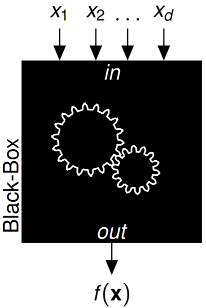
Optimization in Machine Learning

Bayesian Optimization:
Black Box Optimization



Learning goals

- Definition and properties
- Examples
- Naive approaches

STANDARD VS. BLACK-BOX OPTIMIZATION

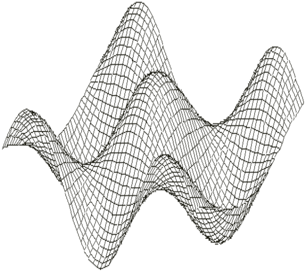
Optimization: Find

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

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

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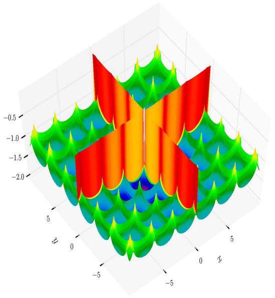

Optimization gets harder ...

- ... 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

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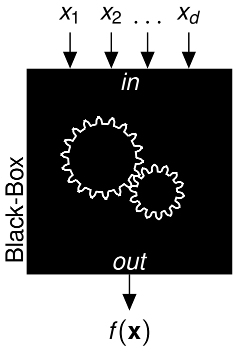
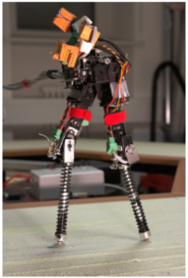


Optimization gets **really hard** if ...

- ... 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**



- **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
- *Calandra et al. (2014). An Experimental Evaluation of Bayesian Optimization on Bipedal Locomotion*

EXAMPLES FOR BAYESIAN OPTIMIZATION

2. Optimization of a cookie recipe

https://www.bettycrocker.com

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	

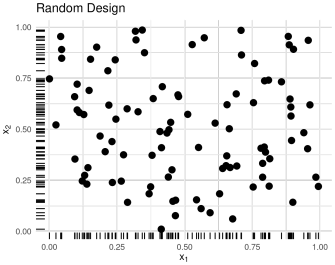
- **Goal:** Find "optimal" composition and amounts of ingredients
- **Evaluation:** Cookies are baked according to the recipe, tested and rated by volunteers
- *Kochanski et al. (2017). Bayesian Optimization for a Better Dessert*

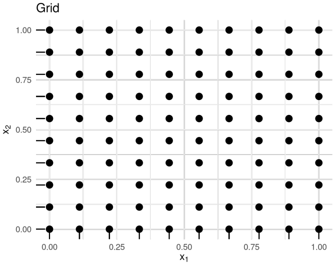
NAIVE APPROACHES

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

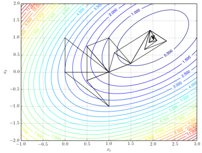


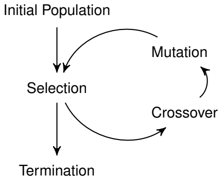


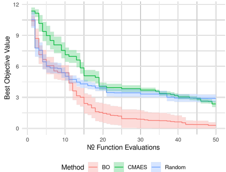
Rug plots of RS vs. GS.

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







Right: BO vs. CMAES vs. RS on 2D Ackley. CMAES initially performs poorly, needs to init itself, not made for expensive regimes.