

# Visualization in Multiobjective Optimization

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# Introduction

### Introduction

Multiobjective optimization problem Minimize

 $\mathbf{f} \colon X \to F$ 

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

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

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 [14]

- 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

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



The Empirical Attainment Function (EAF) [15] or the Average Runtime Attainment Function (aRTA) [3] can be used in such cases

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### This tutorial is not about

- Visualization of a few solutions for decision making purposes (see [29])
- Visualization in the decision space
- General multidimensional visualization methods not previously used on approximation sets

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### This tutorial covers

- Visualization of entire sets in the objective space
  - Single approximation sets [1]
  - Repeated approximation sets [2, 3]

# A taxonomy of visualization methods

Visualizing single

approximation sets



# Methodology

### Evaluating and comparing visualization methods

- No existing 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

### 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

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### Benchmark approximation sets

These two sets are not sufficient for all purposes!

Missing:

- A set with knees
- A set with different relations between objectives, temporarily using [13]:



- A sequence of sets mimicking convergence in time
- ... (possibly others)

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# Desired properties of visualization methods

### Demonstration on the 4-D linear and spherical sets

- Preservation of the
  - Dominance relation between solutions
  - $\cdot$  Front shape
  - $\cdot\,$  Objective range
  - Distribution of solutions
- Robustness
- Handling of large sets
- $\cdot$  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

# Individual solutions (Visualizing solutions independently from each other) $\rightarrow$ Showing original values of solutions

- Scatter plot matrix
- Bubble chart
- Parallel coordinates [19]
- Radar chart
- Chord diagram [22], TBA
- Heat maps [32]
- Interactive decision maps [26]



### 15

17

### 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



# 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





	Preservation of the							
dominance relation	front shape	objective range	distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	*	1	*	1	*	1	×	1

# Parallel coordinates

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



# Parallel coordinates



(	dominance relation	front shape	objective range	distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
Ē	≈	×	1	≈	1	×	×	1	1

### 22

# Parallel coordinates



# Radar chart

- Similar to parallel coordinates
- Additionally connects the two extreme coordinates
- m objectives  $\rightarrow m$  radial axes
- Also called a spider chart, polar chart, star plot, ...

# Radar chart



# Radar chart



# Heat maps

 $\cdot m$  objectives  $\rightarrow m$  columns

- One solution per row
- Each cell colored according to objective value
- $\cdot$  No loss of information



	Preservati	on of the						
dominance relation	front shape	objective range	distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	×	1	×	1	×	×	1	1

# Heat maps



28

0.8

0.7

0.6

0.5

0.4

0.3

0.2

0.1

0.0

 $\mathbf{f}_4$ 

### 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
- $\cdot$  Color used to denote third objective
- Fixed value of the forth objective

### Interactive decision maps



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# Visualizing single approximation sets

Individual solutions (Visualizing solutions independently from each other)  $\rightarrow$  Showing transformed values of solutions

- Radial coordinate visualization [17, 39]
- 3-D Radial coordinate visualization [18], TBA
- Sin approxim (visualizing solutions independently from each other)

Showing original

alues of solutions

Showing transformed

values of solutions

- Tetrahedron coordinates model [6]
- Polar plots [16], TBA
- Hyper-radial visualization [9]
- Level diagrams [7, 8]
- Prosections [1]

### 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



# Tetrahedron coordinates model

- Only for four objectives
- Similar to RadViz
- Objectives treated as anchors, placed at the vertices of a regular tetrahedron
- Solutions attached to anchors with 'springs'
- Spring flexibility proportional to the objective value
- Solution placed where the forces are in equilibrium



Tetrahedron coordinates model Linear Spherical  $f_2$ Preservation of the Handling of Simultaneous front shape objective distribution

Robustness

1

of solutions

 $\approx$ 

range

Х

×

large sets

/isualizatior

dominance

relation

X

# 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

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Scalability

X

Simplicity

1

# Hyper-radial visualization



	Preservati	on of the	I alianationaliana		Handling of	Simultaneous			
relation	front snape	range	of solutions	Robustness	large sets	visualization	Scalability	Simplicity	
×	≈	1	×	1	≈	1	1	1	

# 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



		Preservati	on of the						
	dominance relation	front shape	objective range	distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
Ì	×	*	1	×	1	*	1	1	1

# Level diagrams with asymmetric norm

- Compute an asymmetric norm a (very similar to the  $I_{\varepsilon+}$  indicator) between any solution and the reference point
  - $\cdot a = 0 \Rightarrow$  the solution dominates the reference point
  - +  $a > 0 \Rightarrow$  the solution needs to be moved by a to dominate the reference point
- Use on our benchmark approximation sets
  - The spherical set is used as the reference set
  - $\cdot \ a=0 \Rightarrow$  the solution from the linear set dominates a solution from the spherical set
  - $a > 0 \Rightarrow$  the solution from the linear set needs to be moved by at least a to dominate one solution from the spherical set

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# Level diagrams with asymmetric norm



### Prosections

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





# Visualizing single approximation sets

Set properties (Visualizing solutions dependently from each other)  $\to$  Showing individual solution-based properties  $\to$  Not optimization based

- Distance and distribution charts [5]
- Pareto shells [38]
- Hyper-space diagonal counting [4]
- Treemaps [40], TBA
- Trade-off region maps [31], TBA



### 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
  - $\cdot\,$  Plot distances between consecutive solutions
  - For the first/last solution, compute distance to first/last non-dominated solution
  - ·  $k \text{ solutions} \rightarrow k+1 \text{ distances}$
- $\cdot$  All distances normalized to [0,1]

### Distance and distribution charts



## 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



	Preservati	ion of the				at 1.		
dominance	front shape	objective	distribution	Robustness	Handling of	Simultaneous	Scalability	Simplicity
relation		range	of solutions		large sets	visualization		
1	×	×	×	×	×	1	1	1

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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
  - $\cdot$  Enumerate the bins for objectives  $f_1$  and  $f_2$
  - $\cdot$  Enumerate the bins for objectives  $f_3$  and  $f_4$
  - $\cdot\,$  Plot the number of solutions in each pair of bins

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# Hyper-space diagonal counting



# Visualizing single approximation sets

Set properties (Visualizing solutions dependently from each other)  $\rightarrow$  Showing individual solution-based properties  $\rightarrow$  Optimization based

- Principal component analysis [42]
- Sammon mapping [33, 36]
- Neuroscale [27, 11]
- Multidimensional scaling [39]
- Isomap [34, 24]
- Seriated heatmaps [39]
- Two-stage mapping [23]
- Distance-based and dominance-based mappings [12]



# 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



# Sammon mapping

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

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

• Minimization by gradient descent or other (iterative) methods







# Neuroscale

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



# 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

$$S(\mathbf{a}, \mathbf{b}; \mathbf{z}) = \frac{1}{m} \sum_{i=1}^{m} \left[ I((a_i < z_i) \land (b_i < z_i)) + I((a_i = z_i) \land (b_i = z_i)) + I((a_i > z_i) \land (b_i > z_i)) \right]$$
$$D(\mathbf{a}, \mathbf{b}) = \frac{1}{k-2} \sum_{\mathbf{z} \notin \{\mathbf{a}, \mathbf{b}\}} (1 - S(\mathbf{a}, \mathbf{b}; \mathbf{z}))$$

# Multidimensional scaling



### 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





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### 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 au metric

### Seriated heatmaps





	Preservati	on of the						
dominance relation	front shape	objective range	distribution of solutions	Robustness	Handling of large sets	Simultaneous visualization	Scalability	Simplicity
×	×	×	×	~	×	×	1	×

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### 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



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# Distance- and dominance-based mappings

### Distance- and dominance-based mappings



### Both mappings

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

### Distance-based mapping

### Dominance-based mapping

- Tries to preserve closeness of solutions
- Similarity between solutions defined as dominance similarity
- Solution ordering using spectral seriation
- Aims at preserving dominance relations among solutions
- $\cdot \mbox{ All } \mathbf{x} \prec \mathbf{y}$  can be shown correctly
- Tries to minimize cases where
   x ⊀ y is not shown correctly

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# Visualizing single approximation sets Set properties (Visualizing solutions dependently from each other) → Showing aggregated properties • Self-organizing maps [21, 30] • Aggregation trees [13] • MoGrams [35], TBA

### 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
  - $\cdot \,$  Similar neurons  $\rightarrow$  light color
  - $\cdot~$  Different neurons (cluster boundaries)  $\rightarrow$  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



# Visualizing repeated approximation sets

### Showing performance at a time

• Empirical Attainment Function (EAF) [15]

Average Runtime Attainment Function

### Showing performance over time

(aRTA) [3]



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# Empirical attainment function

### **Goal-attainment**

- Approximation set A
- A point in the objective space **z** is attained by *A* when **z** is weakly dominated by at least one solution from *A*



## Empirical attainment function

### EAF values [15]

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







# Empirical attainment function

### Differences in EAF values [25]

- 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



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### Visualization of 3-D EAF

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

### Exact case

- Attainment surfaces: Visualization of facets
- EAF values: Slicing [2]
- EAF differences: Slicing, Maximum intensity projection [41, 2]

### Approximated case

- Attainment surfaces: Grid-based sampling [20]
- EAF values: Slicing, Direct volume rendering [10, 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



# Exact 3-D EAF differences

### Maximum intensity projection

- $\cdot$  Volume rendering method for spatial data represented by voxels
- $\cdot$  Simple and efficient
- $\cdot\,$  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)
- $\cdot$  Plot on top of previous ones





# Approximated attainment surfaces

### Grid-based sampling

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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



Linear

Spherical

# Approximated EAF values and differences

### Discretization into voxels

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

### Slicing



### Approximated 3-D EAF differences

### Maximum intensity projection

- Plots produced using Voreen [28, 37]
- 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



# Approximated 3-D EAF differences



### Approximated 3-D EAF values

Direct volume rendering of Sph



1/5 and 5/5

### Average Runtime Attainment Function

### aRTA value

- $\cdot$  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

- $\cdot$  Algorithms  ${\cal A}$  and  ${\cal B}$
- $\cdot\,$  Compute ratio between  $\mathsf{aRTA}(\mathbf{z})$  values for  $\mathcal A$  and  $\mathcal B$

Visualization using grid-based sampling [3]

### Approximated aRTA values

Two algorithms on the sphere-sphere problem [3]



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# Approximated aRTA ratios

aRTA ratio between Algorithms  ${\cal A}$  and  ${\cal B}$  [3]









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### Summary

- Visualization in multiobjective optimization useful for various purposes
- Customized methods are needed to address the peculiarities of approximation set visualization
- Many new approaches in the last years



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### SYNERGY

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

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