Bayesian Optimization Tutorial

Why Go Beyond Traditional Optimization?

Joel Paulson
Assistant Professor, Department of Chemical and Biomolecular Engineering, The Ohio State University

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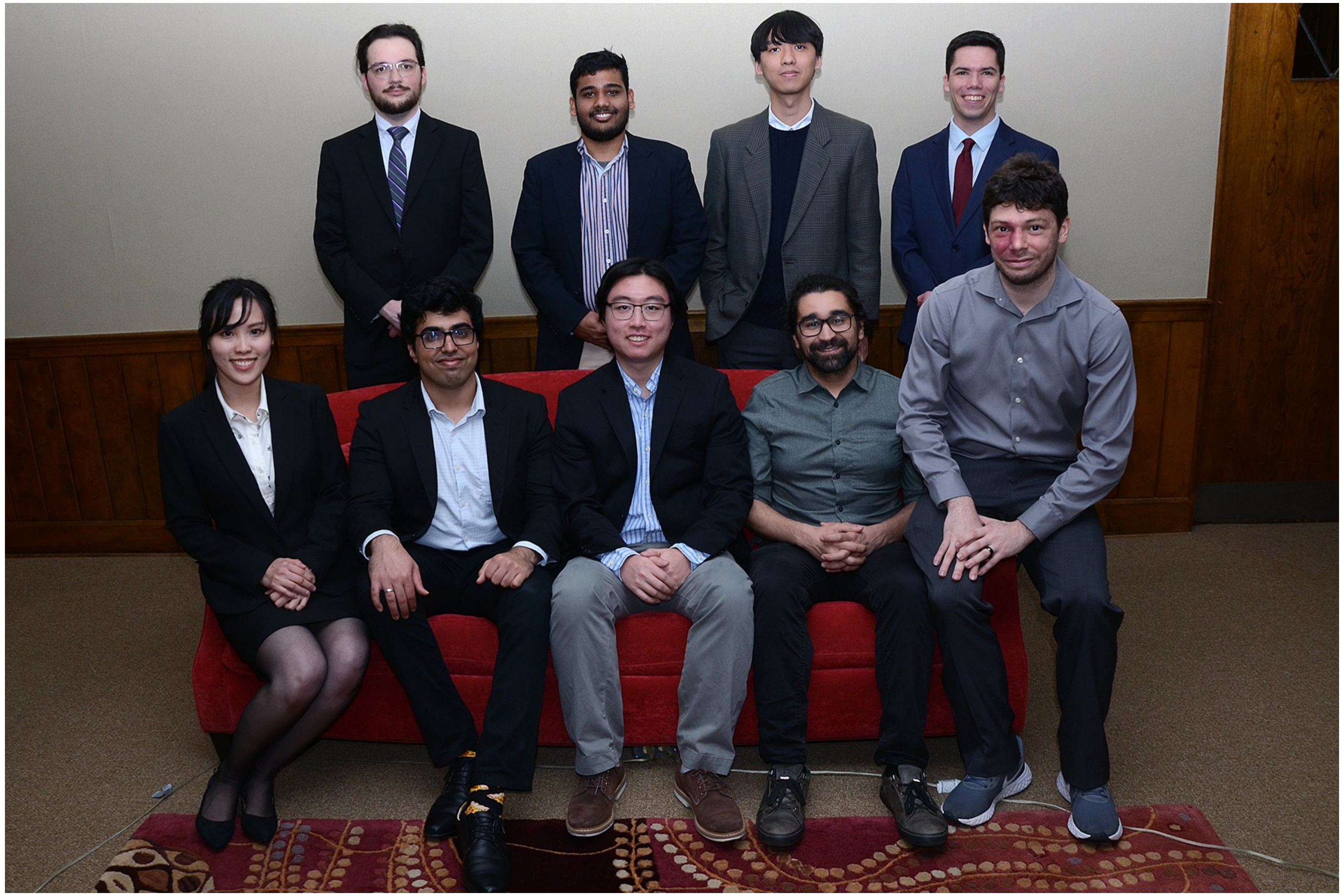
For copies of slides & code, see
https://github.com/joelpaulson/Great_Lakes_PSE_Workshop_2023

Thank you to My Group for Help Developing Materials! (Especially the Code for the Modules)



What is an Optimization Problem?

decision (design) variables

$$\min_{x} \quad f(x)$$

objective function

$$\text{s.t.} \quad x \in \Omega$$

constraints (feasible region)

- Optimization problems are **pervasive** in every application domain
  - differentiate problems based on characteristics → determine what solver to use

- There are a huge number of available optimization algorithms; difficult to *a priori* know the best one but we can eliminate some options

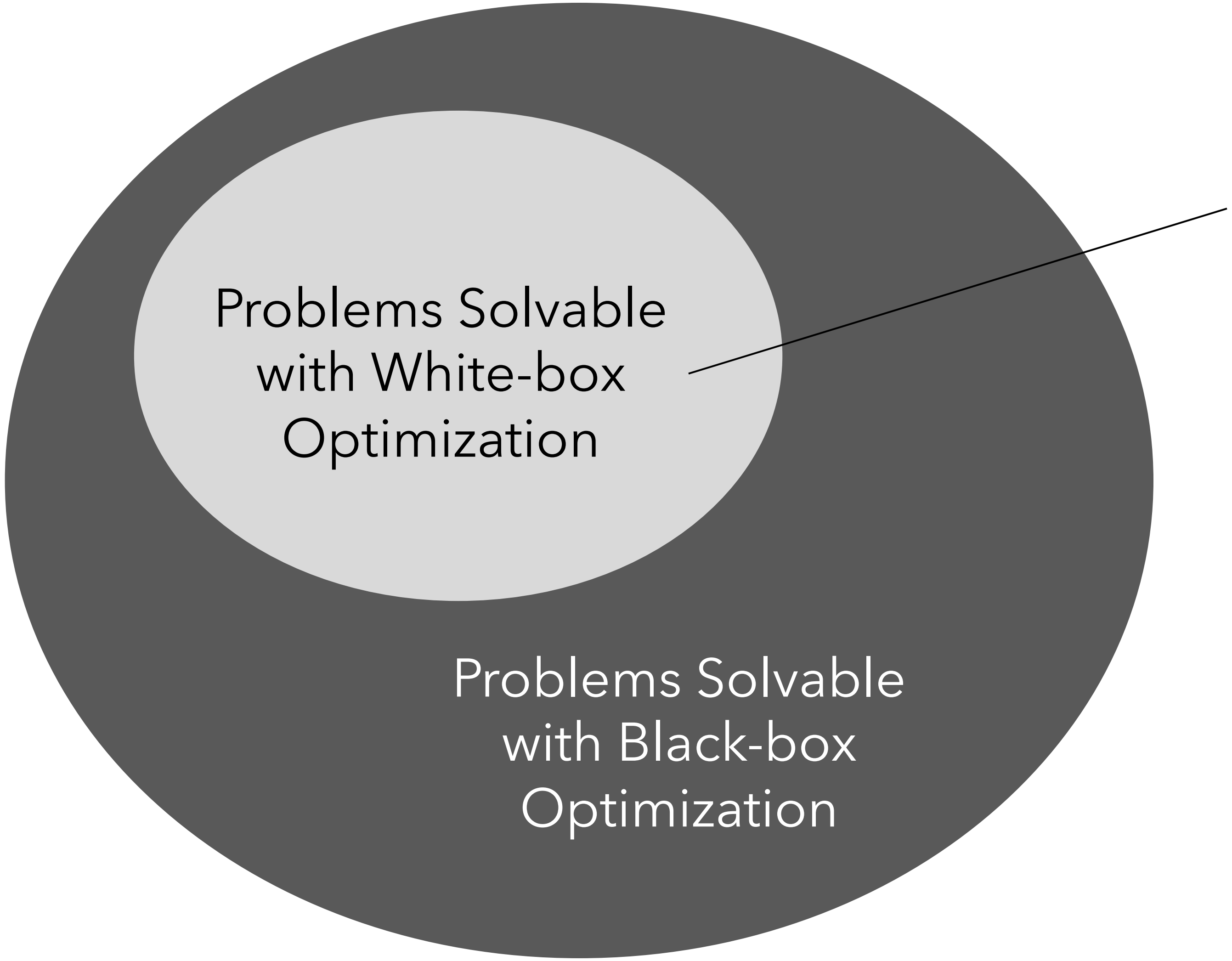
How to Classify Optimization Algorithms?

- A simple way to "partition" the algorithms into two major buckets are "white-box" and "black-box" (i.e., not white box)

- White-box means that we need an "equation-oriented model" of the system so that the mathematical structure of $f(x)$ and Ω satisfy certain important assumptions
  - The exact assumptions depend on the method, but they will typically require the functions to be differentiable and/or easy to build relaxations of them

- Any method that only requires evaluations of $f(x)$ and $x \in \Omega$ at specific points can then be classified as "black box"

How to Classify Optimization Algorithms?



Since white-box algorithms make stronger assumptions, they can only be used to tackle a subset of problems when compared to black-box algorithms

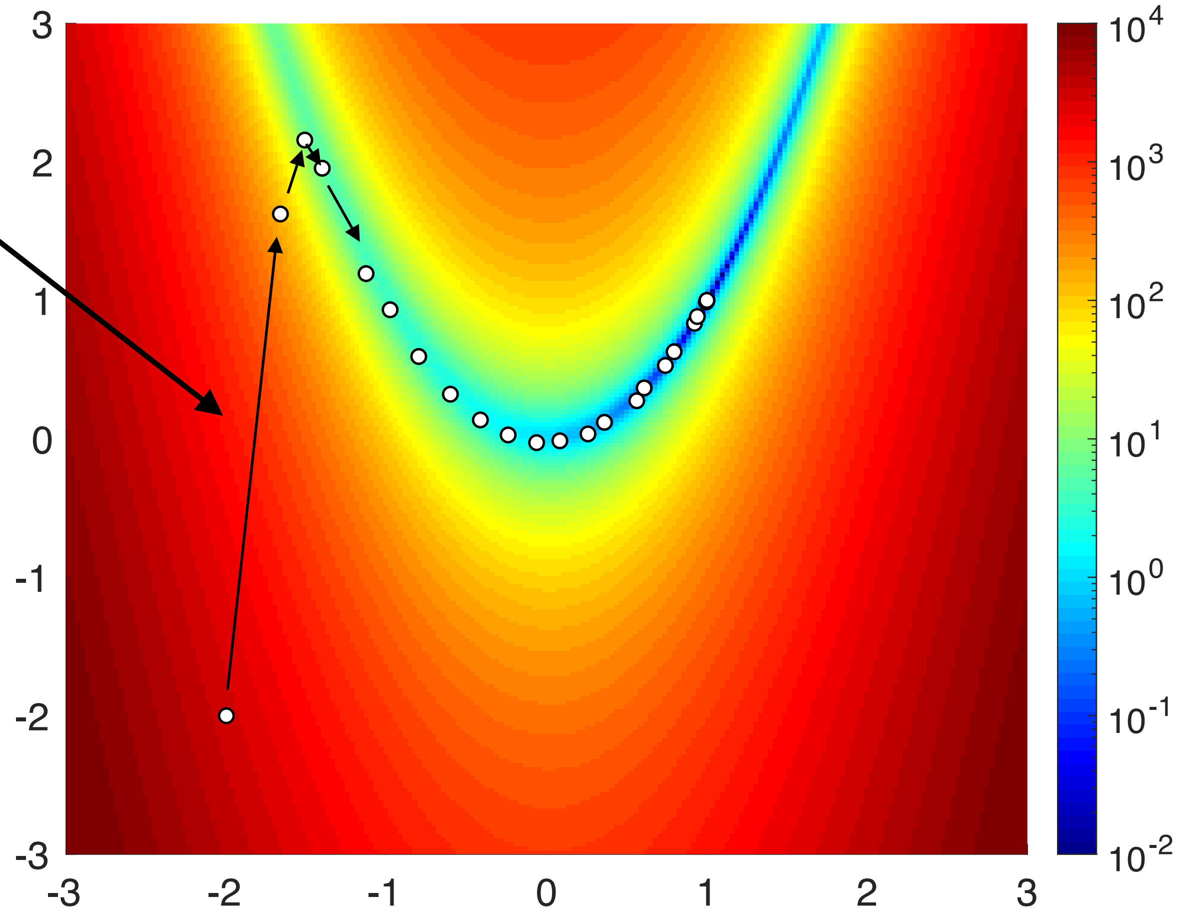
→ The main value of black-box methods are their generality (not necessarily efficient)

Example of White-Box Optimization: Newton's Method

Use derivatives to take step toward reducing objective, i.e.,

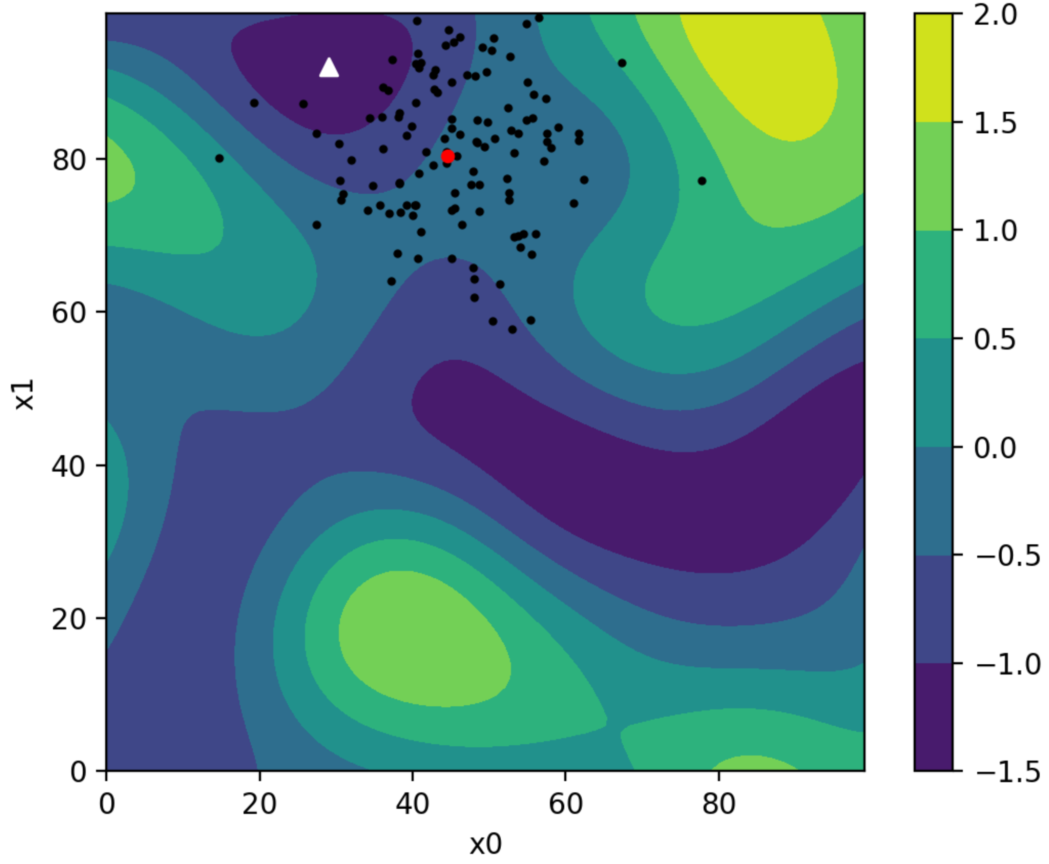
$$x_{k+1} = x_k - \alpha_k \underline{\left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)}$$

This type of algorithm is "local" (requires initial guess) & requires ability to compute derivatives (expensive when the structure of the function is unknown)



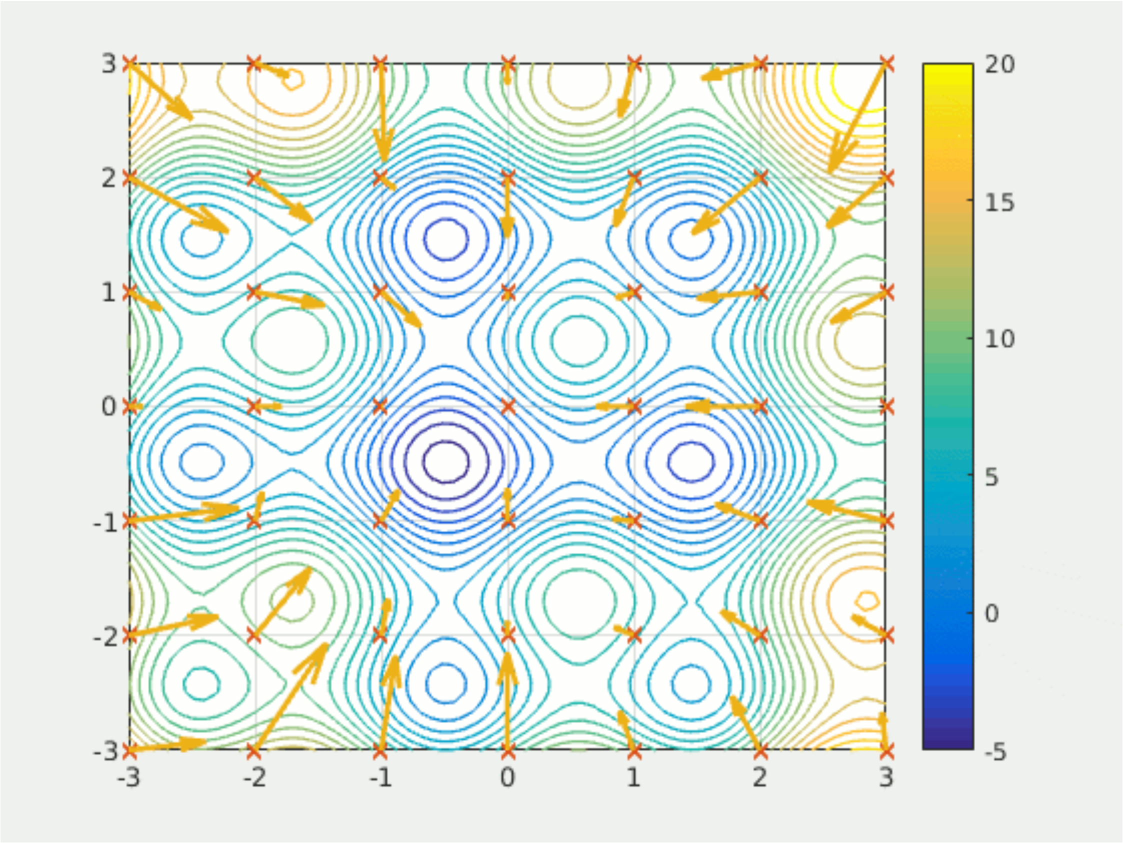
Examples of Black-Box (Derivative-Free) Optimization

Covariance Matrix Adaptive Evolutionary Strategy (CMA-ES)



https://thurinj.github.io/CMA-ES.html

Particle Swarm Optimization (PSO)



https://en.wikipedia.org/wiki/Particle_swarm_optimization

Many derivative-free optimization methods, which to choose?

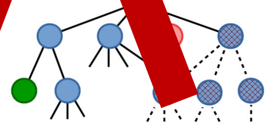
This is really our only option when function evaluations are ***expensive*** (enables us to use all data)

Derivative Free Optimization (DFO)

Deterministic DFO

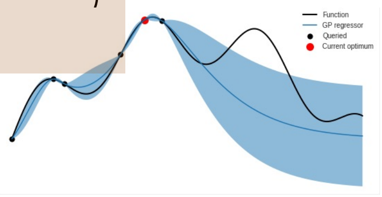
Lipschitzian-based partitioning techniques

- DIRECT Algorithm
- Branch and bound (BB) search



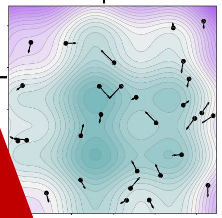
Surrogate-based search algorithms

- Trust-region methods
- Branch & fit algorithm
- Radial basis function (RBF) methods
- ***Bayesian Optimization***



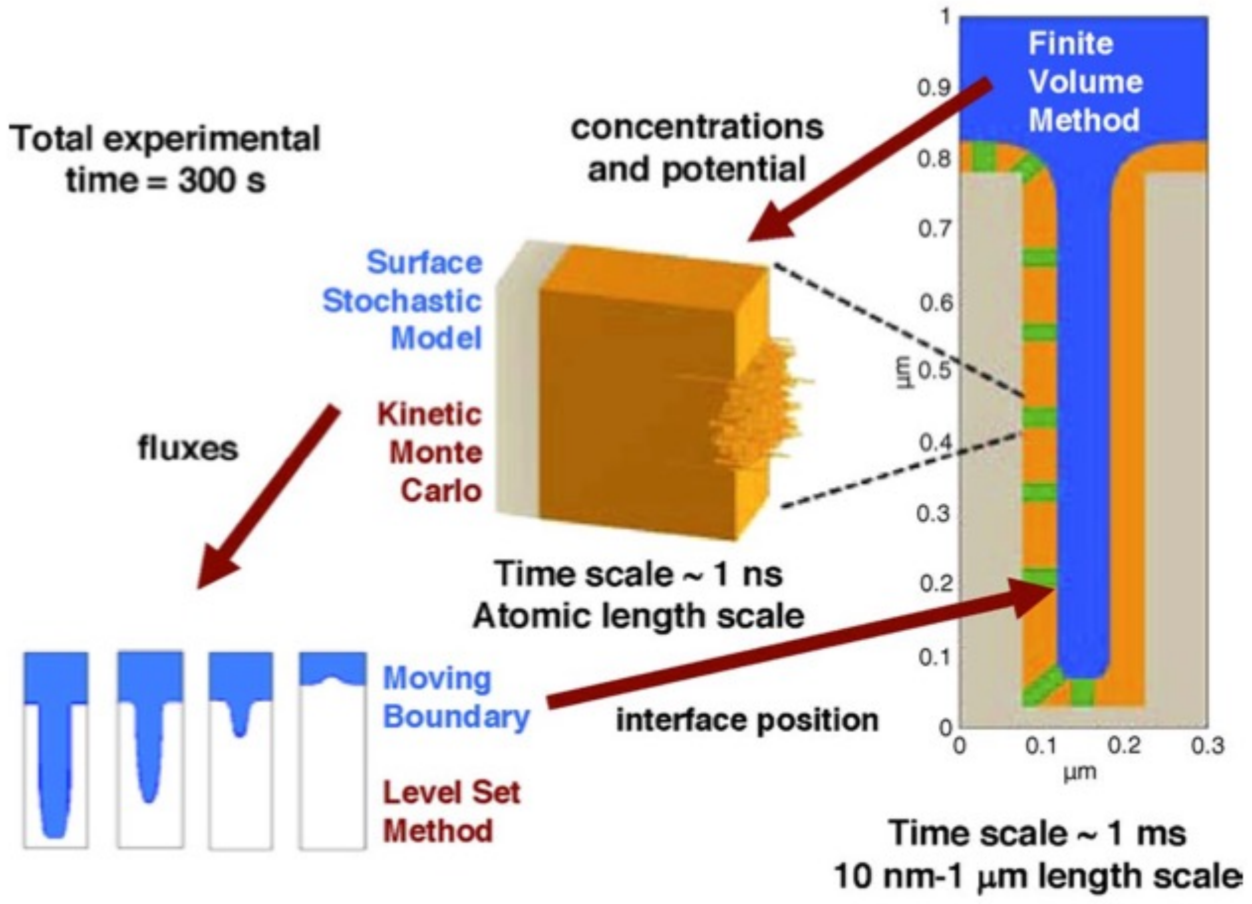
Stochastic DFO

- Hit-and-run
- Simulated annealing
- Genetic Algorithm
- Particle swarm



Expensive functions, they are everywhere

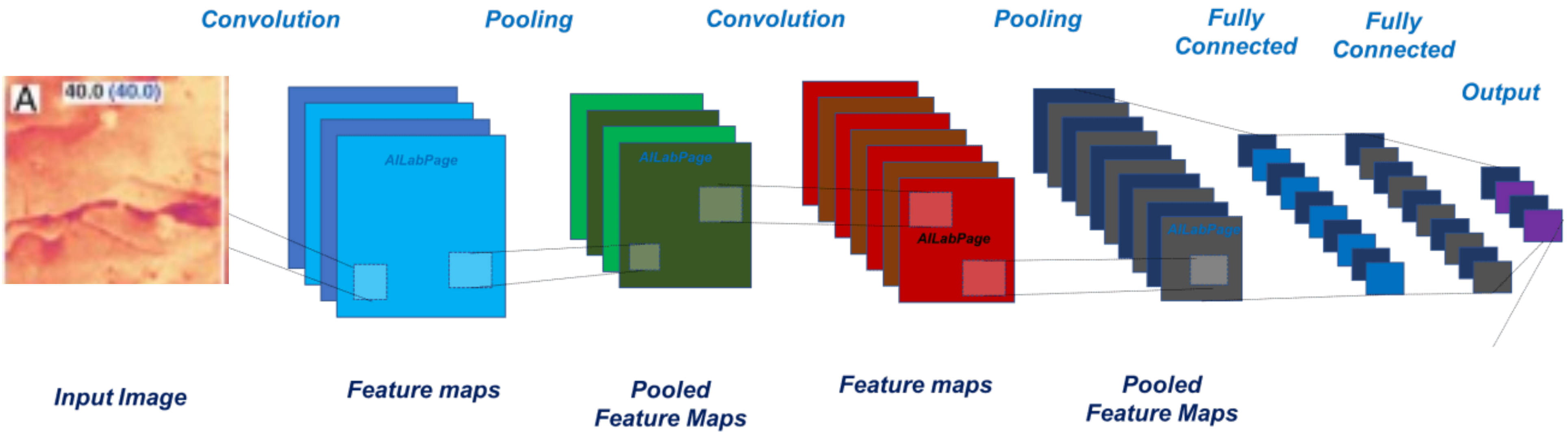
- **Optimizing multi-scale simulation models**



- **Objective:**
  Minimize surface roughness
- **Design variables:**
  Chemical additive concentrations & reaction temperature

Expensive functions, they are everywhere

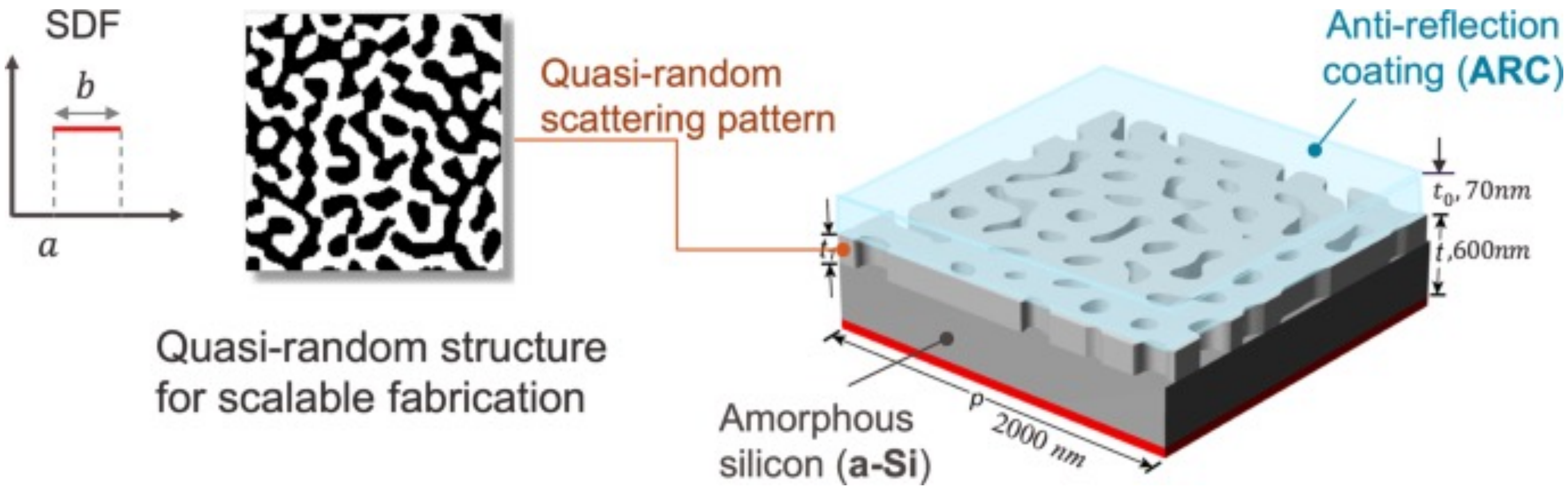
- **Automated machine learning**



- **Objective:** Maximize classification accuracy for image-based chemical sensor
- **Design variables:** Number of layers, number of nodes per layer, learning rates, regularization penalties, activation functions, etc.

Expensive functions, they are everywhere

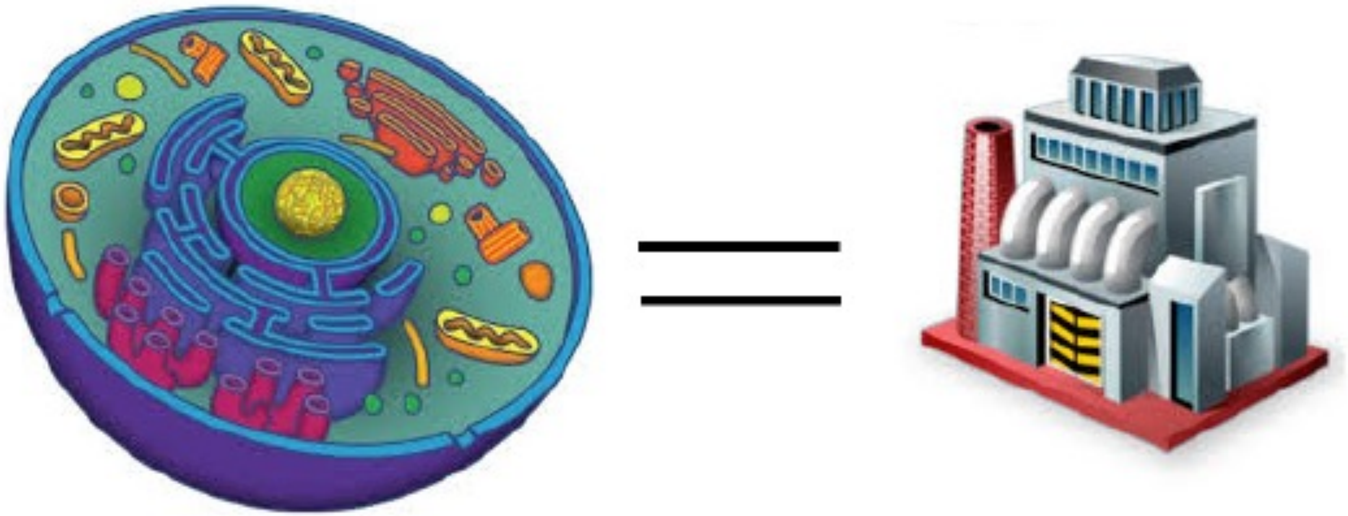
- **Material and drug discovery**



- **Objective:** Maximize light adsorption in quasi-random solar cell
- **Design variables:** Type of amorphous silicon (a-Si), light trapping pattern for fabrication, & overall thickness

Expensive functions, they are everywhere

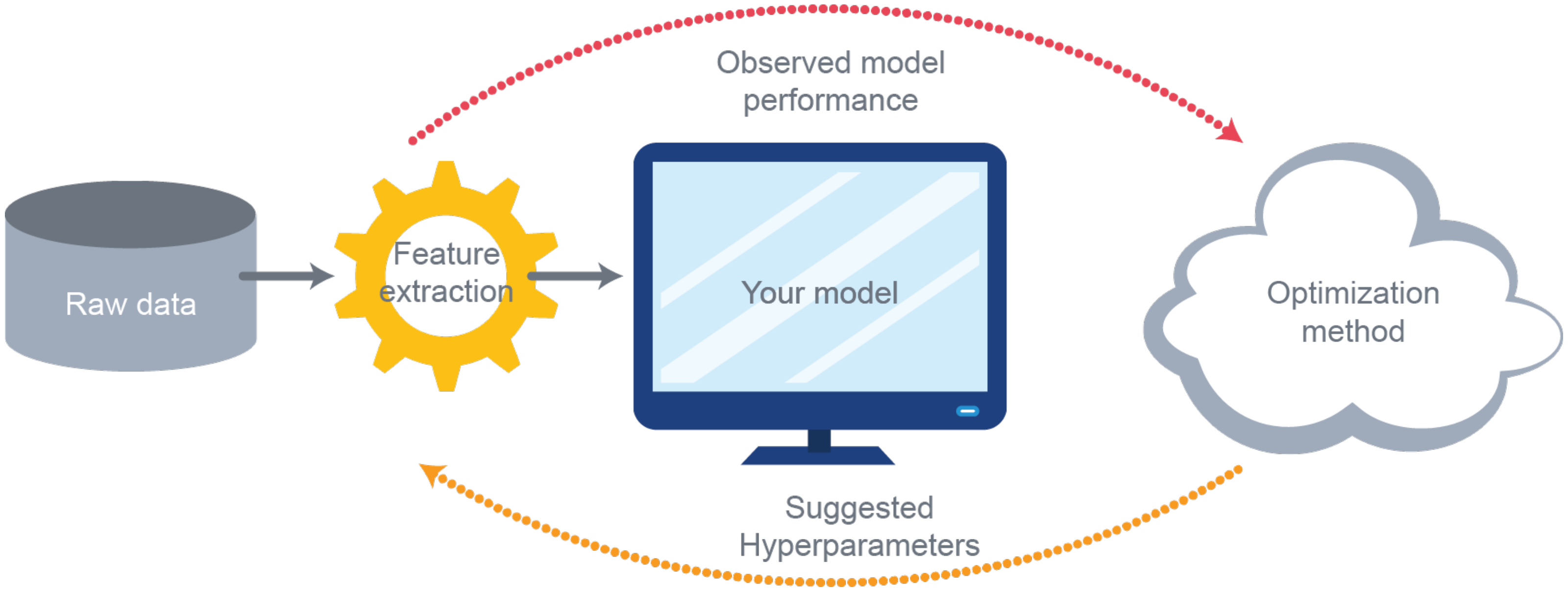
- **Design of experiments: Gene optimization**



  - **Objective:** Maximize efficiency of the cell factory to make product (e.g., proteins)
  - **Design variables:** Gene sequence (e.g., ATTGGTUGA…) & culture conditions (e.g,. pH)

Expensive functions, they are everywhere

- **Tuning hyperparameters in optimization codes**



- **Objective:** Minimize solution time for family of scheduling/planning problems
- **Design variables:** Algorithmic parameters in solver (e.g., CPLEX has 76 design parameters)

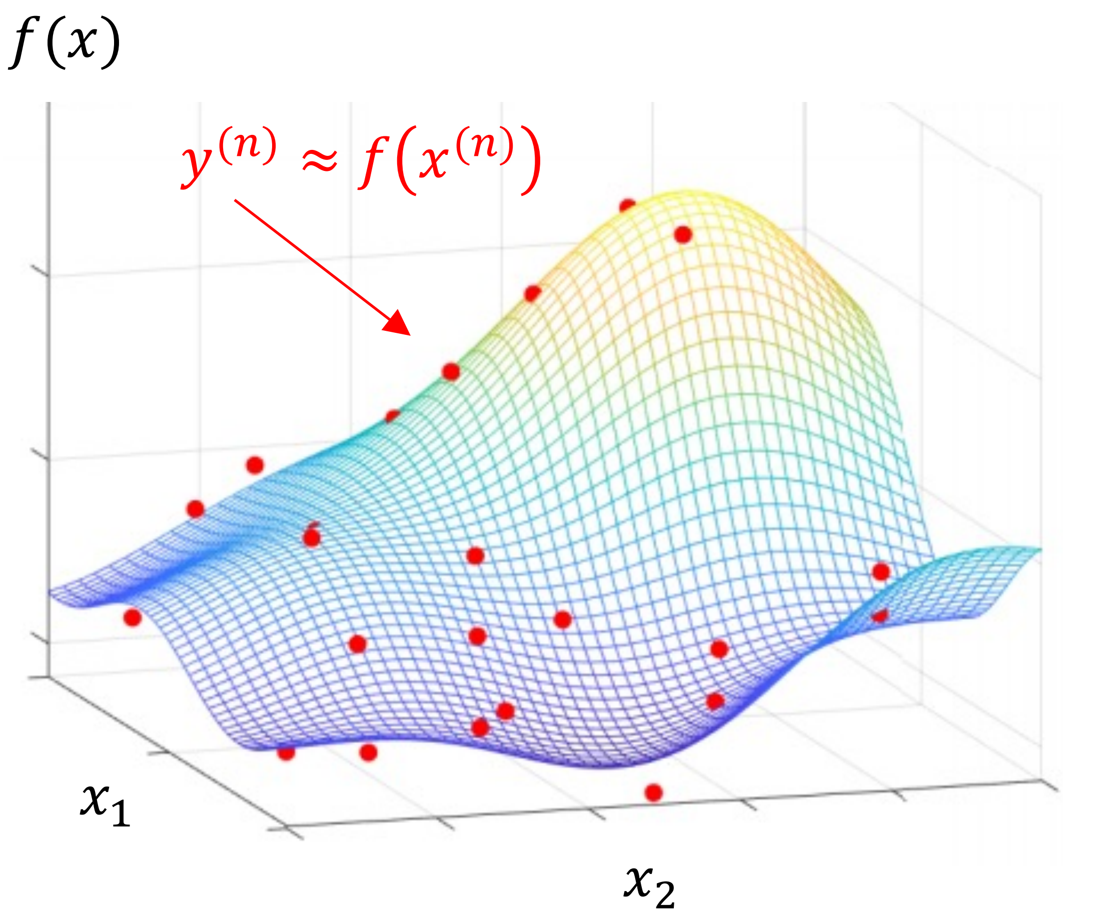
https://sigopt.com/blog/common-problems-in-hyperparameter-optimization/

Expensive functions, they are everywhere

- **Many other problems:**
  - Robotics, aerospace, control, reinforcement learning
  - Tuning websites with A/B testing
  - Calibrating expensive simulators to experimental data
  - etc.…

Standard Goal in Bayesian Optimization:

Optimize functions f : $\mathbb{R}^d \rightarrow \mathbb{R}$ that are:

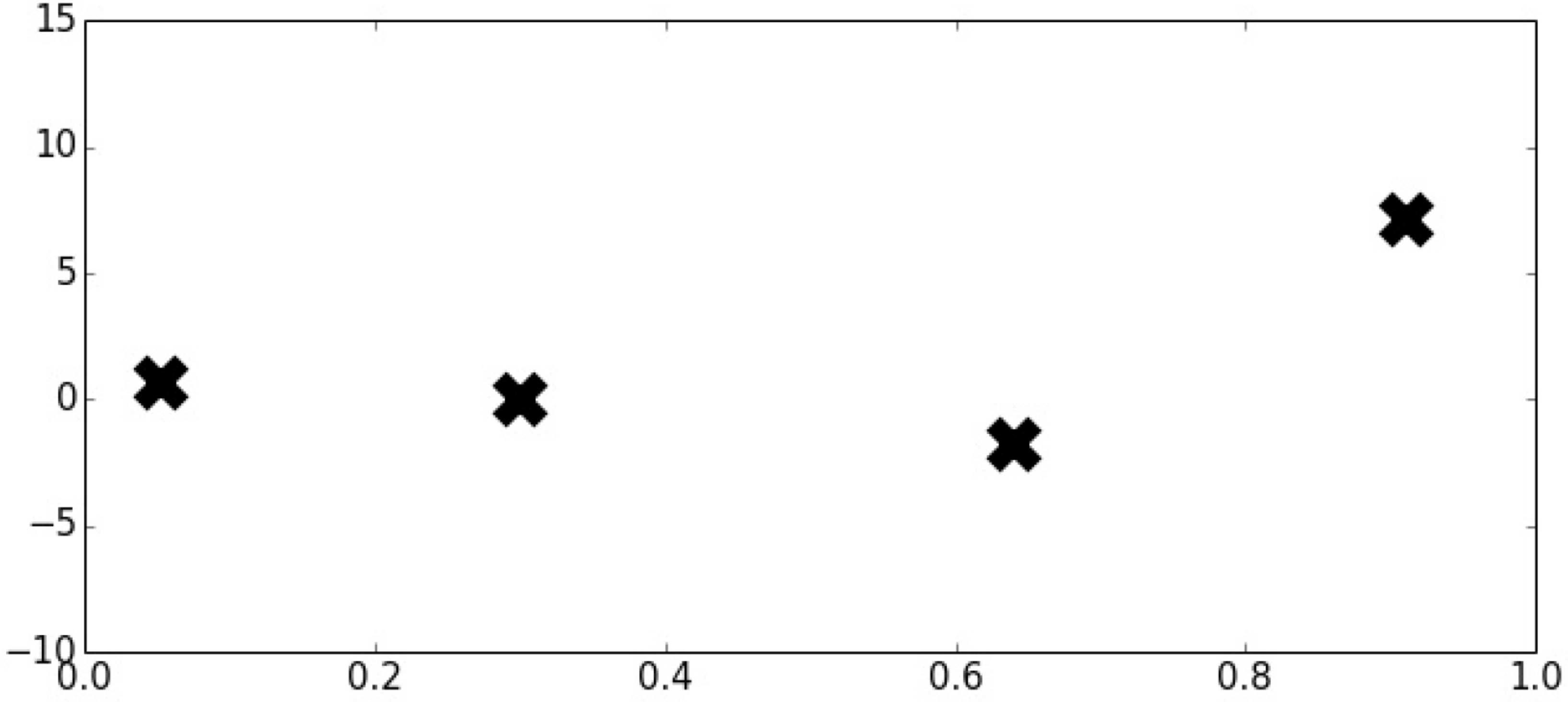


- f(·) is explicitly unknown & non-convex
  - lacks known special structure, e.g., convexity
- f(·) is derivative-free
  - cannot simply get gradients
- f(·) is expensive to evaluate
  - # of evaluations is **severely limited**
- f(·)'s evaluations may be noisy
  - noise independent & ~normally distributed, but unknown variance

*We will deal with black-box constraints later

Illustrative example to build some intuition

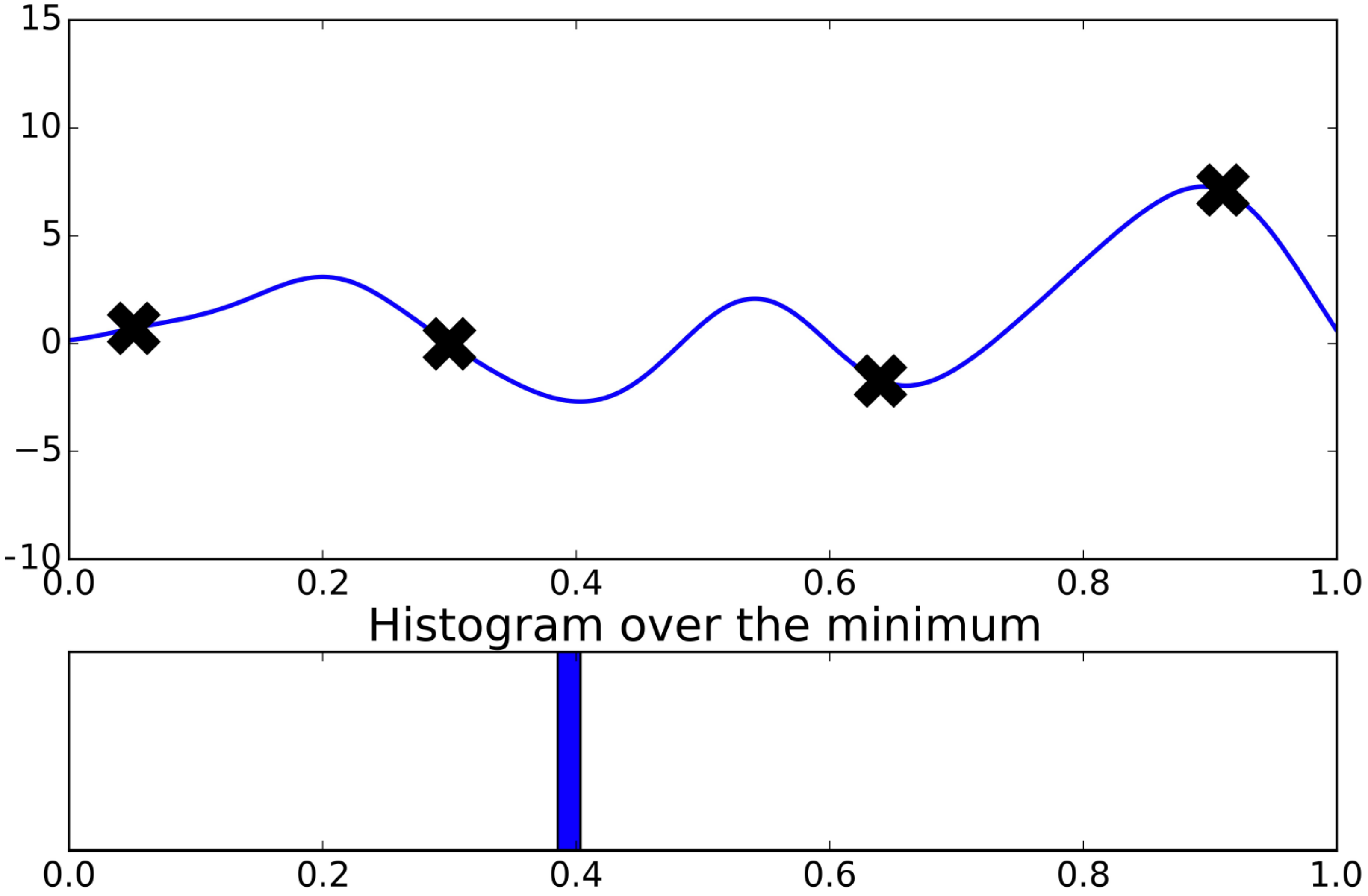
We have four function evaluations



- Where is the minimum of the function f(·)?
- Where should we take our next evaluation?

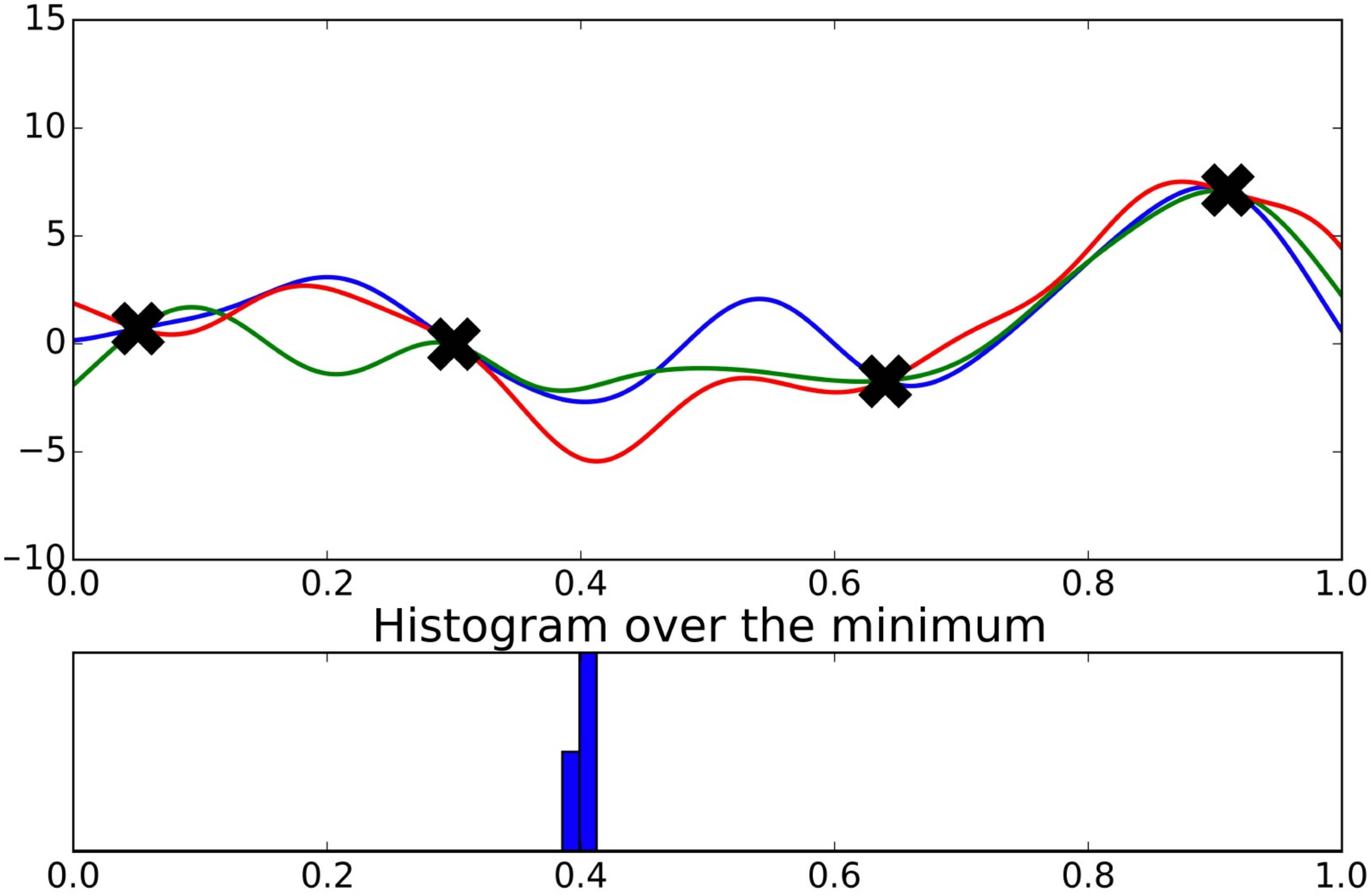
Intuitive solution, fit a surrogate model

One curve; which one should we select?



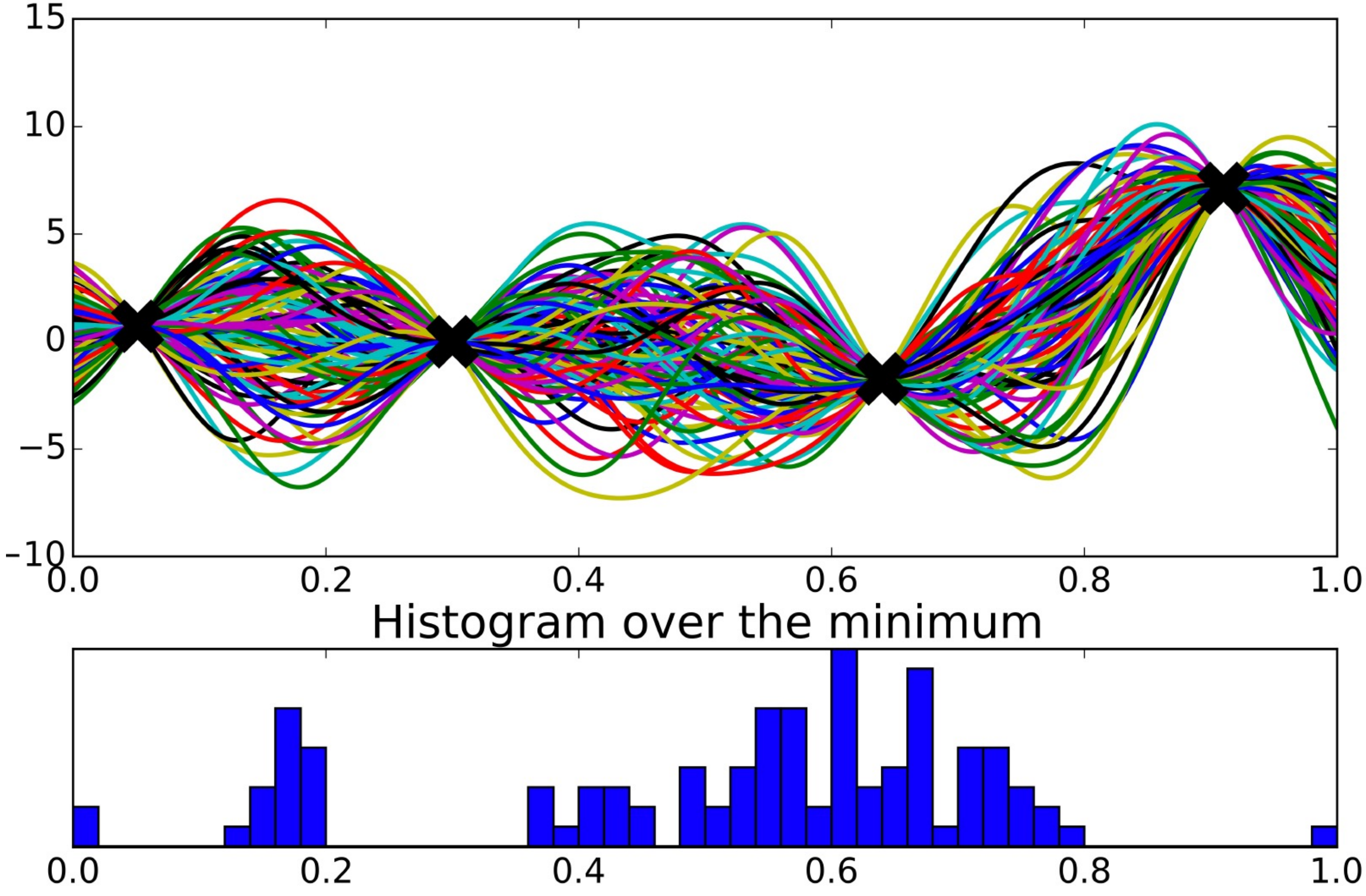
Intuitive solution, fit a surrogate model

Three curves



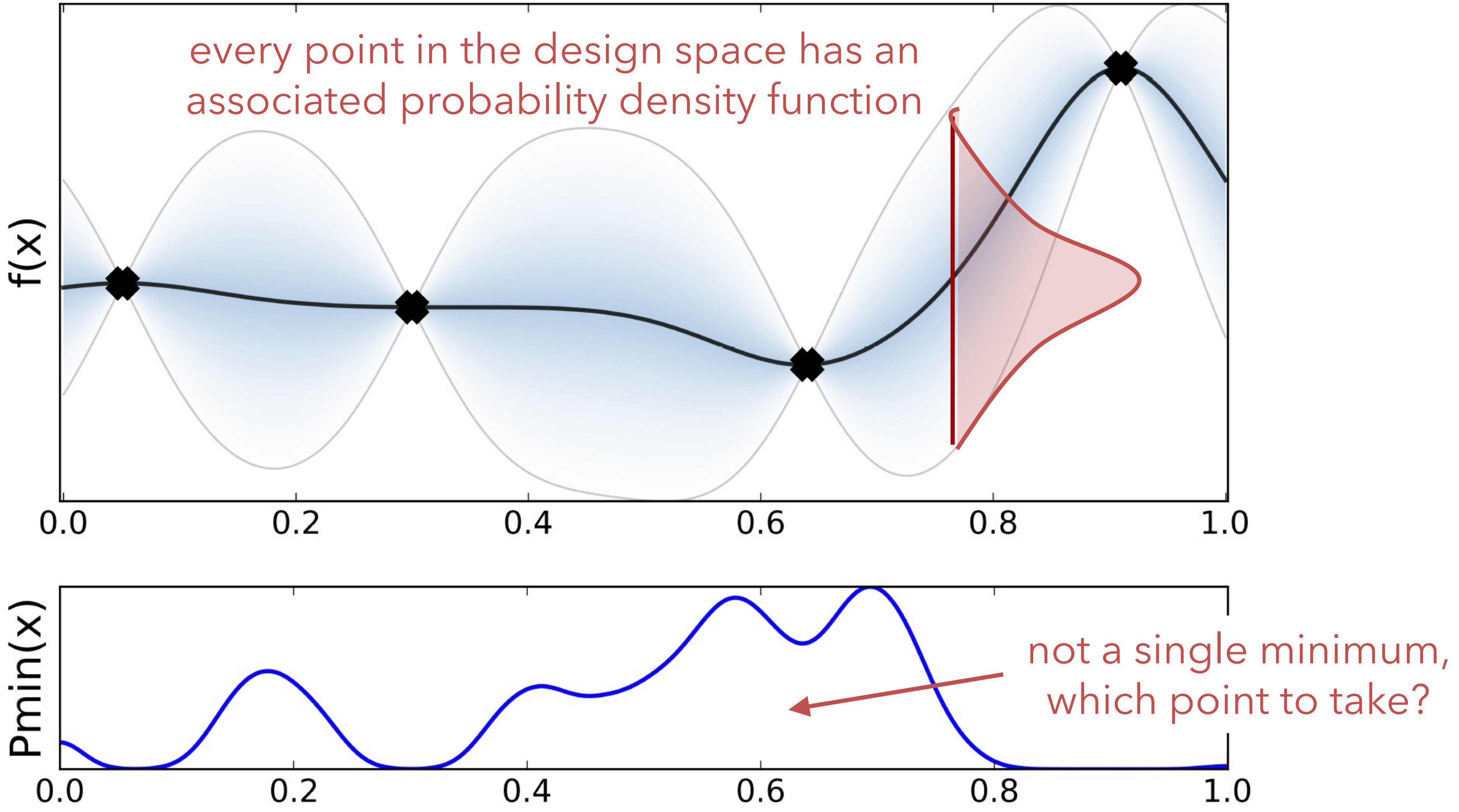
Intuitive solution, fit a surrogate model

One hundred curves



Intuitive solution, fit a surrogate model
Infinite curves

(Need the help of information theory to properly define models + metrics)



Bird's-eye View of Bayesian Optimization

Module 3

while {budget not exhausted}

Module 1

Fit a Bayesian machine learning model
(usually Gaussian process regression)
to observations {x, f(x)}

Find x that maximizes acquisition(x, posterior)

Module 2

Sample x & then observe f(x)

end

More Information

Module 4

Workshop Schedule

9:00 – 9:20	Introduction: Why Go Beyond Traditional Optimization?
9:20 – 10:20	Module 1: Probabilistic Surrogate Modeling*
10:20 – 10:30	Break
10:30 – 11:20	Module 2: Quantifying the Value of Information*
11:20 – 12:20	Module 3: The BO Feedback Loop*
12:20 – 12:30	Break
12:30 – 1:00	Module 4: Beyond Bayesian Optimization

*module includes Python code review / exercises