Introduction

Visualization in Multiobjective Optimization

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GECCO Tutorial, Denver, July 20, 2016

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

Minimize

\[ f: X \rightarrow F \]

\[ f: (x_1, \ldots, x_n) \mapsto (f_1(x_1, \ldots, x_n), \ldots, f_m(x_1, \ldots, x_n)) \]

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

Conflicting objectives → a set of optimal solutions
- Pareto set in the decision space
- Pareto front in the objective space

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

Visualizing solution sets in the objective space

- Interested in sets of mutually non-dominated 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

Visualization can be hard even in 2-D

Stochastic optimization algorithms

- Single run → single approximation set
- Multiple runs → 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]

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

![Benchmark approximation sets](image)

### 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

### 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]

### 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
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

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

<table>
<thead>
<tr>
<th>Dominance relation</th>
<th>Pareto shape</th>
<th>Objective range</th>
<th>Robustness</th>
<th>Handling of large sets</th>
<th>Simultaneous visualization</th>
<th>Scalability</th>
<th>Simplicity</th>
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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

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

#### Heatmaps

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

### Sammon mapping

- A non-linear mapping
- Aims to preserve distances between solutions
  - $d^*_ij$ distance between solutions $x_i$ and $x_j$ in the objective space
  - $d_{ij}$ distance between solutions $x_i$ and $x_j$ 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

- 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

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
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

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

![Principal Component Analysis Graph]

### 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

<table>
<thead>
<tr>
<th>Isomap</th>
<th>Preservation of the</th>
<th>Robustness</th>
<th>Handling of large sets</th>
<th>Simultaneous visualization</th>
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### Additional Information

- **Isomap**
  - First coordinate
  - Second coordinate
  - Third coordinate
  - First principal component
  - Second principal component
  - Linear
  - Spherical
**Summary of the general methods**

<table>
<thead>
<tr>
<th>Method</th>
<th>Preservation of the relation</th>
<th>First shape dominance</th>
<th>Objective range distribution</th>
<th>Robustness</th>
<th>Simplicity</th>
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</tbody>
</table>

**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 \([0, 1]\)
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

Hyper-space diagonal counting

- Inspired by Cantor’s proof that shows \(|\mathbb{N}| = |\mathbb{N}^2| = |\mathbb{N}^3| \ldots \)

\[
\begin{array}{c}
(1, 3) \\
(1, 2) \\
(1, 1)
\end{array} - \begin{array}{c}
(2, 3) \\
(2, 2) \\
(2, 1)
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(3, 2) \\
(3, 1) \\
(3, 1)
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(4, 1)
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\]

- 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
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

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
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

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)
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

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

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

Summary of the specific methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Preservation of dominance relation</th>
<th>Front shape</th>
<th>Objective range</th>
<th>Distribution of solutions</th>
<th>Robustness</th>
<th>Handling of large sets</th>
<th>Simultaneous visualization</th>
<th>Scalability</th>
<th>Simplicity</th>
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</tbody>
</table>
- 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 $z$ is attained by $A$ when $z$ is weakly dominated by at least one solution from $A$

**EAF values** [14]
- Algorithm $A$, approximation sets $A_1, A_2, \ldots, A_r$
- EAF of $z$ is the frequency of attaining $z$ by $A_1, A_2, \ldots, A_r$
- Summary (or $k\%$-) attainment surfaces

**Differences in EAF values** [22]
- Algorithm $A$, approximation sets $A_1, A_2, \ldots, A_r$
- Algorithm $B$, 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
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

Approximated 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

© Christian Lackas
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

Direct volume rendering of Sph-Lin

1/5  2/5  3/5

4/5  5/5  1/5 and 5/5

Direct volume rendering of Sph

1/5 and 5/5
## 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
Acknowledgement

This work was partially funded by the Slovenian Research Agency under research program P2-0209.

This work is part of a project that has received funding from the European Union’s Horizon 2020 research and innovation program under grant agreement No. 692286.

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

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Exploratory analysis of stochastic local search algorithms in biobjective optimization.  

*Interactive Decision Maps: Approximation and Visualization of Pareto Frontier.*  

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Survey of methods to visualize alternatives in multiple criteria decision making problems.  

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Study on effect of MOGA with interactive island model using visualization.