

Hyperparameter Tuning - brute force or smart algorithms?

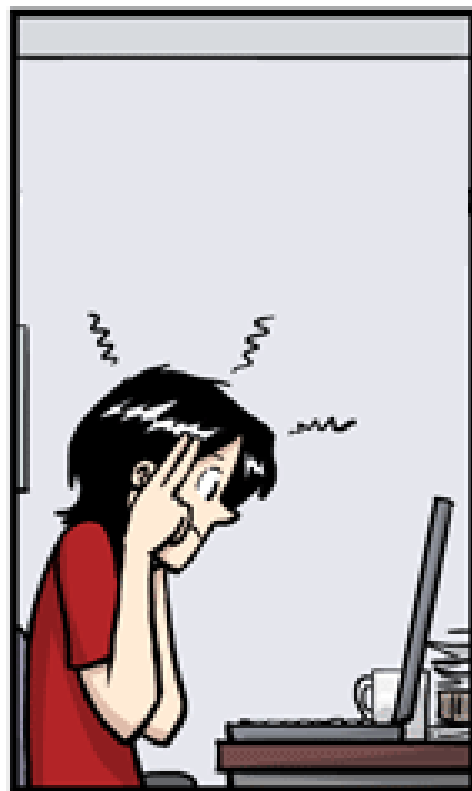
Tobias Rippel

Data Science Meetup, 07.06.2018

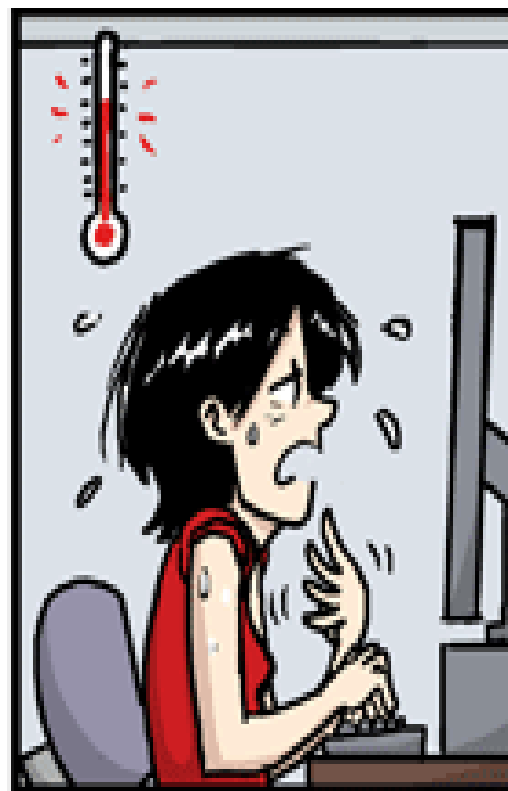
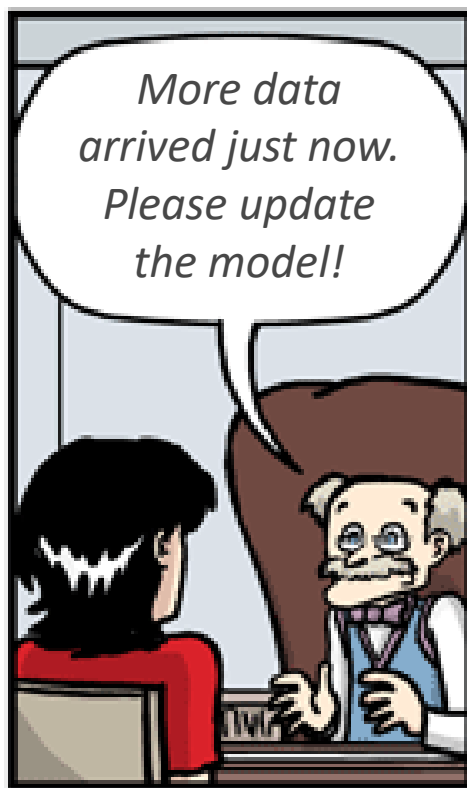
A week in the life of a data scientist



Tuning the model ...



Re-tuning the model ...



Re-tuning the model ...





Manually tuning Machine Learning models is tedious

Manually tuning

- Time consuming, even boring
- Got more data? - *Good for you, now start over!*
- *Fear of missing out*

Automated tuning!

- Test all parameter settings? → ...
- Grid Search → Takes too long
- Random Search → Better, but is that all?
- Smart Algorithms → Sound's interesting!

Smart Algorithm: Basic ideas

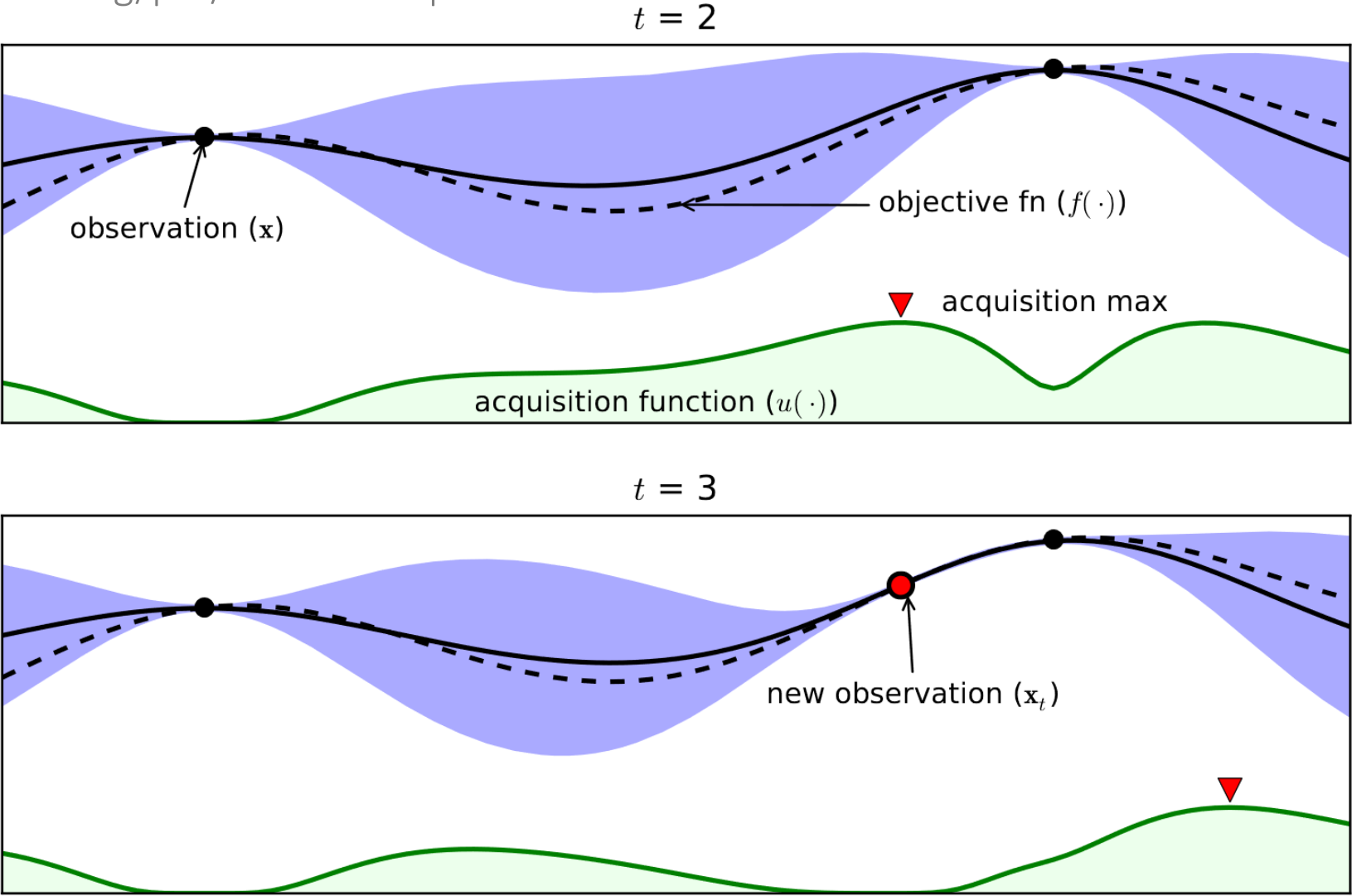


- Gaussian Process
- Tree-structured Parzen Estimator (TPE)
- ...

Gaussian Process



Source: <https://arxiv.org/pdf/1012.2599.pdf>



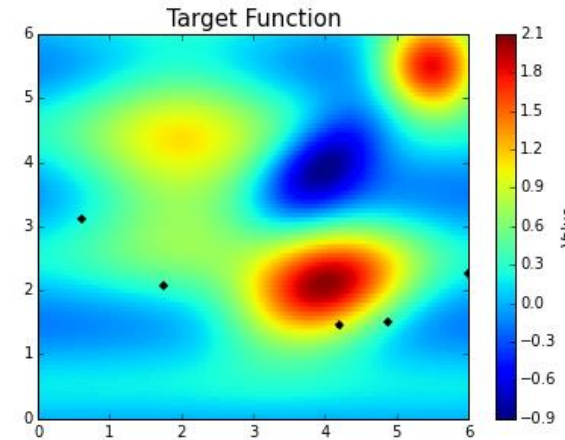
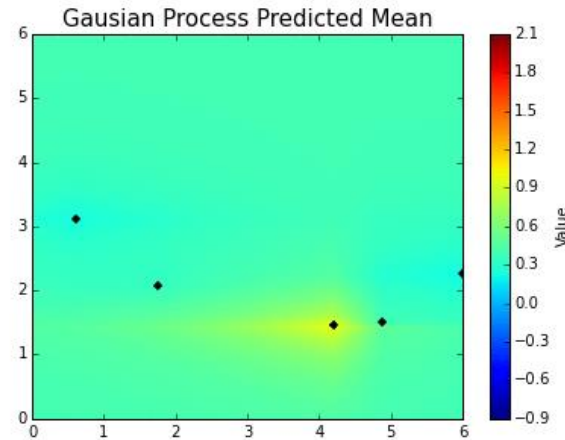
Gaussian Process



Source: <https://github.com/fmfn/BayesianOptimi>

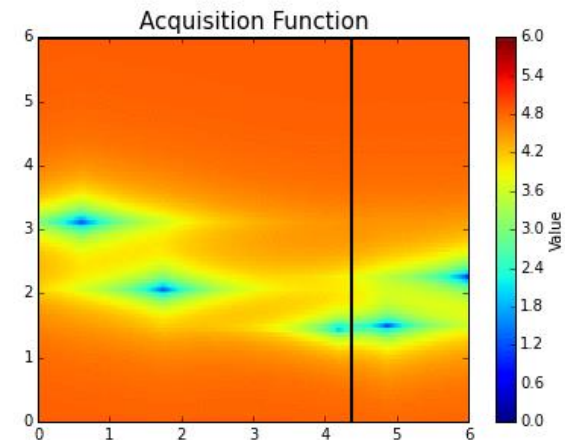
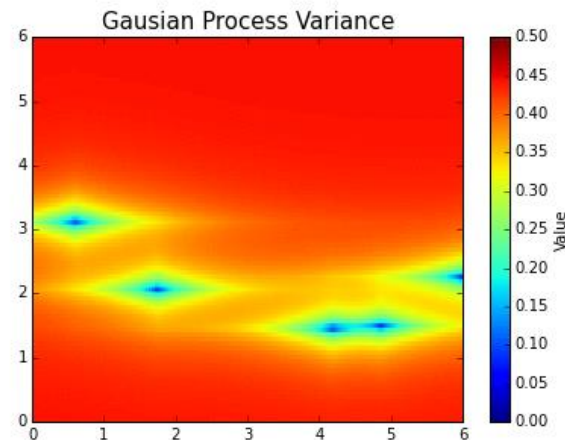
Bayesian Optimization in Action

Bayes Estimation
of Truth



Truth

Variance
Estimation



Data Point
Selector

Benchmark



■ Our benchmark approach:

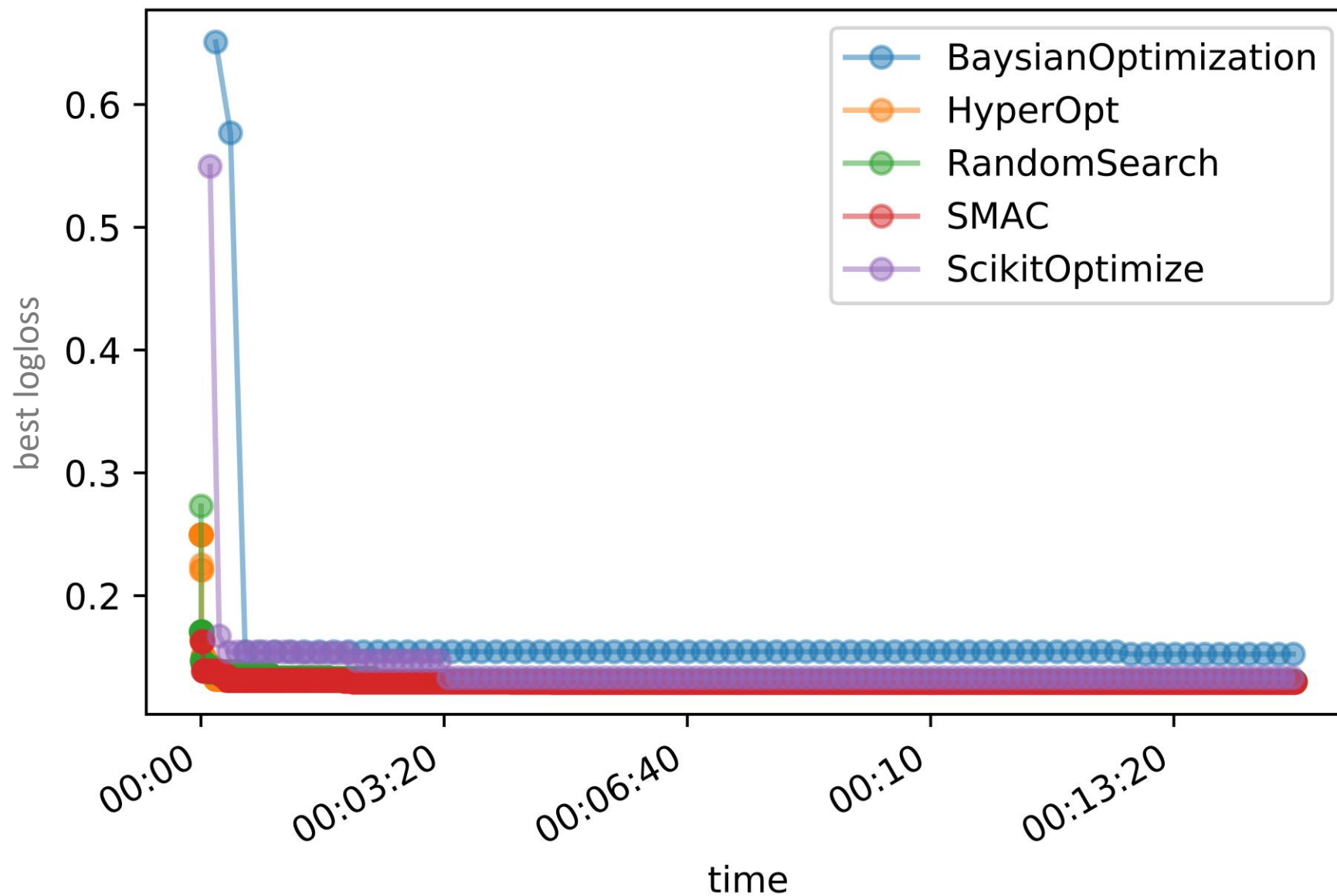
- Limited time (1h)
- Same resources (32 core machine)
- Same ml algorithm (xgboost) optimized on same loss function (log-loss)
- Same datasets (Iris, Real Life Dataset (130k rows, 20 cols)) -> Classification

Category	Hyperparameter Tuning Algorithms
Benchmark	Random Search
Gaussian Process	BayesianOptimization (https://github.com/fmfn/BayesianOptimi)
	Scikit-Optimize (https://github.com/scikit-optimize/scikit-optimize)
Tree-structured Parzen Estimator (TPE)	Hyperopt (https://github.com/hyperopt/hyperopt)
	SMAC (https://github.com/automl/SMAC3)

Results



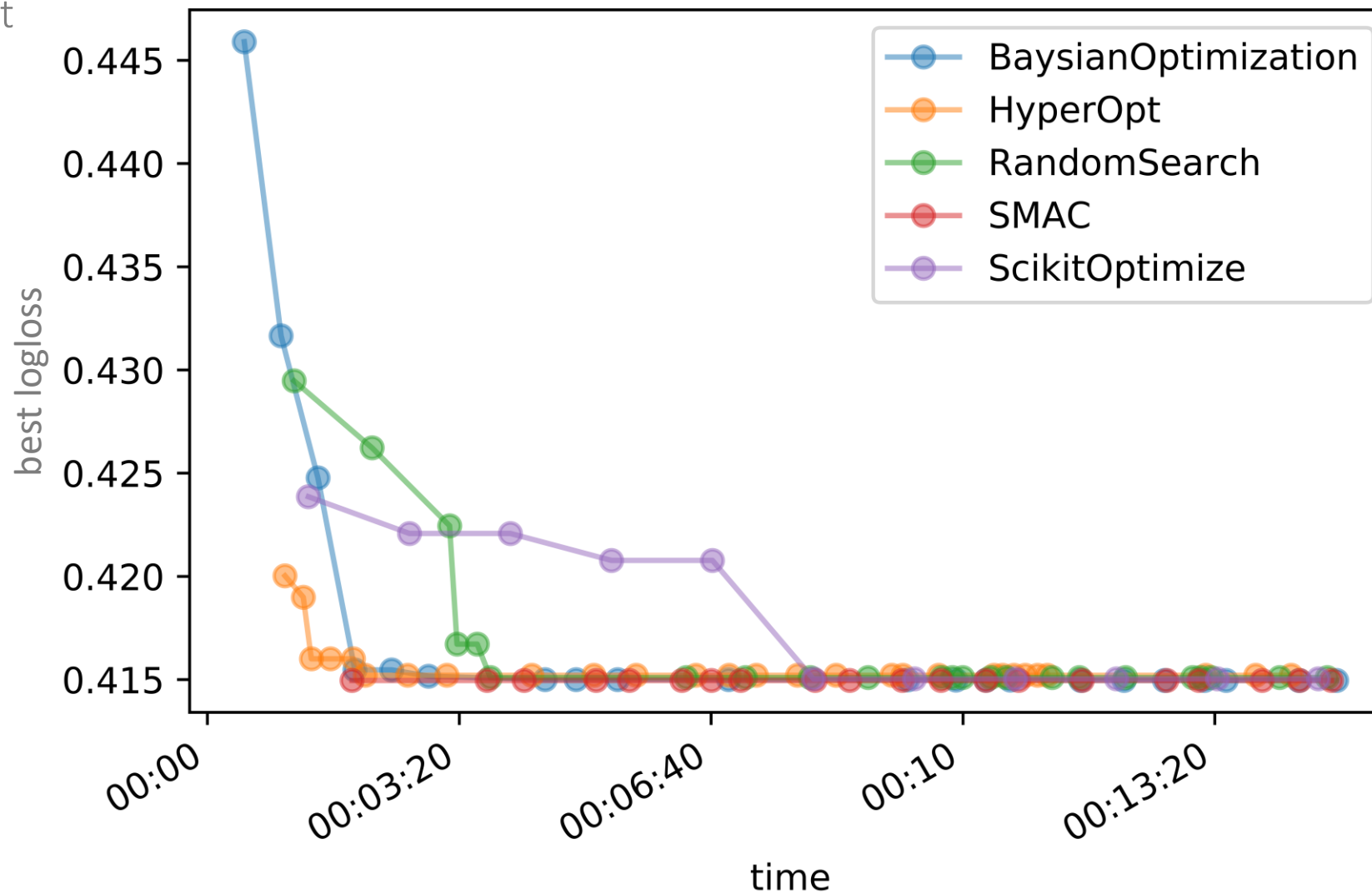
Iris Dataset



Results



Real-Life Dataset





Summary + Take aways

Initial results

- Chosen Smart Algorithms have limited/no benefits over Random search (on our datasets)
- Smart Algorithms have to be parameterized themselves... (BOHHHHH!)

Further experiments

- Test more complex problems (datasets)
- Compare a human expert to these results

Take aways

- Only use Hyperparameter Tuning after you have all the data!
- Spend your time wisely! -> Feature Engineering/ more data are oftentimes more desirable