Visualization in Multiobjective Optimization

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Final version

These slides as well as all the approximation sets used in this tutorial are available at `http://dis.ijs.si/tea/research.htm`

Contents

Introduction

Introduction

Multiobjective optimization problem

Minimize

$$\mathbf{f}\colon X \to F$$
$$\mathbf{f}\colon (x_1, \dots, x_n) \mapsto (f_1(x_1, \dots, x_n), \dots, f_m(x_1, \dots, x_n))$$

- X is an n-dimensional decision space (or search space)
- $F \subseteq \mathbb{R}^m$ is an m-dimensional objective space ($m \geq 2$)

Conflicting objectives $\to$ a set of optimal solutions

- Pareto set in the decision space
- Pareto front in the objective space

Introduction

Visualization in multiobjective optimization

- Solution sets in the decision or objective space (or both)
- Multiobjective landscapes—objective values in the decision space

Visualization of solution sets useful for:

- Analysis of solutions and solution sets
- Decision support in interactive optimization
- Analysis of algorithm performance

Visualization of multiobjective landscapes useful for:

- Revealing problem properties and difficulties
- Identifying basins of attraction of local optima

Introduction

Visualizing solution sets in the decision space

- Problem-specific
- If $X \subseteq \mathbb{R}^m$, any method for visualizing multidimensional solutions can be used
- Not the focus of this tutorial

Visualizing solution sets in the objective space

- Interested in sets of mutually nondominated solutions called approximation sets
- Different from ordinary multidimensional solution sets

Visualization of multiobjective landscapes

- Important for problem understanding, but few approaches exist

Introduction

Challenges of visualizing solution sets in the objective space

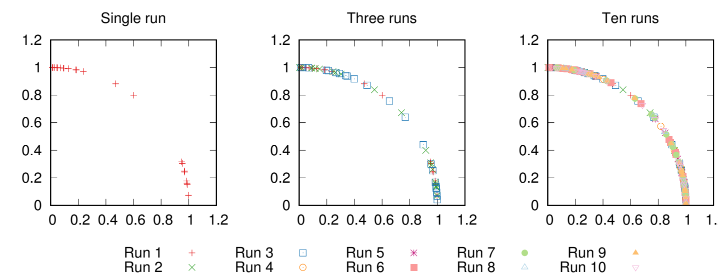
- High dimension and large number of solutions
- Limitations of computing and displaying technologies
- Cognitive limitations

Introduction

Visualization can be hard even in 2-D

Stochastic optimization algorithms

- Single run → single approximation set
- Multiple runs → multiple approximation sets



The Empirical Attainment Function (EAF) [23] or the Average Runtime Attainment Function (aRTA) [10] can be used in such cases

Introduction

This tutorial does not cover

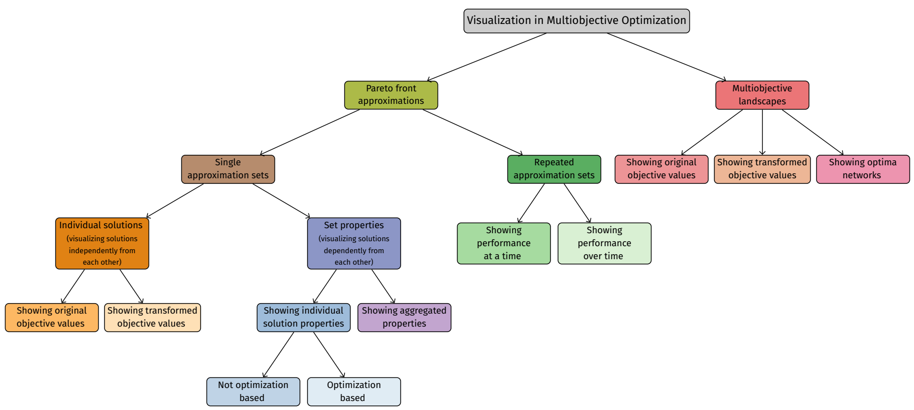
- Visualization of a few solutions for decision making purposes (see [41])
- Visualization of solution sets in the decision space
- General multidimensional visualization methods not previously used on approximation sets

This tutorial covers

- Visualization of solution sets in the objective space
  - Single approximation sets [2]
  - Repeated approximation sets [3, 10]
- Visualization of multiobjective landscapes

A taxonomy of visualization methods

A taxonomy of visualization methods [1]



Visualizing approximation sets

Visualizing approximation sets

Visualizing single approximation sets

Methodology

Evaluating and comparing visualization methods

- No established methodology for evaluating or comparing visualization methods
- Propose benchmark approximation sets (analog to benchmark problems in multiobjective optimization)
- Visualize the sets using different methods
- Observe which set properties are distinguishable after visualization
- Only applicable to methods showing individual solutions or individual solution properties

Benchmark approximation sets

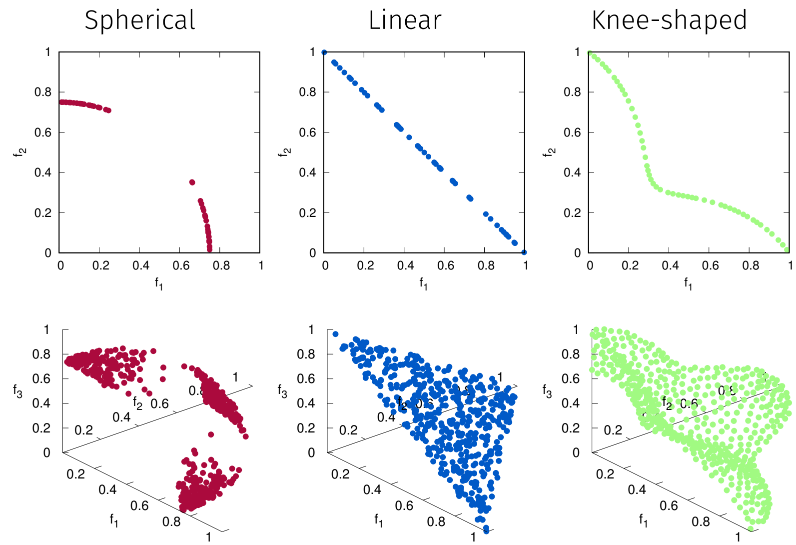
Three different sets that can be instantiated in any dimension

- Spherical with a clustered distribution of solutions (more at the corners and less at the center)
- Linear with a uniform distribution of solutions
- Knee-shaped with an even distribution of solutions

Size of each set

- 2-D: 50 solutions
- 3-D: 500 solutions
- 4-D: 500 solutions

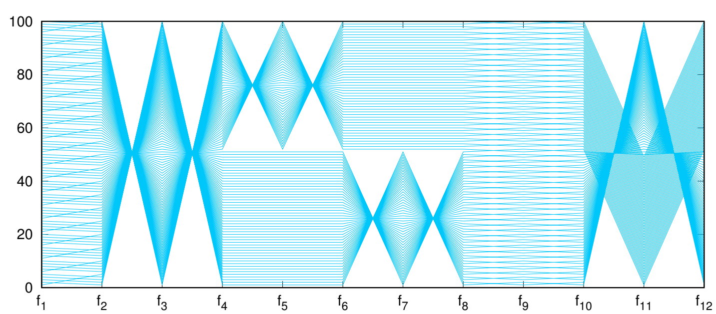
Benchmark approximation sets



Benchmark approximation sets

An additional set with redundant objectives

- Adapted from [21]
- 12 objectives
- Can be instantiated for any number of $10n$ solutions (here 100)



Desired properties of visualization methods

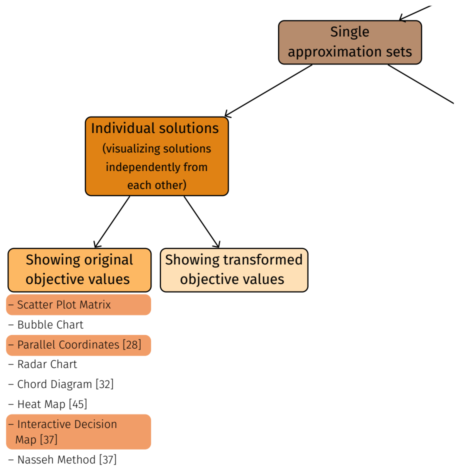
Demonstration on the 4-D spherical, linear and knee-shaped sets

- Preservation of the
  - Dominance relation between solutions
  - Front shape
  - Objective range
  - Distribution of solutions
- Robustness
- Handling of large sets
- Simultaneous visualization of multiple sets
- Scalability in number of objectives
- Simplicity

Demonstration on the 12-D approximation set

- Showing relations between objectives

Visualizing single approximation sets



Scatter plot matrix

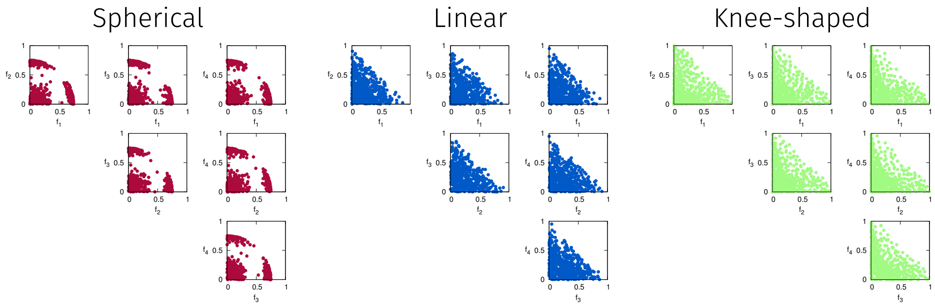
Most often

- Scatter plot in a 2-D space
- Matrix of all possible combinations of objectives
- m objectives $\rightarrow \frac{m(m-1)}{2}$ different combinations

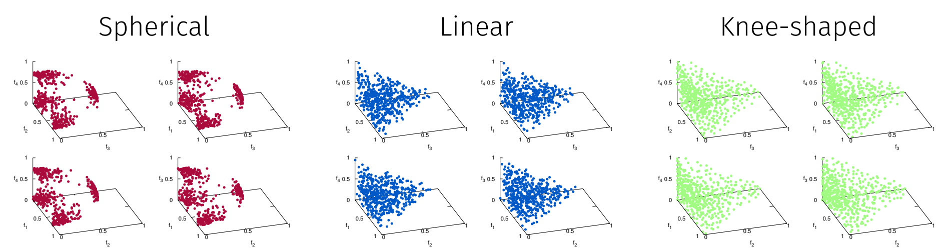
Alternatively

- Scatter plot in a 3-D space
- m objectives $\rightarrow \frac{m(m-1)(m-2)}{6}$ different combinations

Scatter plot matrix



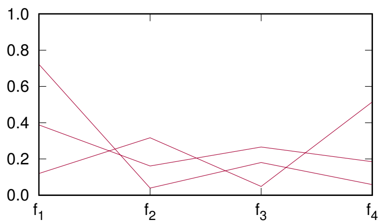
Scatter plot matrix



Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	≈	✓	≈	✓	≈	✓	×	✓

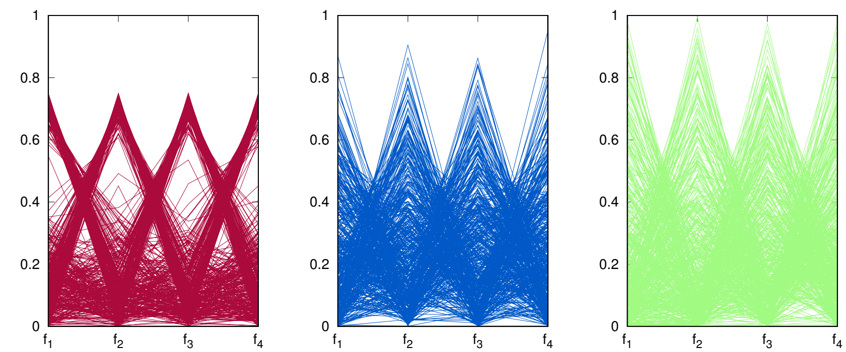
Parallel coordinates

- m objectives $\to$ m parallel axes
- Solution represented as a polyline with vertices on the axes
- Position of each vertex corresponds to that objective value
- No loss of information



Parallel coordinates

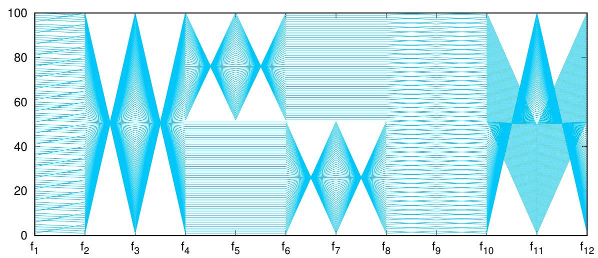
Spherical — Linear — Knee-shaped



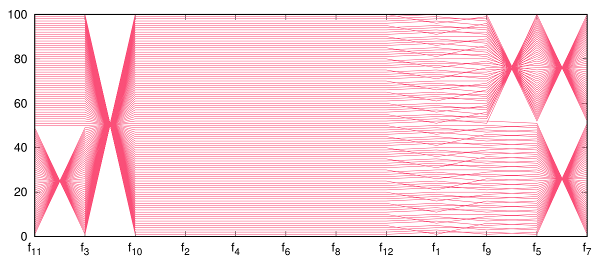
Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
≈	×	✓	≈	✓	×	×	✓	✓

Parallel coordinates

Original



Ordered



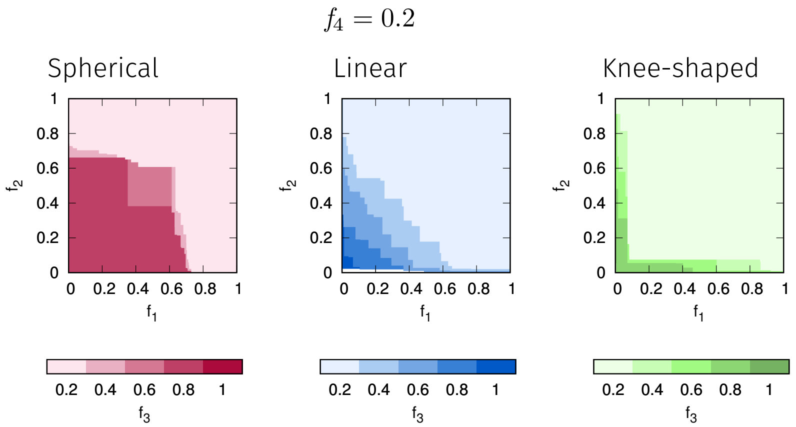
Interactive decision maps

The Edgeworth-Pareto hull (EPH) of an approximation set A contains all points in the objective space that are weakly dominated by any solution in A.

Interactive decision maps

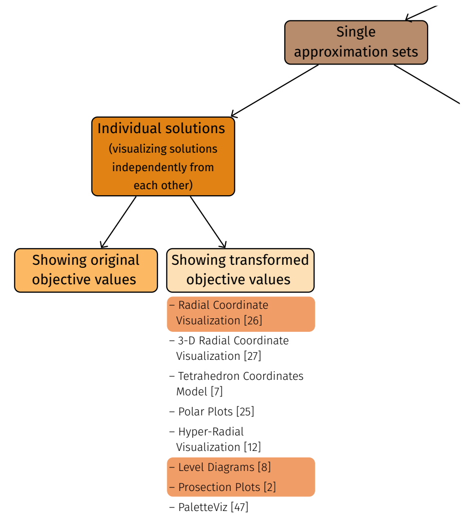
- Visualize the surface of the EPH, not the actual approximation set
- Plot a number of axis-aligned sampling surfaces of the EPH
- Color used to denote third objective
- Fixed value of the forth objective

Interactive decision maps



Preservation of the dominance relation	Preservation of the front shape	Preservation of the objective range	Preservation of the distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	≈	✓	≈	✓	✓	×	×	≈

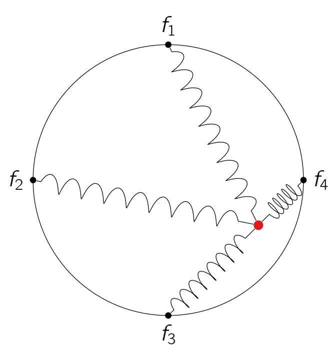
Visualizing single approximation sets



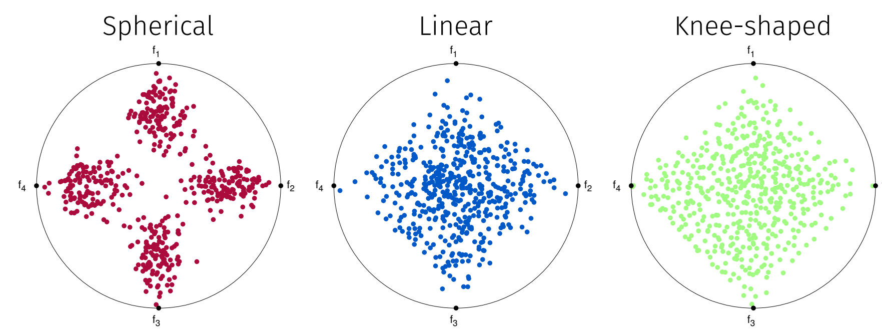
Radial coordinate visualization

Also called RadViz

- Inspired from physics
- Objectives treated as anchors, equally spaced around the circumference of a unit circle
- Solutions attached to anchors with 'springs'
- Spring stiffness proportional to the objective value
- Solution placed where the spring forces are in equilibrium



Radial coordinate visualization



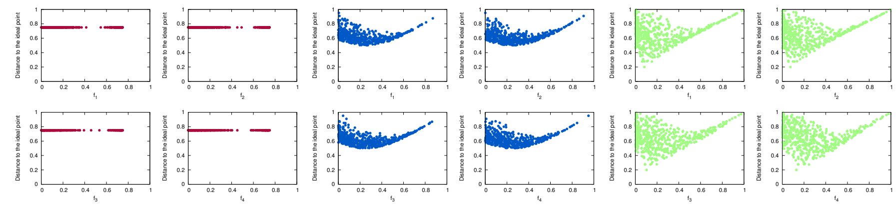
Preservation of the dominance relation	Preservation of the front shape	Preservation of the objective range	Preservation of the distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	×	×	≈	✓	≈	✓	✓	✓

Level diagrams

- m objectives $\rightarrow$ m diagrams
- Plot solutions with objective f_i on the x axis and distance to the ideal point on the y axis

Level diagrams

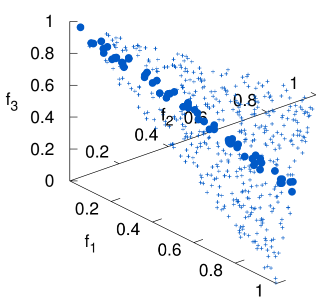
Spherical Linear Knee-shaped



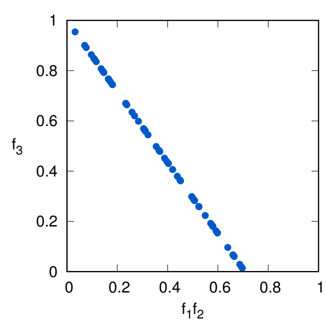
Preservation of the dominance relation	Preservation of the front shape	Preservation of the objective range	Preservation of the distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	≈	✓	×	✓	≈	✓	✓	✓

Prosections

- Visualize only part of the objective space
- Dimensionality reduction by projection of solutions in a section
- Need to choose prosection plane, angle and section width



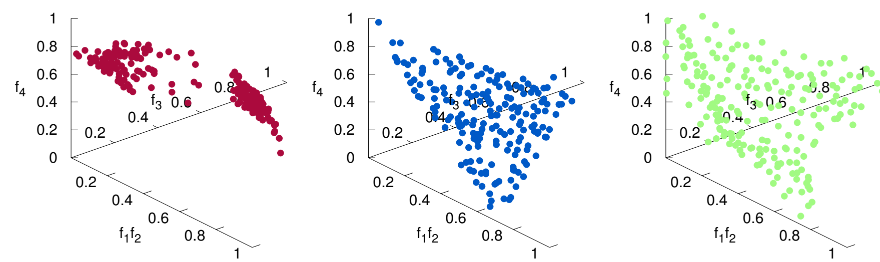
Before prosection



After prosection

Prosections

Spherical Linear Knee-shaped



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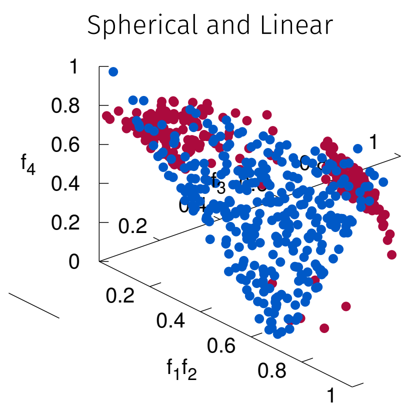
✓	✓	≈	✓	✓	✓	✓	×	≈

Prosections



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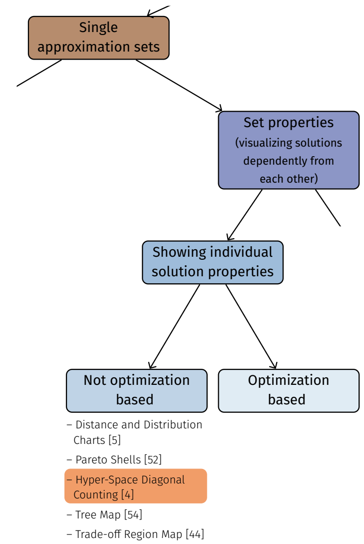
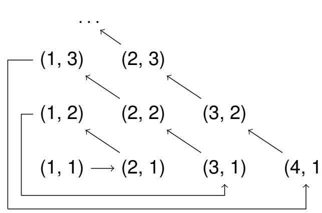
✓	✓	≈	✓	✓	✓	✓	×	≈

Visualizing single approximation sets



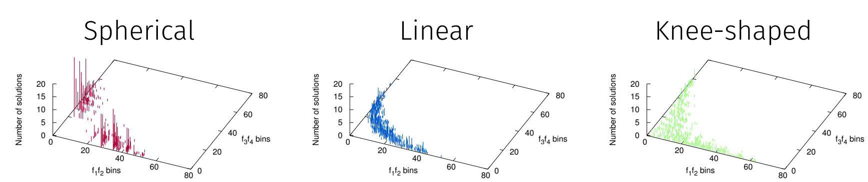
Hyper-space diagonal counting

- Inspired by Cantor's proof that shows $|\mathbb{N}| = |\mathbb{N}^2| = |\mathbb{N}^3| \ldots$



- Discretize each objective (choose a number of bins)
- In the 4-D case
  - Enumerate the bins for objectives f_1 and f_2
  - Enumerate the bins for objectives f_3 and f_4
  - Plot the number of solutions in each pair of bins

Hyper-space diagonal counting



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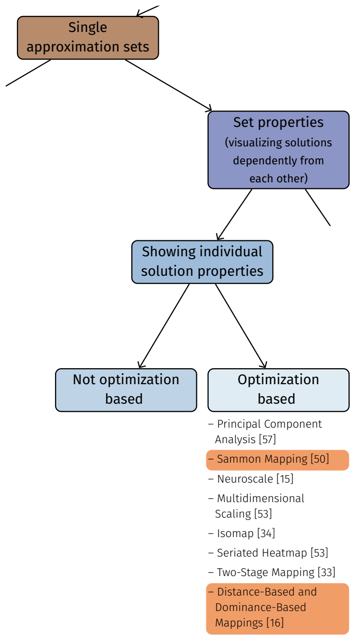
Visualizing single approximation sets



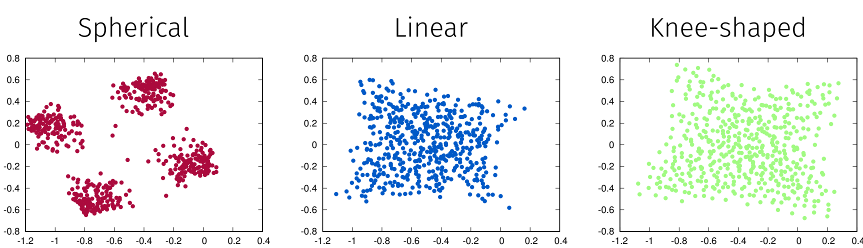
Sammon mapping

- A non-linear mapping
- Aims to preserve distances between solutions
  - d^*_{ij} distance between solutions $\mathbf{x}_i$ and $\mathbf{x}_j$ in the objective space
  - d_{ij} distance between solutions $\mathbf{x}_i$ and $\mathbf{x}_j$ in the visualized space
- Stress function to be minimized

$$S = \sum_i \sum_{j>i} (d^*_{ij} - d_{ij})^2$$

- Minimization by gradient descent or other (iterative) methods

Sammon mapping



Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	×	×	✓	≈	≈	✓	✓	×

Distance- and dominance-based mappings

Both mappings

- Use nondominated sorting to split solutions to fronts
- Project solutions onto the circumference of circles (with circle radius proportional to front number)

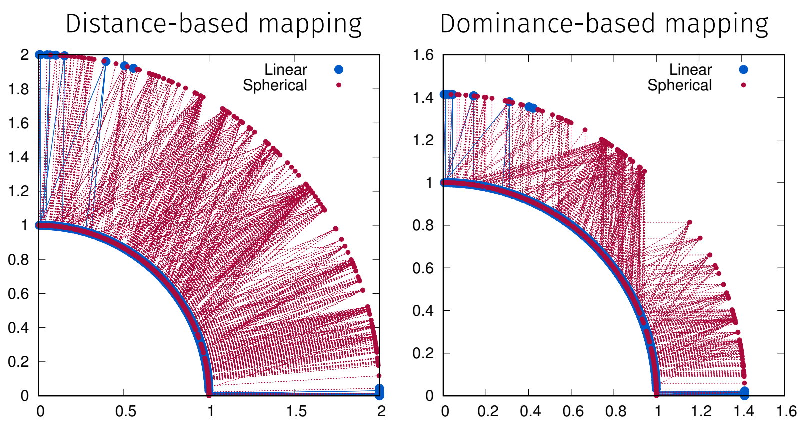
Distance-based mapping

- Tries to preserve closeness of solutions
- Two solutions are very close if their relations to other solutions are mostly equal

Dominance-based mapping

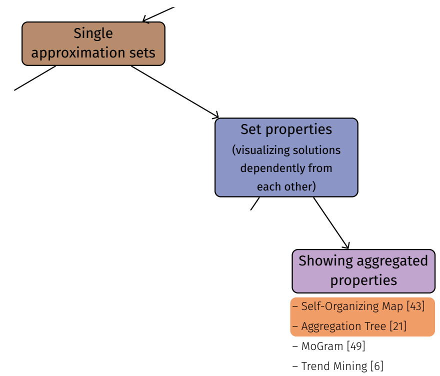
- Aims at preserving dominance relations among solutions
- All $\mathbf{x} \prec \mathbf{y}$ can be shown correctly
- Tries to minimize cases where $\mathbf{x} \not\prec \mathbf{y}$ is not shown correctly

Distance- and dominance-based mappings



Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
× / ✓	×	×	× / ≈	≈	×	✓	✓	×

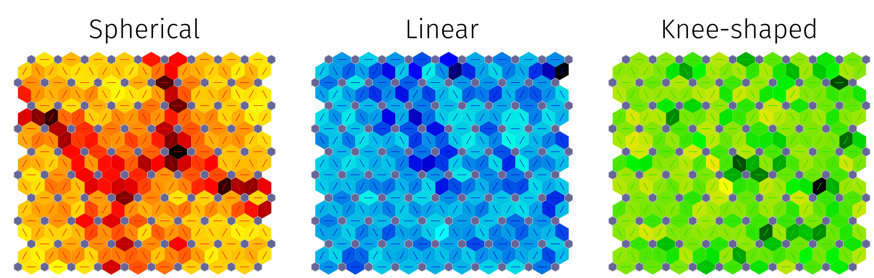
Visualizing single approximation sets



Self-organizing maps

- Self-organizing maps (SOMs) are neural networks
- Nearby solutions are mapped to nearby neurons in the SOM
- A SOM can be visualized using the unified distance matrix
- Distance between adjacent neurons is denoted with color
  - Similar neurons → light color
  - Different neurons (cluster boundaries) → dark color

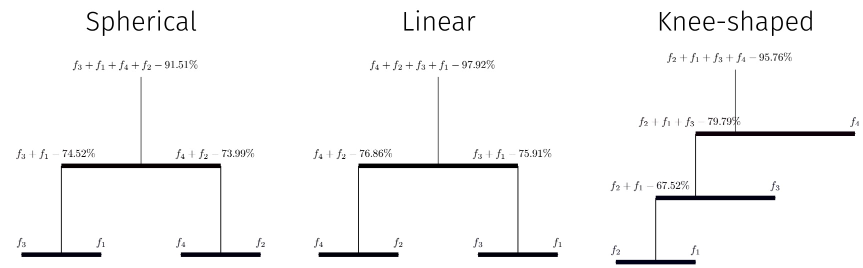
Self-organizing maps



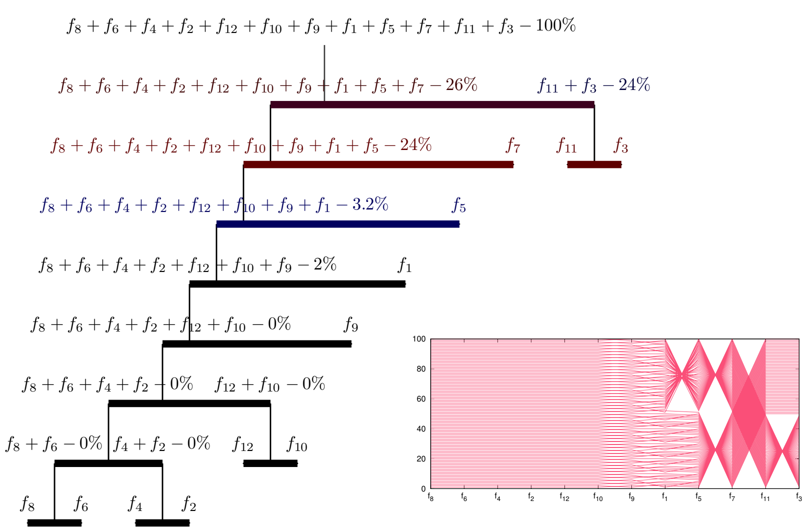
Aggregation trees

- Binary trees that show relationships between objectives
- Iterative clustering of objectives based on their harmony
- Computation of different types of conflict
- Percentages quantify the conflict between objectives
- Colors used to show type of conflict
  - global conflict (black)
  - local conflict on 'good' values (red)
  - local conflict on 'bad' values (blue)
- Can be used to sort objectives in other representations (parallel coordinates, radial charts, heat maps)

Aggregation trees



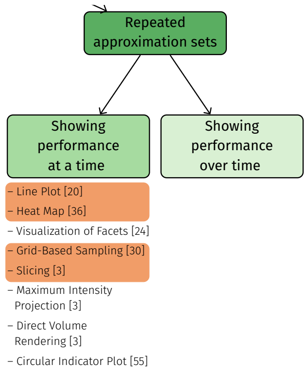
Aggregation trees



Visualizing approximation sets

Visualizing repeated approximation sets

Visualizing repeated approximation sets

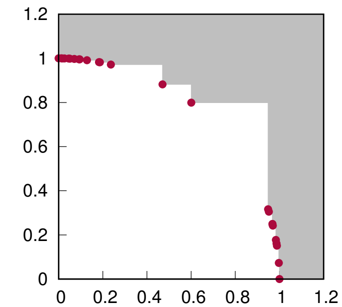


Showing performance at a time with the Empirical Attainment Function (EAF) [23]

Empirical attainment function

Goal-attainment

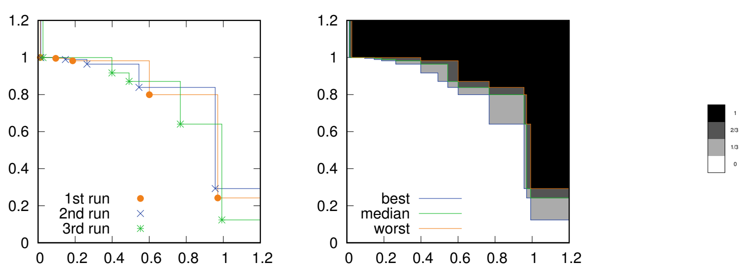
- Approximation set A
- A point in the objective space $\mathbf{z}$ is attained by A when $\mathbf{z}$ is weakly dominated by at least one solution from A



Empirical attainment function

EAF values [23]

- Algorithm $\mathcal{A}$, approximation sets $A_1, A_2, \ldots, A_r$
- EAF of $\mathbf{z}$ is the frequency of attaining $\mathbf{z}$ by $A_1, A_2, \ldots, A_r$
- Summary (or k%-) attainment surfaces

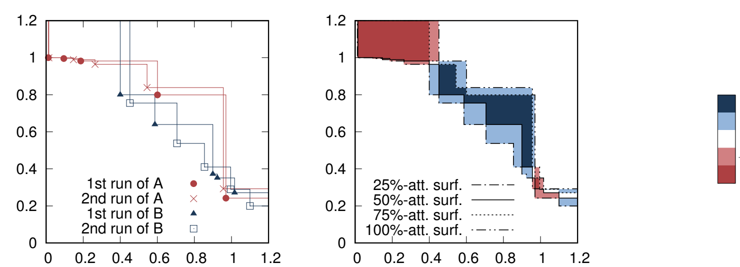


- Visualization with line plots and heat maps

Empirical attainment function

Differences in EAF values [36]

- Algorithm $\mathcal{A}$, approximation sets $A_1, A_2, \ldots, A_r$
- Algorithm $\mathcal{B}$, approximation sets $B_1, B_2, \ldots, B_r$
- Visualize differences between EAF values



- Visualization with heat maps

Visualization of 3-D EAF

Need to compute and visualize a large number (over 10 000) of cuboids

Exact case

- EAF values: Slicing [3], Visualization of facets [13, 24]
- EAF differences: Slicing, Maximum intensity projection [56, 3]

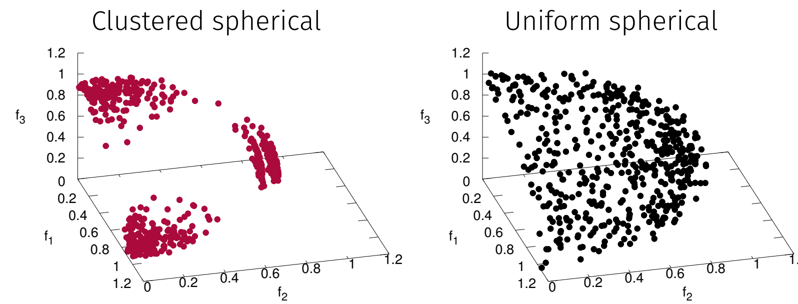
Approximated case

- EAF values: Grid-based sampling [30], Slicing, Direct volume rendering [14, 3]
- EAF differences: Slicing, Maximum intensity projection, Direct volume rendering

Benchmark approximation sets

Two groups of spherical approximation sets

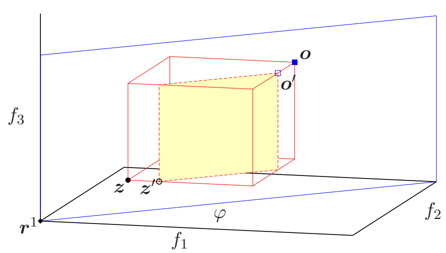
- 5 spherical approximation sets with a clustered distribution of solutions (different radii, 100 solutions in each)
- 5 spherical approximation sets with a uniform distribution of solutions (different radii, 100 solutions in each)



Exact 3-D EAF values and differences

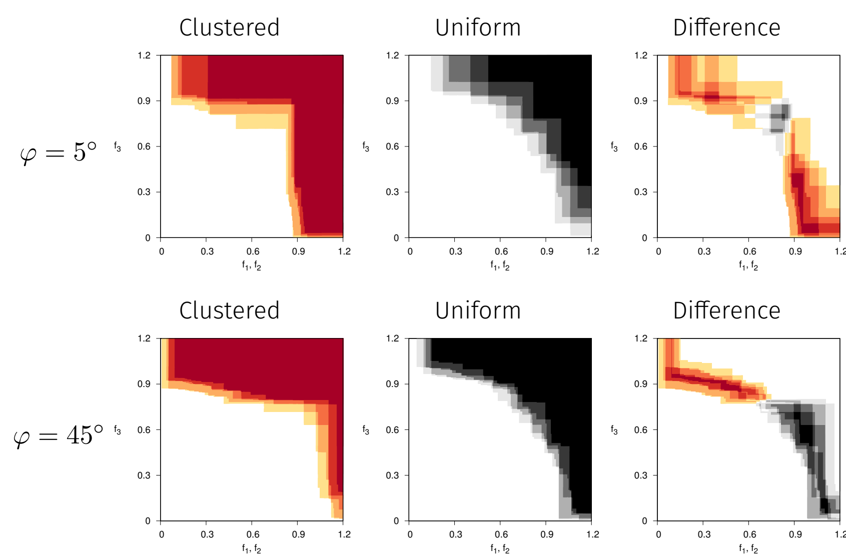
Slicing

- Visualize cuboids intersecting the slicing plane
- Need to choose coordinate and angle



Exact 3-D EAF values and differences

Slicing



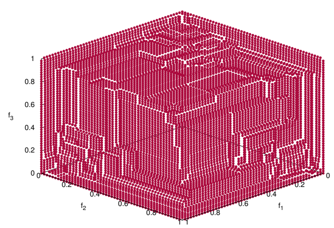
Approximated attainment surfaces

Grid-based sampling

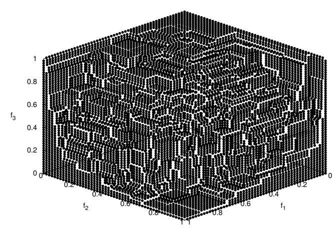
Repeat for all $f_i f_j, i < j$ (i.e. $f_1 f_2, f_1 f_3$ and $f_2 f_3$):

- Construct a $k \times k$ grid on the plane $f_i f_j$
- Compute intersections between the attainment surface and the axis-aligned lines on the grid

Clustered

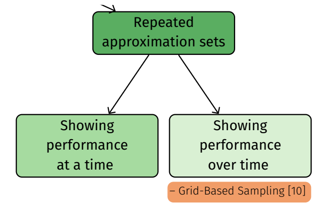


Uniform



Median attainment surfaces

Visualizing repeated approximation sets



Showing performance over time with the Average Runtime Attainment Function (aRTA) [10]

Average Runtime Attainment Function

aRTA value

- Algorithm $\mathcal{A}$ run r times
- All solutions that are nondominated at creation are recorded
- aRTA($\mathbf{z}$) is the average number of evaluations needed to attain $\mathbf{z}$

aRTA ratio

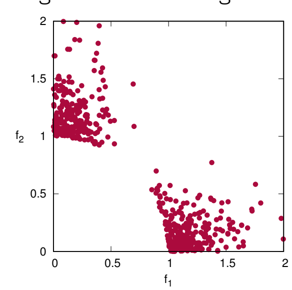
- Algorithms $\mathcal{A}$ and $\mathcal{B}$
- Visualize ratio between aRTA($\mathbf{z}$) values for $\mathcal{A}$ and $\mathcal{B}$

Benchmark approximation sets

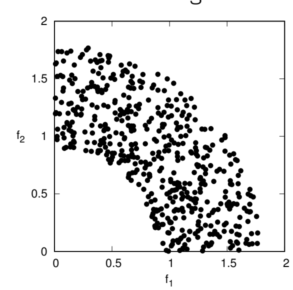
Two groups of sets mimicking convergence to a spherical front

- 5 sets mimicking logarithmic convergence to a spherical front with a clustered distribution (100 solutions each)
- 5 sets mimicking linear convergence to a spherical front with a uniform distribution (100 solutions each)

Clustered with logarithmic convergence



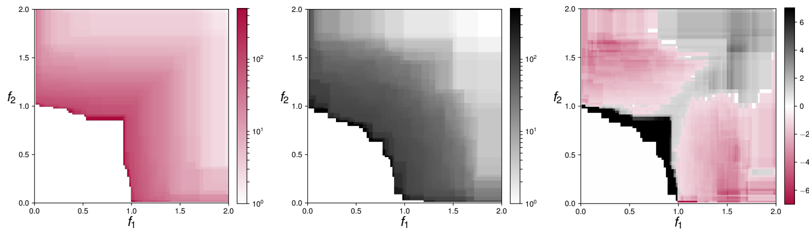
Uniform with linear convergence



Average Runtime Attainment Function

Grid-based sampling

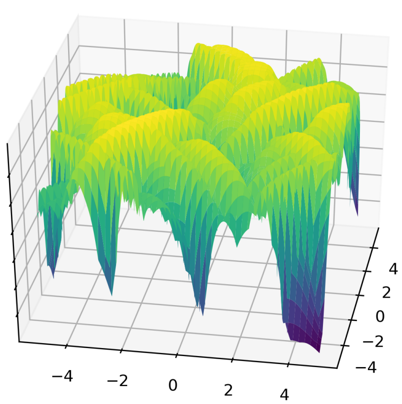
Clustered with logarithmic convergence | Uniform with linear convergence | Ratio



Visualizing multiobjective landscapes

Visualizing problem landscapes

- Single objective: visualize objective values in the decision space
- Multiple objectives: ?



Benchmark problems

The **bbob-biobj** test suite [11]

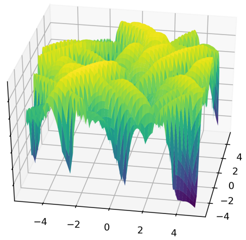
- Each bi-objective function constructed as the combination of two single-objective **bbob** functions
- Problems scalable in the number of decision variables
- Known single-objective optima, but not the Pareto set (or front)
- Included in the COCO platform (`https://github.com/numbbo/coco`)

Benchmark problems with 2-D and 5-D decision spaces

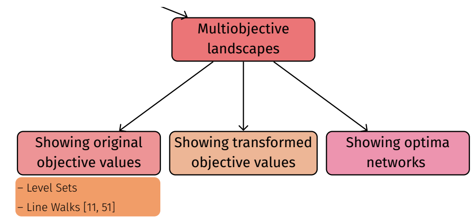
Three bbob-biobj benchmark problems

- Double sphere problem ($F_1 = (f_1, f_1)$ in 2-D and 5-D, instance 1)
- Sphere-Gallagher problem ($F_{10} = (f_1, f_{21})$ in 2-D and 5-D, instance 1)
- Double Gallagher problem ($F_{55} = (f_{21}, f_{21})$ in 2-D and 5-D, instance 1)

*Gallagher = Gallagher's Gaussian 101-me Peaks Function



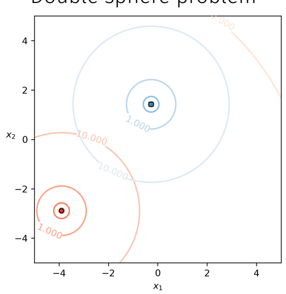
Visualizing multiobjective landscapes



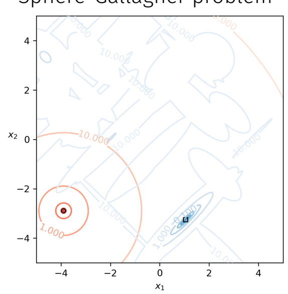
Level sets

- Curves connecting points with the same value
- Orange = first objective, blue = second objective
- Demonstration on the 2-D benchmark problems

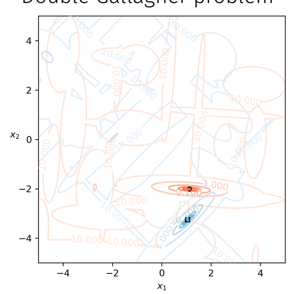
Double sphere problem



Sphere-Gallagher problem



Double Gallagher problem

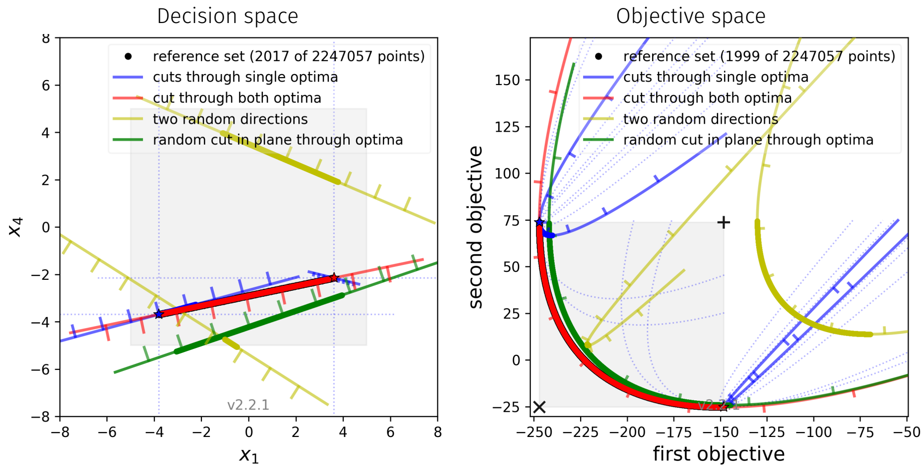


Line walks

- Equidistant sampling of the decision space along a line
- The line does not have to be parallel to an axis
- Not constrained by the decision space dimension
- Two display options
  - Show resulting values for each objective separately
  - Show resulting values in the objective space
- Demonstration on the 5-D benchmark problems

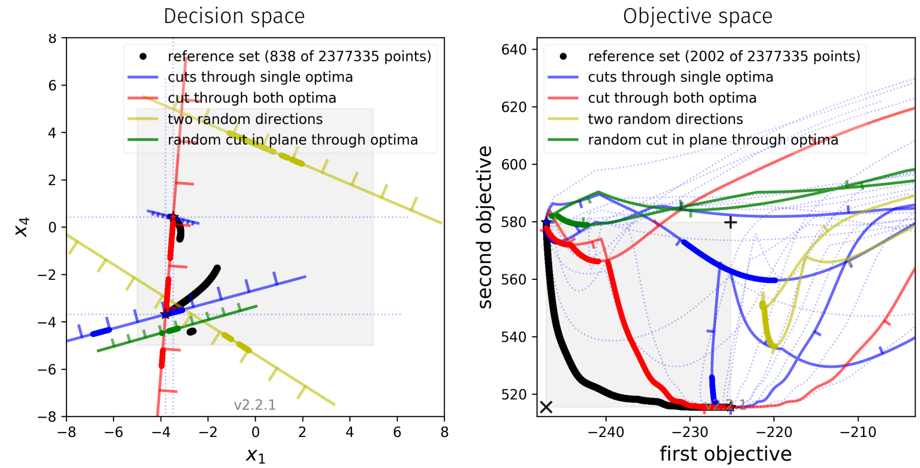
Line walks

Double sphere problem in 5-D



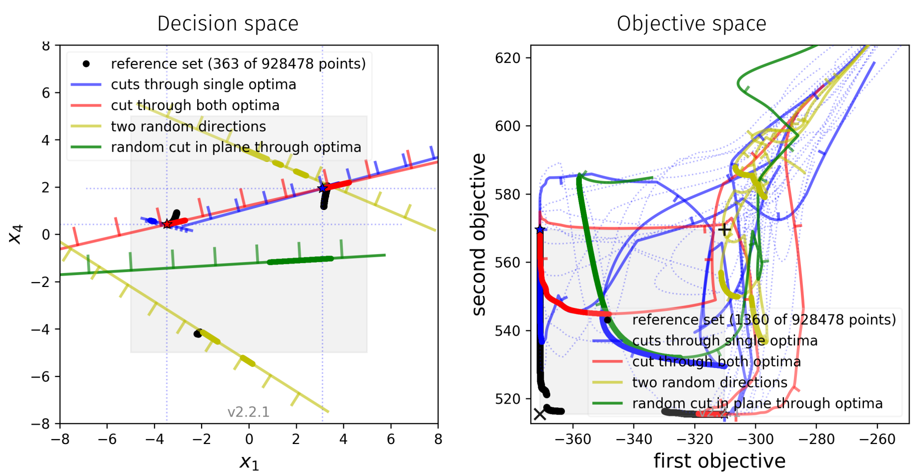
Line walks

Sphere-Gallagher problem in 5-D

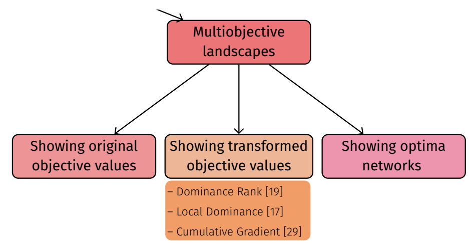


Line walks

Double Gallagher problem in 5-D



Visualizing multiobjective landscapes



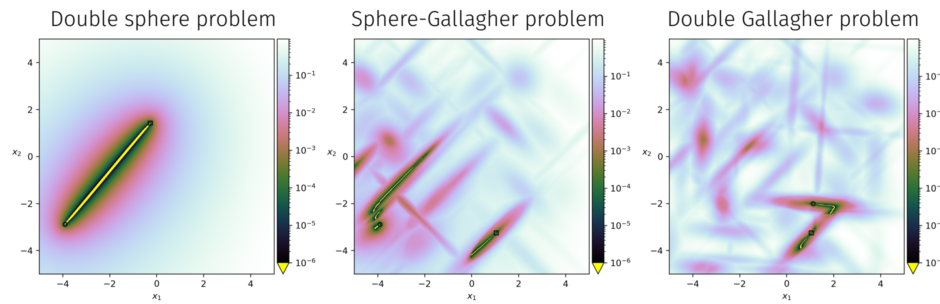
Showing transformed objective values

- Decision space approximated with a grid of points
- Show value using color (contours or the third dimension)
- Suitable only for 2-D decision spaces

Visualizing dominance ranks

- Discretized decision space (1000×1000 grid)
- Rank $=$ number of grid points that dominate the current point
- All nondominted points have a rank of zero
- Visualize normalized ranks in logarithmic scale

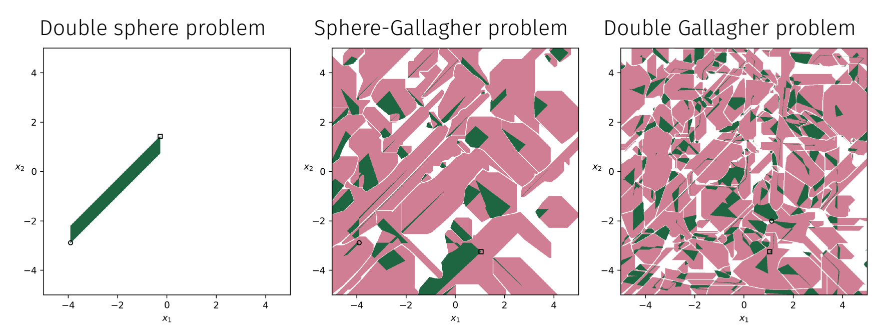
Visualizing dominance ranks



Visualizing local dominance

- Discretized decision space (1000×1000 grid)
- Moore neighborhood = eight surrounding points
- Compute three different kinds of regions
  - **Green** Locally dominance-neutral regions
    - Points that are mutually nondominated with all their neighbors
    - Not equal to local Pareto sets
  - **Pink** Basins of attraction
  - **White** Boundary regions
- Can take a long time to compute

Visualizing local dominance



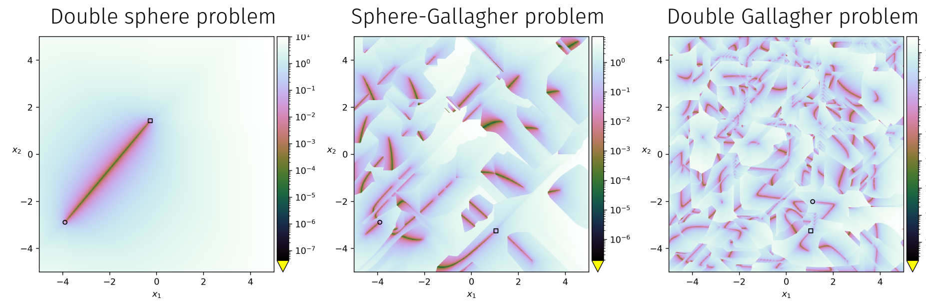
Visualizing cumulative gradients

- Discretized decision space (1000×1000 grid)
- Compute the bi-objective gradient for all grid points

$$v = \frac{v_1}{||v_1||} + \frac{v_2}{||v_2||}$$

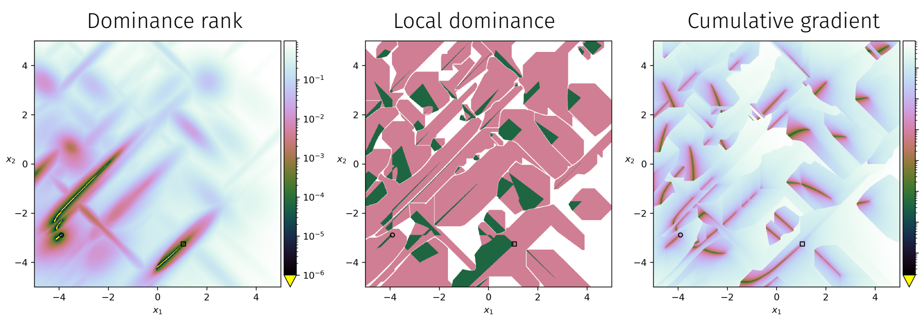
- From a grid point, follow the path in the direction of the bi-objective gradient
- Sum all bi-objective gradient values along the path
- Visualize cumulative gradients in logarithmic scale

Visualizing cumulative gradients



Global vs. local information

Sphere-Gallagher problem



Visualizing multiobjective landscapes

How to handle such visualization when $n > 2$?

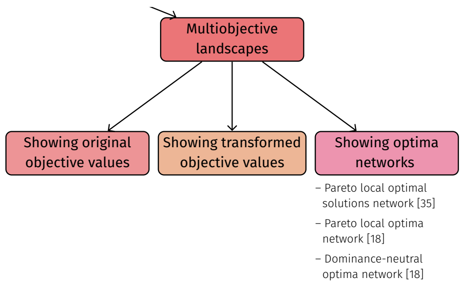
Level sets, dominance ranks, local dominance and cumulative gradients

- Require cuts through the decision space (cf. slicing)
- Challenging to compute and interpret these methods in n-D

Line walks

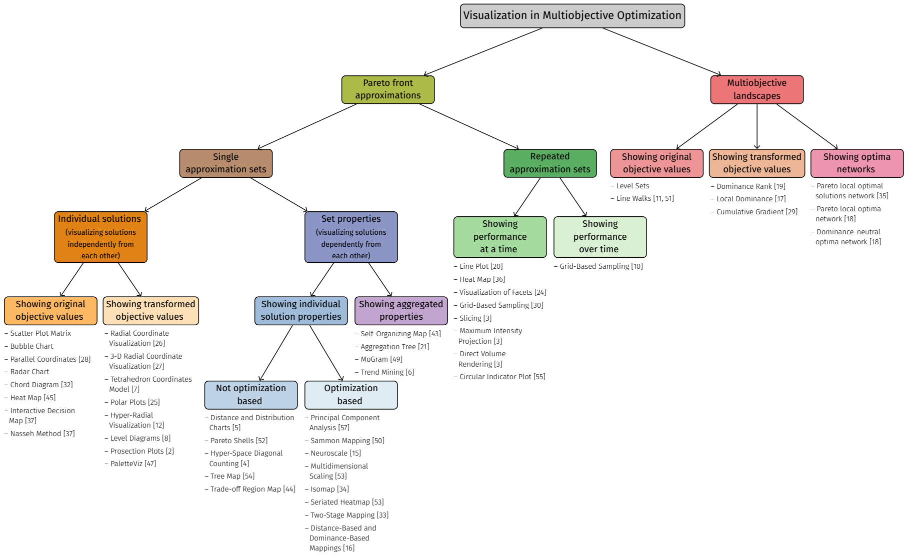
- A useful alternative for high-dimensional decision spaces
- The presented information is very limited

Visualizing multiobjective landscapes



Summary

Summary



Summary

- Visualization in multiobjective optimization useful for various purposes
- Customized methods are needed to address the peculiarities of approximation set visualization as well as multiobjective landscape visualization
- New visualization methods should first be analyzed using approximation sets and problems with known properties
- Visualization methods should also be evaluated with user studies (never done in multiobjective optimization and seldom in evolutionary computation [39])

Acknowledgement

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