkbench model object, and specify the uncertainties and outcomes:

```
[ ]: from ema_workbench import Model, RealParameter, ScalarOutcome, ema_logging, perform_
     ↪experiments

     if __name__ == "__main__":
         # We recommend setting pass_root_logger_level=True when running on a cluster, to␣
     ↪ensure consistent log levels.
         ema_logging.log_to_stderr(level=ema_logging.INFO, pass_root_logger_level=True)

         ema_model = Model("simpleModel", function=some_model)  # instantiate the model

         # specify uncertainties
         ema_model.uncertainties = [
             RealParameter("x1", 0.1, 10),
             RealParameter("x2", -0.01, 0.01),
             RealParameter("x3", -0.01, 0.01),
         ]
         # specify outcomes
         ema_model.outcomes = [ScalarOutcome("y")]
```

2b. Test the model

Now, we can run the model locally to test it:

```
[ ]: from ema_workbench import SequentialEvaluator

     with SequentialEvaluator(ema_model) as evaluator:
         results = perform_experiments(ema_model, 100, evaluator=evaluator)
```

In this stage, you can test your model and make sure it works as expected. You can also check if everything is included in the results and do initial validation on the model, before scaling up to a cluster.

3. Run the model on a MPI cluster

Now that we have a working model, we can run it on a cluster. To do this, we need to import the `MPIEvaluator` class from the `ema_workbench` package, and instantiate it with our model. Then, we can use the `perform_experiments` function as usual, and the MPIEvaluator will take care of distributing the experiments over the cluster. Finally, we can save the results to a tarball, as usual.

[ ]:
```python
# ema_example_model.py
from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    ema_logging,
    perform_experiments,
    MPIEvaluator,
    save_results,
)


def some_model(x1=None, x2=None, x3=None):
    return {"y": x1 * x2 + x3}


if __name__ == "__main__":
    ema_logging.log_to_stderr(level=ema_logging.INFO, pass_root_logger_level=True)

    ema_model = Model("simpleModel", function=some_model)

    ema_model.uncertainties = [
        RealParameter("x1", 0.1, 10),
        RealParameter("x2", -0.01, 0.01),
        RealParameter("x3", -0.01, 0.01),
    ]
    ema_model.outcomes = [ScalarOutcome("y")]

    # Note that we switch to the MPIEvaluator here
    with MPIEvaluator(ema_model) as evaluator:
        results = evaluator.perform_experiments(scenarios=10000)

    # Save the results
    save_results(results, "ema_example_model.tar.gz")
```

To run this script on a cluster, we need to use the `mpiexec` command:

```
mpiexec -n 1 python ema_example_model.py
```

This command will execute the `ema_example_model.py` Python script using MPI. MPI-specific configurations are inferred from default settings or any configurations provided elsewhere, such as in an MPI configuration file or additional flags to `mpiexec` (not shown in the provided command). The number of workers that will be spawned by the MPIEvaluator depends on the MPI universe size. The way this size can be controlled depends on which implementation of MPI you have. See the discussion in the docs of mpi4py for details.

The output of the script will be saved to the `ema_mpi_test.tar.gz` file, which can be loaded and analyzed later as usual.

Example: Running on the DelftBlue supercomputer (with SLURM)

As an example, we'll show how to run the model on the DelftBlue supercomputer, which uses the SLURM scheduler. The DelftBlue supercomputer is a cluster of 218 nodes, each with 2 Intel Xeon Gold E5-6248R CPUs (48 cores total), 192 GB of RAM, and 480 GB of local SSD storage. The nodes are connected with a 100 Gbit/s Infiniband network.

*These steps roughly follow the*DelftBlue Crash-course for absolute beginners*. If you get stuck, you can refer to that guide for more information.*

1. Creating a SLURM script

First, you need to create a SLURM script. This is a bash script that will be executed on the cluster, and it will contain all the necessary commands to run your model. You can create a new file, for example `slurm_script.sh`, and add the following lines:

```
#!/bin/bash

#SBATCH --job-name="Python_test"
#SBATCH --time=00:02:00
#SBATCH --ntasks=10
#SBATCH --cpus-per-task=1
#SBATCH --partition=compute
#SBATCH --mem-per-cpu=4GB
#SBATCH --account=research-tpm-mas

module load 2023r1
module load openmpi
module load python
module load py-numpy
module load py-scipy
module load py-mpi4py
module load py-pip

pip install --user ema_workbench

mpiexec -n 1 python3 example_mpi_lake_model.py
```

Modify the script to suit your needs: - Set the `--job-name` to something descriptive. - Update the maximum `--time` to the expected runtime of your model. The job will be terminated if it exceeds this time limit. - Set the `--ntasks` to the number of cores you want to use. Each node in DelftBlue currently has 48 cores, so for example `--ntasks=96` might use two nodes, but can also be distributed over more nodes. Note that using MPI involves quite some overhead. If you do not plan to use more than 48 cores, you might want to consider using the MultiprocessingEvaluator and request exclusive node access (see below). - Update the memory `--mem-per-cpu` to the amount of memory you need per core. Each node has 192 GB of memory, so you can use up to 4 GB per core. - Add `--exclusive` if you want to claim a full node for your job. In that case, specify `--nodes` next to `--ntasks`. Requesting exclusive access to one or more nodes will delay you scheduling time, because you need to wait for the full nodes to become available. - Set the `--account` to your project account. You can find this on the Accounting and Shares page of the DelftBlue docs.

See Submit Jobs at the DelftBlue docs for more information on the SLURM script configuration.

Then, you need to load the necessary modules. You can find the available modules on the DHPC modules page of the DelftBlue docs. In this example, we're loading the 2023r1 toolchain, which includes Python 3.9, and then we're loading the necessary Python packages.

You might want to install additional Python packages. You can do this with `pip install -U --user`

<package>. Note that you need to use the --user flag, because you don't have root access on the cluster. To install the EMA Workbench, you can use pip install -U --user ema_workbench. If you want to install a development branch, you can use pip install -e -U --user git+https://github.com/quaquel/EMAworkbench@<BRANCH>#egg=ema-workbench, where <BRANCH> is the name of the branch you want to install.

Finally, the script uses mpiexec to run Python script in a way that allows the MPIEvaluator to distribute the experiments over the cluster. The -n 1 argument meanst that we only start a single process. This main process in turn will spawn additional worker processes. The number of worker processes that will spawn defaults to the value of --ntasks - 1.

Note that the bash scripts (sh), including the slurm_script.sh we just created, need LF line endings. If you are using Windows, line endings are CRLF by default, and you need to convert them to LF. You can do this with most text editors, like Notepad++ or Atom for example.

1. Setting up the environment

First, you need to log in on DelftBlue. As an employee, you can login from the command line with:

```
ssh <netid>@login.delftblue.tudelft.nl
```

where <netid> is your TU Delft netid. You can also use an SSH client such as PuTTY.

As a student, you need to jump though an extra hoop:

```
ssh -J <netid>@student-linux.tudelft.nl <netid>@login.delftblue.tudelft.nl
```

Note: Below are the commands for students. If you are an employee, you need to remove the -J <netid>@student-linux.tudelft.nl from all commands below.

Once you're logged in, you want to jump to your scratch directory (note it's not but is not backed up).

```
cd ../../scratch/<netid>
```

Create a new directory for this tutorial, for example mkdir ema_mpi_test and then cd ema_mpi_test

Then, you want to send your Python file and SLURM script to DelftBlue. Open a **new** command line terminal, and then you can do this with scp:

```
scp -J <netid>@student-linux.tudelft.nl ema_example_model.py slurm_script.sh <netid>
↪@login.delftblue.tudelft.nl:/scratch/<netid>/ema_mpi_test
```

Before scheduling the SLURM script, we first have to make it executable:

```
chmod +x slurm_script.sh
```

Then we can schedule it:

```
sbatch slurm_script.sh
```

Now it's scheduled!

You can check the status of your job with squeue:

```
squeue -u <netid>
```

You might want to inspect the log file, which is created by the SLURM script. You can do this with cat:

```
cat slurm-<jobid>.out
```

where <jobid> is the job ID of your job, which you can find with squeue.

When the job is finished, we can download the tarball with our results. Open the command line again (can be the same one as before), and you can copy the results back to your local machine with scp:

```
scp -J <netid>@student-linux.tudelft.nl <netid>@login.delftblue.tudelft.nl:/scratch/
↪<netid>/ema_mpi_test/ema_mpi_test.pickle .
```

Finally, we can clean up the files on DelftBlue, to avoid cluttering the scratch directory:

```
cd ..
rm -rf "ema_mpi_test"
```

[ ]:

1.10 Examples

1.10.1 Output space exploration

Output space exploration is a form of optimization based on novelty search. In the workbench, it relies on the optimization functionality. You can use output space exploration by passing an instance of either OutputSpaceExploration or AutoAdaptiveOutputSpaceExploration as algorithm to evaluator.optimize. The fact that output space exploration uses the optimization functionality also implies that we can track convergence in a similar manner. Epsilon progress is defined identical, but evidently other metrics such as hypervolume might not be applicable in the context of output space exploration.

The difference between OutputSpaceExploration and AutoAdaptiveOutputSpaceExploration is in the evolutionary operators. AutoAdaptiveOutputSpaceExploration uses auto adaptive operator selection as implemented in the BORG MOEA, while OutputSpaceExploration by default uses Simulated Binary crossover with polynomial mutation. Injection of new solutions is handled through auto adaptive population sizing and periodically starting with a new population if search is stalling. Below, examples are given of how to use both algorithms, as well as a a quick visualization of the convergence dynamics.

For this example, we are using a stylized case study frequently used to develop and test decision making under deep uncertainty methods: the shallow lake problem. In this problem, a city has to decide on the amount of pollution they are going to put into a shallow lake per year. The city gets benefits from polluting the lake, but if an unknown threshold is crossed, the lake permanently shifts to an undesirable polluted state. For further details on this case study, see for example Quinn et al, 2017 and Bartholomew et al, 2021.

[1]:
```
from outputspace_exploration_lake_model import lake_problem

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MultiprocessingEvaluator,
    Policy,
    SequentialEvaluator,
```

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```
    OutputSpaceExploration,
)
```

[2]:
```
ema_logging.log_to_stderr(ema_logging.INFO)

# instantiate the model
lake_model = Model("lakeproblem", function=lake_problem)
lake_model.time_horizon = 100

# specify uncertainties
lake_model.uncertainties = [
    RealParameter("b", 0.1, 0.45),
    RealParameter("q", 2.0, 4.5),
    RealParameter("mean", 0.01, 0.05),
    RealParameter("stdev", 0.001, 0.005),
    RealParameter("delta", 0.93, 0.99),
]

# set levers, one for each time step
lake_model.levers = [RealParameter(str(i), 0, 0.1) for i in range(lake_model.time_
↪horizon)]

# specify outcomes
# output space exploration

lake_model.outcomes = [
    ScalarOutcome("max_P", kind=ScalarOutcome.MAXIMIZE),
    ScalarOutcome("utility", kind=ScalarOutcome.MAXIMIZE),
    ScalarOutcome("inertia", kind=ScalarOutcome.MAXIMIZE),
    ScalarOutcome("reliability", kind=ScalarOutcome.MAXIMIZE),
]

# override some of the defaults of the model
lake_model.constants = [Constant("alpha", 0.41), Constant("nsamples", 150)]
```

Above, we have setup the lake problem, specified the uncertainties, policy levers, outcomes of interest and (optionally) some constants. We are now ready to run output space exploration on this model. For this, we use the default optimization functionality of the world bank, but pass the `OutputSpaceExploration` class. Below, we are running output space exploration over the uncertainties, which implies we need to pass a reference policy. We also rerun the algorithm for 5 different seeds. We can track convergence of the outputspace epxloration by tracking ϵ-progress.

The `grid_spec` keyword argument, which is specific to output space exploration specifies the grid structure we are imposing on the output space. There must be a tuple for each outcome of interest. Each tuple specifies the minimum value, the maximum value and the size of the grid cell on this outcome dimension.

[3]:
```
from ema_workbench.em_framework.optimization import EpsilonProgress

# generate some default policy
reference = Policy("nopolicy", **{l.name: 0.02 for l in lake_model.levers})
n_seeds = 5

convergences = []
```

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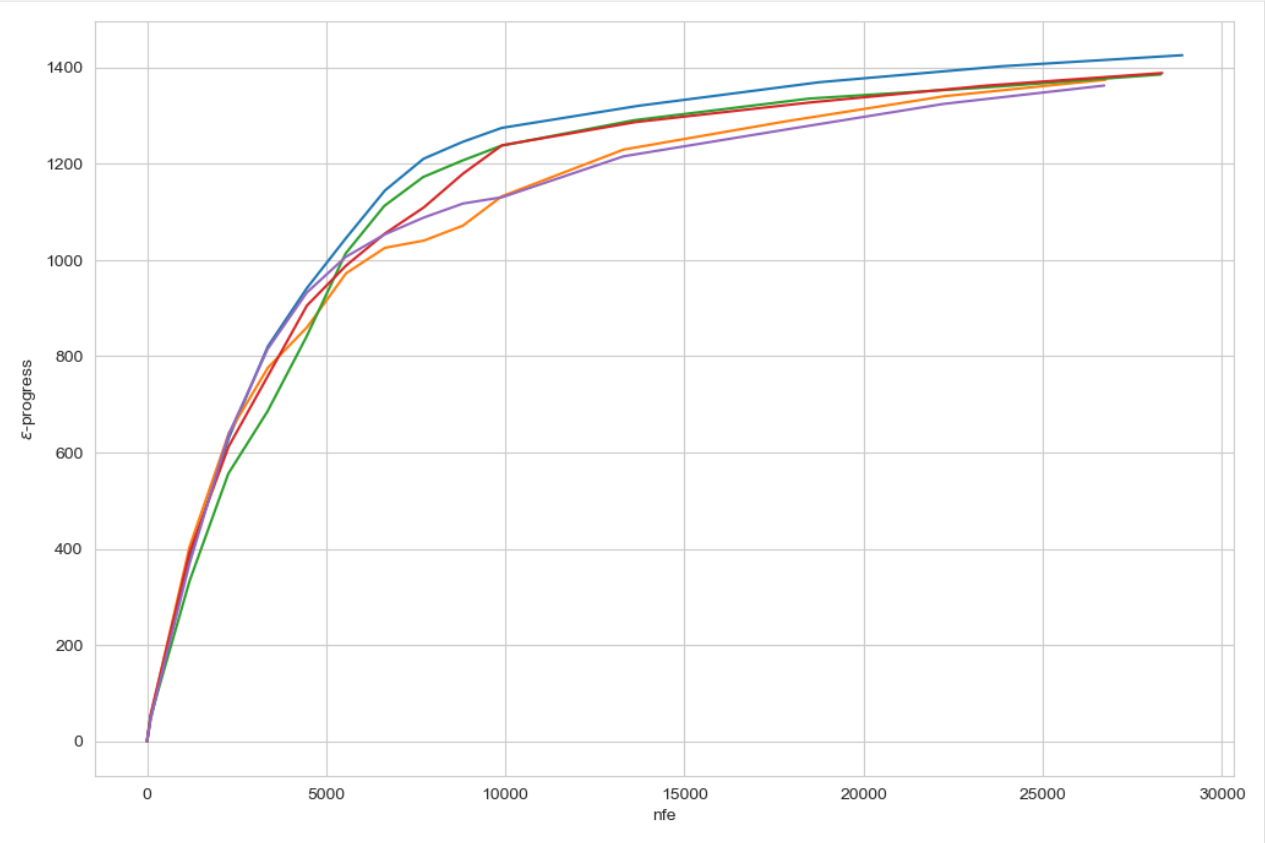
```
with MultiprocessingEvaluator(lake_model) as evaluator:
    for _ in range(n_seeds):
        convergence_metrics = [
            EpsilonProgress(),
        ]
        res, convergence = evaluator.optimize(
            algorithm=OutputSpaceExploration,
            grid_spec=[(0, 12, 0.5), (0, 0.6, 0.05), (0, 1, 0.1), (0, 1, 0.1)],
            nfe=25000,
            searchover="uncertainties",
            reference=reference,
            convergence=convergence_metrics,
        )
        convergences.append(convergence)
```

```
[MainProcess/INFO] pool started with 10 workers
28893it [01:37, 296.69it/s]
[MainProcess/INFO] optimization completed, found 1425 solutions
26750it [01:30, 294.10it/s]
[MainProcess/INFO] optimization completed, found 1374 solutions
28290it [01:35, 297.43it/s]
[MainProcess/INFO] optimization completed, found 1385 solutions
28332it [01:35, 296.93it/s]
[MainProcess/INFO] optimization completed, found 1388 solutions
26712it [01:31, 290.48it/s]
[MainProcess/INFO] optimization completed, found 1362 solutions
[MainProcess/INFO] terminating pool
```

[4]:
```
import matplotlib.pyplot as plt
import seaborn as sns

sns.set_style("whitegrid")
fig, ax = plt.subplots()
for convergence in convergences:
    ax.plot(convergence.nfe, convergence.epsilon_progress)

ax.set_xlabel("nfe")
ax.set_ylabel("$\epsilon$-progress")
plt.show()
```



The figure above shows the ϵ-progress per nfe for each of the five random seeds. As can be seen, the algorithm converges to essentially the same amount of epsilon progress across the seeds. This suggests that the algorithm has converged and thus found all possible output grid cells.

auto adaptive operator selection

The foregoing example used the default version of the output space exploration algorithm. This algorithm uses Simulated Binary Crossover (SBX) with Polynomial Mutation (PM) as its evolutionary operators. However, it is conceivable that for some problems other evolutionary operators might be more suitable. You can pass your own combination of operators if desired using platypus. For general use, however, it can sometimes be easier to let the algorithm itself figure out which operators to use. To support this, we also provide an `AutoAdaptiveOutputSpaceExploration` algorithm. This algorithm uses Auto Adaptive Operator selection as also used in the BORG algorithm. Note that this algorithm is limited to RealParameters only.

[5]:
```
from ema_workbench.em_framework.outputspace_exploration import␣
↪AutoAdaptiveOutputSpaceExploration
from ema_workbench.em_framework.optimization import OperatorProbabilities


convergences = []

with MultiprocessingEvaluator(lake_model) as evaluator:
    for _ in range(5):
        convergence_metrics = [
            EpsilonProgress(),
```

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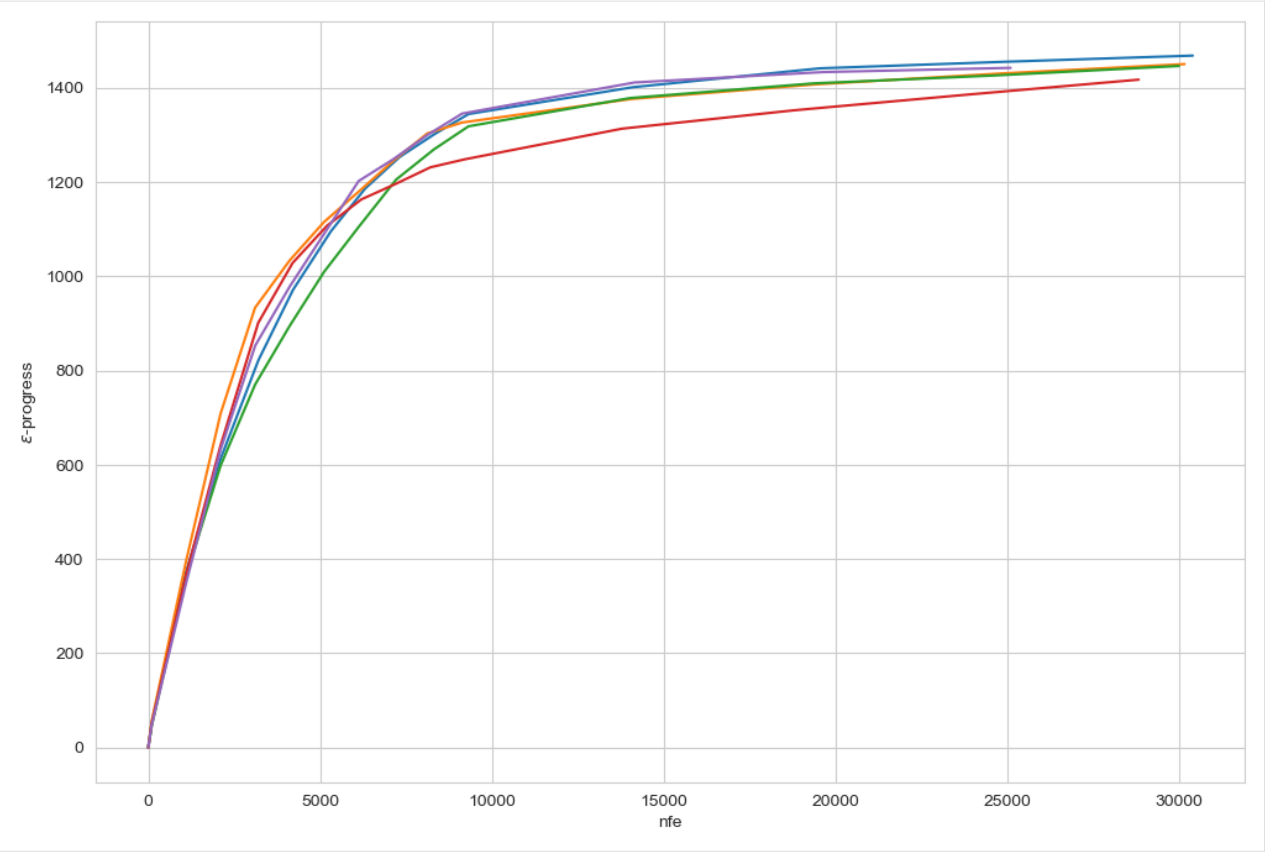
```
            OperatorProbabilities("SBX", 0),
            OperatorProbabilities("PCX", 1),
            OperatorProbabilities("DE", 2),
            OperatorProbabilities("UNDX", 3),
            OperatorProbabilities("SPX", 4),
            OperatorProbabilities("UM", 5),
        ]
        res, convergence = evaluator.optimize(
            algorithm=AutoAdaptiveOutputSpaceExploration,
            grid_spec=[(0, 12, 0.5), (0, 0.6, 0.05), (0, 1, 0.1), (0, 1, 0.1)],
            nfe=25000,
            searchover="uncertainties",
            reference=reference,
            variator=None,
            convergence=convergence_metrics,
        )
        convergences.append(convergence)
```

```
[MainProcess/INFO] pool started with 10 workers
30388it [01:48, 279.93it/s]
[MainProcess/INFO] optimization completed, found 1468 solutions
30150it [01:46, 282.56it/s]
[MainProcess/INFO] optimization completed, found 1450 solutions
29988it [01:48, 275.21it/s]
[MainProcess/INFO] optimization completed, found 1446 solutions
28816it [01:40, 286.94it/s]
[MainProcess/INFO] optimization completed, found 1417 solutions
25088it [01:28, 284.70it/s]
[MainProcess/INFO] optimization completed, found 1442 solutions
[MainProcess/INFO] terminating pool
```

[6]:
```
sns.set_style("whitegrid")
fig, ax = plt.subplots()
for convergence in convergences:
    ax.plot(convergence.nfe, convergence.epsilon_progress)

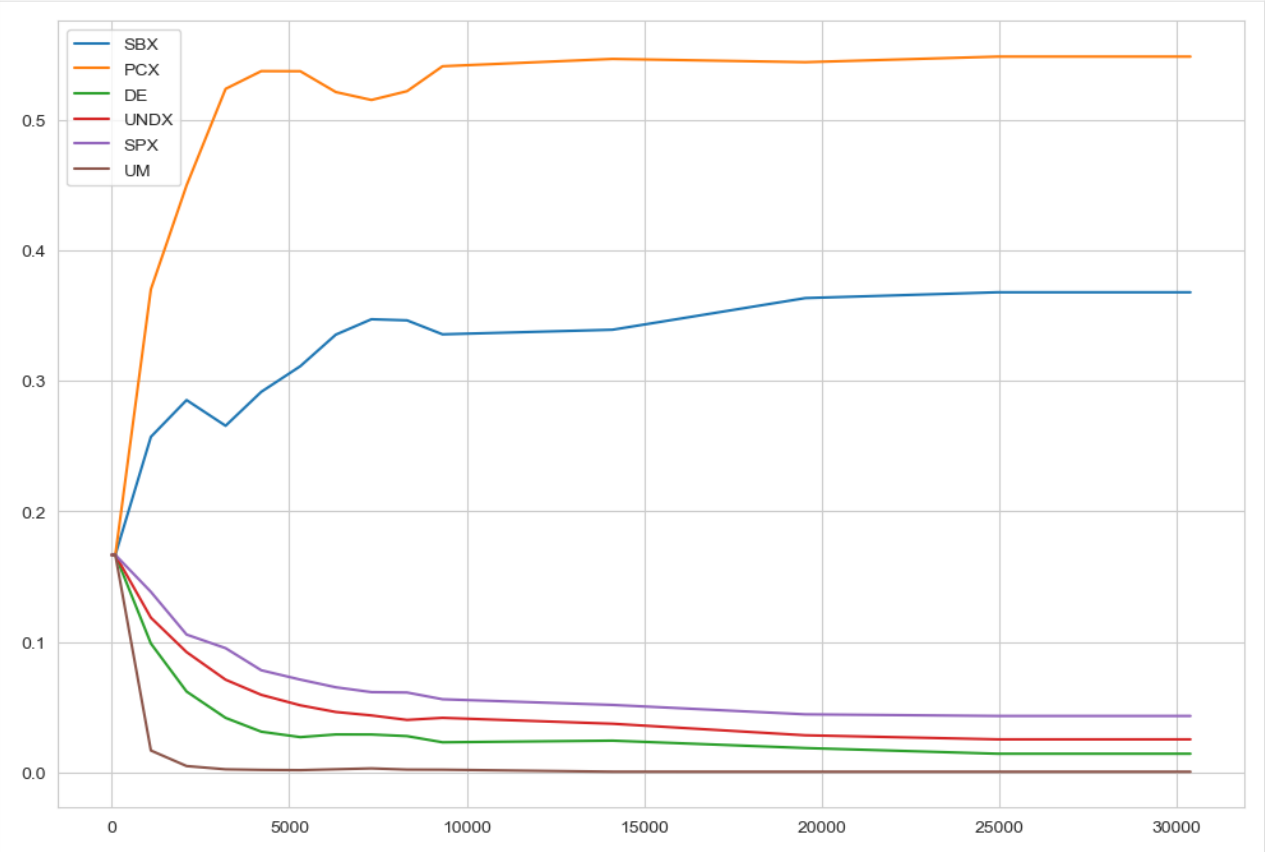
ax.set_xlabel("nfe")
ax.set_ylabel("$\epsilon$-progress")
plt.show()
```

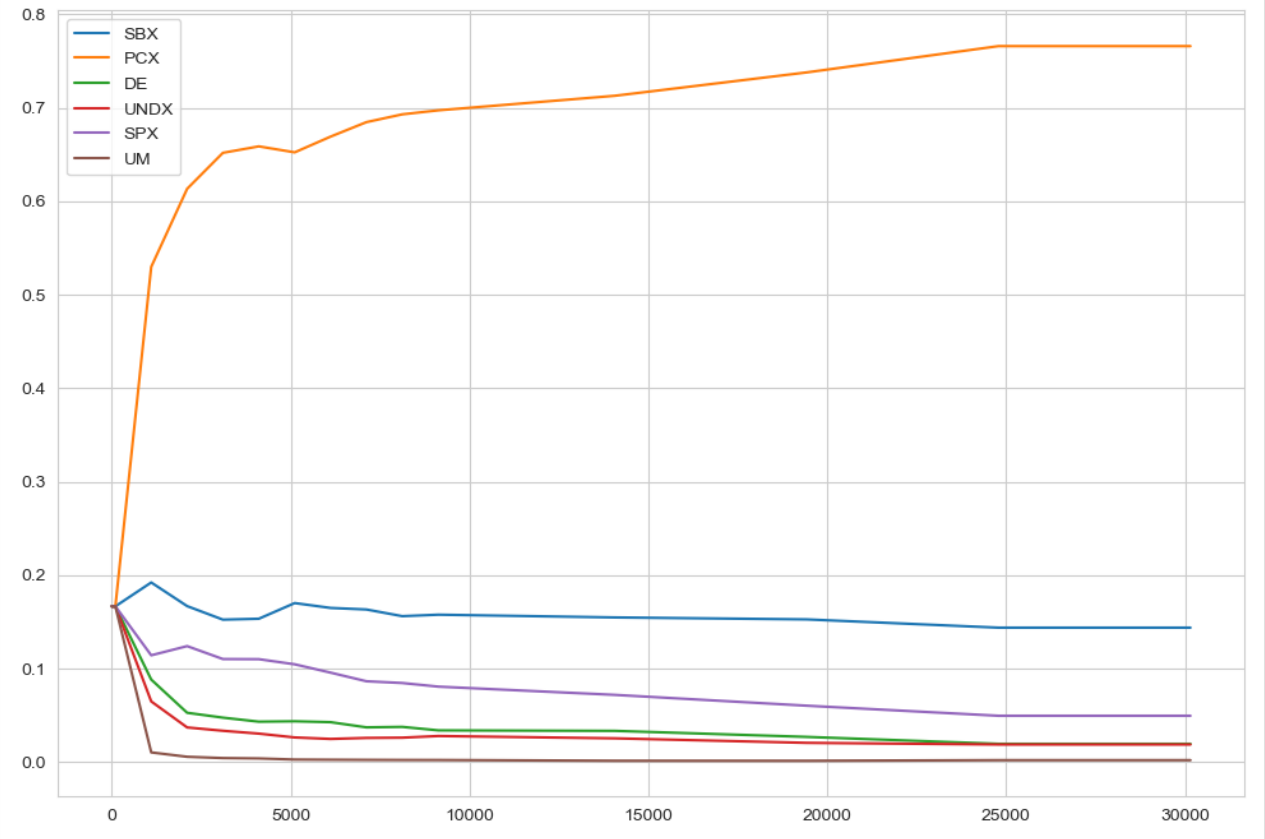


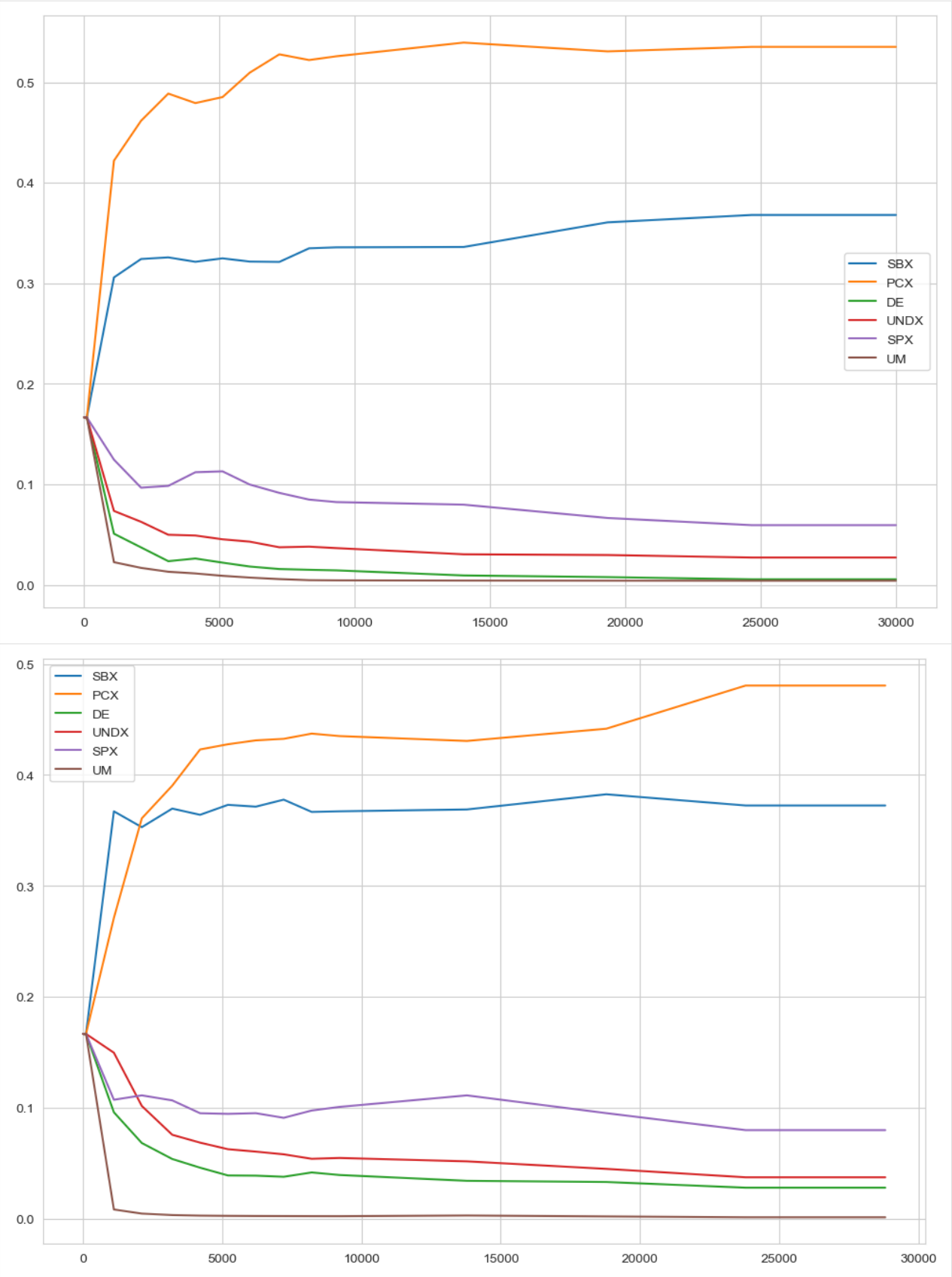
Above, you see the ϵ-convergence for the auto adaptive operator selection version of the outputspace algorithm. Like the normal version, it converges to essential the same number across the different seeds. Note also that the ϵ-progress is slightly higher, and also the total number of identified solutions (see log messages) is higher. That suggests that for even for a relatively simple problem, there is value in using the auto adaptive operator selection.

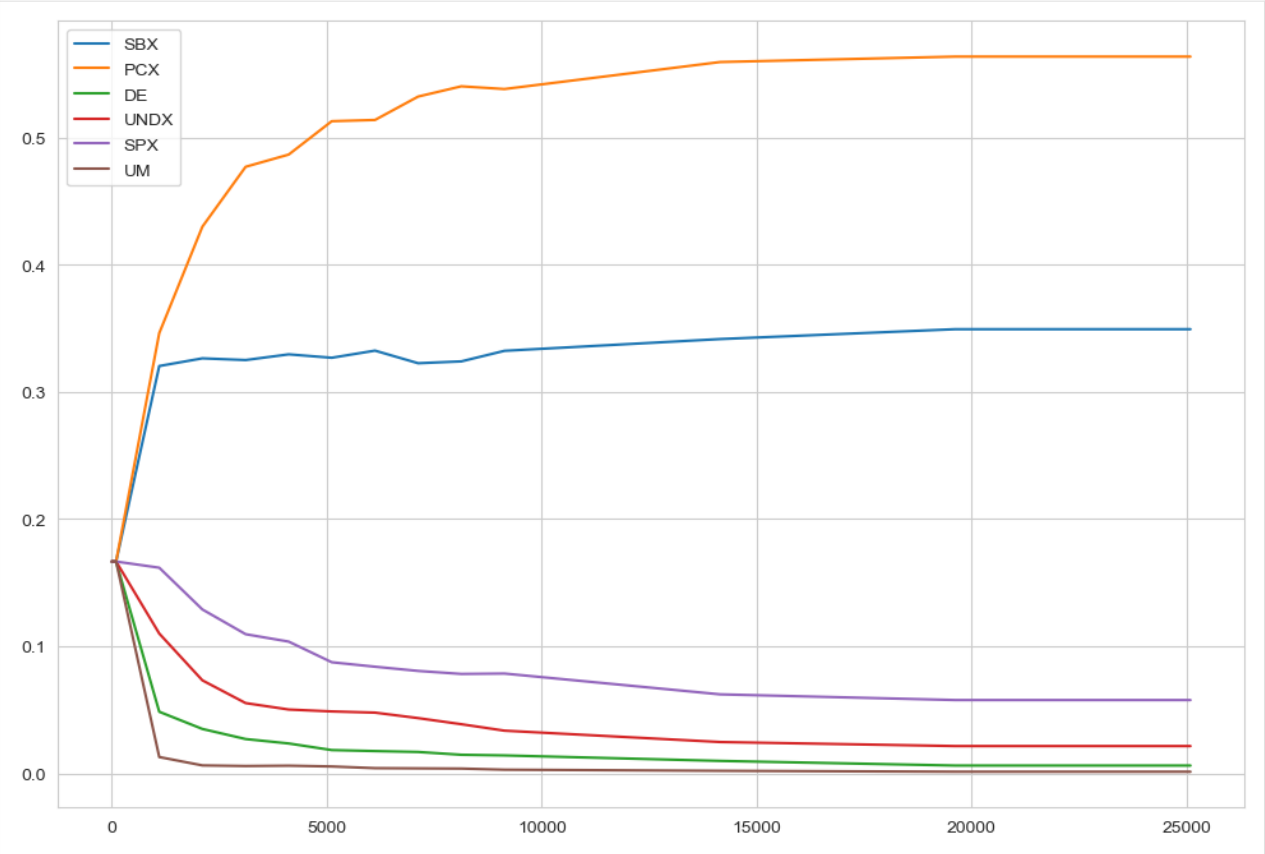
In case of `AutoAdaptiveOutputSpaceExploration` it can sometimes also be revealing to check the dynamics of the operators over the evolution. This is shown below separately for each seed. For the meaning of the abbreviations, check the BORG algorithm.

[7]:
```
for convergence in convergences:
    fig, ax = plt.subplots()
    ax.plot(convergence.nfe, convergence.SBX, label="SBX")
    ax.plot(convergence.nfe, convergence.PCX, label="PCX")
    ax.plot(convergence.nfe, convergence.DE, label="DE")
    ax.plot(convergence.nfe, convergence.UNDX, label="UNDX")
    ax.plot(convergence.nfe, convergence.SPX, label="SPX")
    ax.plot(convergence.nfe, convergence.UM, label="UM")
    ax.legend()
plt.show()
```


SBX
PCX
DE
UNDX
SPX
UM
0.0
0.1
0.2
0.3
0.4
0.5
0
5000
10000
15000
20000
25000
30000


SBX
PCX
DE
UNDX
SPX
UM
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
5000
10000
15000
20000
25000
30000


SBX
PCX
DE
UNDX
SPX
UM
0.0
0.1
0.2
0.3
0.4
0.5
0
5000
10000
15000
20000
25000
30000



LHS

for comparison, let's also generate a Latin Hypercube Sample and compare the results. Since the output space exploration return close to 1500 solutions, we use 1500 for LHS as well.

[8]:
```
with MultiprocessingEvaluator(lake_model) as evaluator:
    experiments, outcomes = evaluator.perform_experiments(scenarios=1500,␣
↪policies=reference)
```

```
[MainProcess/INFO] pool started with 10 workers
[MainProcess/INFO] performing 1500 scenarios * 1 policies * 1 model(s) = 1500 experiments
100%|| 1500/1500 [00:04<00:00, 331.08it/s]
[MainProcess/INFO] experiments finished
[MainProcess/INFO] terminating pool
```

comparison

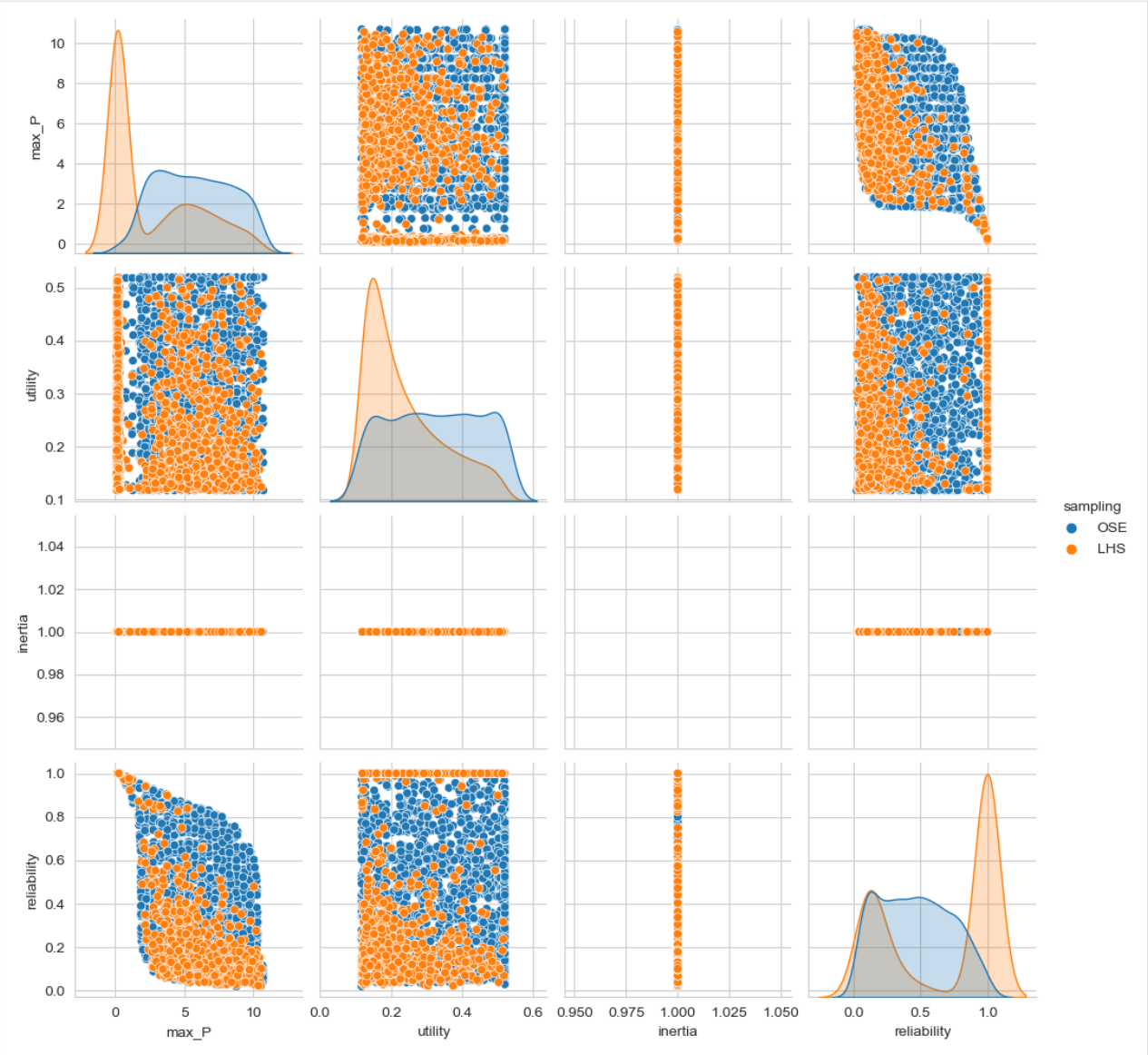
Below we compare the LHS with the last seed of the autoadaptive algorithm. Remember, the purpose of output space exploration is to identify the kinds of behavior that a model can show given a set of uncertain parameters. So, we are creating a pairwise scatter plot of the outcomes for both output space exploration (in blue) and the latin hypercube sampling (in orange).

[9]:
```
outcomes = pd.DataFrame(outcomes)
outcomes["sampling"] = "LHS"
```

[10]:
```
ose = res.iloc[:, 5::].copy()
ose["sampling"] = "OSE"
```

[11]:
```
data = pd.concat([ose, outcomes], axis=0, ignore_index=True)
```

[12]:
```
# sns.pairplot(data, hue='sampling')
sns.pairplot(data, hue="sampling", vars=data.columns[0:4])
plt.show()
```



As you can clearly see, the output space exploration algorithm has uncovered behaviors that were not seen in the 1500 sample LHS.

[ ]:

1.10.2 Performing Scenario Discovery in Python

The purpose of example is to demonstrate how one can do scenario discovery in python. I will demonstrate how we can perform both PRIM in an interactive way, as well as briefly show how to use CART, which is also available in the exploratory modeling workbench. There is ample literature on both CART and PRIM and their relative merits for use in scenario discovery. So I won't be discussing that here in any detail.

In order to demonstrate the use of the exploratory modeling workbench for scenario discovery, I am using a published example. I am using the data used in the original article by Ben Bryant and Rob Lempert where they first introduced 2010. Ben Bryant kindly made this data available and allowed me to share it. The data comes as a csv file. We can

import the data easily using pandas. columns 2 up to and including 10 contain the experimental design, while the classification is presented in column 15

This example is a slightly updated version of a blog post on https://waterprogramming.wordpress.com/2015/08/05/scenario-discovery-in-python/

[1]:
```
import pandas as pd

data = pd.read_csv("./data/bryant et al 2010 data.csv", index_col=False)
x = data.iloc[:, 2:11]
y = data.iloc[:, 15].values
```

The exploratory modeling workbench comes with a separate analysis package. This analysis package contains prim. So let's import prim. The workbench also has its own logging functionality. We can turn this on to get some more insight into prim while it is running.

[2]:
```
from ema_workbench.analysis import prim
from ema_workbench.util import ema_logging

ema_logging.log_to_stderr(ema_logging.INFO);
```

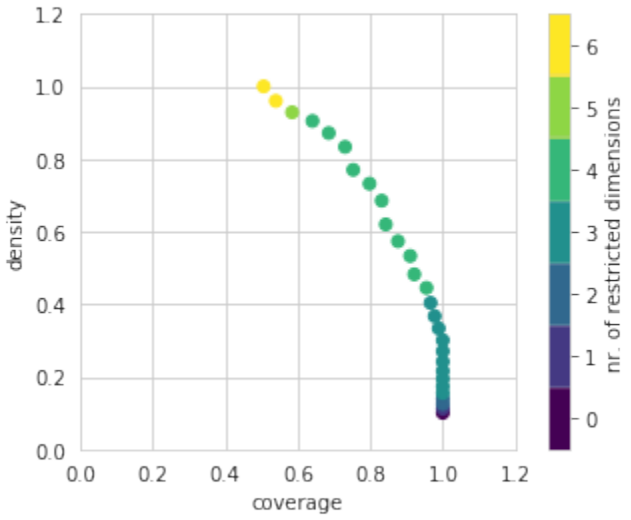
Next, we need to instantiate the prim algorithm. To mimic the original work of Ben Bryant and Rob Lempert, we set the peeling alpha to 0.1. The peeling alpha determines how much data is peeled off in each iteration of the algorithm. The lower the value, the less data is removed in each iteration. The minimum coverage threshold that a box should meet is set to 0.8. Next, we can use the instantiated algorithm to find a first box.

[3]:
```
prim_alg = prim.Prim(x, y, threshold=0.8, peel_alpha=0.1)
box1 = prim_alg.find_box()
```

```
[MainProcess/INFO] 882 points remaining, containing 89 cases of interest
[MainProcess/INFO] mean: 1.0, mass: 0.05102040816326531, coverage: 0.5056179775280899,␣
↪density: 1.0 restricted_dimensions: 6
```

Let's investigate this first box is some detail. A first thing to look at is the trade off between coverage and density. The box has a convenience function for this called `show_tradeoff`.

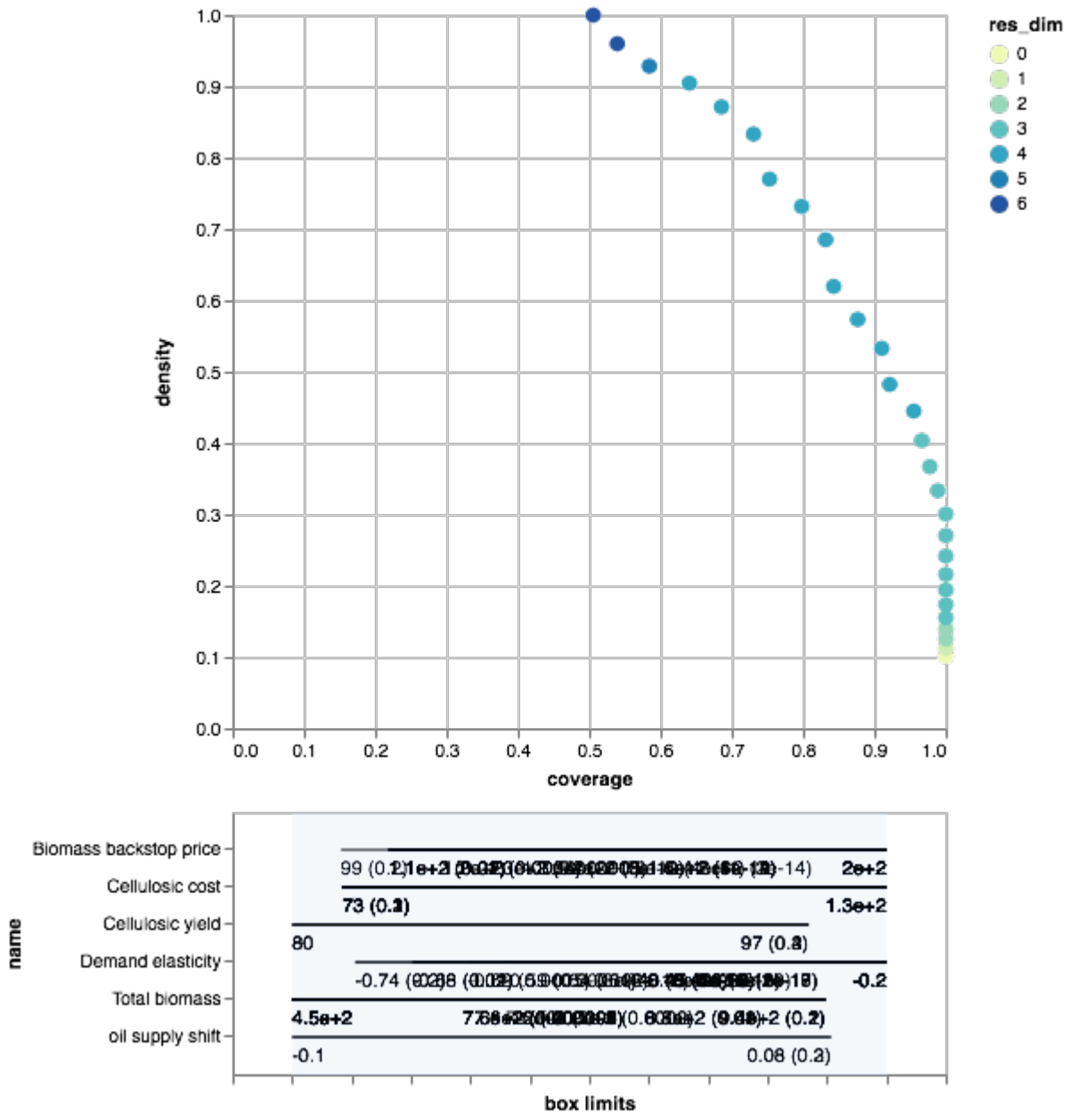
[4]:
```
box1.show_tradeoff()
plt.show()
```



Since we are doing this analysis in a notebook, we can take advantage of the interactivity that the browser offers. A relatively recent addition to the python ecosystem is the library altair. Altair can be used to create interactive plots for use in a browser. Altair is an optional dependency for the workbench. If available, we can create the following visual.

[5]:
```
box1.inspect_tradeoff()
```

[5]:



Here we can interactively explore the boxes associated with each point in the density coverage trade-off. It also offers mouse overs for the various points on the trade off curve. Given the id of each point, we can also use the workbench to manually inpect the peeling trajectory. Following Bryant & Lempert, we inspect box 21.

[6]:
```
box1.resample(21)
```

```
[MainProcess/INFO] resample 0
[MainProcess/INFO] resample 1
```

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```
[MainProcess/INFO] resample 2
[MainProcess/INFO] resample 3
[MainProcess/INFO] resample 4
[MainProcess/INFO] resample 5
[MainProcess/INFO] resample 6
[MainProcess/INFO] resample 7
[MainProcess/INFO] resample 8
[MainProcess/INFO] resample 9
```

[6]:

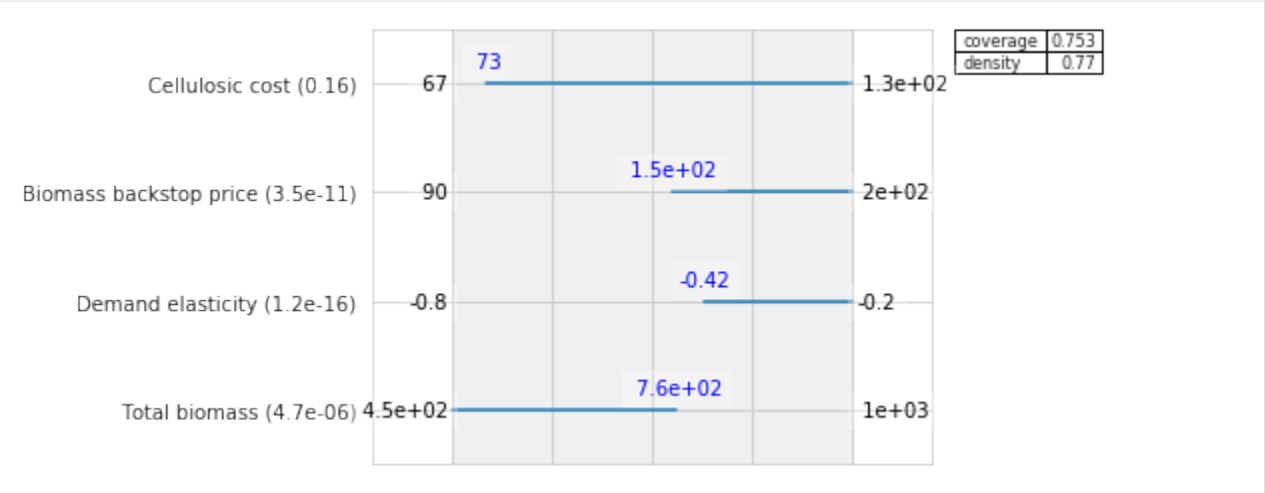
	reproduce coverage	reproduce density
Total biomass	100.0	100.0
Demand elasticity	100.0	100.0
Biomass backstop price	100.0	100.0
Cellulosic cost	90.0	90.0
Cellulosic yield	20.0	20.0
Electricity coproduction	20.0	20.0
Feedstock distribution	0.0	0.0
Oil elasticity	0.0	0.0
oil supply shift	0.0	0.0

[7]:

```
box1.inspect(21)
box1.inspect(21, style="graph")
plt.show()
```

```
coverage     0.752809
density      0.770115
id                 21
mass         0.0986395
mean          0.770115
res_dim              4
Name: 21, dtype: object

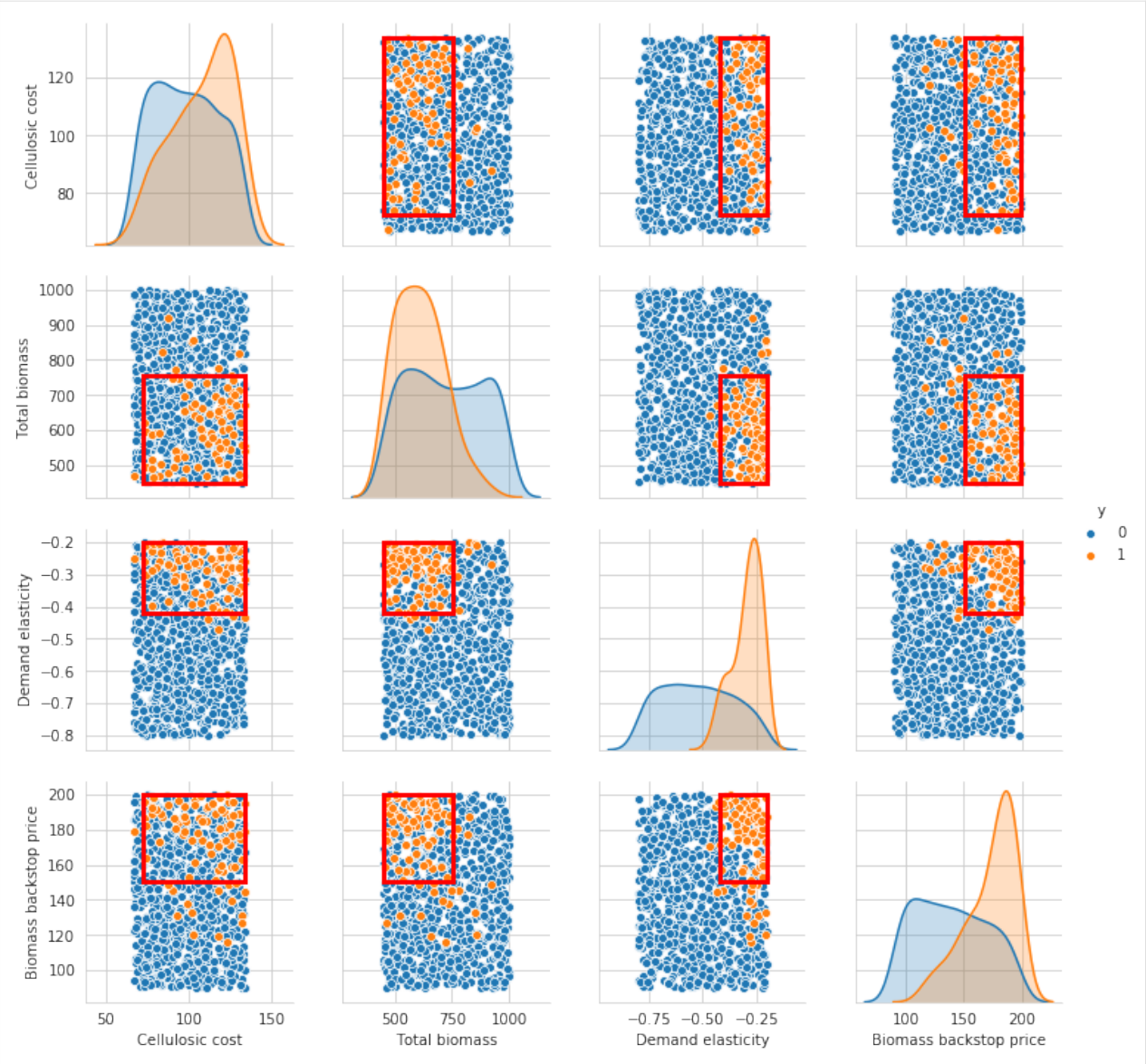
                           box 21
                              min         max                        qp values
Total biomass           450.000000  755.799988   [-1.0, 4.716968553178765e-06]
Demand elasticity        -0.422000   -0.202000  [1.1849299115762218e-16, -1.0]
Biomass backstop price  150.049995  199.600006   [3.515112530263049e-11, -1.0]
Cellulosic cost          72.650002  133.699997     [0.15741333528927348, -1.0]
```



If one where to do a detailed comparison with the results reported in the original article, one would see small numerical differences. These differences arise out of subtle differences in implementation. The most important difference is that the exploratory modeling workbench uses a custom objective function inside prim which is different from the one used in the scenario discovery toolkit. Other differences have to do with details about the hill climbing optimization that is used in prim, and in particular how ties are handled in selected the next step. The differences between the two implementations are only numerical, and don't affect the overarching conclusions drawn from the analysis.

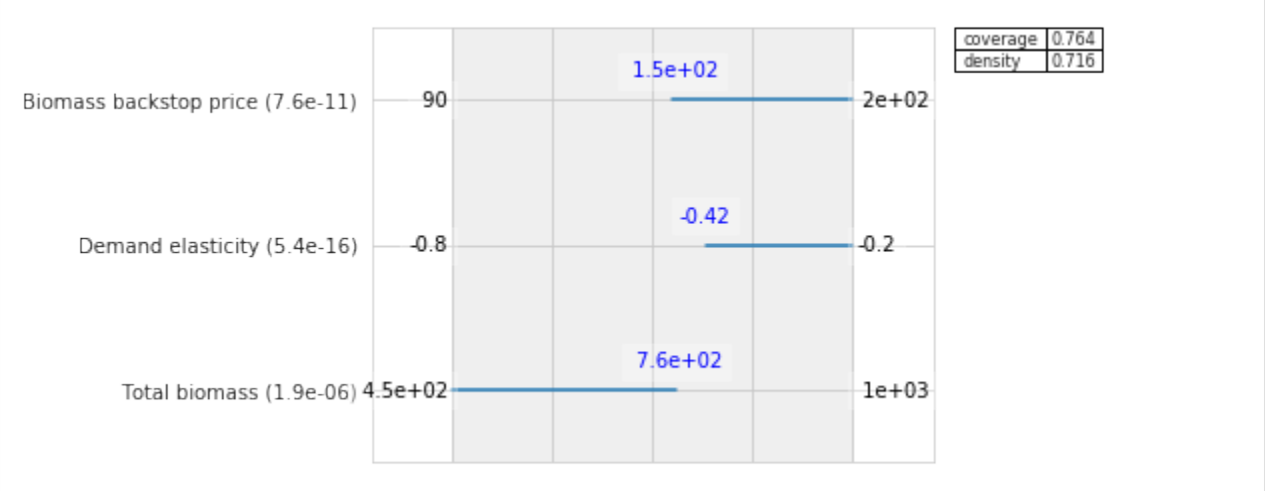
Let's select this 21 box, and get a more detailed view of what the box looks like. Following Bryant et al., we can use scatter plots for this.

[8]:
```
box1.select(21)
fig = box1.show_pairs_scatter(21)
plt.show()
```



Because the last restriction is not significant, we can choose to drop this restriction from the box.

[9]:
```
box1.drop_restriction("Cellulosic cost")
box1.inspect(style="graph")
plt.show()
```



We have now found a first box that explains over 75% of the cases of interest. Let's see if we can find a second box that explains the remainder of the cases.

[10]:
```
box2 = prim_alg.find_box()
```

```
[MainProcess/INFO] 787 points remaining, containing 21 cases of interest
[MainProcess/INFO] box does not meet threshold criteria, value is 0.3541666666666667,␣
↪returning dump box
```

As we can see, we are unable to find a second box. The best coverage we can achieve is 0.35, which is well below the specified 0.8 threshold. Let's look at the final overal results from interactively fitting PRIM to the data. For this, we can use to convenience functions that transform the stats and boxes to pandas data frames.

[11]:
```
prim_alg.stats_to_dataframe()
```

[11]:

	coverage	density	mass	res_dim
box 1	0.764045	0.715789	0.10771	3
box 2	0.235955	0.026684	0.89229	0

[12]:
```
prim_alg.boxes_to_dataframe()
```

[12]:

	box 1		box 2	
	min	max	min	max
Demand elasticity	-0.422000	-0.202000	-0.8	-0.202000
Biomass backstop price	150.049995	199.600006	90.0	199.600006
Total biomass	450.000000	755.799988	450.0	997.799988

CART

The way of interacting with CART is quite similar to how we setup the prim analysis. We import cart from the analysis package. We instantiate the algorithm, and next fit CART to the data. This is done via the `build_tree` method.

[13]:
```
from ema_workbench.analysis import cart

cart_alg = cart.CART(x, y, 0.05)
cart_alg.build_tree()
```

```
/Users/jhkwakkel/miniconda3/lib/python3.6/importlib/_bootstrap.py:219: ImportWarning: can
↪'t resolve package from __spec__ or __package__, falling back on __name__ and __path__
  return f(*args, **kwds)
/Users/jhkwakkel/miniconda3/lib/python3.6/importlib/_bootstrap.py:219: ImportWarning: can
↪'t resolve package from __spec__ or __package__, falling back on __name__ and __path__
  return f(*args, **kwds)
/Users/jhkwakkel/miniconda3/lib/python3.6/importlib/_bootstrap.py:219: ImportWarning: can
↪'t resolve package from __spec__ or __package__, falling back on __name__ and __path__
  return f(*args, **kwds)
```

Now that we have trained CART on the data, we can investigate its results. Just like PRIM, we can use `stats_to_dataframe` and `boxes_to_dataframe` to get an overview.

[14]:
```
cart_alg.stats_to_dataframe()
```

[14]:

	coverage	density	mass	res dim
box 1	0.011236	0.021739	0.052154	2
box 2	0.000000	0.000000	0.546485	2
box 3	0.000000	0.000000	0.103175	2
box 4	0.044944	0.090909	0.049887	2
box 5	0.224719	0.434783	0.052154	2
box 6	0.112360	0.227273	0.049887	3
box 7	0.000000	0.000000	0.051020	3
box 8	0.606742	0.642857	0.095238	2

[15]:
```
cart_alg.boxes_to_dataframe()
```

[15]:

	box 1		box 2		box 3	\
	min	max	min	max	min	
Cellulosic yield	80.0	81.649998	81.649998	99.900002	80.000	
Demand elasticity	-0.8	-0.439000	-0.800000	-0.439000	-0.439	
Biomass backstop price	90.0	199.600006	90.000000	199.600006	90.000	

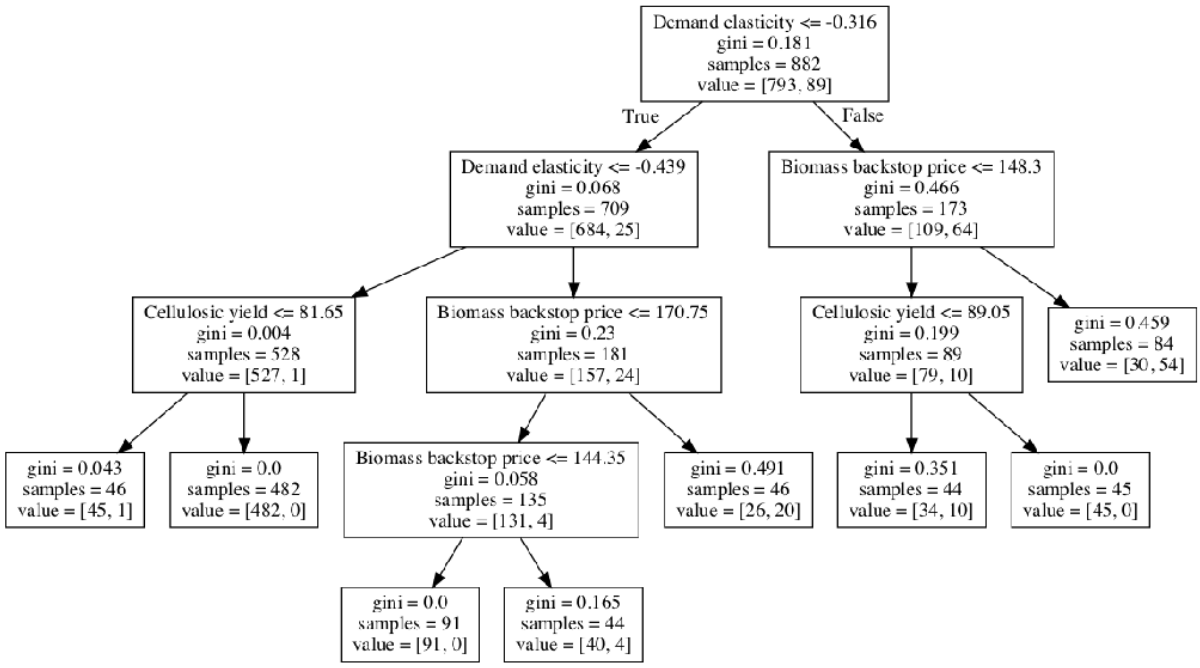
	box 4		box 5	\
	max	min	max	min
Cellulosic yield	99.900002	80.000000	99.900002	80.000
Demand elasticity	-0.316500	-0.439000	-0.316500	-0.439
Biomass backstop price	144.350006	144.350006	170.750000	170.750

	box 6		box 7	\
	max	min	max	min
Cellulosic yield	99.900002	80.0000	89.049999	89.049999
Demand elasticity	-0.316500	-0.3165	-0.202000	-0.316500
Biomass backstop price	199.600006	90.0000	148.300003	90.000000

	box 8		
	max	min	max
Cellulosic yield	99.900002	80.000000	99.900002
Demand elasticity	-0.202000	-0.316500	-0.202000
Biomass backstop price	148.300003	148.300003	199.600006

Alternatively, we might want to look at the classification tree directly. For this, we can use the `show_tree` method.

[16]:
```
fig = cart_alg.show_tree()
fig.set_size_inches((18, 12))
plt.show()
```



[ ]:
```
```

1.10.3 Vadere EMA connector demo

This notebook demonstrates the setup of a Vadere model connection. It uses an example Vadere model, made with Vadere 2.1. Before running the code yourself, please acquire a copy of Vadere from the official Vadere website. For more information on the use of the EMA Workbench, please refer to the official EMA Workbench documentation. This demo is based on the code provided on the documentation pages.

Step 1: imports

The first step is to import the needed modules. This depends on the use and the type of analysis that is intended. The most important one here is the VadereModel from the model connectors. As said, please refer for more information on this to the official EMA Workbench documentation.

[ ]:
```
from ema_workbench import (
    perform_experiments,
    RealParameter,
    ema_logging,
    MultiprocessingEvaluator,
    Samplers,
    ScalarOutcome,
    IntegerParameter,
    RealParameter,
```

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```
)
from ema_workbench.connectors.vadere import VadereModel
import pandas as pd
import numpy as np
```

Step 2: Setting up the model

In this demonstration, we use a simple Vadere model example. The model includes two sources and one target, and spawns a number of pedestrians every second. The model uses the OSM locomotion implementation, and collects the following:

- The average evacuation time -> stored in evacuationTime.txt
- The average speed of all pedestrians each time step -> stored in speed.csv

Note that the EMA connector assumes .txt files for scalar outcomes and .csv files for time series outcomes. Pleasure use these file types, and declare them explicitly in processor_files as shown below.

[2]:
```
# This model saves scalar results to a density.txt and speed.txt file.
# Please acquire your own copy of Vadere, and place the vadere-console.jar in your model/
↪scenarios directory
# Note that the vadere model files and the console.jar should always be placed in a␣
↪separate wd as the python runfile
model = VadereModel(
    "demoModel",
    vadere_jar="vadere-console.jar",
    processor_files=["evacuationTime.txt", "speed.csv"],
    model_file="demo.scenario",
    wd="models/vadereModel/scenarios/",
)
```

[3]:
```
# set the number of replications to handle model stochasticity
model.replications = 5
```

Note that for specifying model uncertainties (and potential levers), the Vadere model class can change any variable present in the model file (Vadere scenario). To realize this, an exact location to the variable of interest in the Vadere scenario file has to be specified. Vadere scenario files follow a nested dictionary structure. Therefore, the exact location of the variable should be passed in a list of argumentes, passed as one string.

See the example below, that variates the following:

- The number of spawned pedestrians from both sources
- The mean of the free flow speed distribution

[4]:
```
model.uncertainties = [
    IntegerParameter(
        name="spawnNumberA",
        lower_bound=1,
        upper_bound=50,
        variable_name=['("scenario", "topography", "sources", 0, "spawnNumber")'],
    ),
    IntegerParameter(
        name="spawnNumberB",
```

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```
        lower_bound=1,
        upper_bound=50,
        variable_name=['("scenario", "topography", "sources", 1, "spawnNumber")'],
    ),
    RealParameter(
        name="FreeFlowSpeed",
        lower_bound=0.7,
        upper_bound=1.5,
        variable_name=[
            '("scenario", "topography", "attributesPedestrian", "speedDistributionMean")'
        ],
    ),
]
```

The model outcomes can be specified by passing the exact name as present in the output file (speed.txt here). The naming convention depends on the used Vadere data processors, but usually follows the name + id of the processor. When in doubt, it is advised to do a demo Vadere run using the Vadere software and to inspect the generated output files. Note that we take the mean of the outcomes here, since we specified multiple replications. Note that we now only focus on scalar outcomes. See the end of this demo for timeseries.

[5]:
```
model.outcomes = [
    ScalarOutcome(name="evacuationTime", variable_name="meanEvacuationTime-PID8",␣
↪function=np.mean)
]
```

Step 3: Performing experiments

The last step is to perform experiment with the Vadere model. Both sequential runs as runs in parallel are supported. Note however that a Vadere run can use a lot of RAM, and using all available CPU cores can lead to performance issues in some cases. Additionally, one Vadere run is by default already multithreaded. It is therefore recommended to not use the full set of available processes.

[6]:
```
# enable EMA logging
ema_logging.log_to_stderr(ema_logging.INFO)
```

[6]:
```
<Logger EMA (DEBUG)>
```

[7]:
```
# run in sequential 2 experiments
results_sequential = perform_experiments(model, scenarios=2, uncertainty_
↪sampling=Samplers.LHS)
```

```
[MainProcess/INFO] performing 2 scenarios * 1 policies * 1 model(s) = 2 experiments
  0%|                                                    | 0/2 [00:00<?, ?it/
↪s][MainProcess/INFO] performing experiments sequentially
100%|| 2/2 [01:03<00:00, 31.75s/it]
[MainProcess/INFO] experiments finished
```

[8]:
```
# run 6 experiments in parallel
with MultiprocessingEvaluator(model, n_processes=-1) as evaluator:
    experiments, outcomes = evaluator.perform_experiments(
        scenarios=4, uncertainty_sampling=Samplers.LHS
    )
```

```
[MainProcess/INFO] pool started with 4 workers
[MainProcess/INFO] performing 4 scenarios * 1 policies * 1 model(s) = 4 experiments
100%|| 4/4 [00:37<00:00,  9.39s/it]
[MainProcess/INFO] experiments finished
[MainProcess/INFO] terminating pool
[ForkPoolWorker-1/INFO] finalizing
[ForkPoolWorker-4/INFO] finalizing
[ForkPoolWorker-3/INFO] finalizing
[ForkPoolWorker-2/INFO] finalizing
```

Inspect the results

we can now look at the results directly. For more extensive exploratory analysis methods, please refer to the official EMA Workbench documentation.

[9]:
```
experiments.head()
```

[9]:

	spawnNumberA	spawnNumberB	FreeFlowSpeed	scenario	policy	model
0	25.0	33.0	0.838960	2	None	demoModel
1	46.0	19.0	1.413804	3	None	demoModel
2	28.0	11.0	0.942684	4	None	demoModel
3	2.0	50.0	1.111305	5	None	demoModel

[10]:
```
pd.DataFrame(outcomes).head()
```

[10]:

	evacuationTime
0	14.268966
1	9.990154
2	11.673846
3	11.155385

Using time series data

It is additionally possible to specify time series output data. See below for an example on how to do this.

Note that this example now uses a different model class, since we do not want to average multiple scalar outcomes but are rather interested in a time series outcome. Hence, the SingleReplicationVadereModel is used. Now, the timeStep and average speeds are collected every step.

[11]:
```
from ema_workbench import TimeSeriesOutcome
from ema_workbench.connectors.vadere import SingleReplicationVadereModel
```

[12]:
```
# This model saves scalar results to a density.txt and speed.txt file.
# Please acquire your own copy of Vadere, and place the vadere-console.jar in your model/
↪scenarios directory
# Note that the vadere model files should always be placed in a separate wd as the␣
↪python runfile
model = SingleReplicationVadereModel(
    "demoModel",
    vadere_jar="vadere-console.jar",
    processor_files=["evacuationTime.txt", "speed.csv"],
```

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```
    model_file="demo.scenario",
    wd="models/vadereModel/scenarios/",
)
```

[13]:
```
model.uncertainties = [
    IntegerParameter(
        name="spawnNumberA",
        lower_bound=1,
        upper_bound=50,
        variable_name=['("scenario", "topography", "sources", 0, "spawnNumber")'],
    ),
    IntegerParameter(
        name="spawnNumberB",
        lower_bound=1,
        upper_bound=50,
        variable_name=['("scenario", "topography", "sources", 1, "spawnNumber")'],
    ),
    RealParameter(
        name="FreeFlowSpeed",
        lower_bound=0.7,
        upper_bound=1.5,
        variable_name=[
            '("scenario", "topography", "attributesPedestrian", "speedDistributionMean")'
        ],
    ),
]
```

[14]:
```
model.outcomes = [TimeSeriesOutcome(name="speedTime", variable_name="areaSpeed-PID5")]
```

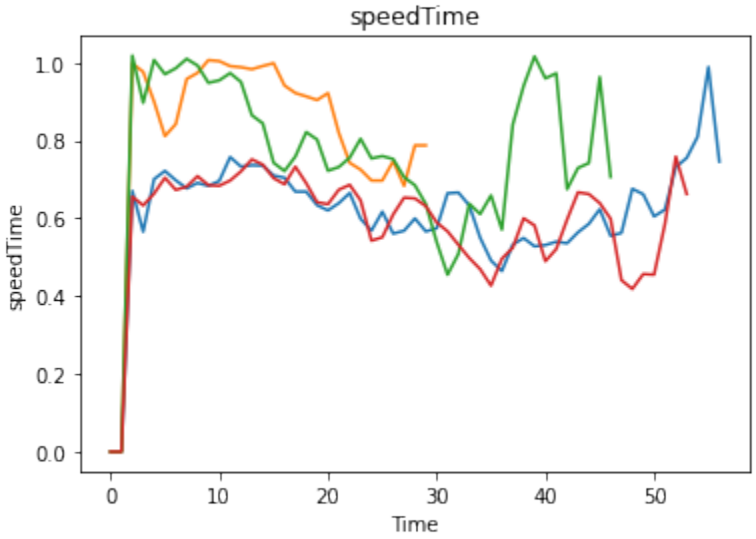
[15]:
```
# Run experiments in parallel with all logical CPU cores except one
with MultiprocessingEvaluator(model, n_processes=-1) as evaluator:
    experiments, outcomes = evaluator.perform_experiments(
        scenarios=4, uncertainty_sampling=Samplers.LHS
    )
```

```
[MainProcess/INFO] pool started with 4 workers
[MainProcess/INFO] performing 4 scenarios * 1 policies * 1 model(s) = 4 experiments
100%|| 4/4 [00:07<00:00,  1.90s/it]
[MainProcess/INFO] experiments finished
[MainProcess/INFO] terminating pool
[ForkPoolWorker-8/INFO] finalizing
[ForkPoolWorker-5/INFO] finalizing
[ForkPoolWorker-6/INFO] finalizing
[ForkPoolWorker-7/INFO] finalizing
```

[16]:
```
from ema_workbench.analysis.plotting import lines

lines(experiments, outcomes, outcomes_to_show="speedTime")
```

[16]:
```
(<Figure size 432x288 with 1 Axes>,
 {'speedTime': <AxesSubplot:title={'center':'speedTime'}, xlabel='Time', ylabel=
↪'speedTime'>})
```



1.10.4 example_eijgenraam.py

```
"""

"""

# Created on 12 Mar 2020
#
# .. codeauthor::  jhkwakkel

import bisect
import functools
import math
import operator

import numpy as np
import scipy as sp

from ema_workbench import Model, RealParameter, ScalarOutcome, ema_logging,␣
↪MultiprocessingEvaluator

##========================================================================
## Implement the model described by Eijgenraam et al. (2012)
# code taken from Rhodium Eijgenraam example
##------------------------------------------------------------------------

# Parameters pulled from the paper describing each dike ring
params = ("c", "b", "lam", "alpha", "eta", "zeta", "V0", "P0", "max_Pf")
raw_data = {
    10: (16.6939, 0.6258, 0.0014, 0.033027, 0.320, 0.003774, 1564.9, 0.00044, 1 / 2000),
    11: (42.6200, 1.7068, 0.0000, 0.032000, 0.320, 0.003469, 1700.1, 0.00117, 1 / 2000),
    15: (125.6422, 1.1268, 0.0098, 0.050200, 0.760, 0.003764, 11810.4, 0.00137, 1 /␣
```

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```
    ↪2000),
    16: (324.6287, 2.1304, 0.0100, 0.057400, 0.760, 0.002032, 22656.5, 0.00110, 1 /␣
    ↪2000),
    22: (154.4388, 0.9325, 0.0066, 0.070000, 0.620, 0.002893, 9641.1, 0.00055, 1 / 2000),
    23: (26.4653, 0.5250, 0.0034, 0.053400, 0.800, 0.002031, 61.6, 0.00137, 1 / 2000),
    24: (71.6923, 1.0750, 0.0059, 0.043900, 1.060, 0.003733, 2706.4, 0.00188, 1 / 2000),
    35: (49.7384, 0.6888, 0.0088, 0.036000, 1.060, 0.004105, 4534.7, 0.00196, 1 / 2000),
    38: (24.3404, 0.7000, 0.0040, 0.025321, 0.412, 0.004153, 3062.6, 0.00171, 1 / 1250),
    41: (58.8110, 0.9250, 0.0033, 0.025321, 0.422, 0.002749, 10013.1, 0.00171, 1 / 1250),
    42: (21.8254, 0.4625, 0.0019, 0.026194, 0.442, 0.001241, 1090.8, 0.00171, 1 / 1250),
    43: (340.5081, 4.2975, 0.0043, 0.025321, 0.448, 0.002043, 19767.6, 0.00171, 1 /␣
    ↪1250),
    44: (24.0977, 0.7300, 0.0054, 0.031651, 0.316, 0.003485, 37596.3, 0.00033, 1 / 1250),
    45: (3.4375, 0.1375, 0.0069, 0.033027, 0.320, 0.002397, 10421.2, 0.00016, 1 / 1250),
    47: (8.7813, 0.3513, 0.0026, 0.029000, 0.358, 0.003257, 1369.0, 0.00171, 1 / 1250),
    48: (35.6250, 1.4250, 0.0063, 0.023019, 0.496, 0.003076, 7046.4, 0.00171, 1 / 1250),
    49: (20.0000, 0.8000, 0.0046, 0.034529, 0.304, 0.003744, 823.3, 0.00171, 1 / 1250),
    50: (8.1250, 0.3250, 0.0000, 0.033027, 0.320, 0.004033, 2118.5, 0.00171, 1 / 1250),
    51: (15.0000, 0.6000, 0.0071, 0.036173, 0.294, 0.004315, 570.4, 0.00171, 1 / 1250),
    52: (49.2200, 1.6075, 0.0047, 0.036173, 0.304, 0.001716, 4025.6, 0.00171, 1 / 1250),
    53: (69.4565, 1.1625, 0.0028, 0.031651, 0.336, 0.002700, 9819.5, 0.00171, 1 / 1250),
}
data = {i: dict(zip(params, raw_data[i])) for i in raw_data}

# Set the ring we are analyzing
ring = 15
max_failure_probability = data[ring]["max_Pf"]


# Compute the investment cost to increase the dike height
def exponential_investment_cost(
    u,  # increase in dike height
    h0,  # original height of the dike
    c,  # constant from Table 1
    b,  # constant from Table 1
    lam,
):  # constant from Table 1
    if u == 0:
        return 0
    else:
        return (c + b * u) * math.exp(lam * (h0 + u))


def eijgenraam_model(
    X1,
    X2,
    X3,
    X4,
    X5,
    X6,
    T1,
    T2,
```

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```
    T3,
    T4,
    T5,
    T6,
    T=300,
    P0=data[ring]["P0"],
    V0=data[ring]["V0"],
    alpha=data[ring]["alpha"],
    delta=0.04,
    eta=data[ring]["eta"],
    gamma=0.035,
    rho=0.015,
    zeta=data[ring]["zeta"],
    c=data[ring]["c"],
    b=data[ring]["b"],
    lam=data[ring]["lam"],
):
    """Python implementation of the Eijgenraam model

    Params
    ------
    Xs : list
         list of dike heightenings
    Ts : list
         time of dike heightenings
    T : int, optional
        planning horizon
    P0 : <>, optional
         constant from Table 1
    V0 : <>, optional
         constant from Table 1
    alpha : <>, optional
            constant from Table 1
    delta : float, optional
            discount rate, mentioned in Section 2.2
    eta : <>, optional
          constant from Table 1
    gamma : float, optional
            paper says this is taken from government report, but no indication
            of actual value
    rho : float, optional
          risk-free rate, mentioned in Section 2.2
    zeta : <>, optional
           constant from Table 1
    c : <>, optional
        constant from Table 1
    b : <>, optional
        constant from Table 1
    lam : <>, optional
         constant from Table 1

    """
```

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```
    Ts = [T1, T2, T3, T4, T5, T6]
    Xs = [X1, X2, X3, X4, X5, X6]

    Ts = [int(Ts[i] + sum(Ts[:i])) for i in range(len(Ts)) if Ts[i] + sum(Ts[:i]) < T]
    Xs = Xs[: len(Ts)]

    if len(Ts) == 0:
        Ts = [0]
        Xs = [0]

    if Ts[0] > 0:
        Ts.insert(0, 0)
        Xs.insert(0, 0)

    S0 = P0 * V0
    beta = alpha * eta + gamma - rho
    theta = alpha - zeta

    # calculate investment
    investment = 0

    for i in range(len(Xs)):
        step_cost = exponential_investment_cost(Xs[i], 0 if i == 0 else sum(Xs[:i]), c,␣
↪b, lam)
        step_discount = math.exp(-delta * Ts[i])
        investment += step_cost * step_discount

    # calculate expected losses
    losses = 0

    for i in range(len(Xs) - 1):
        losses += math.exp(-theta * sum(Xs[: (i + 1)])) * (
            math.exp((beta - delta) * Ts[i + 1]) - math.exp((beta - delta) * Ts[i])
        )

    if Ts[-1] < T:
        losses += math.exp(-theta * sum(Xs)) * (
            math.exp((beta - delta) * T) - math.exp((beta - delta) * Ts[-1])
        )

    losses = losses * S0 / (beta - delta)

    # salvage term
    losses += S0 * math.exp(beta * T) * math.exp(-theta * sum(Xs)) * math.exp(-delta *␣
↪T) / delta

    def find_height(t):
        if t < Ts[0]:
            return 0
        elif t > Ts[-1]:
            return sum(Xs)
        else:
```

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```
            return sum(Xs[: bisect.bisect_right(Ts, t)])

    failure_probability = [
        P0 * np.exp(alpha * eta * t) * np.exp(-alpha * find_height(t)) for t in range(T+ 1)
    ]
    total_failure = 1 - functools.reduce(operator.mul, [1 - p for p in failure_probability], 1)
    mean_failure = sum(failure_probability) / (T + 1)
    max_failure = max(failure_probability)

    return (investment, losses, investment + losses, total_failure, mean_failure, max_failure)


if __name__ == "__main__":
    model = Model("eijgenraam", eijgenraam_model)

    model.responses = [
        ScalarOutcome("TotalInvestment", ScalarOutcome.INFO),
        ScalarOutcome("TotalLoss", ScalarOutcome.INFO),
        ScalarOutcome("TotalCost", ScalarOutcome.MINIMIZE),
        ScalarOutcome("TotalFailureProb", ScalarOutcome.INFO),
        ScalarOutcome("AvgFailureProb", ScalarOutcome.MINIMIZE),
        ScalarOutcome("MaxFailureProb", ScalarOutcome.MINIMIZE),
    ]

    # Set uncertainties
    model.uncertainties = [
        RealParameter.from_dist("P0", sp.stats.lognorm(scale=0.00137, s=0.25)),
        # @UndefinedVariable
        RealParameter.from_dist("alpha", sp.stats.norm(loc=0.0502, scale=0.01)),
        # @UndefinedVariable
        RealParameter.from_dist("eta", sp.stats.lognorm(scale=0.76, s=0.1)),
    ]  # @UndefinedVariable

    # having a list like parameter were values are automagically wrappen
    # into a list can be quite useful.....
    model.levers = [RealParameter(f"X{i}", 0, 500) for i in range(1, 7)] + [
        RealParameter(f"T{i}", 0, 300) for i in range(1, 7)
    ]

    ema_logging.log_to_stderr(ema_logging.INFO)

    with MultiprocessingEvaluator(model, n_processes=-1) as evaluator:
        results = evaluator.perform_experiments(1000, 4)
```

1.10.5 example_excel.py

```
"""
Created on 27 Jul. 2011

This file illustrated the use the EMA classes for a model in Excel.

It used the excel file provided by
`A. Sharov <https://home.comcast.net/~sharov/PopEcol/lec10/fullmod.html>`_

This excel file implements a simple predator prey model.

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
"""

from ema_workbench import RealParameter, TimeSeriesOutcome, ema_logging, perform_
↪experiments

from ema_workbench.connectors.excel import ExcelModel
from ema_workbench.em_framework.evaluators import MultiprocessingEvaluator

if __name__ == "__main__":
    ema_logging.log_to_stderr(level=ema_logging.INFO)

    model = ExcelModel("predatorPrey", wd="./models/excelModel", model_file="excel␣
↪example.xlsx")
    model.uncertainties = [
        RealParameter("K2", 0.01, 0.2),
        # we can refer to a cell in the normal way
        # we can also use named cells
        RealParameter("KKK", 450, 550),
        RealParameter("rP", 0.05, 0.15),
        RealParameter("aaa", 0.00001, 0.25),
        RealParameter("tH", 0.45, 0.55),
        RealParameter("kk", 0.1, 0.3),
    ]

    # specification of the outcomes
    model.outcomes = [
        TimeSeriesOutcome("B4:B1076"),
        # we can refer to a range in the normal way
        TimeSeriesOutcome("P_t"),
    ]  # we can also use named range

    # name of the sheet
    model.default_sheet = "Sheet1"

    with MultiprocessingEvaluator(model) as evaluator:
        results = perform_experiments(model, 100, reporting_interval=1,␣
↪evaluator=evaluator)
```

1.10.6 example_flu.py

```
"""
Created on 20 dec. 2010

This file illustrated the use of the workbench for a model
specified in Python itself. The example is based on `Pruyt & Hamarat <https://www.
↪systemdynamics.org/conferences/2010/proceed/papers/P1253.pdf>`_.
For comparison, run both this model and the flu_vensim_no_policy_example.py and
compare the results.


.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                chamarat <c.hamarat  (at) tudelft (dot) nl>

"""

import matplotlib.pyplot as plt
import numpy as np
from numpy import sin, min, exp

from ema_workbench import Model, RealParameter, TimeSeriesOutcome, perform_experiments,␣
↪ema_logging
from ema_workbench import MultiprocessingEvaluator, SequentialEvaluator
from ema_workbench.analysis import lines, Density

# ========================================================================
#
#    the model itself
#
# ========================================================================

FINAL_TIME = 48
INITIAL_TIME = 0
TIME_STEP = 0.0078125

switch_regions = 1.0
switch_immunity = 1.0
switch_deaths = 1.0
switch_immunity_cap = 1.0


def LookupFunctionX(variable, start, end, step, skew, growth, v=0.5):
    return start + ((end - start) / ((1 + skew * exp(-growth * (variable - step))) ** (1␣
↪/ v)))


def flu_model(
    x11=0,
    x12=0,
    x21=0,
    x22=0,
    x31=0,
```

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```
    x32=0,
    x41=0,
    x51=0,
    x52=0,
    x61=0,
    x62=0,
    x81=0,
    x82=0,
    x91=0,
    x92=0,
    x101=0,
    x102=0,
):
    # Assigning initial values
    additional_seasonal_immune_population_fraction_R1 = float(x11)
    additional_seasonal_immune_population_fraction_R2 = float(x12)

    fatality_rate_region_1 = float(x21)
    fatality_rate_region_2 = float(x22)

    initial_immune_fraction_of_the_population_of_region_1 = float(x31)
    initial_immune_fraction_of_the_population_of_region_2 = float(x32)

    normal_interregional_contact_rate = float(x41)
    interregional_contact_rate = switch_regions * normal_interregional_contact_rate

    permanent_immune_population_fraction_R1 = float(x51)
    permanent_immune_population_fraction_R2 = float(x52)

    recovery_time_region_1 = float(x61)
    recovery_time_region_2 = float(x62)

    susceptible_to_immune_population_delay_time_region_1 = 1
    susceptible_to_immune_population_delay_time_region_2 = 1

    root_contact_rate_region_1 = float(x81)
    root_contact_rate_region_2 = float(x82)

    infection_rate_region_1 = float(x91)
    infection_rate_region_2 = float(x92)

    normal_contact_rate_region_1 = float(x101)
    normal_contact_rate_region_2 = float(x102)

    ######
    susceptible_to_immune_population_flow_region_1 = 0.0
    susceptible_to_immune_population_flow_region_2 = 0.0
    ######

    initial_value_population_region_1 = 6.0 * 10**8
    initial_value_population_region_2 = 3.0 * 10**9

```

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```
    initial_value_infected_population_region_1 = 10.0
    initial_value_infected_population_region_2 = 10.0

    initial_value_immune_population_region_1 = (
        switch_immunity
        * initial_immune_fraction_of_the_population_of_region_1
        * initial_value_population_region_1
    )
    initial_value_immune_population_region_2 = (
        switch_immunity
        * initial_immune_fraction_of_the_population_of_region_2
        * initial_value_population_region_2
    )

    initial_value_susceptible_population_region_1 = (
        initial_value_population_region_1 - initial_value_immune_population_region_1
    )
    initial_value_susceptible_population_region_2 = (
        initial_value_population_region_2 - initial_value_immune_population_region_2
    )

    recovered_population_region_1 = 0.0
    recovered_population_region_2 = 0.0

    infected_population_region_1 = initial_value_infected_population_region_1
    infected_population_region_2 = initial_value_infected_population_region_2

    susceptible_population_region_1 = initial_value_susceptible_population_region_1
    susceptible_population_region_2 = initial_value_susceptible_population_region_2

    immune_population_region_1 = initial_value_immune_population_region_1
    immune_population_region_2 = initial_value_immune_population_region_2

    deceased_population_region_1 = [0.0]
    deceased_population_region_2 = [0.0]
    runTime = [INITIAL_TIME]

    # --End of Initialization--

    Max_infected = 0.0

    for time in range(int(INITIAL_TIME / TIME_STEP), int(FINAL_TIME / TIME_STEP)):
        runTime.append(runTime[-1] + TIME_STEP)
        total_population_region_1 = (
            infected_population_region_1
            + recovered_population_region_1
            + susceptible_population_region_1
            + immune_population_region_1
        )
        total_population_region_2 = (
            infected_population_region_2
            + recovered_population_region_2
```

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```
            + susceptible_population_region_2
            + immune_population_region_2
        )

        infected_population_region_1 = max(0, infected_population_region_1)
        infected_population_region_2 = max(0, infected_population_region_2)

        infected_fraction_region_1 = infected_population_region_1 / total_population_
↪region_1
        infected_fraction_region_2 = infected_population_region_2 / total_population_
↪region_2

        impact_infected_population_on_contact_rate_region_1 = 1 - (
            infected_fraction_region_1 ** (1 / root_contact_rate_region_1)
        )
        impact_infected_population_on_contact_rate_region_2 = 1 - (
            infected_fraction_region_2 ** (1 / root_contact_rate_region_2)
        )

        #        if ((time*TIME_STEP) >= 4) and ((time*TIME_STEP)<=10):
        #            normal_contact_rate_region_1 = float(x101)*(1 - 0.5)
        #        else:normal_contact_rate_region_1 = float(x101)

        normal_contact_rate_region_1 = float(x101) * (
            1 - LookupFunctionX(infected_fraction_region_1, 0, 1, 0.15, 0.75, 15)
        )

        contact_rate_region_1 = (
            normal_contact_rate_region_1 * impact_infected_population_on_contact_rate_
↪region_1
        )
        contact_rate_region_2 = (
            normal_contact_rate_region_2 * impact_infected_population_on_contact_rate_
↪region_2
        )

        recoveries_region_1 = (
            (1 - (fatality_rate_region_1 * switch_deaths))
            * infected_population_region_1
            / recovery_time_region_1
        )
        recoveries_region_2 = (
            (1 - (fatality_rate_region_2 * switch_deaths))
            * infected_population_region_2
            / recovery_time_region_2
        )

        flu_deaths_region_1 = (
            fatality_rate_region_1
            * switch_deaths
            * infected_population_region_1
            / recovery_time_region_1
```

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```
        )
        flu_deaths_region_2 = (
            fatality_rate_region_2
            * switch_deaths
            * infected_population_region_2
            / recovery_time_region_2
        )

        infections_region_1 = (
            susceptible_population_region_1
            * contact_rate_region_1
            * infection_rate_region_1
            * infected_fraction_region_1
        ) + (
            susceptible_population_region_1
            * interregional_contact_rate
            * infection_rate_region_1
            * infected_fraction_region_2
        )
        infections_region_2 = (
            susceptible_population_region_2
            * contact_rate_region_2
            * infection_rate_region_2
            * infected_fraction_region_2
        ) + (
            susceptible_population_region_2
            * interregional_contact_rate
            * infection_rate_region_2
            * infected_fraction_region_1
        )

        infected_population_region_1_NEXT = infected_population_region_1 + (
            TIME_STEP * (infections_region_1 - flu_deaths_region_1 - recoveries_region_1)
        )
        infected_population_region_2_NEXT = infected_population_region_2 + (
            TIME_STEP * (infections_region_2 - flu_deaths_region_2 - recoveries_region_2)
        )

        if infected_population_region_1_NEXT < 0 or infected_population_region_2_NEXT <␣
↪0:
            pass

        recovered_population_region_1_NEXT = recovered_population_region_1 + (
            TIME_STEP * recoveries_region_1
        )
        recovered_population_region_2_NEXT = recovered_population_region_2 + (
            TIME_STEP * recoveries_region_2
        )

        if fatality_rate_region_1 >= 0.025:
            qw = 1.0
        elif fatality_rate_region_1 >= 0.01:
```

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```
            qw = 0.8
        elif fatality_rate_region_1 >= 0.001:
            qw = 0.6
        elif fatality_rate_region_1 >= 0.0001:
            qw = 0.4
        else:
            qw = 0.2

        if (time * TIME_STEP) <= 10:
            normal_immune_population_fraction_region_1 = (
                additional_seasonal_immune_population_fraction_R1 / 2
            ) * sin(4.5 + (time * TIME_STEP / 2)) + (
                (
                    (2 * permanent_immune_population_fraction_R1)
                    + additional_seasonal_immune_population_fraction_R1
                )
                / 2
            )
        else:
            normal_immune_population_fraction_region_1 = max(
                (
                    float(qw),
                    (additional_seasonal_immune_population_fraction_R1 / 2)
                    * sin(4.5 + (time * TIME_STEP / 2))
                    + (
                        (
                            (2 * permanent_immune_population_fraction_R1)
                            + additional_seasonal_immune_population_fraction_R1
                        )
                        / 2
                    ),
                )
            )

        normal_immune_population_fraction_region_2 = switch_immunity_cap * min(
            (
                (
                    sin((time * TIME_STEP / 2) + 1.5)
                    * additional_seasonal_immune_population_fraction_R2
                    / 2
                )
                + (
                    (
                        (2 * permanent_immune_population_fraction_R2)
                        + additional_seasonal_immune_population_fraction_R2
                    )
                    / 2
                ),
                (
                    permanent_immune_population_fraction_R1
                    + additional_seasonal_immune_population_fraction_R1
                ),
```

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```
            ),
        ) + (
            (1 - switch_immunity_cap)
            * (
                (
                    sin((time * TIME_STEP / 2) + 1.5)
                    * additional_seasonal_immune_population_fraction_R2
                    / 2
                )
                + (
                    (
                        (2 * permanent_immune_population_fraction_R2)
                        + additional_seasonal_immune_population_fraction_R2
                    )
                    / 2
                )
            )
        )

        normal_immune_population_region_1 = (
            normal_immune_population_fraction_region_1 * total_population_region_1
        )
        normal_immune_population_region_2 = (
            normal_immune_population_fraction_region_2 * total_population_region_2
        )

        if switch_immunity == 1:
            susminreg1_1 = (
                normal_immune_population_region_1 - immune_population_region_1
            ) / susceptible_to_immune_population_delay_time_region_1
            susminreg1_2 = (
                susceptible_population_region_1
                / susceptible_to_immune_population_delay_time_region_1
            )
            susmaxreg1 = -(
                immune_population_region_1 / susceptible_to_immune_population_delay_time_
↪region_1
            )
            if (susmaxreg1 >= susminreg1_1) or (susmaxreg1 >= susminreg1_2):
                susceptible_to_immune_population_flow_region_1 = susmaxreg1
            elif (susminreg1_1 < susminreg1_2) and (susminreg1_1 > susmaxreg1):
                susceptible_to_immune_population_flow_region_1 = susminreg1_1
            elif (susminreg1_2 < susminreg1_1) and (susminreg1_2 > susmaxreg1):
                susceptible_to_immune_population_flow_region_1 = susminreg1_2
        else:
            susceptible_to_immune_population_flow_region_1 = 0

        if switch_immunity == 1:
            susminreg2_1 = (
                normal_immune_population_region_2 - immune_population_region_2
            ) / susceptible_to_immune_population_delay_time_region_2
            susminreg2_2 = (
```

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```
                susceptible_population_region_2
                / susceptible_to_immune_population_delay_time_region_2
            )
            susmaxreg2 = -(
                immune_population_region_2 / susceptible_to_immune_population_delay_time_
↪region_2
            )
            if (susmaxreg2 >= susminreg2_1) or (susmaxreg2 >= susminreg2_2):
                susceptible_to_immune_population_flow_region_2 = susmaxreg2
            elif (susminreg2_1 < susminreg2_2) and (susminreg2_1 > susmaxreg2):
                susceptible_to_immune_population_flow_region_2 = susminreg2_1
            elif (susminreg2_2 < susminreg2_1) and (susminreg2_2 > susmaxreg2):
                susceptible_to_immune_population_flow_region_2 = susminreg2_2
        else:
            susceptible_to_immune_population_flow_region_2 = 0

        susceptible_population_region_1_NEXT = susceptible_population_region_1 - (
            TIME_STEP * (infections_region_1 + susceptible_to_immune_population_flow_
↪region_1)
        )
        susceptible_population_region_2_NEXT = susceptible_population_region_2 - (
            TIME_STEP * (infections_region_2 + susceptible_to_immune_population_flow_
↪region_2)
        )

        immune_population_region_1_NEXT = immune_population_region_1 + (
            TIME_STEP * susceptible_to_immune_population_flow_region_1
        )
        immune_population_region_2_NEXT = immune_population_region_2 + (
            TIME_STEP * susceptible_to_immune_population_flow_region_2
        )

        deceased_population_region_1_NEXT = deceased_population_region_1[-1] + (
            TIME_STEP * flu_deaths_region_1
        )
        deceased_population_region_2_NEXT = deceased_population_region_2[-1] + (
            TIME_STEP * flu_deaths_region_2
        )

        # Updating integral values
        if Max_infected < (
            infected_population_region_1_NEXT
            / (
                infected_population_region_1_NEXT
                + recovered_population_region_1_NEXT
                + susceptible_population_region_1_NEXT
                + immune_population_region_1_NEXT
            )
        ):
            Max_infected = infected_population_region_1_NEXT / (
                infected_population_region_1_NEXT
                + recovered_population_region_1_NEXT
```

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```
                + susceptible_population_region_1_NEXT
                + immune_population_region_1_NEXT
            )

        recovered_population_region_1 = recovered_population_region_1_NEXT
        recovered_population_region_2 = recovered_population_region_2_NEXT

        infected_population_region_1 = infected_population_region_1_NEXT
        infected_population_region_2 = infected_population_region_2_NEXT

        susceptible_population_region_1 = susceptible_population_region_1_NEXT
        susceptible_population_region_2 = susceptible_population_region_2_NEXT

        immune_population_region_1 = immune_population_region_1_NEXT
        immune_population_region_2 = immune_population_region_2_NEXT

        deceased_population_region_1.append(deceased_population_region_1_NEXT)
        deceased_population_region_2.append(deceased_population_region_2_NEXT)

        # End of main code

    return {"TIME": runTime, "deceased_population_region_1": deceased_population_region_
↪1}


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = Model("mexicanFlu", function=flu_model)
    model.uncertainties = [
        RealParameter("x11", 0, 0.5),
        RealParameter("x12", 0, 0.5),
        RealParameter("x21", 0.0001, 0.1),
        RealParameter("x22", 0.0001, 0.1),
        RealParameter("x31", 0, 0.5),
        RealParameter("x32", 0, 0.5),
        RealParameter("x41", 0, 0.9),
        RealParameter("x51", 0, 0.5),
        RealParameter("x52", 0, 0.5),
        RealParameter("x61", 0, 0.8),
        RealParameter("x62", 0, 0.8),
        RealParameter("x81", 1, 10),
        RealParameter("x82", 1, 10),
        RealParameter("x91", 0, 0.1),
        RealParameter("x92", 0, 0.1),
        RealParameter("x101", 0, 200),
        RealParameter("x102", 0, 200),
    ]

    model.outcomes = [TimeSeriesOutcome("TIME"), TimeSeriesOutcome("deceased_population_
↪region_1")]

```

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```
    nr_experiments = 500

    with SequentialEvaluator(model) as evaluator:
        results = perform_experiments(model, nr_experiments, evaluator=evaluator)

    print("laat")

    lines(
        results,
        outcomes_to_show="deceased_population_region_1",
        show_envelope=True,
        density=Density.KDE,
        titles=None,
        experiments_to_show=np.arange(0, nr_experiments, 10),
    )
    plt.show()
```

1.10.7 example_lake_model.py

```
"""
An example of the lake problem using the ema workbench.

The model itself is adapted from the Rhodium example by Dave Hadka,
see https://gist.github.com/dhadka/a8d7095c98130d8f73bc

"""

import math

import numpy as np
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MultiprocessingEvaluator,
)
from ema_workbench.em_framework.evaluators import Samplers


def lake_problem(
    b=0.42,  # decay rate for P in lake (0.42 = irreversible)
    q=2.0,  # recycling exponent
    mean=0.02,  # mean of natural inflows
    stdev=0.001,  # future utility discount rate
    delta=0.98,  # standard deviation of natural inflows
    alpha=0.4,  # utility from pollution
```

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```
    nsamples=100,  # Monte Carlo sampling of natural inflows
    **kwargs,
):
    try:
        decisions = [kwargs[str(i)] for i in range(100)]
    except KeyError:
        decisions = [0] * 100
        print("No valid decisions found, using 0 water release every year as default")

    nvars = len(decisions)
    decisions = np.array(decisions)

    # Calculate the critical pollution level (Pcrit)
    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)

    # Generate natural inflows using lognormal distribution
    natural_inflows = np.random.lognormal(
        mean=math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
        sigma=math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
        size=(nsamples, nvars),
    )

    # Initialize the pollution level matrix X
    X = np.zeros((nsamples, nvars))

    # Loop through time to compute the pollution levels
    for t in range(1, nvars):
        X[:, t] = (
            (1 - b) * X[:, t - 1]
            + (X[:, t - 1] ** q / (1 + X[:, t - 1] ** q))
            + decisions[t - 1]
            + natural_inflows[:, t - 1]
        )

    # Calculate the average daily pollution for each time step
    average_daily_P = np.mean(X, axis=0)

    # Calculate the reliability (probability of the pollution level being below Pcrit)
    reliability = np.sum(X < Pcrit) / float(nsamples * nvars)

    # Calculate the maximum pollution level (max_P)
    max_P = np.max(average_daily_P)

    # Calculate the utility by discounting the decisions using the discount factor␣
↪(delta)
    utility = np.sum(alpha * decisions * np.power(delta, np.arange(nvars)))

    # Calculate the inertia (the fraction of time steps with changes larger than 0.02)
    inertia = np.sum(np.abs(np.diff(decisions)) > 0.02) / float(nvars - 1)

    return max_P, utility, inertia, reliability

```

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```

if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    lake_model.time_horizon = 100

    # specify uncertainties
    lake_model.uncertainties = [
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("mean", 0.01, 0.05),
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("delta", 0.93, 0.99),
    ]

    # set levers, one for each time step
    lake_model.levers = [RealParameter(str(i), 0, 0.1) for i in range(lake_model.time_
↪horizon)]

    # specify outcomes
    lake_model.outcomes = [
        ScalarOutcome("max_P"),
        ScalarOutcome("utility"),
        ScalarOutcome("inertia"),
        ScalarOutcome("reliability"),
    ]

    # override some of the defaults of the model
    lake_model.constants = [Constant("alpha", 0.41), Constant("nsamples", 150)]

    # generate some random policies by sampling over levers
    n_scenarios = 1000
    n_policies = 4

    with MultiprocessingEvaluator(lake_model) as evaluator:
        res = evaluator.perform_experiments(n_scenarios, n_policies, lever_
↪sampling=Samplers.MC)
```

1.10.8 example_mesa.py

```
"""

This example is a proof of principle for how MESA models can be
controlled using the ema_workbench.

"""

# Import EMA Workbench modules
```

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```
from ema_workbench import (
    ReplicatorModel,
    RealParameter,
    BooleanParameter,
    IntegerParameter,
    Constant,
    ArrayOutcome,
    perform_experiments,
    save_results,
    ema_logging,
)

# Necessary packages for the model
import math
from enum import Enum
import mesa
import networkx as nx

# MESA demo model "Virus on a Network", from https://github.com/projectmesa/mesa-
↪examples/blob/d16736778fdb500a3e5e05e082b27db78673b562/examples/virus_on_network/virus_
↪on_network/model.py


class State(Enum):
    SUSCEPTIBLE = 0
    INFECTED = 1
    RESISTANT = 2


def number_state(model, state):
    return sum(1 for a in model.grid.get_all_cell_contents() if a.state is state)


def number_infected(model):
    return number_state(model, State.INFECTED)


def number_susceptible(model):
    return number_state(model, State.SUSCEPTIBLE)


def number_resistant(model):
    return number_state(model, State.RESISTANT)


class VirusOnNetwork(mesa.Model):
    """A virus model with some number of agents"""

    def __init__(
        self,
        num_nodes=10,
        avg_node_degree=3,
```

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```
        initial_outbreak_size=1,
        virus_spread_chance=0.4,
        virus_check_frequency=0.4,
        recovery_chance=0.3,
        gain_resistance_chance=0.5,
    ):
        self.num_nodes = num_nodes
        prob = avg_node_degree / self.num_nodes
        self.G = nx.erdos_renyi_graph(n=self.num_nodes, p=prob)
        self.grid = mesa.space.NetworkGrid(self.G)
        self.schedule = mesa.time.RandomActivation(self)
        self.initial_outbreak_size = (
            initial_outbreak_size if initial_outbreak_size <= num_nodes else num_nodes
        )
        self.virus_spread_chance = virus_spread_chance
        self.virus_check_frequency = virus_check_frequency
        self.recovery_chance = recovery_chance
        self.gain_resistance_chance = gain_resistance_chance

        self.datacollector = mesa.DataCollector(
            {
                "Infected": number_infected,
                "Susceptible": number_susceptible,
                "Resistant": number_resistant,
            }
        )

        # Create agents
        for i, node in enumerate(self.G.nodes()):
            a = VirusAgent(
                i,
                self,
                State.SUSCEPTIBLE,
                self.virus_spread_chance,
                self.virus_check_frequency,
                self.recovery_chance,
                self.gain_resistance_chance,
            )
            self.schedule.add(a)
            # Add the agent to the node
            self.grid.place_agent(a, node)

        # Infect some nodes
        infected_nodes = self.random.sample(list(self.G), self.initial_outbreak_size)
        for a in self.grid.get_cell_list_contents(infected_nodes):
            a.state = State.INFECTED

        self.running = True
        self.datacollector.collect(self)

    def resistant_susceptible_ratio(self):
        try:
```

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```
            return number_state(self, State.RESISTANT) / number_state(self, State.
↪SUSCEPTIBLE)
        except ZeroDivisionError:
            return math.inf

    def step(self):
        self.schedule.step()
        # collect data
        self.datacollector.collect(self)

    def run_model(self, n):
        for i in range(n):
            self.step()


class VirusAgent(mesa.Agent):
    def __init__(
        self,
        unique_id,
        model,
        initial_state,
        virus_spread_chance,
        virus_check_frequency,
        recovery_chance,
        gain_resistance_chance,
    ):
        super().__init__(unique_id, model)

        self.state = initial_state

        self.virus_spread_chance = virus_spread_chance
        self.virus_check_frequency = virus_check_frequency
        self.recovery_chance = recovery_chance
        self.gain_resistance_chance = gain_resistance_chance

    def try_to_infect_neighbors(self):
        neighbors_nodes = self.model.grid.get_neighborhood(self.pos, include_
↪center=False)
        susceptible_neighbors = [
            agent
            for agent in self.model.grid.get_cell_list_contents(neighbors_nodes)
            if agent.state is State.SUSCEPTIBLE
        ]
        for a in susceptible_neighbors:
            if self.random.random() < self.virus_spread_chance:
                a.state = State.INFECTED

    def try_gain_resistance(self):
        if self.random.random() < self.gain_resistance_chance:
            self.state = State.RESISTANT

    def try_remove_infection(self):
```

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```
        # Try to remove
        if self.random.random() < self.recovery_chance:
            # Success
            self.state = State.SUSCEPTIBLE
            self.try_gain_resistance()
        else:
            # Failed
            self.state = State.INFECTED

    def try_check_situation(self):
        if (self.random.random() < self.virus_check_frequency) and (self.state is State.
↪INFECTED):
            self.try_remove_infection()

    def step(self):
        if self.state is State.INFECTED:
            self.try_to_infect_neighbors()
        self.try_check_situation()


# Setting up the model as a function
def model_virus_on_network(
    num_nodes=1,
    avg_node_degree=1,
    initial_outbreak_size=1,
    virus_spread_chance=1,
    virus_check_frequency=1,
    recovery_chance=1,
    gain_resistance_chance=1,
    steps=10,
):
    # Initialising the model
    virus_on_network = VirusOnNetwork(
        num_nodes=num_nodes,
        avg_node_degree=avg_node_degree,
        initial_outbreak_size=initial_outbreak_size,
        virus_spread_chance=virus_spread_chance,
        virus_check_frequency=virus_check_frequency,
        recovery_chance=recovery_chance,
        gain_resistance_chance=gain_resistance_chance,
    )

    # Run the model steps times
    virus_on_network.run_model(steps)

    # Get model outcomes
    outcomes = virus_on_network.datacollector.get_model_vars_dataframe()

    # Return model outcomes
    return {
        "Infected": outcomes["Infected"].tolist(),
        "Susceptible": outcomes["Susceptible"].tolist(),
```

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```
        "Resistant": outcomes["Resistant"].tolist(),
    }


if __name__ == "__main__":
    # Initialize logger to keep track of experiments run
    ema_logging.log_to_stderr(ema_logging.INFO)

    # Instantiate and pass the model
    model = ReplicatorModel("VirusOnNetwork", function=model_virus_on_network)

    # Define model parameters and their ranges to be sampled
    model.uncertainties = [
        IntegerParameter("num_nodes", 10, 100),
        IntegerParameter("avg_node_degree", 2, 8),
        RealParameter("virus_spread_chance", 0.1, 1),
        RealParameter("virus_check_frequency", 0.1, 1),
        RealParameter("recovery_chance", 0.1, 1),
        RealParameter("gain_resistance_chance", 0.1, 1),
    ]

    # Define model parameters that will remain constant
    model.constants = [Constant("initial_outbreak_size", 1), Constant("steps", 30)]

    # Define model outcomes
    model.outcomes = [
        ArrayOutcome("Infected"),
        ArrayOutcome("Susceptible"),
        ArrayOutcome("Resistant"),
    ]

    # Define the number of replications
    model.replications = 5

    # Run experiments with the aforementioned parameters and outputs
    results = perform_experiments(models=model, scenarios=20)

    # Get the results
    experiments, outcomes = results
```

1.10.9 example_mpi_lake_model.py

```
"""
An example of the lake problem using the ema workbench.

The model itself is adapted from the Rhodium example by Dave Hadka,
see https://gist.github.com/dhadka/a8d7095c98130d8f73bc

"""

```

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```
import math
import time

import numpy as np
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MPIEvaluator,
    save_results,
)


def lake_problem(
    b=0.42,  # decay rate for P in lake (0.42 = irreversible)
    q=2.0,  # recycling exponent
    mean=0.02,  # mean of natural inflows
    stdev=0.001,  # future utility discount rate
    delta=0.98,  # standard deviation of natural inflows
    alpha=0.4,  # utility from pollution
    nsamples=100,  # Monte Carlo sampling of natural inflows
    **kwargs,
):
    try:
        decisions = [kwargs[str(i)] for i in range(100)]
    except KeyError:
        decisions = [0] * 100
        print("No valid decisions found, using 0 water release every year as default")

    nvars = len(decisions)
    decisions = np.array(decisions)

    # Calculate the critical pollution level (Pcrit)
    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)

    # Generate natural inflows using lognormal distribution
    natural_inflows = np.random.lognormal(
        mean=math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
        sigma=math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
        size=(nsamples, nvars),
    )

    # Initialize the pollution level matrix X
    X = np.zeros((nsamples, nvars))

    # Loop through time to compute the pollution levels
    for t in range(1, nvars):
        X[:, t] = (
```

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```
            (1 - b) * X[:, t - 1]
            + (X[:, t - 1] ** q / (1 + X[:, t - 1] ** q))
            + decisions[t - 1]
            + natural_inflows[:, t - 1]
        )

    # Calculate the average daily pollution for each time step
    average_daily_P = np.mean(X, axis=0)

    # Calculate the reliability (probability of the pollution level being below Pcrit)
    reliability = np.sum(X < Pcrit) / float(nsamples * nvars)

    # Calculate the maximum pollution level (max_P)
    max_P = np.max(average_daily_P)

    # Calculate the utility by discounting the decisions using the discount factor␣
↪(delta)
    utility = np.sum(alpha * decisions * np.power(delta, np.arange(nvars)))

    # Calculate the inertia (the fraction of time steps with changes larger than 0.02)
    inertia = np.sum(np.abs(np.diff(decisions)) > 0.02) / float(nvars - 1)

    return max_P, utility, inertia, reliability


if __name__ == "__main__":
    import ema_workbench

    # run with mpiexec -n 1 -usize {ntasks} python example_mpi_lake_model.py
    starttime = time.perf_counter()

    ema_logging.log_to_stderr(ema_logging.INFO, pass_root_logger_level=True)
    ema_logging.get_rootlogger().info(f"{ema_workbench.__version__}")

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    lake_model.time_horizon = 100

    # specify uncertainties
    lake_model.uncertainties = [
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("mean", 0.01, 0.05),
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("delta", 0.93, 0.99),
    ]

    # set levers, one for each time step
    lake_model.levers = [RealParameter(str(i), 0, 0.1) for i in range(lake_model.time_
↪horizon)]

    # specify outcomes
```

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```
    lake_model.outcomes = [
        ScalarOutcome("max_P"),
        ScalarOutcome("utility"),
        ScalarOutcome("inertia"),
        ScalarOutcome("reliability"),
    ]

    # override some of the defaults of the model
    lake_model.constants = [Constant("alpha", 0.41), Constant("nsamples", 150)]

    # generate some random policies by sampling over levers
    n_scenarios = 10000
    n_policies = 4

    with MPIEvaluator(lake_model) as evaluator:
        res = evaluator.perform_experiments(n_scenarios, n_policies, chunksize=250)

    save_results(res, "test.tar.gz")

    print(time.perf_counter() - starttime)
```

1.10.10 example_netlogo.py

```
"""

This example is a proof of principle for how NetLogo models can be
controlled using pyNetLogo and the ema_workbench. Note that this
example uses the NetLogo 6 version of the predator prey model that
comes with NetLogo. If you are using NetLogo 5, replace the model file
with the one that comes with NetLogo.

"""

import numpy as np

from ema_workbench import (
    RealParameter,
    ema_logging,
    ScalarOutcome,
    TimeSeriesOutcome,
    MultiprocessingEvaluator,
)
from ema_workbench.connectors.netlogo import NetLogoModel

# Created on 20 mrt. 2013
#
# .. codeauthor::  jhkwakkel


if __name__ == "__main__":
```

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```
    # turn on logging
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = NetLogoModel(
        "predprey", wd="./models/predatorPreyNetlogo", model_file="Wolf Sheep Predation.
↪nlogo"
    )
    model.run_length = 100
    model.replications = 10

    model.uncertainties = [
        RealParameter("grass-regrowth-time", 1, 99),
        RealParameter("initial-number-sheep", 50, 100),
        RealParameter("initial-number-wolves", 50, 100),
        RealParameter("sheep-reproduce", 5, 10),
        RealParameter("wolf-reproduce", 5, 10),
    ]

    model.outcomes = [
        ScalarOutcome("sheep", variable_name="count sheep", function=np.mean),
        TimeSeriesOutcome("wolves"),
        TimeSeriesOutcome("grass"),
    ]

    # perform experiments
    n = 10

    with MultiprocessingEvaluator(model, n_processes=-1, maxtasksperchild=4) as␣
↪evaluator:
        results = evaluator.perform_experiments(n)

    print()
```

1.10.11 example_pysd_teacup.py

```
"""


"""

# Created on Jul 23, 2016
#
# .. codeauthor::jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>

from ema_workbench import RealParameter, TimeSeriesOutcome, ema_logging, perform_
↪experiments

from ema_workbench.connectors.pysd_connector import PysdModel

if __name__ == "__main__":
```

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```
    ema_logging.log_to_stderr(ema_logging.INFO)

    mdl_file = "./models/pysd/Teacup.mdl"

    model = PysdModel("teacup", mdl_file=mdl_file)

    model.uncertainties = [
        RealParameter("room_temperature", 33, 120, variable_name="Room Temperature")
    ]
    model.outcomes = [TimeSeriesOutcome("teacup_temperature", variable_name="Teacup␣
↪Temperature")]

    perform_experiments(model, 100)
```

1.10.12 example_python.py

```
"""
Created on 20 dec. 2010

This file illustrated the use the EMA classes for a contrived example
It's main purpose has been to test the parallel processing functionality

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
"""

from ema_workbench import Model, RealParameter, ScalarOutcome, ema_logging, perform_
↪experiments


def some_model(x1=None, x2=None, x3=None):
    return {"y": x1 * x2 + x3}


if __name__ == "__main__":
    ema_logging.LOG_FORMAT = "[%(name)s/%(levelname)s/%(processName)s] %(message)s"
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = Model("simpleModel", function=some_model)  # instantiate the model

    # specify uncertainties
    model.uncertainties = [
        RealParameter("x1", 0.1, 10),
        RealParameter("x2", -0.01, 0.01),
        RealParameter("x3", -0.01, 0.01),
    ]
    # specify outcomes
    model.outcomes = [ScalarOutcome("y")]

    results = perform_experiments(model, 100)
```

1.10.13 example_simio.py

```
"""
Created on 27 Jun 2019

@author: jhkwakkel
"""

from ema_workbench import ema_logging, CategoricalParameter, MultiprocessingEvaluator,␣
↪ScalarOutcome

from ema_workbench.connectors.simio_connector import SimioModel

if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = SimioModel(
        "simioDemo", wd="./model_bahareh", model_file="SupplyChainV3.spfx", main_model=
↪"Model"
    )

    model.uncertainties = [
        CategoricalParameter("DemandDistributionParameter", (20, 30, 40, 50, 60)),
        CategoricalParameter("DemandInterarrivalTime", (0.25, 0.5, 0.75, 1, 1.25, 1.5, 1.
↪75, 2)),
    ]

    model.levers = [
        CategoricalParameter("InitialInventory", (500, 600, 700, 800, 900)),
        CategoricalParameter("ReorderPoint", (100, 200, 300, 400, 500)),
        CategoricalParameter("OrderUpToQuantity", (500, 600, 700, 800, 900)),
        CategoricalParameter("ReviewPeriod", (3, 4, 5, 6, 7)),
    ]

    model.outcomes = [ScalarOutcome("AverageInventory"), ScalarOutcome(
↪"AverageServiceLevel")]

    n_scenarios = 10
    n_policies = 2

    with MultiprocessingEvaluator(model) as evaluator:
        results = evaluator.perform_experiments(n_scenarios, n_policies)
```

1.10.14 example_vensim.py

```
"""
Created on 3 Jan. 2011

This file illustrated the use the EMA classes for a contrived vensim
example


.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                chamarat <c.hamarat (at) tudelft (dot) nl>
"""

from ema_workbench import TimeSeriesOutcome, perform_experiments, RealParameter, ema_
↪logging

from ema_workbench.connectors.vensim import VensimModel

if __name__ == "__main__":
    # turn on logging
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate a model
    wd = "./models/vensim example"
    vensimModel = VensimModel("simpleModel", wd=wd, model_file="model.vpm")
    vensimModel.uncertainties = [RealParameter("x11", 0, 2.5), RealParameter("x12", -2.5,
↪ 2.5)]

    vensimModel.outcomes = [TimeSeriesOutcome("a")]

    results = perform_experiments(vensimModel, 1000)
```

1.10.15 example_vensim_advanced_flu.py

```
"""
Created on 20 May, 2011

This module shows how you can use vensim models directly
instead of coding the model in Python. The underlying case
is the same as used in fluExample

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                epruyt <e.pruyt (at) tudelft (dot) nl>
"""

import numpy as np

from ema_workbench import (
    TimeSeriesOutcome,
    ScalarOutcome,
    ema_logging,
```

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```
    Policy,
    MultiprocessingEvaluator,
    save_results,
)
from ema_workbench.connectors.vensim import VensimModel
from ema_workbench.em_framework.parameters import parameters_from_csv


def time_of_max(infected_fraction, time):
    index = np.where(infected_fraction == np.max(infected_fraction))
    timing = time[index][0]
    return timing


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = VensimModel("fluCase", wd="./models/flu", model_file="FLUvensimV1basecase.vpm
↪")

    # outcomes
    model.outcomes = [
        TimeSeriesOutcome(
            "deceased_population_region_1", variable_name="deceased population region 1"
        ),
        TimeSeriesOutcome("infected_fraction_R1", variable_name="infected fraction R1"),
        ScalarOutcome(
            "max_infection_fraction", variable_name="infected fraction R1", function=np.
↪max
        ),
        ScalarOutcome(
            "time_of_max", variable_name=["infected fraction R1", "TIME"], function=time_
↪of_max
        ),
    ]

    # create uncertainties based on csv
    # FIXME csv is missing
    model.uncertainties = parameters_from_csv("./models/flu/flu_uncertainties.csv")

    # add policies
    policies = [
        Policy("no policy", model_file="FLUvensimV1basecase.vpm"),
        Policy("static policy", model_file="FLUvensimV1static.vpm"),
        Policy("adaptive policy", model_file="FLUvensimV1dynamic.vpm"),
    ]

    with MultiprocessingEvaluator(model, n_processes=-1) as evaluator:
        results = evaluator.perform_experiments(1000, policies=policies)

    save_results(results, "./data/1000 flu cases with policies.tar.gz")
```

1.10.16 example_vensim_energy.py

```
"""
Created on 27 Jan 2014

@author: jhkwakkel
"""

from ema_workbench import (
    RealParameter,
    TimeSeriesOutcome,
    ema_logging,
    MultiprocessingEvaluator,
    ScalarOutcome,
    perform_experiments,
    CategoricalParameter,
    save_results,
    Policy,
)
from ema_workbench.connectors.vensim import VensimModel
from ema_workbench.em_framework.evaluators import SequentialEvaluator


def get_energy_model():
    model = VensimModel(
        "energyTransition",
        wd="./models",
        model_file="RB_V25_ets_1_policy_modified_adaptive_extended_outcomes.vpm",
    )

    model.outcomes = [
        TimeSeriesOutcome(
            "cumulative_carbon_emissions", variable_name="cumulative carbon emissions"
        ),
        TimeSeriesOutcome(
            "carbon_emissions_reduction_fraction",
            variable_name="carbon emissions reduction fraction",
        ),
        TimeSeriesOutcome("fraction_renewables", variable_name="fraction renewables"),
        TimeSeriesOutcome("average_total_costs", variable_name="average total costs"),
        TimeSeriesOutcome("total_costs_of_electricity", variable_name="total costs of␣
↪electricity"),
    ]

    model.uncertainties = [
        RealParameter(
            "demand_fuel_price_elasticity_factor",
            0,
            0.5,
            variable_name="demand fuel price elasticity factor",
        ),
        RealParameter(
            "economic_lifetime_biomass", 30, 50, variable_name="economic lifetime biomass
```

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```
↪"
        ),
        RealParameter("economic_lifetime_coal", 30, 50, variable_name="economic lifetime␣
↪coal"),
        RealParameter("economic_lifetime_gas", 25, 40, variable_name="economic lifetime␣
↪gas"),
        RealParameter("economic_lifetime_igcc", 30, 50, variable_name="economic lifetime␣
↪igcc"),
        RealParameter("economic_lifetime_ngcc", 25, 40, variable_name="economic lifetime␣
↪ngcc"),
        RealParameter(
            "economic_lifetime_nuclear", 50, 70, variable_name="economic lifetime nuclear
↪"
        ),
        RealParameter("economic_lifetime_pv", 20, 30, variable_name="economic lifetime pv
↪"),
        RealParameter("economic_lifetime_wind", 20, 30, variable_name="economic lifetime␣
↪wind"),
        RealParameter("economic_lifetime_hydro", 50, 70, variable_name="economic␣
↪lifetime hydro"),
        RealParameter(
            "uncertainty_initial_gross_fuel_costs",
            0.5,
            1.5,
            variable_name="uncertainty initial gross fuel costs",
        ),
        RealParameter(
            "investment_proportionality_constant",
            0.5,
            4,
            variable_name="investment proportionality constant",
        ),
        RealParameter(
            "investors_desired_excess_capacity_investment",
            0.2,
            2,
            variable_name="investors desired excess capacity investment",
        ),
        RealParameter(
            "price_demand_elasticity_factor",
            -0.07,
            -0.001,
            variable_name="price demand elasticity factor",
        ),
        RealParameter(
            "price_volatility_global_resource_markets",
            0.1,
            0.2,
            variable_name="price volatility global resource markets",
        ),
        RealParameter("progress_ratio_biomass", 0.85, 1, variable_name="progress ratio␣
↪biomass"),
```

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```
        RealParameter("progress_ratio_coal", 0.9, 1.05, variable_name="progress ratio coal"),
        RealParameter("progress_ratio_gas", 0.85, 1, variable_name="progress ratio gas"),
        RealParameter("progress_ratio_igcc", 0.9, 1.05, variable_name="progress ratio igcc"),
        RealParameter("progress_ratio_ngcc", 0.85, 1, variable_name="progress ratio ngcc"),
        RealParameter("progress_ratio_nuclear", 0.9, 1.05, variable_name="progress ratio nuclear"),
        RealParameter("progress_ratio_pv", 0.75, 0.9, variable_name="progress ratio pv"),
        RealParameter("progress_ratio_wind", 0.85, 1, variable_name="progress ratio wind"),
        RealParameter("progress_ratio_hydro", 0.9, 1.05, variable_name="progress ratio hydro"),
        RealParameter(
            "starting_construction_time", 0.1, 3, variable_name="starting construction time"
        ),
        RealParameter(
            "time_of_nuclear_power_plant_ban",
            2013,
            2100,
            variable_name="time of nuclear power plant ban",
        ),
        RealParameter(
            "weight_factor_carbon_abatement", 1, 10, variable_name="weight factor carbon abatement"
        ),
        RealParameter(
            "weight_factor_marginal_investment_costs",
            1,
            10,
            variable_name="weight factor marginal investment costs",
        ),
        RealParameter(
            "weight_factor_technological_familiarity",
            1,
            10,
            variable_name="weight factor technological familiarity",
        ),
        RealParameter(
            "weight_factor_technological_growth_potential",
            1,
            10,
            variable_name="weight factor technological growth potential",
        ),
        RealParameter(
            "maximum_battery_storage_uncertainty_constant",
            0.2,
            3,
            variable_name="maximum battery storage uncertainty constant",
        ),
```

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```
        RealParameter(
            "maximum_no_storage_penetration_rate_wind",
            0.2,
            0.6,
            variable_name="maximum no storage penetration rate wind",
        ),
        RealParameter(
            "maximum_no_storage_penetration_rate_pv",
            0.1,
            0.4,
            variable_name="maximum no storage penetration rate pv",
        ),
        CategoricalParameter(
            "SWITCH_lookup_curve_TGC", (1, 2, 3, 4), variable_name="SWITCH lookup curve␣
↪TGC"
        ),
        CategoricalParameter(
            "SWTICH_preference_carbon_curve", (1, 2), variable_name="SWTICH preference␣
↪carbon curve"
        ),
        CategoricalParameter(
            "SWITCH_economic_growth", (1, 2, 3, 4, 5, 6), variable_name="SWITCH economic␣
↪growth"
        ),
        CategoricalParameter(
            "SWITCH_electrification_rate",
            (1, 2, 3, 4, 5, 6),
            variable_name="SWITCH electrification rate",
        ),
        CategoricalParameter(
            "SWITCH_Market_price_determination",
            (1, 2),
            variable_name="SWITCH Market price determination",
        ),
        CategoricalParameter(
            "SWITCH_physical_limits", (1, 2), variable_name="SWITCH physical limits"
        ),
        CategoricalParameter(
            "SWITCH_low_reserve_margin_price_markup",
            (1, 2, 3, 4),
            variable_name="SWITCH low reserve margin price markup",
        ),
        CategoricalParameter(
            "SWITCH_interconnection_capacity_expansion",
            (1, 2, 3, 4),
            variable_name="SWITCH interconnection capacity expansion",
        ),
        CategoricalParameter(
            "SWITCH_storage_for_intermittent_supply",
            (1, 2, 3, 4, 5, 6, 7),
            variable_name="SWITCH storage for intermittent supply",
        ),
```

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```
        CategoricalParameter("SWITCH_carbon_cap", (1, 2, 3), variable_name="SWITCH␣
↪carbon cap"),
        CategoricalParameter(
            "SWITCH_TGC_obligation_curve", (1, 2, 3), variable_name="SWITCH TGC␣
↪obligation curve"
        ),
        CategoricalParameter(
            "SWITCH_carbon_price_determination",
            (1, 2, 3),
            variable_name="SWITCH carbon price determination",
        ),
    ]
    return model


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)
    model = get_energy_model()

    policies = [
        Policy("no policy", model_file="RB_V25_ets_1_extended_outcomes.vpm"),
        Policy("static policy", model_file="ETSPolicy.vpm"),
        Policy(
            "adaptive policy",
            model_file="RB_V25_ets_1_policy_modified_adaptive_extended_outcomes.vpm",
        ),
    ]

    n = 100000
    with MultiprocessingEvaluator(model) as evaluator:
        experiments, outcomes = evaluator.perform_experiments(n, policies=policies)
    #
    # outcomes.pop("TIME")
    # results = experiments, outcomes
    # save_results(results, f"./data/{n}_lhs.tar.gz")
```

1.10.17 example_vensim_flu.py

```
"""
Created on 20 May, 2011

This module shows how you can use vensim models directly
instead of coding the model in Python. The underlying case
is the same as used in fluExample

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                epruyt <e.pruyt (at) tudelft (dot) nl>
"""

import numpy as np
```

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```

from ema_workbench import (
    RealParameter,
    TimeSeriesOutcome,
    ema_logging,
    ScalarOutcome,
    perform_experiments,
    Policy,
    save_results,
)
from ema_workbench.connectors.vensim import VensimModel

if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = VensimModel("fluCase", wd=r"./models/flu", model_file=r"FLUvensimV1basecase.vpm")

    # outcomes
    model.outcomes = [
        TimeSeriesOutcome(
            "deceased_population_region_1", variable_name="deceased population region 1"
        ),
        TimeSeriesOutcome("infected_fraction_R1", variable_name="infected fraction R1"),
        ScalarOutcome(
            "max_infection_fraction", variable_name="infected fraction R1", function=np.max
        ),
    ]

    # Plain Parametric Uncertainties
    model.uncertainties = [
        RealParameter(
            "additional_seasonal_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R1",
        ),
        RealParameter(
            "additional_seasonal_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R2",
        ),
        RealParameter(
            "fatality_ratio_region_1", 0.0001, 0.1, variable_name="fatality ratio region 1"
        ),
        RealParameter(
            "fatality_rate_region_2", 0.0001, 0.1, variable_name="fatality rate region 2"
        ),
        RealParameter(
```

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```
            "initial_immune_fraction_of_the_population_of_region_1",
            0,
            0.5,
            variable_name="initial immune fraction of the population of region 1",
        ),
        RealParameter(
            "initial_immune_fraction_of_the_population_of_region_2",
            0,
            0.5,
            variable_name="initial immune fraction of the population of region 2",
        ),
        RealParameter(
            "normal_interregional_contact_rate",
            0,
            0.9,
            variable_name="normal interregional contact rate",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="permanent immune population fraction R1",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="permanent immune population fraction R2",
        ),
        RealParameter("recovery_time_region_1", 0.1, 0.75, variable_name="recovery time␣
↪region 1"),
        RealParameter("recovery_time_region_2", 0.1, 0.75, variable_name="recovery time␣
↪region 2"),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_1",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 1",
        ),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_2",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 2",
        ),
        RealParameter(
            "root_contact_rate_region_1", 0.01, 5, variable_name="root contact rate␣
↪region 1"
        ),
        RealParameter(
            "root_contact_ratio_region_2", 0.01, 5, variable_name="root contact ratio␣
↪region 2"
```

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```
        ),
        RealParameter(
            "infection_ratio_region_1", 0, 0.15, variable_name="infection ratio region 1"
        ),
        RealParameter("infection_rate_region_2", 0, 0.15, variable_name="infection rate␣
↪region 2"),
        RealParameter(
            "normal_contact_rate_region_1", 10, 100, variable_name="normal contact rate␣
↪region 1"
        ),
        RealParameter(
            "normal_contact_rate_region_2", 10, 200, variable_name="normal contact rate␣
↪region 2"
        ),
    ]

    # add policies
    policies = [
        Policy("no policy", model_file=r"FLUvensimV1basecase.vpm"),
        Policy("static policy", model_file=r"FLUvensimV1static.vpm"),
        Policy("adaptive policy", model_file=r"FLUvensimV1dynamic.vpm"),
    ]

    results = perform_experiments(model, 1000, policies=policies)
    save_results(results, "./data/1000 flu cases with policies.tar.gz")
```

1.10.18 example_vensim_lookup.py

```
"""
Created on Oct 1, 2012

This is a simple example of the lookup uncertainty provided for
use in conjunction with vensim models. This example is largely based on
`Eker et al. (2014) <https://onlinelibrary.wiley.com/doi/10.1002/sdr.1518/suppinfo>`_

@author: sibeleker
@author: jhkwakkel
"""

import matplotlib.pyplot as plt

from ema_workbench import TimeSeriesOutcome, perform_experiments, ema_logging
from ema_workbench.analysis import lines, Density
from ema_workbench.connectors.vensim import LookupUncertainty, VensimModel


class Burnout(VensimModel):
    model_file = r"\BURNOUT.vpm"
    outcomes = [
        TimeSeriesOutcome("accomplishments_to_date", variable_name="Accomplishments to␣
```

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```
↪Date"),
        TimeSeriesOutcome("energy_level", variable_name="Energy Level"),
        TimeSeriesOutcome("hours_worked_per_week", variable_name="Hours Worked Per Week
↪"),
        TimeSeriesOutcome("accomplishments_per_hour", variable_name="accomplishments per␣
↪hour"),
    ]

    def __init__(self, working_directory, name):
        super().__init__(working_directory, name)

        self.uncertainties = [
            LookupUncertainty(
                "hearne2",
                [(-1, 3), (-2, 1), (0, 0.9), (0.1, 1), (0.99, 1.01), (0.99, 1.01)],
                "accomplishments per hour lookup",
                self,
                0,
                1,
            ),
            LookupUncertainty(
                "hearne2",
                [(-0.75, 0.75), (-0.75, 0.75), (0, 1.5), (0.1, 1.6), (-0.3, 1.5), (0.25,␣
↪2.5)],
                "fractional change in expectations from perceived adequacy lookup",
                self,
                -1,
                1,
            ),
            LookupUncertainty(
                "hearne2",
                [(-2, 2), (-1, 2), (0, 1.5), (0.1, 1.6), (0.5, 2), (0.5, 2)],
                "effect of perceived adequacy on energy drain lookup",
                self,
                0,
                10,
            ),
            LookupUncertainty(
                "hearne2",
                [(-2, 2), (-1, 2), (0, 1.5), (0.1, 1.6), (0.5, 1.5), (0.1, 2)],
                "effect of perceived adequacy of hours worked lookup",
                self,
                0,
                2.5,
            ),
            LookupUncertainty(
                "hearne2",
                [(-1, 1), (-1, 1), (0, 0.9), (0.1, 1), (0.5, 1.5), (1, 1.5)],
                "effect of energy levels on hours worked lookup",
                self,
                0,
                1.5,
```

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```
            ),
            LookupUncertainty(
                "hearne2",
                [(-1, 1), (-1, 1), (0, 0.9), (0.1, 1), (0.5, 1.5), (1, 1.5)],
                "effect of high energy on further recovery lookup",
                self,
                0,
                1.25,
            ),
            LookupUncertainty(
                "hearne2",
                [(-2, 2), (-1, 1), (0, 100), (20, 120), (0.5, 1.5), (0.5, 2)],
                "effect of hours worked on energy recovery lookup",
                self,
                0,
                1.5,
            ),
            LookupUncertainty(
                "approximation",
                [(-0.5, 0.35), (3, 5), (1, 10), (0.2, 0.4), (0, 120)],
                "effect of hours worked on energy drain lookup",
                self,
                0,
                3,
            ),
            LookupUncertainty(
                "hearne1",
                [(0, 1), (0, 0.15), (1, 1.5), (0.75, 1.25)],
                "effect of low energy on further depletion lookup",
                self,
                0,
                1,
            ),
        ]

        self._delete_lookup_uncertainties()


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)
    model = Burnout(r"./models/burnout", "burnout")

    # run policy with old cases
    results = perform_experiments(model, 100)
    lines(results, "Energy Level", density=Density.BOXPLOT)
    plt.show()
```

1.10.19 example_vensim_no_policy_flu.py

```
"""
Created on 20 May, 2011

This module shows how you can use vensim models directly
instead of coding the model in Python. The underlying case
is the same as used in fluExample

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                epruyt <e.pruyt (at) tudelft (dot) nl>
"""

from ema_workbench import (
    RealParameter,
    TimeSeriesOutcome,
    ema_logging,
    perform_experiments,
    MultiprocessingEvaluator,
    save_results,
)

from ema_workbench.connectors.vensim import VensimModel

if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    model = VensimModel("fluCase", wd=r"./models/flu", model_file=r"FLUvensimV1basecase.
↪vpm")

    # outcomes
    model.outcomes = [
        TimeSeriesOutcome(
            "deceased_population_region_1", variable_name="deceased population region 1"
        ),
        TimeSeriesOutcome("infected_fraction_R1", variable_name="infected fraction R1"),
    ]

    # Plain Parametric Uncertainties
    model.uncertainties = [
        RealParameter(
            "additional_seasonal_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R1",
        ),
        RealParameter(
            "additional_seasonal_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="additional seasonal immune population fraction R2",
        ),
        RealParameter(
```

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```
            "fatality_ratio_region_1", 0.0001, 0.1, variable_name="fatality ratio region 1"
        ),
        RealParameter(
            "fatality_rate_region_2", 0.0001, 0.1, variable_name="fatality rate region 2"
        ),
        RealParameter(
            "initial_immune_fraction_of_the_population_of_region_1",
            0,
            0.5,
            variable_name="initial immune fraction of the population of region 1",
        ),
        RealParameter(
            "initial_immune_fraction_of_the_population_of_region_2",
            0,
            0.5,
            variable_name="initial immune fraction of the population of region 2",
        ),
        RealParameter(
            "normal_interregional_contact_rate",
            0,
            0.9,
            variable_name="normal interregional contact rate",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R1",
            0,
            0.5,
            variable_name="permanent immune population fraction R1",
        ),
        RealParameter(
            "permanent_immune_population_fraction_R2",
            0,
            0.5,
            variable_name="permanent immune population fraction R2",
        ),
        RealParameter("recovery_time_region_1", 0.1, 0.75, variable_name="recovery time region 1"),
        RealParameter("recovery_time_region_2", 0.1, 0.75, variable_name="recovery time region 2"),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_1",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 1",
        ),
        RealParameter(
            "susceptible_to_immune_population_delay_time_region_2",
            0.5,
            2,
            variable_name="susceptible to immune population delay time region 2",
        ),
```

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```
        RealParameter(
            "root_contact_rate_region_1", 0.01, 5, variable_name="root contact rate␣
↪region 1"
        ),
        RealParameter(
            "root_contact_ratio_region_2", 0.01, 5, variable_name="root contact ratio␣
↪region 2"
        ),
        RealParameter(
            "infection_ratio_region_1", 0, 0.15, variable_name="infection ratio region 1"
        ),
        RealParameter("infection_rate_region_2", 0, 0.15, variable_name="infection rate␣
↪region 2"),
        RealParameter(
            "normal_contact_rate_region_1", 10, 100, variable_name="normal contact rate␣
↪region 1"
        ),
        RealParameter(
            "normal_contact_rate_region_2", 10, 200, variable_name="normal contact rate␣
↪region 2"
        ),
    ]

    nr_experiments = 1000
    with MultiprocessingEvaluator(model) as evaluator:
        results = perform_experiments(model, nr_experiments, evaluator=evaluator)

    save_results(results, "./data/1000 flu cases no policy.tar.gz")
```

1.10.20 example_vensim_scarcity.py

```
"""
Created on 8 mrt. 2011

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                epruyt <e.pruyt (at) tudelft (dot) nl>
"""

from math import exp

from ema_workbench.connectors.vensim import VensimModel
from ema_workbench.em_framework import (
    RealParameter,
    CategoricalParameter,
    TimeSeriesOutcome,
    perform_experiments,
)
from ema_workbench.util import ema_logging


```

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```
class ScarcityModel(VensimModel):
    def returnsToScale(self, x, speed, scale):
        return (x * 1000, scale * 1 / (1 + exp(-1 * speed * (x - 50))))

    def approxLearning(self, x, speed, scale, start):
        x = x - start
        loc = 1 - scale
        a = (x * 10000, scale * 1 / (1 + exp(speed * x)) + loc)
        return a

    def f(self, x, speed, loc):
        return (x / 10, loc * 1 / (1 + exp(speed * x)))

    def priceSubstite(self, x, speed, begin, end):
        scale = 2 * end
        start = begin - scale / 2

        return (x + 2000, scale * 1 / (1 + exp(-1 * speed * x)) + start)

    def run_model(self, scenario, policy):
        """Method for running an instantiated model structure"""
        kwargs = scenario
        loc = kwargs.pop("lookup_shortage_loc")
        speed = kwargs.pop("lookup_shortage_speed")
        lookup = [self.f(x / 10, speed, loc) for x in range(0, 100)]
        kwargs["shortage price effect lookup"] = lookup

        speed = kwargs.pop("lookup_price_substitute_speed")
        begin = kwargs.pop("lookup_price_substitute_begin")
        end = kwargs.pop("lookup_price_substitute_end")
        lookup = [self.priceSubstite(x, speed, begin, end) for x in range(0, 100, 10)]
        kwargs["relative price substitute lookup"] = lookup

        scale = kwargs.pop("lookup_returns_to_scale_speed")
        speed = kwargs.pop("lookup_returns_to_scale_scale")
        lookup = [self.returnsToScale(x, speed, scale) for x in range(0, 101, 10)]
        kwargs["returns to scale lookup"] = lookup

        scale = kwargs.pop("lookup_approximated_learning_speed")
        speed = kwargs.pop("lookup_approximated_learning_scale")
        start = kwargs.pop("lookup_approximated_learning_start")
        lookup = [self.approxLearning(x, speed, scale, start) for x in range(0, 101, 10)]
        kwargs["approximated learning effect lookup"] = lookup

        super().run_model(kwargs, policy)


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.DEBUG)

    model = ScarcityModel("scarcity", wd="./models/scarcity", model_file="MetalsEMA.vpm")

```

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```
    model.outcomes = [
        TimeSeriesOutcome("relative_market_price", variable_name="relative market price
↪"),
        TimeSeriesOutcome("supply_demand_ratio", variable_name="supply demand ratio"),
        TimeSeriesOutcome("real_annual_demand", variable_name="real annual demand"),
        TimeSeriesOutcome(
            "produced_of_intrinsically_demanded", variable_name="produced of␣
↪intrinsically demanded"
        ),
        TimeSeriesOutcome("supply", variable_name="supply"),
        TimeSeriesOutcome(
            "Installed_Recycling_Capacity", variable_name="Installed Recycling Capacity"
        ),
        TimeSeriesOutcome(
            "Installed_Extraction_Capacity", variable_name="Installed Extraction Capacity
↪"
        ),
    ]

    model.uncertainties = [
        RealParameter(
            "price_elasticity_of_demand", 0, 0.5, variable_name="price elasticity of␣
↪demand"
        ),
        RealParameter(
            "fraction_of_maximum_extraction_capacity_used",
            0.6,
            1.2,
            variable_name="fraction of maximum extraction capacity used",
        ),
        RealParameter(
            "initial_average_recycling_cost", 1, 4, variable_name="initial average␣
↪recycling cost"
        ),
        RealParameter(
            "exogenously_planned_extraction_capacity",
            0,
            15000,
            variable_name="exogenously planned extraction capacity",
        ),
        RealParameter(
            "absolute_recycling_loss_fraction",
            0.1,
            0.5,
            variable_name="absolute recycling loss fraction",
        ),
        RealParameter("normal_profit_margin", 0, 0.4, variable_name="normal profit margin
↪"),
        RealParameter(
            "initial_annual_supply", 100000, 120000, variable_name="initial annual supply
↪"
        ),
```

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```
        RealParameter("initial_in_goods", 1500000, 2500000, variable_name="initial in_
↪goods"),
        RealParameter(
            "average_construction_time_extraction_capacity",
            1,
            10,
            variable_name="average construction time extraction capacity",
        ),
        RealParameter(
            "average_lifetime_extraction_capacity",
            20,
            40,
            variable_name="average lifetime extraction capacity",
        ),
        RealParameter(
            "average_lifetime_recycling_capacity",
            20,
            40,
            variable_name="average lifetime recycling capacity",
        ),
        RealParameter(
            "initial_extraction_capacity_under_construction",
            5000,
            20000,
            variable_name="initial extraction capacity under construction",
        ),
        RealParameter(
            "initial_recycling_capacity_under_construction",
            5000,
            20000,
            variable_name="initial recycling capacity under construction",
        ),
        RealParameter(
            "initial_recycling_infrastructure",
            5000,
            20000,
            variable_name="initial recycling infrastructure",
        ),
        # order of delay
        CategoricalParameter(
            "order_in_goods_delay", (1, 4, 10, 1000), variable_name="order in goods delay
↪"
        ),
        CategoricalParameter(
            "order_recycling_capacity_delay",
            (1, 4, 10),
            variable_name="order recycling capacity delay",
        ),
        CategoricalParameter(
            "order_extraction_capacity_delay",
            (1, 4, 10),
            variable_name="order extraction capacity delay",
```

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```
        ),
        # uncertainties associated with lookups
        RealParameter("lookup_shortage_loc", 20, 50, variable_name="lookup shortage loc
↪"),
        RealParameter("lookup_shortage_speed", 1, 5, variable_name="lookup shortage speed
↪"),
        RealParameter(
            "lookup_price_substitute_speed", 0.1, 0.5, variable_name="lookup price␣
↪substitute speed"
        ),
        RealParameter(
            "lookup_price_substitute_begin", 3, 7, variable_name="lookup price␣
↪substitute begin"
        ),
        RealParameter(
            "lookup_price_substitute_end", 15, 25, variable_name="lookup price␣
↪substitute end"
        ),
        RealParameter(
            "lookup_returns_to_scale_speed",
            0.01,
            0.2,
            variable_name="lookup returns to scale speed",
        ),
        RealParameter(
            "lookup_returns_to_scale_scale", 0.3, 0.7, variable_name="lookup returns to␣
↪scale scale"
        ),
        RealParameter(
            "lookup_approximated_learning_speed",
            0.01,
            0.2,
            variable_name="lookup approximated learning speed",
        ),
        RealParameter(
            "lookup_approximated_learning_scale",
            0.3,
            0.6,
            variable_name="lookup approximated learning scale",
        ),
        RealParameter(
            "lookup_approximated_learning_start",
            30,
            60,
            variable_name="lookup approximated learning start",
        ),
    ]

    results = perform_experiments(model, 1000)
```

1.10.21 feature_scoring_flu.py

```
"""
Created on 30 Oct 2018

@author: jhkwakkel
"""

import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import feature_scoring

ema_logging.log_to_stderr(level=ema_logging.INFO)

# load data
fn = r"./data/1000 flu cases with policies.tar.gz"
x, outcomes = load_results(fn)

# we have timeseries so we need scalars
y = {
    "deceased population": outcomes["deceased_population_region_1"][:, -1],
    "max. infected fraction": np.max(outcomes["infected_fraction_R1"], axis=1),
}

scores = feature_scoring.get_feature_scores_all(x, y)
sns.heatmap(scores, annot=True, cmap="viridis")
plt.show()
```

1.10.22 feature_scoring_flu_confidence.py

```
"""
Created on 30 Oct 2018

@author: jhkwakkel
"""

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis.feature_scoring import get_ex_feature_scores,␣
↪RuleInductionType

ema_logging.log_to_stderr(level=ema_logging.INFO)

# load data
```

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```
fn = r"./data/1000 flu cases no policy.tar.gz"
x, outcomes = load_results(fn)

x = x.drop(["model", "policy"], axis=1)
y = np.max(outcomes["infected_fraction_R1"], axis=1)

all_scores = []
for i in range(100):
    indices = np.random.choice(np.arange(0, x.shape[0]), size=x.shape[0])
    selected_x = x.iloc[indices, :]
    selected_y = y[indices]

    scores = get_ex_feature_scores(selected_x, selected_y, mode=RuleInductionType.
↪REGRESSION)[0]
    all_scores.append(scores)
all_scores = pd.concat(all_scores, axis=1, sort=False)

sns.boxplot(data=all_scores.T)
plt.show()
```

1.10.23 feature_scoring_flu_overtime.py

```
"""
Created on 30 Oct 2018

@author: jhkwakkel
"""

import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import get_ex_feature_scores, RuleInductionType

ema_logging.log_to_stderr(level=ema_logging.INFO)

# load data
fn = r"./data/1000 flu cases no policy.tar.gz"

x, outcomes = load_results(fn)
x = x.drop(["model", "policy"], axis=1)

y = outcomes["deceased_population_region_1"]

all_scores = []

# we only want to show those uncertainties that are in the top 5
# most sensitive parameters at any time step
top_5 = set()
```

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```
for i in range(2, y.shape[1], 8):
    data = y[:, i]
    scores = get_ex_feature_scores(x, data, mode=RuleInductionType.REGRESSION)[0]
    # add the top five for this time step to the set of top5s
    top_5 |= set(scores.nlargest(5, 1).index.values)
    scores = scores.rename(columns={1: outcomes["TIME"][0, i]})
    all_scores.append(scores)

all_scores = pd.concat(all_scores, axis=1, sort=False)
all_scores = all_scores.loc[top_5, :]

fig, ax = plt.subplots()
sns.heatmap(all_scores, ax=ax, cmap="viridis")
plt.show()
```

1.10.24 optimization_lake_model_dps.py

```
"""
This example replicates Quinn, J.D., Reed, P.M., Keller, K. (2017)
Direct policy search for robust multi-objective management of deeply
uncertain socio-ecological tipping points. Environmental Modelling &
Software 92, 125-141.

It also show cases how the workbench can be used to apply the MORDM extension
suggested by Watson, A.A., Kasprzyk, J.R. (2017) Incorporating deeply uncertain
factors into the many objective search process. Environmental Modelling &
Software 89, 159-171.

"""

import math

import numpy as np
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MultiprocessingEvaluator,
    CategoricalParameter,
    Scenario,
)

from ema_workbench.em_framework.optimization import ArchiveLogger, EpsilonProgress


# Created on 1 Jun 2017
```

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```
#
# .. codeauthor::jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>


def get_antropogenic_release(xt, c1, c2, r1, r2, w1):
    """

    Parameters
    ----------
    xt : float
         pollution in lake at time t
    c1 : float
         center rbf 1
    c2 : float
         center rbf 2
    r1 : float
         ratius rbf 1
    r2 : float
         ratius rbf 2
    w1 : float
         weight of rbf 1

    note:: w2 = 1 - w1

    """

    rule = w1 * (abs(xt - c1) / r1) ** 3 + (1 - w1) * (abs(xt - c2) / r2) ** 3
    at1 = max(rule, 0.01)
    at = min(at1, 0.1)

    return at


def lake_problem(
    b=0.42,  # decay rate for P in lake (0.42 = irreversible)
    q=2.0,  # recycling exponent
    mean=0.02,  # mean of natural inflows
    stdev=0.001,  # future utility discount rate
    delta=0.98,  # standard deviation of natural inflows
    alpha=0.4,  # utility from pollution
    nsamples=100,  # Monte Carlo sampling of natural inflows
    myears=1,  # the runtime of the simulation model
    c1=0.25,
    c2=0.25,
    r1=0.5,
    r2=0.5,
    w1=0.5,
):
    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)

    X = np.zeros(myears)
    average_daily_P = np.zeros(myears)
```

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```
    reliability = 0.0
    inertia = 0
    utility = 0

    for _ in range(nsamples):
        X[0] = 0.0
        decision = 0.1

        decisions = np.zeros(myears)
        decisions[0] = decision

        natural_inflows = np.random.lognormal(
            math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
            math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
            size=myears,
        )

        for t in range(1, myears):
            # here we use the decision rule
            decision = get_antropogenic_release(X[t - 1], c1, c2, r1, r2, w1)
            decisions[t] = decision

            X[t] = (
                (1 - b) * X[t - 1]
                + X[t - 1] ** q / (1 + X[t - 1] ** q)
                + decision
                + natural_inflows[t - 1]
            )
            average_daily_P[t] += X[t] / nsamples

        reliability += np.sum(X < Pcrit) / (nsamples * myears)
        inertia += np.sum(np.absolute(np.diff(decisions) < 0.02)) / (nsamples * myears)
        utility += np.sum(alpha * decisions * np.power(delta, np.arange(myears))) /␣
↪nsamples
    max_P = np.max(average_daily_P)

    return max_P, utility, inertia, reliability


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    # specify uncertainties
    lake_model.uncertainties = [
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("mean", 0.01, 0.05),
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("delta", 0.93, 0.99),
    ]
```

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```
    # set levers
    lake_model.levers = [
        RealParameter("c1", -2, 2),
        RealParameter("c2", -2, 2),
        RealParameter("r1", 0, 2),
        RealParameter("r2", 0, 2),
        CategoricalParameter("w1", np.linspace(0, 1, 10)),
    ]
    # specify outcomes
    lake_model.outcomes = [
        ScalarOutcome("max_P", kind=ScalarOutcome.MINIMIZE),
        ScalarOutcome("utility", kind=ScalarOutcome.MAXIMIZE),
        ScalarOutcome("inertia", kind=ScalarOutcome.MAXIMIZE),
        ScalarOutcome("reliability", kind=ScalarOutcome.MAXIMIZE),
    ]

    # override some of the defaults of the model
    lake_model.constants = [
        Constant("alpha", 0.41),
        Constant("nsamples", 100),
        Constant("myears", 100),
    ]

    # reference is optional, but can be used to implement search for
    # various user specified scenarios along the lines suggested by
    # Watson and Kasprzyk (2017)
    reference = Scenario("reference", b=0.4, q=2, mean=0.02, stdev=0.01)

    convergence_metrics = [
        ArchiveLogger(
            "./data",
            [l.name for l in lake_model.levers],
            [o.name for o in lake_model.outcomes],
            base_filename="lake_model_dps_archive.tar.gz",
        ),
        EpsilonProgress(),
    ]

    with MultiprocessingEvaluator(lake_model) as evaluator:
        results, convergence = evaluator.optimize(
            searchover="levers",
            nfe=100000,
            epsilons=[0.1] * len(lake_model.outcomes),
            reference=reference,
            convergence=convergence_metrics,
        )
```

1.10.25 optimization_lake_model_intertemporal.py

```
"""
An example of the lake problem using the ema workbench.

The model itself is adapted from the Rhodium example by Dave Hadka,
see https://gist.github.com/dhadka/a8d7095c98130d8f73bc

"""

import math

import numpy as np
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    ema_logging,
    MultiprocessingEvaluator,
    Constraint,
)
from ema_workbench.em_framework.optimization import HyperVolume, EpsilonProgress


def lake_problem(
    b=0.42,
    q=2.0,
    mean=0.02,
    stdev=0.0017,
    delta=0.98,
    alpha=0.4,
    nsamples=100,
    l0=0,
    l1=0,
    l2=0,
    l3=0,
    l4=0,
    l5=0,
    l6=0,
    l7=0,
    l8=0,
    l9=0,
    l10=0,
    l11=0,
    l12=0,
    l13=0,
    l14=0,
    l15=0,
    l16=0,
    l17=0,
    l18=0,
```

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```
    119=0,
    120=0,
    121=0,
    122=0,
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    124=0,
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    129=0,
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    l71=0,
    l72=0,
    l73=0,
    l74=0,
    l75=0,
    l76=0,
    l77=0,
    l78=0,
    l79=0,
    l80=0,
    l81=0,
    l82=0,
    l83=0,
    l84=0,
    l85=0,
    l86=0,
    l87=0,
    l88=0,
    l89=0,
    l90=0,
    l91=0,
    l92=0,
    l93=0,
    l94=0,
    l95=0,
    l96=0,
    l97=0,
    l98=0,
    l99=0,
):
    decisions = np.array(
        [
            l0,
            l1,
            l2,
            l3,
            l4,
            l5,
            l6,
            l7,
            l8,
            l9,
            l10,
            l11,
            l12,
            l13,
            l14,
            l15,
            l16,
            l17,
            l18,
            l19,
```

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```

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```
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            196,
            197,
            198,
            199,
        ]
    )

    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)
    nvars = len(decisions)
    X = np.zeros((nvars,))
    average_daily_P = np.zeros((nvars,))
    decisions = np.array(decisions)
    reliability = 0.0

    for _ in range(nsamples):
        X[0] = 0.0

        natural_inflows = np.random.lognormal(
            math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
            math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
            size=nvars,
        )

        for t in range(1, nvars):
            X[t] = (
                (1 - b) * X[t - 1]
                + X[t - 1] ** q / (1 + X[t - 1] ** q)
                + decisions[t - 1]
```

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```
                + natural_inflows[t - 1]
            )
            average_daily_P[t] += X[t] / float(nsamples)

        reliability += np.sum(X < Pcrit) / float(nsamples * nvars)

    max_P = np.max(average_daily_P)
    utility = np.sum(alpha * decisions * np.power(delta, np.arange(nvars)))
    inertia = np.sum(np.abs(np.diff(decisions)) > 0.02) / float(nvars - 1)

    return max_P, utility, inertia, reliability


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    lake_model.time_horizon = 100  # used to specify the number of timesteps

    # specify uncertainties
    lake_model.uncertainties = [
        RealParameter("mean", 0.01, 0.05),
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("delta", 0.93, 0.99),
    ]

    # set levers, one for each time step
    lake_model.levers = [RealParameter(f"l{i}", 0, 0.1) for i in range(lake_model.time_
↪horizon)]

    # specify outcomes
    # specify outcomes
    lake_model.outcomes = [
        ScalarOutcome("max_P", kind=ScalarOutcome.MINIMIZE, expected_range=(0, 5)),
        ScalarOutcome("utility", kind=ScalarOutcome.MAXIMIZE, expected_range=(0, 2)),
        ScalarOutcome("inertia", kind=ScalarOutcome.MAXIMIZE, expected_range=(0, 1)),
        ScalarOutcome("reliability", kind=ScalarOutcome.MAXIMIZE, expected_range=(0, 1)),
    ]

    convergence_metrics = [EpsilonProgress()]

    constraints = [
        Constraint("max pollution", outcome_names="max_P", function=lambda x: max(0, x -␣
↪5))
    ]

    with MultiprocessingEvaluator(lake_model) as evaluator:
        results, convergence = evaluator.optimize(
            nfe=5000,
```

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```
            searchover="levers",
            epsilons=[0.125, 0.05, 0.01, 0.01],
            convergence=convergence_metrics,
            constraints=constraints,
        )
```

1.10.26 outputspace_exploration_lake_model.py

```
"""
An example of using output space exploration on the lake problem

The lake problem itself is adapted from the Rhodium example by Dave Hadka,
see https://gist.github.com/dhadka/a8d7095c98130d8f73bc

"""

import math

import numpy as np
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MultiprocessingEvaluator,
    Policy,
)

from ema_workbench.em_framework.outputspace_exploration import OutputSpaceExploration


def lake_problem(
    b=0.42,  # decay rate for P in lake (0.42 = irreversible)
    q=2.0,  # recycling exponent
    mean=0.02,  # mean of natural inflows
    stdev=0.001,  # future utility discount rate
    delta=0.98,  # standard deviation of natural inflows
    alpha=0.4,  # utility from pollution
    nsamples=100,  # Monte Carlo sampling of natural inflows
    **kwargs,
):
    try:
        decisions = [kwargs[str(i)] for i in range(100)]
    except KeyError:
        decisions = [
            0,
        ] * 100
```

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```
    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)
    nvars = len(decisions)
    X = np.zeros((nvars,))
    average_daily_P = np.zeros((nvars,))
    decisions = np.array(decisions)
    reliability = 0.0

    for _ in range(nsamples):
        X[0] = 0.0

        natural_inflows = np.random.lognormal(
            math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
            math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
            size=nvars,
        )

        for t in range(1, nvars):
            X[t] = (
                (1 - b) * X[t - 1]
                + X[t - 1] ** q / (1 + X[t - 1] ** q)
                + decisions[t - 1]
                + natural_inflows[t - 1]
            )
            average_daily_P[t] += X[t] / float(nsamples)

        reliability += np.sum(X < Pcrit) / float(nsamples * nvars)

    max_P = np.max(average_daily_P)
    utility = np.sum(alpha * decisions * np.power(delta, np.arange(nvars)))
    inertia = np.sum(np.absolute(np.diff(decisions)) < 0.02) / float(nvars - 1)

    return max_P, utility, inertia, reliability


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    lake_model.time_horizon = 100

    # specify uncertainties
    lake_model.uncertainties = [
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("mean", 0.01, 0.05),
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("delta", 0.93, 0.99),
    ]

    # set levers, one for each time step
```

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```
    lake_model.levers = [RealParameter(str(i), 0, 0.1) for i in range(lake_model.time_
↪horizon)]

    # specify outcomes
    # note that outcomes of kind INFO will be ignored
    lake_model.outcomes = [
        ScalarOutcome("max_P", kind=ScalarOutcome.MAXIMIZE),
        ScalarOutcome("utility", kind=ScalarOutcome.MAXIMIZE),
        ScalarOutcome("inertia", kind=ScalarOutcome.MAXIMIZE),
        ScalarOutcome("reliability", kind=ScalarOutcome.MAXIMIZE),
    ]

    # override some of the defaults of the model
    lake_model.constants = [Constant("alpha", 0.41), Constant("nsamples", 150)]

    # generate a reference policy
    n_scenarios = 1000
    reference = Policy("nopolicy", **{l.name: 0.02 for l in lake_model.levers})

    # we are doing output space exploration given a reference
    # policy, so we are exploring the output space over the uncertainties
    # grid spec specifies the grid structure imposed on the output space
    # each tuple is associated with an outcome. It gives the minimum
    # maximum, and epsilon value.
    with MultiprocessingEvaluator(lake_model) as evaluator:
        res = evaluator.optimize(
            algorithm=OutputSpaceExploration,
            grid_spec=[
                (0, 12, 0.5),
                (0, 1, 0.05),
                (0, 1, 0.1),
                (0, 1, 0.1),
            ],
            nfe=1000,
            searchover="uncertainties",
            reference=reference,
        )
```

1.10.27 plotting_envelopes_flu.py

```
"""
Created on Jul 8, 2014

@author: jhkwakkel@tudelft.net
"""

import matplotlib.pyplot as plt

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import envelopes, Density
```

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```

ema_logging.log_to_stderr(ema_logging.INFO)

file_name = r"./data/1000 flu cases with policies.tar.gz"
experiments, outcomes = load_results(file_name)

# the plotting functions return the figure and a dict of axes
fig, axes = envelopes(experiments, outcomes, group_by="policy", density=Density.KDE,␣
↪fill=True)

# we can access each of the axes and make changes
for key, value in axes.items():
    # the key is the name of the outcome for the normal plot
    # and the name plus '_density' for the endstate distribution
    if key.endswith("_density"):
        value.set_xscale("log")

plt.show()
```

1.10.28 plotting_envelopes_with_lines_flu.py

```
"""
Created on Jul 8, 2014

@author: jhkwakkel@tudelft.net
"""

import matplotlib.pyplot as plt
import numpy as np

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import lines, Density

ema_logging.log_to_stderr(ema_logging.INFO)

file_name = r"./data/1000 flu cases with policies.tar.gz"
experiments, outcomes = load_results(file_name)

# let's specify a few scenarios that we want to show for
# each of the policies
scenario_ids = np.arange(0, 1000, 100)
experiments_to_show = experiments["scenario_id"].isin(scenario_ids)

# the plotting functions return the figure and a dict of axes
fig, axes = lines(
    experiments,
    outcomes,
    group_by="policy",
    density=Density.KDE,
    show_envelope=True,
```

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```
    experiments_to_show=experiments_to_show,
)

# we can access each of the axes and make changes
for key, value in axes.items():
    # the key is the name of the outcome for the normal plot
    # and the name plus '_density' for the endstate distribution
    if key.endswith("_density"):
        value.set_xscale("log")

plt.show()
```

1.10.29 plotting_kdeovertime_flu.py

```
"""
Created on Jul 8, 2014

@author: jhkwakkel@tudelft.net
"""

import matplotlib.pyplot as plt

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis.plotting import kde_over_time

ema_logging.log_to_stderr(ema_logging.INFO)

# file_name = r'./data/1000 runs scarcity.tar.gz'
file_name = "./data/1000 flu cases no policy.tar.gz"
experiments, outcomes = load_results(file_name)

# the plotting functions return the figure and a dict of axes
fig, axes = kde_over_time(experiments, outcomes, log=True)

plt.show()
```

1.10.30 plotting_lines_flu.py

```
"""
Created on Jul 8, 2014

@author: jhkwakkel@tudelft.net
"""

import matplotlib.pyplot as plt

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import lines, Density

```

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```
ema_logging.log_to_stderr(ema_logging.INFO)

file_name = r"./data/1000 flu cases no policy.tar.gz"
experiments, outcomes = load_results(file_name)

# the plotting functions return the figure and a dict of axes
fig, axes = lines(experiments, outcomes, density=Density.VIOLIN)

# we can access each of the axes and make changes
for key, value in axes.items():
    # the key is the name of the outcome for the normal plot
    # and the name plus '_density' for the endstate distribution
    if key.endswith("_density"):
        value.set_xscale("log")

plt.show()
```

1.10.31 plotting_multiple_densities_flu.py

```
"""
Created on Jul 8, 2014

@author: jhkwakkel@tudelft.net
"""

import math

import matplotlib.pyplot as plt

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import multiple_densities, Density

ema_logging.log_to_stderr(ema_logging.INFO)

file_name = "./data/1000 flu cases with policies.tar.gz"
experiments, outcomes = load_results(file_name)

# pick points in time for which we want to see a
# density subplot
time = outcomes["TIME"][0, :]
times = time[1 :: math.ceil(time.shape[0] / 6)].tolist()

multiple_densities(
    experiments,
    outcomes,
    log=True,
    points_in_time=times,
    group_by="policy",
    density=Density.KDE,
    fill=True,
```

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```
)

plt.show()
```

1.10.32 plotting_pairsplot_flu.py

```
"""
Created on 20 sep. 2011

.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
"""

import matplotlib.pyplot as plt
import numpy as np

from ema_workbench import load_results, ema_logging
from ema_workbench.analysis.pairs_plotting import pairs_lines, pairs_scatter, pairs_
↪density

ema_logging.log_to_stderr(level=ema_logging.DEFAULT_LEVEL)

# load the data
fh = "./data/1000 flu cases no policy.tar.gz"
experiments, outcomes = load_results(fh)

# transform the results to the required format
# that is, we want to know the max peak and the casualties at the end of the
# run
tr = {}

# get time and remove it from the dict
time = outcomes.pop("TIME")

for key, value in outcomes.items():
    if key == "deceased_population_region_1":
        tr[key] = value[:, -1]  # we want the end value
    else:
        # we want the maximum value of the peak
        max_peak = np.max(value, axis=1)
        tr["max peak"] = max_peak

        # we want the time at which the maximum occurred
        # the code here is a bit obscure, I don't know why the transpose
        # of value is needed. This however does produce the appropriate results
        logical = value.T == np.max(value, axis=1)
        tr["time of max"] = time[logical.T]

pairs_scatter(experiments, tr, filter_scalar=False)
pairs_lines(experiments, outcomes)
pairs_density(experiments, tr, filter_scalar=False)
plt.show()
```

1.10.33 regional_sa_flu.py

```
""" A simple example of performing regional sensitivity analysis


"""

import matplotlib.pyplot as plt

from ema_workbench.analysis import regional_sa
from ema_workbench import ema_logging, load_results

fn = "./data/1000 flu cases with policies.tar.gz"
results = load_results(fn)
x, outcomes = results

y = outcomes["deceased population region 1"][:, -1] > 1000000

fig = regional_sa.plot_cdfs(x, y)

plt.show()
```

1.10.34 robust_optimization_lake_model_dps.py

```
"""
This example takes the direct policy search formulation of the lake problem as
found in Quinn et al (2017), but embeds in in a robust optimization.

Quinn, J.D., Reed, P.M., Keller, K. (2017)
Direct policy search for robust multi-objective management of deeply
uncertain socio-ecological tipping points. Environmental Modelling &
Software 92, 125-141.


"""

import math

import numpy as np
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MultiprocessingEvaluator,
)
from ema_workbench.em_framework.samplers import sample_uncertainties

```

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```
# Created on 1 Jun 2017
#
# .. codeauthor::jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>

__all__ = []


def get_antropogenic_release(xt, c1, c2, r1, r2, w1):
    """

    Parameters
    ----------
    xt : float
         pollution in lake at time t
    c1 : float
         center rbf 1
    c2 : float
         center rbf 2
    r1 : float
         ratius rbf 1
    r2 : float
         ratius rbf 2
    w1 : float
         weight of rbf 1

    note:: w2 = 1 - w1

    """

    rule = w1 * (abs(xt - c1 / r1)) ** 3 + (1 - w1) * (abs(xt - c2 / r2) ** 3)
    at1 = max(rule, 0.01)
    at = min(at1, 0.1)

    return at


def lake_problem(
    b=0.42,  # decay rate for P in lake (0.42 = irreversible)
    q=2.0,  # recycling exponent
    mean=0.02,  # mean of natural inflows
    stdev=0.001,  # future utility discount rate
    delta=0.98,  # standard deviation of natural inflows
    alpha=0.4,  # utility from pollution
    nsamples=100,  # Monte Carlo sampling of natural inflows
    myears=1,  # the runtime of the simulation model
    c1=0.25,
    c2=0.25,
    r1=0.5,
    r2=0.5,
    w1=0.5,
):
    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)
```

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```
    X = np.zeros(myears)
    average_daily_P = np.zeros(myears)
    reliability = 0.0
    inertia = 0
    utility = 0

    for _ in range(nsamples):
        X[0] = 0.0
        decision = 0.1

        decisions = np.zeros(myears)
        decisions[0] = decision

        natural_inflows = np.random.lognormal(
            math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
            math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
            size=myears,
        )

        for t in range(1, myears):
            # here we use the decision rule
            decision = get_antropogenic_release(X[t - 1], c1, c2, r1, r2, w1)
            decisions[t] = decision

            X[t] = (
                (1 - b) * X[t - 1]
                + X[t - 1] ** q / (1 + X[t - 1] ** q)
                + decision
                + natural_inflows[t - 1]
            )
            average_daily_P[t] += X[t] / nsamples

        reliability += np.sum(X < Pcrit) / (nsamples * myears)
        inertia += np.sum(np.absolute(np.diff(decisions) < 0.02)) / (nsamples * myears)
        utility += np.sum(alpha * decisions * np.power(delta, np.arange(myears))) /␣
↪nsamples
    max_P = np.max(average_daily_P)

    return max_P, utility, inertia, reliability


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    # specify uncertainties
    lake_model.uncertainties = [
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("mean", 0.01, 0.05),
```

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```
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("delta", 0.93, 0.99),
    ]

    # set levers
    lake_model.levers = [
        RealParameter("c1", -2, 2),
        RealParameter("c2", -2, 2),
        RealParameter("r1", 0, 2),
        RealParameter("r2", 0, 2),
        RealParameter("w1", 0, 1),
    ]

    # specify outcomes
    lake_model.outcomes = [
        ScalarOutcome("max_P"),
        ScalarOutcome("utility"),
        ScalarOutcome("inertia"),
        ScalarOutcome("reliability"),
    ]

    # override some of the defaults of the model
    lake_model.constants = [
        Constant("alpha", 0.41),
        Constant("nsamples", 100),
        Constant("myears", 100),
    ]

    # setup and execute the robust optimization
    def signal_to_noise(data):
        mean = np.mean(data)
        std = np.std(data)
        sn = mean / std
        return sn

    MAXIMIZE = ScalarOutcome.MAXIMIZE  # @UndefinedVariable
    MINIMIZE = ScalarOutcome.MINIMIZE  # @UndefinedVariable
    robustnes_functions = [
        ScalarOutcome("mean p", kind=MINIMIZE, variable_name="max_P", function=np.mean),
        ScalarOutcome("std p", kind=MINIMIZE, variable_name="max_P", function=np.std),
        ScalarOutcome(
            "sn reliability", kind=MAXIMIZE, variable_name="reliability",␣
↪function=signal_to_noise
        ),
    ]
    n_scenarios = 10
    scenarios = sample_uncertainties(lake_model, n_scenarios)
    nfe = 1000

    with MultiprocessingEvaluator(lake_model) as evaluator:
        evaluator.robust_optimize(
            robustnes_functions,
```

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```
            scenarios,
            nfe=nfe,
            epsilons=[0.1] * len(robustnes_functions),
            population_size=5,
        )
```

1.10.35 sample_jointly_lake_model.py

```
"""
An example of the lake problem using the ema workbench. This example
illustrated how you can control more finely how samples are being generated.
In this particular case, we want to apply Sobol analysis over both the
uncertainties and levers at the same time.

"""

import math

import numpy as np
import pandas as pd
from SALib.analyze import sobol
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MultiprocessingEvaluator,
    Scenario,
)
from ema_workbench.em_framework import get_SALib_problem, sample_parameters
from ema_workbench.em_framework import SobolSampler

# from ema_workbench.em_framework.evaluators import Samplers


def get_antropogenic_release(xt, c1, c2, r1, r2, w1):
    """

    Parameters
    ----------
    xt : float
         pollution in lake at time t
    c1 : float
         center rbf 1
    c2 : float
         center rbf 2
    r1 : float
```

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```
        ratius rbf 1
    r2 : float
        ratius rbf 2
    w1 : float
        weight of rbf 1

    note:: w2 = 1 - w1

    """

    rule = w1 * (abs(xt - c1) / r1) ** 3 + (1 - w1) * (abs(xt - c2) / r2) ** 3
    at1 = max(rule, 0.01)
    at = min(at1, 0.1)

    return at


def lake_problem(
    b=0.42,  # decay rate for P in lake (0.42 = irreversible)
    q=2.0,  # recycling exponent
    mean=0.02,  # mean of natural inflows
    stdev=0.001,  # future utility discount rate
    delta=0.98,  # standard deviation of natural inflows
    alpha=0.4,  # utility from pollution
    nsamples=100,  # Monte Carlo sampling of natural inflows
    myears=1,  # the runtime of the simulation model
    c1=0.25,
    c2=0.25,
    r1=0.5,
    r2=0.5,
    w1=0.5,
):
    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)

    X = np.zeros((myears,))
    average_daily_P = np.zeros((myears,))
    reliability = 0.0
    inertia = 0
    utility = 0

    for _ in range(nsamples):
        X[0] = 0.0
        decision = 0.1

        decisions = np.zeros(myears)
        decisions[0] = decision

        natural_inflows = np.random.lognormal(
            math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
            math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
            size=myears,
        )
```

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```
        for t in range(1, myears):
            # here we use the decision rule
            decision = get_antropogenic_release(X[t - 1], c1, c2, r1, r2, w1)
            decisions[t] = decision

            X[t] = (
                (1 - b) * X[t - 1]
                + X[t - 1] ** q / (1 + X[t - 1] ** q)
                + decision
                + natural_inflows[t - 1]
            )
            average_daily_P[t] += X[t] / nsamples

        reliability += np.sum(X < Pcrit) / (nsamples * myears)
        inertia += np.sum(np.absolute(np.diff(decisions) < 0.02)) / (nsamples * myears)
        utility += np.sum(alpha * decisions * np.power(delta, np.arange(myears))) /␣
↪nsamples
    max_P = np.max(average_daily_P)

    return max_P, utility, inertia, reliability


def analyze(results, ooi):
    """analyze results using SALib sobol, returns a dataframe"""

    _, outcomes = results

    parameters = lake_model.uncertainties.copy() + lake_model.levers.copy()

    problem = get_SALib_problem(parameters)
    y = outcomes[ooi]
    sobol_indices = sobol.analyze(problem, y)
    sobol_stats = {key: sobol_indices[key] for key in ["ST", "ST_conf", "S1", "S1_conf"]}
    sobol_stats = pd.DataFrame(sobol_stats, index=problem["names"])
    sobol_stats.sort_values(by="ST", ascending=False)
    s2 = pd.DataFrame(sobol_indices["S2"], index=problem["names"], columns=problem["names
↪"])
    s2_conf = pd.DataFrame(
        sobol_indices["S2_conf"], index=problem["names"], columns=problem["names"]
    )

    return sobol_stats, s2, s2_conf


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    # specify uncertainties
    lake_model.uncertainties = [
```

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```
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("mean", 0.01, 0.05),
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("delta", 0.93, 0.99),
    ]

    # set levers
    lake_model.levers = [
        RealParameter("c1", -2, 2),
        RealParameter("c2", -2, 2),
        RealParameter("r1", 0, 2),
        RealParameter("r2", 0, 2),
        RealParameter("w1", 0, 1),
    ]
    # specify outcomes
    lake_model.outcomes = [
        ScalarOutcome("max_P", kind=ScalarOutcome.MINIMIZE),
        # @UndefinedVariable
        ScalarOutcome("utility", kind=ScalarOutcome.MAXIMIZE),
        # @UndefinedVariable
        ScalarOutcome("inertia", kind=ScalarOutcome.MAXIMIZE),
        # @UndefinedVariable
        ScalarOutcome("reliability", kind=ScalarOutcome.MAXIMIZE),
    ]  # @UndefinedVariable

    # override some of the defaults of the model
    lake_model.constants = [
        Constant("alpha", 0.41),
        Constant("nsamples", 100),
        Constant("myears", 100),
    ]

    # combine parameters and uncertainties prior to sampling
    n_scenarios = 1000
    parameters = lake_model.uncertainties + lake_model.levers
    scenarios = sample_parameters(parameters, n_scenarios, SobolSampler(), Scenario)

    with MultiprocessingEvaluator(lake_model) as evaluator:
        results = evaluator.perform_experiments(scenarios)

    sobol_stats, s2, s2_conf = analyze(results, "max_P")
    print(sobol_stats)
    print(s2)
    print(s2_conf)
```

1.10.36 sample_sobol_lake_model.py

```
"""
An example of the lake problem using the ema workbench.

The model itself is adapted from the Rhodium example by Dave Hadka,
see https://gist.github.com/dhadka/a8d7095c98130d8f73bc

"""

import math

import numpy as np
import pandas as pd
from SALib.analyze import sobol
from scipy.optimize import brentq

from ema_workbench import (
    Model,
    RealParameter,
    ScalarOutcome,
    Constant,
    ema_logging,
    MultiprocessingEvaluator,
    Policy,
)
from ema_workbench.em_framework import get_SALib_problem
from ema_workbench.em_framework.evaluators import Samplers


def lake_problem(
    b=0.42,  # decay rate for P in lake (0.42 = irreversible)
    q=2.0,  # recycling exponent
    mean=0.02,  # mean of natural inflows
    stdev=0.001,  # future utility discount rate
    delta=0.98,  # standard deviation of natural inflows
    alpha=0.4,  # utility from pollution
    nsamples=100,  # Monte Carlo sampling of natural inflows
    **kwargs,
):
    try:
        decisions = [kwargs[str(i)] for i in range(100)]
    except KeyError:
        decisions = [0] * 100

    Pcrit = brentq(lambda x: x**q / (1 + x**q) - b * x, 0.01, 1.5)
    nvars = len(decisions)
    X = np.zeros((nvars,))
    average_daily_P = np.zeros((nvars,))
    decisions = np.array(decisions)
    reliability = 0.0

    for _ in range(nsamples):
```

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```
        X[0] = 0.0

        natural_inflows = np.random.lognormal(
            math.log(mean**2 / math.sqrt(stdev**2 + mean**2)),
            math.sqrt(math.log(1.0 + stdev**2 / mean**2)),
            size=nvars,
        )

        for t in range(1, nvars):
            X[t] = (
                (1 - b) * X[t - 1]
                + X[t - 1] ** q / (1 + X[t - 1] ** q)
                + decisions[t - 1]
                + natural_inflows[t - 1]
            )
            average_daily_P[t] += X[t] / float(nsamples)

        reliability += np.sum(X < Pcrit) / float(nsamples * nvars)

    max_P = np.max(average_daily_P)
    utility = np.sum(alpha * decisions * np.power(delta, np.arange(nvars)))
    inertia = np.sum(np.absolute(np.diff(decisions)) < 0.02) / float(nvars - 1)

    return max_P, utility, inertia, reliability


def analyze(results, ooi):
    """analyze results using SALib sobol, returns a dataframe"""

    _, outcomes = results

    problem = get_SALib_problem(lake_model.uncertainties)
    y = outcomes[ooi]
    sobol_indices = sobol.analyze(problem, y)
    sobol_stats = {key: sobol_indices[key] for key in ["ST", "ST_conf", "S1", "S1_conf"]}
    sobol_stats = pd.DataFrame(sobol_stats, index=problem["names"])
    sobol_stats.sort_values(by="ST", ascending=False)
    s2 = pd.DataFrame(sobol_indices["S2"], index=problem["names"], columns=problem["names
↪"])
    s2_conf = pd.DataFrame(
        sobol_indices["S2_conf"], index=problem["names"], columns=problem["names"]
    )

    return sobol_stats, s2, s2_conf


if __name__ == "__main__":
    ema_logging.log_to_stderr(ema_logging.INFO)

    # instantiate the model
    lake_model = Model("lakeproblem", function=lake_problem)
    lake_model.time_horizon = 100
```

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```
    # specify uncertainties
    lake_model.uncertainties = [
        RealParameter("b", 0.1, 0.45),
        RealParameter("q", 2.0, 4.5),
        RealParameter("mean", 0.01, 0.05),
        RealParameter("stdev", 0.001, 0.005),
        RealParameter("delta", 0.93, 0.99),
    ]

    # set levers, one for each time step
    lake_model.levers = [RealParameter(str(i), 0, 0.1) for i in range(lake_model.time_
↪horizon)]

    # specify outcomes
    lake_model.outcomes = [
        ScalarOutcome("max_P"),
        ScalarOutcome("utility"),
        ScalarOutcome("inertia"),
        ScalarOutcome("reliability"),
    ]

    # override some of the defaults of the model
    lake_model.constants = [Constant("alpha", 0.41), Constant("nsamples", 150)]

    # generate sa single default no release policy
    policy = Policy("no release", **{str(i): 0.1 for i in range(100)})

    n_scenarios = 1000

    with MultiprocessingEvaluator(lake_model) as evaluator:
        results = evaluator.perform_experiments(
            n_scenarios, policy, uncertainty_sampling=Samplers.SOBOL
        )

    sobol_stats, s2, s2_conf = analyze(results, "max_P")
    print(sobol_stats)
    print(s2)
    print(s2_conf)
```

1.10.37 sd_boostedtrees_flu.py

```
"""

"""

import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns
from matplotlib.collections import CircleCollection
```

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```
from sklearn.ensemble import AdaBoostClassifier
from sklearn.tree import DecisionTreeClassifier

from ema_workbench import load_results, ema_logging
from ema_workbench.analysis import feature_scoring

ema_logging.log_to_stderr(ema_logging.INFO)


def plot_factormap(x1, x2, ax, bdt, nominal):
    """helper function for plotting a 2d factor map"""
    x_min, x_max = x[:, x1].min(), x[:, x1].max()
    y_min, y_max = x[:, x2].min(), x[:, x2].max()
    xx, yy = np.meshgrid(np.linspace(x_min, x_max, 500), np.linspace(y_min, y_max, 500))

    grid = np.ones((xx.ravel().shape[0], x.shape[1])) * nominal
    grid[:, x1] = xx.ravel()
    grid[:, x2] = yy.ravel()

    Z = bdt.predict(grid)
    Z = Z.reshape(xx.shape)

    ax.contourf(xx, yy, Z, cmap=plt.cm.Paired, alpha=0.5)  # @UndefinedVariable

    for i in (0, 1):
        idx = y == i
        ax.scatter(x[idx, x1], x[idx, x2], s=5)
    ax.set_xlabel(columns[x1])
    ax.set_ylabel(columns[x2])


def plot_diag(x1, ax):
    x_min, x_max = x[:, x1].min(), x[:, x1].max()
    for i in (0, 1):
        idx = y == i
        ax.hist(x[idx, x1], range=(x_min, x_max), alpha=0.5)


# load data
experiments, outcomes = load_results("./data/1000 flu cases with policies.tar.gz")

# transform to numpy array with proper recoding of cateogorical variables
x, columns = feature_scoring._prepare_experiments(experiments)
y = outcomes["deceased_population_region 1"][:, -1] > 1000000

# establish mean case for factor maps
# this is questionable in particular in case of categorical dimensions
minima = x.min(axis=0)
maxima = x.max(axis=0)
nominal = minima + (maxima - minima) / 2

# fit the boosted tree
```

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```
bdt = AdaBoostClassifier(DecisionTreeClassifier(max_depth=3), algorithm="SAMME", n_
↪estimators=200)
bdt.fit(x, y)

# determine which dimensions are most important
sorted_indices = np.argsort(bdt.feature_importances_)[::-1]

# do the actual plotting
# this is a quick hack, tying it to seaborn Pairgrid is probably
# the more elegant solution, but is tricky with what arguments
# can be passed to the plotting function
fig, axes = plt.subplots(ncols=5, nrows=5, figsize=(15, 15))

for i, row in enumerate(axes):
    for j, ax in enumerate(row):
        if i > j:
            plot_factormap(sorted_indices[j], sorted_indices[i], ax, bdt, nominal)
        elif i == j:
            plot_diag(sorted_indices[j], ax)
        else:
            ax.set_xticks([])
            ax.set_yticks([])
            ax.axis("off")

        if j > 0:
            ax.set_yticklabels([])
            ax.set_ylabel("")
        if i < len(axes) - 1:
            ax.set_xticklabels([])
            ax.set_xlabel("")

# add the legend
# Draw a full-figure legend outside the grid
handles = [
    CircleCollection([10], color=sns.color_palette()[0]),
    CircleCollection([10], color=sns.color_palette()[1]),
]

legend = fig.legend(handles, ["False", "True"], scatterpoints=1)

plt.tight_layout()
plt.show()
```

1.10.38 sd_cart_flu.py

```
"""
Created on May 26, 2015

@author: jhkwakkel
"""

import matplotlib.pyplot as plt

import ema_workbench.analysis.cart as cart
from ema_workbench import ema_logging, load_results

ema_logging.log_to_stderr(level=ema_logging.INFO)


def classify(data):
    # get the output for deceased population
    result = data["deceased_population_region_1"]

    # if deceased population is higher then 1.000.000 people,
    # classify as 1
    classes = result[:, -1] > 1000000

    return classes


# load data
fn = "./data/1000 flu cases with policies.tar.gz"
results = load_results(fn)
experiments, outcomes = results

# extract results for 1 policy
logical = experiments["policy"] == "no policy"
new_experiments = experiments[logical]
new_outcomes = {}
for key, value in outcomes.items():
    new_outcomes[key] = value[logical]

results = (new_experiments, new_outcomes)

# perform cart on modified results tuple

cart_alg = cart.setup_cart(results, classify, mass_min=0.05)
cart_alg.build_tree()

# print cart to std_out
print(cart_alg.stats_to_dataframe())
print(cart_alg.boxes_to_dataframe())

# visualize
cart_alg.show_boxes(together=False)
cart_alg.show_tree()
```

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```
plt.show()
```

1.10.39 sd_cart_wcm.py

```
"""
Created on May 26, 2015

@author: jhkwakkel
"""

import matplotlib.pyplot as plt

import ema_workbench.analysis.cart as cart
from ema_workbench import ema_logging, load_results

ema_logging.log_to_stderr(level=ema_logging.INFO)

default_flow = 2.178849944502783e7

# load data
fn = "./data/5000 runs WCM.tar.gz"
results = load_results(fn)
x, outcomes = results

ooi = "throughput Rotterdam"
outcome = outcomes[ooi] / default_flow
y = outcome < 1

cart_alg = cart.CART(x, y)
cart_alg.build_tree()

# print cart to std_out
print(cart_alg.stats_to_dataframe())
print(cart_alg.boxes_to_dataframe())

# visualize
cart_alg.show_boxes(together=False)
cart_alg.show_tree()
plt.show()
```

1.10.40 sd_dimensional_stacking_flu.py

```
"""

This file illustrated the use of the workbench for using dimensional
stacking for scenario discovery


.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
```

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```

"""

import matplotlib.pyplot as plt

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import dimensional_stacking

ema_logging.log_to_stderr(level=ema_logging.INFO)

# load data
fn = "./data/1000 flu cases no policy.tar.gz"
x, outcomes = load_results(fn)

y = outcomes["deceased_population_region_1"][:, -1] > 1000000

fig = dimensional_stacking.create_pivot_plot(x, y, 2, bin_labels=True)

plt.show()
```

1.10.41 sd_logit_flu_example.py

```
"""

"""

import matplotlib.pyplot as plt
import seaborn as sns

import ema_workbench.analysis.logistic_regression as logistic_regression
from ema_workbench import load_results

# Created on 14 Mar 2019
#
# .. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>


experiments, outcomes = load_results("./data/1000 flu cases no policy.tar.gz")

x = experiments.drop(["model", "policy"], axis=1)
y = outcomes["deceased_population_region_1"][:, -1] > 1000000

logit = logistic_regression.Logit(x, y)
logit.run()

logit.show_tradeoff()

# when we change the default threshold, the tradeoff curve is
# recalculated
logit.threshold = 0.8
```

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```
logit.show_tradeoff()

# we can also look at the tradeoff across threshold values
# for a given model
logit.show_threshold_tradeoff(3)

# inspect shows the threshold tradeoff for the model
# as well as the statistics of the model
logit.inspect(3)

# we can also visualize the performance of the model
# using a pairwise scatter plot
sns.set_style("white")
logit.plot_pairwise_scatter(3)

plt.show()
```

1.10.42 sd_prim_PCA_flu.py

```
"""

This file illustrated the use of the workbench for doing
a PRIM analysis with PCA preprocessing

The data was generated using a system dynamics models implemented in Vensim.
See flu_example.py for the code.


"""

import matplotlib.pyplot as plt

import ema_workbench.analysis.prim as prim
from ema_workbench import ema_logging, load_results

#
# .. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>

ema_logging.log_to_stderr(level=ema_logging.INFO)

# load data
fn = r"./data/1000 flu cases no policy.tar.gz"
x, outcomes = load_results(fn)

# specify y
y = outcomes["deceased_population_region_1"][:, -1] > 1000000

rotated_experiments, rotation_matrix = prim.pca_preprocess(x, y, exclude=["model",
↪"policy"])

```

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```
# perform prim on modified results tuple
prim_obj = prim.Prim(rotated_experiments, y, threshold=0.8)
box = prim_obj.find_box()

box.show_tradeoff()
box.inspect(22)
plt.show()
```

1.10.43 sd_prim_bryant_and_lempert.py

```
"""
Created on 12 Nov 2018

@author: jhkwakkel
"""

import matplotlib.pyplot as plt
import pandas as pd

from ema_workbench.analysis import prim
from ema_workbench.util import ema_logging

ema_logging.log_to_stderr(ema_logging.INFO)

data = pd.read_csv("./data/bryant et al 2010 data.csv", index_col=False)
x = data.iloc[:, 2:11]
y = data.iloc[:, 15].values

prim_alg = prim.Prim(x, y, threshold=0.8, peel_alpha=0.1)
box1 = prim_alg.find_box()

box1.show_tradeoff()
print(box1.resample(21))
box1.inspect(21)
box1.inspect(21, style="graph")
box1.show_pairs_scatter(21)

plt.show()
```

1.10.44 sd_prim_constrained.py

```
"""
a short example on how to use the constrained prim function.

for more details see Kwakkel (2019) A generalized many-objective optimization
approach for scenario discovery, doi: https://doi.org/10.1002/ffo2.8

"""

```

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```
import matplotlib.pyplot as plt
import pandas as pd

from ema_workbench.analysis import prim
from ema_workbench.util import ema_logging

ema_logging.log_to_stderr(ema_logging.INFO)

data = pd.read_csv("./data/bryant et al 2010 data.csv", index_col=False)
x = data.iloc[:, 2:11]
y = data.iloc[:, 15].values

box = prim.run_constrained_prim(x, y, peel_alpha=0.1)

box.show_tradeoff()
box.inspect(35)
box.inspect(35, style="graph")

plt.show()
```

1.10.45 sd_prim_flu.py

```
"""

This file illustrated the use of the workbench for doing
a PRIM analysis.

The data was generated using a system dynamics models implemented in Vensim.
See flu_example.py for the code.


.. codeauthor:: jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
                chamarat <c.hamarat  (at) tudelft (dot) nl>

"""

import matplotlib.pyplot as plt

import ema_workbench.analysis.prim as prim
from ema_workbench import ema_logging, load_results

ema_logging.log_to_stderr(level=ema_logging.INFO)


def classify(data):
    # get the output for deceased population
    ooi = data["deceased_population_region_1"]
    return ooi[:, -1] > 1000000


```

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```
# load data
fn = r"./data/1000 flu cases no policy.tar.gz"
results = load_results(fn)

# perform prim on modified results tuple
prim_obj = prim.setup_prim(results, classify, threshold=0.8, threshold_type=1)

box_1 = prim_obj.find_box()
box_1.show_ppt()
box_1.show_tradeoff()
# box_1.inspect([5, 6], style="graph", boxlim_formatter="{: .2f}")

fig, axes = plt.subplots(nrows=2, ncols=1)

box_1.inspect([5, 6], style="graph", boxlim_formatter="{: .2f}", ax=axes)
plt.show()

box_1.inspect(5)
box_1.select(5)
box_1.write_ppt_to_stdout()
box_1.show_pairs_scatter(5)

# print prim to std_out
print(prim_obj.stats_to_dataframe())
print(prim_obj.boxes_to_dataframe())

# visualize
prim_obj.show_boxes()
plt.show()
```

1.10.46 sd_prim_wcm.py

```
"""
Created on Feb 13, 2014

This example demonstrates the use of PRIM. The dataset was generated
using the world container model

(Tavasszy et al 2011; https://dx.doi.org/10.1016/j.jtrangeo.2011.05.005)


"""

import matplotlib.pyplot as plt

from ema_workbench import ema_logging, load_results
from ema_workbench.analysis import prim

ema_logging.log_to_stderr(ema_logging.INFO)

```

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```
default_flow = 2.178849944502783e7


def classify(outcomes):
    ooi = "throughput Rotterdam"
    outcome = outcomes[ooi]
    outcome = outcome / default_flow

    classes = outcome < 1
    return classes


fn = r"./data/5000 runs WCM.tar.gz"
results = load_results(fn)

prim_obj = prim.setup_prim(results, classify, mass_min=0.05, threshold=0.75)

# let's find a first box
box1 = prim_obj.find_box()

# let's analyze the peeling trajectory
box1.show_ppt()
box1.show_tradeoff()
box1.inspect_tradeoff()

box1.write_ppt_to_stdout()

# based on the peeling trajectory, we pick entry number 44
box1.select(44)

# show the resulting box
prim_obj.show_boxes()
prim_obj.boxes_to_dataframe()

plt.show()
```

1.10.47 timeseries_clustering_flu.py

```
"""
Created on 11 Apr 2019

@author: jhkwakkel
"""

import matplotlib.pyplot as plt
import seaborn as sns

from ema_workbench import load_results
from ema_workbench.analysis import clusterer, plotting, Density

```

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```
experiments, outcomes = load_results("./data/1000 flu cases no policy.tar.gz")
data = outcomes["infected_fraction_R1"]

# calculate distances
distances = clusterer.calculate_cid(data)

# plot dedrog
clusterer.plot_dendrogram(distances)

# do agglomerative clustering on the distances
clusters = clusterer.apply_agglomerative_clustering(distances, n_clusters=5)

# show the clusters in the output space
x = experiments.copy()
x["clusters"] = clusters.astype("object")
plotting.lines(x, outcomes, group_by="clusters", density=Density.BOXPLOT)

# show the input space
sns.pairplot(
    x,
    hue="clusters",
    vars=[
        "infection ratio region 1",
        "root contact rate region 1",
        "normal contact rate region 1",
        "recovery time region 1",
        "permanent immune population fraction R1",
    ],
    plot_kws=dict(s=7),
)
plt.show()
```

1.11 Best practices

1.11.1 Separate experimentation and analysis

It is strongly recommended to cleanly separate the various steps in your exploratory modeling pipeline. So, separately execute your experiments or perform your optimization, save the results, and next analyze these results. Moreover, since parallel execution can be troublesome within the Jupyter Lab / notebook environment, I personally run my experiments and optimizations either from the command line or through an IDE using a normal python file. Jupyter Lab is then used to analyze the results.

1.11.2 Keeping things organized

A frequently recurring cause of problems when using the workbench stems from not properly organizing your files. In particular when using multiprocessing it is key that you keep things well organized. The way the workbench works with multiprocessing is that it copies the entire working directory of the model to a temporary folder for each subprocess. This temporary folder is located in the same folder as the python or notebook file from which you are running. If the working directory of your model is the same as the directory in which the run file resized, you can easily fill up your hard disk in minutes. To avoid these kinds of problems, I suggest to use a directory structure as outlined below.

```
project
├─ model_files
      ├── a_model.nlogo
      └── some_input.csv
├─ results
      ├── 100k_nfe_seed1.csv
      └── 1000_experiments.tar.gz
├─ figures
      └── pairwise_scatter.png
├─experiments.py
├─optimization.py
├─analysis.ipynb
└─model_definition.py
```

Also, if you are not familiar with absolute and relative paths, please read up on that first and only use relative paths when using the workbench. Not only will this reduce the possibility for errors, it will also mean that moving your code from one machine to another will be a lot easier.

1.12 Vensim Tips and Tricks

1.12.1 Debugging a model

A common occurring problem is that some of the runs of a Vensim model do not complete correctly. In the logger, we see a message stating that a run did not complete correct, with a description of the case that did not complete correctly attached to it. Typically, this error is due to a division by zero somewhere in the model during the simulation. The easiest way of finding the source of the division by zero is via Vensim itself. However, this requires that the model is parameterized as specified by the case that created the error. It is of course possible to set all the parameters by hand, however this becomes annoying on larger models, or if one has to do it multiple times. Since the Vensim DLL does not have a way to save a model, we cannot use the DLL. Instead, we can use the fact that one can save a Vensim model as a text file. By changing the required parameters in this text file via the workbench, we can then open the modified model in Vensim and spot the error.

The following script can be used for this purpose.

```
"""
Created on 11 aug. 2011
```

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```
3
4  .. codeauthor:: wauping <w.auping (at) student (dot) tudelft (dot) nl>
5                   jhkwakkel <j.h.kwakkel (at) tudelft (dot) nl>
6
7
8  To be able to debug the Vensim model, a few steps are needed:
9
10     1.  The case that gave a bug, needs to be saved in a text  file. The entire
11         case description should be on a single line.
12     2.  Reform and clean your model ( In the Vensim menu: Model, Reform and
13         Clean). Choose
14
15          * Equation Order: Alphabetical by group (not really necessary)
16          * Equation Format: Terse
17
18     3.  Save your model as text (File, Save as..., Save as Type: Text Format
19         Models
20     4.  Run this script
21     5.  If the print in the end is not set([]), but set([array]), the array
22         gives the values that where not found and changed
23     5.  Run your new model (for example 'new text.mdl')
24     6.  Vensim tells you about your critical mistake
25
26 """
27
28 fileSpecifyingError = ""
29
30 pathToExistingModel = "/salinization/Verzilting_aanpassingen incorrect.mdl"
31 pathToNewModel = "/models/salinization/Verzilting_aanpassingen correct.mdl"
32 newModel = open(pathToNewModel, "w")
33
34 # line = open(fileSpecifyingError).read()
35
36 line = "rainfall : 0.154705633188; adaptation time from non irrigated agriculture : 0.
   ↪915157119079; salt effect multiplier : 1.11965969891; adaptation time to non irrigated␣
   ↪agriculture : 0.48434342934; adaptation time to irrigated agriculture : 0.330990830832;
   ↪ water shortage multiplier : 0.984356102036; delay time salt seepage : 6.0; adaptation␣
   ↪time : 6.90258192256; births multiplier : 1.14344734715; diffusion lookup : [(0, 8.0),␣
   ↪(10, 8.0), (20, 8.0), (30, 8.0), (40, 7.9999999999999005), (50, 4.0), (60, 9.
   ↪982194802803703e-14), (70, 1.2455526635140464e-27), (80, 1.5541686655435471e-41), (90,␣
   ↪1.9392517969836692e-55)]; salinity effect multiplier : 1.10500381093; technological␣
   ↪developments in irrigation : 0.0117979353255; adaptation time from irrigated␣
   ↪agriculture : 1.58060947607; food shortage multiplier : 0.955325345996; deaths␣
   ↪multiplier : 0.875605669911; "
37
38 # we assume the case specification was copied from the logger
39 splitOne = line.split(",")
40 variable = {}
41 for n in range(len(splitOne) - 1):
42     splitTwo = splitOne[n].split(":")
43     variableElement = splitTwo[0]
44     # Delete the spaces and other rubish on the sides of the variable name
```

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```
    variableElement = variableElement.lstrip()
    variableElement = variableElement.lstrip("'")
    variableElement = variableElement.rstrip()
    variableElement = variableElement.rstrip("'")
    print(variableElement)
    valueElement = splitTwo[1]
    valueElement = valueElement.lstrip()
    valueElement = valueElement.rstrip()
    variable[variableElement] = valueElement
print(variable)

# This generates a new (text-formatted) model
changeNextLine = False
settedValues = []
for line in open(pathToExistingModel):
    if line.find("=") != -1:
        elements = line.split("=")
        value = elements[0]
        value = value.strip()
        if value in variable:
            elements[1] = variable.get(value)
            line = elements[0] + " = " + elements[1]
            settedValues.append(value)

    newModel.write(line)
newModel.close()  # in order to be able to open the model in Vensim
notSet = set(variable.keys()) - set(settedValues)
print(notSet)
```

1.13 Glossary

parameter uncertainty
: An uncertainty is a parameter uncertainty if the range is continuous from the lower bound to the upper bound. A parameter uncertainty can be either real valued or discrete valued.

categorical uncertainty
: An uncertainty is categorical if there is not a range but a set of possibilities over which one wants to sample.

lookup uncertainty
: vensim specific extension to categorical uncertainty for handling lookups in various ways

uncertainty space
: the space created by the set of uncertainties

ensemble
: a python class responsible for running a series of computational experiments.

model interface
: a python class that provides an interface to an underlying model

working directory
: a directory that contains files that a model needs

classification trees
a category of machine learning algorithms for rule induction

prim (patient rule induction method)
a rule induction algorithm

coverage
a metric developed for scenario discovery

density
a metric developed for scenario discovery

scenario discovery
a use case of EMA

case
A case specifies the input parameters for a run of a model. It is a dict instance, with the names of the uncertainties as key, and their sampled values as value.

experiment
An experiment is a complete specification for a run. It specifies the case, the name of the policy, and the name of the model.

policy
a policy is by definition an object with a name attribute. So, policy['name'] most return the name of the policy

result
the combination of an experiment and the associated outcomes for the experiment

outcome
the data of interest produced by a model given an experiment

1.14 EMA Modules

1.14.1 Exploratory modeling framework

model

This module specifies the abstract base class for interfacing with models. Any model that is to be controlled from the workbench is controlled via an instance of an extension of this abstract base class.

`class ema_workbench.em_framework.model.AbstractModel(name)`

`ModelStructureInterface` is one of the the two main classes used for performing EMA. This is an abstract base class and cannot be used directly.

`uncertainties`

list of parameter instances

Type
list

`levers`

list of parameter instances

Type
list

outcomes

list of outcome instances

Type
list

name

alphanumerical name of model structure interface

Type
str

output

this should be a dict with the names of the outcomes as key

Type
dict

When extending this class :meth:`model_init` and

:meth:`run_model` have to be implemented.

as_dict()

returns a dict representation of the model

cleanup()

This model is called after finishing all the experiments, but just prior to returning the results. This method gives a hook for doing any cleanup, such as closing applications.

In case of running in parallel, this method is called during the cleanup of the pool, just prior to removing the temporary directories.

initialized(*policy*)

check if model has been initialized

Parameters
policy (*a Policy instance*)

model_init(*policy*)

Method called to initialize the model.

Parameters
policy (*dict*) – policy to be run.

Note: This method should always be implemented. Although in simple cases, a simple pass can suffice.

---

reset_model()

Method for resetting the model to its initial state. The default implementation only sets the outputs to an empty dict.

retrieve_output()

Method for retrieving output after a model run. Deprecated, will be removed in version 3.0 of the EMA-workbench.

Return type
dict with the results of a model run.

run_model(*scenario*, *policy*)

Method for running an instantiated model structure.

Parameters

- **scenario** (*Scenario instance*)
- **policy** (*Policy instance*)

class ema_workbench.em_framework.model.**FileModel**(*name*, *wd=None*, *model_file=None*)

as_dict()

returns a dict representation of the model

class ema_workbench.em_framework.model.**Model**(*name*, *function=None*)

class ema_workbench.em_framework.model.**Replicator**(*name*)

run_model(*scenario*, *policy*)

Method for running an instantiated model structure.

Parameters

- **scenario** (*Scenario instance*)
- **policy** (*Policy instance*)

class ema_workbench.em_framework.model.**ReplicatorModel**(*name*, *function=None*)

class ema_workbench.em_framework.model.**SingleReplication**(*name*)

run_model(*scenario*, *policy*)

Method for running an instantiated model structure.

Parameters

- **scenario** (*Scenario instance*)
- **policy** (*Policy instance*)

parameters

parameters and related helper classes and functions

class ema_workbench.em_framework.parameters.**BooleanParameter**(*name*, *default=None*, *variable_name=None*, *pff=False*)

boolean model input parameter

A BooleanParameter is similar to a CategoricalParameter, except the category values can only be True or False.

Parameters

- **name** (*str*)
- **variable_name** (*str, or list of str*)

class ema_workbench.em_framework.parameters.**CategoricalParameter**(*name*, *categories*, *default=None*, *variable_name=None*, *pff=False*, *multivalue=False*)

categorical model input parameter

Parameters

- **name** (*str*)
- **categories** (*collection of obj*)
- **variable_name** (*str, or list of str*)
- **multivalue** (*boolean*) – if categories have a set of values, for each variable_name a different one.
- **TODO** (*#*)
- **TODO**

cat_for_index(*index*)

return category given index

Parameters
index (*int*)

Return type
object

from_dist(*name*, *dist*)

alternative constructor for creating a parameter from a frozen scipy.stats distribution directly

Parameters

- **dist** (*scipy stats frozen dist*)
- ****kwargs** (*valid keyword arguments for Parameter instance*)

index_for_cat(*category*)

return index of category

Parameters
category (*object*)

Return type
int

class ema_workbench.em_framework.parameters.**Constant**(*name*, *value*)

Constant class,

can be used for any parameter that has to be set to a fixed value

class ema_workbench.em_framework.parameters.**IntegerParameter**(*name*, *lower_bound*, *upper_bound*, *resolution=None*, *default=None*, *variable_name=None*, *pff=False*)

integer valued model input parameter

Parameters

- **name** (*str*)
- **lower_bound** (*int*)
- **upper_bound** (*int*)
- **resolution** (*iterable*)
- **variable_name** (*str, or list of str*)
- **pff** (*bool*) – if true, sample over this parameter using resolution in case of partial factorial sampling

Raises

- **ValueError** – if lower bound is larger than upper bound
- **ValueError** – if entries in resolution are outside range of lower_bound and upper_bound, or not an integer instance
- **ValueError** – if lower_bound or upper_bound is not an integer instance

classmethod from_dist(*name*, *dist*, ***kwargs*)

alternative constructor for creating a parameter from a frozen scipy.stats distribution directly

Parameters

- **dist** (*scipy stats frozen dist*)
- ****kwargs** (*valid keyword arguments for Parameter instance*)

class ema_workbench.em_framework.parameters.**Parameter**(*name*, *lower_bound*, *upper_bound*, *resolution=None*, *default=None*, *variable_name=None*, *pff=False*)

Base class for any model input parameter

Parameters

- **name** (*str*)
- **lower_bound** (*int or float*)
- **upper_bound** (*int or float*)
- **resolution** (*collection*)
- **pff** (*bool*) – if true, sample over this parameter using resolution in case of partial factorial sampling

Raises

- **ValueError** – if lower bound is larger than upper bound
- **ValueError** – if entries in resolution are outside range of lower_bound and upper_bound

classmethod from_dist(*name*, *dist*, ***kwargs*)

alternative constructor for creating a parameter from a frozen scipy.stats distribution directly

Parameters

- **dist** (*scipy stats frozen dist*)
- ****kwargs** (*valid keyword arguments for Parameter instance*)

class ema_workbench.em_framework.parameters.**RealParameter**(*name*, *lower_bound*, *upper_bound*, *resolution=None*, *default=None*, *variable_name=None*, *pff=False*)

real valued model input parameter

Parameters

- **name** (*str*)
- **lower_bound** (*int or float*)
- **upper_bound** (*int or float*)
- **resolution** (*iterable*)
- **variable_name** (*str, or list of str*)

- **pff** (*bool*) – if true, sample over this parameter using resolution in case of partial factorial sampling

Raises

- **ValueError** – if lower bound is larger than upper bound
- **ValueError** – if entries in resolution are outside range of lower_bound and upper_bound

classmethod from_dist(*name*, *dist*, ***kwargs*)

alternative constructor for creating a parameter from a frozen scipy.stats distribution directly

Parameters

- **dist** (*scipy stats frozen dist*)
- ****kwargs** (*valid keyword arguments for Parameter instance*)

ema_workbench.em_framework.parameters.**parameters_from_csv**(*uncertainties*, ***kwargs*)

Helper function for creating many Parameters based on a DataFrame or csv file

Parameters

- **uncertainties** (*str, DataFrame*)
- ****kwargs** (*dict, arguments to pass to pandas.read_csv*)

Return type
list of Parameter instances

This helper function creates uncertainties. It assumes that the DataFrame or csv file has a column titled 'name', optionally a type column {int, real, cat}, can be included as well. the remainder of the columns are handled as values for the parameters. If type is not specified, the function will try to infer type from the values.

Note that this function does not support the resolution and default kwargs on parameters.

An example of a csv:

NAME,TYPE,,, a_real,real,0,1.1, an_int,int,1,9, a_categorical,cat,a,b,c

this CSV file would result in

[RealParameter('a_real', 0, 1.1, resolution=[], default=None),
IntegerParameter('an_int', 1, 9, resolution=[], default=None), CategoricalParameter('a_categorical', ['a', 'b', 'c'], default=None)]

ema_workbench.em_framework.parameters.**parameters_to_csv**(*parameters*, *file_name*)

Helper function for writing a collection of parameters to a csv file

Parameters

- **parameters** (*collection of Parameter instances*)
- **file_name** (*str*)

The function iterates over the collection and turns these into a data frame prior to storing them. The resulting csv can be loaded using the parameters_from_csv function. Note that currently we don't store resolution and default attributes.

outcomes

Module for outcome classes

class ema_workbench.em_framework.outcomes.**AbstractOutcome**(*name*, *kind=0*, *variable_name=None*, *function=None*, *expected_range=None*, *shape=None*, *dtype=None*)

Base Outcome class

Parameters

- **name** (*str*) – Name of the outcome.
- **kind** (*{INFO, MINIMIZE, MAXIMIZE}, optional*)
- **variable_name** (*str, optional*) – if the name of the outcome in the underlying model is different from the name of the outcome, you can supply the variable name as an optional argument, if not provided, defaults to name
- **function** (*callable, optional*) – a callable to perform postprocessing on data retrieved from model
- **expected_range** (*2 tuple, optional*) – expected min and max value for outcome, used by HyperVolume convergence metric
- **shape** (*{tuple, None} optional*) – must be used in conjunction with dtype. Enables pre-allocation of data structure for storing results.
- **dtype** (*datatype, optional*) – must be used in conjunction with shape. Enables pre-allocation of data structure for storing results.

name

Type
str

kind

Type
int

variable_name

Type
str

function

Type
callable

shape

Type
tuple

dtype

Type
dataype

abstract classmethod from_disk(*filename*, *archive*)

helper function for loading from disk

Parameters

- **filename** (*str*)
- **archive** (*Tarfile*)

abstract classmethod to_disk(*values*)

helper function for writing outcome to disk

Parameters
values (*obj*) – data to store

Return type
BytesIO

class ema_workbench.em_framework.outcomes.**ArrayOutcome**(*name*, *variable_name=None*, *function=None*, *expected_range=None*, *shape=None*, *dtype=None*)

Array Outcome class for n-dimensional arrays

Parameters

- **name** (*str*) – Name of the outcome.
- **variable_name** (*str, optional*) – if the name of the outcome in the underlying model is different from the name of the outcome, you can supply the variable name as an optional argument, if not provided, defaults to name
- **function** (*callable, optional*) – a callable to perform postprocessing on data retrieved from model
- **expected_range** (*2 tuple, optional*) – expected min and max value for outcome, used by HyperVolume convergence metric
- **shape** (*{tuple, None} optional*) – must be used in conjunction with dtype. Enables pre-allocation of data structure for storing results.
- **dtype** (*datatype, optional*) – must be used in conjunction with shape. Enables pre-allocation of data structure for storing results.

name

Type
str

kind

Type
int

variable_name

Type
str

function

Type
callable

shape

Type
tuple

expected_range

Type
tuple

dtype

Type
datatype

classmethod from_disk(*filename*, *archive*)

helper function for loading from disk

Parameters

- **filename** (*str*)
- **archive** (*Tarfile*)

classmethod to_disk(*values*)

helper function for writing outcome to disk

Parameters
values (*ND array*)

Returns

- *BytesIO*
- *filename*

class ema_workbench.em_framework.outcomes.**Constraint**(*name*, *parameter_names=None*, *outcome_names=None*, *function=None*)

Constraints class that can be used when defining constrained optimization problems.

Parameters

- **name** (*str*)
- **parameter_names** (*str or collection of str*)
- **outcome_names** (*str or collection of str*)
- **function** (*callable*)

name

Type
str

parameter_names

name(s) of the uncertain parameter(s) and/or lever parameter(s) to which the constraint applies

Type
str, list of str

outcome_names

name(s) of the outcome(s) to which the constraint applies

Type
str, list of str

function

The function should return the distance from the feasibility threshold, given the model outputs with a variable name. The distance should be 0 if the constraint is met.

Type
callable

class ema_workbench.em_framework.outcomes.**ScalarOutcome**(*name*, *kind=0*, *variable_name=None*, *function=None*, *expected_range=None*, *dtype=None*)

Scalar Outcome class

Parameters

- **name** (*str*) – Name of the outcome.
- **kind** (*{INFO, MINIMIZE, MAXIMIZE}, optional*)
- **variable_name** (*str, optional*) – if the name of the outcome in the underlying model is different from the name of the outcome, you can supply the variable name as an optional argument, if not provided, defaults to name
- **function** (*callable, optional*) – a callable to perform post processing on data retrieved from model
- **expected_range** (*collection, optional*) – expected min and max value for outcome, used by HyperVolume convergence metric
- **dtype** (*datatype, optional*) – Enables pre-allocation of data structure for storing results.

name

Type
str

kind

Type
int

variable_name

Type
str

function

Type
callable

shape

Type
tuple

expected_range

Type
tuple

dtype

Type
datatype

classmethod from_disk(*filename*, *archive*)

helper function for loading from disk

Parameters

- **filename** (*str*)
- **archive** (*Tarfile*)

classmethod to_disk(*values*)

helper function for writing outcome to disk

Parameters
values (*1D array*)

Returns

- *BytesIO*
- *filename*

class ema_workbench.em_framework.outcomes.**TimeSeriesOutcome**(*name*, *variable_name=None*, *function=None*, *expected_range=None*, *shape=None*, *dtype=None*)

TimeSeries Outcome class for 1D arrays

Parameters

- **name** (*str*) – Name of the outcome.
- **variable_name** (*str, optional*) – if the name of the outcome in the underlying model is different from the name of the outcome, you can supply the variable name as an optional argument, if not provided, defaults to name
- **function** (*callable, optional*) – a callable to perform postprocessing on data retrieved from model
- **expected_range** (*2 tuple, optional*) – expected min and max value for outcome, used by HyperVolume convergence metric
- **shape** (*{tuple, None} optional*) – must be used in conjunction with dtype. Enables pre-allocation of data structure for storing results.
- **dtype** (*datatype, optional*) – must be used in conjunction with shape. Enables pre-allocation of data structure for storing results.

name

Type
str

kind

Type
int

variable_name

Type
str

function

Type
callable

shape

Type
tuple

expected_range

Type
tuple

dtype

Type
datatype

Notes

Time series outcomes are currently assumed to be 1D arrays. If you are dealing with higher dimensional outputs (e.g., multiple replications resulting in 2D arrays), use ArrayOutcome instead.

classmethod from_disk(*filename*, *archive*)

helper function for loading from disk

Parameters

- **filename** (*str*)
- **archive** (*Tarfile*)

classmethod to_disk(*values*)

helper function for writing outcome to disk

Parameters
values (*DataFrame*)

Returns

- *StringIO*
- *filename*

evaluators

collection of evaluators for performing experiments, optimization, and robust optimization

class ema_workbench.em_framework.evaluators.**Samplers**(*value*, *names=None*, **values*, *module=None*, *qualname=None*, *type=None*, *start=1*, *boundary=None*)

Enum for different kinds of samplers

class ema_workbench.em_framework.evaluators.**SequentialEvaluator**(*msis*)

evaluate_experiments(*scenarios*, *policies*, *callback*, *combine='factorial'*)

used by ema_workbench

finalize()

finalize the evaluator

initialize()

initialize the evaluator

ema_workbench.em_framework.evaluators.**optimize**(*models*, *algorithm=<class 'platypus.algorithms.EpsNSGAII'>*, *nfe=10000*, *searchover='levers'*, *evaluator=None*, *reference=None*, *convergence=None*, *constraints=None*, *convergence_freq=1000*, *logging_freq=5*, *variator=None*, ***kwargs*)

optimize the model

Parameters

- **models** (*1 or more Model instances*)
- **algorithm** (*a valid Platypus optimization algorithm*)
- **nfe** (*int*)
- **searchover** (*{'uncertainties', 'levers'}*)
- **evaluator** (*evaluator instance*)
- **reference** (*Policy or Scenario instance, optional*) – overwrite the default scenario in case of searching over levers, or default policy in case of searching over uncertainties
- **convergence** (*function or collection of functions, optional*)
- **constraints** (*list, optional*)
- **convergence_freq** (*int*) – nfe between convergence check
- **logging_freq** (*int*) – number of generations between logging of progress
- **variator** (*platypus GAOperator instance, optional*) – if None, it falls back on the defaults in platypus-opts which is SBX with PM
- **kwargs** (*any additional arguments will be passed on to algorithm*)

Return type
pandas DataFrame

Raises

- **EMAError if searchover is not one of 'uncertainties' or 'levers'** –
- **NotImplementedError if len(models) > 1** –

ema_workbench.em_framework.evaluators.**perform_experiments**(*models*, *scenarios=0*, *policies=0*, *evaluator=None*, *reporting_interval=None*, *reporting_frequency=10*, *uncertainty_union=False*, *lever_union=False*, *outcome_union=False*, *uncertainty_sampling=Samplers.LHS*, *lever_sampling=Samplers.LHS*, *callback=None*, *return_callback=False*, *combine='factorial'*, *log_progress=False*, ***kwargs*)

sample uncertainties and levers, and perform the resulting experiments on each of the models

Parameters

- **models** (*one or more AbstractModel instances*)
- **scenarios** (*int or collection of Scenario instances, optional*)
- **policies** (*int or collection of Policy instances, optional*)
- **evaluator** (*Additional keyword arguments are passed on to evaluate_experiments of the*)
- **reporting_interval** (*int, optional*)
- **reporting_frequency** (*int, optional*)
- **uncertainty_union** (*boolean, optional*)
- **lever_union** (*boolean, optional*)
- **outcome_union** (*boolean, optional*)
- **uncertainty_sampling** (*{LHS, MC, FF, PFF, SOBOL, MORRIS, FAST}, optional*)
- **lever_sampling** (*{LHS, MC, FF, PFF, SOBOL, MORRIS, FAST}, optional TODO:: update doc*)
- **callback** (*Callback instance, optional*)
- **return_callback** (*boolean, optional*)
- **log_progress** (*bool, optional*)
- **combine** (*{'factorial', 'zipover'}, optional*) – how to combine uncertainties and levers? In case of 'factorial', both are sampled separately using their respective samplers. Next the resulting designs are combined in a full factorial manner. In case of 'zipover', both are sampled separately and then combined by cycling over the shortest of the the two sets of designs until the longest set of designs is exhausted.
- **evaluator**

Returns

the experiments as a dataframe, and a dict with the name of an outcome as key, and the associated values as numpy array. Experiments and outcomes are aligned on index.

Return type

tuple

optimization

class ema_workbench.em_framework.optimization.**ArchiveLogger**(*directory*, *decision_varnames*, *outcome_varnames*, *base_filename='archives.tar.gz'*)

Helper class to write the archive to disk at each iteration

Parameters

- **directory** (*str*)
- **decision_varnames** (*list of str*)
- **outcome_varnames** (*list of str*)
- **base_filename** (*str, optional*)

classmethod load_archives(*filename*)

load the archives stored with the ArchiveLogger

Parameters
filename (*str*) – relative path to file

Return type
dict with nfe as key and dataframe as vlaue

class ema_workbench.em_framework.optimization.**Convergence**(*metrics*, *max_nfe*, *convergence_freq=1000*, *logging_freq=5*, *log_progress=False*)

helper class for tracking convergence of optimization

class ema_workbench.em_framework.optimization.**EpsilonIndicatorMetric**(*reference_set*, *problem*, ***kwargs*)

EpsilonIndicator metric

Parameters

- **reference_set** (*DataFrame*)
- **problem** (*PlatypusProblem instance*)

this is a thin wrapper around EpsilonIndicator as provided by platypus to make it easier to use in conjunction with the workbench.

class ema_workbench.em_framework.optimization.**EpsilonProgress**

epsilon progress convergence metric class

class ema_workbench.em_framework.optimization.**GenerationalDistanceMetric**(*reference_set*, *problem*, ***kwargs*)

GenerationalDistance metric

Parameters

- **reference_set** (*DataFrame*)
- **problem** (*PlatypusProblem instance*)
- **d** (*int, default=1*) – the power in the intergenerational distance function

This is a thin wrapper around GenerationalDistance as provided by platypus to make it easier to use in conjunction with the workbench.

see https://link.springer.com/content/pdf/10.1007/978-3-319-15892-1_8.pdf for more information

class ema_workbench.em_framework.optimization.**HypervolumeMetric**(*reference_set*, *problem*, ***kwargs*)

Hypervolume metric

Parameters

- **reference_set** (*DataFrame*)
- **problem** (*PlatypusProblem instance*)

this is a thin wrapper around Hypervolume as provided by platypus to make it easier to use in conjunction with the workbench.

class ema_workbench.em_framework.optimization.**InvertedGenerationalDistanceMetric**(*reference_set*, *problem*, ***kwargs*)

InvertedGenerationalDistance metric

Parameters

- **reference_set** (*DataFrame*)
- **problem** (*PlatypusProblem instance*)
- **d** (*int, default=1*) – the power in the inverted intergenerational distance function

This is a thin wrapper around InvertedGenerationalDistance as provided by platypus to make it easier to use in conjunction with the workbench.

see https://link.springer.com/content/pdf/10.1007/978-3-319-15892-1_8.pdf for more information

class ema_workbench.em_framework.optimization.**OperatorProbabilities**(*name*, *index*)

OperatorProbabiliy convergence tracker for use with auto adaptive operator selection.

Parameters

- **name** (*str*)
- **index** (*int*)

State of the art MOEAs like Borg (and GenerationalBorg provided by the workbench) use autoadaptive operator selection. The algorithm has multiple different evolutionary operators. Over the run, it tracks how well each operator is doing in producing fitter offspring. The probability of the algorithm using a given evolutionary operator is proportional to how well this operator has been doing in producing fitter offspring in recent generations. This class can be used to track these probabilities over the run of the algorithm.

class ema_workbench.em_framework.optimization.**Problem**(*searchover*, *parameters*, *outcome_names*, *constraints*, *reference=None*)

small extension to Platypus problem object, includes information on the names of the decision variables, the names of the outcomes, and the type of search

class ema_workbench.em_framework.optimization.**RobustProblem**(*parameters*, *outcome_names*, *scenarios*, *robustness_functions*, *constraints*)

small extension to Problem object for robust optimization, adds the scenarios and the robustness functions

class ema_workbench.em_framework.optimization.**SpacingMetric**(*problem*)

Spacing metric

Parameters

problem (*PlatypusProblem instance*)

this is a thin wrapper around Spacing as provided by platypus to make it easier to use in conjunction with the workbench.

ema_workbench.em_framework.optimization.**epsilon_nondominated**(*results*, *epsilons*, *problem*)

Merge the list of results into a single set of non dominated results using the provided epsilon values

Parameters

- **results** (*list of DataFrames*)
- **epsilons** (*epsilon values for each objective*)
- **problem** (*PlatypusProblem instance*)

Return type
DataFrame

Notes

this is a platypus based alternative to pareto.py (https://github.com/matthewjwoodruff/pareto.py)

ema_workbench.em_framework.optimization.**rebuild_platypus_population**(*archive*, *problem*)

rebuild a population of platypus Solution instances

Parameters

- **archive** (*DataFrame*)
- **problem** (*PlatypusProblem instance*)

Return type
list of platypus Solutions

ema_workbench.em_framework.optimization.**to_problem**(*model*, *searchover*, *reference=None*, *constraints=None*)

helper function to create Problem object

Parameters

- **model** (*AbstractModel instance*)
- **searchover** (*str*)
- **reference** (*Policy or Scenario instance, optional*) – overwrite the default scenario in case of searching over levers, or default policy in case of searching over uncertainties
- **constraints** (*list, optional*)

Return type
Problem instance

ema_workbench.em_framework.optimization.**to_robust_problem**(*model*, *scenarios*, *robustness_functions*, *constraints=None*)

helper function to create RobustProblem object

Parameters

- **model** (*AbstractModel instance*)
- **scenarios** (*collection*)
- **robustness_functions** (*iterable of ScalarOutcomes*)
- **constraints** (*list, optional*)

Return type
RobustProblem instance

outputspace_exploration

Provides a genetic algorithm based on novelty search for output space exploration.

The algorithm is inspired by Chérel et al (2015). In short, from Chérel et al, we have taken the idea of the HitBox. Basically, this is an epsilon archive where one keeps track of how many solutions have fallen into each grid cell. Next, tournament selection based on novelty is used as the selective pressure. Novelty is defined as 1/nr. of solutions in same grid cell. This is then combined with auto-adaptive population sizing as used in e-NSGAII. This replaces the use of adaptive Cauchy mutation as used by Chérel et al. There is also an more sophisticated algorithm that adds auto-adaptive operator selection as used in BORG.

The algorithm can be used in combination with the optimization functionality of the workbench. Just pass an OutputSpaceExploration instance as algorithm to optimize.

class ema_workbench.em_framework.outputspace_exploration.**AutoAdaptiveOutputSpaceExploration**(*problem*, *grid_spec=No*
pop-
u-
la-
tion_size=100,
gen-
er-
a-
tor=<platypus
ob-
ject>,
vari-
a-
tor=None,
***kwargs*)

A combination of auto-adaptive operator selection with OutputSpaceExploration.

The parametrization of all operators is based on the default values as used in Borg 1.9.

Parameters

- **problem** (*a platypus Problem instance*)
- **grid_spec** (*list of tuples*) – with min, max, and epsilon for each outcome of interest
- **population_size** (*int, optional*)

Notes

Limited to RealParameters only.

class ema_workbench.em_framework.outputspace_exploration.**OutputSpaceExploration**(*problem*, *grid_spec=None*, *population_size=100*, *generator=<platypus.operators.Rand object>*, *variator=None*, ***kwargs*)

Basic genetic algorithm for output space exploration using novelty search.

Parameters

- **problem** (*a platypus Problem instance*)
- **grid_spec** (*list of tuples*) – with min, max, and epsilon for each outcome of interest
- **population_size** (*int, optional*)

The algorithm defines novelty using an epsilon-like grid in the output space. Novelty is one divided by the number of seen solutions in a given grid cell. Tournament selection using novelty is used to create offspring. Crossover is done using simulated binary crossover and mutation is done using polynomial mutation.

The epsilon like grid structure for tracking novelty is implemented using an archive, the Hit Box. Per epsilon grid cell, a single solution closes to the centre of the cell is maintained. This makes the algorithm behave virtually identical to -NSGAII. The archive is returned as results and epsilon progress is defined.

To deal with a stalled search, adaptive time continuation, identical to -NSGAII is used.

Notes

Output space exploration relies on the optimization functionality of the workbench. Therefore, outcomes of kind INFO are ignored. For output space exploration the direction (i.e. minimize or maximize) does not matter.

samplers

This module contains various classes that can be used for specifying different types of samplers. These different samplers implement basic sampling techniques including Full Factorial sampling, Latin Hypercube sampling, and Monte Carlo sampling.

class ema_workbench.em_framework.samplers.**AbstractSampler**

Abstract base class from which different samplers can be derived.

In the simplest cases, only the sample method needs to be overwritten. generate_designs` is the only method called from outside. The other methods are used internally to generate the designs.

generate_designs(*parameters*, *nr_samples*)

external interface for Sampler. Returns the computational experiments over the specified parameters, for the given number of samples for each parameter.

Parameters

- **parameters** (*list*) – a list of parameters for which to generate the experimental designs
- **nr_samples** (*int*) – the number of samples to draw for each parameter

Returns

- *generator* – a generator object that yields the designs resulting from combining the parameters
- *int* – the number of experimental designs

generate_samples(*parameters*, *size*)

The main method of :class: *~sampler.Sampler* and its children. This will call the sample method for each of the parameters and return the resulting designs.

Parameters

- **parameters** (*collection*) – a collection of RealParameter, IntegerParameter, and CategoricalParameter instances.
- **size** (*int*) – the number of samples to generate.

Returns
dict with the parameter.name as key, and the sample as value

Return type
dict

sample(*distribution*, *size*)

method for sampling a number of samples from a particular distribution. The various samplers differ with respect to their implementation of this method.

Parameters

- **distribution** (*scipy frozen distribution*)
- **size** (*int*) – the number of samples to generate

Returns
the samples for the distribution and specified parameters

Return type
numpy array

class ema_workbench.em_framework.samplers.**DefaultDesigns**(*designs*, *parameters*, *n*)

iterable for the experimental designs

class ema_workbench.em_framework.samplers.**FullFactorialSampler**

generates a full factorial sample.

If the parameter is non categorical, the resolution is set the number of samples. If the parameter is categorical, the specified value for samples will be ignored and each category will be used instead.

determine_nr_of_designs(*sampled_parameters*)

Helper function for determining the number of experiments that will be generated given the sampled parameters.

Parameters
sampled_parameters (*list*) – a list of sampled parameters, as the values return by generate_samples

Returns
the total number of experimental design

Return type
int

generate_designs(*parameters*, *nr_samples*)

This method provides an alternative implementation to the default implementation provided by Sampler. This version returns a full factorial design across the parameters.

Parameters

- **parameters** (*list*) – a list of parameters for which to generate the experimental designs
- **nr_samples** (*int*) – the number of intervals to use on each Parameter. Categorical parameters always return all their categories

Returns

- *generator* – a generator object that yields the designs resulting from combining the parameters
- *int* – the number of experimental designs

generate_samples(*parameters*, *size*)

The main method of :class: *~sampler.Sampler* and its children. This will call the sample method for each of the parameters and return the resulting samples

Parameters

- **parameters** (*collection*) – a collection of Parameter instances
- **size** (*int*) – the number of samples to generate.

Returns
with the paramertainty.name as key, and the sample as value

Return type
dict

class ema_workbench.em_framework.samplers.**LHSSampler**

generates a Latin Hypercube sample for each of the parameters

sample(*distribution*, *size*)

generate a Latin Hypercube Sample.

Parameters

- **distribution** (*scipy frozen distribution*)
- **size** (*int*) – the number of samples to generate

Returns
with the paramertainty.name as key, and the sample as value

Return type
dict

class ema_workbench.em_framework.samplers.**MonteCarloSampler**

generates a Monte Carlo sample for each of the parameters.

sample(*distribution*, *size*)

generate a Monte Carlo Sample.

Parameters

- **distribution** (*scipy frozen distribution*)
- **size** (*int*) – the number of samples to generate

Returns
with the paramertainty.name as key, and the sample as value

Return type
dict

class ema_workbench.em_framework.samplers.**UniformLHSSampler**

generate_samples(*parameters*, *size*)

Parameters

- **parameters** (*collection*)
- **size** (*int*)

Returns
dict with the parameter.name as key, and the sample as value

Return type
dict

ema_workbench.em_framework.samplers.**determine_parameters**(*models*, *attribute*, *union=True*)

determine the parameters over which to sample

Parameters

- **models** (*a collection of AbstractModel instances*)
- **attribute** (*{'uncertainties', 'levers'}*)
- **union** (*bool, optional*) – in case of multiple models, sample over the union of levers, or over the intersection of the levers

Return type
collection of Parameter instances

ema_workbench.em_framework.samplers.**sample_levers**(*models*, *n_samples*, *union=True*, *sampler=<ema_workbench.em_framework.samplers.LHSSampler object>*)

generate policies by sampling over the levers

Parameters

- **models** (*a collection of AbstractModel instances*)
- **n_samples** (*int*)
- **union** (*bool, optional*) – in case of multiple models, sample over the union of levers, or over the intersection of the levers
- **sampler** (*Sampler instance, optional*)

Return type
generator yielding Policy instances

ema_workbench.em_framework.samplers.**sample_parameters**(*parameters*, *n_samples*, *sampler=<ema_workbench.em_framework.samplers.LHSSampler object>*, *kind=<class 'ema_workbench.em_framework.points.Point'>*)

generate cases by sampling over the parameters

Parameters

- **parameters** (*collection of AbstractParameter instances*)

- **n_samples** (*int*)
- **sampler** (*Sampler instance, optional*)
- **kind** (*{Case, Scenario, Policy}, optional*) – the class into which the samples are collected

Return type
generator yielding Case, *Scenario*, or Policy instances

ema_workbench.em_framework.samplers.**sample_uncertainties**(*models*, *n_samples*, *union=True*, *sampler=<ema_workbench.em_framework.samplers.LHSSample object>*)

generate scenarios by sampling over the uncertainties

Parameters

- **models** (*a collection of AbstractModel instances*)
- **n_samples** (*int*)
- **union** (*bool, optional*) – in case of multiple models, sample over the union of uncertainties, or over the intersection of the uncertainties
- **sampler** (*Sampler instance, optional*)

Return type
generator yielding Scenario instances

salib_samplers

Samplers for working with SALib

class ema_workbench.em_framework.salib_samplers.**FASTSampler**(*m=4*)

Sampler generating a Fourier Amplitude Sensitivity Test (FAST) using SALib

Parameters
m (*int (default: 4)*) – The interference parameter, i.e., the number of harmonics to sum in the Fourier series decomposition

class ema_workbench.em_framework.salib_samplers.**MorrisSampler**(*num_levels=4*, *optimal_trajectories=None*, *local_optimization=True*)

Sampler generating a morris design using SALib

Parameters

- **num_levels** (*int*) – The number of grid levels
- **grid_jump** (*int*) – The grid jump size
- **optimal_trajectories** (*int, optional*) – The number of optimal trajectories to sample (between 2 and N)
- **local_optimization** (*bool, optional*) – Flag whether to use local optimization according to Ruano et al. (2012) Speeds up the process tremendously for bigger N and num_levels. Stating this variable to be true causes the function to ignore gurobi.

class ema_workbench.em_framework.salib_samplers.**SobolSampler**(*second_order=True*)

Sampler generating a Sobol design using SALib

Parameters
second_order (*bool, optional*) – indicates whether second order effects should be included

ema_workbench.em_framework.salib_samplers.**get_SALib_problem**(*uncertainties*)
returns a dict with a problem specification as required by SALib

experiment_runner

helper module for running experiments and keeping track of which model has been initialized with which policy.

class ema_workbench.em_framework.experiment_runner.**ExperimentRunner**(*msis*)
Helper class for running the experiments

This class contains the logic for initializing models properly, running the experiment, getting the results, and cleaning up afterwards.

Parameters
- **msis** (*dict*)
- **model_kwargs** (*dict*)

msi_initializiation
keeps track of which model is initialized with which policy.

Type
dict

msis
models indexed by name

Type
dict

model_kwargs
keyword arguments for model_init

Type
dict

run_experiment(*experiment*)
The logic for running a single experiment. This code makes sure that model(s) are initialized correctly.

Parameters
experiment (*Case instance*)

Returns
- **experiment_id** (*int*)
- **case** (*dict*)
- **policy** (*str*)
- **model_name** (*str*)
- **result** (*dict*)

Raises
- ***EMAError*** – if the model instance raises an EMA error, these are reraised.
- **Exception** – Catch all for all other exceptions being raised by the model. These are reraised.

callbacks

This module provides an abstract base class for a callback and a default implementation.

If you want to store the data in a way that is different from the functionality provided by the default callback, you can write your own extension of callback. For example, you can easily implement a callback that stores the data in e.g. a NoSQL file.

The only method to implement is the __call__ magic method. To use logging of progress, always call super.

class ema_workbench.em_framework.callbacks.**AbstractCallback**(*uncertainties*, *levers*, *outcomes*, *nr_experiments*, *reporting_interval=None*, *reporting_frequency=10*, *log_progress=False*)

Abstract base class from which different call back classes can be derived. Callback is responsible for storing the results of the runs.

Parameters

- **uncertainties** (*list*) – list of uncertain parameters
- **levers** (*list*) – list of lever parameters
- **outcomes** (*list*) – a list of outcomes
- **nr_experiments** (*int*) – the total number of experiments to be executed
- **reporting_interval** (*int, optional*) – the interval between progress logs
- **reporting_frequency** (*int, optional*) – the total number of progress logs
- **log_progress** (*bool, optional*) – if true, progress is logged, if false, use tqdm progress bar.

i

a counter that keeps track of how many experiments have been saved

Type
int

nr_experiments

Type
int

outcomes

Type
list

parameters

combined list of uncertain parameters and lever parameters

Type
list

reporting_interval

the interval between progress logs

Type
int,

abstract get_results()

method for retrieving the results. Called after all experiments have been completed. Any extension of AbstractCallback needs to implement this method.

class ema_workbench.em_framework.callbacks.**DefaultCallback**(*uncertainties*, *levers*, *outcomes*, *nr_experiments*, *reporting_interval=100*, *reporting_frequency=10*, *log_progress=False*)

Default callback class

Parameters

- **uncertainties** (*list*) – list of uncertain parameters
- **levers** (*list*) – list of lever parameters
- **outcomes** (*list*) – a list of outcomes
- **nr_experiments** (*int*) – the total number of experiments to be executed
- **reporting_interval** (*int, optional*) – the interval between progress logs
- **reporting_frequency** (*int, optional*) – the total number of progress logs
- **log_progress** (*bool, optional*) – if true, progress is logged, if false, use tqdm progress bar.

Callback can be used in perform_experiments as a means for specifying the way in which the results should be handled. If no callback is specified, this default implementation is used. This one can be overwritten or replaced with a callback of your own design. For example if you prefer to store the result in a database or write them to a text file.

get_results()

method for retrieving the results. Called after all experiments have been completed. Any extension of AbstractCallback needs to implement this method.

class ema_workbench.em_framework.callbacks.**FileBasedCallback**(*uncertainties*, *levers*, *outcomes*, *nr_experiments*, *reporting_interval=100*, *reporting_frequency=10*)

Callback that stores data in csv files while running th model

Parameters

- **uncertainties** (*list*) – list of uncertain parameters
- **levers** (*list*) – list of lever parameters
- **outcomes** (*list*) – a list of outcomes
- **nr_experiments** (*int*) – the total number of experiments to be executed
- **reporting_interval** (*int, optional*) – the interval between progress logs
- **reporting_frequency** (*int, optional*) – the total number of progress logs
- **log_progress** (*bool, optional*) – if true, progress is logged, if false, use tqdm progress bar.

Warning: This class is still in beta. the data is stored in ./temp, relative to the current working directory. If this directory already exists, it will be overwritten.

get_results()

method for retrieving the results. Called after all experiments have been completed. Any extension of AbstractCallback needs to implement this method.

points

classes for representing points in parameter space, as well as associated hellper functions

class ema_workbench.em_framework.points.**Experiment**(*name*, *model_name*, *policy*, *scenario*, *experiment_id*)

A convenience object that contains a specification of the model, policy, and scenario to run

name

Type
str

model_name

Type
str

policy

Type
Policy instance

scenario

Type
Scenario instance

experiment_id

Type
int

class ema_workbench.em_framework.points.**ExperimentReplication**(*scenario*, *policy*, *constants*, *replication=None*)

helper class that combines scenario, policy, any constants, and replication information (seed etc) into a single dictionary.

This class represent the complete specification of parameters to run for a given experiment.

class ema_workbench.em_framework.points.**Point**(*name=None*, *unique_id=None*, ***kwargs*)

class ema_workbench.em_framework.points.**Policy**(*name=None*, ***kwargs*)

Helper class representing a policy

name

Type
str, int, or float

id

Type
int

all keyword arguments are wrapped into a dict.

class ema_workbench.em_framework.points.**Scenario**(*name=None*, ***kwargs*)

Helper class representing a scenario

name

Type
str, int, or float

id

Type
int

all keyword arguments are wrapped into a dict.

ema_workbench.em_framework.points.**combine_cases_factorial**(**point_collections*)

Combine collections of cases in a full factorial manner

Parameters
point_collections (*collection of collections of Point instances*)

Yields
Point

ema_workbench.em_framework.points.**combine_cases_sampling**(**point_collection*)

Combine collections of cases by iterating over the longest collection while sampling with replacement from the others

Parameters
point_collection (*collection of collection of Point instances*)

Yields
Point

ema_workbench.em_framework.points.**experiment_generator**(*scenarios*, *model_structures*, *policies*, *combine='factorial'*)

generator function which yields experiments

Parameters

- **scenarios** (*iterable of dicts*)
- **model_structures** (*list*)
- **policies** (*list*)
- **{'factorial** (*combine =*) – controls how to combine scenarios, policies, and model_structures into experiments.
- **sample'}** – controls how to combine scenarios, policies, and model_structures into experiments.

Notes

if combine is 'factorial' then this generator is essentially three nested loops: for each model structure, for each policy, for each scenario, return the experiment. This means that designs should not be a generator because this will be exhausted after the running the first policy on the first model. if combine is 'zipover' then this generator cycles over scenarios, policies and model structures until the longest of the three collections is exhausted.

futures_multiprocessing

support for using the multiprocessing library in combination with the workbench

class ema_workbench.em_framework.futures_multiprocessing.**MultiprocessingEvaluator**(*msis*, *n_processes=None*, *max-tasksper-child=None*, ***kwargs*)

evaluator for experiments using a multiprocessing pool

Parameters

- **msis** (*collection of models*)
- **n_processes** (*int (optional)*) – A negative number can be inputted to use the number of logical cores minus the negative cores. For example, on a 12 thread processor, -2 results in using 10 threads.
- **max_tasks** (*int (optional)*)

note that the maximum number of available processes is either multiprocessing.cpu_count() and in case of windows, this never can be higher then 61

evaluate_experiments(*scenarios*, *policies*, *callback*, *combine='factorial'*)

used by ema_workbench

finalize()

finalize the evaluator

initialize()

initialize the evaluator

futures_ipyparallel

This module provides functionality for combining the EMA workbench with IPython parallel.

class ema_workbench.em_framework.futures_ipyparallel.**IpyparallelEvaluator**(*msis*, *client*, ***kwargs*)

evaluator for using an ipypparallel pool

evaluate_experiments(*scenarios*, *policies*, *callback*, *combine='factorial'*, ***kwargs*)

used by ema_workbench

finalize()

finalize the evaluator

initialize()

initialize the evaluator

futures_mpi

class ema_workbench.em_framework.futures_mpi.**MPIEvaluator**(*msis*, *n_processes=None*, ***kwargs*)

Evaluator for experiments using MPI Pool Executor from mpi4py

evaluate_experiments(*scenarios*, *policies*, *callback*, *combine='factorial'*, ***kwargs*)

used by ema_workbench

finalize()

finalize the evaluator

initialize()

initialize the evaluator

futures_util

ema_workbench.em_framework.futures_util.**finalizer**(*experiment_runner*)

cleanup

ema_workbench.em_framework.futures_util.**setup_working_directories**(*models*, *root_dir*)

copies the working directory of each model to a process specific temporary directory and update the working directory of the model

Parameters

- **models** (*list*)
- **root_dir** (*str*)

util

utilities used throughout em_framework

class ema_workbench.em_framework.util.**Counter**(*startfrom=0*)

helper function for generating counter based names for NamedDicts

class ema_workbench.em_framework.util.**NamedDict**(*name=<function representation>*, ***kwargs*)

class ema_workbench.em_framework.util.**ProgressTrackingMixIn**(*N*, *reporting_interval*, *logger*, *log_progress=False*, *log_func=<function ProgressTrackingMixIn.<lambda>>*)

Mixin for monitoring progress

Parameters

- **N** (*int*) – total number of experiments
- **reporting_interval** (*int*) – nfe between logging progress
- **logger** (*logger instance*)
- **log_progress** (*bool, optional*)
- **log_func** (*callable, optional*) – function called with self as only argument, should invoke self._logger with custom log message

i

Type
int

reporting_interval

Type
int

log_progress

Type
bool

log_func

Type
callable

pbar
if log_progress is true, None, if false tqdm.tqdm instance

Type
{None, tqdm.tqdm instance}

ema_workbench.em_framework.util.**combine**(**args*)
combine scenario and policy into a single experiment dict

Parameters
args (*two or more dicts that need to be combined*)

Return type
a single unified dict containing the entries from all dicts

Raises
EMAError – if a keyword argument exists in more than one dict

ema_workbench.em_framework.util.**determine_objects**(*models*, *attribute*, *union=True*)
determine the parameters over which to sample

Parameters

- **models** (*a collection of AbstractModel instances*)
- **attribute** (*{'uncertainties', 'levers', 'outcomes'}*)
- **union** (*bool, optional*) – in case of multiple models, sample over the union of levers, or over the intersection of the levers

Return type
collection of Parameter instances

ema_workbench.em_framework.util.**representation**(*named_dict*)
helper function for generating repr based names for NamedDicts

1.14.2 Connectors

vensim

vensimDLLwrapper

pysd_connector

netlogo

simio

excel

This module provides a base class that can be used to perform EMA on Excel models. It relies on win32com

class ema_workbench.connectors.excel.**ExcelModel**(*name*, *wd=None*, *model_file=None*, *default_sheet=None*, *pointers=None*)

1.14.3 Analysis

prim

A scenario discovery oriented implementation of PRIM.

The implementation of prim provided here is data type aware, so categorical variables will be handled appropriately. It also uses a non-standard objective function in the peeling and pasting phase of the algorithm. This algorithm looks at the increase in the mean divided by the amount of data removed. So essentially, it uses something akin to the first order derivative of the original objective function.

The implementation is designed for interactive use in combination with the jupyter notebook.

class ema_workbench.analysis.prim.**PRIMObjectiveFunctions**(*value*, *names=None*, **values*, *module=None*, *qualname=None*, *type=None*, *start=1*, *boundary=None*)

class ema_workbench.analysis.prim.**Prim**(*x*, *y*, *threshold*, *obj_function=PRIMObjectiveFunctions.LENIENT1*, *peel_alpha=0.05*, *paste_alpha=0.05*, *mass_min=0.05*, *threshold_type=1*, *mode=RuleInductionType.BINARY*, *update_function='default'*)

Patient rule induction algorithm

The implementation of Prim is tailored to interactive use in the context of scenario discovery

Parameters

- **x** (*DataFrame*) – the independent variables
- **y** (*1d ndarray*) – the dependent variable
- **threshold** (*float*) – the density threshold that a box has to meet
- **obj_function** (*{LENIENT1, LENIENT2, ORIGINAL}*) – the objective function used by PRIM. Defaults to a lenient objective function based on the gain of mean divided by the loss of mass.

- **peel_alpha** (*float, optional*) – parameter controlling the peeling stage (default = 0.05).
- **paste_alpha** (*float, optional*) – parameter controlling the pasting stage (default = 0.05).
- **mass_min** (*float, optional*) – minimum mass of a box (default = 0.05).
- **threshold_type** (*{ABOVE, BELOW}*) – whether to look above or below the threshold value
- **mode** (*{RuleInductionType.BINARY, RuleInductionType.REGRESSION}, optional*) – indicated whether PRIM is used for regression, or for scenario classification in which case y should be a binary vector
- **{'default'** (*update_function =*) – controls behavior of PRIM after having found a first box. use either the default behavior were all points are removed, or the procedure suggested by guivarch et al (2016) doi:10.1016/j.envsoft.2016.03.006 to simply set all points to be no longer of interest (only valid in binary mode).
- **'guivarch'}** – controls behavior of PRIM after having found a first box. use either the default behavior were all points are removed, or the procedure suggested by guivarch et al (2016) doi:10.1016/j.envsoft.2016.03.006 to simply set all points to be no longer of interest (only valid in binary mode).
- **optional** – controls behavior of PRIM after having found a first box. use either the default behavior were all points are removed, or the procedure suggested by guivarch et al (2016) doi:10.1016/j.envsoft.2016.03.006 to simply set all points to be no longer of interest (only valid in binary mode).

See also:

`cart`

property boxes

Property for getting a list of box limits

determine_coi(*indices*)

Given a set of indices on y, how many cases of interest are there in this set.

Parameters
indices (*ndarray*) – a valid index for y

Returns
the number of cases of interest.

Return type
int

Raises
ValueError – if threshold_type is not either ABOVE or BELOW

find_box()

Execute one iteration of the PRIM algorithm. That is, find one box, starting from the current state of Prim.

property stats

property for getting a list of dicts containing the statistics for each box

class ema_workbench.analysis.prim.**PrimBox**(*prim*, *box_lims*, *indices*)

A class that holds information for a specific box

coverage

coverage of currently selected box

Type
float

density

density of currently selected box

Type
float

mean

mean of currently selected box

Type
float

res_dim

number of restricted dimensions of currently selected box

Type
int

mass

mass of currently selected box

Type
float

peeling_trajectory

stats for each box in peeling trajectory

Type
DataFrame

box_lims

list of box lims for each box in peeling trajectory

Type
list

by default, the currently selected box is the last box on the peeling trajectory, unless this is changed via *PrimBox.select()*.

drop_restriction(*uncertainty=''*, *i=-1*)

Drop the restriction on the specified dimension for box i

Parameters

- **i** (*int, optional*) – defaults to the currently selected box, which defaults to the latest box on the trajectory
- **uncertainty** (*str*)

Replace the limits in box i with a new box where for the specified uncertainty the limits of the initial box are being used. The resulting box is added to the peeling trajectory.

inspect(*i=None*, *style='table'*, *ax=None*, ***kwargs*)

Write the stats and box limits of the user specified box to standard out. If i is not provided, the last box will be printed

Parameters

- **i** (*int or list of ints, optional*) – the index of the box, defaults to currently selected box
- **style** (*{'table', 'graph', 'data'}*) – the style of the visualization. 'table' prints the stats and boxlim. 'graph' creates a figure. 'data' returns a list of tuples, where each tuple contains the stats and the box_lims.
- **ax** (*axes or list of axes instances, optional*) – used in conjunction with *graph* style, allows you to control the axes on which graph is plotted if i is list, axes should be list of equal length. If axes is None, each i_j in i will be plotted in a separate figure.
- **that** (*additional kwargs are passed to the helper function*)
- **graph** (*generates the table or*)

resample(*i=None*, *iterations=10*, *p=0.5*)

Calculate resample statistics for candidate box i

Parameters

- **i** (*int, optional*)
- **iterations** (*int, optional*)
- **p** (*float, optional*)

Return type
DataFrame

select(*i*)

select an entry from the peeling and pasting trajectory and update the prim box to this selected box.

Parameters
i (*int*) – the index of the box to select.

show_pairs_scatter(*i=None*, *dims=None*, *diag_kind=DiagKind.KDE*, *upper='scatter'*, *lower='contour'*, *fill_subplots=True*)

Make a pair wise scatter plot of all the restricted dimensions with color denoting whether a given point is of interest or not and the boxlims superimposed on top.

Parameters

- **i** (*int, optional*)
- **dims** (*list of str, optional*) – dimensions to show, defaults to all restricted dimensions
- **diag_kind** (*{DiagKind.KDE, DiagKind.CDF}*) – Plot diagonal as kernel density estimate ('kde') or cumulative density function ('cdf').
- **upper** (*string, optional*) – Use either 'scatter', 'contour', or 'hist' (bivariate histogram) plots for upper and lower triangles. Upper triangle can also be 'none' to eliminate redundancy. Legend uses lower triangle style for markers.
- **lower** (*string, optional*) – Use either 'scatter', 'contour', or 'hist' (bivariate histogram) plots for upper and lower triangles. Upper triangle can also be 'none' to eliminate redundancy. Legend uses lower triangle style for markers.
- **fill_subplots** (*Boolean, optional*) – if True, subplots are resized to fill their respective axes. This removes unnecessary whitespace, but may be undesirable for some variable combinations.

Return type
seaborn PairGrid

show_ppt()

show the peeling and pasting trajectory in a figure

show_tradeoff(*cmap=<matplotlib.colors.ListedColormap object>*, *annotated=False*)

Visualize the trade off between coverage and density. Color is used to denote the number of restricted dimensions.

Parameters

- **cmap** (*valid matplotlib colormap*)
- **annotated** (*bool, optional. Shows point labels if True.*)

Return type
a Figure instance

update(*box_lims*, *indices*)

update the box to the provided box limits.

Parameters

- **box_lims** (*DataFrame*) – the new box_lims
- **indices** (*ndarray*) – the indices of y that are inside the box

write_ppt_to_stdout()

write the peeling and pasting trajectory to stdout

ema_workbench.analysis.prim.**pca_preprocess**(*experiments*, *y*, *subsets=None*, *exclude={}*)

perform PCA to preprocess experiments before running PRIM

Pre-process the data by performing a pca based rotation on it. This effectively turns the algorithm into PCA-PRIM as described in Dalal et al (2013)

Parameters

- **experiments** (*DataFrame*)
- **y** (*ndarray*) – one dimensional binary array
- **subsets** (*dict, optional*) – expects a dictionary with group name as key and a list of uncertainty names as values. If this is used, a constrained PCA-PRIM is executed
- **exclude** (*list of str, optional*) – the uncertainties that should be excluded from the rotation

Returns

- *rotated_experiments* – DataFrame
- *rotation_matrix* – DataFrame

Raises
RuntimeError – if mode is not binary (i.e. y is not a binary classification). if X contains non numeric columns

ema_workbench.analysis.prim.**run_constrained_prim**(*experiments*, *y*, *issignificant=True*, ***kwargs*)

Run PRIM repeatedly while constraining the maximum number of dimensions available in x

Improved usage of PRIM as described in Kwakkel (2019).

Parameters

- **x** (*DataFrame*)
- **y** (*numpy array*)
- **issignificant** (*bool, optional*) – if True, run prim only on subsets of dimensions that are significant for the initial PRIM on the entire dataset.
- ****kwargs** (*any additional keyword arguments are passed on to PRIM*)

Return type
PrimBox instance

ema_workbench.analysis.prim.**setup_prim**(*results*, *classify*, *threshold*, *incl_unc=[]*, ***kwargs*)

Helper function for setting up the prim algorithm

Parameters

- **results** (*tuple*) – tuple of DataFrame and dict with numpy arrays the return from `perform_experiments()`.
- **classify** (*str or callable*) – either a string denoting the outcome of interest to use or a function.
- **threshold** (*double*) – the minimum score on the density of the last box on the peeling trajectory. In case of a binary classification, this should be between 0 and 1.
- **incl_unc** (*list of str, optional*) – list of uncertainties to include in prim analysis
- **kwargs** (*dict*) – valid keyword arguments for prim.Prim

Return type
a Prim instance

Raises

- **PrimException** – if data resulting from classify is not a 1-d array.
- **TypeError** – if classify is not a string or a callable.

cart

A scenario discovery oriented implementation of CART. It essentially is a wrapper around scikit-learn's version of CART.

class ema_workbench.analysis.cart.**CART**(*x*, *y*, *mass_min=0.05*, *mode=RuleInductionType.BINARY*)

CART algorithm

can be used in a manner similar to PRIM. It provides access to the underlying tree, but it can also show the boxes described by the tree in a table or graph form similar to prim.

Parameters

- **x** (*DataFrame*)
- **y** (*1D ndarray*)
- **mass_min** (*float, optional*) – a value between 0 and 1 indicating the minimum fraction of data points in a terminal leaf. Defaults to 0.05, identical to prim.
- **mode** (*{BINARY, CLASSIFICATION, REGRESSION}*) – indicates the mode in which CART is used. Binary indicates binary classification, classification is multiclass, and regression is regression.

boxes

list of DataFrame box lims

Type
list

stats

list of dicts with stats

Type
list

Notes

This class is a wrapper around scikit-learn's CART algorithm. It provides an interface to CART that is more oriented towards scenario discovery, and shared some methods with PRIM

See also:

prim

property boxes

rtype: list with boxlims for each terminal leaf

build_tree()

train CART on the data

show_tree(*mplfig=True*, *format='png'*)

return a png (defaults) or svg of the tree

On Windows, graphviz needs to be installed with conda.

Parameters

- **mplfig** (*bool, optional*) – if true (default) returns a matplotlib figure with the tree, otherwise, it returns the output as bytes
- **format** (*{'png', 'svg'}, default 'png'*) – Gives a format of the output.

property stats

rtype: list with scenario discovery statistics for each terminal leaf

ema_workbench.analysis.cart.**setup_cart**(*results*, *classify*, *incl_unc=None*, *mass_min=0.05*)

helper function for performing cart in combination with data generated by the workbench.

Parameters

- **results** (*tuple of DataFrame and dict with numpy arrays*) – the return from perform_experiments().
- **classify** (*string, function or callable*) – either a string denoting the outcome of interest to use or a function.
- **incl_unc** (*list of strings, optional*)
- **mass_min** (*float, optional*)

Raises
TypeError – if classify is not a string or a callable.

clusterer

This module provides time series clustering functionality using complex invariant distance. For details see Steinmann et al (2020)

ema_workbench.analysis.clusterer.**apply_agglomerative_clustering**(*distances*, *n_clusters*, *metric='precomputed'*, *linkage='average'*)

apply agglomerative clustering to the distances

Parameters

- **distances** (*ndarray*)
- **n_clusters** (*int*)
- **metric** (*str, optional. The distance metric to use. The default is 'precomputed'. For a list of available metrics, see the documentation of scipy.spatial.distance.pdist.*)
- **linkage** (*{'average', 'complete', 'single'}*)

Return type
1D ndarray with cluster assignment

ema_workbench.analysis.clusterer.**calculate_cid**(*data*, *condensed_form=False*)

calculate the complex invariant distance between all rows

Parameters

- **data** (*2d ndarray*)
- **condensed_form** (*bool, optional*)

Returns
a 2D ndarray with the distances between all time series, or condensed form similar to scipy.spatial.distance.pdist¶

Return type
distances

ema_workbench.analysis.clusterer.**plot_dendrogram**(*distances*)

plot dendrogram for distances

logistic_regression

This module implements logistic regression for scenario discovery.

The module draws its inspiration from Quinn et al (2018) 10.1029/2018WR022743 and Lamontagne et al (2019). The implementation here generalizes their work and embeds it in a more typical scenario discovery workflow with a posteriori selection of the appropriate number of dimensions to include. It is modeled as much as possible on the api used for PRIM and CART.

class ema_workbench.analysis.logistic_regression.**Logit**(*x*, *y*, *threshold=0.95*)

Implements an interactive version of logistic regression using BIC based forward selection

Parameters

- **x** (*DataFrame*)
- **y** (*numpy Array*)

- **threshold** (*float*)

coverage

coverage of currently selected model

Type
float

density

density of currently selected model

Type
float

res_dim

number of restricted dimensions of currently selected model

Type
int

peeling_trajectory

stats for each model in peeling trajectory

Type
DataFrame

models

list of models associated with each model on the peeling trajectory

Type
list

inspect(*i*, *step=0.1*)

Inspect one of the models by showing the threshold tradeoff and summary2

Parameters

- **i** (*int*)
- **step** (*float between [0, 1]*)

plot_pairwise_scatter(*i*, *threshold=0.95*)

plot pairwise scatter plot of data points, with contours as background

Parameters

- **i** (*int*)
- **threshold** (*float*)

Return type
Figure instance

The lower triangle background is a binary contour based on the specified threshold. All axis not shown are set to a default value in the middle of their range

The upper triangle shows a contour map with the conditional probability, again setting all non shown dimensions to a default value in the middle of their range.

run(***kwargs*)

run logistic regression using forward selection using a Bayesian Information Criterion for selecting whether and if so which dimension to add

Parameters

- **details** (*kwargs are passed on to model.fit. For*)
- **https** (*see*)

show_threshold_tradeoff(*i*, *cmap=<matplotlib.colors.ListedColormap object>*, *step=0.1*)

Visualize the trade off between coverage and density for a given model i across the range of threshold values

Parameters

- **i** (*int*)
- **cmap** (*valid matplotlib colormap*)
- **step** (*float, optional*)

Return type
a Figure instance

show_tradeoff(*cmap=<matplotlib.colors.ListedColormap object>*, *annotated=False*)

Visualize the trade off between coverage and density. Color is used to denote the number of restricted dimensions.

Parameters

- **cmap** (*valid matplotlib colormap*)
- **annotated** (*bool, optional. Shows point labels if True.*)

Return type
a Figure instance

update(*model*, *selected*)

helper function for adding a model to the collection of models and update the associated attributes

Parameters

- **model** (*statsmodel fitted logit model*)
- **selected** (*list of str*)

dimensional_stacking

This module provides functionality for doing dimensional stacking of uncertain factors in order to reveal patterns in the values for a single outcome of interests. It is inspired by the work reported here with one deviation.

Rather than using association rules to identify the uncertain factors to use, this code uses random forest based feature scoring instead. It is also possible to use the code provided here in combination with any other feature scoring or factor prioritization technique instead, or by simply selecting uncertain factors in some other manner.

ema_workbench.analysis.dimensional_stacking.**create_pivot_plot**(*x*, *y*, *nr_levels=3*, *labels=True*, *categories=True*, *nbins=3*, *bin_labels=False*)

convenience function for easily creating a pivot plot

Parameters

- **x** (*DataFrame*)
- **y** (*1d ndarray*)
- **nr_levels** (*int, optional*) – the number of levels in the pivot table. The number of uncertain factors included in the pivot table is two times the number of levels.
- **labels** (*bool, optional*) – display names of uncertain factors

- **categories** (*bool, optional*) – display category names for each uncertain factor
- **nbins** (*int, optional*) – number of bins to use when discretizing continuous uncertain factors
- **bin_labels** (*bool, optional*) – if True show bin interval / name, otherwise show only a number

Return type
Figure

This function performs feature scoring using random forests, selects a number of high scoring factors based on the specified number of levels, creates a pivot table, and visualizes the table. This is a convenience function. For more control over the process, use the code in this function as a template.

regional_sa

Module offers support for performing basic regional sensitivity analysis. The module can be used to perform regional sensitivity analysis on all uncertainties specified in the experiment array, as well as the ability to zoom in on any given uncertainty in more detail.

ema_workbench.analysis.regional_sa.**plot_cdfs**(*x*, *y*, *ccdf=False*)

plot cumulative density functions for each column in x, based on the classification specified in y.

Parameters

- **x** (*DataFrame*) – the experiments to use in the cdfs
- **y** (*ndaray*) – the categorization for the data
- **ccdf** (*bool, optional*) – if true, plot a complementary cdf instead of a normal cdf.

Return type
a matplotlib Figure instance

feature_scoring

Feature scoring functionality

ema_workbench.analysis.feature_scoring.**CHI2**(*X*, *y*)

Compute chi-squared stats between each non-negative feature and class.

This score can be used to select the *n_features* features with the highest values for the test chi-squared statistic from X, which must contain only **non-negative features** such as booleans or frequencies (e.g., term counts in document classification), relative to the classes.

Recall that the chi-square test measures dependence between stochastic variables, so using this function "weeds out" the features that are the most likely to be independent of class and therefore irrelevant for classification.

Read more in the User Guide.

Parameters

- **X** (*{array-like, sparse matrix} of shape (n_samples, n_features)*) – Sample vectors.
- **y** (*array-like of shape (n_samples,)*) – Target vector (class labels).

Returns

- **chi2** (*ndarray of shape (n_features,)*) – Chi2 statistics for each feature.

- **p_values** (*ndarray of shape (n_features,)*) – P-values for each feature.

See also:

f_classif
ANOVA F-value between label/feature for classification tasks.

f_regression
F-value between label/feature for regression tasks.

Notes

Complexity of this algorithm is O(n_classes * n_features).

Examples

```
>>> import numpy as np
>>> from sklearn.feature_selection import chi2
>>> X = np.array([[1, 1, 3],
...               [0, 1, 5],
...               [5, 4, 1],
...               [6, 6, 2],
...               [1, 4, 0],
...               [0, 0, 0]])
>>> y = np.array([1, 1, 0, 0, 2, 2])
>>> chi2_stats, p_values = chi2(X, y)
>>> chi2_stats
array([15.3...,  6.5       ,  8.9...])
>>> p_values
array([0.0004..., 0.0387..., 0.0116... ])
```

ema_workbench.analysis.feature_scoring.**F_CLASSIFICATION**(*X*, *y*)

Compute the ANOVA F-value for the provided sample.

Read more in the User Guide.

Parameters

- **X** (*{array-like, sparse matrix} of shape (n_samples, n_features)*) – The set of regressors that will be tested sequentially.
- **y** (*array-like of shape (n_samples,)*) – The target vector.

Returns

- **f_statistic** (*ndarray of shape (n_features,)*) – F-statistic for each feature.
- **p_values** (*ndarray of shape (n_features,)*) – P-values associated with the F-statistic.

See also:

chi2
Chi-squared stats of non-negative features for classification tasks.

f_regression
F-value between label/feature for regression tasks.

Examples

```
>>> from sklearn.datasets import make_classification
>>> from sklearn.feature_selection import f_classif
>>> X, y = make_classification(
...     n_samples=100, n_features=10, n_informative=2, n_clusters_per_class=1,
...     shuffle=False, random_state=42
... )
>>> f_statistic, p_values = f_classif(X, y)
>>> f_statistic
array([2.2...e+02, 7.0...e-01, 1.6...e+00, 9.3...e-01,
       5.4...e+00, 3.2...e-01, 4.7...e-02, 5.7...e-01,
       7.5...e-01, 8.9...e-02])
>>> p_values
array([7.1...e-27, 4.0...e-01, 1.9...e-01, 3.3...e-01,
       2.2...e-02, 5.7...e-01, 8.2...e-01, 4.5...e-01,
       3.8...e-01, 7.6...e-01])
```

ema_workbench.analysis.feature_scoring.**F_REGRESSION**(*X*, *y*, *, *center=True*, *force_finite=True*)

Univariate linear regression tests returning F-statistic and p-values.

Quick linear model for testing the effect of a single regressor, sequentially for many regressors.

This is done in 2 steps:

1. The cross correlation between each regressor and the target is computed using `r_regression()` as:

```
E[(X[:, i] - mean(X[:, i])) * (y - mean(y))] / (std(X[:, i]) * std(y))
```

2. It is converted to an F score and then to a p-value.

`f_regression()` is derived from `r_regression()` and will rank features in the same order if all the features are positively correlated with the target.

Note however that contrary to `f_regression()`, `r_regression()` values lie in [-1, 1] and can thus be negative. `f_regression()` is therefore recommended as a feature selection criterion to identify potentially predictive feature for a downstream classifier, irrespective of the sign of the association with the target variable.

Furthermore `f_regression()` returns p-values while `r_regression()` does not.

Read more in the User Guide.

Parameters

- **X** (*{array-like, sparse matrix} of shape (n_samples, n_features)*) – The data matrix.
- **y** (*array-like of shape (n_samples,)*) – The target vector.
- **center** (*bool, default=True*) – Whether or not to center the data matrix *X* and the target vector *y*. By default, *X* and *y* will be centered.
- **force_finite** (*bool, default=True*) – Whether or not to force the F-statistics and associated p-values to be finite. There are two cases where the F-statistic is expected to not be finite:
  - when the target *y* or some features in *X* are constant. In this case, the Pearson's R correlation is not defined leading to obtain *np.nan* values in the F-statistic and p-value. When *force_finite=True*, the F-statistic is set to *0.0* and the associated p-value is set to *1.0*.

– when a feature in *X* is perfectly correlated (or anti-correlated) with the target *y*. In this case, the F-statistic is expected to be *np.inf*. When *force_finite=True*, the F-statistic is set to *np.finfo(dtype).max* and the associated p-value is set to *0.0*.

Added in version 1.1.

Returns

- **f_statistic** (*ndarray of shape (n_features,)*) – F-statistic for each feature.
- **p_values** (*ndarray of shape (n_features,)*) – P-values associated with the F-statistic.

See also:

`r_regression`
Pearson's R between label/feature for regression tasks.

`f_classif`
ANOVA F-value between label/feature for classification tasks.

`chi2`
Chi-squared stats of non-negative features for classification tasks.

`SelectKBest`
Select features based on the k highest scores.

`SelectFpr`
Select features based on a false positive rate test.

`SelectFdr`
Select features based on an estimated false discovery rate.

`SelectFwe`
Select features based on family-wise error rate.

`SelectPercentile`
Select features based on percentile of the highest scores.

Examples

```
>>> from sklearn.datasets import make_regression
>>> from sklearn.feature_selection import f_regression
>>> X, y = make_regression(
...     n_samples=50, n_features=3, n_informative=1, noise=1e-4, random_state=42
... )
>>> f_statistic, p_values = f_regression(X, y)
>>> f_statistic
array([1.2...+00, 2.6...+13, 2.6...+00])
>>> p_values
array([2.7..., 1.5..., 1.0...])
```

ema_workbench.analysis.feature_scoring.**get_ex_feature_scores**(*x*, *y*, *mode=RuleInductionType.CLASSIFICATION*, *nr_trees=100*, *max_features=None*, *max_depth=None*, *min_samples_split=2*, *min_samples_leaf=None*, *min_weight_fraction_leaf=0*, *max_leaf_nodes=None*, *bootstrap=True*, *oob_score=True*, *random_state=None*)

Get feature scores using extra trees

Parameters

- **x** (*DataFrame*)
- **y** (*1D nd.array*)
- **mode** ({*RuleInductionType.CLASSIFICATION, RuleInductionType.REGRESSION*})
- **nr_trees** (*int, optional*) – nr. of trees in forest (default=250)
- **max_features** (*int, float, string or None, optional*) – by default, it will use number of features/3, following Jaxa-Rozen & Kwakkel (2018) doi: 10.1016/j.envsoft.2018.06.011 see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **max_depth** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **min_samples_split** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **min_samples_leaf** (*int, optional*) – defaults to 1 for N=1000 or lower, from there on proportional to sqrt of N (see discussion in Jaxa-Rozen & Kwakkel (2018) doi: 10.1016/j.envsoft.2018.06.011) see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **min_weight_fraction_leaf** (*float, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **max_leaf_nodes** (*int or None, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **bootstrap** (*bool, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **oob_score** (*bool, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html
- **random_state** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html

Returns

- *pandas DataFrame* – sorted in descending order of tuples with uncertainty and feature scores
- *object* – either ExtraTreesClassifier or ExtraTreesRegressor

ema_workbench.analysis.feature_scoring.**get_feature_scores_all**(*x*, *y*, *alg='extra trees'*, *mode=RuleInductionType.REGRESSION*, ***kwargs*)

perform feature scoring for all outcomes using the specified feature scoring algorithm

Parameters

- **x** (*DataFrame*)
- **y** (*dict of 1d numpy arrays*) – the outcomes, with a string as key, and a 1D array for each outcome
- **alg** (*{'extra trees', 'random forest', 'univariate'}, optional*)
- **mode** (*{RuleInductionType.REGRESSION, RuleInductionType.CLASSIFICATION}, optional*)
- **kwargs** (*dict, optional*) – any remaining keyword arguments will be passed to the specific feature scoring algorithm

Return type
DataFrame instance

ema_workbench.analysis.feature_scoring.**get_rf_feature_scores**(*x*, *y*, *mode=RuleInductionType.CLASSIFICATION*, *nr_trees=250*, *max_features='sqrt'*, *max_depth=None*, *min_samples_split=2*, *min_samples_leaf=1*, *bootstrap=True*, *oob_score=True*, *random_state=None*)

Get feature scores using a random forest

Parameters

- **x** (*DataFram,e*)
- **y** (*1D nd.array*)
- **mode** (*{RuleInductionType.CLASSIFICATION, RuleInductionType.REGRESSION}*)
- **nr_trees** (*int, optional*) – nr. of trees in forest (default=250)
- **max_features** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
- **max_depth** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
- **min_samples** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
- **min_samples_leaf** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
- **bootstrap** (*bool, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
- **oob_score** (*bool, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
- **random_state** (*int, optional*) – see https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html

Returns

- *pandas DataFrame* – sorted in descending order of tuples with uncertainty and feature scores
- *object* – either RandomForestClassifier or RandomForestRegressor

ema_workbench.analysis.feature_scoring.**get_univariate_feature_scores**(*x*, *y*, *score_func=<function f_classif>*)

calculate feature scores using univariate statistical tests. In case of categorical data, chi square or the Anova F value is used. In case of continuous data the Anova F value is used.

Parameters

- **x** (*DataFrame*)
- **y** (*1D nd.array*)
- **score_func** (*{F_CLASSIFICATION, F_REGRESSION, CHI2}*) – the score function to use, one of f_regression (regression), or f_classification or chi2 (classification).

Returns
sorted in descending order of tuples with uncertainty and feature scores (i.e. p values in this case).

Return type
pandas DataFrame

plotting

this module provides functions for generating some basic figures. The code can be used as is, or serve as an example for writing your own code.

ema_workbench.analysis.plotting.**envelopes**(*experiments*, *outcomes*, *outcomes_to_show=None*, *group_by=None*, *grouping_specifiers=None*, *density=None*, *fill=False*, *legend=True*, *titles={}*, *ylabels={}*, *log=False*)

Make envelop plots.

An envelope shows over time the minimum and maximum value for a set of runs over time. It is thus to be used in case of time series data. The function will try to find a result labeled "TIME". If this is present, these values will be used on the X-axis. In case of Vensim models, TIME is present by default.

Parameters

- **experiments** (*DataFrame*)
- **outcomes** (*OutcomesDict*)
- **outcomes_to_show**
- **str** (*list of*)
- **str**
- **optional**
- **group_by** (*str, optional*) – name of the column in the experimentsto group results by. Alternatively, *index* can be used to use indexing arrays as the basis for grouping.
- **grouping_specifiers** (*iterable or dict, optional*) – set of categories to be used as a basis for grouping by. Grouping_specifiers is only meaningful if group_by is provided as well. In case of grouping by index, the grouping specifiers should be in a dictionary where the key denotes the name of the group.
- **density** (*{None, HIST, KDE, VIOLIN, BOXPLOT}, optional*)

- **fill** (*bool, optional*)
- **legend** (*bool, optional*)
- **titles** (*dict, optional*) – a way for controlling whether each of the axes should have a title. There are three possibilities. If set to None, no title will be shown for any of the axes. If set to an empty dict, the default, the title is identical to the name of the outcome of interest. If you want to override these default names, provide a dict with the outcome of interest as key and the desired title as value. This dict need only contain the outcomes for which you want to use a different title.
- **ylabels** (*dict, optional*) – way for controlling the ylabels. Works identical to titles.
- **log** (*bool, optional*) – log scale density plot

Returns

- **Figure** (*Figure instance*)
- **axes** (*dict*) – dict with outcome as key, and axes as value. Density axes' are indexed by the outcome followed by _density.

Note: the current implementation is limited to seven different categories in case of group_by, categories, and/or discretesize. This limit is due to the colors specified in COLOR_LIST.

Examples

```
>>> import util as util
>>> data = util.load_results(r'1000 flu cases.cPickle')
>>> envelopes(data, group_by='policy')
```

will show an envelope for three three different policies, for all the outcomes of interest. while

```
>>> envelopes(data, group_by='policy', categories=['static policy',
              'adaptive policy'])
```

will only show results for the two specified policies, ignoring any results associated with 'no policy'.

ema_workbench.analysis.plotting.**kde_over_time**(*experiments*, *outcomes*, *outcomes_to_show=None*, *group_by=None*, *grouping_specifiers=None*, *colormap='viridis'*, *log=True*)

Plot a KDE over time. The KDE is is visualized through a heatmap

Parameters

- **experiments** (*DataFrame*)
- **outcomes** (*OutcomesDict*)
- **outcomes_to_show** (*list of str, optional*) – list of outcome of interest you want to plot. If empty, all outcomes are plotted. **Note**: just names.
- **group_by** (*str, optional*) – name of the column in the cases array to group results by. Alternatively, *index* can be used to use indexing arrays as the basis for grouping.
- **grouping_specifiers** (*iterable or dict, optional*) – set of categories to be used as a basis for grouping by. Grouping_specifiers is only meaningful if group_by is provided

as well. In case of grouping by index, the grouping specifiers should be in a dictionary where the key denotes the name of the group.

- **colormap** (*str, optional*) – valid matplotlib color map name
- **log** (*bool, optional*)

Returns

- *list of Figure instances* – a figure instance for each group for each outcome
- *dict* – dict with outcome as key, and axes as value. Density axes' are indexed by the outcome followed by _density

ema_workbench.analysis.plotting.**lines**(*experiments*, *outcomes*, *outcomes_to_show=[]*, *group_by=None*, *grouping_specifiers=None*, *density=''*, *legend=True*, *titles={}*, *ylabels={}*, *experiments_to_show=None*, *show_envelope=False*, *log=False*)

This function takes the results from `perform_experiments()` and visualizes these as line plots. It is thus to be used in case of time series data. The function will try to find a result labeled "TIME". If this is present, these values will be used on the X-axis. In case of Vensim models, TIME is present by default.

Parameters

- **experiments** (*DataFrame*)
- **outcomes** (*OutcomesDict*)
- **outcomes_to_show** (*list of str, optional*) – list of outcome of interest you want to plot. If empty, all outcomes are plotted. **Note**: just names.
- **group_by** (*str, optional*) – name of the column in the cases array to group results by. Alternatively, *index* can be used to use indexing arrays as the basis for grouping.
- **grouping_specifiers** (*iterable or dict, optional*) – set of categories to be used as a basis for grouping by. Grouping_specifiers is only meaningful if group_by is provided as well. In case of grouping by index, the grouping specifiers should be in a dictionary where the key denotes the name of the group.
- **density** (*{None, HIST, KDE, VIOLIN, BOXPLOT}, optional*)
- **legend** (*bool, optional*)
- **titles** (*dict, optional*) – a way for controlling whether each of the axes should have a title. There are three possibilities. If set to None, no title will be shown for any of the axes. If set to an empty dict, the default, the title is identical to the name of the outcome of interest. If you want to override these default names, provide a dict with the outcome of interest as key and the desired title as value. This dict need only contain the outcomes for which you want to use a different title.
- **ylabels** (*dict, optional*) – way for controlling the ylabels. Works identical to titles.
- **experiments_to_show** (*ndarray, optional*) – indices of experiments to show lines for, defaults to None.
- **show_envelope** (*bool, optional*) – show envelope of outcomes. This envelope is the based on the minimum at each column and the maximum at each column.
- **log** (*bool, optional*) – log scale density plot

Returns

- **fig** (*Figure instance*)

- **axes** (*dict*) – dict with outcome as key, and axes as value. Density axes' are indexed by the outcome followed by _density.

Note: the current implementation is limited to seven different categories in case of group_by, categories, and/or discretesize. This limit is due to the colors specified in COLOR_LIST.

---

ema_workbench.analysis.plotting.**multiple_densities**(*experiments*, *outcomes*, *points_in_time=None*, *outcomes_to_show=None*, *group_by=None*, *grouping_specifiers=None*, *density=Density.KDE*, *legend=True*, *titles={}*, *ylabels={}*, *experiments_to_show=None*, *plot_type=PlotType.ENVELOPE*, *log=False*, ***kwargs*)

Make an envelope plot with multiple density plots over the run time

Parameters

- **experiments** (*DataFrame*)
- **outcomes** (*OutcomesDict*)
- **points_in_time** (*list*) – a list of points in time for which you want to see the density. At the moment up to 6 points in time are supported
- **outcomes_to_show** (*list of str, optional*) – list of outcome of interest you want to plot. If empty, all outcomes are plotted. **Note**: just names.
- **group_by** (*str, optional*) – name of the column in the cases array to group results by. Alternatively, *index* can be used to use indexing arrays as the basis for grouping.
- **grouping_specifiers** (*iterable or dict, optional*) – set of categories to be used as a basis for grouping by. Grouping_specifiers is only meaningful if group_by is provided as well. In case of grouping by index, the grouping specifiers should be in a dictionary where the key denotes the name of the group.
- **density** (*{Density.KDE, Density.HIST, Density.VIOLIN, Density.BOXPLOT},*) – optional
- **legend** (*bool, optional*)
- **titles** (*dict, optional*) – a way for controlling whether each of the axes should have a title. There are three possibilities. If set to None, no title will be shown for any of the axes. If set to an empty dict, the default, the title is identical to the name of the outcome of interest. If you want to override these default names, provide a dict with the outcome of interest as key and the desired title as value. This dict need only contain the outcomes for which you want to use a different title.
- **ylabels** (*dict, optional*) – way for controlling the ylabels. Works identical to titles.
- **experiments_to_show** (*ndarray, optional*) – indices of experiments to show lines for, defaults to None.
- **plot_type** (*{PlotType.ENVELOPE, PlotType.ENV_LIN, PlotType.LINES}, optional*)
- **log** (*bool, optional*)

Returns

- **fig** (*Figure instance*)

- **axes** (*dict*) – dict with outcome as key, and axes as value. Density axes' are indexed by the outcome followed by _density.

Note: the current implementation is limited to seven different categories in case of group_by, categories, and/or discretesize. This limit is due to the colors specified in COLOR_LIST.

Note: the connection patches are for some reason not drawn if log scaling is used for the density plots. This appears to be an issue in matplotlib itself.

---

pairs_plotting

This module provides R style pairs plotting functionality.

ema_workbench.analysis.pairs_plotting.**pairs_density**(*experiments*, *outcomes*, *outcomes_to_show=[]*, *group_by=None*, *grouping_specifiers=None*, *ylabels={}*, *point_in_time=-1*, *log=True*, *gridsize=50*, *colormap='coolwarm'*, *filter_scalar=True*)

Generate a R style pairs hexbin density multiplot. In case of time-series data, the end states are used.

hexbin makes hexagonal binning plot of x versus y, where x, y are 1-D sequences of the same length, N. If C is None (the default), this is a histogram of the number of occurrences of the observations at (x[i],y[i]). For further detail see matplotlib on hexbin

Parameters

- **experiments** (*DataFrame*)
- **outcomes** (*dict*)
- **outcomes_to_show** (*list of str, optional*) – list of outcome of interest you want to plot.
- **group_by** (*str, optional*) – name of the column in the cases array to group results by. Alternatively, *index* can be used to use indexing arrays as the basis for grouping.
- **grouping_specifiers** (*dict, optional*) – dict of categories to be used as a basis for grouping by. Grouping_specifiers is only meaningful if group_by is provided as well. In case of grouping by index, the grouping specifiers should be in a dictionary where the key denotes the name of the group.
- **ylabels** (*dict, optional*) – ylabels is a dictionary with the outcome names as keys, the specified values will be used as labels for the y axis.
- **point_in_time** (*float, optional*) – the point in time at which the scatter is to be made. If None is provided (default), the end states are used. point_in_time should be a valid value on time
- **log** (*bool, optional*) – indicating whether density should be log scaled. Defaults to True.
- **gridsize** (*int, optional*) – controls the gridsize for the hexagonal bining. (default = 50)
- **cmap** (*str*) – color map that is to be used in generating the hexbin. For details on the available maps, see pylab. (Defaults = coolwarm)

- **filter_scalar** (*bool, optional*) – remove the non-time-series outcomes. Defaults to True.

Returns

- *fig* – the figure instance
- *dict* – key is tuple of names of outcomes, value is associated axes instance

ema_workbench.analysis.pairs_plotting.**pairs_lines**(*experiments*, *outcomes*, *outcomes_to_show=[]*, *group_by=None*, *grouping_specifiers=None*, *ylabels={}*, *legend=True*, ***kwargs*)

Generate a R style pairs lines multiplot. It shows the behavior of two outcomes over time against each other. The origin is denoted with a circle and the end is denoted with a '+'.

Parameters

- **experiments** (*DataFrame*)
- **outcomes** (*dict*)
- **outcomes_to_show** (*list of str, optional*) – list of outcome of interest you want to plot.
- **group_by** (*str, optional*) – name of the column in the cases array to group results by. Alternatively, *index* can be used to use indexing arrays as the basis for grouping.
- **grouping_specifiers** (*dict, optional*) – dict of categories to be used as a basis for grouping by. Grouping_specifiers is only meaningful if group_by is provided as well. In case of grouping by index, the grouping specifiers should be in a dictionary where the key denotes the name of the group.
- **ylabels** (*dict, optional*) – ylabels is a dictionary with the outcome names as keys, the specified values will be used as labels for the y axis.
- **legend** (*bool, optional*) – if true, and group_by is given, show a legend.
- **point_in_time** (*float, optional*) – the point in time at which the scatter is to be made. If None is provided (default), the end states are used. point_in_time should be a valid value on time

Returns

- *fig* – the figure instance
- *dict* – key is tuple of names of outcomes, value is associated axes instance

ema_workbench.analysis.pairs_plotting.**pairs_scatter**(*experiments*, *outcomes*, *outcomes_to_show=[]*, *group_by=None*, *grouping_specifiers=None*, *ylabels={}*, *legend=True*, *point_in_time=-1*, *filter_scalar=False*, ***kwargs*)

Generate a R style pairs scatter multiplot. In case of time-series data, the end states are used.

Parameters

- **experiments** (*DataFrame*)
- **outcomes** (*dict*)
- **outcomes_to_show** (*list of str, optional*) – list of outcome of interest you want to plot.
- **group_by** (*str, optional*) – name of the column in the cases array to group results by. Alternatively, *index* can be used to use indexing arrays as the basis for grouping.

- **grouping_specifiers** (*dict, optional*) – dict of categories to be used as a basis for grouping by. Grouping_specifiers is only meaningful if group_by is provided as well. In case of grouping by index, the grouping specifiers should be in a dictionary where the key denotes the name of the group.
- **ylabels** (*dict, optional*) – ylabels is a dictionary with the outcome names as keys, the specified values will be used as labels for the y axis.
- **legend** (*bool, optional*) – if true, and group_by is given, show a legend.
- **point_in_time** (*float, optional*) – the point in time at which the scatter is to be made. If None is provided (default), the end states are used. point_in_time should be a valid value on time
- **filter_scalar** (*bool, optional*) – remove the non-time-series outcomes. Defaults to True.

Returns

- **fig** (*Figure instance*) – the figure instance
- **axes** (*dict*) – key is tuple of names of outcomes, value is associated axes instance
- *.. note:: the current implementation is limited to seven different* – categories in case of column, categories, and/or discretesize. This limit is due to the colors specified in COLOR_LIST.

parcoords

This module offers a general purpose parallel coordinate plotting Class using matplotlib.

class ema_workbench.analysis.parcoords.**ParallelAxes**(*limits*, *formatter=None*, *fontsize=14*, *rot=90*)

Base class for creating a parallel axis plot.

Parameters

- **limits** (*DataFrame*) – A DataFrame specifying the limits for each dimension in the data set. For categorical data, the first cell should contain all categories. See get_limits for more details.
- **formattter** (*dict , optional*) – dict with precision format strings for minima and maxima, use column name as key. If column is not present, or no formatter dict is provided, precision formatting defaults to .2f
- **fontsize** (*int, optional*) – fontsize for defaults text items
- **rot** (*float, optional*) – rotation of axis labels

limits

A DataFrame specifying the limits for each dimension in the data set. For categorical data, the first cell should contain all categories.

Type
DataFrame

recoding

non numeric columns are converting to integer variables

Type
dict

flipped_axes
set of Axes that are to be shown flipped

Type
set

axis_labels

Type
list of str

fontsize

Type
int

fig

Type
a matplotlib Figure instance

axes

Type
list of matplotlib Axes instances

ticklabels

Type
list of str

datalabels
labels associated with lines

Type
list of str

Notes

The basic setup of the Parallel Axis plot is a row of mpl Axes instances, with all whitespace in between removed. The number of Axes is the number of columns - 1.

invert_axis(*axis*)
flip direction for specified axis

Parameters
axis (*str or list of str*)

legend()
add a legend to the figure

plot(*data*, *color=None*, *label=None*, ***kwargs*)
plot data on parallel axes

Parameters

- **data** (*DataFrame or Series*)
- **color** (*valid mpl color, optional*)
- **label** (*str, optional*)

- **plot** (*any additional kwargs will be passed to matplotlib's*)
- **method.**
- **initializing** (*Data is normalized using the limits specified when*)
- **ParallelAxis.**

ema_workbench.analysis.parcoords.**get_limits**(*data*)

helper function to get limits of a FataFrame that can serve as input to ParallelAxis

Parameters
data (*DataFrame*)

Return type
DataFrame

b_and_w_plotting

This module offers basic functionality for converting a matplotlib figure to black and white. The provided functionality is largely determined by what is needed for the workbench.

ema_workbench.analysis.b_and_w_plotting.**set_fig_to_bw**(*fig*, *style='hatching'*, *line_style='continuous'*)

TODO it would be nice if for lines you can select either markers, gray scale, or simple black

Take each axes in the figure and transform its content to black and white. Lines are transformed based on different line styles. Fills such as can be used in *meth*:envelopes are gray-scaled. Heathmaps are also gray-scaled.

derived from and expanded for my use from: https://stackoverflow.com/questions/7358118/matplotlib-black-white-colormap-with-dashes-dots-etc

Parameters

- **fig** (*figure*) – the figure to transform to black and white
- **style** (*{HATCHING, GREYSCALE}*) – parameter controlling how collections are transformed.
- **line_style** (*str, {'continuous', 'black', None}*)

plotting_util

Plotting utility functions

ema_workbench.analysis.plotting_util.**COLOR_LIST = [(0.12156862745098039, 0.4666666666666667, 0.7058823529411765), (1.0, 0.4980392156862745, 0.054901960784313725), (0.17254901960784313, 0.6274509803921569, 0.17254901960784313), (0.8392156862745098, 0.15294117647058825, 0.1568627450980392), (0.5803921568627451, 0.403921568627451, 0.7411764705882353), (0.5490196078431373, 0.3372549019607843, 0.29411764705882354), (0.8901960784313725, 0.4666666666666667, 0.7607843137254902), (0.4980392156862745, 0.4980392156862745, 0.4980392156862745), (0.7372549019607844, 0.7411764705882353, 0.13333333333333333), (0.09019607843137255, 0.7450980392156863, 0.8117647058823529)]**

Default color list

class ema_workbench.analysis.plotting_util.**Density**(*value*, *names=None*, **values*, *module=None*, *qualname=None*, *type=None*, *start=1*, *boundary=None*)

Enum for different types of density plots

BOXENPLOT = 'boxenplot'

constant for plotting density as a boxenplot

BOXPLOT = 'boxplot'

constant for plotting density as a boxplot

HIST = 'hist'

constant for plotting density as a histogram

KDE = 'kde'

constant for plotting density as a kernel density estimate

VIOLIN = 'violin'

constant for plotting density as a violin plot, which combines a Gaussian density estimate with a boxplot

class ema_workbench.analysis.plotting_util.**LegendEnum**(*value*, *names=None*, **values*, *module=None*, *qualname=None*, *type=None*, *start=1*, *boundary=None*)

Enum for different styles of legends

class ema_workbench.analysis.plotting_util.**PlotType**(*value*, *names=None*, **values*, *module=None*, *qualname=None*, *type=None*, *start=1*, *boundary=None*)

ENVELOPE = 'envelope'

constant for plotting envelopes

ENV_LIN = 'env_lin'

constant for plotting envelopes with lines

LINES = 'lines'

constant for plotting lines

scenario_discovery_util

Scenario discovery utilities used by both `cart` and `prim`

class ema_workbench.analysis.scenario_discovery_util.**RuleInductionType**(*value*, *names=None*, **values*, *module=None*, *qualname=None*, *type=None*, *start=1*, *boundary=None*)

BINARY = 'binary'

constant indicating binary classification mode. This is the most common used mode in scenario discovery

CLASSIFICATION = 'classification'

constant indicating classification mode

REGRESSION = 'regression'

constant indicating regression mode

1.14.4 Util

ema_exceptions

Exceptions and warning used internally by the EMA workbench. In line with advice given in PEP 8.

exception ema_workbench.util.ema_exceptions.**CaseError**(*message*, *case*, *policy=None*)

error to be used when a particular run creates an error. The character of the error can be specified as the message, and the actual case that gave rise to the error.

exception ema_workbench.util.ema_exceptions.**EMAError**(**args*)

Base EMA error

exception ema_workbench.util.ema_exceptions.**EMAParallelError**(**args*)

parallel EMA error

exception ema_workbench.util.ema_exceptions.**EMAWarning**(**args*)

base EMA warning class

ema_logging

This module contains code for logging EMA processes. It is modeled on the default logging approach that comes with Python. This logging system will also work in case of multiprocessing.

ema_workbench.util.ema_logging.**get_rootlogger**()

Returns root logger used by the EMA workbench

Return type
the logger of the EMA workbench

ema_workbench.util.ema_logging.**log_to_stderr**(*level=None*, *pass_root_logger_level=False*)

Turn on logging and add a handler which prints to stderr

Parameters

- **level** (*int*) – minimum level of the messages that will be logged
- **pas_root_logger_level** (*bool, optional. Default False*) – if true, all module loggers will be set to the same logging level as the root logger. Recommended True when using the MPIEvaluator.

ema_workbench.util.ema_logging.**temporary_filter**(*name='EMA'*, *level=0*, *functname=None*)

temporary filter log message

Parameters

- **name** (*str or list of str, optional*) – logger on which to apply the filter.
- **level** (*int, or list of int, optional*) – don't log message of this level or lower
- **funcname** (*str or list of str, optional*) – don't log message of this function
- **logger** (*all modules have their own unique*)
- **ema_workbench.analysis.prim)** ((*e.g.*)

utilities

This module provides various convenience functions and classes.

ema_workbench.util.utilities.**load_results**(*file_name*)

load the specified bz2 file. the file is assumed to be saves using save_results.

Parameters
file_name (*str*) – the path to the file

Raises
IOError if file not found –

ema_workbench.util.utilities.**merge_results**(*results1*, *results2*)

convenience function for merging the return from `perform_experiments()`.

The function merges results2 with results1. For the experiments, it generates an empty array equal to the size of the sum of the experiments. As dtype is uses the dtype from the experiments in results1. The function assumes that the ordering of dtypes and names is identical in both results.

A typical use case for this function is in combination with `experiments_to_cases()`. Using `experiments_to_cases()` one extracts the cases from a first set of experiments. One then performs these cases on a different model or policy, and then one wants to merge these new results with the old result for further analysis.

Parameters

- **results1** (*tuple*) – first results to be merged
- **results2** (*tuple*) – second results to be merged

Return type
the merged results

ema_workbench.util.utilities.**process_replications**(*data*, *aggregation_func=<function mean>*)

Convenience function for processing the replications of a stochastic model's outcomes.

The default behavior is to take the mean of the replications. This reduces the dimensionality of the outcomes from (experiments * replications * outcome_shape) to (experiments * outcome_shape), where outcome_shape is 0-d for scalars, 1-d for time series, and 2-d for arrays.

The function can take either the outcomes (dictionary: keys are outcomes of interest, values are arrays of data) or the results (tuple: experiments as DataFrame, outcomes as dictionary) of a set of simulation experiments.

Parameters

- **data** (*dict, tuple*) – outcomes or results of a set of experiments
- **aggregation_func** (*callabale, optional*) – aggregation function to be applied, defaults to np.mean.

Return type
dict, tuple

ema_workbench.util.utilities.**save_results**(*results*, *file_name*)

save the results to the specified tar.gz file.

The way in which results are stored depends. Experiments are saved as csv. Outcomes depend on the outcome type. Scalar, and <3D arrays are saved as csv files. Higher dimensional arrays are stored as .npy files.

Parameters

- **results** (*tuple*) – the return of perform_experiments

- **file_name** (*str*) – the path of the file

Raises
IOError if file not found –

1.15 Indices and tables

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