Optimization in Machine Learning
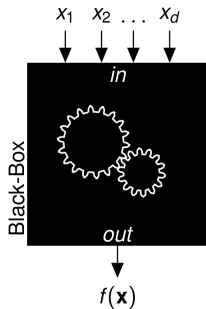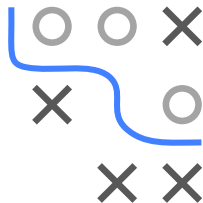
Bayesian Optimization
Black Box Optimization

Learning goals

- Definition and properties
- Examples
- Naive approaches

STANDARD VS. BLACK-BOX OPTIMIZATION

Optimization: Find

$$\min_{\boldsymbol{x}\in\mathcal{S}} f(\boldsymbol{x})$$

with objective function

$$f:\ \mathcal{S}\to\mathbb{R},$$

where $\mathcal{S}$ is usually box constrained.

If we are lucky ...

- ... we have an analytic description of $f:\ \mathcal{S}\to\mathbb{R}$
- ... we can calculate gradients and use gradient-based methods (e.g. gradient descent) for optimization
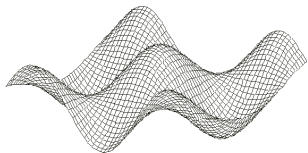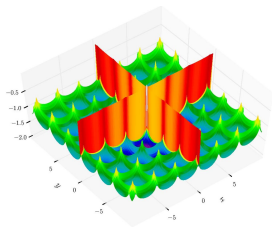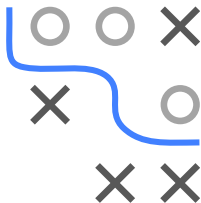
STANDARD VS. BLACK-BOX OPTIMIZATION

Optimization: Find

$$\min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x})$$

with objective function

$$f : \ \mathcal{S} \to \mathbb{R},$$

where $\mathcal{S}$ is usually box constrained.

Optimization gets harder ...

- ... if we cannot calculate gradients (because f is not differentiable or f is not known to us)
- ... but as long as evaluations of f are cheap, we can use standard derivative-free optimization methods (e.g. Nelder-Mead, simulated annealing, EAs)
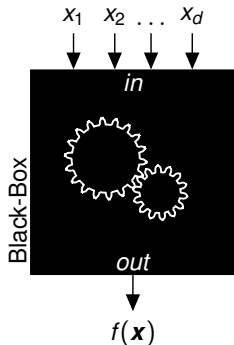
STANDARD VS. BLACK-BOX OPTIMIZATION

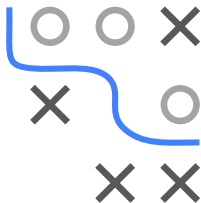**Optimization:** Find

$$\min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x})$$

with objective function

$$f : \ \mathcal{S} \to \mathbb{R},$$

where $\mathcal{S}$ is usually box constrained.

Optimization gets **really hard** if ...

- ... there is no analytic description of $f : \ \mathcal{S} \to \mathbb{R}$ (**black box**)
- ... evaluations of f for given values of $\mathbf{x}$ are **time consuming**

EXAMPLES FOR BAYESIAN OPTIMIZATION

1. Robot Gait Optimization: The robot's gait is controlled by a **parameterized controller** ▸ Calandra et al. 2014

- **Goal:** Find parameters s.t. average velocity (directional speed) of the robot is maximized
- Parameters of the gait control e.g. joints of ankles and knees
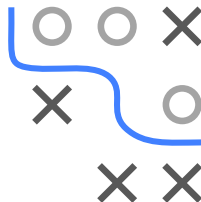
EXAMPLES FOR BAYESIAN OPTIMIZATION

❷ Optimization of a cookie recipe ▸ Kochanski et al. 2017

▸ Click for source

Ingredient	Salt (tsp)†	Total Sugar (g)	Brown Sugar (%)	Vanilla (tsp)†	Chip Quantity (g)	Chip Type
Min	0	150	0	0.25	114	{Dark, Milk, White}
Max	0.5	500	1	1	228	

- **Goal:** Find "optimal" composition and amounts of ingredients
- **Evaluation:** Cookies are baked according to the recipe, tested and rated by volunteers
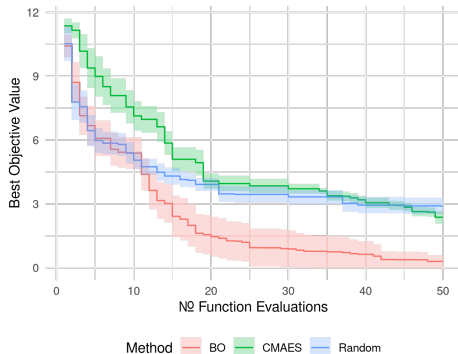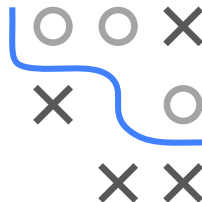
NAIVE APPROACHES

1. Empirical knowledge / manual tuning
   - Select parameters based on "expert" knowledge
   - **Advantages:** Can lead to fairly good outcomes for known problems
   - **Disadvantages:** Very (!) inefficient, poor reproducibility, chosen solution can also be far away from a global optimum

NAIVE APPROACHES

2 Random search / Grid search

- Random search: Evaluate uniformly sampled inputs
- Grid search: Exhaustive search of a predefined grid of inputs
- **Advantages:** Easy, intuitive, parallelization is trivial
- **Disadvantages:** Inefficient, search large irrelevant areas

Rug plots of RS vs. GS.

NAIVE APPROACHES

3 Traditional black-box optimization

- Traditional approaches that do not require derivatives
- E.g. Nelder-Mead, simulated annealing, EAs
- **Advantages:** Truly iterative, focuses on relevant regions
- **Disadvantages:** Still inefficient; usually lots of evaluations are needed to produce good outcomes

BO vs. CMAES vs. RS on 2D Ackley.