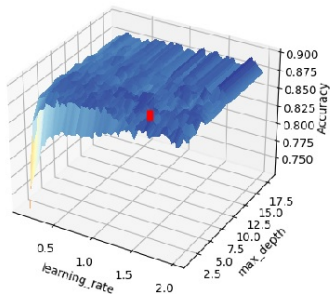


Optimization in Machine Learning

Optimization Problems

Other optimization problems



(a) vehicle

Learning goals

- Discrete / feature selection
- Black-box / hyperparameter optimization
- Noisy
- Multi-objective

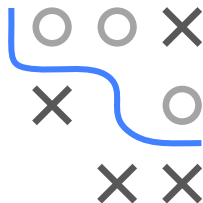
OTHER CLASSES OF OPTIMIZATION PROBLEMS

So far: “nice” (un)constrained problems:

- Problem defined on continuous domain \mathcal{S}
- Analytical objectives (and constraints)

Other characteristics:

- Discrete domain \mathcal{S}
- f **black-box**: Objective not available in analytical form; computer program to evaluate
- f **noisy**: Objective can be queried but evaluations are noisy
$$f(\mathbf{x}) = f_{\text{true}}(\mathbf{x}) + \epsilon, \quad \epsilon \sim F$$
- f **expensive**: Single query takes time / resources
- f multi-objective: $f(\mathbf{x}) : \mathcal{S} \rightarrow \mathbb{R}^m, f(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_m(\mathbf{x}))$



These make the problem typically much harder to solve!

EXAMPLE 1: BEST SUBSET SELECTION

Let $\mathcal{D} = \left(\left(\mathbf{x}^{(i)}, y^{(i)} \right) \right)_{1 \leq i \leq n}$, $\mathbf{x}^{(i)} \in \mathbb{R}^p$. Fit LM based on best feature subset.

$$\min_{\theta \in \Theta} \left(y^{(i)} - \theta^\top \mathbf{x}^{(i)} \right)^2, \|\theta\|_0 \leq k$$

Problem characteristics:

- White-box: Objective available in analytical form
- Discrete: \mathcal{S} is mixed continuous and discrete
- Constrained

The problem is even **NP-hard** (Bin et al., 1997, The Minimum Feature Subset Selection Problem)!

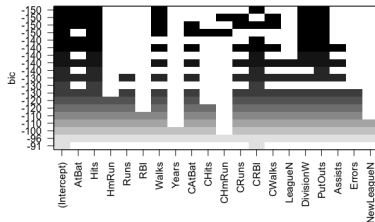
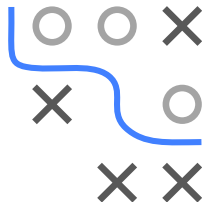


Figure: Source: RPubS, Subset Selection Methods

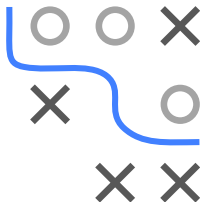


EXAMPLE 3: FEATURE SEL. (MULTIOBJECTIVE)

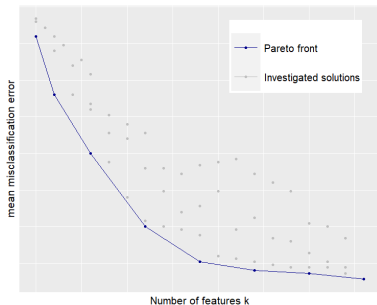
Feature selection is usually inherently multi-objective, with model sparsity as a 2nd trade-off target:

$$\min_{\mathbf{s} \in \{0,1\}^p} \left(\widehat{\text{GE}}(\mathcal{I}, \mathcal{J}, \rho, \mathbf{s}), \sum_{i=1}^p s_i \right).$$

$\widehat{\text{GE}}$ general. err. with metric ρ and estim. with resampling splits \mathcal{J}



- Multiobjective
- black box
eval by program
- S is discrete / binary
- expensive
1 eval: 1 or multiple ERM(s)!
- noisy
uses data / resampling

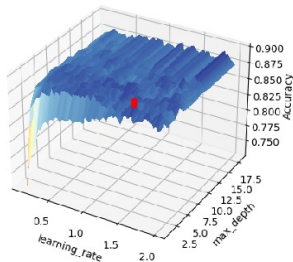
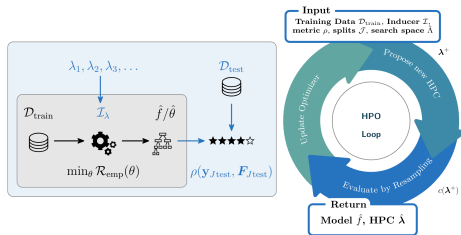
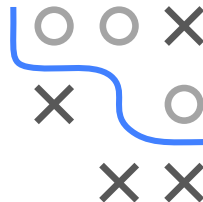


EXAMPLE 4: HYPERPARAMETER OPTIMIZATION

- Learner \mathcal{I} usually configurable by hyperparameters $\lambda \in \Lambda$.
- Find best HP configuration λ^*

$$\lambda^* \in \arg \min_{\lambda \in \Lambda} c(\lambda) = \arg \min \widehat{\text{GE}}(\mathcal{I}, \mathcal{J}, \rho, \lambda)$$

$\widehat{\text{GE}}$ general. err. with metric ρ and estim. with resampling splits \mathcal{J}



(a) vehicle

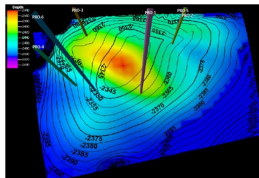
XGBoost HP landscape; source:

ceur-ws.org/Vol-2846/paper22.pdf

MORE BLACK-BOX PROBLEMS

Black-box problems from engineering: **oil well placement**

- The goal is to determine the optimal locations and operation parameters for wells in oil reservoirs
- Basic premise: achieving maximum revenue from oil while minimizing operating costs
- In addition, the objective function is subject to complex combinations of geological, economical, petrophysical and fluid dynamical constraints
- Each function evaluation requires several computationally expensive reservoir simulations while taking uncertainty in the reservoir description into account



Oil saturation at various depths with possible location of wells.

Source: [https://doi.org/10.1007/](https://doi.org/10.1007/s13202-019-0710-1)

s13202-019-0710-1

