Scaling up complexity

Big data tools for Physics and Astronomy, CWI Amsterdam

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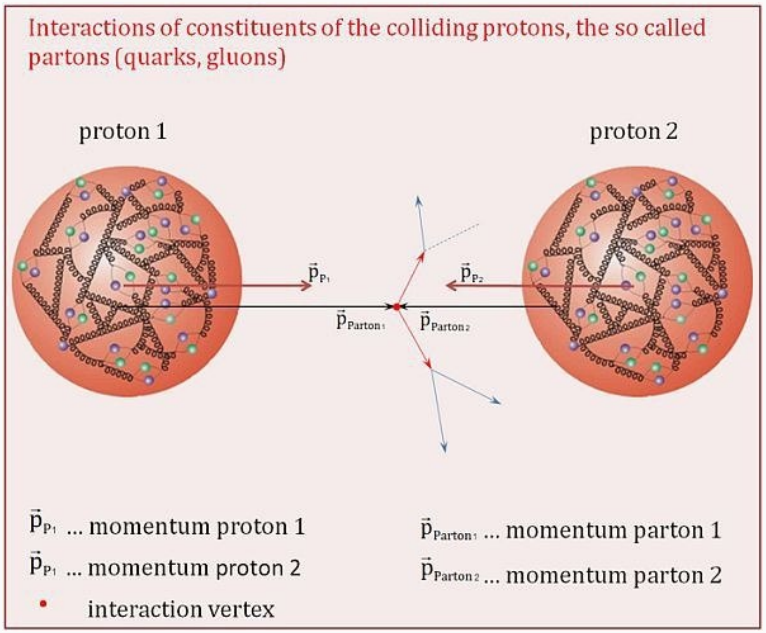
UNIVERSITA
DEGLI STUDI
DI TORINO

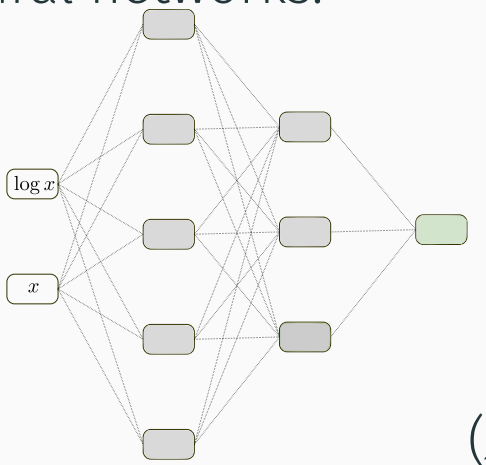
NNPDF in two slides

- I work in the NNPDF collaboration.
- We provide predictions for LHC processes. Specifically, we determine the *Parton Distribution functions* of the proton.
- Think of it as the probability density of sampling given quark or a gluon with a momentum p_{parton_1} (+quantum corrections).



NNPDF innovations related to statistical learning[1]

- Do not assume an overly restricted model for the PDFs. Paramterize them with neural networks.



$$pdf(x, Q_0) = Cx^{-\alpha}(1-x)^{\beta} \times \qquad (x = p_{\text{parton1}}/p_{p1})$$

- A method to propagate uncertainty on the experimental inputs: Psudorreplica sampling.
- A method to validate the methodology: Closure testing.

[1] See talk on IML workshop last Friday

Motivating example: NNPDF 3.1

- NNPDF 3.0 released at the end of 2014.
- NNPDF 3.1 (released last month arxiv:1706.00428) was planned as a small update:
  - Add a bunch of new data (mostly for LHC experiments)
  - Improvement in methodology (fitting the charm quark PDF).
- How difficult can it be?
  - *A lot*![2] LHC data provide very precise constraints.
  - At this precision a lot of previously neglected effects become important (think interpolation accuracy, Monte Carlo integration).
- Problem not fundamentally different but requires more complex scrutiny.
- Need to test compare and understand precisely all our inputs
  $\longrightarrow$ Need powerful analysis code.

[2] See talk at HiggsTools Turin last month

This talk

Alternative title *“How I wanted to make a plotting tool and ended up building a compiler”*

What we want

- Flexible analysis framework.

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- Flexible analysis framework.
  - *Plot X as a function of Y without many assumptions on what they are.*
- High level declarative input: *What you want, not how.*
- Initialization stage: Check all the inputs
- Results as reproducible and backwards compatible as possible.
- Loops are important. Make them first class.

Reportengine

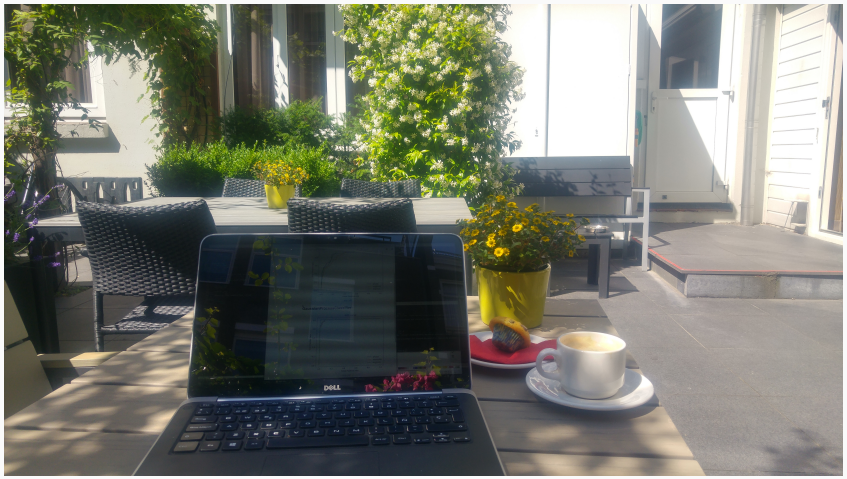
https://github.com/NNPDF/reportengine

A *framework* for scientific code.

- Advanced configuration parser.
- Call graph generator and executor.
- Supports for contracts.
- General command support (e.g. colors, error handlers).
- A report application built on top of it.
- How difficult can be?

The Iris flower dataset

- 150 samples from 3 species of *Iris flowers*, from a single pasture in the Gaspé Peninsula.
- Measured 4 features: Sepal width and height, petal width and height.
- Popularized by Fisher, in works on Linear Discriminant analysis.



Example application: flowers

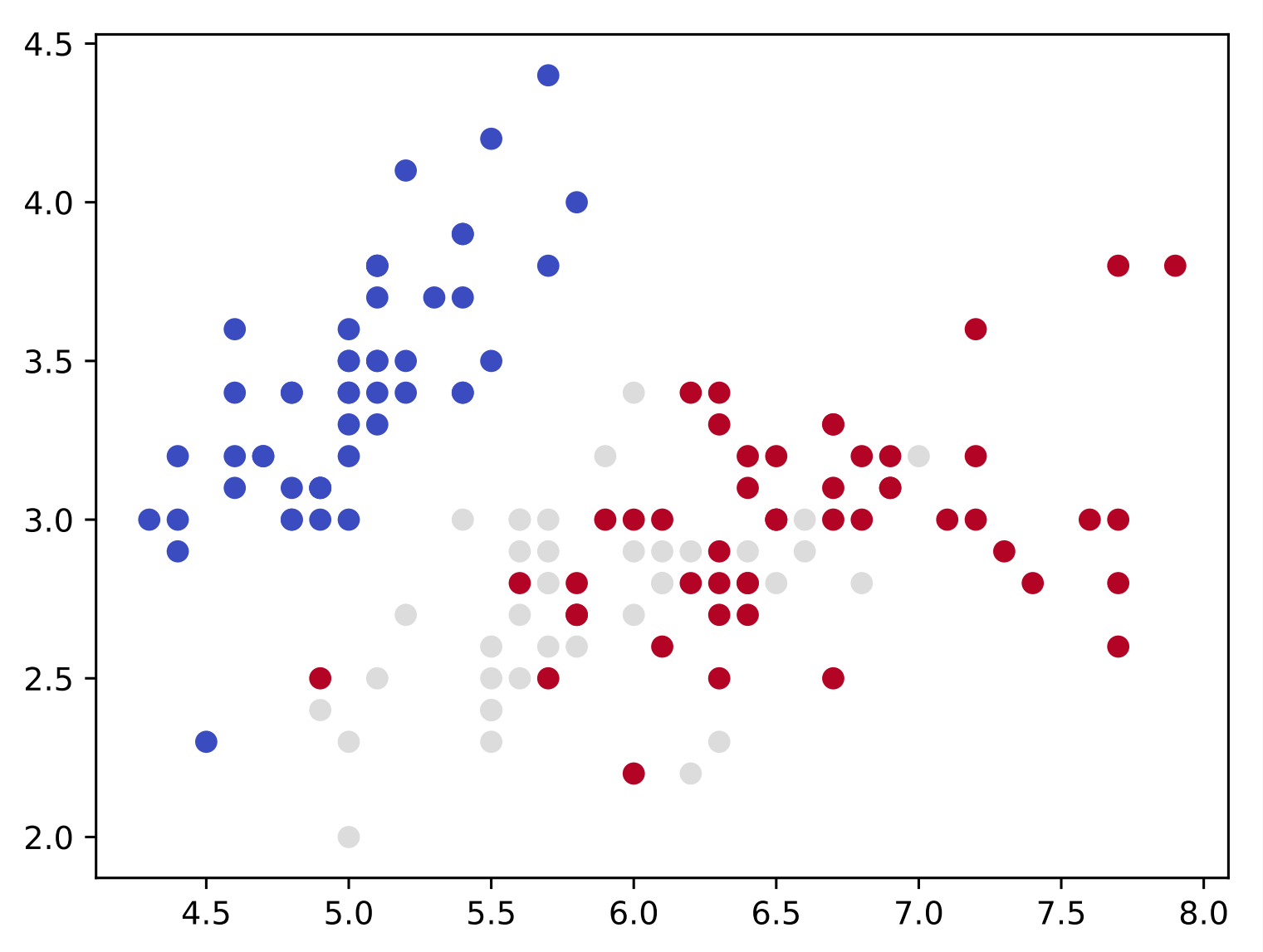
- An example app to study the IRIS dataset.
- Objectives:
  - Demonstrate design requirements and main features of the framework.
  - Examples that fit on a slide.
- Non objectives:
  - Usefulness.
  - Nice plots.
- Using scikits-learn because it has a nice API.

Simple input

```
#input.yaml
xaxis: "sepal length (cm)"
yaxis: "sepal width (cm)"

actions_:
    - - plot_2d
```

Simple output



Let’s implement it all!

A little boilerplate

```
#flowers/app.py An IRIS study application
from reportengine.app import App
from reportengine.report import Config
from reportengine.configparser import ConfigError
class FlowersConfig(Config):
    ...
class FlowersApp(App):
    config_class = FlowersConfig
def main():
    a = FlowersApp(name="Flowers",
        default_providers=['flowers.actions',
        'reportengine.report'])
    a.main()

if __name__ == '__main__':
    main()
```

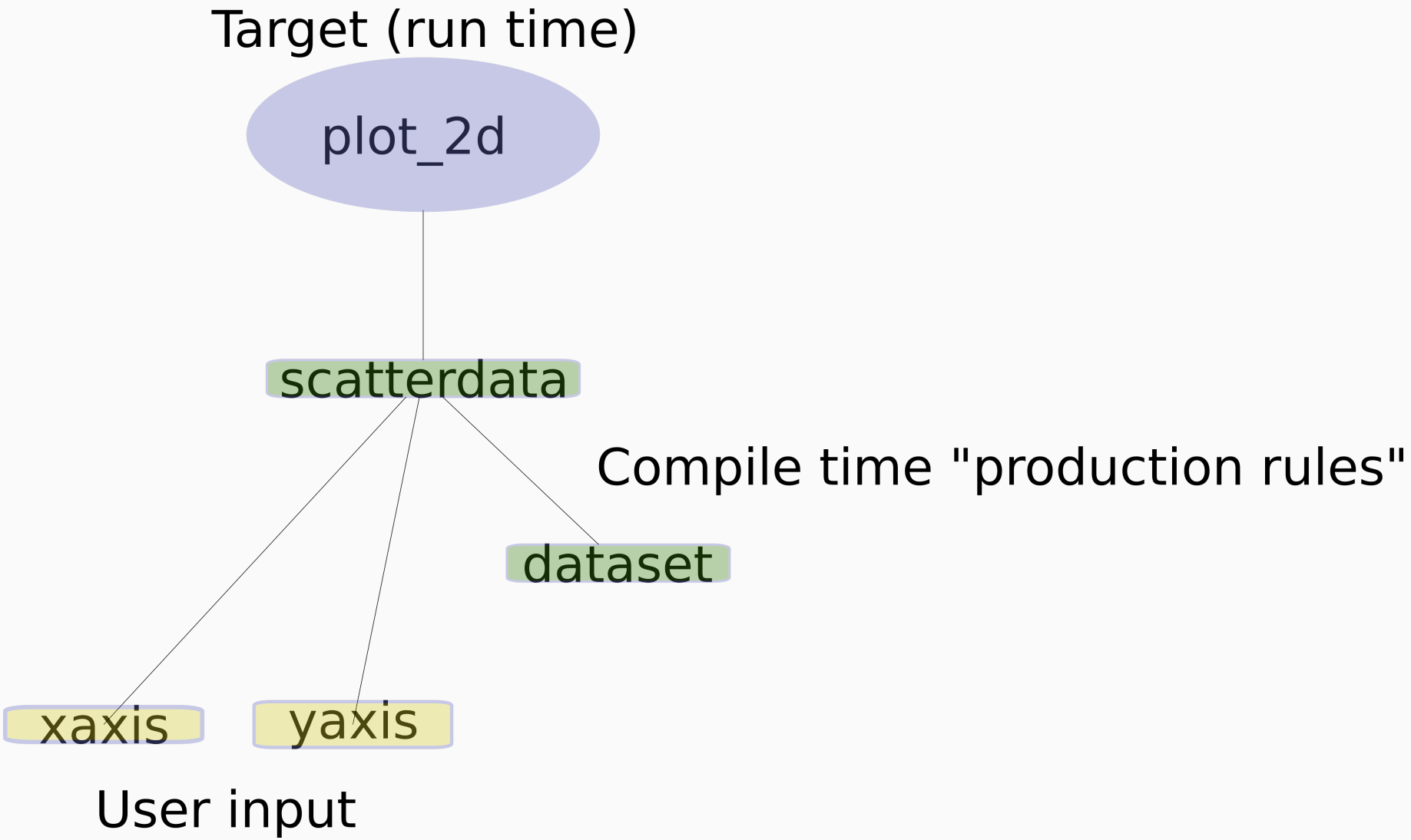
Basic API elements

- Config class
  - “Compile time” functionality. Parses inputs and generates resources before the slow functions run.
  - Two types of functions:

    Input parsers “parse_<KEY>” Take KEY as argument from the input card and produce a result.

    Production rules “produce_<KEY>” take zero or more inputs and produce the resource KEY based on them.
- Provider modules
  - Just normal python modules!
  - Containing functions executed at runtime.

Compilation and execution plan



Argument binding by name

- In reportengine *f*(*argname*), means that to execute *f* we must find a resource called *argname*
- *argname* Could be
  - An input parameter
  - A production rule
  - A runtime function

Config

```
class FlowersConfig(Config):
    def produce_dataset(self):
        """Produce the IRIS dataset"""
        return sklearn.datasets.load_iris()
    def parse_xaxis(self, feature:str):
        """Feature in the X axis"""
        return feature
    def parse_yaxis(self, feature:str):
        """Feature in the Y axis"""
        return feature
    def produce_scatterdata(self, dataset, xaxis, yaxis):
        """Check that features exist and return the data values"""
        def ind(name):
            try:
                 return dataset.feature_names.index(name)
            except ValueError as e:
                raise ConfigError(f'No such feature', bad_item=name,
                    alternatives=dataset.feature_names) from e
        i,j = ind(xaxis), ind(yaxis)
        return dataset.data[:, i], dataset.data[:,j], dataset.target
```

Provider

```
#flowers/actions.py Tools to analyze the IRIS dataset
from reportengine.figure import figure
@figure
def plot_2d(scatterdata):
    """Generate scatter plot of the values of xaxis vs yaxis"""
    x,y,category = scatterdata
    fig, ax = plt.subplots()
    ax.scatter(x,y, c=category, cmap=plt.cm.coolwarm)
    return fig
```

Done!

```
$ flowers input.yaml  -o output
[INFO]: All requirements processed and checked successfully.
Executing actions.
$ ls output/figures/
plot_2d.pdf  plot_2d.png
```

Much more than giving the correct result: Errors

```
$ cat typo.yaml
xaxis: "sepal lenght (cm)"
yaxis: "sepal width (cm)"
actions_:
    - - plot_2d
$ flowers typo.yaml
[ERROR]: Bad configuration encountered:
No such feature
Instead of 'sepal lenght (cm)', did you mean one of the following?
 - sepal length (cm)
 - petal length (cm)
 - sepal width (cm)

$ head -1 badtype.yaml
xaxis: 43
$ flowers badtype.yaml
[ERROR]: Bad configuration encountered:
Bad input type for parameter 'xaxis': Value '43' is not of type
str, but of type 'int'.
```

Much more than giving the correct result: Help

```
$ flowers --help plot_2d
Defined in: flowers.actions
Generates: figure
plot_2d(scatterdata)
Generate scatter plot of the values of xaxis vs yaxis
The following resources are read from the configuration:
    xaxis(str): Feature in the X axis   [Used by scatterdata]
    yaxis(str): Feature in the Y axis   [Used by scatterdata]
```

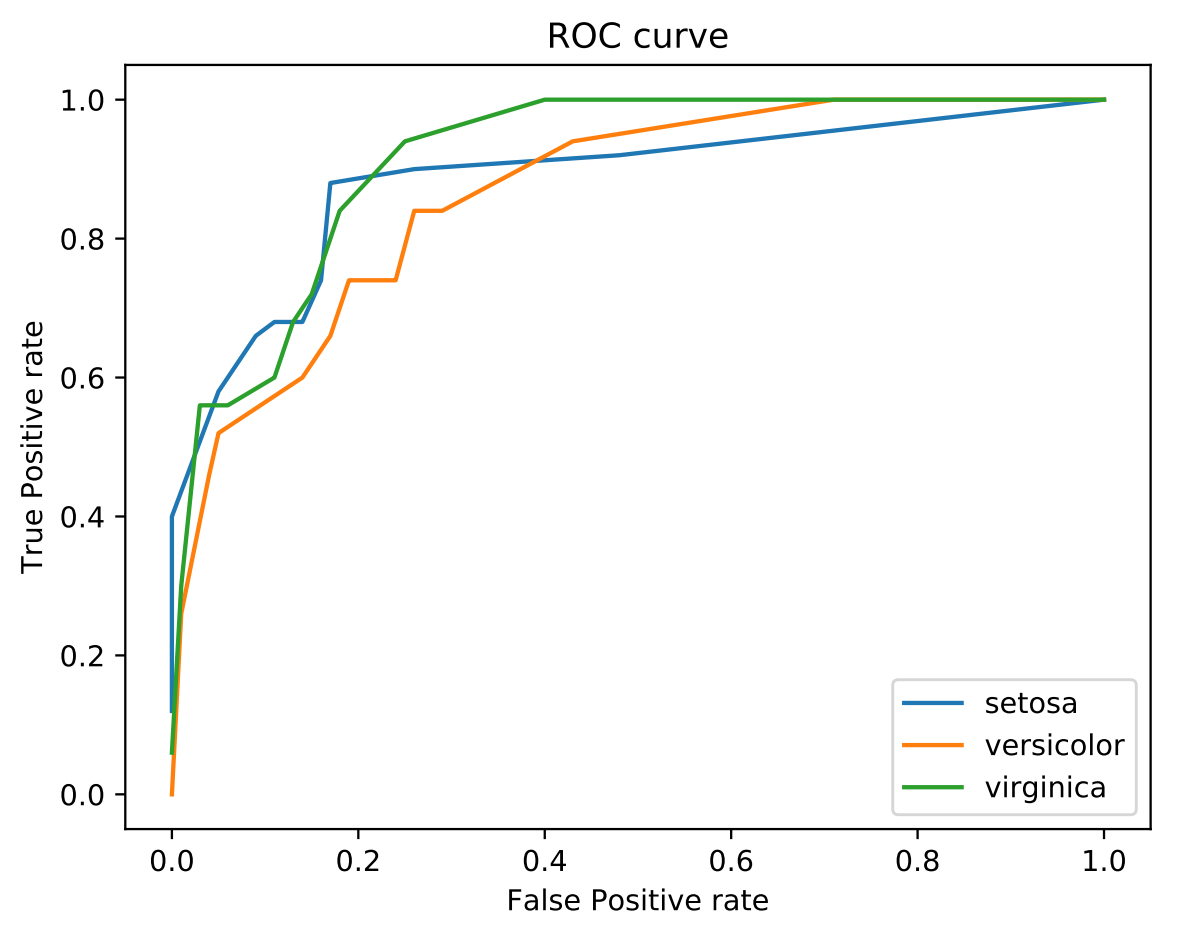
```
#app.py
ALGORITHMS = {
    'svc': sklearn.svm.SVC,
    'gp': sklearn.gaussian_process.GaussianProcessClassifier,
    'random_forest': sklearn.ensemble.RandomForestClassifier
}
#class Config
    def parse_algorithm(self, alg:str):
        """The name of the classification algorithms"""
        ...

#actions.py
def fit_result(algorithm, dataset):
    """Fit to a sample of the dataset where some labels have been
    shuffled  using the default algorithm
    parameters"""
    ...

@figure
def plot_roc(fit_result, algorithm, dataset):
    ...
```

Random Forest ROC curve

```
$ cat input.yaml
algorithm: random_forest
actions_:
    - - plot_roc
$ flowers input.yaml
```



Support vector: Crash!

```
$ cat input.yaml
algorithm: svc
actions_:
    - - plot_roc
$ flowers input.yaml
[INFO]: All requirements processed and checked successfully.
Executing actions.
----
Traceback (most recent call last):
...
AttributeError: predict_proba is not available when
probability=False
----
[CRITICAL]: A critical error oucurred. It has been logged in
/tmp/Flowers-crash-svp6cymq
```

What happened

- Support Vector Machines is (by default) a categorical classifier so the ROC curve doesn't make sense.
- Fitting the data itself makes perfect sense, but the ROC action should require probabilistic algorithms.
    - Let's assume we don't want to use the probabilistic version of SVC.
- We should require it at initialization time, not after the expensive fitting.

Contracts

- Executed at initialization time.
- Can execute arbitrary logic on whatever is known at that moment.

```
from reportengine.checks import make_argcheck, CheckError
@make_argcheck
def _check_can_predict_probabilities(algorithm):
    res = hasattr(algorithm().fit([[0],[1]], [0,1]), 'predict_proba')
    if not res:
        raise CheckError(f"Algorithm {algorithm.__name__}"
            "doesn't support 'predict_proba'")

@figure
@_check_can_predict_probabilities
def plot_roc(fit_result, algorithm, dataset):
    ...
```

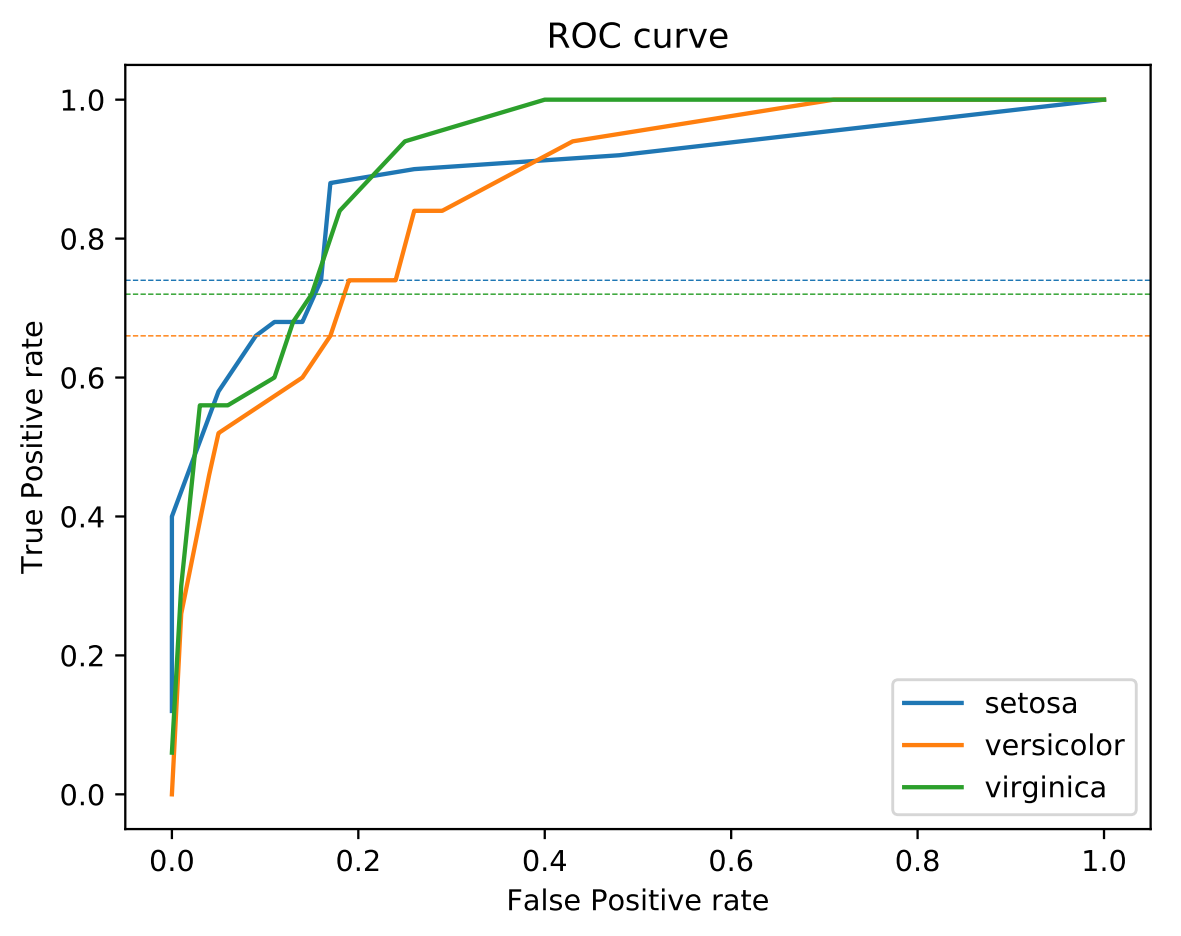
Parameters

- Read from input directly.
- Automatically type checked.
- Can have defaults, and further checks.

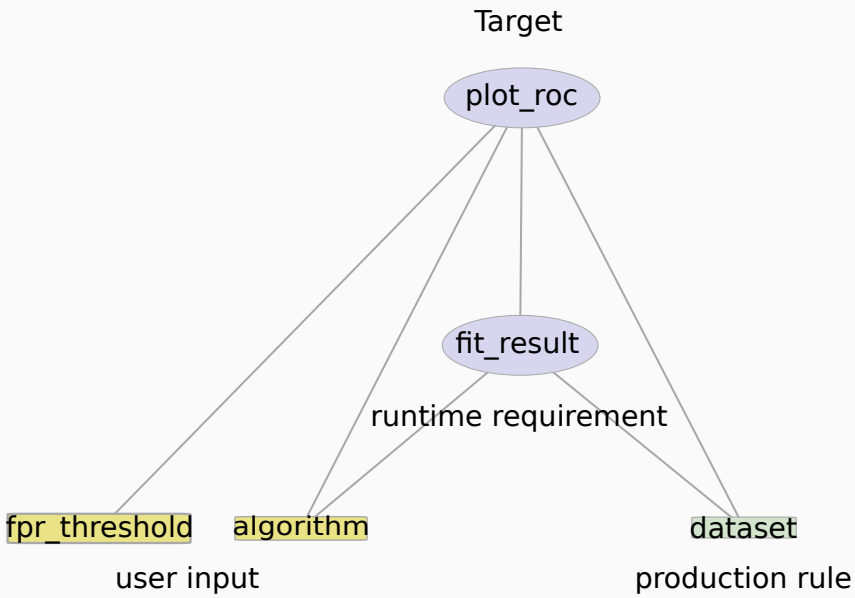
```
@make_argcheck
def _check_fpr_threshold(fpr_threshold):
    """Check that it's in (0,1) if given"""
    ...
@figure
@_check_fpr_threshold
@_check_can_predict_probabilities
def plot_roc(fit_result, algorithm, dataset,
        fpr_threshold:(float, type(None))=None):
    """Plot the ROC curve for each category. Mark the true positive
    rate at the ``fpr_threshold`` if given"""
    ...
```

Plot with parameter

```
#input.yaml
fpr_threshold: 0.15
algorithm: random_forest
actions_:
    - - plot_roc
```



Graph building and execution



Roughly when a runtime node is required:

1. Find requirements.
2. Verify requirements recursively.
3. Execute checks (contracts).
4. Requirement is satisfied.

Execute runtime nodes (in dependency order) when all *targets* (user requested actions) have been verified.

Loops and reports. But which algorithm is better?

- We would like to find out whether Gaussian Processes or Random Forests produce a better ROC curve.
  - We want to compute it for each.
  - Need a way to express loops (and in general namespaces) in a declarative way.
- We would like to see the results organized together.

Report application

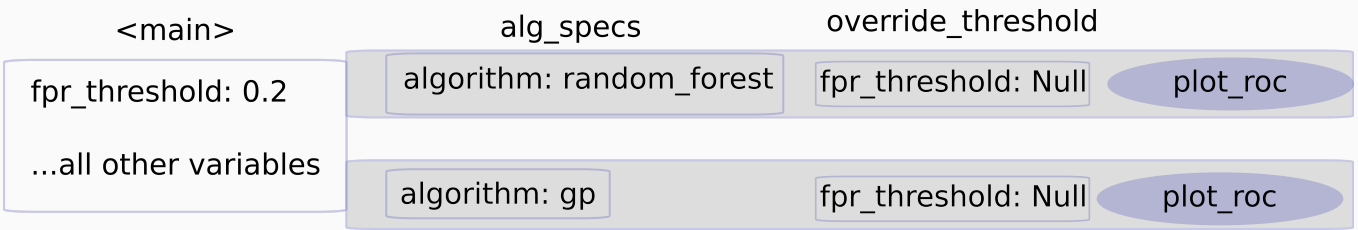
- Special tags {@@} are evaluated and used to infer *targets*.
- Targets are validated and then executed, just as described.
- Text is substituted, and the resulting *markdown* is passed to PANDOC to generate HTML.

An example

```
fpr_threshold: 0.2
#any name
override_threshold:
    fpr_threshold: Null
#any name
alg_specs:
    - algorithm: random_forest
    - algorithm: gp
template_text: |
    % IRIS dataset with some shuffled labels
    % Zahari Kassabov
    {@with alg_specs::override_threshold@}
    {@algorithm@}
    ------------
    {@plot_roc@}
    {@endwith@}
actions_:
    - - report:
            main: True
```

Stack frame aggregation

- Associate a list of elements to each target:
  - This is what “{@with ...@}” does. E.g. plot_roc is “associated” to [’alg_specs’, ’override_threshold’]
- If an element:
  - is a mapping, push its variables to the stack
  - is a list of mappings, do the Cartesian product and execute the action for each possible stack.
- Repeat the text between {@with ...@} and {@endwith@} for each possibility.



Output

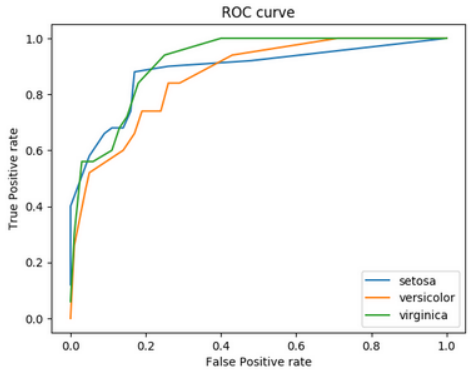
file:///home/zah/phd/reportengine/example/output/index.html 67% Search

IRIS dataset with some shuffled labels

Zahari Kassabov

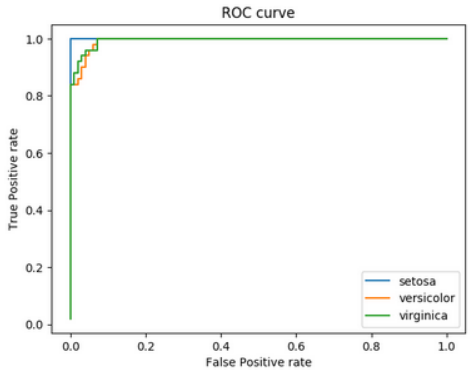
- RandomForestClassifier
- GaussianProcessClassifier

RandomForestClassifier



.png .pdf

GaussianProcessClassifier



.png .pdf

Powered by reportengine

Automatic lists

- If we know how to parse X, we know how to parse a list of X!

```
from reportengine.configparser import element_of
#class Config
    @element_of('algorithms')
    def parse_algorithm(self, alg:str):
        """The name of the classification algorithms"""
        ...
```

- Can shorten “alg_specs” from before:

```
algorithms:
  - random_forest
  - gp
```

Putting things together

```
from reportengine import collect
fit_results = collect(fit_result, ['algorithms'])
```

“Execute fit_result for each namespace in [’algorithms’] and put the flattened result in a list”

```
import pandas as pd
from sklearn.metrics import hamming_loss
from reportenfine.table import table
@table
def hamming_loss_table(algorithms, fit_results, dataset):
    records = []
    for algorithm, res in zip(algorithms, fit_results):
        records.append({'algorithm': algorithm.__name__, "Hamming "
                "loss": hamming_loss(dataset.target,
                    res.predict(dataset.data))})
    return pd.DataFrame(records)
```

Simple input

```
#report.yaml
algorithms:
    - random_forest
    - gp

template_text: |
    % IRIS dataset with some shuffled labels
    % Zahari Kassabov
    Hamming loss
    ============
    {@hamming_loss_table@}
    ROC curves
    ==========
    {@with algorithms@}
    {@algorithm@}
    ------------
    {@plot_roc@}
    {@endwith@}

actions_:
    - - report:
            main: True
```

Complex output

file:///home/zah/phd/reportengine/example/output/index.html 90% Search

IRIS dataset with some shuffled labels — Zahari Kassabov

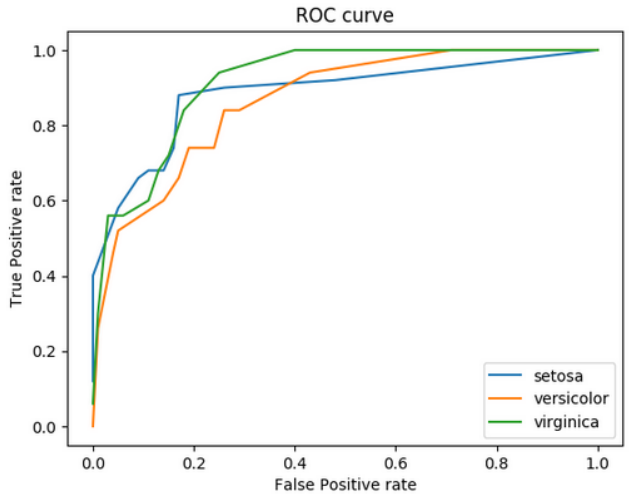
- Hamming loss
- ROC curves
  - RandomForestClassifier
  - GaussianProcessClassifier

Hamming loss

	Hamming loss	algorithm
0	0.313333	RandomForestClassifier
1	0.046667	GaussianProcessClassifier

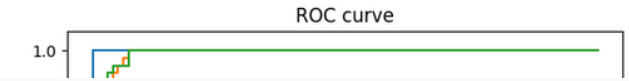
ROC curves

RandomForestClassifier



.png .pdf

GaussianProcessClassifier



Thank you!