Applications of Machine Learning in Engineering

(and Parameter Tuning)

Lars Kotthoff

University of Wyoming
larsko@uwyo.edu

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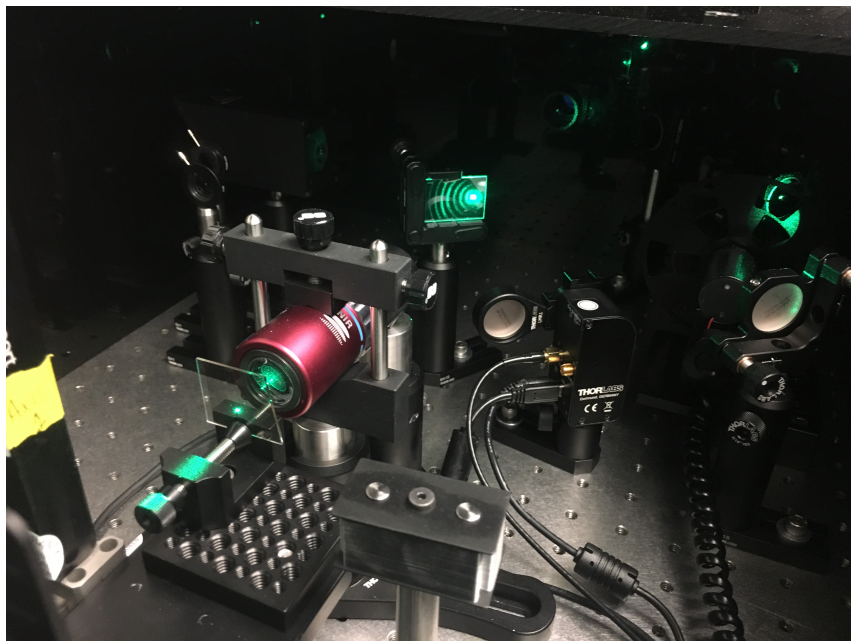
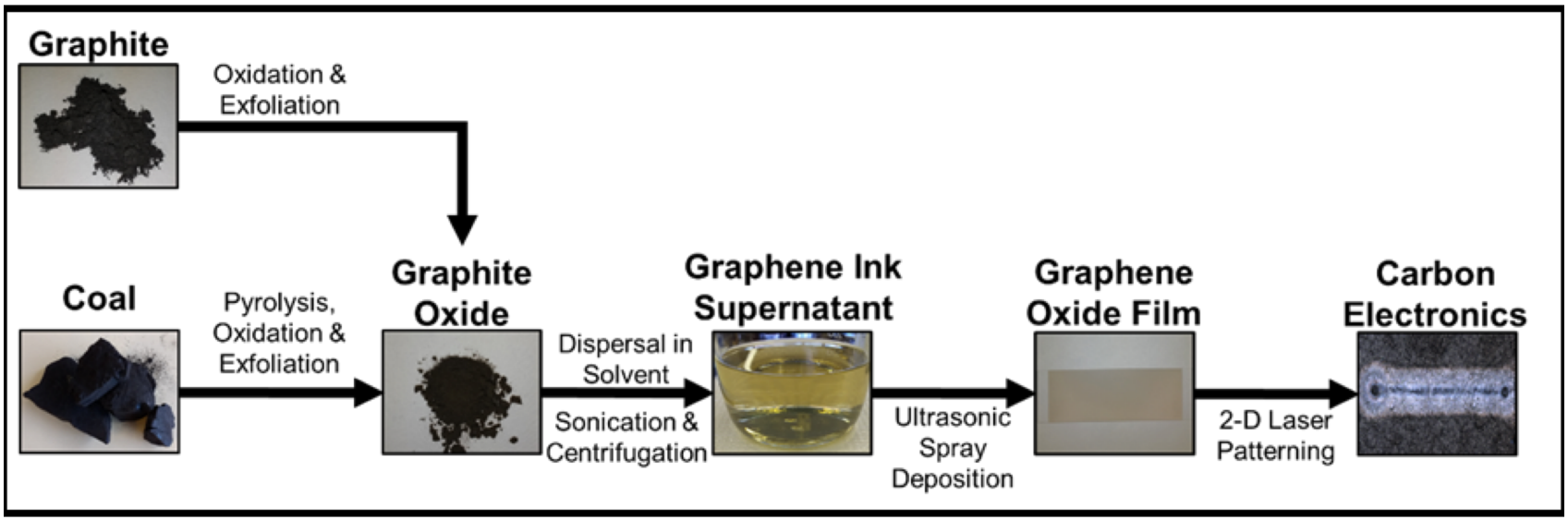
slides available at https://www.cs.uwyo.edu/~larsko/slides/rmacc19.pdf

Optimizing Graphene Oxide Reduction

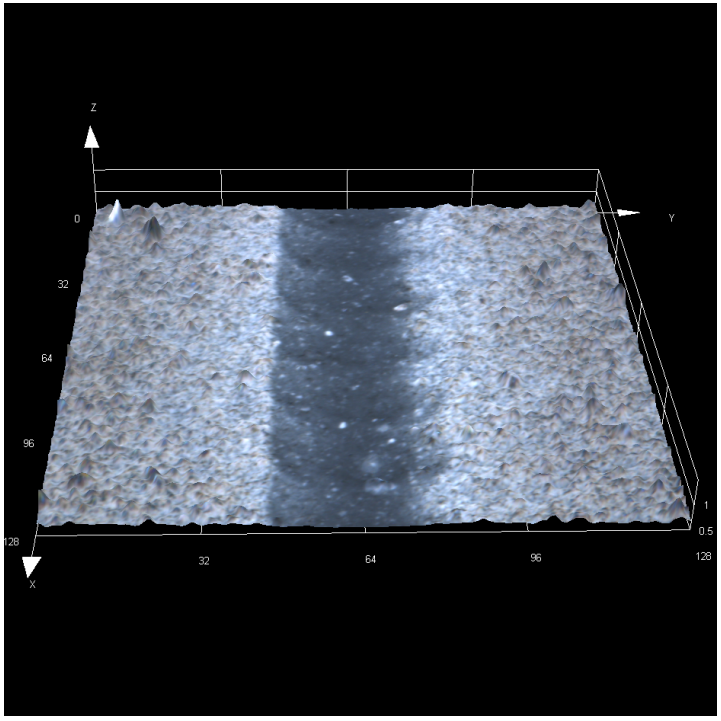
- ▷ reduce graphene oxide to graphene through laser irradiation
- ▷ allows to create electrically conductive lines in insulating material
- ▷ laser parameters need to be tuned carefully to achieve good results

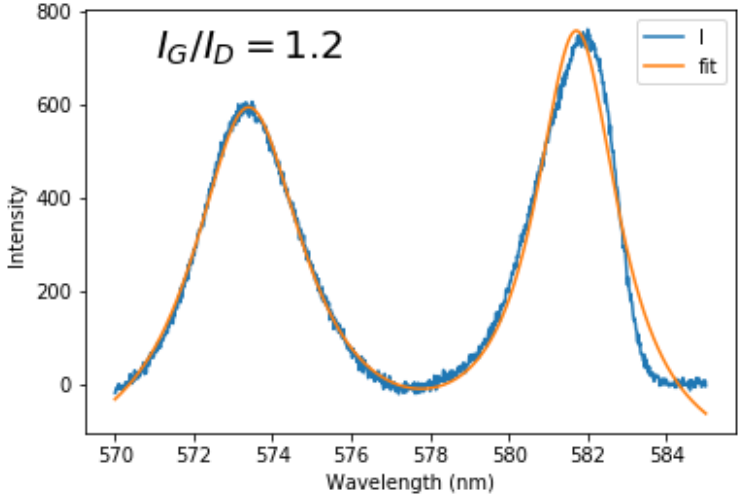


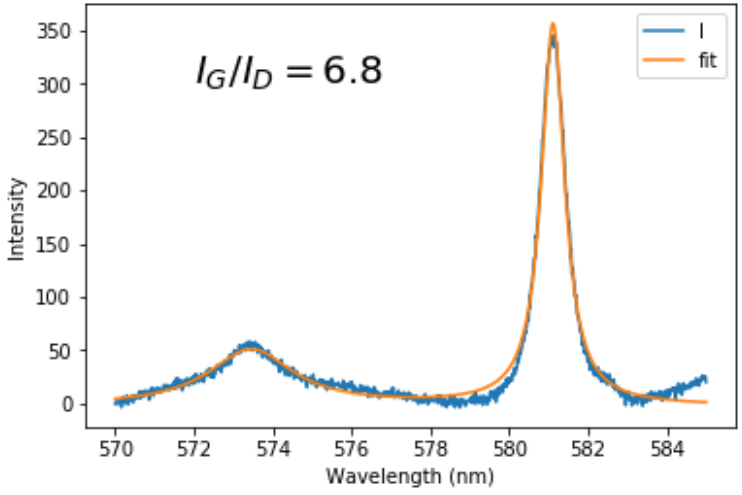
From Graphite/Coal to Carbon Electronics



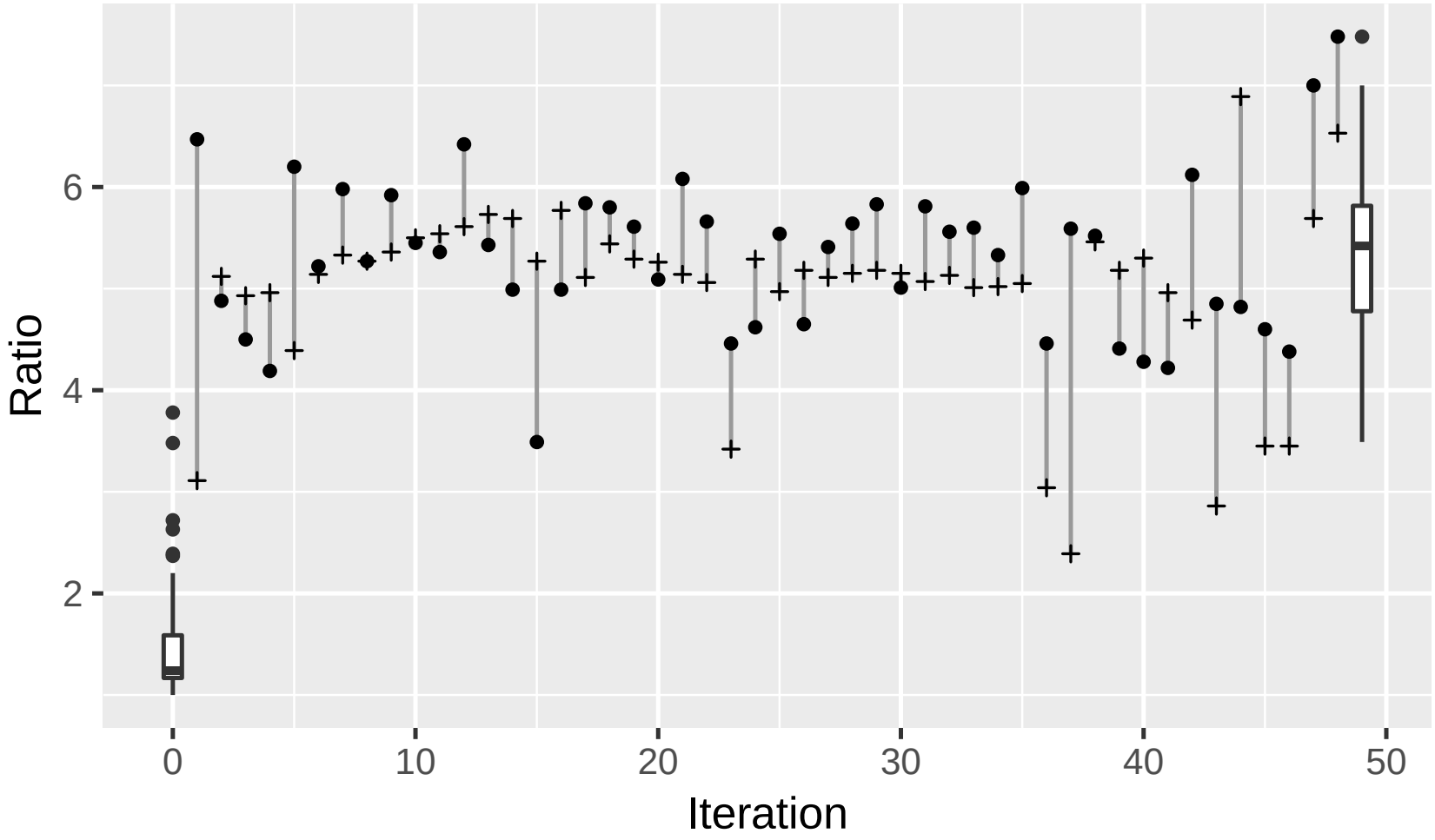
Evaluation of Irradiated Material







ML-Optimized Laser Parameters



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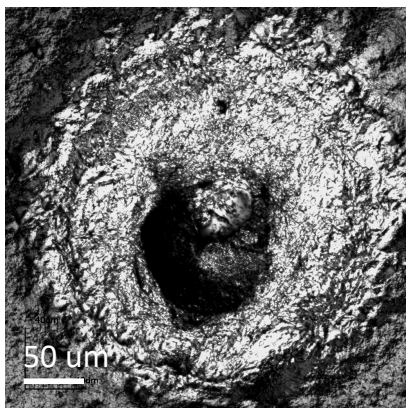
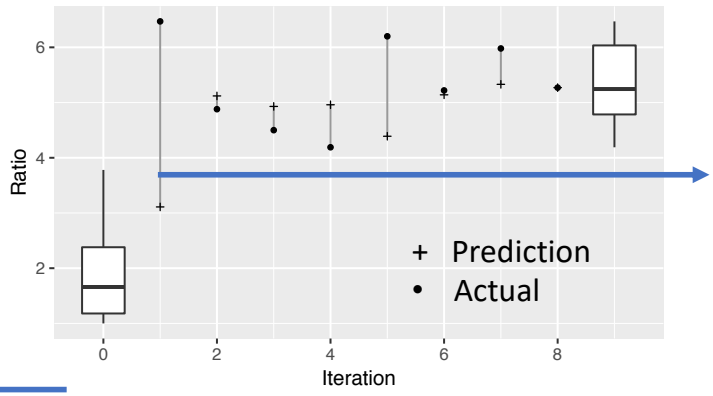
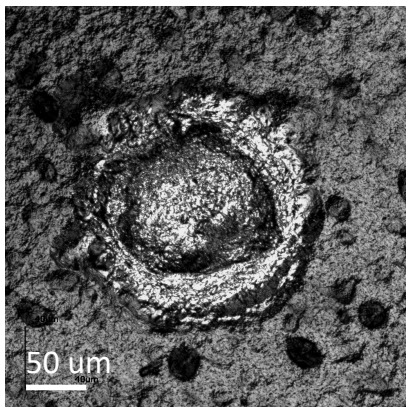




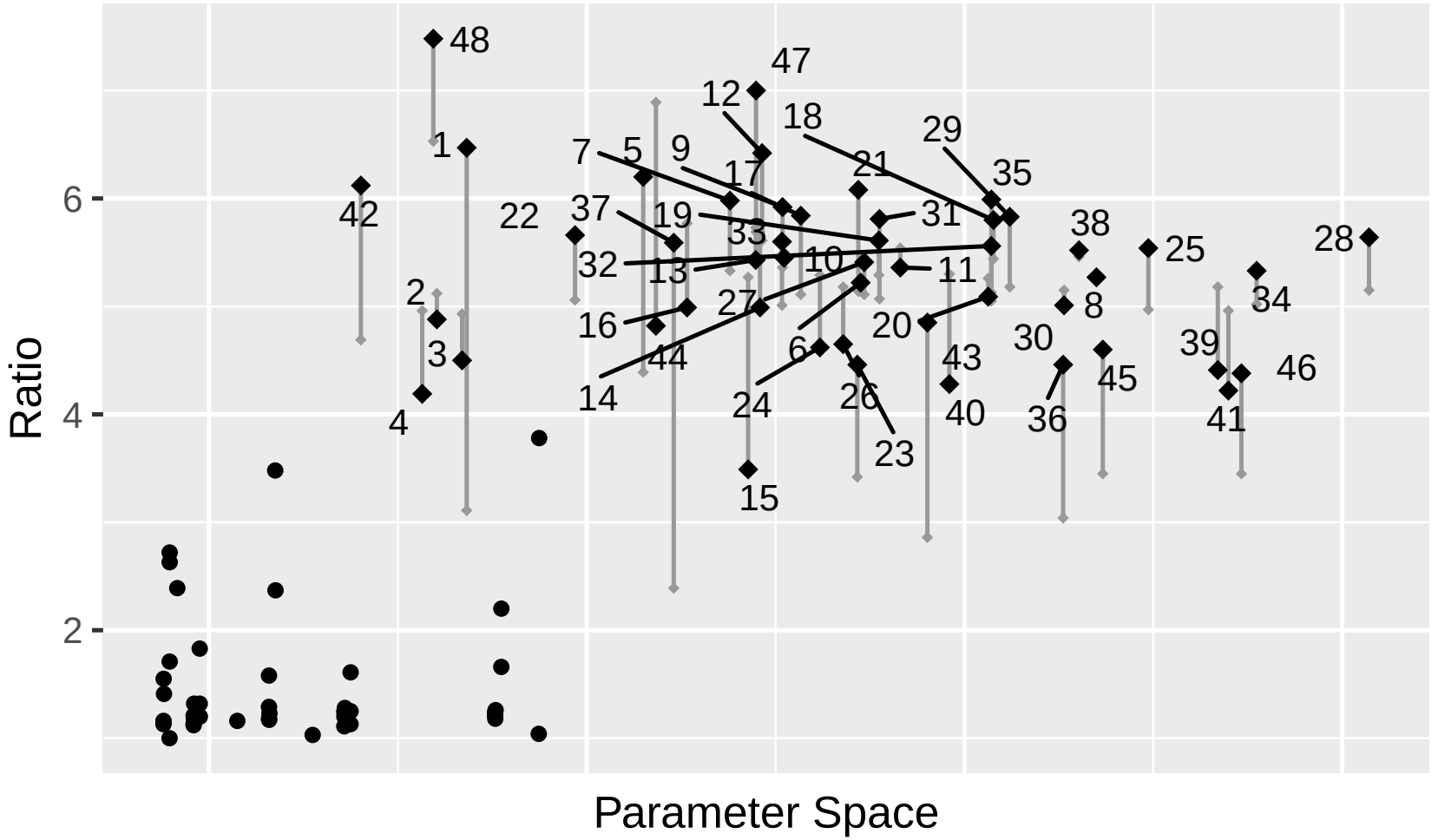


During Training

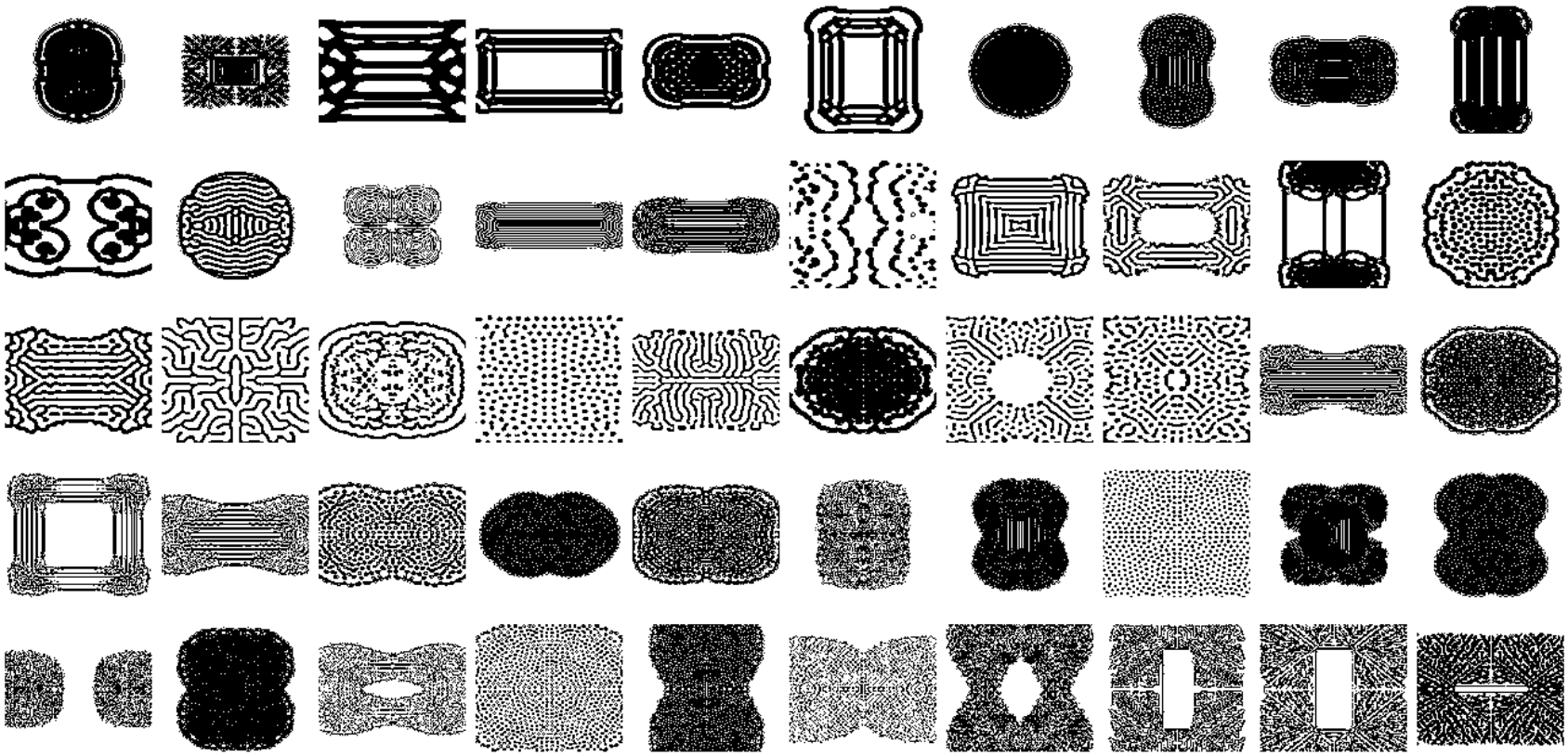
After 1st prediction

- Predictions work even with small training dataset (19 points)
- AI Model achieved I_G/I_D ratio (>6) after 1st prediction

Explored Parameter Space



Design of New Materials



- optimize parameters of pattern generator for energy absorption of material

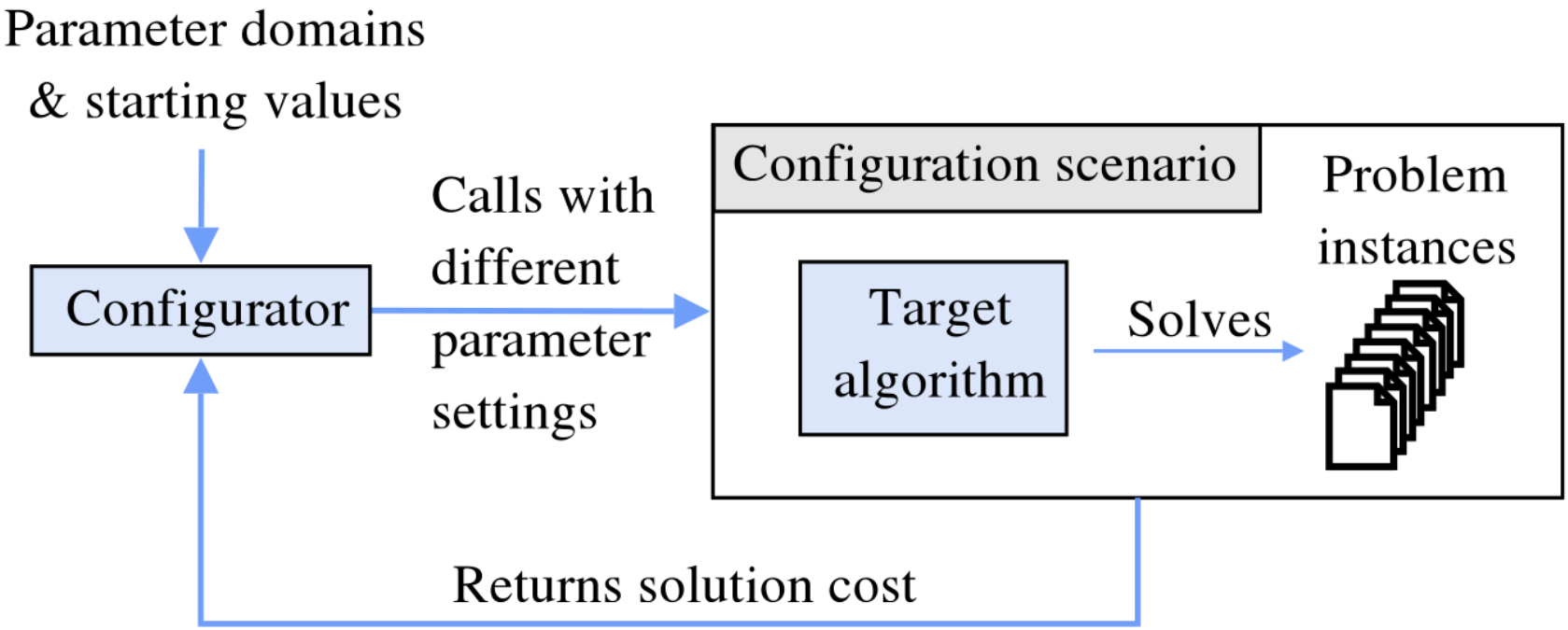
Big Picture

- advance the state of the art through meta-algorithmic techniques
- rather than inventing new things, use existing things more intelligently – automatically
- invent new things through combinations of existing things

What to Tune – Parameters

- ▷ anything you can change that makes sense to change
- ▷ e.g. heuristic, power of a laser, kernel for a machine learning method
- ▷ not random seed, whether to enable debugging, etc.
- ▷ some will affect performance, others will have no effect at all

Automated Parameter Tuning



Frank Hutter and Marius Lindauer, "Algorithm Configuration: A Hands on Tutorial", AAAI 2016

General Approach

- ▷ evaluate algorithm as black-box function
- ▷ observe effect of parameters without knowing the inner workings
- ▷ decide where to evaluate next
- ▷ balance diversification/exploration and intensification/exploitation
- ▷ repeat until satisfied

When are we done?

- ▷ most approaches incomplete
- ▷ cannot prove optimality, not guaranteed to find optimal solution (with finite time)
- ▷ performance highly dependent on configuration space

⟶ How do we know when to stop?

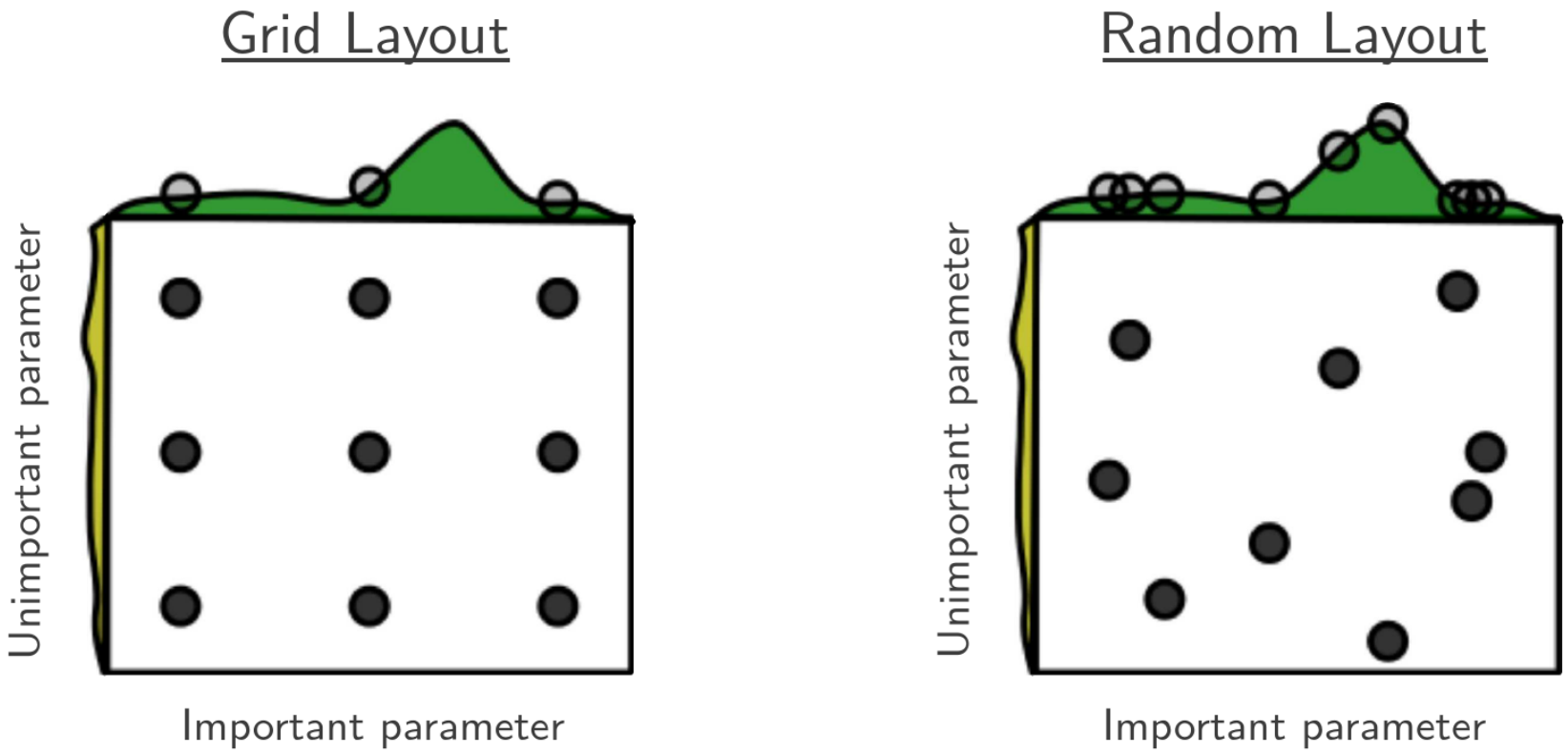
Resource Budget

How much time/how many function evaluations?

- ▷ too much ⟶▷ wasted resources
- ▷ too little ⟶▷ suboptimal result
- ▷ use statistical tests
- ▷ evaluate on parts of the instance set
- ▷ for runtime: adaptive capping

Grid and Random Search

- evaluate certain points in parameter space



Bergstra, James, and Yoshua Bengio. "Random Search for Hyper-Parameter Optimization." J. Mach. Learn. Res. 13, no. 1 (February 2012): 281–305.

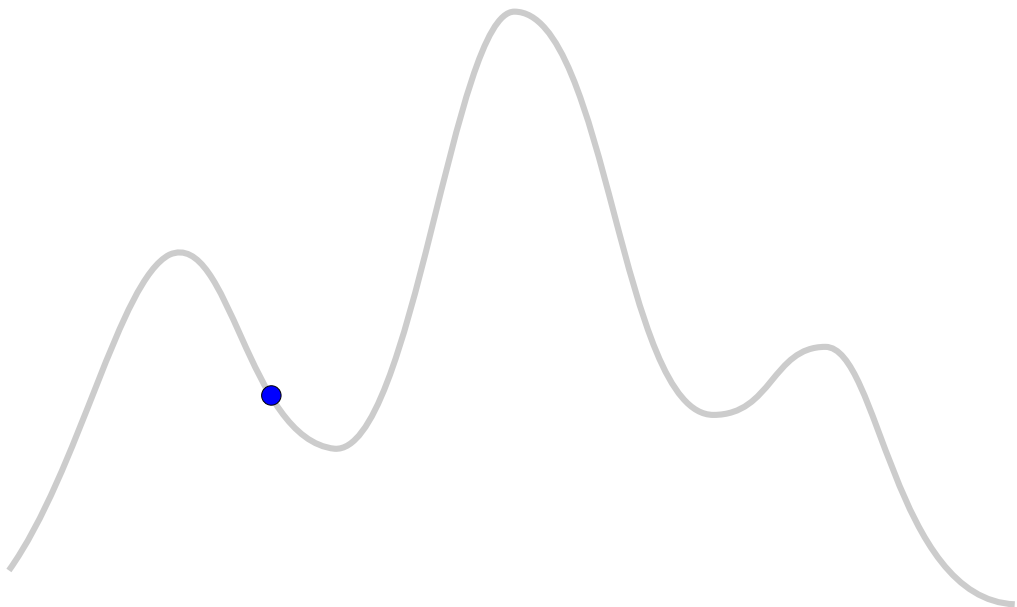
Local Search

- start with random configuration
- change a single parameter (local search step)
- if better, keep the change, else revert
- repeat, stop when resources exhausted or desired solution quality achieved
- restart occasionally with new random configurations

Local Search Example

graphics by Holger Hoos

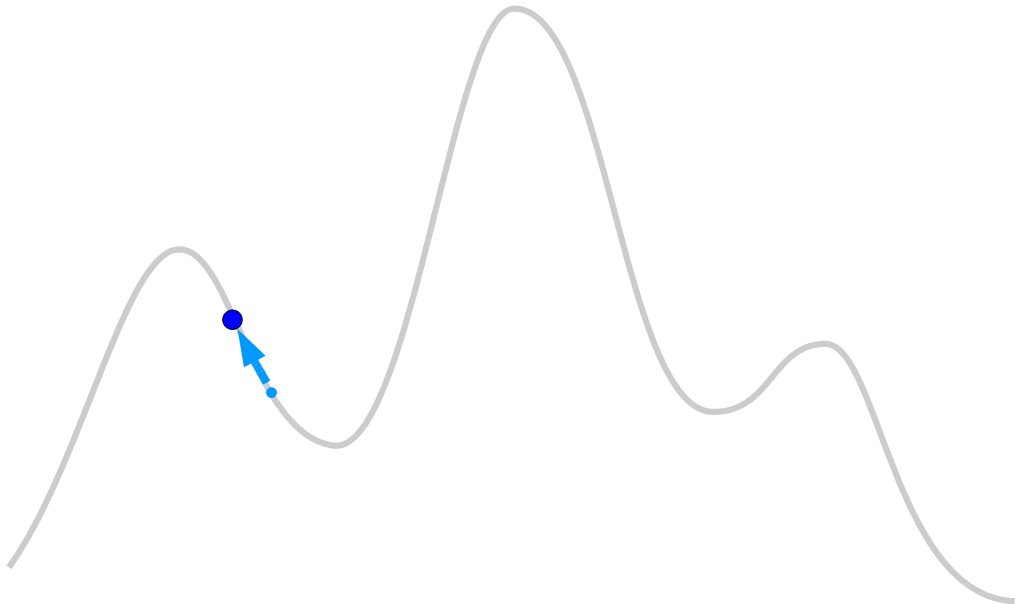
Local Search Example



Initialisation

graphics by Holger Hoos

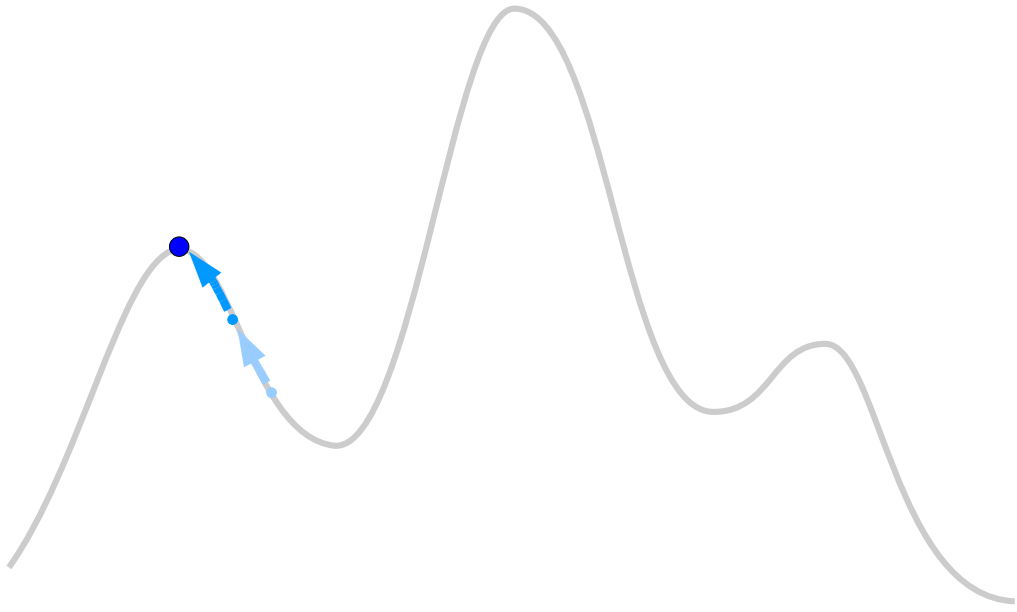
Local Search Example



Local Search

graphics by Holger Hoos

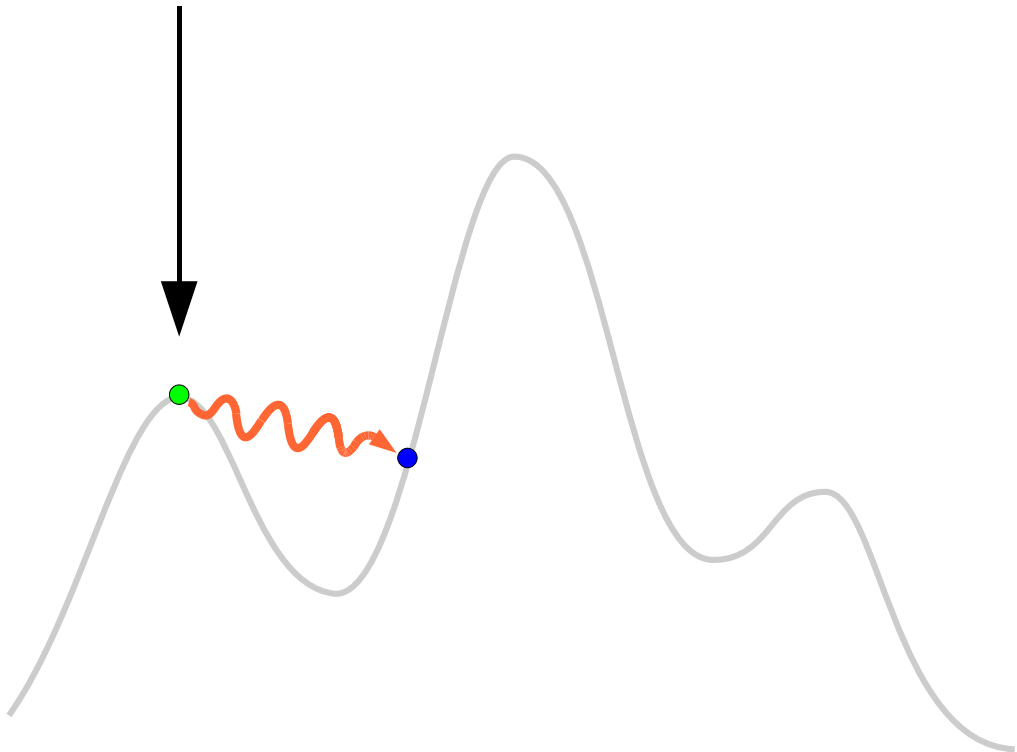
Local Search Example



Local Search

graphics by Holger Hoos

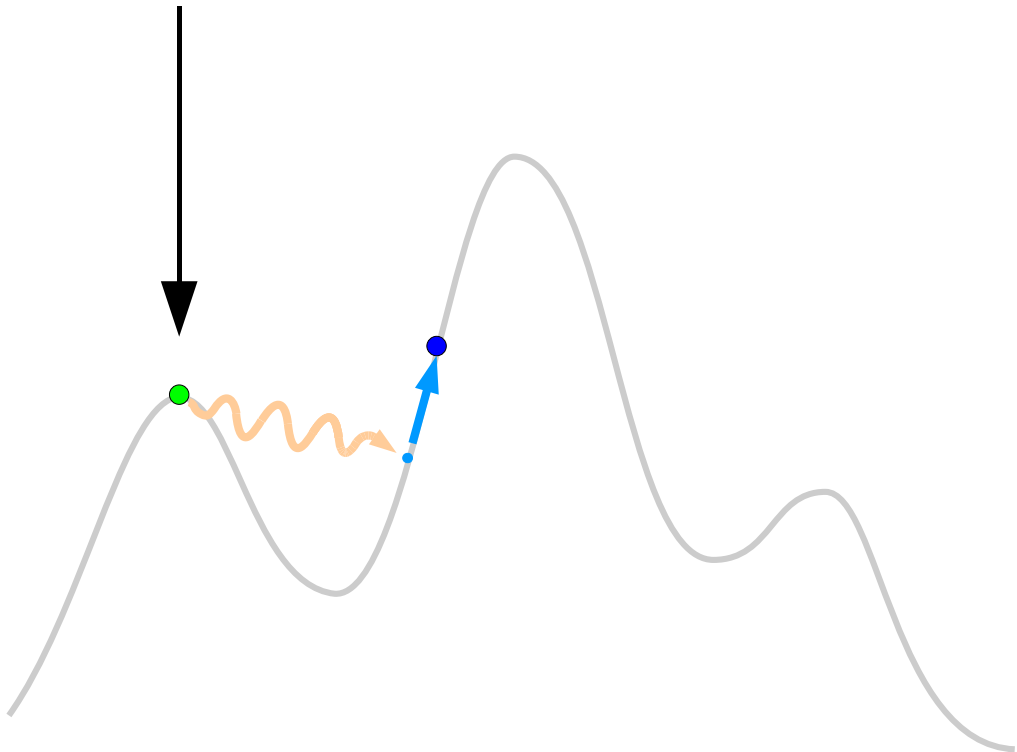
Local Search Example



Perturbation

graphics by Holger Hoos

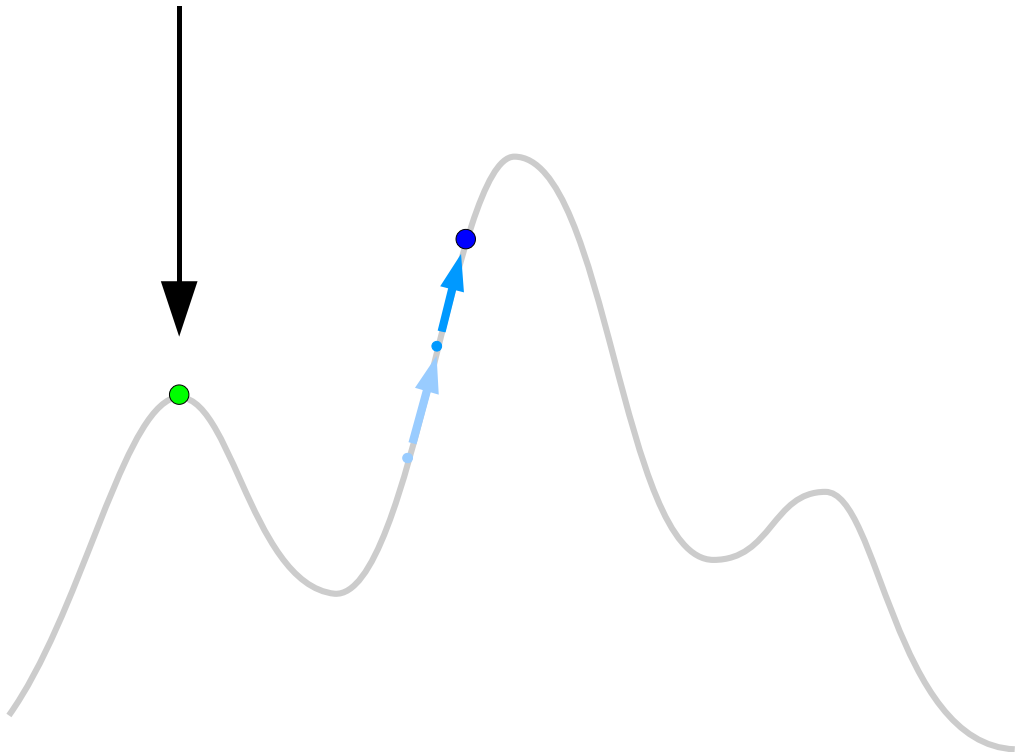
Local Search Example



Local Search

graphics by Holger Hoos

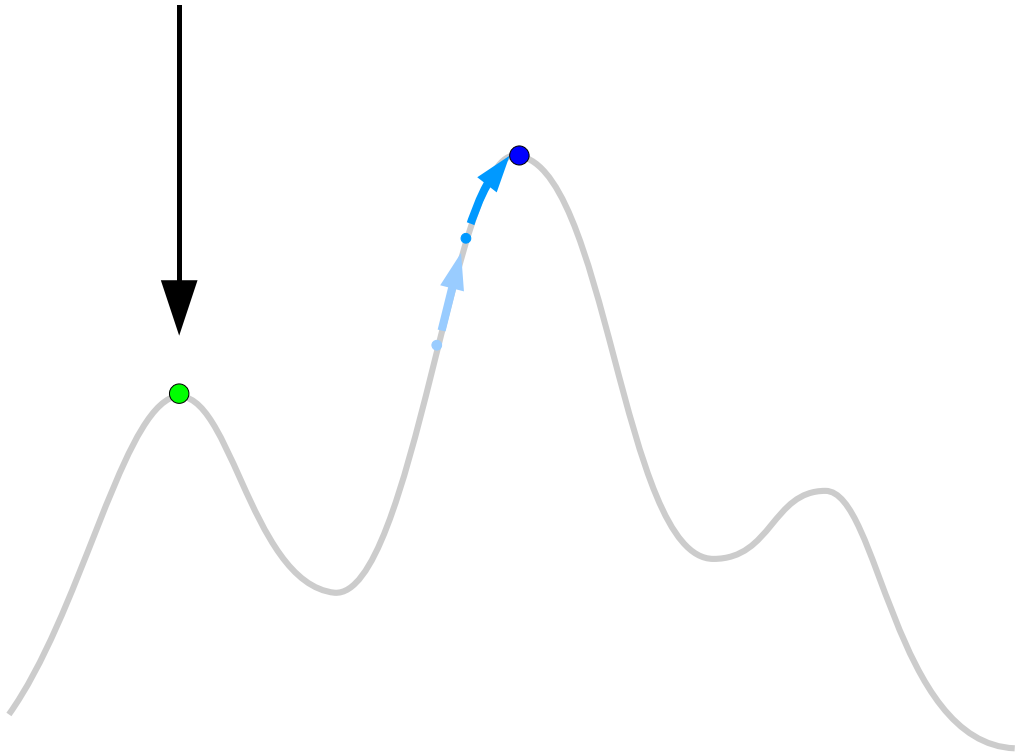
Local Search Example



Local Search

graphics by Holger Hoos

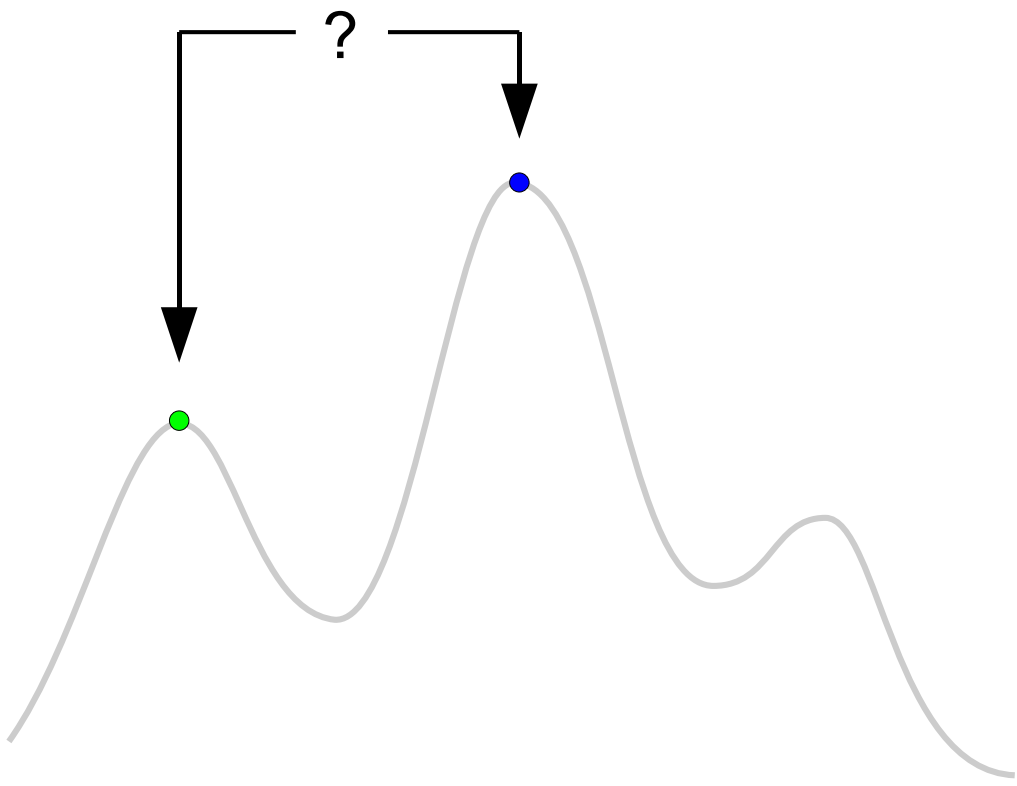
Local Search Example



Local Search

graphics by Holger Hoos

Local Search Example



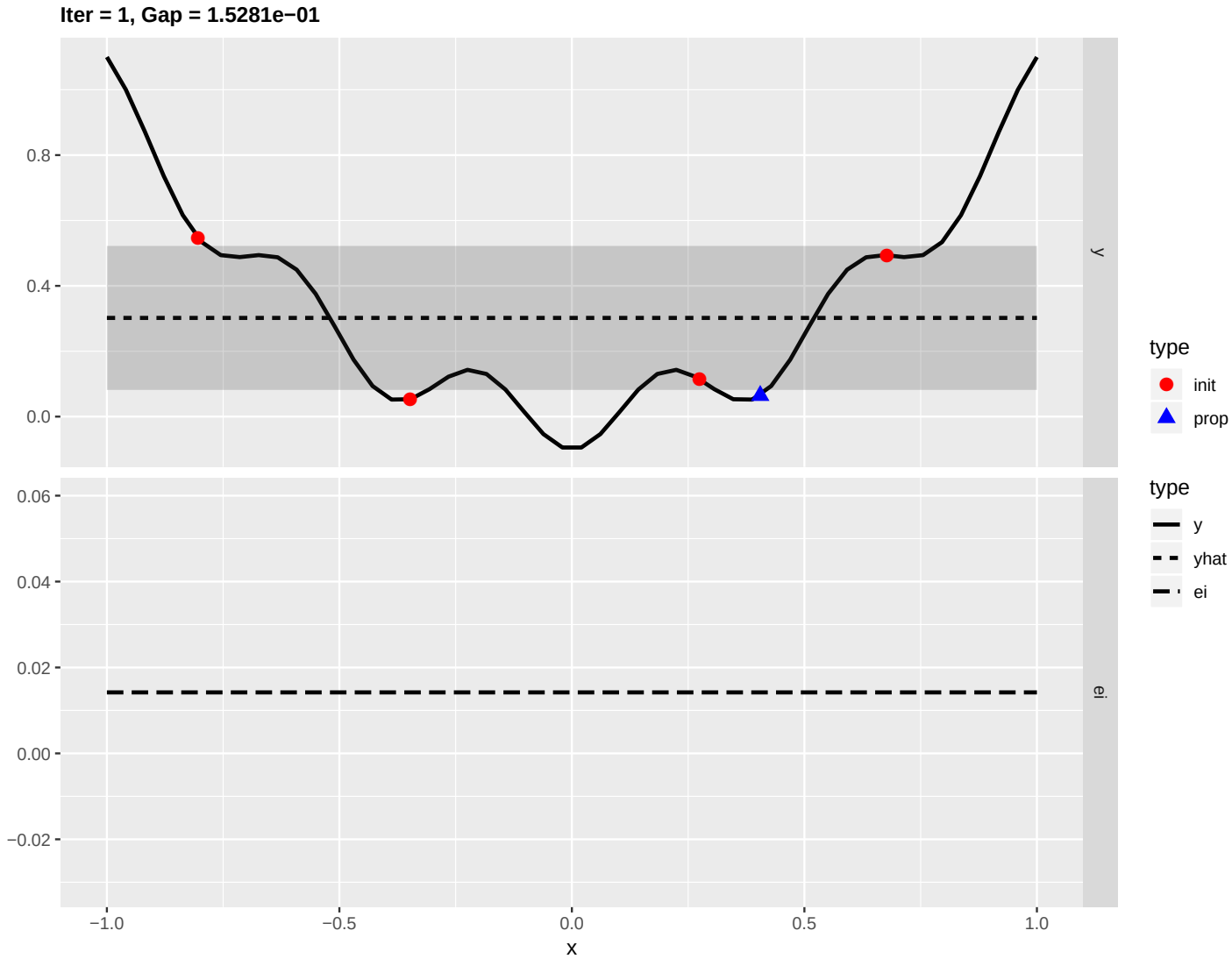
Selection (using Acceptance Criterion)

graphics by Holger Hoos

Surrogate-Model-Based Search

- ▷ evaluate small number of initial (random) configurations
- ▷ build surrogate model of parameter-performance surface based on this
- ▷ use model to predict where to evaluate next
- ▷ repeat, stop when resources exhausted or desired solution quality achieved
- ▷ allows targeted exploration of promising configurations

Surrogate-Model-Based Search Example



Bischl, Bernd, Jakob Richter, Jakob Bossek, Daniel Horn, Janek Thomas, and Michel Lang. "MlrMBO: A Modular Framework for Model-Based Optimization of Expensive Black-Box Functions," March 9, 2017. http://arxiv.org/abs/1703.03373.

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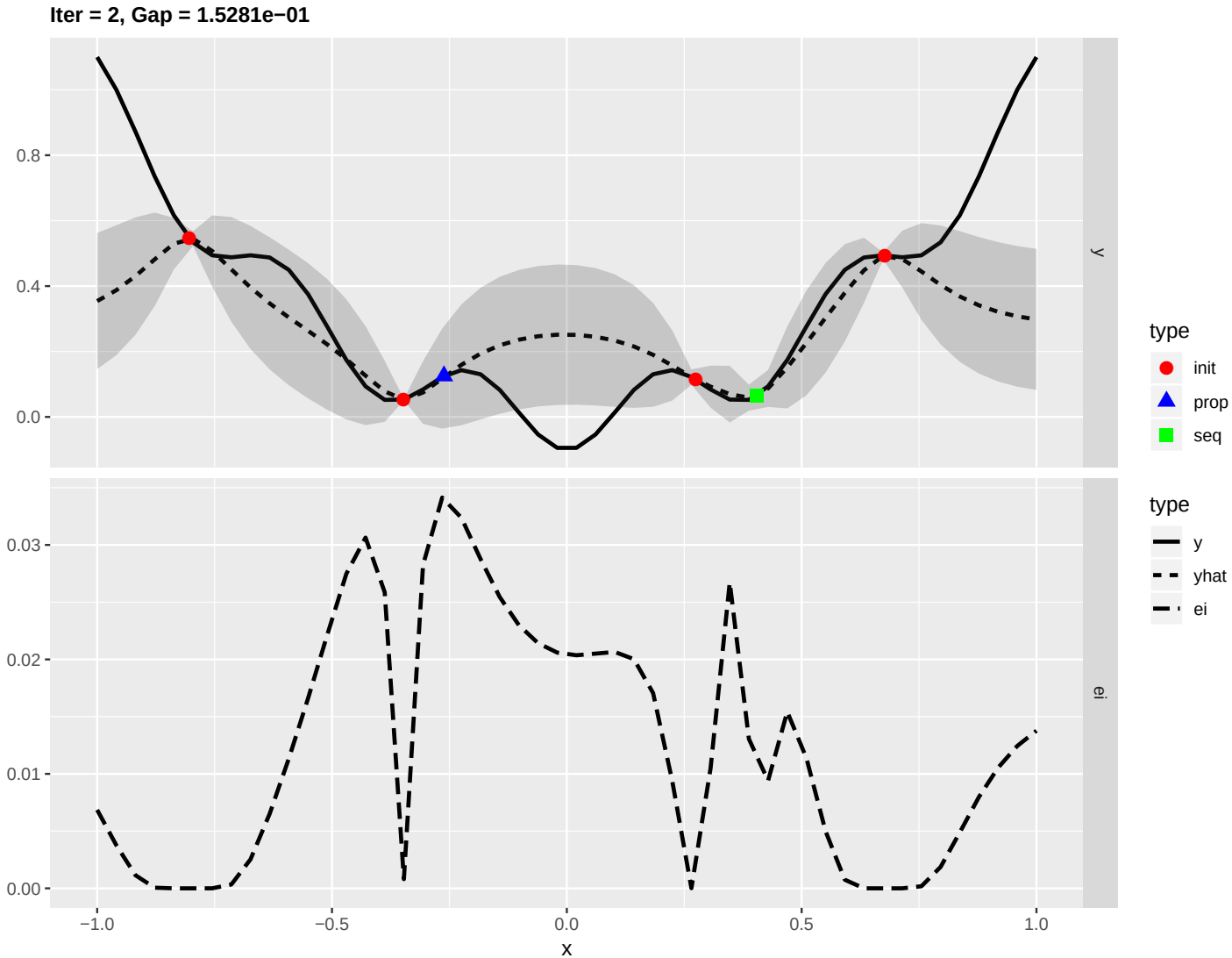

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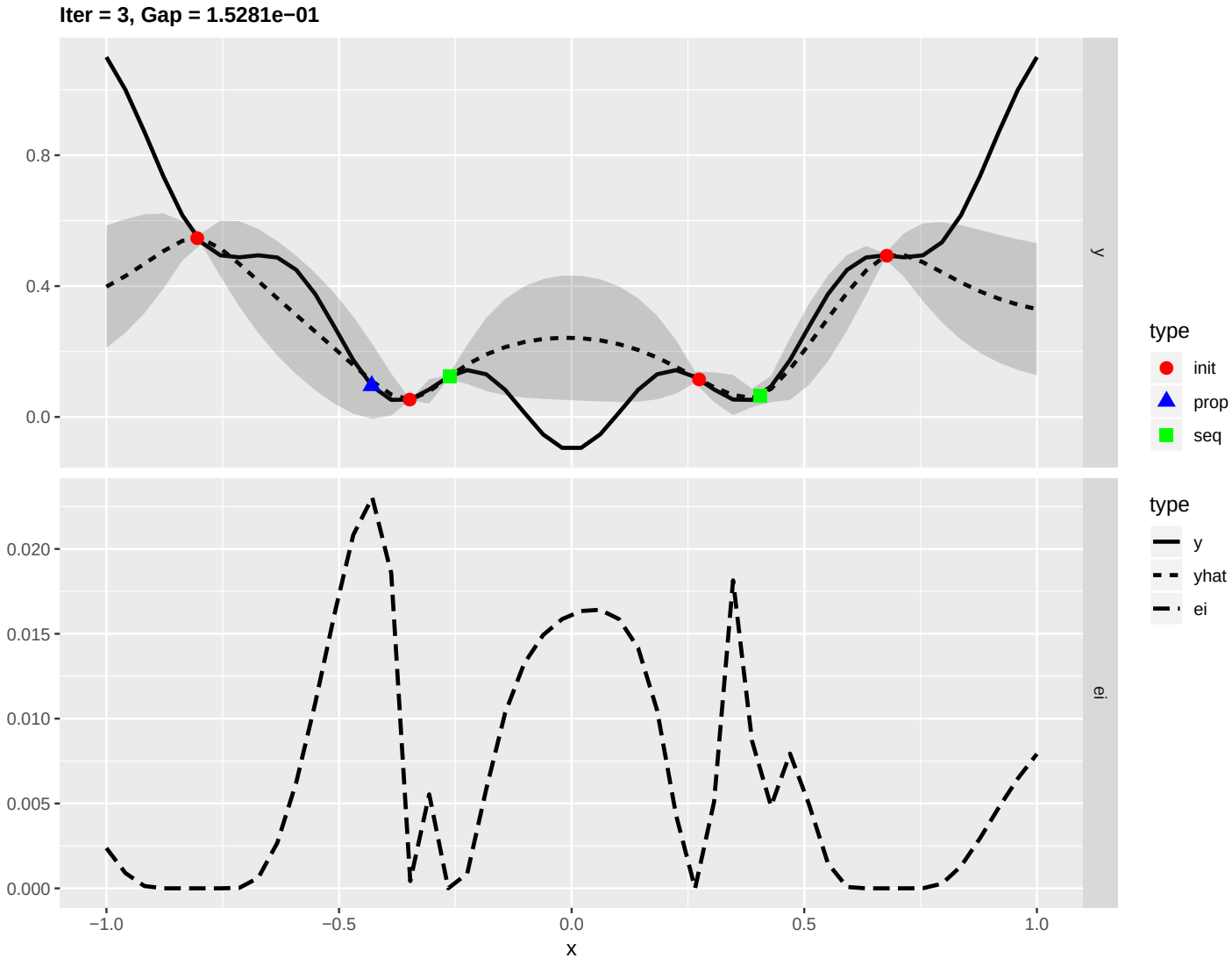

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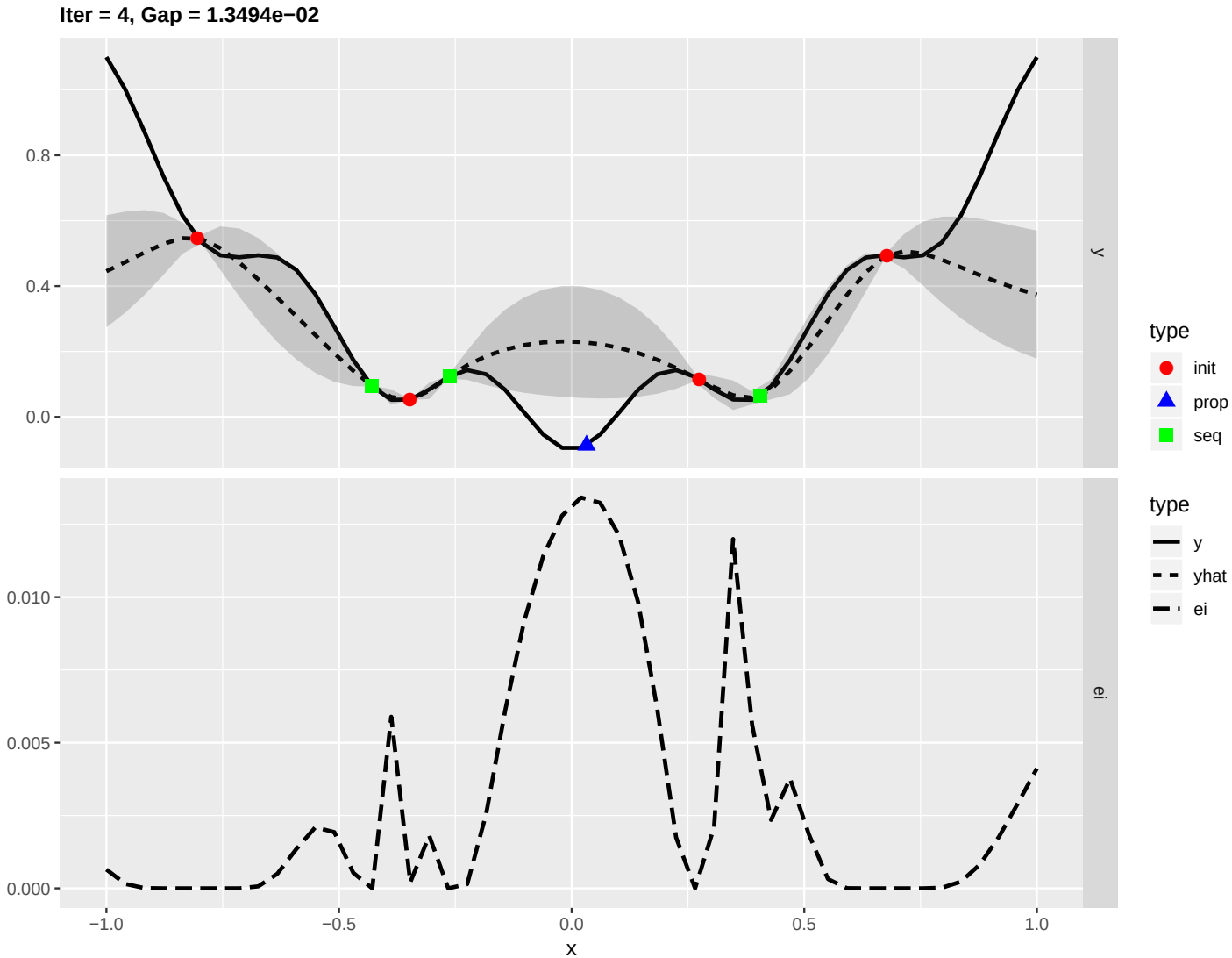

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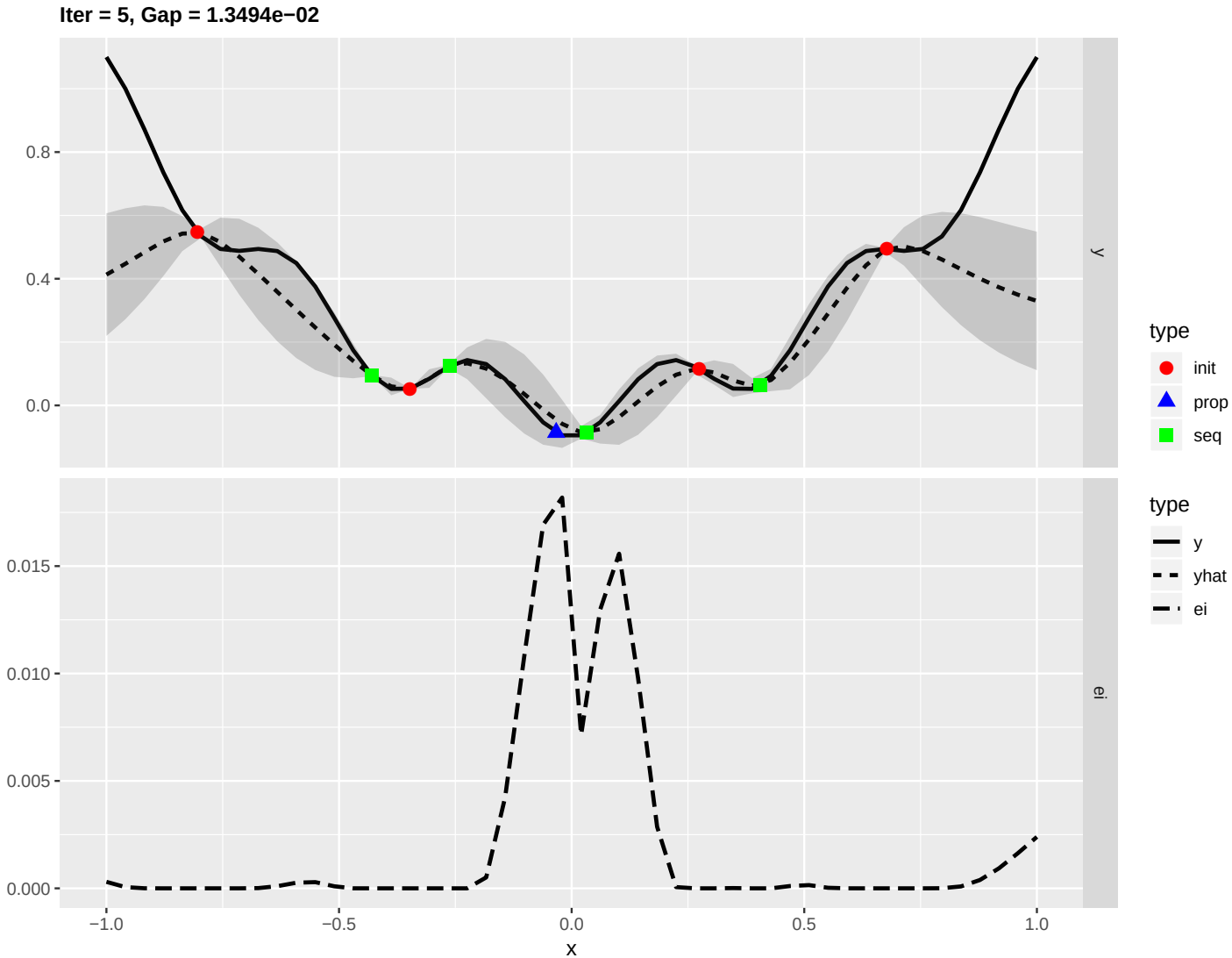

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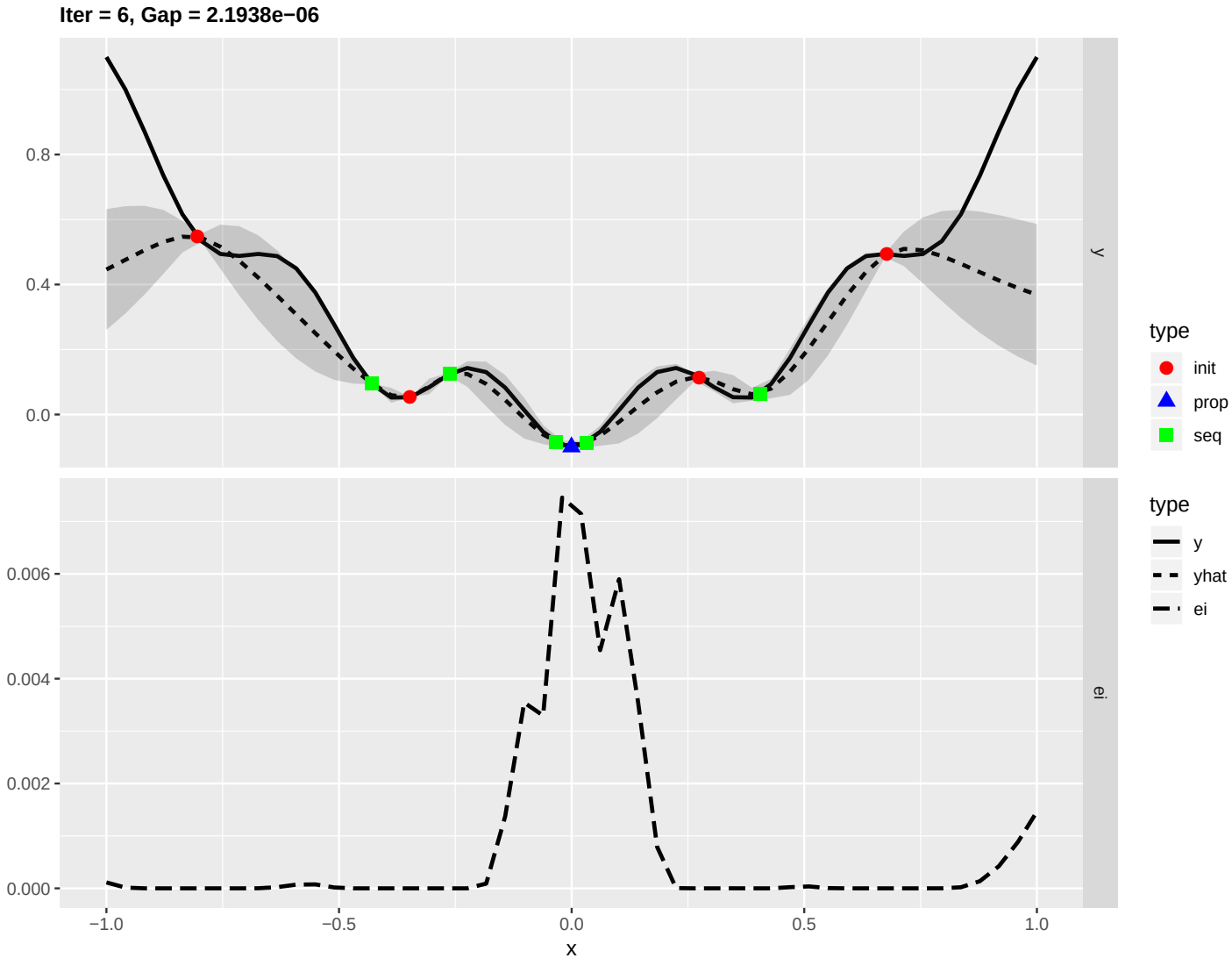

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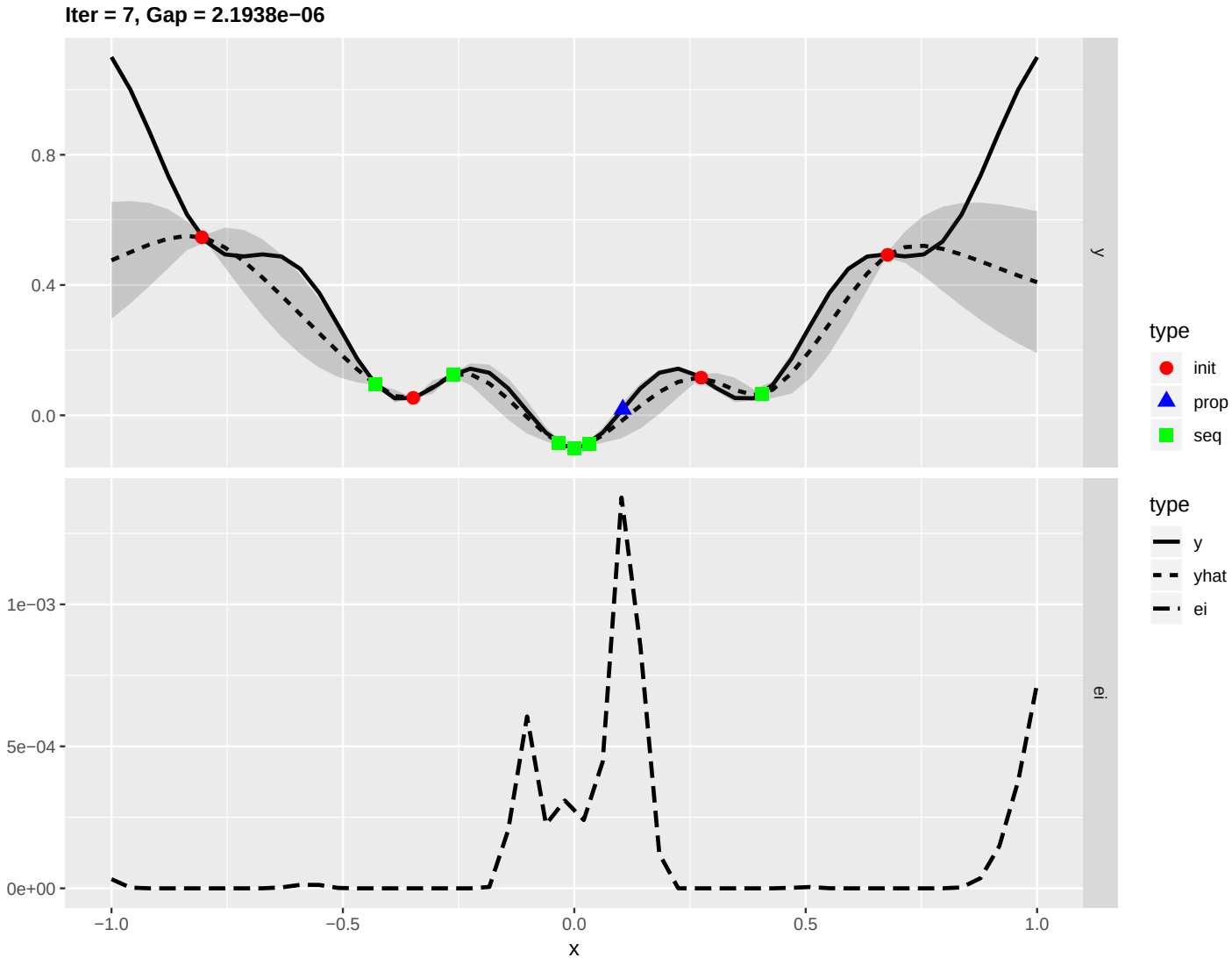

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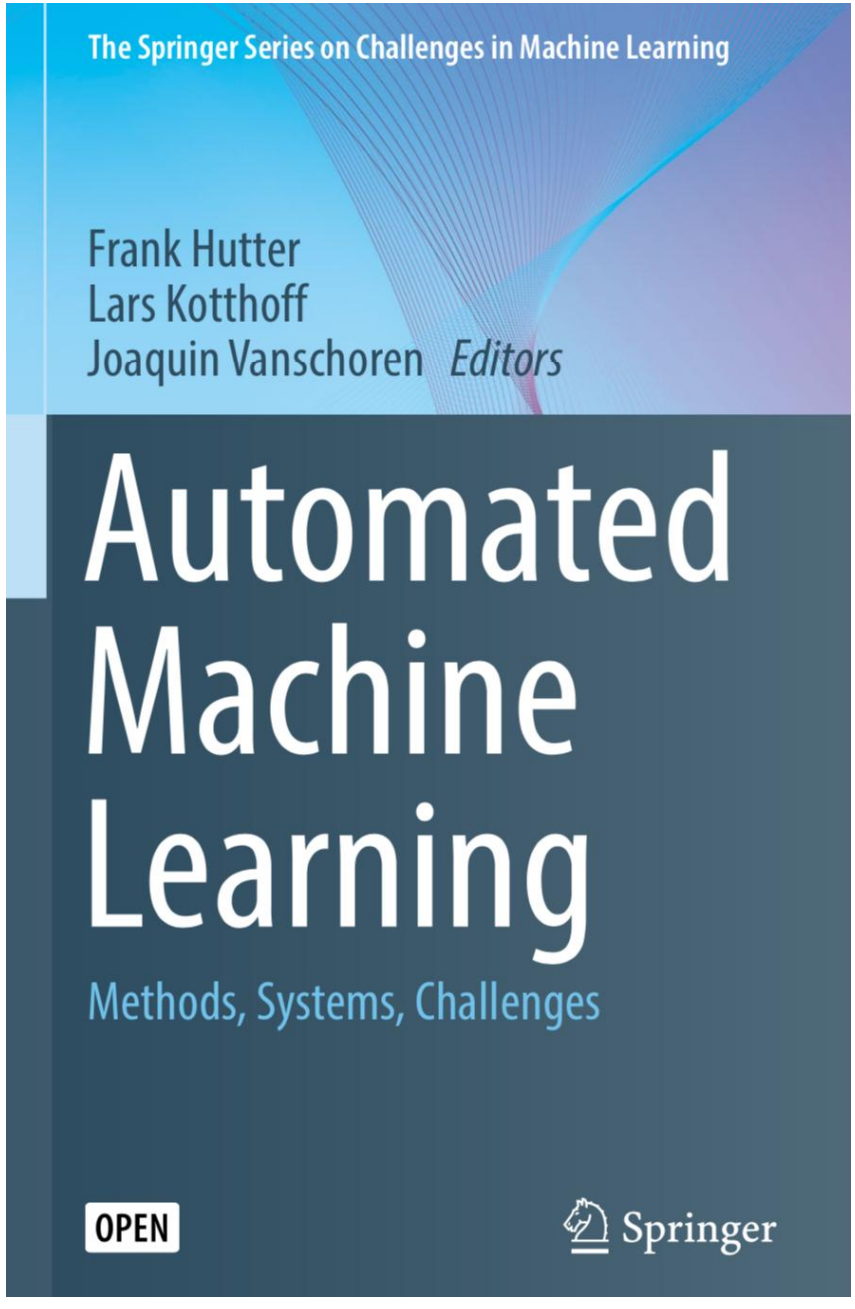
Tools and Resources

iRace	`http://iridia.ulb.ac.be/irace/`
TPOT	`https://github.com/EpistasisLab/tpot`
mlrMBO	`https://github.com/mlr-org/mlrMBO`
SMAC	`http://www.cs.ubc.ca/labs/beta/Projects/SMAC/`
Spearmint	`https://github.com/HIPS/Spearmint`
TPE	`https://jaberg.github.io/hyperopt/`

COSEAL group for COnfiguration and SElection of ALgorithms: `https://www.coseal.net/`

Further reading: Jones, Donald R., Matthias Schonlau, and William J. Welch. "Efficient Global Optimization of Expensive Black-Box Functions." J. of Global Optimization 13, no. 4 (December 1998): 455–92.



https://www.automl.org/book/

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NSF

Exercises

- (install python and/or scikit-learn)
- download `https://www.cs.uwyo.edu/~larsko/mbo/mbo.py` and run it
- try a different data set
- try tuning different/more parameters
- ...

Two-Slide MBO

```
# https://www.cs.uwyo.edu/~larsko/mbo/mbo.py
params = { 'C': np.logspace(-2, 10, 13),
           'gamma': np.logspace(-9, 3, 13) }
param_grid = [ { 'C': x, 'gamma': y } for x in params['C']
                                       for y in params['gamma'] ]
# [{'C': 0.01, 'gamma': 1e-09}, {'C': 0.01, 'gamma': 1e-08}...]

initial_samples = 3
evals = 10
random.seed(1)

def est_acc(pars):
    clf = svm.SVC(**pars)
    return np.median(cross_val_score(clf, iris.data, iris.target, cv = 10))

data = []
for pars in random.sample(param_grid, initial_samples):
    acc = est_acc(pars)
    data += [ list(pars.values()) + [ acc ] ]
# [[1.0, 0.1, 1.0],
#  [1000000000.0, 1e-07, 1.0],
#  [0. 1, 1e-06,0.9333333333333333]]
```

Two-Slide MBO

```
regr = RandomForestRegressor(random_state = 0)
for evals in range(0, evals):
    df = np.array(data)
    regr.fit(df[:,0:2], df[:,2])

    preds = regr.predict([ list(pars.values()) for pars in param_grid ])
    i = preds.argmax()

    acc = est_acc(param_grid[i])
    data += [ list(param_grid[i].values()) + [ acc ] ]
    print("{}: best predicted {} for {}, actual {}"
            .format(evals, round(preds[i], 2), param_grid[i], round(acc, 2)))

i = np.array(data)[:,2].argmax()
print("Best accuracy ({}) for parameters {}".format(data[i][2], data[i][0:2]))
```

Two-Slide MBO (slide 3)

```
0: best predicted 0.99 for {'C': 1.0, 'gamma': 1e-09}, actual 0.93
1: best predicted 0.99 for {'C': 1000000000.0, 'gamma': 1e-09}, actual 0.93
2: best predicted 0.99 for {'C': 1000000000.0, 'gamma': 0.1}, actual 0.93
3: best predicted 0.97 for {'C': 1.0, 'gamma': 0.1}, actual 1.0
4: best predicted 0.99 for {'C': 1.0, 'gamma': 0.1}, actual 1.0
5: best predicted 1.0 for {'C': 1.0, 'gamma': 0.1}, actual 1.0
6: best predicted 1.0 for {'C': 1.0, 'gamma': 0.1}, actual 1.0
7: best predicted 1.0 for {'C': 1.0, 'gamma': 0.1}, actual 1.0
8: best predicted 1.0 for {'C': 0.01, 'gamma': 0.1}, actual 0.93
9: best predicted 1.0 for {'C': 1.0, 'gamma': 0.1}, actual 1.0
Best accuracy (1.0) for parameters [1.0, 0.1]
```