Multiobjective Optimization

taste

...

costs

cooking time

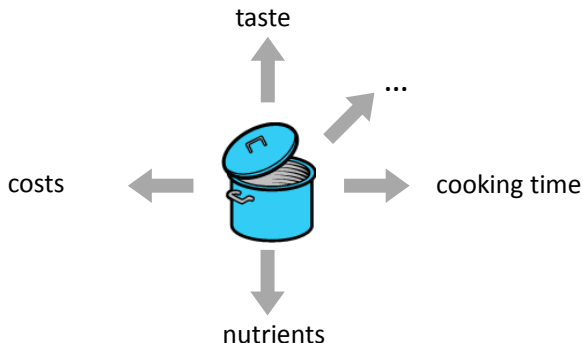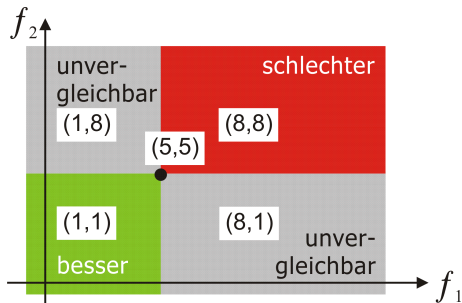nutrients

Real-world problems: various demands on problem solution
⇒ multiple conflictive objective functions

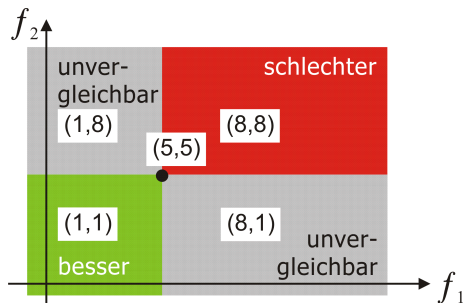# Multiobjective Optimization

Multiobjective Problem

$f : S \subseteq \mathbb{R}^n \to Z \subseteq \mathbb{R}^d, \quad \min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_d(\mathbf{x}))$

How to relate vectors?

Pareto Dominance

partial order among vectors in $\mathbb{R}^d$ and thus in $\mathbb{R}^n$

$(1,1) \prec (5,5) \prec (8,8)$

$(1,8) \parallel (5,5) \parallel (8,1)$

$\mathbf{a} \preceq \mathbf{b}$, $\mathbf{a}$ weakly dominates $\mathbf{b}$: $\iff \forall i \in \{1, \ldots, d\} : a_i \leq b_i$

$\mathbf{a} \prec \mathbf{b}$, $\mathbf{a}$ dominates $\mathbf{b}$: $\iff \mathbf{a} \preceq \mathbf{b}$ and $\mathbf{a} \neq \mathbf{b}$, i.e., $\exists i \in \{1, \ldots, d\} : a_i < b_i$

$\mathbf{a} \| \mathbf{b}$, $\mathbf{a}$ and $\mathbf{b}$ are incomparable: $\iff$ neither $\mathbf{a} \preceq \mathbf{b}$ nor $\mathbf{b} \preceq \mathbf{a}$.

Aim of Optimization

Pareto front: set of optimal solution vectors in $\mathbb{R}^d$, i.e.,
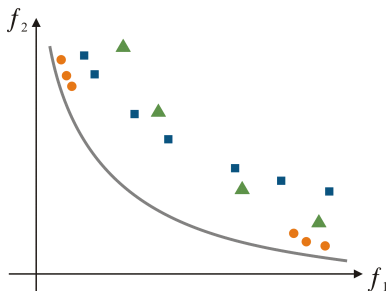$$PF = \{\mathbf{x} \in Z \mid \nexists \mathbf{x}' \in Z \text{ with } \mathbf{x}' \prec \mathbf{x}\}$$

Aim of optimization: find Pareto front?
  PF maybe infinitively large
  PF hard to hit exactly in continuous space
  $\Rightarrow$ too ambitious!

Aim of optimization: approximate Pareto front!

Scalarization
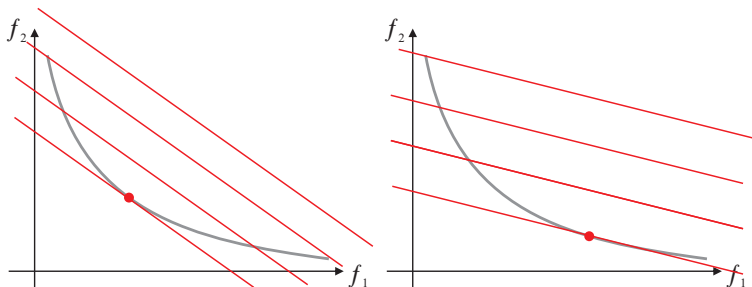
Isn't there an easier way?

Scalarize objectives to single-objective function:
$$f : S \subseteq \mathbb{R}^n \to Z \subseteq \mathbb{R}^2 \Rightarrow \quad f_{scal} = w_1 f_1(\mathbf{x}) + w_2 f_2(\mathbf{x})$$

Result: single solution
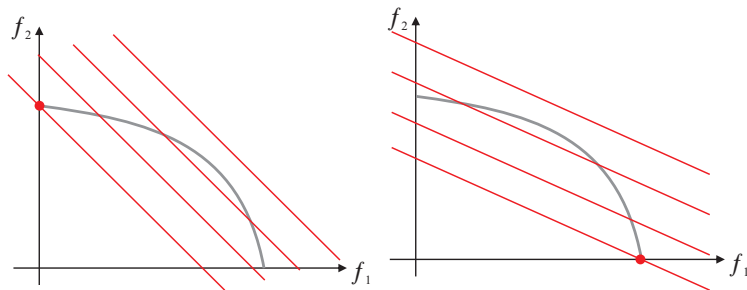Specify desired solution by choice of w_1, w_2

Scalarization

Previous example: convex Pareto front

Consider concave Pareto front
  ↯ only boundary solutions are optimal
  ⇒ scalarization by simple weighting is not a good idea

Classification

a-priori approach
first specify preferences, then optimize

more advanced scalarization techniques (e.g. Tschebyscheff)
allow to access all elements of PF

remaining difficulty:
how to express your desires through parameter values!?
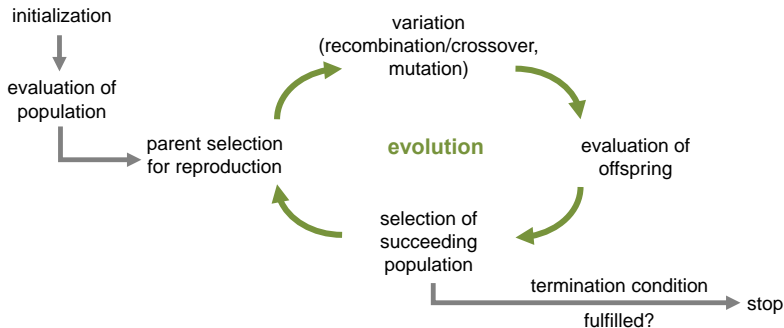
a-posteriori approach
first optimize (approximate Pareto front), then choose solution

⇒back to a-posteriori approach
⇒state-of-the-art methods: evolutionary algorithms

Evolutionary Algorithms

Evolutionary Multiobjective Optimization Algorithms (EMOA)
Multiobjective Optimization Evolutionary Algorithms (MOEA)

What to change in case of multiobjective optimization?
Selection!
Remaining operators may work on search space only

Selection in EMOA

Selection requires sortable population to choose best individuals

How to sort d-dimensional objective vectors?

Primary selection criterion:
use Pareto dominance relation to sort comparable individuals

Secondary selection criterion:
apply additional measure to incomparable individuals to enforce order

Non-dominated Sorting
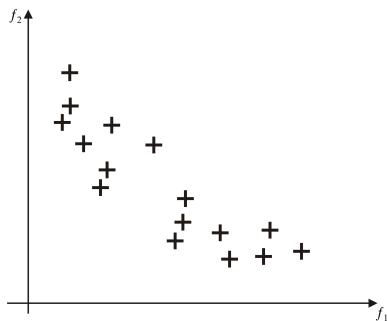
Example for primary selection criterion

partition population into sets of mutually incomparable solutions (antichains)

non-dominated set: best elements of set
NDS(M) = $\{\mathbf{x} \in M \mid \nexists \mathbf{x}' \in M \text{ with } \mathbf{x}' \prec \mathbf{x}\}$

Simple algorithm:
iteratively remove non-dominated set until population empty

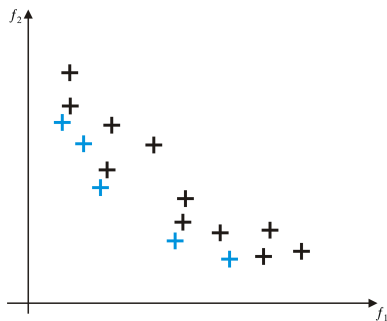# Non-dominated Sorting

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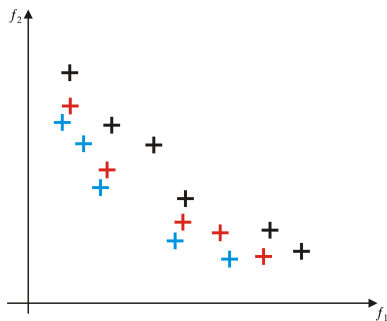
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NSGA-II

Popular EMOA: Non-dominated Sorting Genetic Algorithm II

$(\mu + \mu)$-selection:

1. perform non-dominated sorting on all $\mu + \mu$ individuals
2. take best subsets as long as they can be included completely
3. if population size μ not reached but next subset does not fit in completely:
   apply secondary selection criterion *crowding distance* to that subset
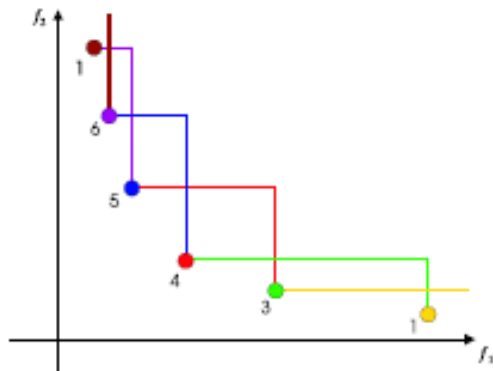4. fill up population with best ones w.r.t. the *crowding distance*

NSGA-II

Crowding distance:

  1/2 perimeter of empty bounding box around point
  value of infinity for boundary points
  large values good

Difficulties of Selection

imagine point in the middle of the search space
  $d = 2$: 1/4 better, 1/4 worse, 1/2 incomparable
  $d = 3$: 1/8 better, 1/8 worse, 3/4 incomparable
  general: fraction 2^{-d+1} comparable, decreases exponentially

⇒typical case: all individuals incomparable
⇒mainly secondary selection criterion in operation

Drawback of crowding distance:
rewards spreading of points, does not reward approaching the Pareto front
⇒NSGA-II diverges for large d, difficulties already for $d = 3$

Difficulties of Selection

Secondary selection criterion has to be meaningful!

Desired: choose best subset of size μ from individuals

How to compare sets of partially incomparable points?
$\Rightarrow$use quality indicators for sets
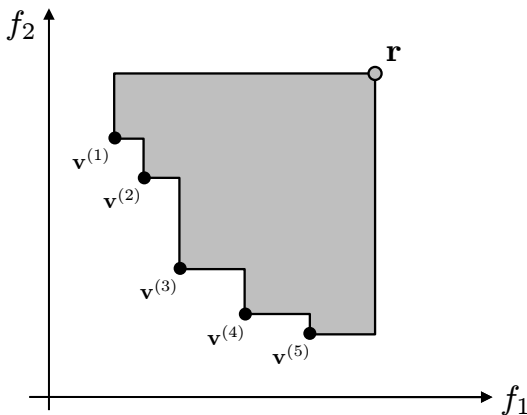
One approach for selection
$\Rightarrow$for each point: determine contribution to quality value of set
$\Rightarrow$sort points according to contribution

Hypervolumen (S-metric) as Quality Measure

dominated hypervolume:
size of dominated space bounded by reference point

$$H(M, \mathbf{r}) := \mathsf{Leb}\left(\bigcup_{i=1}^{m} [\mathbf{v}^{(i)}, \mathbf{r}]\right)$$

$$M = \{\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \dots, \mathbf{v}^{(m)}\}$$
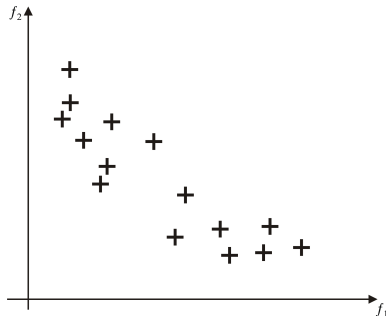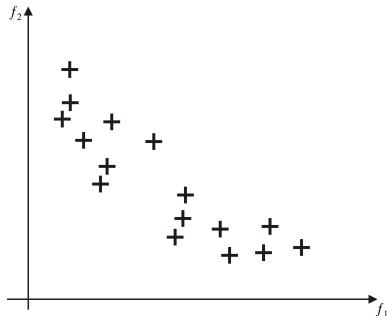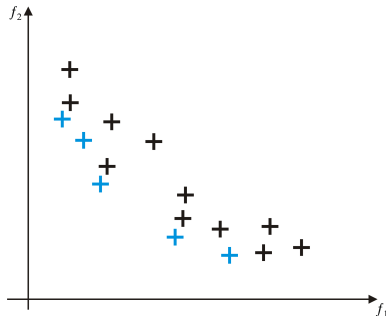
$\mathbf{r}$ reference point

to be maximized

SMS(S-Metric Selection)-EMOA

State-of-the-art EMOA

$(\mu + 1)$-selection

1. non-dominated sorting
2. in case of incomparability: contributions to hypervolume of subset

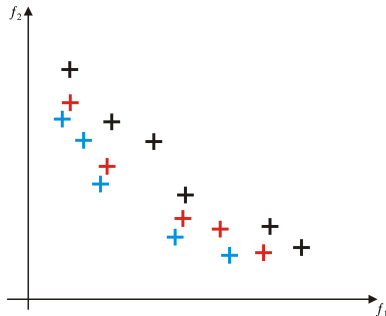# SMS(S-Metric Selection)-EMOA

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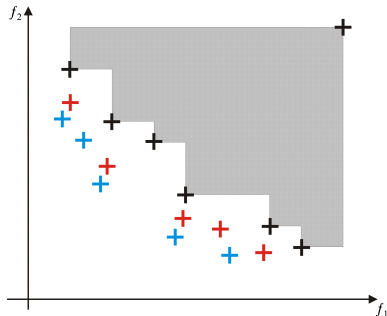2. in case of incomparability: contributions to hypervolume of subset

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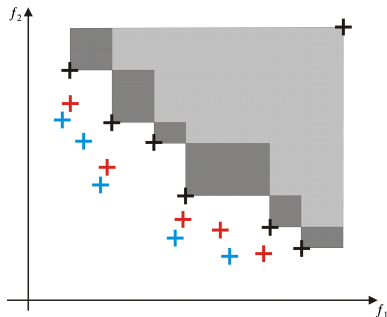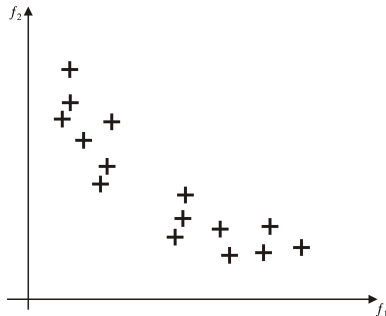2. in case of incomparability: contributions to hypervolume of subset

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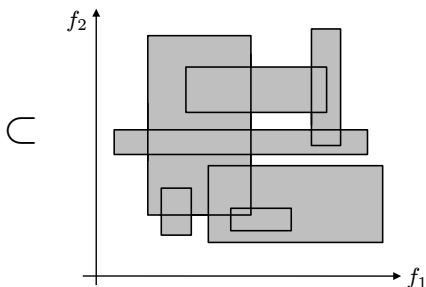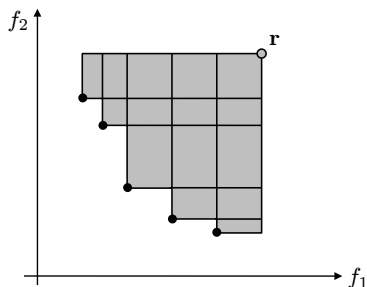
Computational complexity of hypervolume

Lower Bound
$\Omega(m \log m)$

Upper Bound
$O(m^{d/2} \cdot 2^{O(\log^* m)})$

proof: hypervolume as special case of Klee's measure problem

Conclusions on EMOA

NSGA-II
  only suitable in case of d=2 objective functions
  otherwise no convergence to Pareto front

SMS-EMOA
  also effective for $d > 2$ due to hypervolume
  hypervolume calculation time-consuming
  $\Rightarrow$use approximation of hypervolume

Other state-of-the-art EMOA, e.g.

- MO-CMA-ES: CMA-ES + hypervolume selection

- ϵ-MOEA: objective space partitioned into grid, only 1 point per cell

- MSOPS: selection acc. to ranks of different scalarizations

Conclusions

- real-world problems are often multiobjective
- Pareto dominance only a partial order
- a priory: parameterization difficult
- a posteriori: choose solution after knowing possible compromises
- state-of-the-art a posteriori methods: EMOA, MOEA
- EMOA require sortable population for selection
- use quality measures as secondary selection criterion
- hypervolume: excellent quality measure, but computationally intensive
- use state-of-the-art EMOA, other may fail completely