Bayesian optimization with Scikit-Optimize

Gilles Louppe

@glouppe NYU

PyData Amsterdam 2017

Pause café?

You have an espresso machine with many buttons and knobs to tweak.

Your task is to **brew the best cup of espresso** before dying of caffeine overdose.

$$x^* = \arg\max_x f(x)$$

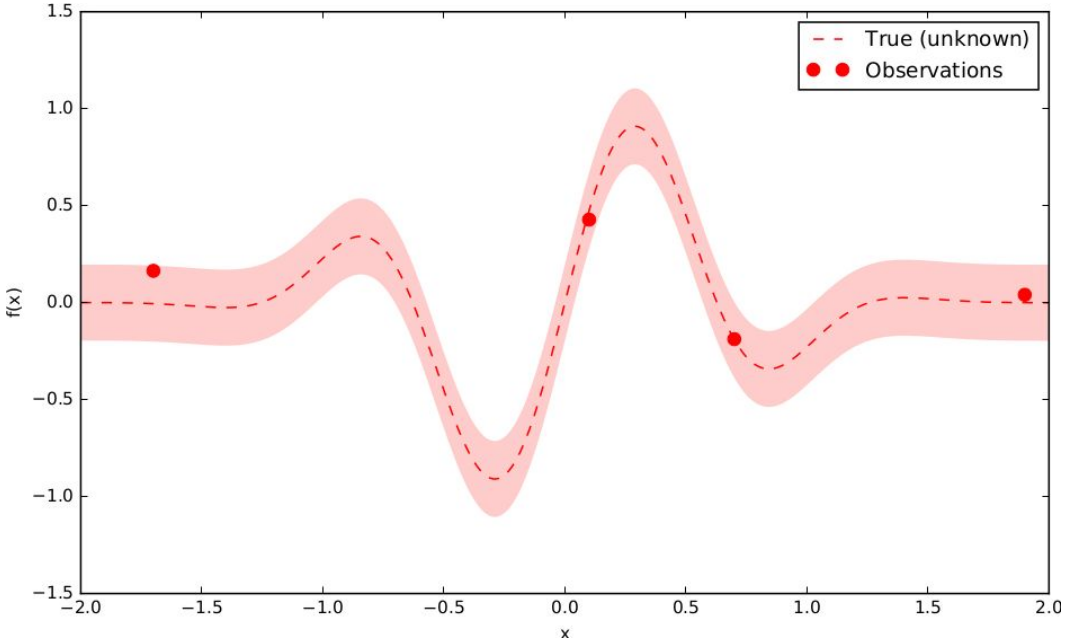
- f is a black box function, with no closed form nor gradients.
- f is expensive to evaluate.
- You may only have noisy observations of f.

If you do not have these constraints, **do not** use Bayesian optimization.

Bayesian optimisation, step-by-step

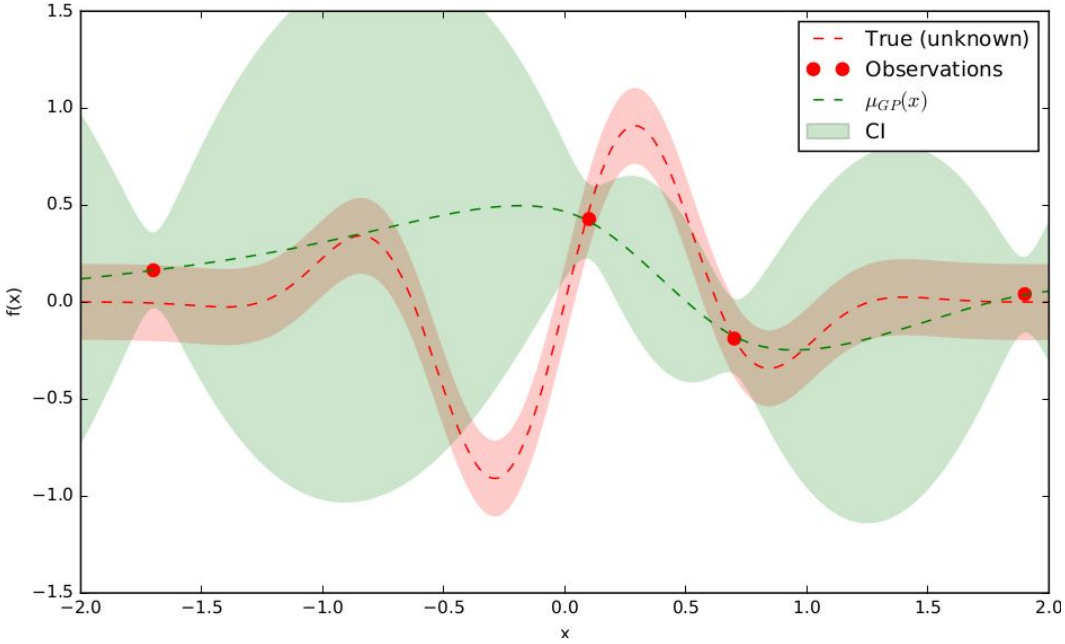
Start with observations of the objective f:

$$\{(x_i, f(x_i))|i = 1, \ldots, t\}$$



Bayesian optimisation, step-by-step

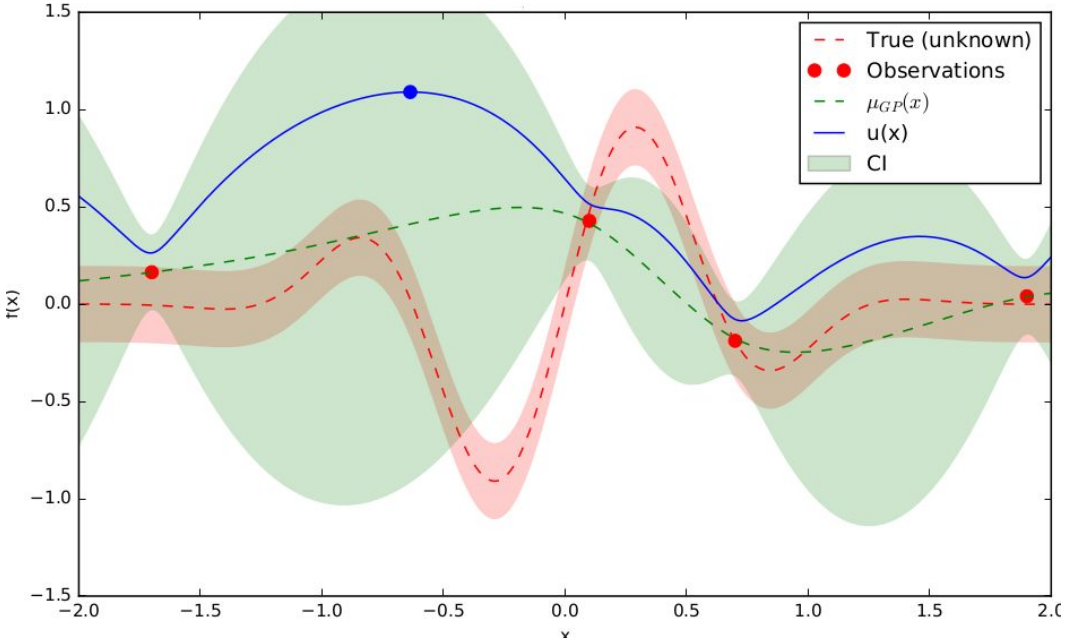
Build a probabilistic model for f (typically, a Gaussian process).



Bayesian optimisation, step-by-step

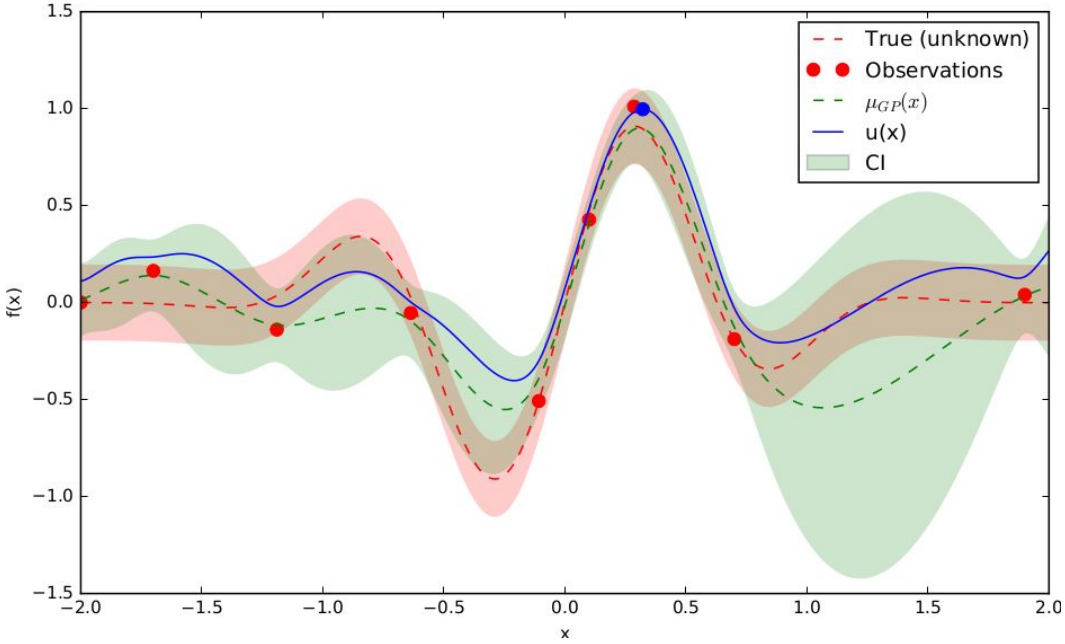
Optimize a cheap utility function u based on the posterior distribution for sampling the next point.

$$x_{t+1} = \arg\max_x u(x)$$



Bayesian optimisation, step-by-step

Evaluate f and repeat.



What is Bayesian about Bayesian optimization?

- The unknown objective is considered as a *random function* (a stochastic process) on which we place a **prior** (here defined by a Gaussian process capturing our beliefs about the function behaviour).

- Function evaluations are treated as data and used to update the prior to form the **posterior** distribution over the objective function.

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Scikit-Optimize

A simple library for black-box optimization with a `scipy.optimize` interface.

Sprouted from a (never-ending) Scikit-Learn pull request.

https://scikit-optimize.github.io

```
pip install scikit-optimize
```

Objective function

- Takes a list of values as argument.
- Returns a scalar (the lower, the better)

```
from sklearn.datasets import load_boston
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.model_selection import cross_val_score

boston = load_boston()
X, y = boston.data, boston.target

def objective(params):
    # Unpack parameters
    learning_rate = 10. ** params[0]
    max_depth = params[1]
    min_samples_split = params[2]
    max_features = params[3]

    # Build regressor
    reg = GradientBoostingRegressor(
        n_estimators=50,
        learning_rate=learning_rate,
        max_depth=max_depth,
        min_samples_split=min_samples_split,
        max_features=max_features,
        random_state=1)

    # The lower the better
    return -np.mean(cross_val_score(reg, X, y, cv=5, n_jobs=-1,
                                    scoring="neg_mean_absolute_error"))
```

Minimize

- Takes the objective function and the bounds of the parameter space.
- That's it!

- The `r` tuple contains all the results (final and intermediate).

```
from skopt import gp_minimize

space  = [(-5.0, 0.0),      # learning_rate
          (1, 5),           # max_depth
          (2, 100),         # min_samples_split
          (1, X.shape[1])]  # max_features

r = gp_minimize(objective, space, n_calls=50, random_state=1)
```

```
r.x
```

```
[-0.96542858133704623, 5, 9, 7]
```

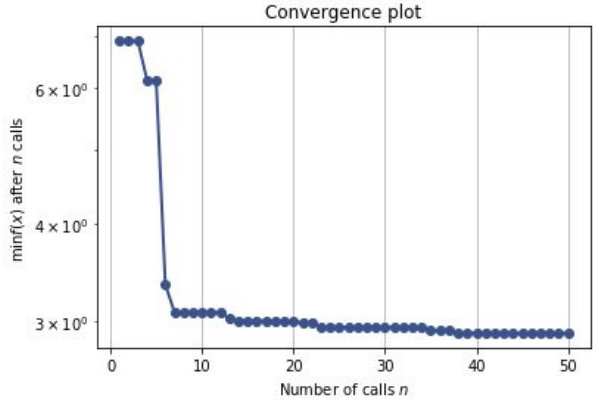
```
r.fun
```

```
2.8944939733595256
```

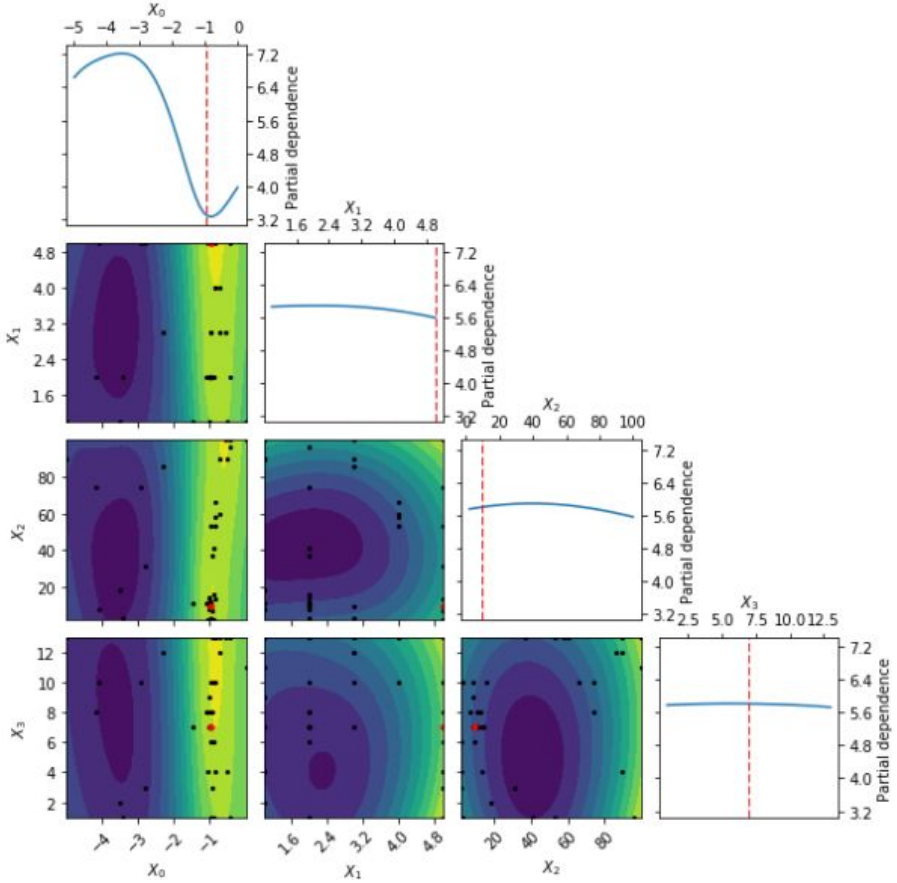
Visualization

- Convergence plot
- Pairwise partial dependence plot of the surrogate objective.

```
from skopt.plots import plot_convergence
plot_convergence(r, yscale="log")
```




```
from skopt.plots import plot_objective
plot_objective(r)
```

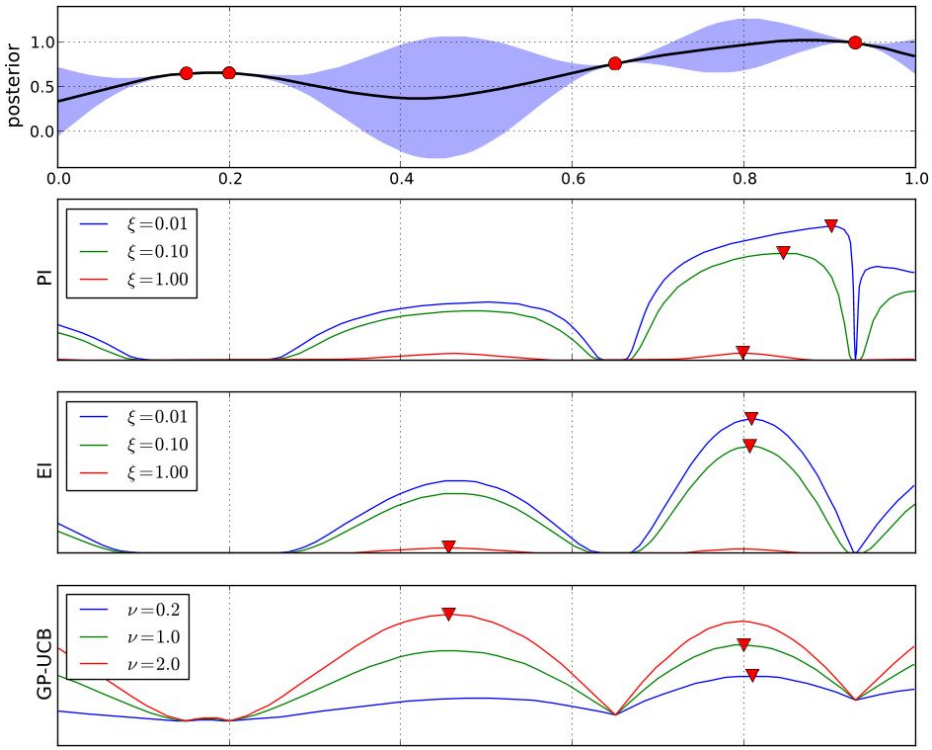


Credits: arXiv:1012.2599

Acquisition function

Specifies the next sample x.

- Upper confidence bound
  $$\mathrm{UCB}(x) = \mu_{GP}(x) + \kappa\sigma_{GP}(x)$$
- Probability of improvement
  $$\mathrm{PI}(x) = P(f(x) \geq f(x_t^+) + \kappa)$$
- Expected improvement
  $$\mathrm{EI}(x) = \mathbb{E}[f(x) - f(x_t^+)]$$



κ provides a knob for controlling the exploration-exploitation trade-off.

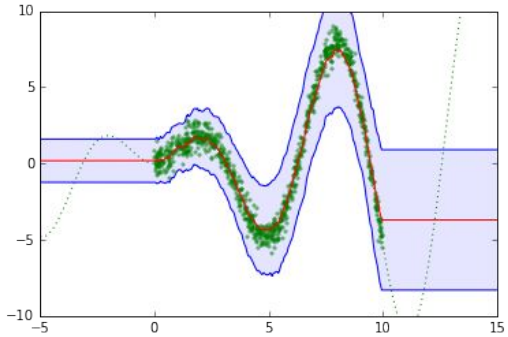
Surrogate model

The probabilistic model for f is usually built as a Gaussian Process.

Scikit-Optimize supports any Scikit-Learn regressor that can also return the variance of the predictions (`return_std=True`).

- Random forests / Extra-trees
- Gradient boosting

Tree-based optimization is fast and usually better on discontinuous high-dimensional spaces.



Random forests as a probabilistic model.

```
from skopt import forest_minimize
r = forest_minimize(objective, space)
```

```
r.x
```

```
[-0.89303546067450945, 5, 33, 9]
```

```
r.fun
```

```
2.8175239612455112
```

Is this better than **random**?

Was this actually worth it?

Random search

- If nothing works, try random search.
- Works surprisingly well, often only slightly worse than “smart” algorithms.

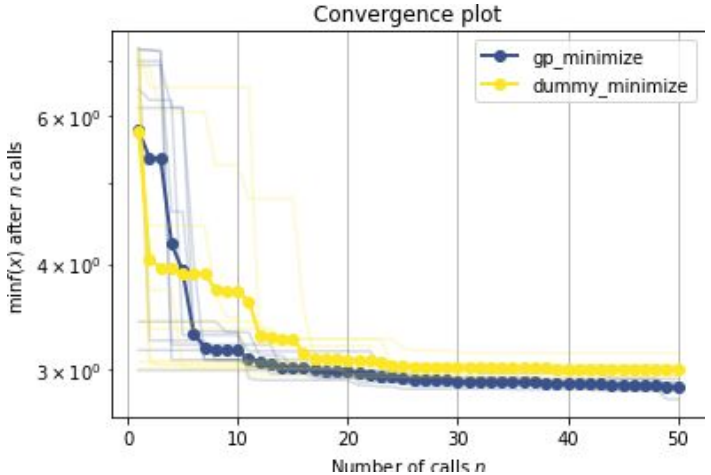
```
from skopt import dummy_minimize
r_dummy = dummy_minimize(objective, space, n_calls=50)
```

```
r_dummy.x
```

```
[-0.46028641219053501, 4, 80, 11]
```

```
r_dummy.fun
```

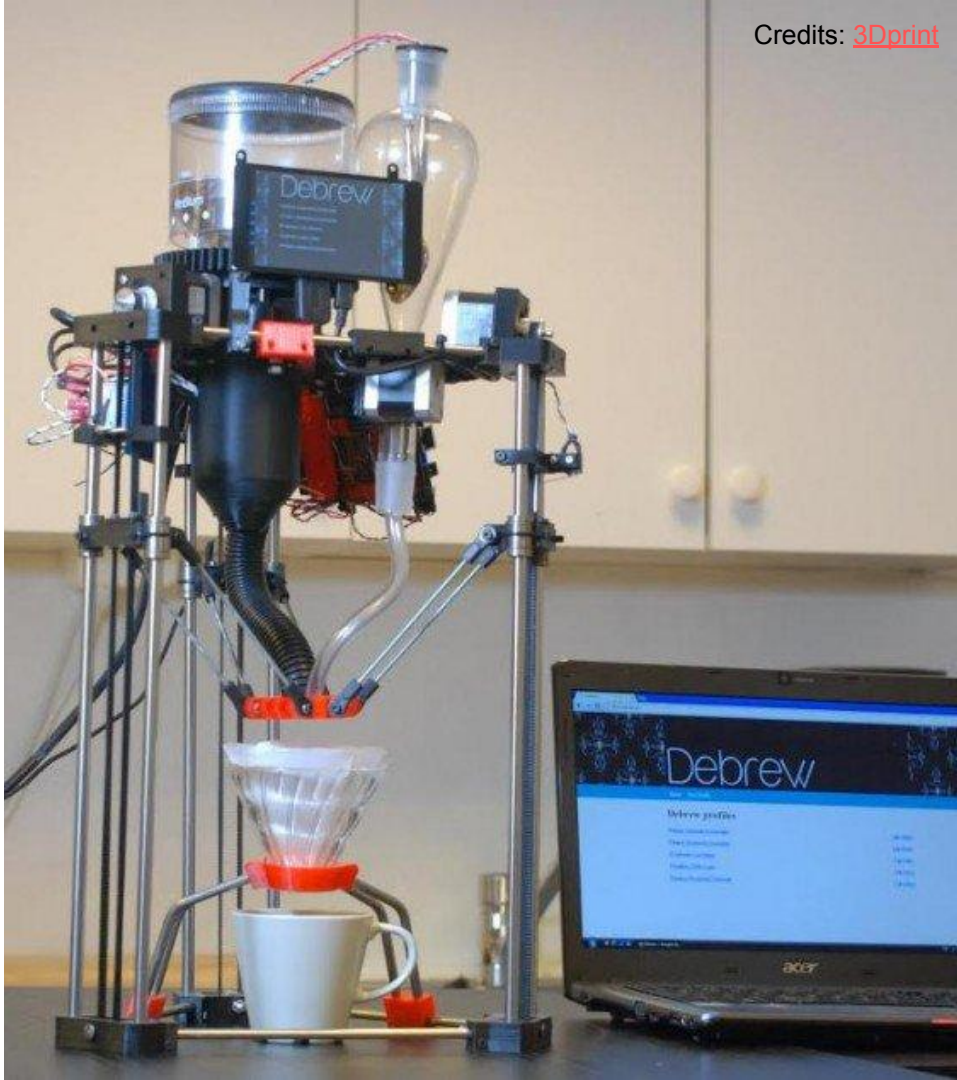
```
3.1180178726663654
```



Ouf!

Wait.

That’s nice, but how do I put my coffee maker into a Python function?



Credits: 3Dprint

Ask and tell API

- Factor out the evaluation of the objective function.
- `ask`: query next point to evaluate
  `tell`: provide function value
- Resume long optimization by pickling/unpickling the `Optimizer` object.

```
from skopt import Optimizer
opt = Optimizer(space, gp)
```

```
# Next query point
next_x = opt.ask()
next_x
```

```
[-0.69339327310821286, 3, 74, 3]
```

```
# Tell value at x
r = opt.tell(next_x, objective(next_x))
```

```
# Shortcut for ask() + tell()
r = opt.run(objective, n_iter=50)
```

```
r.x
```

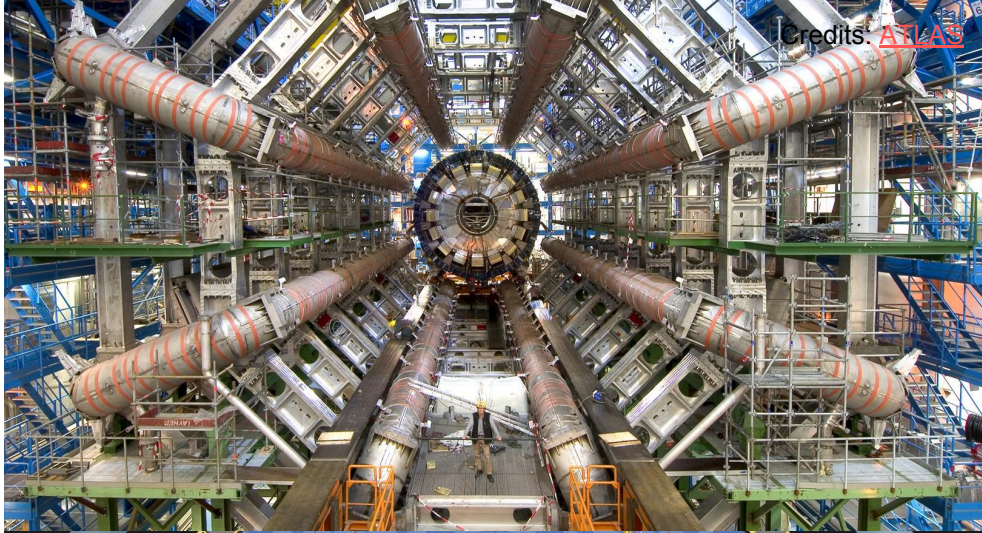
```
[-0.867784969421451, 5, 37, 9]
```

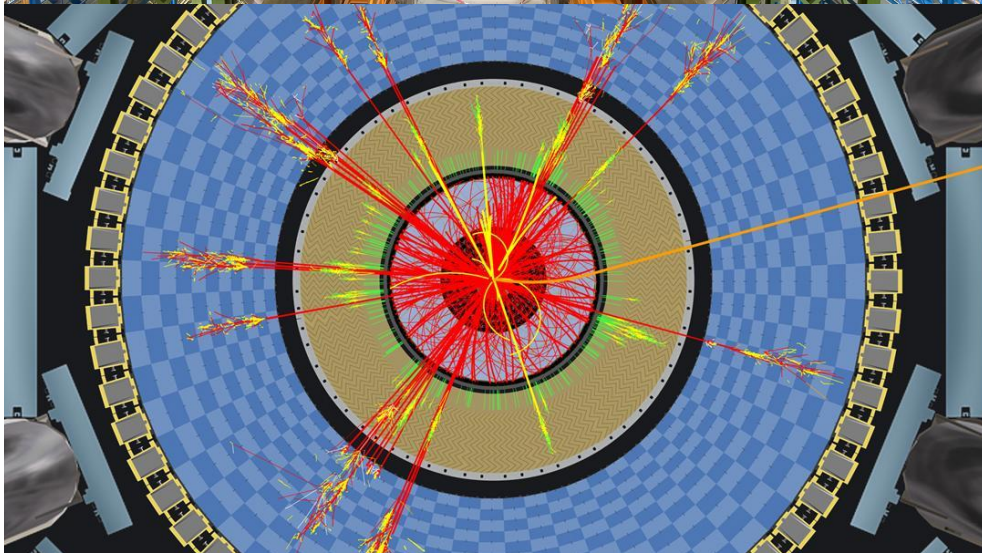
```
r.fun
```

```
2.736335329599823
```

Beyond coffee (or ML)

Tuning high energy physics simulators to match experimental data (e.g., 1610.08328)





Good coffee is expensive and does not come with gradients.
Bayesian optimisation can help.

Summary

- Bayesian optimisation is a principled approach for optimising an expensive function f.

- Scikit-Optimize provides an easy-to-use set of tools for this.

We want you!

Help us improve Scikit-Optimize

https://github.com/scikit-optimize/scikit-optimize