



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>

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Introduction

Multiobjective optimization problem

Minimize

$$\mathbf{f}: X \rightarrow F$$

$$\mathbf{f}: (x_1, \dots, x_n) \mapsto (f_1(x_1, \dots, x_n), \dots, f_m(x_1, \dots, x_n))$$

- 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 \rightarrow a set of optimal solutions

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

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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

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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

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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

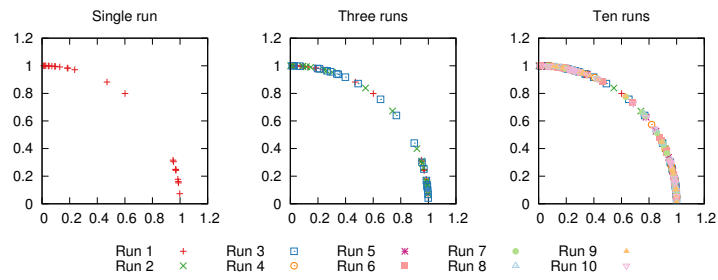
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Introduction

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)** [20] or the **Average Runtime Attainment Function (aRTA)** [9] can be used in such cases

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Introduction

This tutorial does not cover

- Visualization of a few solutions for decision making purposes (see [36])
- 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, 9]
- Visualization of multiobjective landscapes

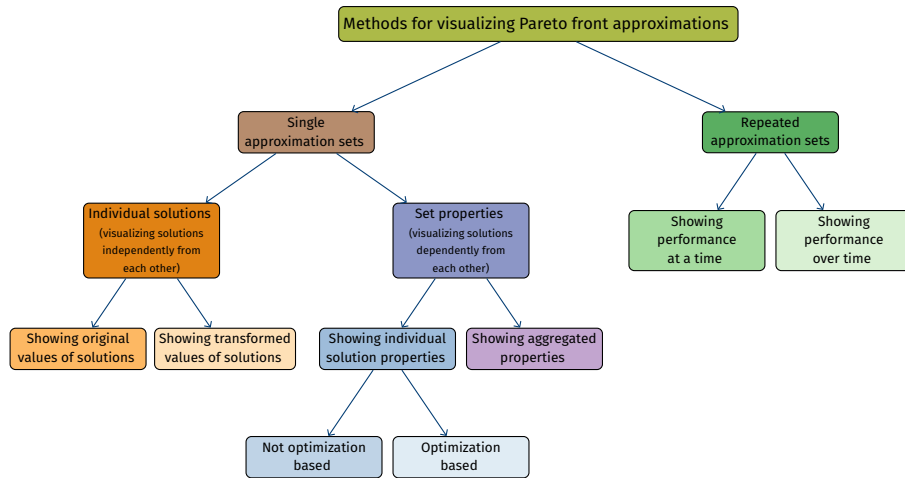
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Visualizing approximation sets

Visualizing approximation sets

A taxonomy of visualization methods

A taxonomy of visualization methods [1]



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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

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Benchmark approximation sets

Three different sets that can be instantiated in any dimension

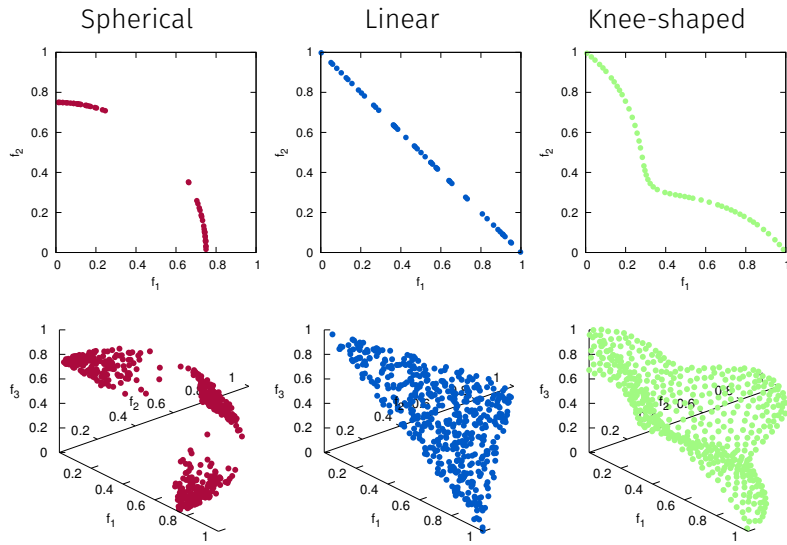
- **Spherical** with a **clustered distribution** of solutions (more at the corners and less at the center)
- **Linear** with a **uniform distribution** of solutions
- **Knee-shaped** with an **even distribution** of solutions

Size of each set

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

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Benchmark approximation sets

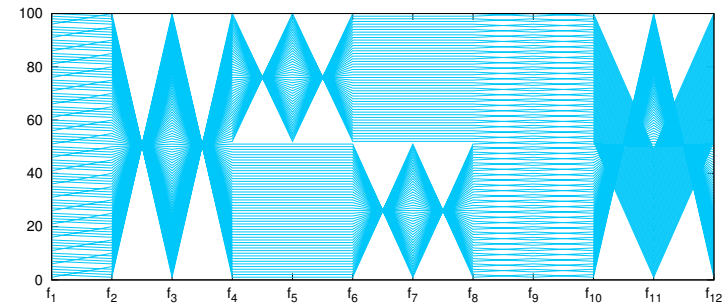


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Benchmark approximation sets

An additional set with redundant objectives

- Adapted from [18]
- 12 objectives
- Can be instantiated for any number of $10n$ solutions (here 100)



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Desired properties of visualization methods

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

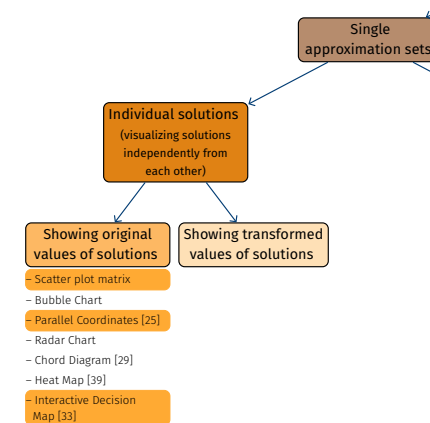
- Preservation of the
 - Dominance relation between solutions
 - Front shape
 - Objective range
 - Distribution of solutions
- Robustness
- Handling of large sets
- Simultaneous visualization of multiple sets
- Scalability in number of objectives
- Simplicity

Demonstration on the 12-D approximation set

- Showing relations between objectives

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Visualizing single approximation sets



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Scatter plot matrix

Most often

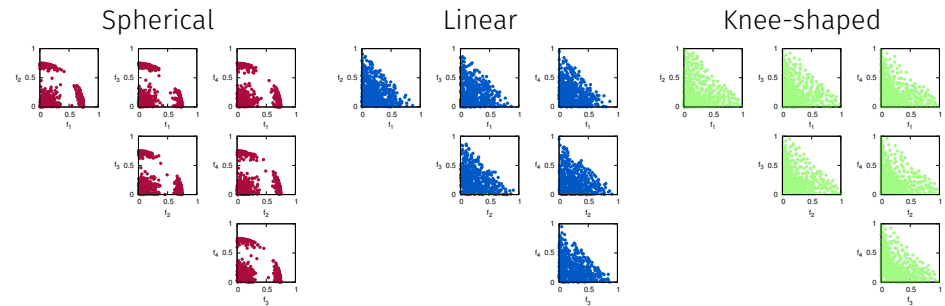
- Scatter plot in a 2-D space
- Matrix of all possible combinations of objectives
- m objectives $\rightarrow \frac{m(m-1)}{2}$ different combinations

Alternatively

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

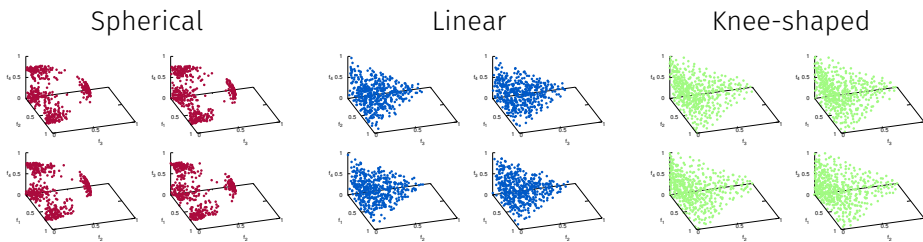
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Scatter plot matrix



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Scatter plot matrix

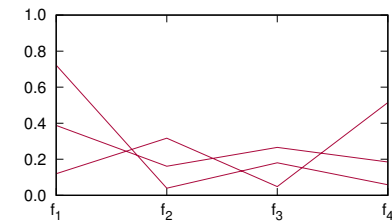


dominance relation	Preservation of the			Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
	front shape	objective range	distribution of solutions					
×	≈	✓	≈	✓	≈	✓	×	✓

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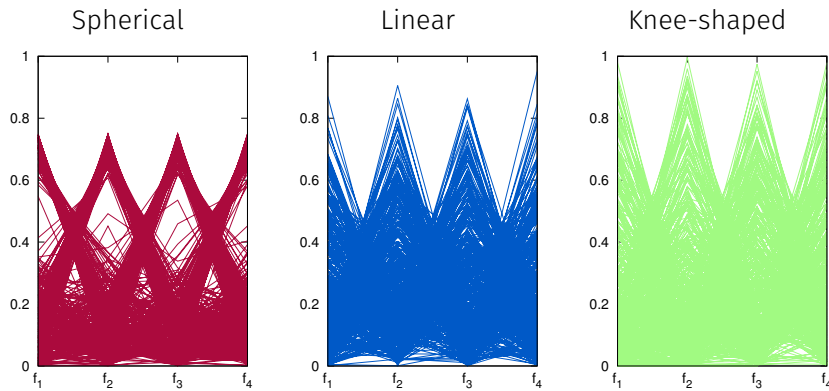
Parallel coordinates

- m objectives $\rightarrow m$ 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



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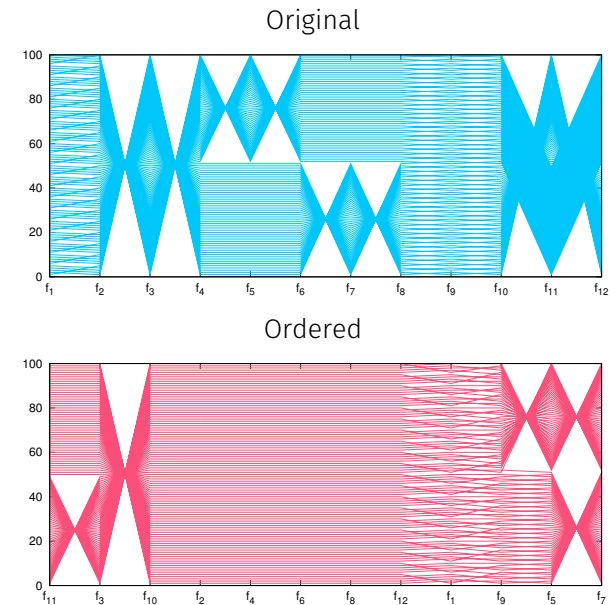
Parallel coordinates



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

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Parallel coordinates



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Interactive decision maps

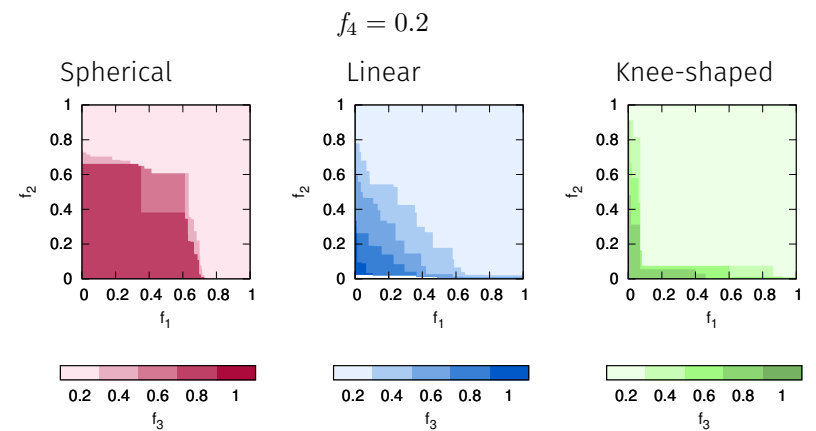
The **Edgeworth-Pareto hull (EPH)** of an approximation set A contains all points in the objective space that are weakly dominated by any solution in A .

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 fourth objective

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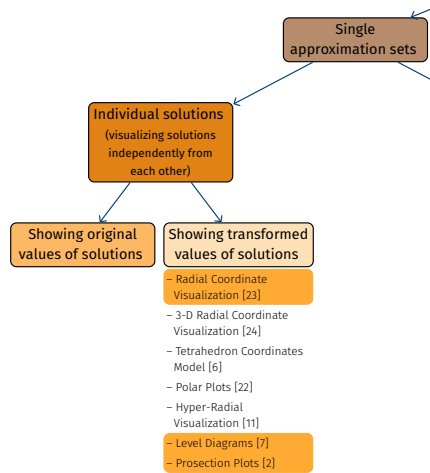
Interactive decision maps



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

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Visualizing single approximation sets

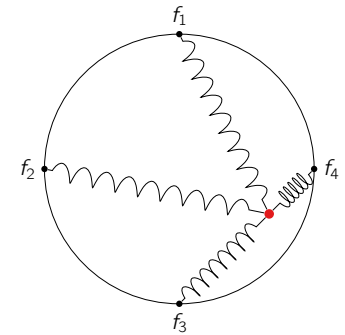


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Radial coordinate visualization

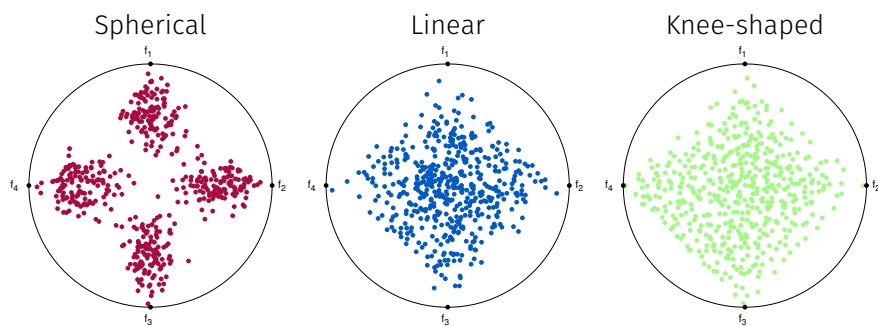
Also called **RadViz**

- 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



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Radial coordinate visualization



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

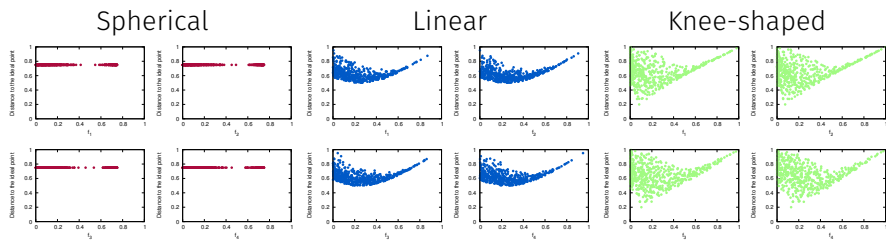
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Level diagrams

- 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

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Level diagrams

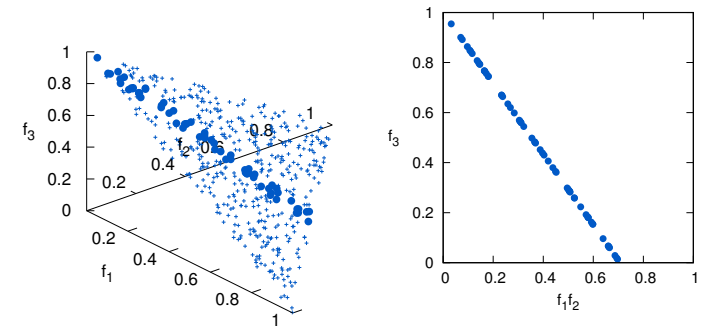


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	≈	✓	×	✓	≈	✓	✓	✓

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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

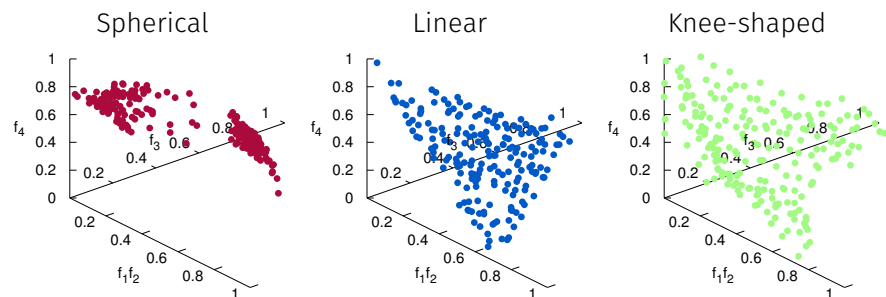


Before prosection

After prosection

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Prosections

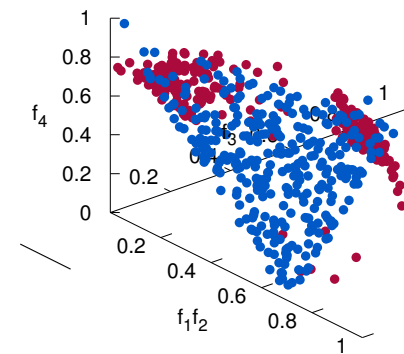


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
✓	✓	≈	✓	✓	✓	✓	×	≈

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Prosections

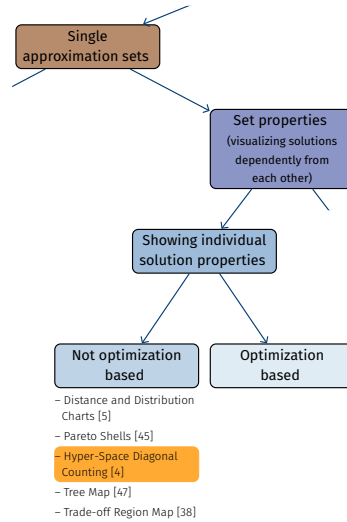
Spherical and Linear



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

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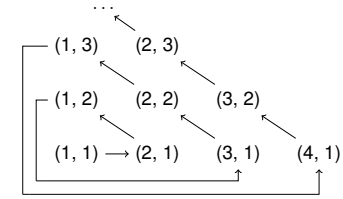
Visualizing single approximation sets



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Hyper-space diagonal counting

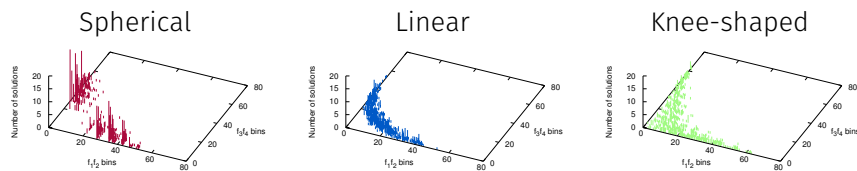
- Inspired by Cantor's proof that shows $|\mathbb{N}| = |\mathbb{N}^2| = |\mathbb{N}^3| \dots$



- 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

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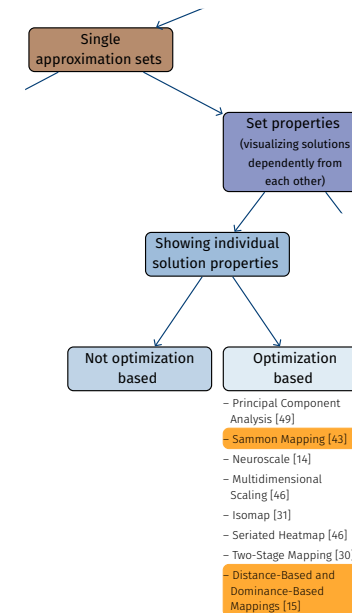
Hyper-space diagonal counting



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

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Visualizing single approximation sets



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Sammon mapping

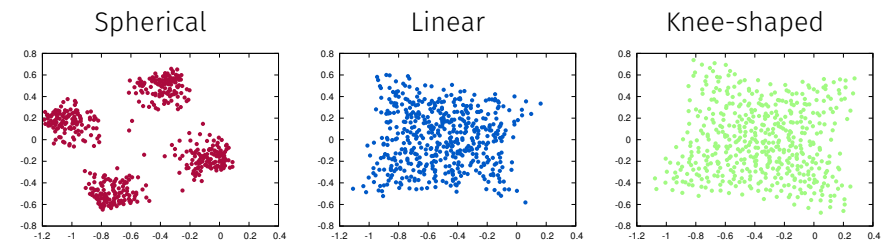
- A non-linear mapping
- Aims to preserve distances between solutions
 - d_{ij}^* distance between solutions \mathbf{x}_i and \mathbf{x}_j in the objective space
 - d_{ij} distance between solutions \mathbf{x}_i and \mathbf{x}_j in the visualized space
- Stress function to be minimized

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

- Minimization by gradient descent or other (iterative) methods

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Sammon mapping



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

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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

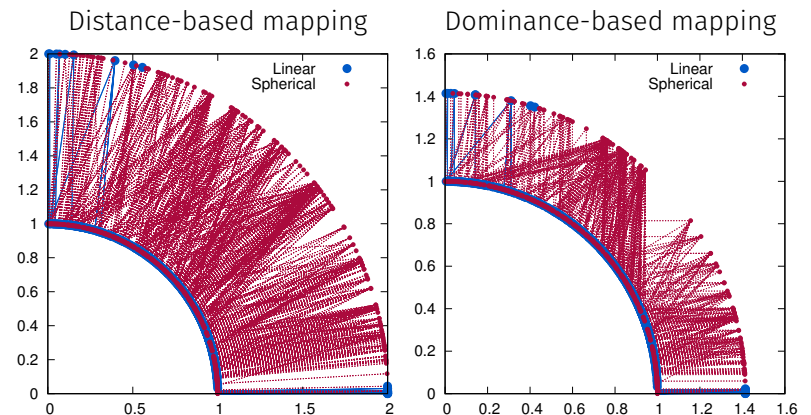
- Tries to preserve closeness of solutions
- Two solutions are very close if their relations to other solutions are mostly equal

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

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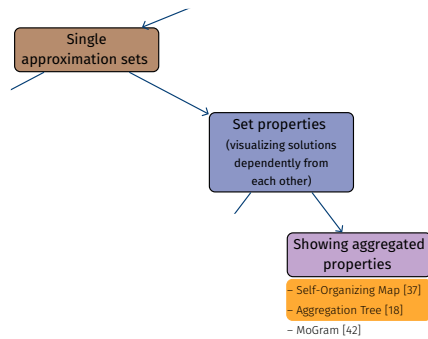
Distance- and dominance-based mappings



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

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Visualizing single approximation sets



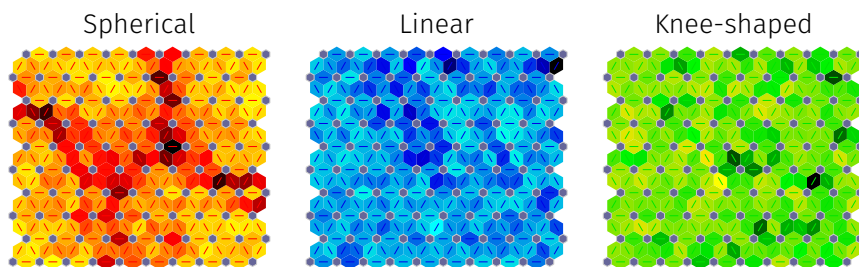
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Self-organizing maps

- 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

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Self-organizing maps



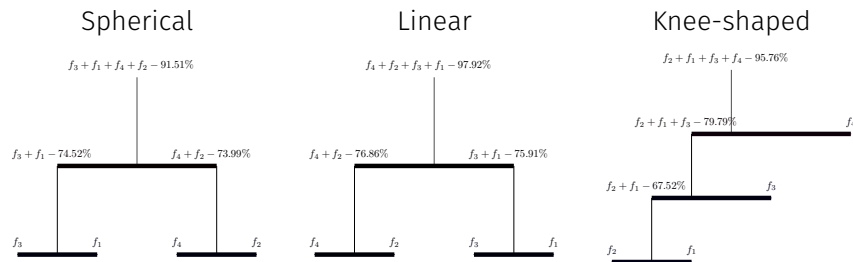
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Aggregation trees

- 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)

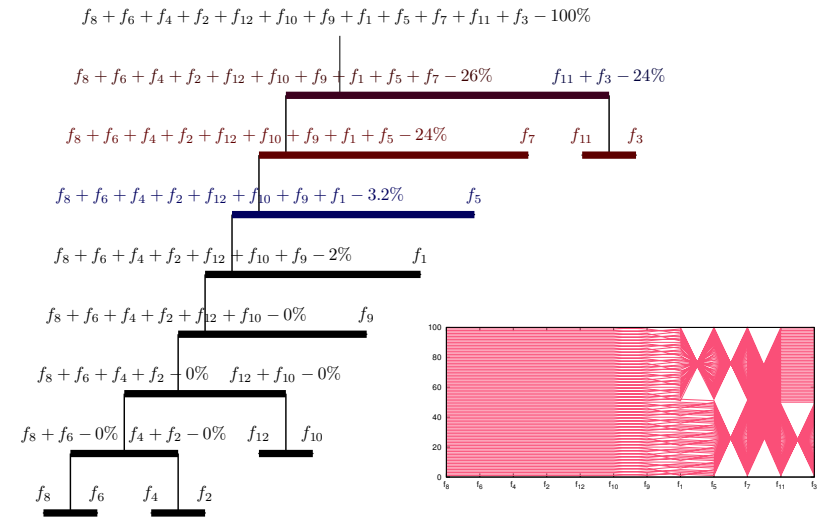
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Aggregation trees



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Aggregation trees

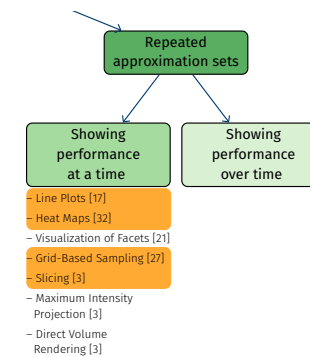


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Visualizing approximation sets

Visualizing repeated approximation sets

Visualizing repeated approximation sets



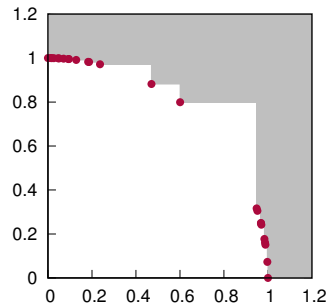
- Showing performance at a time with the **Empirical Attainment Function (EAF)** [20]
- Showing performance over time with the **Average Runtime Attainment Function (aRTA)** [9]

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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

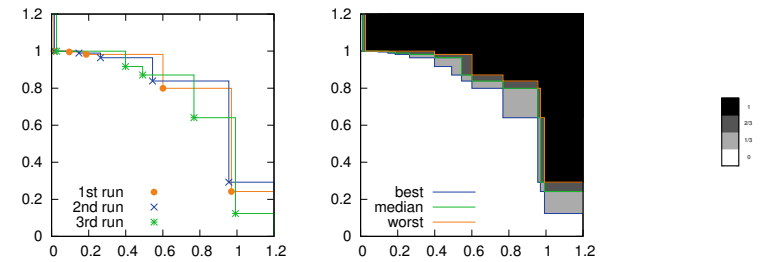


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Empirical attainment function

EAF values [20]

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



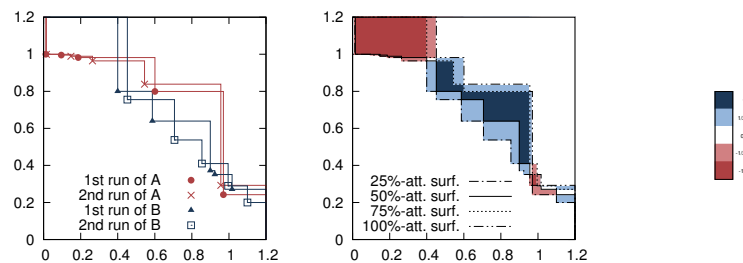
- Visualization with line plots and heat maps

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Empirical attainment function

Differences in EAF values [32]

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



- Visualization with heat maps

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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 [12, 21]
- EAF differences: **Slicing**, Maximum intensity projection [48, 3]

Approximated case

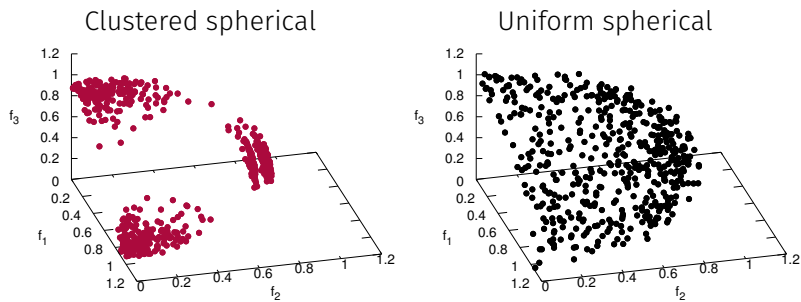
- EAF values: **Grid-based sampling** [27], Slicing, Direct volume rendering [13, 3]
- EAF differences: Slicing, Maximum intensity projection, Direct volume rendering

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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)

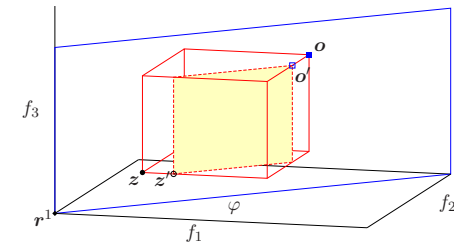


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Exact 3-D EAF values and differences

Slicing

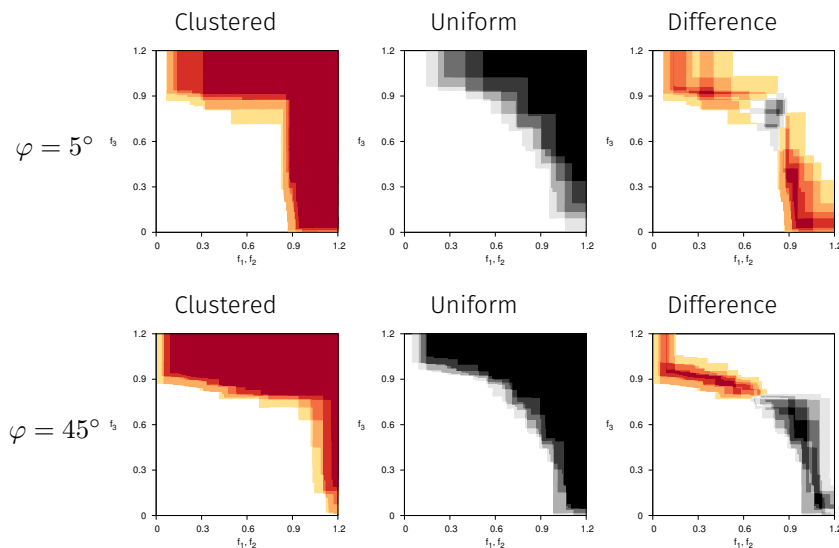
- Visualize cuboids intersecting the slicing plane
- Need to choose coordinate and angle



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Exact 3-D EAF values and differences

Slicing



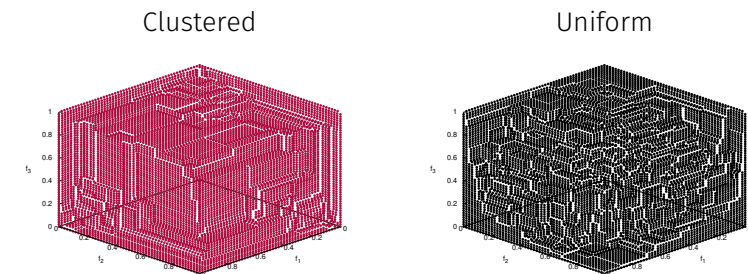
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Approximated attainment surfaces

Grid-based sampling

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

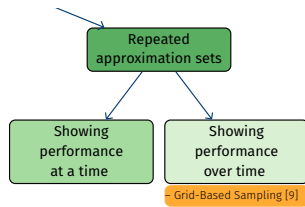
- Construct a $k \times k$ grid on the plane $f_i f_j$
- Compute intersections between the attainment surface and the axis-aligned lines on the grid



Median attainment surfaces

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Visualizing repeated approximation sets



- Showing performance at a time with the **Empirical Attainment Function (EAF)** [20]
- Showing performance over time with the **Average Runtime Attainment Function (aRTA)** [9]

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Average Runtime Attainment Function

aRTA value

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

aRTA ratio

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

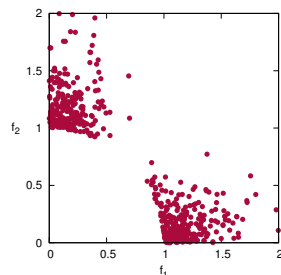
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Benchmark approximation sets

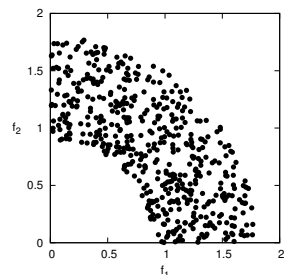
Two groups of sets mimicking convergence to a spherical front

- 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 **linear distribution** (100 solutions each)

Clustered spherical with logarithmic convergence



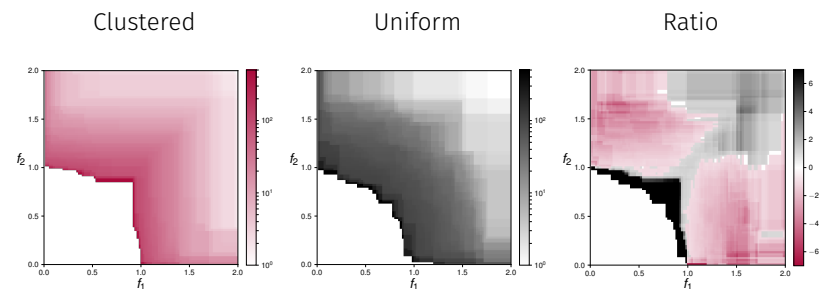
Uniform spherical with linear convergence



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Average Runtime Attainment Function

Grid-based sampling

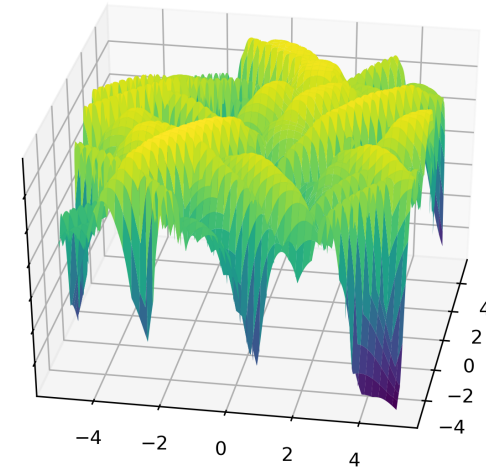


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Visualizing multiobjective landscapes

Visualizing multiobjective landscapes

Visualize objective values in the decision space



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Visualizing multiobjective landscapes

General idea (for 2-D decision spaces)

- Decision space approximated with a grid of points
- Show **some value** using color, contours or the third dimension

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

Visualizing multiobjective landscapes

Methods for visualizing multiobjective landscapes

- Level sets
- Normalized ranks [16]
- Cumulative gradients [26]
- Line walks [10, 44]

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Benchmark problems

The **bbob-biobj** test suite [10]

- 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>)

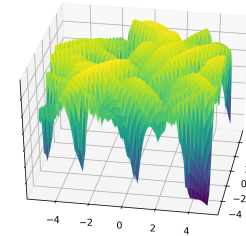
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2-D benchmark problems

Three **bbob-biobj** benchmark problems

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

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

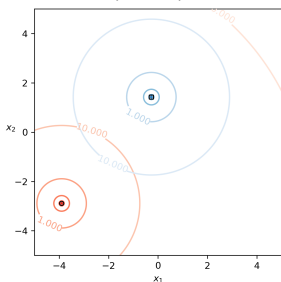


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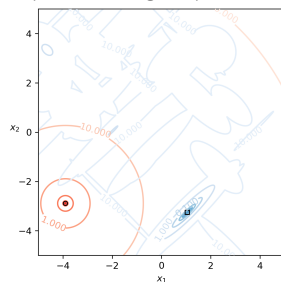
Level sets

- Curves connecting points with the same value
- Orange = first objective, blue = second objective

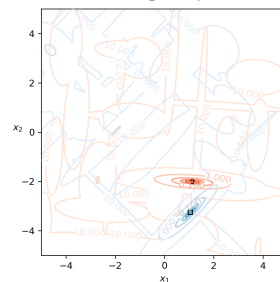
Double sphere problem



Sphere-Gallagher problem



Double Gallagher problem



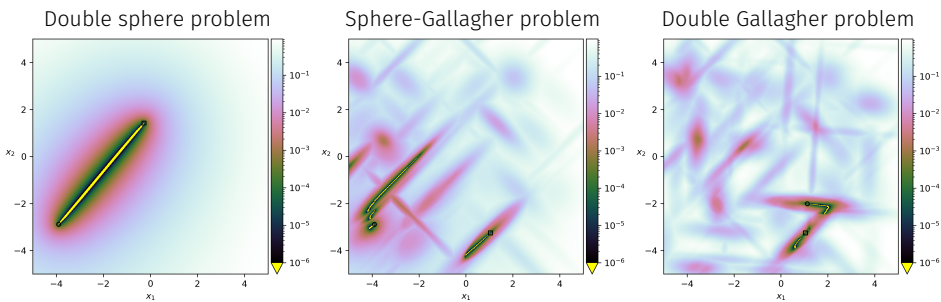
65

Visualizing normalized ranks

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

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Visualizing normalized ranks



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Visualizing cumulative gradients

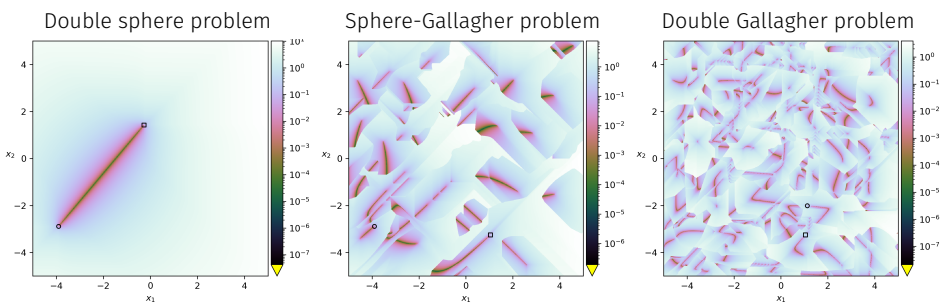
- Discretized decision space (1000 × 1000 grid)
- Compute the bi-objective gradient for all grid points

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

- 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

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Visualizing cumulative gradients

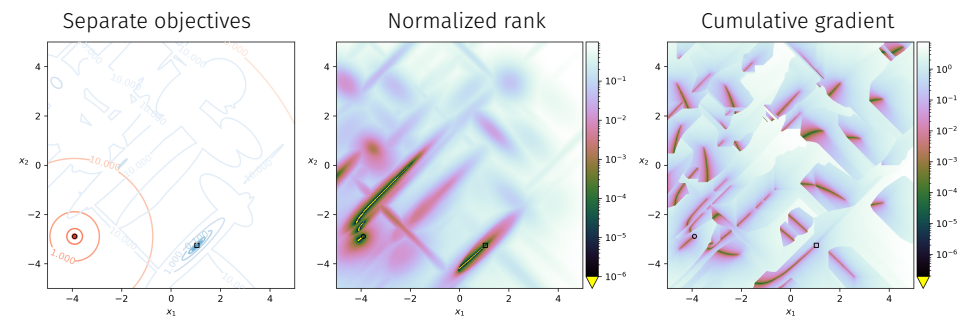


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Visualizing bi-objective landscapes

Global vs. local information

Sphere-Gallagher problem



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Visualizing multiobjective landscapes

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

Normalized ranks or cumulative gradients

- Requires cuts through the decision space (cf. slicing)
- Challenging to compute and interpret normalized ranks and cumulative gradients in n -D

Alternative: line walks

- Show objective values along a line

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5-D benchmark problems

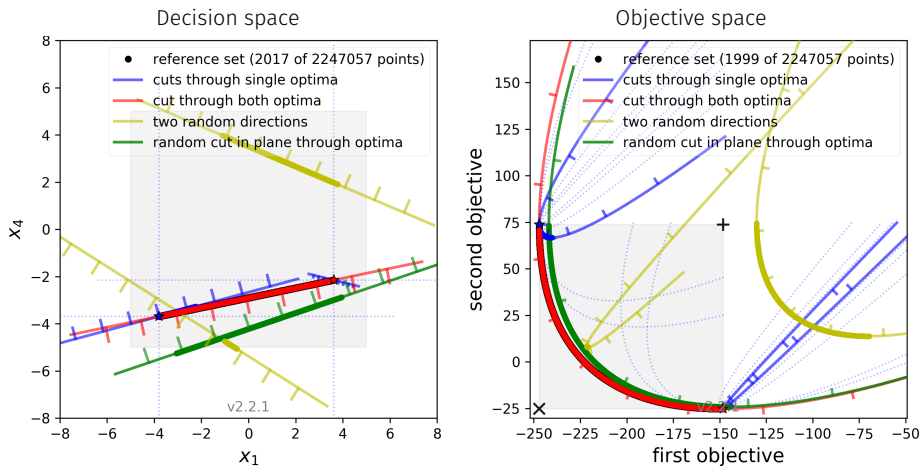
Three **bbob-biobj** benchmark problems

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

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Line walks

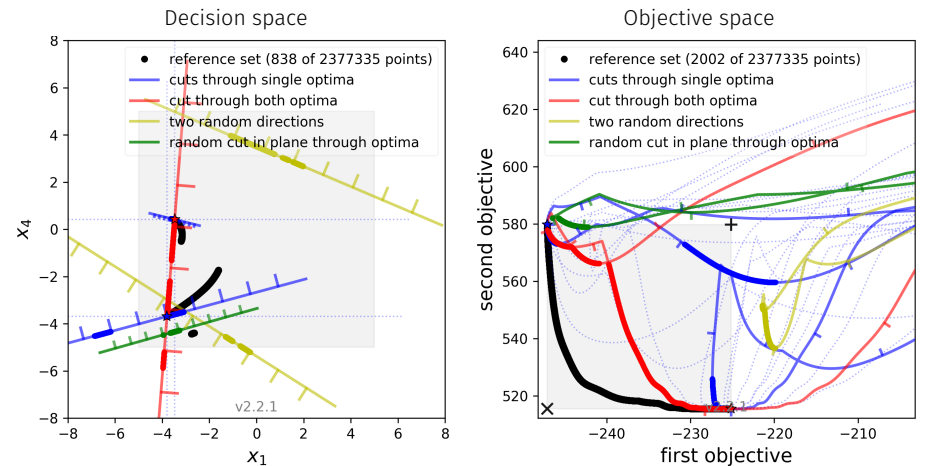
Double sphere problem



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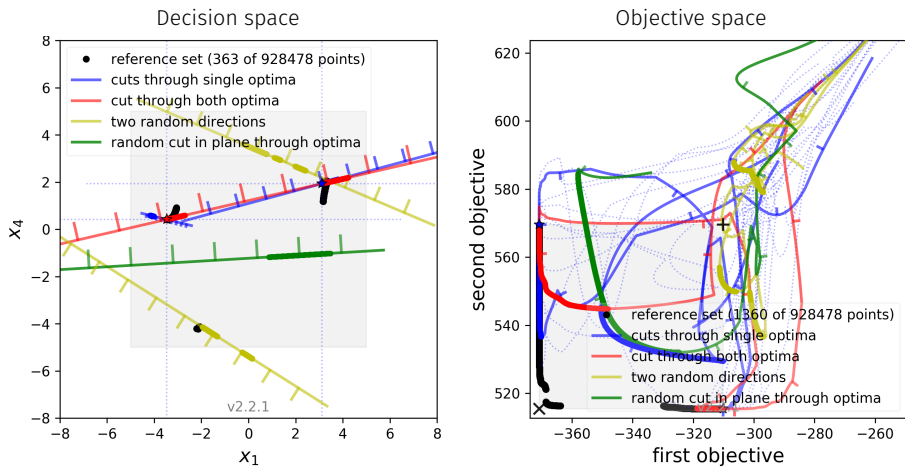
Line walks

Sphere-Gallagher problem



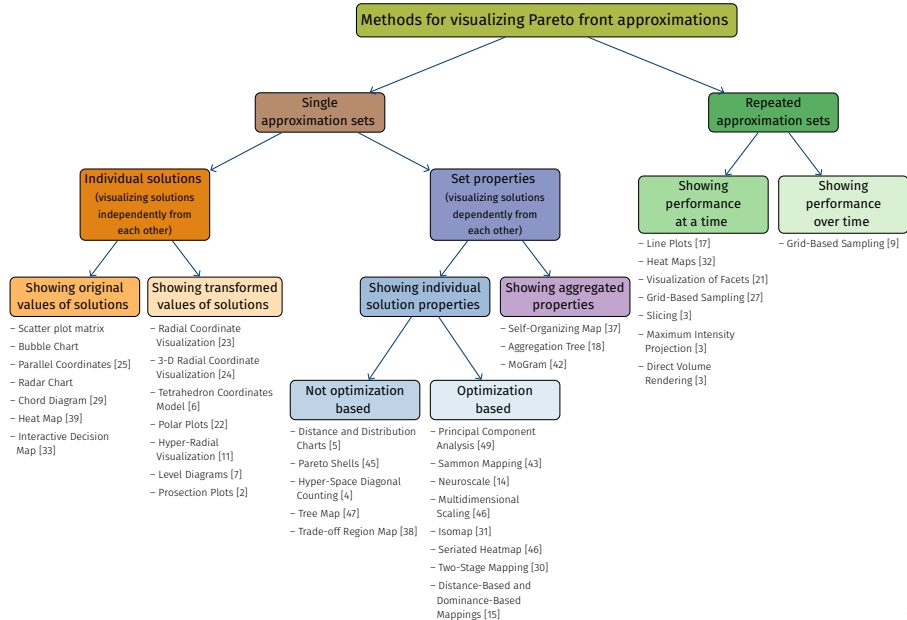
74

Double Gallagher problem



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

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