Visualization in Multiobjective Optimization

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Final version

Tutorial slides are available at
http://dis.ijs.si/tea/research.htm

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Introduction

Introduction

Multiobjective optimization problem

Minimize

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

- X is an n-dimensional decision 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

Introduction

Visualization in multiobjective optimization

Useful for different purposes [13]

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

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

Introduction

Visualizing solution sets in the objective space

- Interested in sets of mutually nondominated solutions called approximation sets
- Different from ordinary multidimensional solution sets
- The focus of this tutorial

Challenges

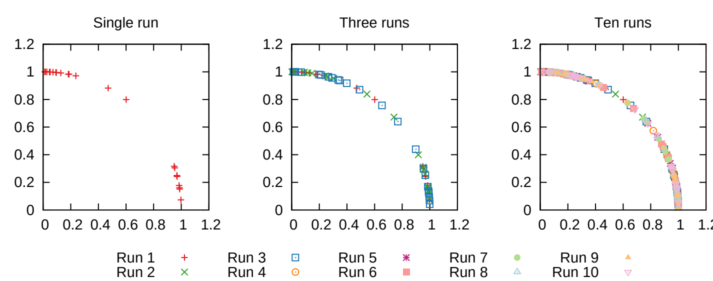
- High dimension and large number of solutions
- Limitations of computing and displaying technologies
- Cognitive limitations

Introduction

Visualization can be hard even in 2-D

Stochastic optimization algorithms

- Single run $\rightarrow$ single approximation set
- Multiple runs $\rightarrow$ multiple approximation sets



Visualization of the Empirical Attainment Function (EAF) can be used in such cases

Introduction

This tutorial is not about

- Visualization for decision making purposes [26]
- Visualization in the decision space
- General multidimensional visualization methods not previously used on approximation sets

This tutorial covers

- Visualization in the objective space
- Visualization of separate approximation sets [1]
- Visualization of EAF values and differences in EAF values [2]

Visualizing approximation sets

Methodology

Comparing visualization methods

- No existing methodology for 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

Benchmark approximation sets

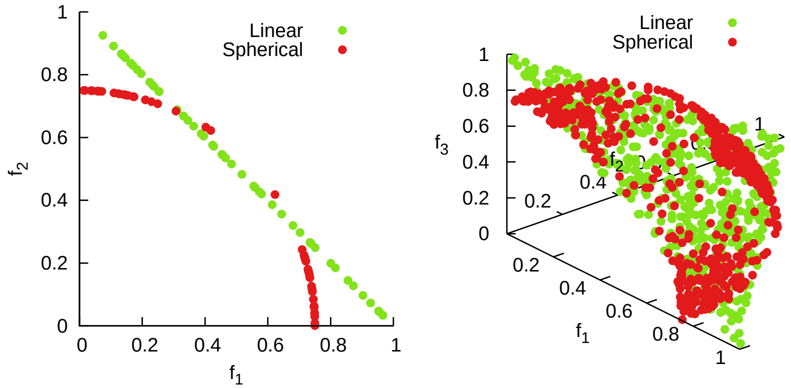
Two different sets that can be instantiated in any dimension [1]

- Linear with a uniform distribution of solutions
- Spherical with a nonuniform distribution of solutions (more at the corners and less at the center)
- Sets are intertwined

Size of each set

- 2-D: 50 solutions
- 3-D: 500 solutions
- 4-D: only 300 solutions since most methods cannot handle more

Benchmark approximation sets



Visualizing approximation sets

Desired properties of visualization methods

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

Visualizing approximation sets

Existing methods

Showing only methods previously used in multiobjective optimization

- General methods
- Specific methods – designed for visualizing approximation sets

Demonstration on 4-D benchmark approximation sets

General methods

- Scatter plot matrix
- Bubble chart
- Radial coordinate visualization [16, 36]
- Parallel coordinates [17]
- Heatmaps [29]
- Sammon mapping [30, 33]
- Neuroscale [24, 10]
- Self-organizing maps [18, 27]
- Principal component analysis [39]
- Isomap [31, 21]

Scatter plot matrix

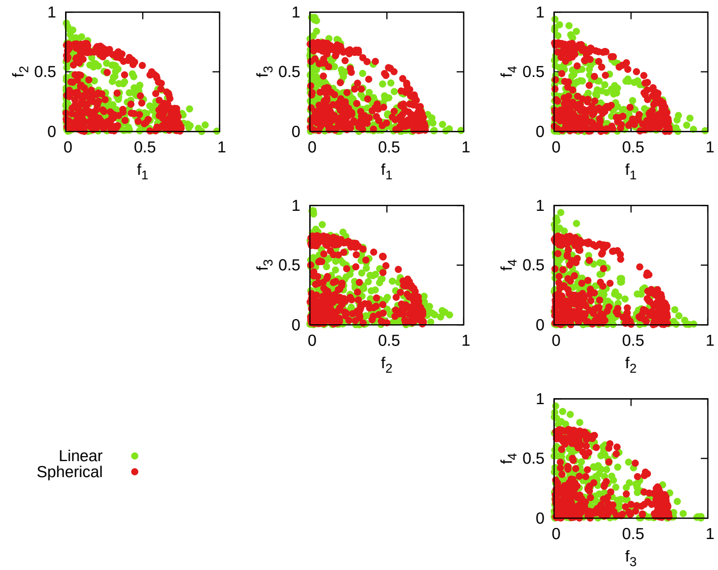
Most often

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

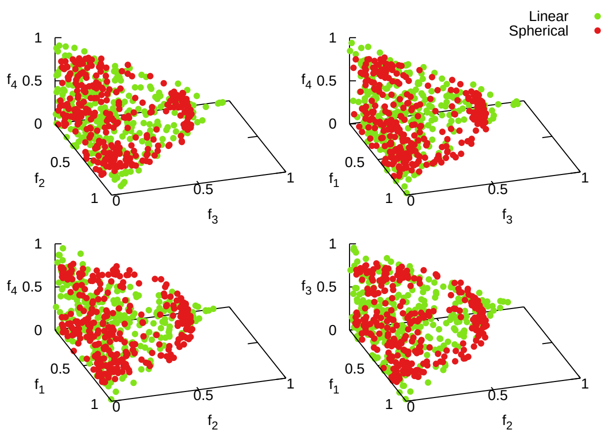
Alternatively

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

Bubble chart

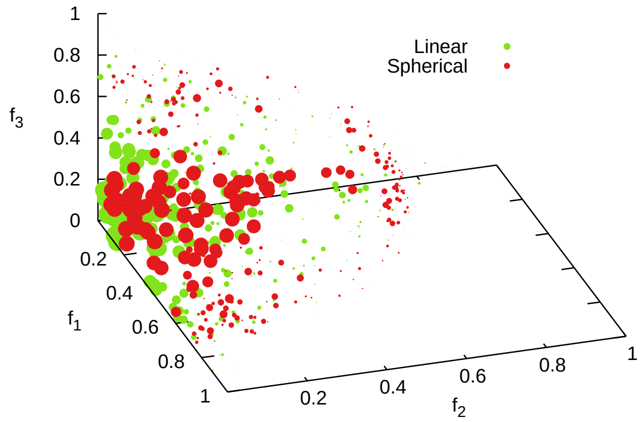
4-D objective space

- Similar to a 3-D scatter plot
- Fourth objective visualized with point size

5-D objective space

- Fifth objective visualized with colors

Bubble chart

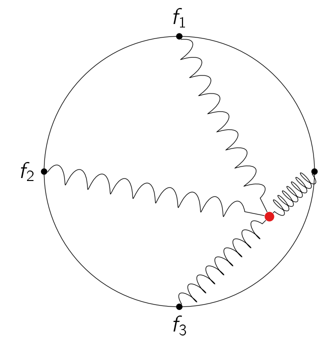


Preservation of the dominance relation	Preservation of the front shape	Preservation of the objective range	Preservation of the distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	≈	✓	≈	✓	≈	✓	×	✓

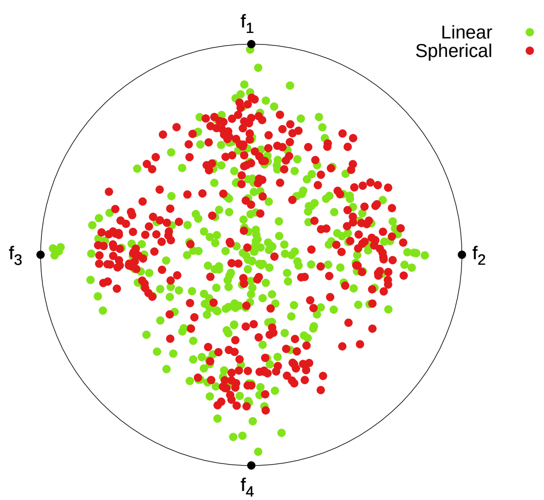
Radial coordinate visualization

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



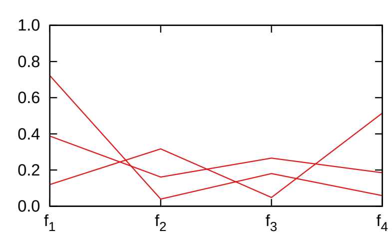
Radial coordinate visualization



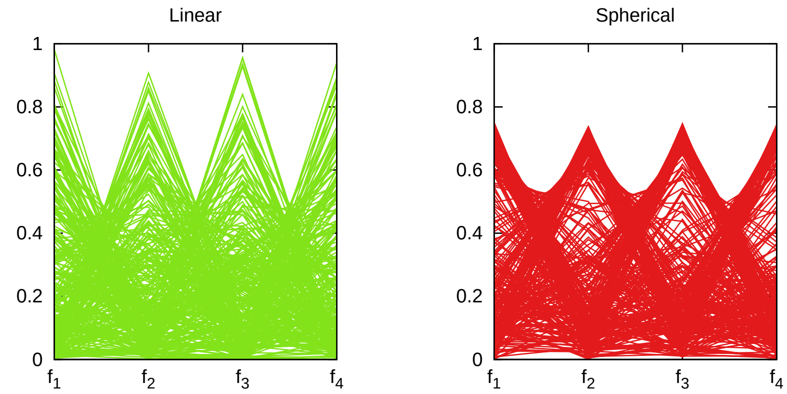
Preservation of the dominance relation	Preservation of the front shape	Preservation of the objective range	Preservation of the distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	×	×	≈	✓	≈	✓	✓	✓

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



Parallel coordinates

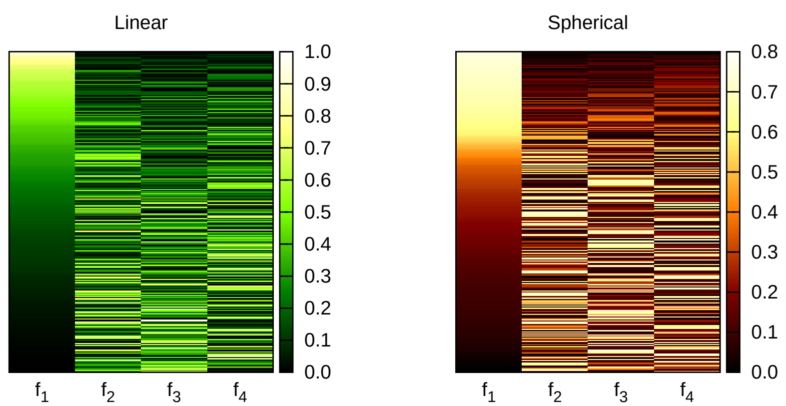


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
≈	×	✓	≈	✓	×	×	✓	✓

Heatmaps

- m objectives $\rightarrow$ m columns
- One solution per row
- Each cell colored according to objective value
- No loss of information

Heatmaps



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

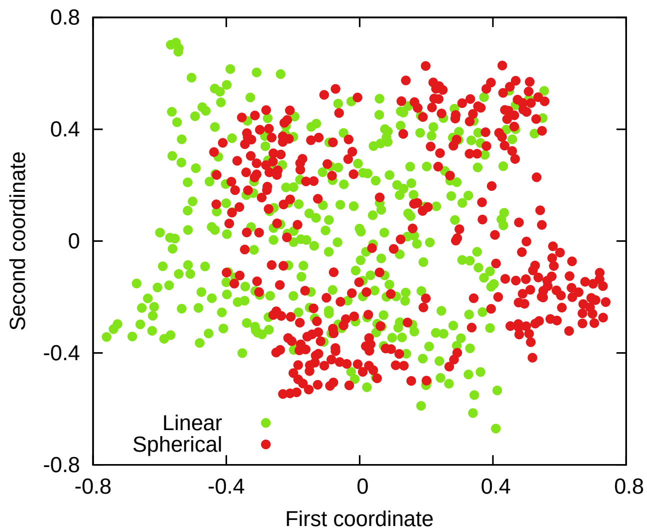
Sammon mapping

- 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

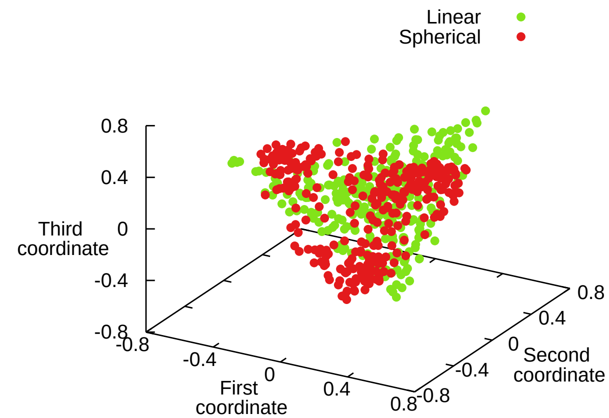
$$S = \sum_i \sum_{j>i} (d^*_{ij} - d_{ij})^2$$

- Minimization by gradient descent or other (iterative) methods

Sammon mapping



Sammon mapping

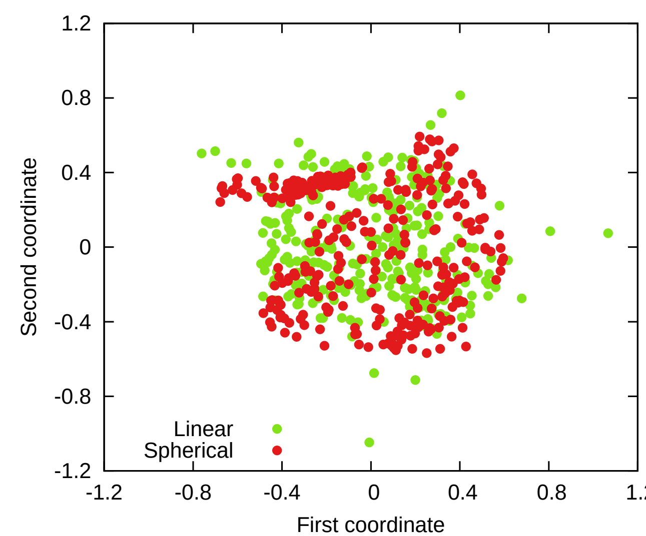


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	×	×	✓	≈	≈	✓	✓	×

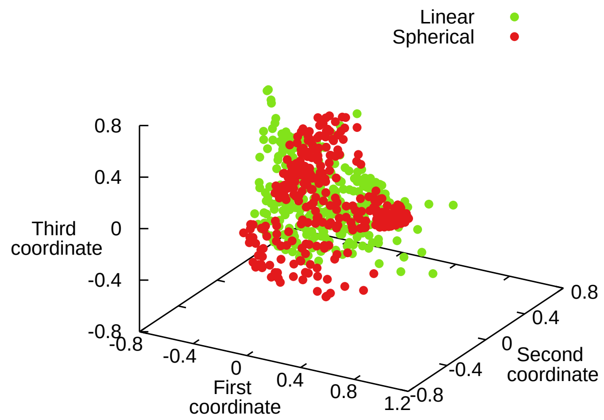
Neuroscale

- A non-linear mapping
- Aims to minimize the same stress function as Sammon mapping
- Uses a radial basis function neural network to model the projection

Neuroscale



Neuroscale

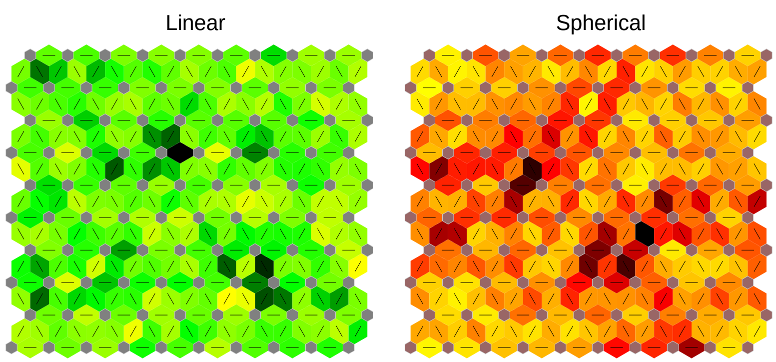


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	×	×	×	≈	≈	✓	✓	×

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

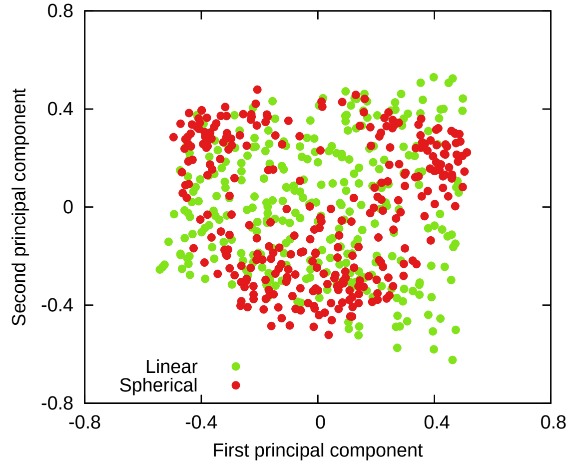


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	×	×	×	≈	✓	×	✓	×

Principal component analysis

- Principal components are linear combinations of objectives that maximize variance (and are uncorrelated with already chosen components)
- They are the eigenvectors with the highest eigenvalues of the covariance matrix

Principal component analysis

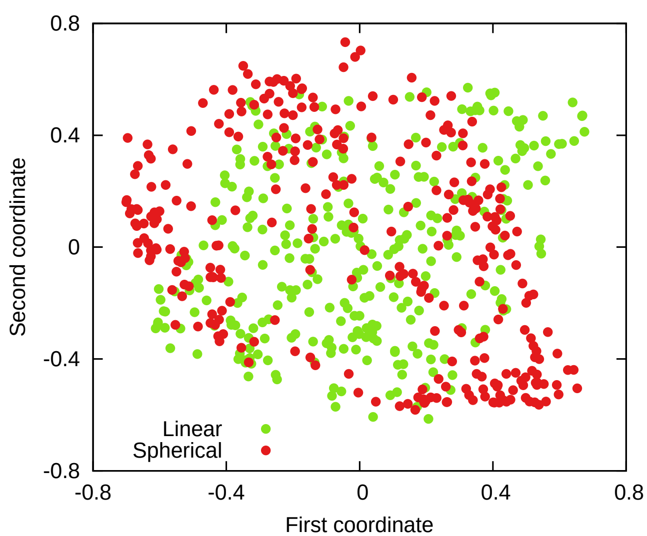


Preservation of the dominance relation	Preservation of the front shape	Preservation of the objective range	Preservation of the distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	×	×	×	≈	≈	✓	✓	×

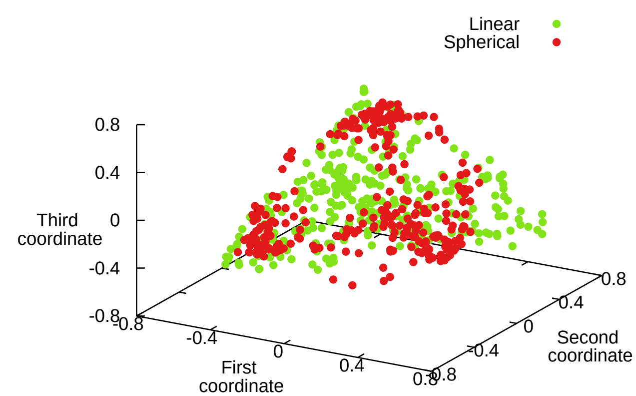
Isomap

- Assumes solutions lie on some low-dimensional manifold and the distances along this manifold should be preserved
- Creates a graph of solutions, where only the neighboring solutions are linked
- The geodesic distance between any two solutions is calculated as the sum of Euclidean distances on the shortest path between the two solutions
- Uses multidimensional scaling to perform the mapping based on these distances

Isomap



Isomap



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
×	×	×	≈	≈	≈	✓	✓	×

Summary of the general methods

Method	Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
	dominance relation	front shape	objective range	distribution of solutions					
Scatter plot matrix	×	≈	✓	≈	✓	≈	✓	×	✓
Bubble chart	×	≈	✓	≈	✓	≈	✓	×	✓
Radial coordinate visual.	×	×	×	≈	✓	≈	✓	✓	✓
Parallel coordinates	≈	×	✓	≈	✓	×	×	✓	✓
Heatmaps	×	×	✓	×	✓	×	×	✓	✓
Sammon mapping	×	×	×	✓	≈	≈	✓	✓	×
Neuroscale	×	×	×	×	≈	≈	✓	✓	×
Self-organizing maps	×	×	×	×	≈	✓	×	✓	×
Principal component analysis	×	×	×	×	≈	≈	✓	✓	×
Isomap	×	×	×	≈	≈	≈	✓	✓	×

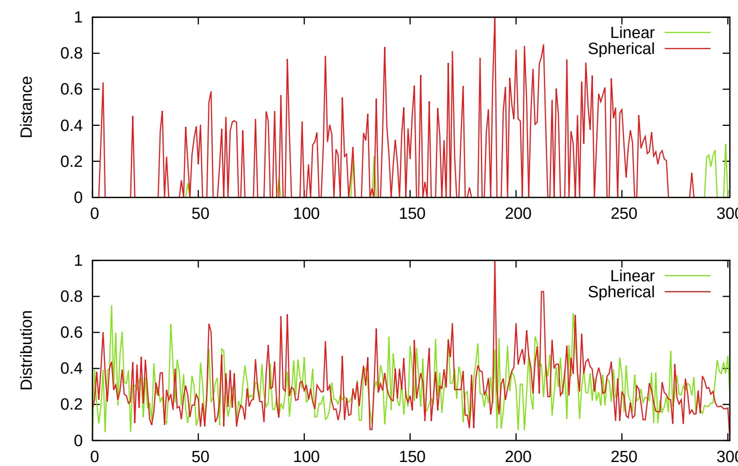
Specific methods

- Distance and distribution charts [4]
- Interactive decision maps [23]
- Hyper-space diagonal counting [3]
- Two-stage mapping [20]
- Level diagrams [6]
- Hyper-radial visualization [8]
- Pareto shells [35]
- Seriated heatmaps [36]
- Multidimensional scaling [36]
- Prosections [1]

Distance and distribution charts

- Plot solutions against their distance to the Pareto front and distance to other solutions
- Distance chart
  - Plot distance to the nearest non-dominated solution
- Distribution chart
  - Sort solutions w.r.t. first objective
  - Plot distances between consecutive solutions
  - For the first/last solution, compute distance to first/last non-dominated solution
  - k solutions $\rightarrow k+1$ distances
- All distances normalized to $[0, 1]$

Distance and distribution charts



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

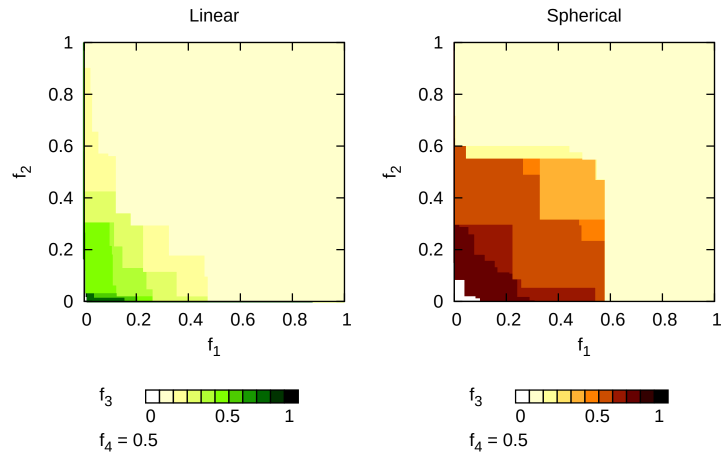
Interactive decision maps

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

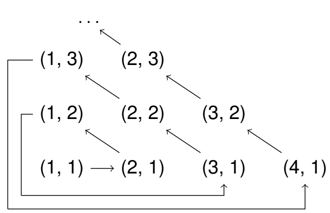
Interactive decision maps



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

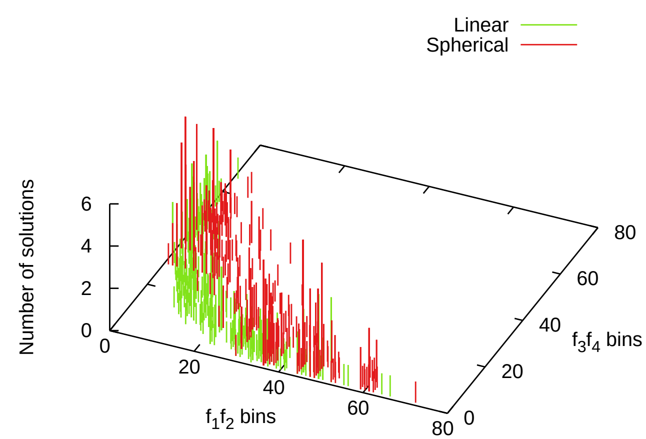
Hyper-space diagonal counting

- 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



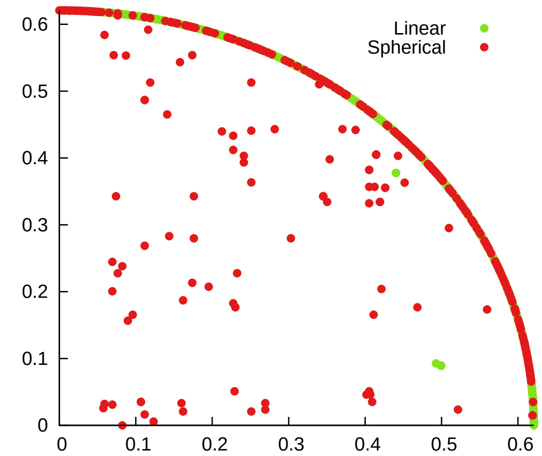
Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	×	×	≈	✓	✓	✓	✓	≈

Two-stage mapping

Steps

- Split solutions to nondominated and dominated solutions
- Compute r as the average norm of nondominated solutions
- Find a permutation of nondominated solutions that minimizes implicit dominance errors and sum of distances between consecutive solutions
- First stage: distribute nondominated solutions on the circumference of a quarter-circle with radius r in the order of the permutation and with distances proportional to their distances in the objective space
- Second stage: map each dominated solution to the minimal point of all nondominated solutions that dominate it

Two-stage mapping

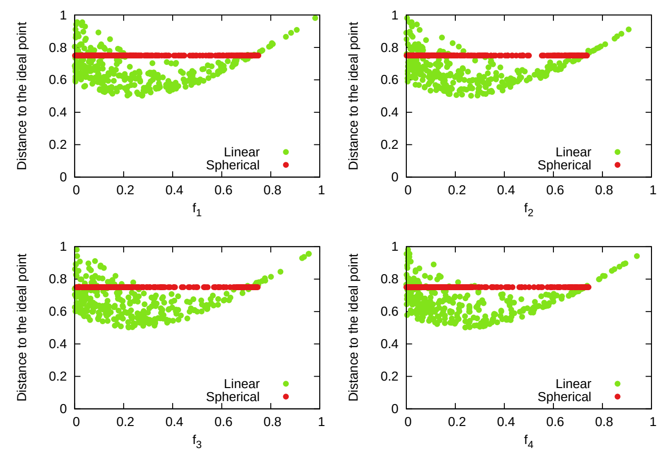


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
≈	×	×	×	×	×	✓	≈	×

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

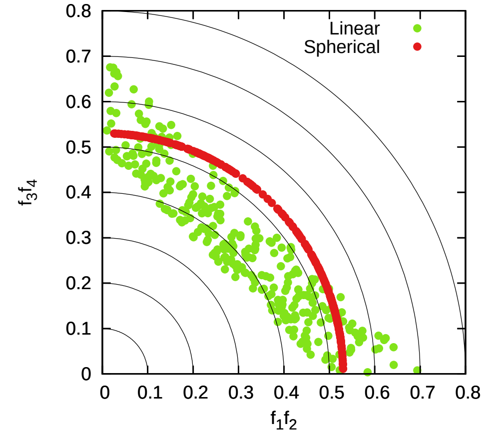


Preservation of the				Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
dominance relation	front shape	objective range	distribution of solutions					
×	≈	✓	×	✓	≈	✓	✓	✓

Hyper-radial visualization

- Solutions preserve distance (hyper-radius) to the ideal point
- Distances are computed separately for two subsets of objectives
- Indifference curves denote points with the same preference

Hyper-radial visualization

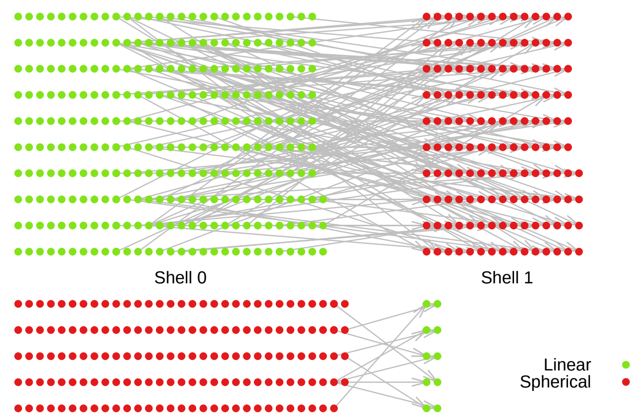


Preservation of the: dominance relation	front shape	objective range	distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	≈	✓	×	✓	≈	✓	✓	✓

Pareto shells

- Use nondominated sorting to split solutions to Pareto shells
- Represent solutions in a graph
- Connect dominated solutions to those that dominate them (we show only one arrow per dominated solution)

Pareto shells

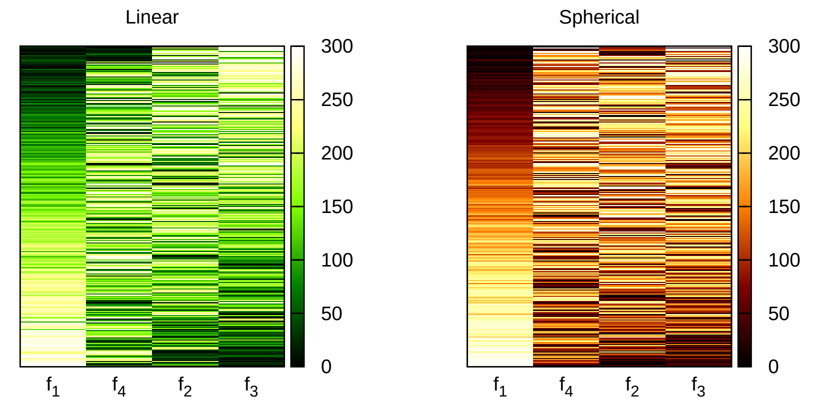


Preservation of the: dominance relation	front shape	objective range	distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
✓	×	×	×	×	×	✓	✓	✓

Seriated heatmaps

- Heatmaps with rearranged objectives and solutions
- Similar objectives and similar solutions are placed together
- Ranks are used instead of actual objective values for a more uniform color usage
- Similarity can be computed using
  - Euclidean distance
  - Spearman's footrule
  - Kendall's τ metric

Seriated heatmaps



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
×	×	×	×	≈	×	×	✓	×

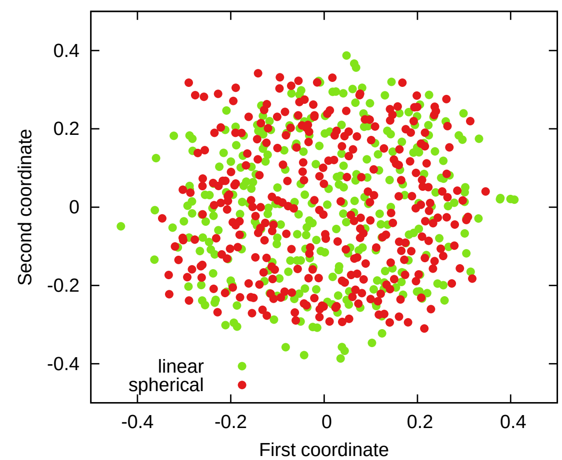
Multidimensional scaling

- Classical multidimensional scaling aims at preserving similarities between solutions
- Here, dominance distance is used to measure similarity
- Two solutions are similar if they share dominance relationships with a third solution

$$S(\mathbf{a}, \mathbf{b}; \mathbf{z}) = \frac{1}{m} \sum_{i=1}^{m} [I((a_i < z_i) \wedge (b_i < z_i)) + I((a_i = z_i) \wedge (b_i = z_i)) + I((a_i > z_i) \wedge (b_i > z_i))]$$

$$D(\mathbf{a}, \mathbf{b}) = \frac{1}{k-2} \sum_{\mathbf{z} \notin \{\mathbf{a}, \mathbf{b}\}} (1 - S(\mathbf{a}, \mathbf{b}; \mathbf{z}))$$

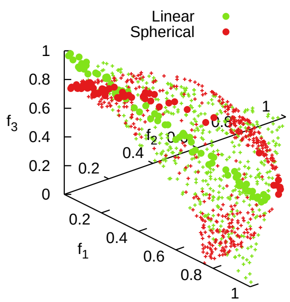
Multidimensional scaling



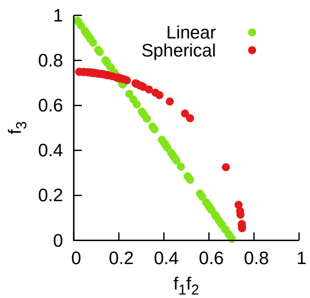
Preservation of the: dominance relation	Preservation of the: front shape	Preservation of the: objective range	Preservation of the: distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	×	×	×	×	≈	✓	✓	×

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



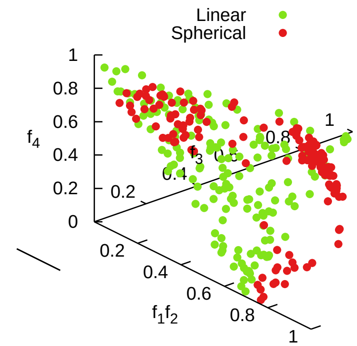
Before prosection



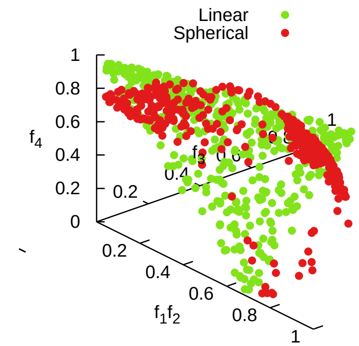
After prosection

Prosections

300 solutions



3000 solutions



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
✓	✓	≈	✓	✓	✓	✓	×	≈

Summary of the specific methods

Method	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
Distance and distrib. charts	≈	×	×	×	✓	×	✓	✓	≈
Interactive decision maps	×	≈	✓	≈	✓	✓	×	×	≈
Hyper-space diagonal count.	×	×	×	≈	✓	✓	✓	✓	≈
Two-stage mapping	≈	×	×	×	×	×	✓	≈	×
Level diagrams	×	≈	✓	×	✓	≈	✓	✓	✓
Hyper-radial visualization	×	≈	✓	×	✓	≈	✓	✓	✓
Pareto shells	✓	×	×	×	×	×	✓	✓	✓
Seriated heatmaps	×	×	×	×	≈	×	×	✓	×
Multidimensional scaling	×	×	×	×	×	≈	✓	✓	×
Prosections	✓	✓	≈	✓	✓	✓	✓	×	≈

Other (newer) methods

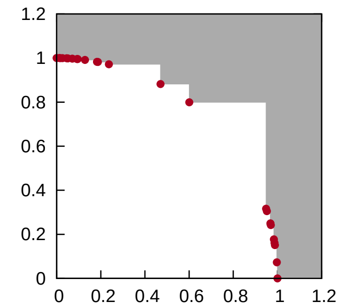
- Tetrahedron coordinates model [5]
- Distance-based and dominance-based mappings [11]
- Aggregation trees [12]
- Trade-off region maps [28]
- Treemaps [37]
- MoGrams [32]
- Polar plots [15]
- Level diagrams with asymmetric norm [7]
- Visualization following Shneiderman mantra [19]

Visualizing EAF values and differences

Empirical attainment function

Goal-attainment

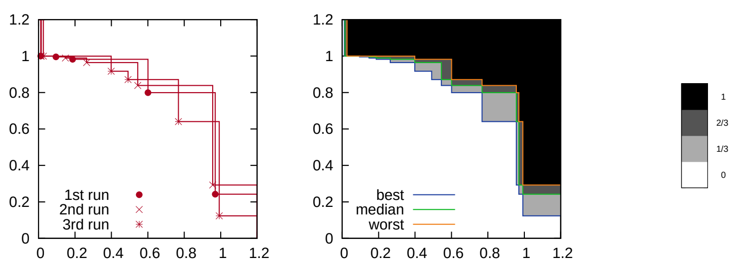
- Approximation set A
- A point in the objective space $\mathbf{z}$ is attained by A when $\mathbf{z}$ is weakly dominated by at least one solution from A



Empirical attainment function

EAF values [14]

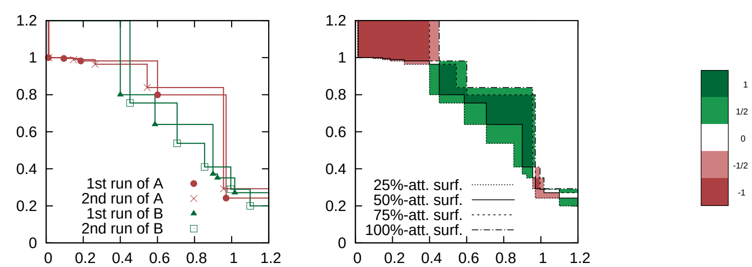
- Algorithm $\mathcal{A}$, approximation sets $A_1, A_2, \ldots, A_r$
- EAF of $\mathbf{z}$ is the frequency of attaining $\mathbf{z}$ by $A_1, A_2, \ldots, A_r$
- Summary (or $k\%$-) attainment surfaces



Empirical attainment function

Differences in EAF values [22]

- 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 of 3-D EAF

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

Exact case

- EAF values: Slicing [2]
- EAF differences: Slicing, Maximum intensity projection [38, 2]

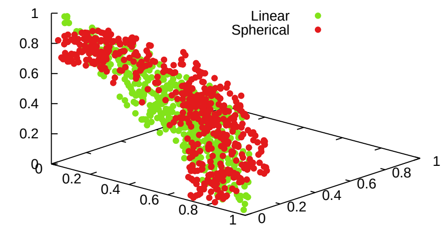
Approximated case

- EAF values: Slicing, Direct volume rendering [9, 2]
- EAF differences: Slicing, Maximum intensity projection, Direct volume rendering

Benchmark approximation sets

Sets of approximation sets

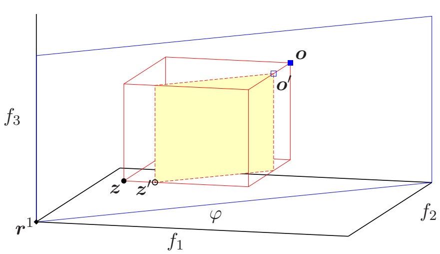
- 5 linear approximation sets with a uniform distribution of solutions (100 solutions in each)
- 5 spherical approximation sets with a nonuniform distribution of solutions (100 solutions in each)



Exact 3-D EAF values and differences

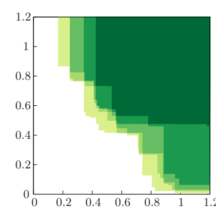
Slicing

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

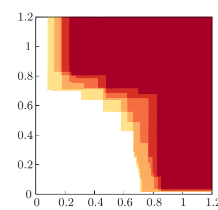


Exact 3-D EAF values and differences

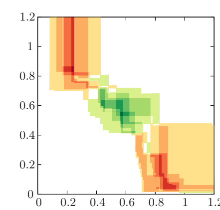
Slicing



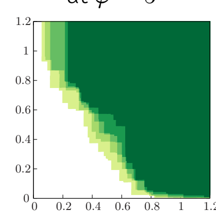
Slice of Lin at $\varphi = 5°$



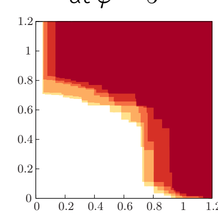
Slice of Sph at $\varphi = 5°$



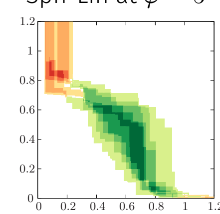
Slice of Lin-Sph and Sph-Lin at $\varphi = 5°$



Slice of Lin at $\varphi = 45°$



Slice of Sph at $\varphi = 45°$

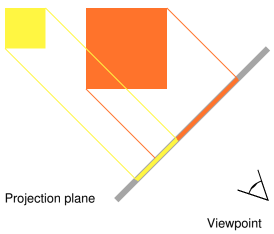


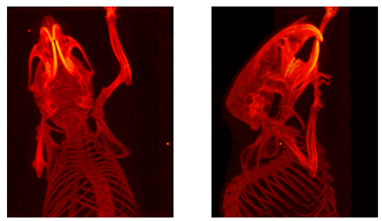
Slice of Lin-Sph and Sph-Lin at $\varphi = 45°$

Exact 3-D EAF differences

Maximum intensity projection

- Volume rendering method for spatial data represented by voxels
- Simple and efficient
- No sense of depth, cannot distinguish between front and back





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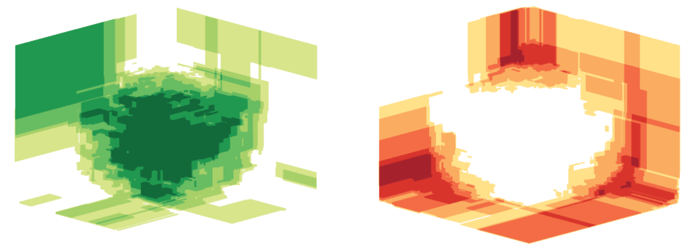
Exact 3-D EAF differences

Maximum intensity projection

- Suitable for visualizing EAF differences (focus on large differences)
- Sorting w.r.t. EAF differences (smaller to larger)
- Plot on top of previous ones

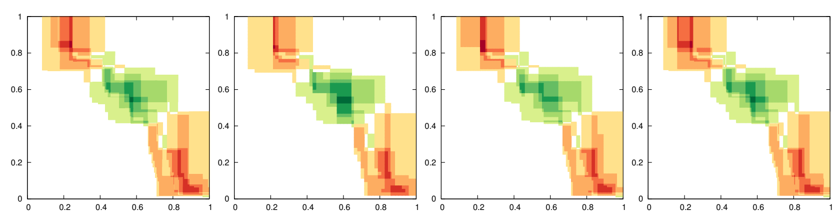


The approximated case

Discretization into voxels

- Discretization of cuboids
- Discretization from the space of EAF values/differences

Slicing

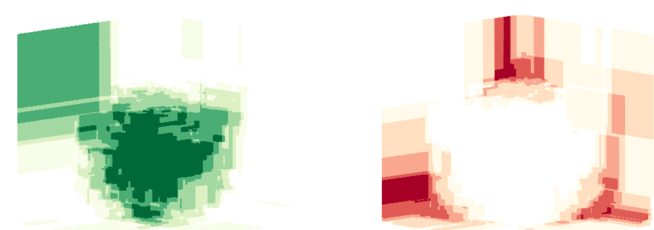


Exact | 64^3 voxels | 128^3 voxels | 256^3 voxels

Approximated 3-D EAF differences

Maximum intensity projection

- Plots produced using Voreen [25, 34]
- Some loss of information



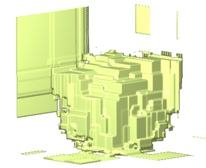
Approximated 3-D EAF values and differences

Direct volume rendering

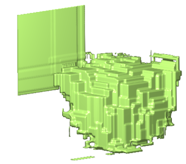
- Volume rendering method for spatial data represented by voxels
- A transfer function assigns color and opacity to voxel values
- Enables to see “inside the volume”
- Requires the definition of the transfer function

Approximated 3-D EAF differences

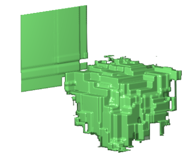
Direct volume rendering of Lin-Sph



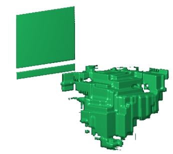
1/5



2/5

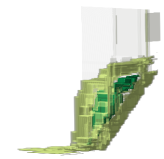


3/5



4/5

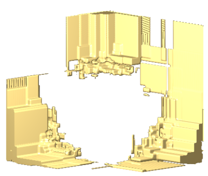
5/5



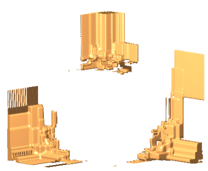
1/5 and 5/5

Approximated 3-D EAF differences

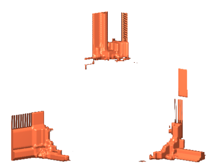
Direct volume rendering of Sph-Lin



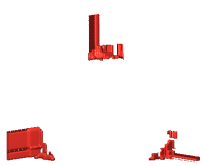
1/5



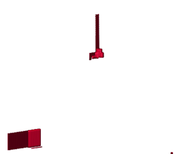
2/5



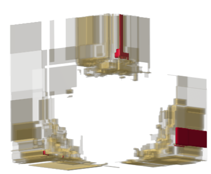
3/5



4/5



5/5



1/5 and 5/5

Approximated 3-D EAF values

Direct volume rendering of Sph

1/5 and 5/5

Summary

Summary – Visualization of approximation sets

General methods

- Scatter plot matrix
- Bubble chart
- Radial coordinate visualization
- Parallel coordinates
- Heatmaps
- Sammon mapping
- Neuroscale
- Self-organizing maps
- Principal component analysis
- Isomap

Specific methods

- Distance and distribution charts
- Interactive decision maps
- Hyper-space diagonal counting
- Two-stage mapping
- Level diagrams
- Hyper-radial visualization
- Pareto shells
- Seriated heatmaps
- Multidimensional scaling
- Prosections

Summary – Visualization of EAFs

Exact 3-D case

EAF values

- Slicing

EAF differences

- Slicing
- Maximum intensity projection

Approximated 3-D case

EAF values

- Slicing
- Direct volume rendering

EAF differences

- Slicing
- Maximum intensity projection
- Direct volume rendering

Summary

- Visualization in multiobjective optimization needed for various purposes
- General methods fail to address the peculiarities of approximation set visualization
- Customized methods give more information and are currently gaining attentions

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SYNERGY
Synergy for Smart Multi-Objective Optimization
`www.synergy-twinning.eu`

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