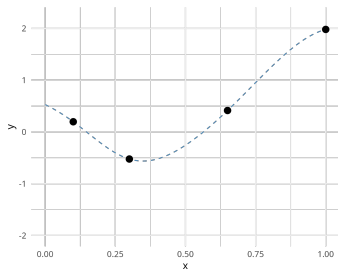


Optimization in Machine Learning

Bayesian Optimization

Basic BO Loop and Surrogate Modelling



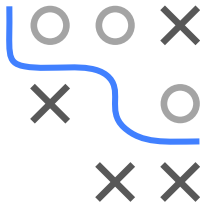
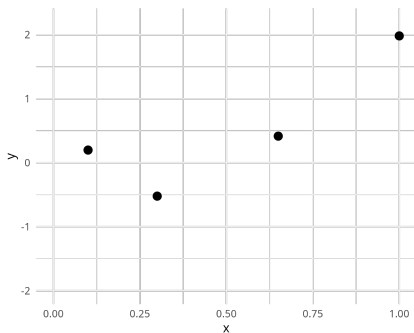
Learning goals

- Initial design
- Surrogate modeling
- Basic loop

OPTIMIZATION VIA SURROGATE MODELING

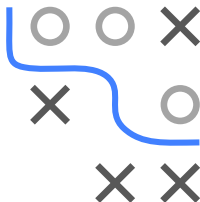
Starting point:

- We do not know the objective function $f : \mathcal{S} \rightarrow \mathbb{R}$
- But we can evaluate f for a few different inputs $\mathbf{x} \in \mathcal{S}$
- For now we assume that those evaluations are noise-free
- **Idea:** Use the data $\mathcal{D}^{[t]} = \{(\mathbf{x}^{[i]}, y^{[i]})\}_{i=1, \dots, t}$, $y^{[i]} := f(\mathbf{x}^{[i]})$, to derive properties about the unknown function f



INITIAL DESIGN

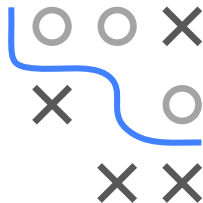
- Should cover / explore input space sufficiently:
 - Random design
 - Latin hypercube sampling
 - Sobol sampling
- Type of design usually has not the largest effect
- A more important choice is the **size** of the initial design
 - Should neither be too small (bad initial fit) nor too large (spending too much budget without doing “intelligent” optimization)
 - Rule of thumb: $4d$



LATIN HYPERCUBE SAMPLING

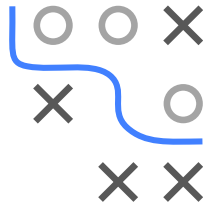
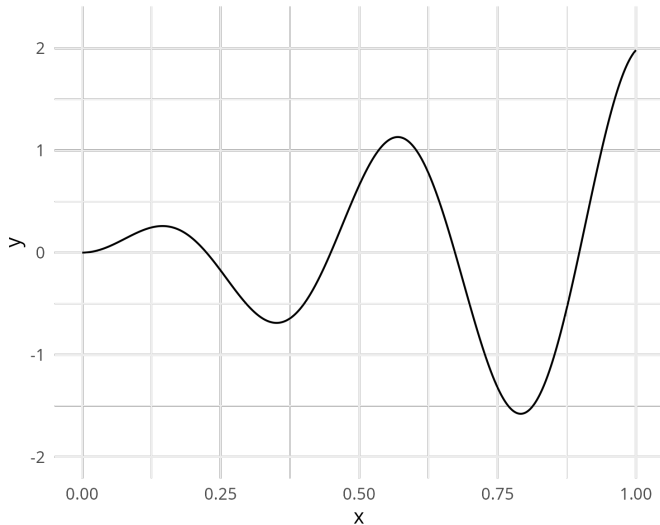
Actual sampling of points, e.g., constructed via **Maximin**:

- The minimum distance between any two points in \mathcal{D} is $2q = \min_{\mathbf{x} \in \mathcal{D}, \mathbf{x}' \in \mathcal{D}} \rho(\mathbf{x}, \mathbf{x}')$ (ρ any metric, e.g., Euclidean distance)
- q is the packing radius - the radius of the largest ball that can be placed around every design point such that no two balls overlap
- Goal: Find \mathcal{D} that maximizes $2q$: $\max_{\mathcal{D}} \min_{\mathbf{x} \in \mathcal{D}, \mathbf{x}' \in \mathcal{D}} \rho(\mathbf{x}, \mathbf{x}')$
- Ensures that the design points in \mathcal{D} are as far apart from each other as possible



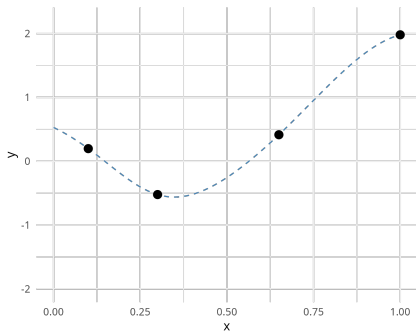
SURROGATE MODELING

Running example = minimize this “black-box”:

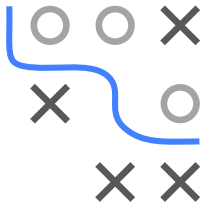


SURROGATE MODELING

- ❶ Fit a **regression model** $\hat{f} : \mathcal{D}^{[t]} \rightarrow \mathbb{R}$ (blue) to extract maximum information from the design points (black) and learn properties of f

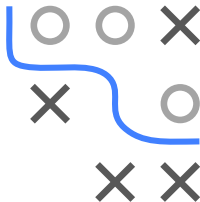
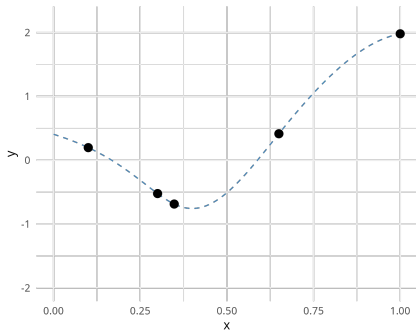


As we can eval f without noise, we fit an interpolator



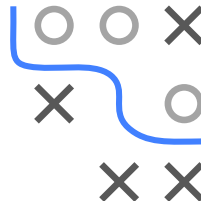
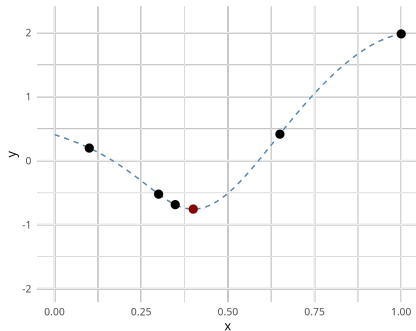
SURROGATE MODELING

- After evaluation of the new point, we **adjust** the model on the expanded dataset via (slower) refitting or a (cheaper) online update



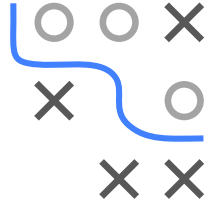
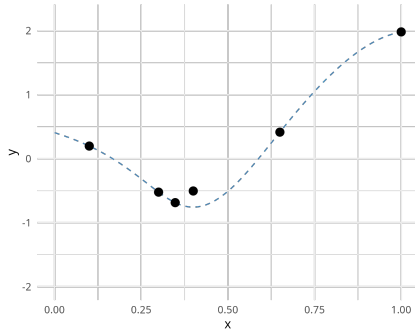
SURROGATE MODELING

- We again obtain a new candidate point (red) by optimizing the cheap surrogate model function (blue) ...



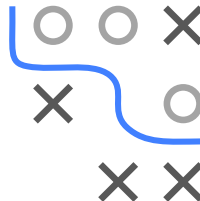
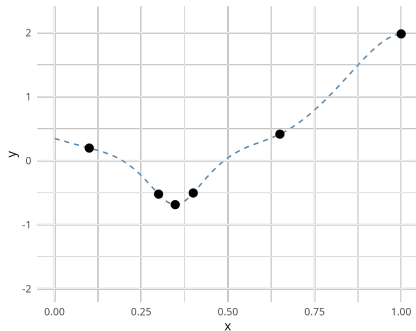
SURROGATE MODELING

- ... and evaluate that candidate



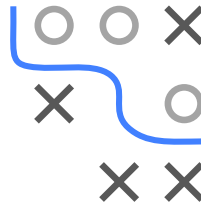
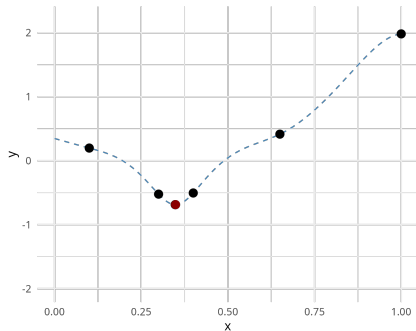
SURROGATE MODELING

- We repeat: (i) **fit** the model



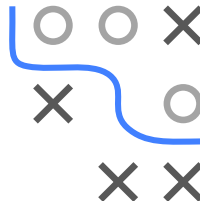
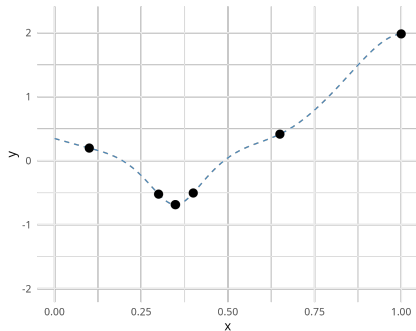
SURROGATE MODELING

- (ii) **propose** a new point



SURROGATE MODELING

- (iii) **evaluate** that point

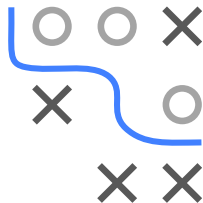


- We observe that the algorithm converged

BASIC LOOP

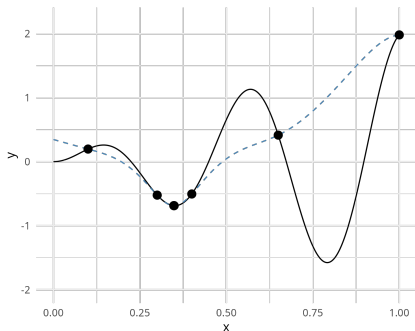
The basic loop of our sequential optimization procedure is:

- 1 Fit surrogate model \hat{f} on previous evaluations
 $\mathcal{D}^{[t]} = \{(\mathbf{x}^{[i]}, y^{[i]})\}_{i=1, \dots, t}$
- 2 Optimize the surrogate model \hat{f} to obtain a new point
 $\mathbf{x}^{[t+1]} := \arg \min_{\mathbf{x} \in \mathcal{S}} \hat{f}(\mathbf{x})$
- 3 Evaluate $\mathbf{x}^{[t+1]}$ and update data
 $\mathcal{D}^{[t+1]} = \mathcal{D}^{[t]} \cup \{(\mathbf{x}^{[t+1]}, f(\mathbf{x}^{[t+1]}))\}$



EXPLORATION VS. EXPLOITATION

We see: We ran into a local minimum. We did not “explore” the most crucial areas and **missed** the global minimum.



- Better ways to propose points based on our model exist, so-called **acquisition functions**
- Optimizing SM directly corresponds to raw / mean prediction as AQF
- Results in **high exploitation but low exploration**

