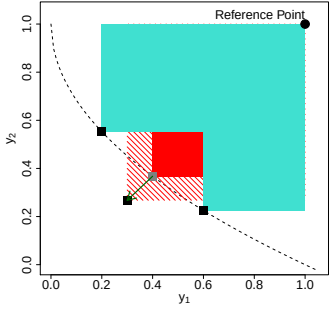
Optimization in Machine Learning

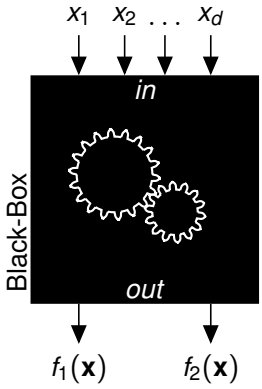
Bayesian Optimization
Multicriteria Bayesian Optimization

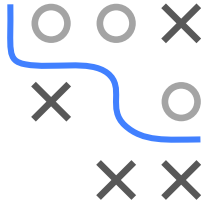


Learning goals

- Multicriteria Optimization
- Taxonomy
- ParEGO, SMS-EGO, EHI

MULTICRITERIA BAYESIAN OPTIMIZATION





$$f : \mathcal{S} \to \mathbb{R}^m$$
$$\min_{\mathbf{x} \in \mathcal{S}} \quad f(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_m(\mathbf{x}))$$

- A configuration **x dominates** ($\prec$) $\tilde{\mathbf{x}}$ if

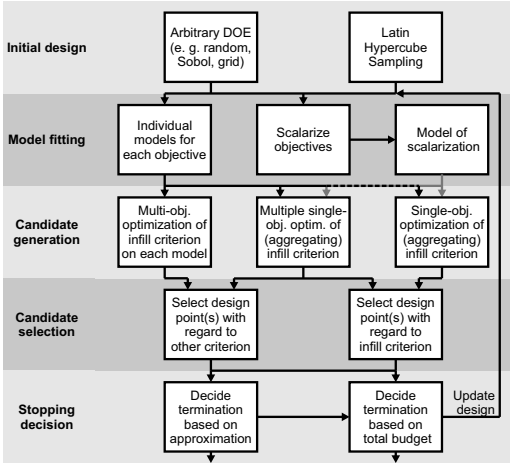
$$\forall i \in \{1, ..., m\} : \quad f_i(\mathbf{x}) \leq f_i(\tilde{\mathbf{x}})$$
$$\text{and } \exists j \in \{1, ..., m\} : \quad f_j(\mathbf{x}) < f_j(\tilde{\mathbf{x}})$$

- Set of non-dominated solutions:

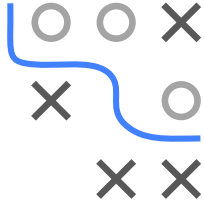
$$\mathcal{P} := \{\mathbf{x} \in \mathcal{S} | \nexists \tilde{\mathbf{x}} \in \mathcal{S} : \tilde{\mathbf{x}} \prec \mathbf{x}\}$$

- Pareto set $\mathcal{P}$, Pareto front $\mathcal{F} = f(\mathcal{P})$
- Goal: Find $\hat{\mathcal{P}}$ of non-dominated points that estimates the true Pareto set $\mathcal{P}$

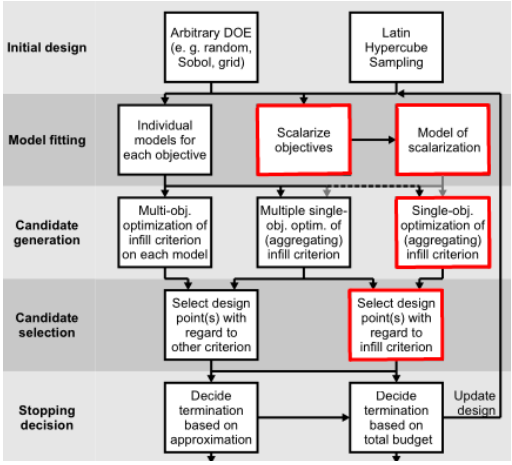
TAXONOMY

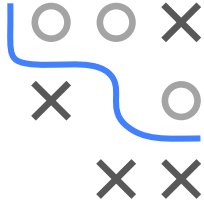


Horn, Wagner, Bischl et al. (2014).

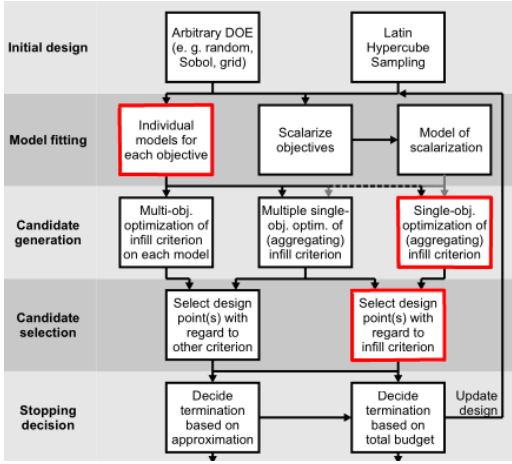


PAREGO


Initial design
Arbitrary DOE (e. g. random, Sobol, grid)
Latin Hypercube Sampling
Model fitting
Individual models for each objective
Scalarize objectives
Model of scalarization
Candidate generation
Multi-obj. optimization of infill criterion on each model
Multiple single-obj. optim. of (aggregating) infill criterion
Single-obj. optimization of (aggregating) infill criterion
Candidate selection
Select design point(s) with regard to other criterion
Select design point(s) with regard to infill criterion
Stopping decision
Decide termination based on approximation
Decide termination based on total budget
Update design



SMS-EGO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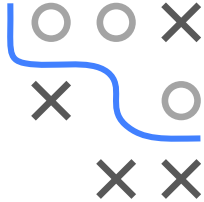
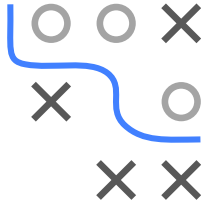


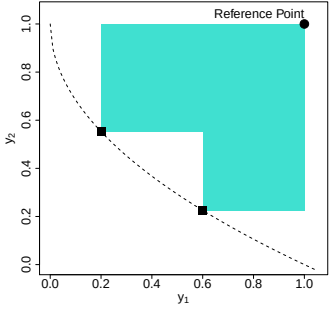
SMS-EGO

Individual models for each objective f_i

Single-objective optimization of aggregating acquisition function:
Calculate contribution of the confidence bound of candidate to the current front approximation



- Calculate LCB for each objective
- Measure contribution with regard to the hypervolume improvement
- For ε-dominated ($\prec_\varepsilon$) solutions, a penalty is added



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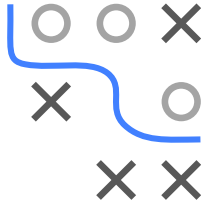

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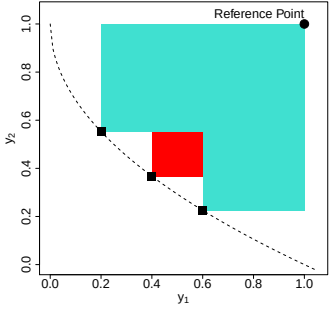
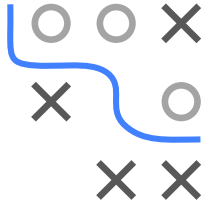


SMS-EGO



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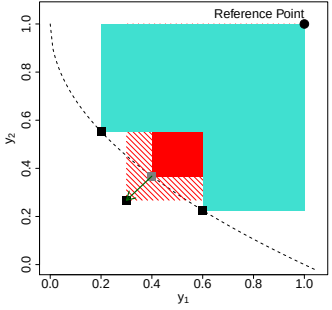

OUTLOOK

Many more options exist:

- Expected Hypervolume Improvement
- Multi-EGO
- Entropy based: PESMO, MESMO
- ...