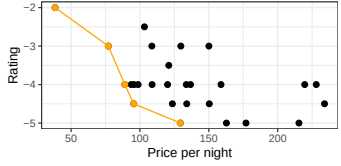
Optimization in Machine Learning

Multi-criteria Optimization

Introduction

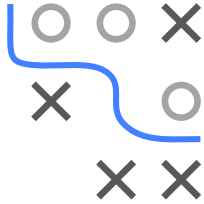


find cheap room with good rating

Learning goals

- What is multi-criteria optimization?
- Motivating examples
- Pareto optimality

INTRODUCTORY EXAMPLE



Often we want to solve optimization problems concerning several goals.

General applications:

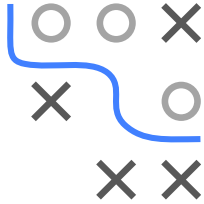
- Medicine: maximum effect, but minimum side effect of a drug.
- Finances: maximum return, but minimum risk of an equity portfolio.
- Production planning: maximum revenue, but minimum costs.
- Booking a hotel: maximum rating, but minimum costs.

In machine learning:

- Sparse models: maximum predictive performance, but minimal number of features.
- Fast models: maximum predictive performance, but short prediction time.
- ...

INTRODUCTORY EXAMPLE

Example: Choose the best hotel by maximizing ratings subject to a maximum price per night.

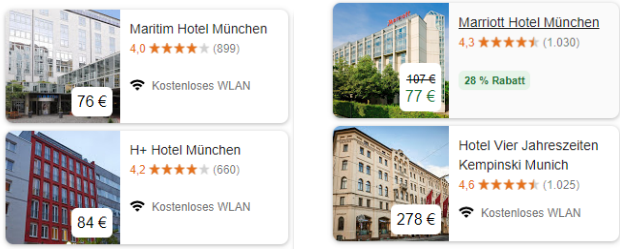


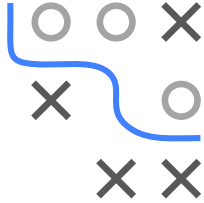
Problems:

- The result depends on how we select the maximum price; different price bounds give different solutions.
- We could also choose a minimum rating and optimize the price.
- The more objectives we include, the harder it gets to fix cutoffs like these.

Goal: Find a more general approach to solve multi-criteria problems.

INTRODUCTORY EXAMPLE



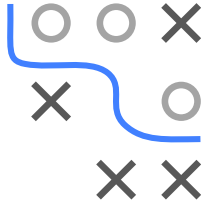


When booking a hotel: find the hotel with

- minimum price per night (**costs**), and
- maximum user rating (**performance**).

Since our standard is to minimize objectives, we minimize negative ratings.

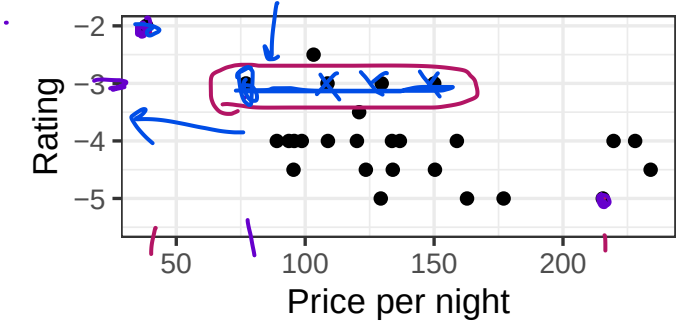
INTRODUCTORY EXAMPLE



The objectives often conflict with each other:

- Lower price $\rightarrow$ usually lower hotel rating.
- Better rating $\rightarrow$ usually higher price.

Example: (negative) average rating by hotel guests (1–5) vs. average price per night.



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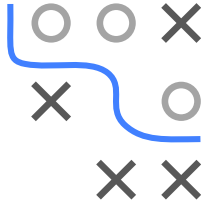
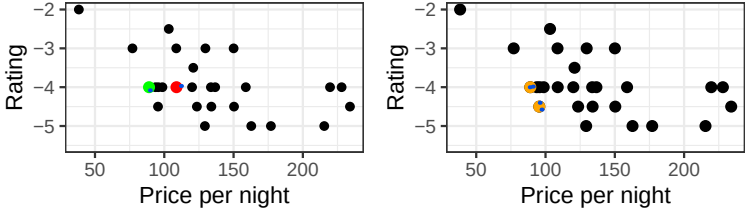


We cannot directly establish a total order on the objective space:

- Left: A hotel with rating 4 for 89 Euro ($f^{(1)} = (89, -4.0)$) is better than a hotel for 108 Euro with the same rating ($f^{(2)} = (108, -4.0)$).
- Right: How to decide if $f^{(1)} = (89, -4.0)$ is better or worse than $f^{(2)} = (95, -4.5)$?
- How much is one *rating point* worth?



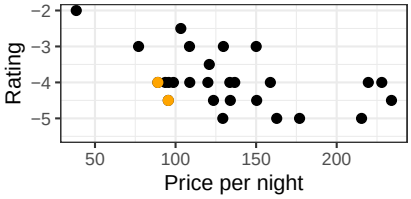
Let $f = (\text{price}, -\text{rating})$. The candidate $f^{(1)} = (89, -4.0)$ dominates $f^{(2)} = (108, -4.0)$. That is, $f^{(1)}$ is at least as good in every dimension, and strictly better in one dimension. Hence $f^{(2)} \prec f^{(1)}$. But for $f^{(1)} = (89, -4.0)$ and $f^{(2)} = (95, -4.5)$ we cannot say any is strictly better.

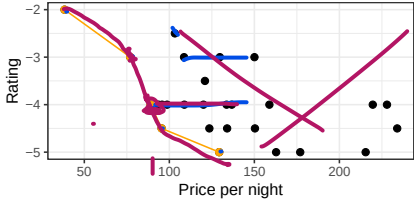
HOW TO DEFINE OPTIMALITY?

- We call these **incomparable** (or *equivalent* in the Pareto sense):

$$f^{(1)} \not\prec f^{(2)} \quad \text{and} \quad f^{(2)} \not\prec f^{(1)}.$$

- All such non-dominated points form the **Pareto front**.





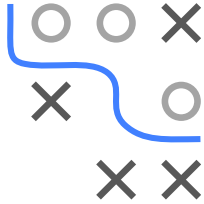
DEFINITION: MULTI-CRITERIA OPTIMIZATION

A **multi-criteria optimization problem** is defined by

$$\min_{\boldsymbol{x} \in \mathcal{S}} \boldsymbol{f}(\boldsymbol{x}) \quad \Leftrightarrow \quad \min_{\boldsymbol{x} \in \mathcal{S}} \big(f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x})\big),$$

with $\mathcal{S} \subset \mathbb{R}^n$ and a multi-criteria objective function $f : \mathcal{S} \to \mathbb{R}^m,\ m \geq 2$.

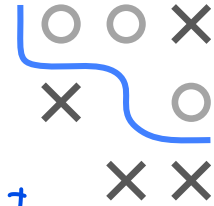
- **Goal:** minimize multiple target functions simultaneously.
- $(f_1(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x}))^\top$ maps each candidate $\boldsymbol{x}$ into the objective space $\mathbb{R}^m$.
- Typically no single best solution exists, as the objectives are often in conflict and cannot be totally ordered in $\mathbb{R}^m$.
- W.l.o.g. we always minimize.
- Also called multi-objective optimization, Pareto optimization, etc.



PARETO SETS AND PARETO OPTIMALITY

Definition:
Given

$$\min_{\boldsymbol{x}\in\mathcal{S}} \big(f_1(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x})\big), \quad f_i : \mathcal{S} \to \mathbb{R}.$$



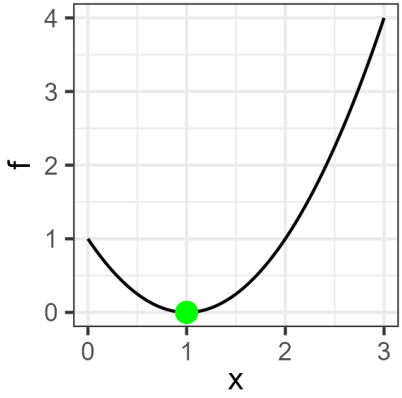
- A candidate $\boldsymbol{x}^{(1)}$ **(Pareto-)dominates** $\boldsymbol{x}^{(2)}$ if $f(\boldsymbol{x}^{(1)}) \prec f(\boldsymbol{x}^{(2)})$, i.e.:
  1. $f_i(\boldsymbol{x}^{(1)}) \leq f_i(\boldsymbol{x}^{(2)})$ for all i, for all obj. functions at least
  2. $f_j(\boldsymbol{x}^{(1)}) < f_j(\boldsymbol{x}^{(2)})$ for at least one j. as good for at least one obj.
- A candidate $\boldsymbol{x}^*$ not dominated by any other candidate is **Pareto optimal**. better
  if we can't find a point that dominate the given point, then it's optimal
- The set of all Pareto optimal candidates is the **Pareto set** $\mathcal{P} = \{\boldsymbol{x} \in \mathcal{S} \mid \nexists\, \tilde{\boldsymbol{x}} : f(\tilde{\boldsymbol{x}}) \prec f(\boldsymbol{x})\}$.
- $\mathcal{F} = f(\mathcal{P})$, the **Pareto front**, is the image of that set in objective space.

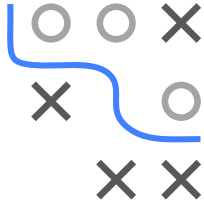
EXAMPLE: ONE OBJECTIVE FUNCTION

We consider

$$\min_x f(x) = (x-1)^2, \quad 0 \leq x \leq 3.$$

The optimum is at $x^* = 1$.

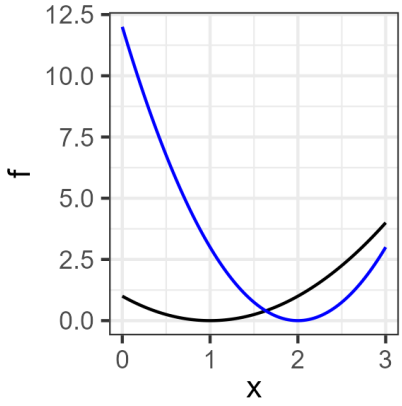


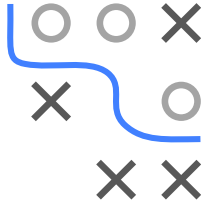


EXAMPLE: TWO TARGET FUNCTIONS

We extend the above problem to two objectives $f_1(x) = (x-1)^2$ and $f_2(x) = 3(x-2)^2$. Thus

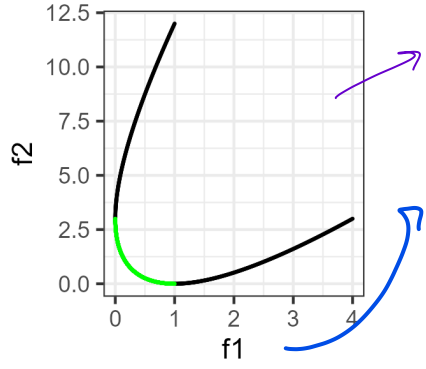
$$\min_x f(x) = \big(f_1(x),\, f_2(x)\big), \quad 0 \leq x \leq 3.$$





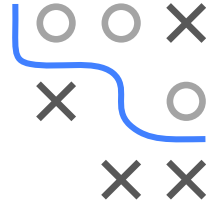
EXAMPLE: TWO TARGET FUNCTIONS

Visualizing both objectives: $\big(f_1(x),\ f_2(x)\big)$ for all $x \in [0, 3]$ in the objective space:



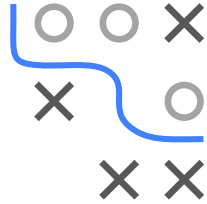
Todo Understand this

axes are the func. values



The Pareto front is shown in green.

A-PRIORI VS. A-POSTERIORI



- The Pareto set is a set of equally valid solutions.
- Often, we only want a **single** solution in practice.
- Without extra info, there is no unique best solution: one must choose based on further criteria (cost constraints, business preference, etc.).

Two overall strategies:

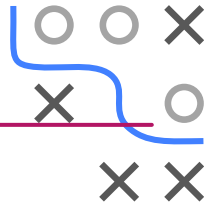
- **A-priori approach**: incorporate user preferences *before* the optimization.
- **A-posteriori approach**: first find (an approximation of) the entire Pareto set, then let the user choose.

A-PRIORI PROCEDURE

Example: Weighted total

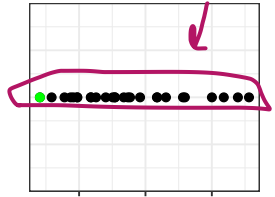
boil down to single criteria

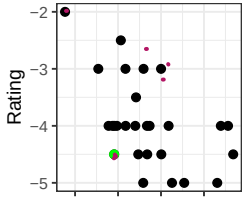
$$\min_{\boldsymbol{x}} \sum_{i=1}^{m} w_i f_i(\boldsymbol{x})$$



Prior knowledge: “One rating point is worth 50 Euro to this customer.”

$$\min_{\text{Hotel}} (\text{Price}) \; - \; 50 \times (\text{Rating})$$

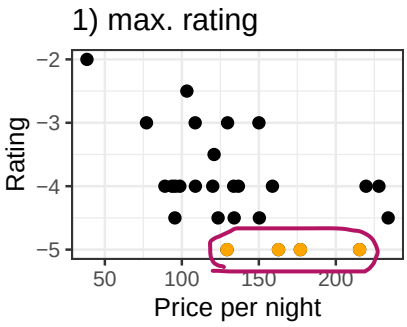


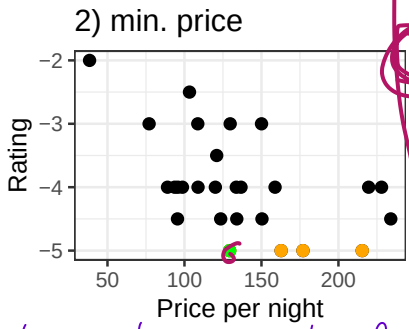


A-PRIORI PROCEDURE

Example: Lexicographic method

Prior knowledge: The rating is more important than the price. Hence we optimize the rating first, then the price among those best ratings:





opt. wrt to 1st obj., then 2nd . . .
(depends on how we order)

A-PRIORI PROCEDURE

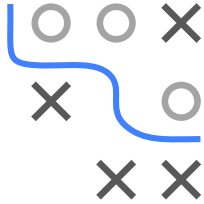
Lexicographic approach in general:

$$f_1^* = \min_{\boldsymbol{x} \in \mathcal{S}} f_1(\boldsymbol{x}),$$

$$f_2^* = \min_{\substack{\boldsymbol{x} \in \mathcal{S}: \\ f_1(\boldsymbol{x}) = f_1^*}} f_2(\boldsymbol{x}),$$

$$f_3^* = \min_{\substack{\boldsymbol{x} \in \mathcal{S}: \\ f_1(\boldsymbol{x}) = f_1^*,\, f_2(\boldsymbol{x}) = f_2^*}} f_3(\boldsymbol{x}),$$

$$\vdots$$



But different orderings yield different solutions.

Summary (a-priori):

- Implicit assumption: single-objective optimization is “easy.”
- We get only *one* solution, which depends strongly on the chosen weighting/order/etc.
- Varying these parameters systematically can produce several solutions, but may miss large parts of the non-dominated set.

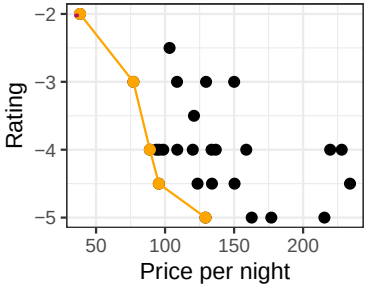
A-POSTERIORI PROCEDURE

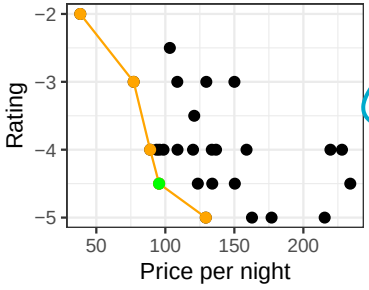
A-posteriori methods aim to

- find *all* optimal candidates (or a good approximation of them),
- let the user pick a single solution based on personal preferences or additional info (e.g. hotel location).

Hence, a-posteriori methods are more general.

Example: All Pareto-optimal hotels are shown on the left. User then picks from that subset on the right, based on hidden preferences (location, brand loyalty, etc.):





EVALUATION OF SOLUTIONS

A common measure for the performance of a set of candidates $\mathcal{P} \subset \boldsymbol{\mathcal{S}}$ is the **dominated hypervolume**:

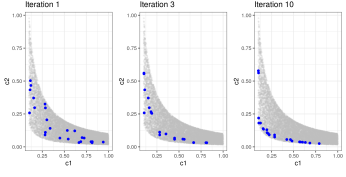
$$S(\mathcal{P}, R) = \lambda\Big(\bigcup_{\boldsymbol{x} \in \mathcal{P}} \{\, \boldsymbol{x} \mid \tilde{\boldsymbol{x}} \prec \boldsymbol{x} \prec R\}\Big),$$

where $\lambda(\cdot)$ is the Lebesgue measure and R a pre-specified reference point every point in the set must dominate

- HV is measured w.r.t. the reference point R, often chosen so each component is a known "worst" (upper bound) for that objective.
- HV is also called the **S-metric**.
- Its computation is $\mathcal{O}(n^{m-1})$ in the number of points and dimension m.
- Efficient algorithms exist for small m. In ML, we rarely exceed $m = 3$ in practice.

Optimization in Machine Learning

Multi-criteria Optimization
Evolutionary Approaches

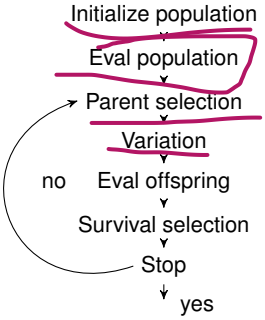


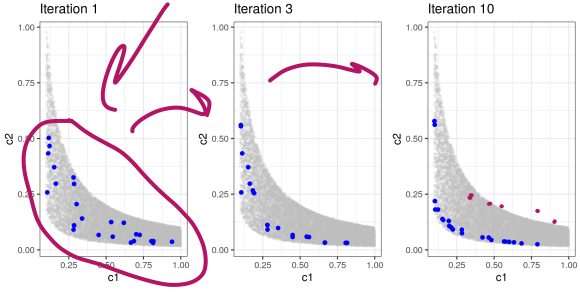
Learning goals

- EMOAs and population-based approach
- NSGA-II
- SMS-EMOA

A-POSTERIORI METHODS AND EVOLUTIONARY ALGORITHMS

Evolutionary multi-objective algorithms (EMOAs) evolve a diverse population over time to approximate the Pareto front.



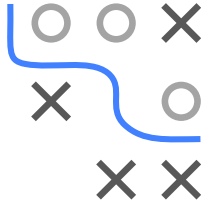


- Population-based search approximates a whole Pareto set in one run.
- The main steps (initialize, select, vary, survive, repeat) mirror standard EAs but must handle multiple objectives.

BASIC EA TEMPLATE LOOP

Algorithm 1: Basic EA template loop

1 Initialize and evaluate population $\mathcal{P}_0 \subset \mathcal{S}$ with $|\mathcal{P}_0| = \mu$
2 $t \leftarrow 0$
3 **repeat**
4 Select parents from $\mathcal{P}_t$ and generate offspring $\mathcal{Q}_t$, with $|\mathcal{Q}_t| = \lambda$
5 Select μ survivors to form $\mathcal{P}_{t+1}$
6 $t \leftarrow t + 1$
7 **until** *Stop criterion is fulfilled*

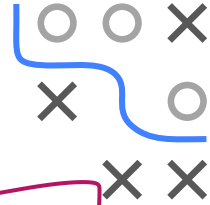


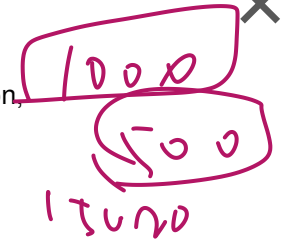
- As in standard EAs, we have parent selection, variation, and survival selection.
- For multi-objective EAs (EMOAs), ranking solutions by "fitness" is no longer straightforward. We need special selection strategies (non-dominated sorting, etc.).

NSGA-II

The **non-dominated sorting genetic algorithm (NSGA-II)** was published by Deb et al. 2002.

- Follows a $(\mu + \lambda)$ strategy for survival.
- Any standard variation operators (like polynomial mutation, SBX) can be used.
- Parent and survival selection both use:
  1. **Non-dominated sorting (NDS)** as the main ranking criterion,
  2. **Crowding distance** as a tie-break.

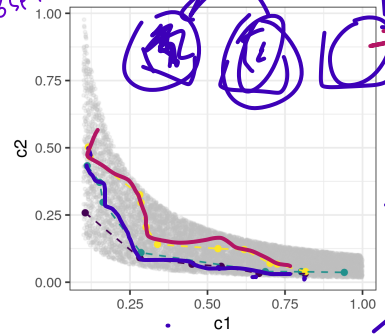




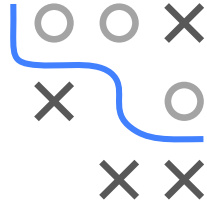
NSGA-II: NON-DOMINATED SORTING (I)

NDS partitions an objective space set into fronts $\mathcal{F}_1 \prec \mathcal{F}_2 \prec \mathcal{F}_3 \prec \ldots$.

- $\mathcal{F}_1$ is non-dominated, each $\boldsymbol{x} \in \mathcal{F}_2$ is dominated, but only by points in $\mathcal{F}_1$, each $\boldsymbol{x} \in \mathcal{F}_3$ is dominated, but only by points in $\mathcal{F}_1$ and $\mathcal{F}_2$, and so on.
- We can easily compute the partitioning by computing all non-dominated points $\mathcal{F}_1$, removing them, then computing the next layer of non-dominated points $\mathcal{F}_2$, and so on.

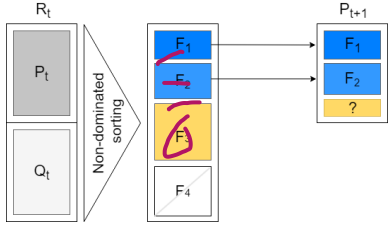


NSGA-II: NON-DOMINATED SORTING (II)



For **survival** in $(\mu + \lambda)$ selection:

- We rank all $\mu + \lambda$ individuals by front index.
- We start filling the next population from $\mathcal{F}_1$ upward.
- If front $\mathcal{F}_i$ cannot fully fit (because we would exceed μ), we partially fill with a subset of $\mathcal{F}_i$.

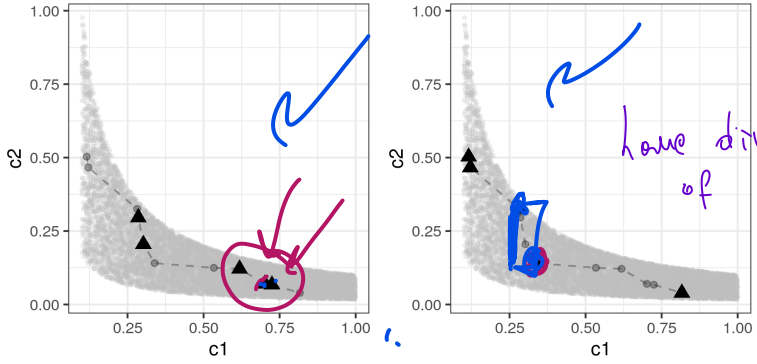


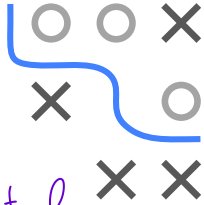
But: Which individuals survive from this partially included front? $\rightarrow$ *crowding distance* sorting.

(NDS is also used for parent selection with binary tournaments.)

NSGA-II: CROWDING DISTANCE (I)

Idea: Prefer individuals that are more "spread out" (less crowded).





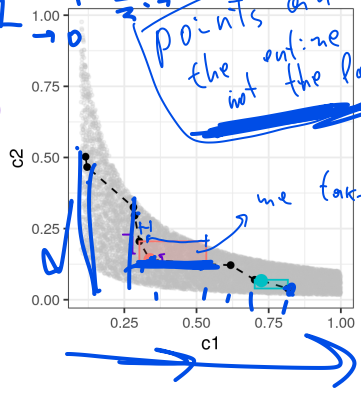
Left: not good, solutions bunched up. Right: better spread.

NSGA-II: CROWDING DISTANCE (II)

Crowding distance:
For each objective f_j:

- Sort points by f_j (in ascending order).
- Normalize f_j values to [0, 1].
- "Border" points (lowest/highest f_j) get infinite distance (ensuring they always survive if possible).
- For internal points, distance is difference in f_j-values between next neighbors.

Then sum (or average) across all m objectives to get the final crowding score.



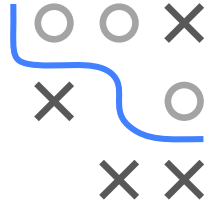
Red: High CD Blue: Low CD

HYPERVOLUME CONTRIBUTION

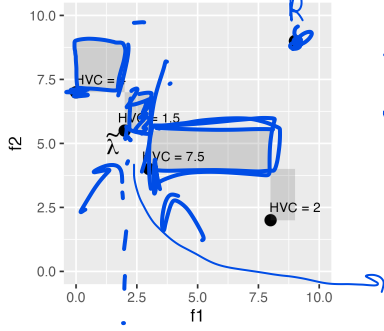
S-Metric-Selection uses the *hypervolume contribution* $\Delta s(\boldsymbol{x}, \mathcal{P})$ of each individual:

$$\Delta s(\boldsymbol{x}, \mathcal{P}) = S(\mathcal{P}, R) - S\big(\mathcal{P} \setminus \{\boldsymbol{x}\},\, R\big),$$

where $S(\cdot, R)$ is the dominated HV w.r.t. reference point R.



- Dark rectangles: unique HV part dominated only by that dot
- Gray cross: reference point R.
- The individual with the smallest HV contribution is "least important" for covering objective space.
- This is used by the SMS-EMOA to remove individuals in survival selection.

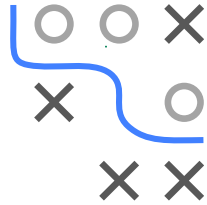


SMS-EMOA ALGORITHM

Algorithm 2: SMS-EMOA

1 Generate initial population $\mathcal{P}_0$ of size μ
2 $t \leftarrow 0$
3 **repeat**
4 Create exactly one offspring $\mathbf{q}$ by recombination + mutation
5 Perform non-dominated sorting on $(\mathcal{P}_t \cup \{\mathbf{q}\})$
6 Let $\mathcal{F}_k$ be the last front
7 $\tilde{\boldsymbol{x}} \leftarrow \arg\min_{\boldsymbol{x} \in \mathcal{F}_k} \Delta s(\boldsymbol{x}, \mathcal{F}_k)$
8 $\mathcal{P}_{t+1} \leftarrow \left(\mathcal{P}_t \cup \{\mathbf{q}\}\right) \setminus \{\tilde{\boldsymbol{x}}\}$
9 $t \leftarrow t + 1$
10 **until** *Termination*

- As soon as we exceed size $\mu + 1$, remove the worst HV contributor from the *last front*.
- That way, each iteration keeps exactly μ individuals.
- Ranking is primarily by front membership; hypervolume contrib. is the tiebreak.

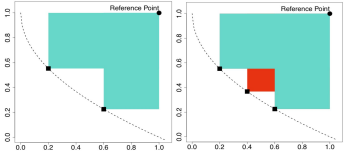


for last layer we use HVC as a tiebreaker

Adding more than 1 point will make deciding which points to remove an NP hard problem

Optimization in Machine Learning

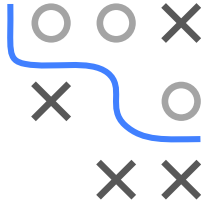
Multi-criteria Optimization
Bayesian Optimization



Learning goals

- Single-criteria recap
- Multi-criteria introduction
- Scalarization vs. HV-based methods

RECAP: BAYESIAN OPTIMIZATION



Advantages of BO

- Sample efficient
- Can handle noise
- Native incorporation of priors
- Does not require gradients
- Theoretical guarantees

We will now extend BO to multiple cost functions.

RECAP: BAYESIAN OPTIMIZATION

Algorithm 0: Bayesian optimization loop

Require: Search space $\mathcal{S}$, cost function f, acquisition function u, predictive model $\hat{f}$, maximal number of function evaluations T

Result : Best configuration $\hat{\boldsymbol{x}}$ (based on $\mathcal{D}$ or $\hat{f}$)

1 Initialize data $\mathcal{D}^{(0)}$ with initial observations

2 **for** $t \leftarrow 1$ **to** T **do**

3 Fit predictive model $\hat{f}^{(t)}$ on $\mathcal{D}^{(t-1)}$

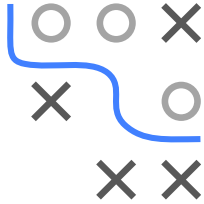
4 Select next query point:

$$\boldsymbol{x}^{(t)} \in \arg\max_{\boldsymbol{x} \in \mathcal{S}} u\left(\boldsymbol{x}; \mathcal{D}^{(t-1)}, \hat{f}^{(t)}\right)$$

5 Query $f(\boldsymbol{x}^{(t)})$

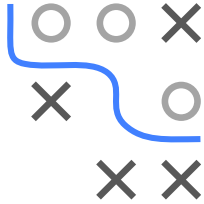
6 Update data:

$$\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \{\langle \boldsymbol{x}^{(t)}, f(\boldsymbol{x}^{(t)}) \rangle\}$$



MULTI-CRITERIA BAYESIAN OPTIMIZATION

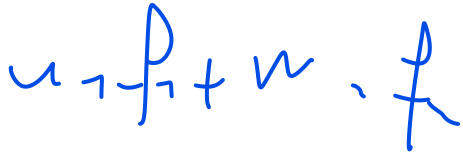
Goal: Extend Bayesian optimization to multiple cost functions



$$\min_{\boldsymbol{x}\in\mathcal{S}} f(\boldsymbol{x}) \quad \Leftrightarrow \quad \min_{\boldsymbol{x}\in\mathcal{S}} \big(f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x})\big).$$

There are two basic approaches:

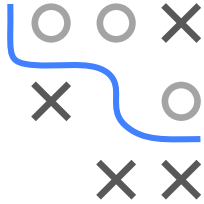
1. Simplify the problem by scalarizing the cost functions, or
2. define acquisition functions for multiple cost functions.



SCALARIZATION

Idea: Aggregate all cost functions

$$\min_{\boldsymbol{x} \in \mathcal{S}} \sum_{i=1}^{m} w_i f_i(\boldsymbol{x}) \qquad \text{with} \quad w_i \geq 0$$



- **Obvious problem:** How to choose $w_1, \ldots, w_m$?
  - Expert knowledge?
  - Systematic variation?
  - Random variation?
- If expert knowledge is not available a-priori, we need to ensure that different trade-offs between cost functions are explored.
- Simplifies multi-criteria optimization problem to single-objective $\longrightarrow$ standard Bayesian optimization can be used without adapting the general algorithm.

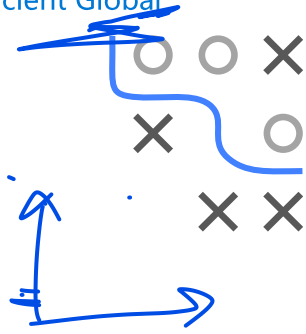
SCALARIZATION: PAREGO

Knowles 2006

ParEGO (Pareto Efficient Global Optimization)

Scalarize the cost functions using the augmented Chebychev norm / achievement function

$$f = \max_{i=1,\dots,m} \left(w_i f_i(\boldsymbol{x})\right) + \rho \sum_{i=1}^{m} w_i f_i(\boldsymbol{x}),$$



- The weights $w \in W$ are drawn from

$$W = \left\{ w = (w_1, \dots, w_m) \,\middle|\, \sum_{i=1}^{m} w_i = 1,\ w_i = \frac{l}{s},\ l \in \{0, \dots, s\} \right\},$$

with $|W| = \binom{s+m-1}{m-1}$.

- New weights are drawn in every BO iteration.
- ρ is a small parameter (e.g. 0.05).
- s controls how many distinct weight vectors exist.

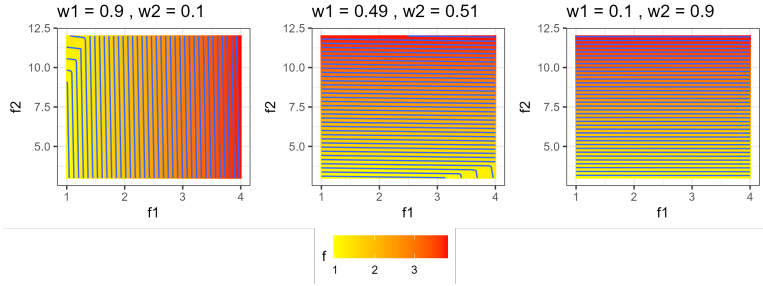
Weights are randomly varied

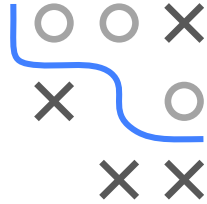
We do one iter of single crit BO

0.99

0.01

WHY THE CHEBYCHEV NORM?





$$f = \max_{i=1,\dots,m}\left(w_i f_i(\boldsymbol{x})\right) + \rho \sum_{i=1}^{m} w_i f_i(\boldsymbol{x}),$$

- The norm consists of two components:
  - $\max_i\left(w_i f_i(\boldsymbol{x})\right)$ considers only the maximum weighted cost.
  - $\sum_i w_i f_i(\boldsymbol{x})$ is the weighted sum of all costs.
- ρ controls the trade-off between these parts.
- By randomizing the weights w in each iteration (and keeping ρ small), extreme points in single cost functions can be explored.
- One can prove that every solution of this scalarized problem is Pareto-optimal.

PAREGO ALGORITHM

ParEGO loop

Require: Search space $\mathcal{S}$, cost function f, acquisition function u, predictive model $\hat{f}$, maximal number of function evaluations T, ρ, l, s

Result : Best configuration $\hat{\boldsymbol{x}}$ (according to $\mathcal{D}$ or $\hat{f}$)

1 Initialize data $\mathcal{D}^{(0)}$ with initial observations

2 **for** $t = 1$ **to** T **do**

3 Sample $w \in W = \left\{(w_1, \ldots, w_m) \mid \sum w_i = 1,\ w_i = \frac{l}{s}, l \in \{0, \ldots, s\}\right\}$

4 Compute scalarization: $c^{(t)} = \max_i \left(w_i f_i(\boldsymbol{x})\right) + \rho \sum_i w_i f_i(\boldsymbol{x})$

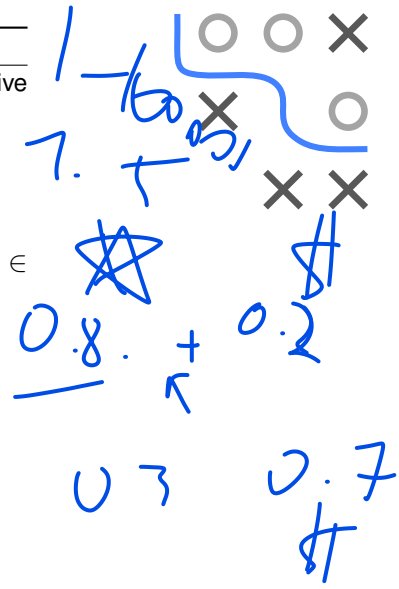
5 Fit predictive model $\hat{f}^{(t)}$ on $\mathcal{D}^{(t-1)}$

6 Select next query point: $\boldsymbol{x}^{(t)} \in \arg\max_{\boldsymbol{x} \in \mathcal{S}} u(\boldsymbol{x}; \mathcal{D}^{(t-1)}, \hat{f}^{(t)})$

7 Query $f(\boldsymbol{x}^{(t)})$

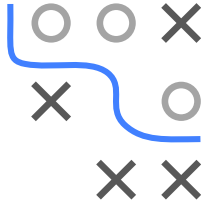
8 Update data:

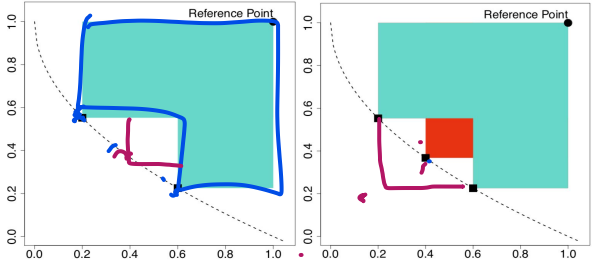
$$\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \{\langle \boldsymbol{x}^{(t)}, f(\boldsymbol{x}^{(t)})\rangle\}$$



HV BASED ACQUISITION FUNCTIONS

Idea: Define acquisition function that directly models the contribution to the dominated hypervolume (HV):
$\max(0,\ S(\mathcal{P} \cup \boldsymbol{x}, R)\ -\ S(\mathcal{P}, R))$



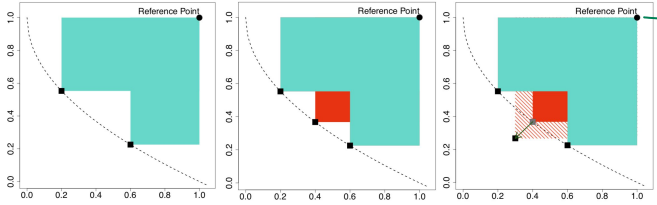


- Fit m single-objective surrogate models $\hat{f}_1, \ldots, \hat{f}_m$.
- Acquisition function uses all surrogate models simultaneously.
- Still a single-objective optimization problem (of acquisition itself).

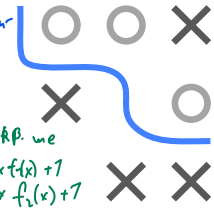
S-METRIC SELECTION-BASED EGO

Using the ~~Lower Confidence Bound~~ $u_{\text{LCB},1}(\boldsymbol{x}), \ldots, u_{\text{LCB},m}(\boldsymbol{x})$, one can form an *optimistic* estimate of the hypervolume contribution:

we want to incorporate the uncertainty



if we don't have RP. we can just peak $\max f(x) + 1$ $\max f_2(x) + 1$



Problem: HV-contribution can be zero across large regions where the lower confidence bound is already dominated.

- Large zero-plateaus make optimization of the acquisition harder.
- SMS-EGO adds an adaptive penalty in such dominated regions.

This method is referred to as ▸ Ponweiser et al. 2008.

if points are in the box, then we won't have any HVC so we need to figure out what to do

FURTHER HV ACQUISITION FUNCTIONS

Expected Hypervolume Improvement (EHI) ▸ Yang et al. 2019:

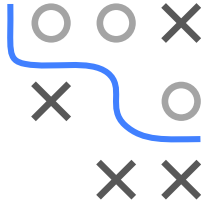
$$u_{EI,\mathcal{H}}(\boldsymbol{x}) = \int_{-\infty}^{\infty} p(f \mid \boldsymbol{x}) \times \left[S(\mathcal{P} \cup \boldsymbol{x}, R) \; - \; S(\mathcal{P}, R) \right] df$$

- Direct extension of u_{EI} to the hypervolume criterion.
- $p(f \mid \boldsymbol{x})$ is the joint predictive density of all surrogate models at $\boldsymbol{x}$.
- With independent GPs per objective, this factorizes over m univariate normals.
- Exact integral feasible for $m \leq 3$, else simulation-based.

Further HV-based acquisitions:

- **Stepwise Uncertainty Reduction (SUR)** w.r.t. the probability of improvement.
- **Expected Maximin Improvement (EMI)** w.r.t. the ϵ-indicator.

HYPERVOLUME BASED BO ALGORITHM



Hypervolume-based Bayesian optimization loop

Require: Search space $\mathcal{S}$, cost function f, acquisition function u, predictive model(s) $\hat{f}_1, \ldots, \hat{f}_m$, maximal number of function evaluations T

Result : Best configuration $\hat{\boldsymbol{x}}$

Initialize data $\mathcal{D}^{(0)}$ with initial observations

for $t = 1$ **to** T **do**

  Fit predictive models $\hat{f}_1^{(t)}, \ldots, \hat{f}_m^{(t)}$ on $\mathcal{D}^{(t-1)}$

  Select next query point:

$$\boldsymbol{x}^{(t)} \in \arg\max_{\boldsymbol{x} \in \mathcal{S}} u\left(\boldsymbol{x};\, \mathcal{D}^{(t-1)},\, \hat{f}_1^{(t)}, \ldots, \hat{f}_m^{(t)}\right)$$

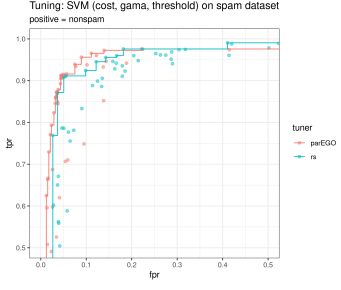
  Query $f(\boldsymbol{x}^{(t)})$

  Update data:

$$\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \left\{ \langle \boldsymbol{x}^{(t)}, f(\boldsymbol{x}^{(t)}) \rangle \right\}$$

Optimization in Machine Learning

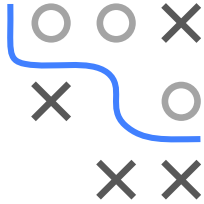
Multi-criteria Optimization
Practical Applications



Learning goals

- ROC optimization
- Efficient models
- Fairness considerations

PRACTICAL APPLICATIONS IN MACHINE LEARNING



ROC Optimization: Balance *true positive* and *false positive* rates

- Typically used in unbalanced classification with unspecified costs.
- Could also consider other ROC metrics, e.g., *positive predicted value* or *false discovery rate*

Efficient Models: Balance *predictive performance* with *prediction time*, *energy consumption*, and/or *model size*.

- Time: production models need to predict fast.
- Size / Energy: model might be deployed on a mobile/edge device with power constraints

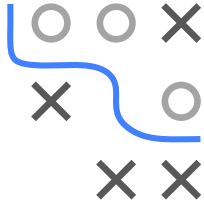
Sparse Models: Balance *predictive performance* and *number of used features*—for cost efficiency or interpretability.

Fair Models: Balance *predictive performance* and *fairness*.

- Model should not disadvantage certain subgroups (e.g. by gender).
- Multiple approaches exist to quantify fairness

ROC OPTIMIZATION - SETUP

Again, we want to train a *spam detector* on the popular Spam dataset[1].



- Learner: SVM with RBF kernel
- Hyperparameters:

`cost`	$[2^{-15}, 2^{15}]$
γ	$[2^{-15}, 2^{15}]$
Threshold t	$[0, 1]$

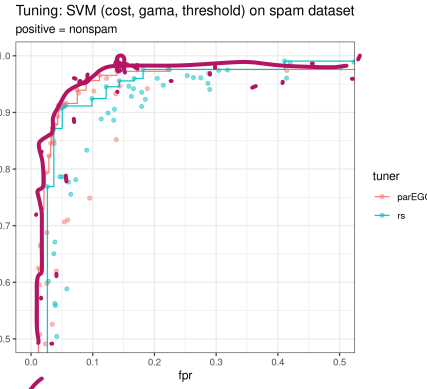
- Objective: *minimize* false positive rate (FPR) and *maximize* true positive rate (TPR), via 5-fold CV
- Optimizer: multi-criteria Bayesian optimization
  - ParEGO with $\rho = 0.05$, $s = 100000$
  - Acquisition: Confidence Bound ($\alpha = 2$)
  - Budget: 100 evaluations
- Tuning is done on a training holdout, and the hyperparameter configs on the estimated Pareto front are validated on external test set.

The threshold t could also be optimized post-hoc separately.

[1] `https://archive.ics.uci.edu/ml/datasets/spambase`

ROC OPTIMIZATION - RESULT I

- Compared to *random search*, many *ParEGO* evaluations lie on the Pareto front.
- The *ParEGO* Pareto front dominates most random-search solutions.
- Dominated hypervolume (w.r.t. reference point $(0, 1)$):
  ParEGO: 0.965
  random: 0.959



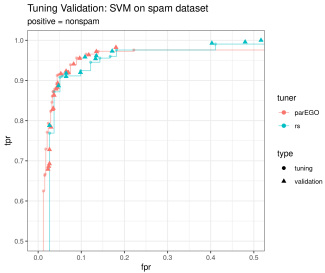
ROC OPTIMIZATION - RESULT II

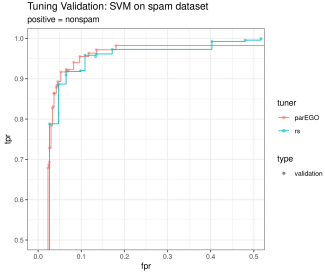
Validate configurations on the estimated Pareto front:

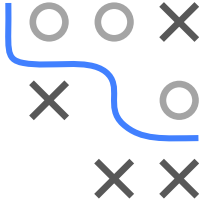
- The performance changes slightly on a new holdout set.
- TPR improved a bit, but FPR got slightly worse.
- Some configs become dominated once tested on the new holdout.
- Dominated hypervolume on the validation set:

  ParEGO: 0.960

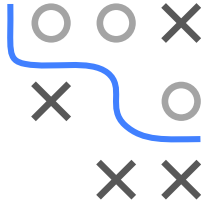
  random: 0.961





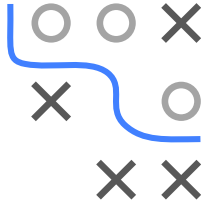


EFFICIENT MODELS - OVERVIEW



- “Efficiency” can refer to:
  - Memory consumption
  - Training or prediction time
  - Number of features used
  - Energy consumption
  - . . .
- Some hyperparameters strongly impact efficiency:
  - Number of trees (RF, GBDT)
  - Number, size, type of layers (NN)
  - L1 regularization strength
- Others might have no direct influence on efficiency.
- Typical scenario: searching over multiple algorithms with different cost–performance trade-offs.

EFFICIENT MODELS - EXAMPLE: FEATURE SELECTION I

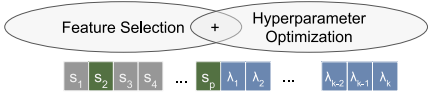


Goal: Identify an informative subset of features with minimal drop in performance vs. using all features.

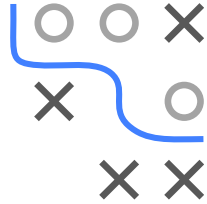
$$\min_{\boldsymbol{x} \in \mathcal{S},\ s \in \{0,1\}^p} \left(\widehat{GE}\big(\mathcal{I}(\mathcal{D}, \boldsymbol{x}, s)\big),\ \frac{1}{p} \sum_{i=1}^{p} s_i \right).$$

fraction of feat. used

- Typically, feature selection and hyperparameter tuning happen in separate steps.
- Alternatively, search a good subset s and hyperparams $\boldsymbol{x}$ *simultaneously*.

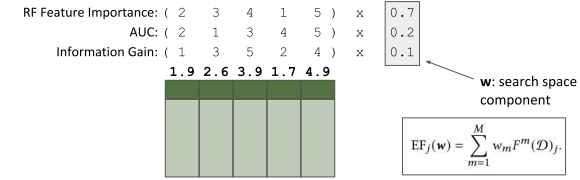


EFFICIENT MODELS - EXAMPLE: FEATURE SELECTION II



Idea: *Multi-Objective Hyperparameter Tuning and Feature Selection using Filter Ensembles* ▸ Binder et al. 2020.

- Pre-calculate multiple *feature-filter* rank vectors.



- New hyperparameter vector: $\boldsymbol{x} = (\tilde{\boldsymbol{x}}, w_1, \ldots, w_p, \tau)$
  - $\tilde{\boldsymbol{x}}$: learner hyperparameters
  - $(w_1, \ldots, w_p)$: weights for each filter ranking
  - $\tau \in [0, 1]$: fraction of features to keep

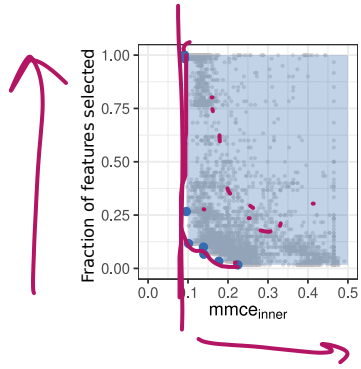
EFFICIENT MODELS - EXAMPLE: FEATURE SELECTION III

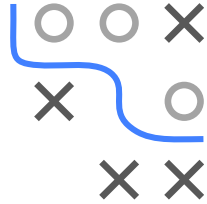
Joint FS + HP search on `Sonar` data[2]:

- Learner: SVM (RBF kernel).
- Hyperparams:

$$\begin{aligned} \texttt{cost} &\quad [2^{-10}, 2^{10}] \\ \gamma &\quad [2^{-10}, 2^{10}] \\ (w_1, \ldots, w_p) &\quad [0,1]^p \\ \tau &\quad [0,1] \end{aligned}$$

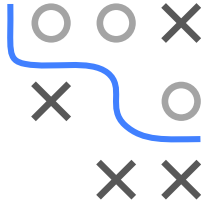
- Objective: minimize misclassification + fraction of selected features.
- Optimizer: ParEGO + random forest surrogate + LCB acquisition, 15 batch proposals, budget 2000 evals.





[2] Only tuning error is shown

EFFICIENT MODELS - EXAMPLE: FLOPS



Goal: Optimize *accuracy* vs. *FLOPS* (floating-point ops) Wang et al. 2019.

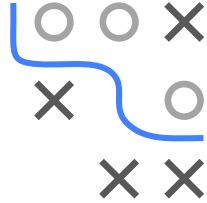
Data: CIFAR-10 (image classification).

Learner: *DenseNet* Huang et al. 2017:

- 4 dense blocks, each with multiple convolution layers that feed into each other.
- Blocks connected by convolution + max-pooling layers.

Training: 300 epochs, batch size 128, initial LR 0.1.

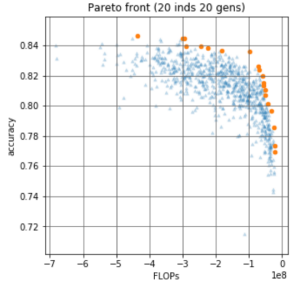
EFFICIENT MODELS - EXAMPLE: FLOPS (CONT.)



- Objectives: *accuracy* vs. *FLOPS per observation*.
- Search space:

`growth rate` (k)	$[8, 32]$
`layers in 1st block`	$[4, 6]$
`layers in 2nd block`	$[4, 12]$
`layers in 3rd block`	$[4, 24]$
`layers in 4th block`	$[4, 16]$

- Tuner: *Particle Swarm Optimization*, population 20, budget 400.

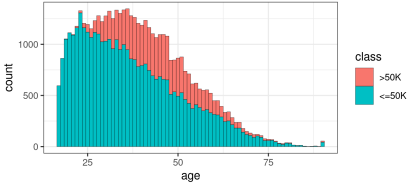


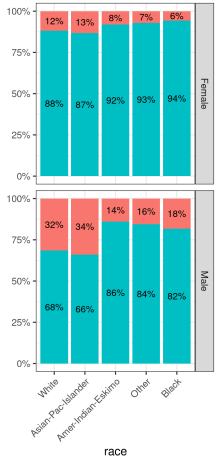
"Growth rate" = # of feature maps added each layer.

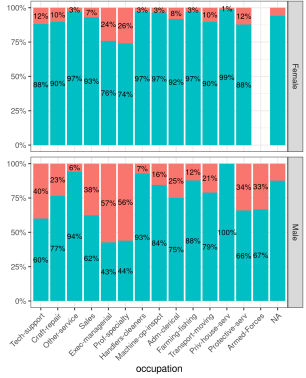
FAIR MODELS - THE ADULT DATASET

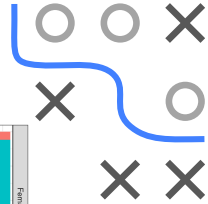
Dataset: Adult

- Source: US Census database, 1994, https://www.openml.org/d/1590.
- 48842 observations
- Target: binary, income above 50k
- 14 features: age, education, hours.per.week, marital.status, native.country, occupation, race, relationship, sex, ...

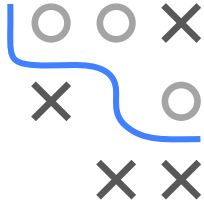








FAIR MODELS - SETUP



A toy example: build a "fair" model for predicting income (binary).

- Learner: XGBoost
- Hyperparams:

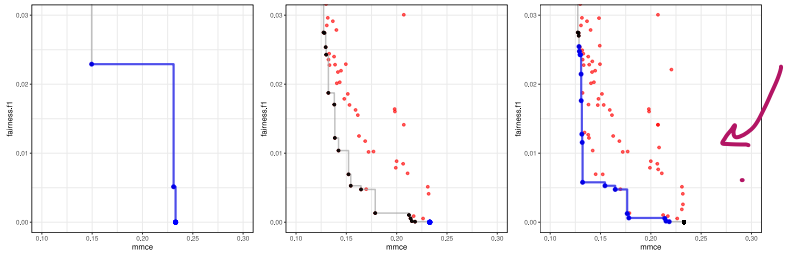
`eta`	$[0.01, 0.2]$
`gamma`	$[2^{-7}, 2^{6}]$
`max_depth`	$\{2, \ldots, 20\}$
`colsample_bytree`	$[0.5, 1]$
`colsample_bylevel`	$[0.5, 1]$
`lambda`	$[2^{-10}, 2^{10}]$
`alpha`	$[2^{-10}, 2^{10}]$
`subsample`	$[0.5, 1]$

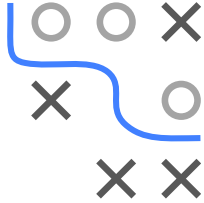
- Objective: *misclassification error* vs. *unfairness*.
- We define "unfairness" as the absolute difference in F1-scores between male/female sub-populations:

$$L_{\text{fair}} := \left| \text{F1}(y_f, \hat{f}(\mathbf{x}_f)) \; - \; \text{F1}(y_m, \hat{f}(\mathbf{x}_m)) \right|.$$

Note: This is a simplistic example. Real fairness questions often need more careful definitions and domain knowledge.

FAIR MODELS - RESULTS





- Optimizer: ParEGO + random forest surrogate, restricting $[w_i]$ to $[0.1, 0.9]$ if we only care about moderate fairness/performance ranges.
- In this example, hyperparams do indeed influence the fairness measure.
- But in practice, changing standard HPs often *won't* suffice to ensure fairness.