Visualization and Performance Metric in Many-Objective Optimization

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IEEE Transactions on Evolutionary Computation, Vol. 20, No. 3, June 2016

> Presented by Drew Buck 10/4/2016



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### **Multi-objective Optimization**

A multi-objective optimization problem (MOP) is of the form

 $\begin{array}{ll} \text{minimize} & \{f_1(\mathbf{x}), \dots, f_k(\mathbf{x})\}\\ \text{subject to} & \mathbf{x} \in S \end{array}$ 

Where

- $f_i: \mathbb{R}^n \to \mathbb{R}$  is an <u>objective function</u>
- $k (\geq 2)$  is the number of (conflicting) objective functions
- $\mathbf{x} = (x_1, \dots, x_n)$  is a <u>decision vector</u>
- $\mathbf{z} = f(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_k(\mathbf{x})) = (z_1, \dots, z_k)$  is an <u>objective vector</u>
- S is the <u>feasible region</u> formed by constraints
- Z (= f(S)) is the <u>feasible objective region</u> of the objective space



A maximization objective  $f_i(\mathbf{x})$  can be converted to a minimization objective  $f'_i(\mathbf{x})$  by setting  $f'_i(\mathbf{x}) = -f_i(\mathbf{x})$ .





### Pareto Dominance



A solution vector  $\mathbf{x}$  *dominates* another solution vector  $\mathbf{y}$  if and only if:

- $f_i(\mathbf{x})$  is not worse than  $f_i(\mathbf{y}), \forall i = 1, 2, ..., k$
- $f_j(\mathbf{x})$  is better than  $f_j(\mathbf{y})$  for at least one j = 1, 2, ..., k

Obviously, an ideal solution to a MOP should not be dominated by any other solution.





A decision vector  $\mathbf{x}^*$  is <u>*Pareto optimal*</u> if and only if there does not exist another decision vector  $\mathbf{x} \in S$  such that  $f_i(\mathbf{x}) \leq f_i(\mathbf{x}^*)$  for all i = 1, ..., k and  $f_i(\mathbf{x}) < f_i(\mathbf{x}^*)$  for at least one index j.

An objective vector  $\mathbf{z}^* = f(\mathbf{x}^*)$  is <u>*Pareto optimal*</u> if and only if there does not exist another objective vector  $\mathbf{z} \in Z$  such that  $z_i \leq z_i^*$  for all i = 1, ..., k and  $z_j^* < z_j$  for at least one index j.



### The Pareto Optimal Set



The set of Pareto optimal solutions forms the Pareto optimal (PO) set.

- In objective space, the PO set is called the <u>Pareto front</u>.
- There may be many (infinite) solutions within the PO set.
- Computing all solutions within the PO set may be infeasible.

The <u>ideal objective vector</u>  $\mathbf{z}^* \in \mathbb{R}^k$  represents the best possible solution, obtained by minimizing each objective independently.

• The ideal objective vector is typically not in the feasible objective region.

The <u>nadir objective vector</u>  $z^{nad}$  is formed from the upper bounds of the PO set.

• The nadir objective vector may or may not be in the feasible objective region.



# Finding the Pareto Optimal Set

- Multi-objective evolutionary algorithms (MOEAs) are well-suited for solving MOPs.
- The goal of a MOEA is to return a set of solutions that is a good approximation of the true PO set:
  - Close to the theoretical true Pareto front.
  - Well distributed over the entire theoretical true Pareto front.

Considerations:

- No longer a single optimal solution
  - How to assign fitness, perform selection, and do crossover and mutation?
- Need to maintain population diversity
  - Don't let the population converge to a single point.





### **Performance Metrics**

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- Given a set of solutions, how well does it approximate the true Pareto optimal set?
- 5 broad categories of performance metrics:
  - Methods that assess the number of Pareto optimal solutions in the set
    - Example: Ratio of Nondominated Individuals (RNI)
      - Measures the proportion of nondominated solutions to population size
  - Methods that measure how close solutions are to the theoretical true Pareto front
    - Example: Inverted Generational Distance (IGD)
      - Measures the distance between solutions on the true Pareto front and their closest neighbors on the approximate Pareto front
  - Methods that quantify the distribution of the set
    - · Example: How evenly are the solutions distributed?
  - Methods that are concerned with the spread of the set
    - Example: Maximum Spread (MS)
      - Measures how well the true Pareto front is covered by the approximation set
  - Methods that consider both closeness to the theoretical true Pareto front and solution diversity simultaneously
    - Example: Hypervolume (S-metric)
      - Calculates the volume or area of the region covered by the approximation set with respect to a given reference point



- Two common metrics are compared in this paper:
  - Inverted Generational Distance (IGD) measures the average distance between points on the true Pareto front and the closest point in the approximation set.
  - Hypervolume (S-metric) measures the volume covered by the set with respect to a given reference point.



## Shape of the Pareto Front

There are three basic shapes of Pareto fronts: convex, linear, and concave. The shape is determined by the feasible objective region of the problem.



The Pareto front can also consist of a mixed front, which is a combination of the three basic types, or be discontinuous.

## Why Does Shape Matter?

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- The shape of the Pareto front can affect how well an optimization algorithm performs.
- Consider the common strategy of choosing a weight vector to reduce the multi-objective problem to a single objective:
  - Given a weight vector  $\mathbf{w} = (w_1, ..., w_k)$ , pick the solution  $\mathbf{z} \in Z$  that minimizes  $\sum_{i=1}^k w_i z_i$
- If the Pareto front is concave, linear weighting will only produce solutions at the edges.



# Generalized Weighted Metric

- Different solutions can be obtained by using a weighted  $L_p$  metric:
  - Pick the solution  $\mathbf{z} \in Z$  that minimizes  $\left(\sum_{i=1}^{k} w_i | z_i z_i^*|^p\right)^{\frac{1}{p}}$
- The  $L_{\infty}$  metric is also called the Tchebycheff metric:
  - Pick the solution  $\mathbf{z} \in Z$  that minimizes  $\max_{i=1,\dots,k} w_i |z_i z_i^*|$



## Many-Objective Optimization

- If k ≥ 4, the problem is considered a many-objective optimization problem (MaOP).
- Difficulties in handling many objectives:
  - A large fraction of the population is nondominated
    - It becomes difficult for a solution to be the best in all objectives
  - Evaluation of diversity measure becomes computationally expensive
    - Need to find neighbors in k-dimensional space
  - Recombination operation may be inefficient
    - Children may be very far from parents
  - Representation of trade-off surface is difficult
    - Exponentially more points are required
  - Performance metrics are computationally expensive to compute
    - Example: calculating hypervolume has exponential complexity with respect to number of dimensions
  - Visualization is difficult
    - Hard to display >3 dimensional space

What proportion of randomly distributed individuals are nondominated in highdimensional spaces?



Proportion of non-dominated individuals within a population.







Many-Objective Evolutionary Algorithms (MaOEAs) are optimized for solving problems with many objectives.

- This paper compares five state-of-the art MaOEAs:
  - MÖEÁ/D
    - MOEA based on decomposition
  - NSGA-III
    - Reference-point based many-objective nondominated sorting genetic algorithm (NSGA)-II
  - ε-MŎEA
    - ε-domination-based MOEA
  - НурЕ
    - Hypervolume estimation algorithm for multi-objective optimization
  - GrEÁ
    - Grid-based evolutionary algorithm







- MOEA/D is a multiobjective evolutionary algorithm based • on decomposition.
  - Simplify the problem into several different single-objective problems using different scalarization functions.
  - Solve these problems using traditional optimization techniques.
- The main algorithm is:
  - 1. Create a uniformly distributed set of weight vectors
  - 2. Define the neighborhood region around each weight vector (e.g. 10) nearest neighbors)
  - 3. Create an initial population by solving the single-objective problem defined by each weight vector
  - 4. Each iteration, for each weight vector
    - a. Select two solutions from the neighborhood of the weight vector and generate a new solution using genetic operators
      b. Perform a problem specific repair/improvement heuristic

    - If the new solution dominates its neighbors, use it as the representative C. solution for this weight vector
    - d. Update the archive population with the set of nondominated solutions







- Generate a new population using binary tournament selection.
- Sort individuals based on dominance depth.
- Partitions that fit into the new population are copied directly.
- The last partition is further sorted based on crowding distance.
  - In high-dimensional spaces, this is often the first front!
- Individuals with the largest distance are added until the new population is filled.



Dominance Depth Partitioning



### NSGA-III



- Uses the same dominance based partitioning as NSGA-II.
- Instead of using crowding distance to accept solutions from the last front, NSGA-III uses uniformly distributed reference vectors, similar to MOEA/D.
- Each individual is associated with the nearest reference point, and niching is used to ensure that the subsequent generation contains a relatively uniform distribution of individuals.
- This also ensures that the population has a good distribution and spread over the entire Pareto front.









- Same approach as NSGA-II for generating a new population and partitioning into nondominated fronts.
- For the last front, compute the fitness of each individual using the hypervolume indicator, using Monte Carlo sampling to estimate the value in high-dimensional space, and move only the individuals with the best fitness to the new population. (Ex. 10,000 sample points)
  - Fitness is based on how much the hypervolume would change if this individual were removed from the front.
  - Approximate values are okay since only the rank of the individuals is important.



 ε-MOEA is a steady-state algorithm that uses two co-evolving populations: an EA population *P* and an archive population *A* containing the best εnondominated solutions.

ε-ΜΟΕΑ

- A random solution *p* is picked from *P* using binary dominance selection and a solution *e* is picked from *A* randomly.
- The child of *p* and *e* is accepted into the population *P* if it dominates an existing individual, which it replaces.
- The child is accepted into the archive population only if it is ε-nondominated.
  - Only one solution is allowed in each εsized grid cell, ensuring population diversity.









- Grid rank:  $GR(\mathbf{x}) = \sum_{k=1}^{M} G_k(\mathbf{x})$ , where  $G_k(\mathbf{x})$  is the grid coordinate of  $\mathbf{x}$  in objective k.
- Density:  $GCD(\mathbf{x}) = \sum_{\mathbf{y} \in N(\mathbf{x})} (M GD(\mathbf{x}, \mathbf{y}))$ , where \_  $GD(\mathbf{x}, \mathbf{y}) = \sum_{k=1}^{M} |G_k(\mathbf{x}) - G_k(\mathbf{y})|$  and  $\mathbf{y} \in N(\mathbf{x}) \Leftrightarrow GD(\mathbf{x}, \mathbf{y}) < M$ .

Grid-based Evolutionary Algorithm

Each iteration:

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Hyperbox distance:  $GCPD(\mathbf{x}) = \sqrt{\sum_{k=1}^{M} \left(\frac{\left(F_k(\mathbf{x}) - \left(lb_k + G_k(\mathbf{x}) \times d_k\right)\right)}{d_k}\right)^2},$ 

where  $G_k(\mathbf{x})$  and  $F_k(\mathbf{x})$  denote the grid coordinate and actual objective value of x for objective k.  $lb_k$  and  $d_k$  are the lower boundary and grid width for objective k.

- Generate new individuals using binary tournament ٠ selection and a hierarchy of the fitness values.
- Partition the new solutions into nondominated fronts as in ٠ NSGA-II and for the last front, use the computed fitness values to decide which solutions to add.
  - The fitness of neighbor solutions is adjusted as solutions are selected and removed from the previous population.







GrEA

### **Visualizing MaOPs**

- In low-dimensional space, a scatter plot can show the location, distribution, and shape of the approximated front.
  - Each axis represents one objective
  - Limited to 2 or 3 objectives
  - A bundle chart also plots size and color, extending the number of possible objectives to 5.
- Most existing approaches can be categorized as...
  - Methods based on a parallel coordinate system:
    - Parallel coordinates
    - Heatmap
  - Methods based on mapping:
    - Sammon mapping
    - Neuroscale
    - RadViz
    - Self-Organizing Map (SOM)
    - Isomap









# Parallel Coordinate Methods



### Parallel Coordinates

Each M-dimensional vector is represented as a polyline that connects points on parallel axes.

- Shows dependencies between objectives
- Many individuals leads to overcrowded lines



### <u>Heatmap</u>

Each individual is a row in the image. Color indicates objective value. Rows are clustered based on similarity.

- Used to display microarray data
- High information density
- Difficult to see tradeoff between objectives

Stress Minimization Methods

The points are mapped from a high-dimensional space to a low-dimensional space in a way that preserves the distances between points.



Uses gradient descent or other iterative methods to minimize a stress function of the form  $E = \frac{1}{\sum_{i < j} d_{ij}^*} \sum_{i < j} \frac{\left(d_{ij}^* - d_{ij}\right)^2}{d_{ij}^*}$ , where  $d_{ij}$  and  $d_{ij}^*$  are distances between the  $i^{th}$  and  $j^{th}$  points in the original and projected spaces respectively.

Similarly, minimizes a stress function using an RBF neural network to generalize the projection transformation to unseen data points.









- Individuals in a high-dimensional space are mapped onto a grid of neurons arranged in a (usually 2D) topology.
- When trained, nearby vectors in the high-dimensional space are mapped onto nearby neurons in the SOM.
- Regional clusters in the SOM represent similar feature vectors.

## **Other Mapping Methods**



- Objectives are represented as anchors on a circle.
- Individuals are connected to each anchor with "springs" that are weighted according to the relative objective values.
- Preserves the distribution of vectors, but does not show the shape of the Pareto front.

- Topological geometry of the highdimensional space is preserved by linking points only to their nearest neighbors.
- Distance between points is computed as the shortest path through the topology.
- Multidimensional scaling is applied to map points to 2D while preserving pairwise distances.



# Proposed Visualization Method

- The proposed visualization method maps individuals from a highdimensional Cartesian space into a 2D polar coordinate system.
  - Angular coordinates show the distribution of individuals on the approximated Pareto front and the crowdedness in each subregion of high-dimensional space.
  - Radial coordinates show the convergence status toward the theoretical true Pareto front.





### Angular Coordinate

- The high-dimensional objective space is evenly divided into subregions.
- Each subregion is represented by one direction vector and assigned an angular coordinate.
- Individuals in the original objective space are mapped onto the closest direction vector and assigned the same angular coordinate.







### MAPPING FROM 3-D TO 2-D SPACES



## **Radial Coordinate**

- The radial coordinate indicates how close an individual is to the theoretical true Pareto front.
- For each of the three basic front shapes, there is a constant *r* that can be used to characterize the shape of the front:
  - Concave:  $\sum_{m=1}^{M} f_m(\mathbf{x})^2 = r^2$
  - Convex:  $\sum_{m=1}^{M} (r f_m(\mathbf{x}))^2 = r^2$
  - Linear:  $\sum_{m=1}^{M} f_m(\mathbf{x}) = r$
- Smaller values of *r* indicate better convergence performance.
- Individuals are assigned a radial coordinate based on closeness to the true Pareto front.
- Each quadrant of the mapped space represents a subfront of the objective space.





r in concave front:  $\sum_{m=1}^{M} (f_m(x))^2 = r^2$ 

r in convex front:  $\sum_{m=1}^{M} (r - f_m(x))^2 = r^2$ 





### **Visualization Process**

- Precompute a set of equally distributed direction vectors in highdimensional space and assign a fixed angular-coordinate to each.
- 2. Map each individual to the nearest direction vector in objective space and assign it the corresponding angular coordinate.
- 3. Determine the shape of the approximate front by solving for *r* using the three possible shapes.
- If most individuals achieve the same value of r under one shape, use this shape as the approximate front. Otherwise consider a mixed front and treat each subpart independently.
- 5. Assign the radial coordinate for each individual based on the closeness to the approximate front.







### **Visualization Examples**



### **More Examples**









Visualizing mixed Pareto front.







- Individuals are mapped from a high-dimensional objective space into a 2D polar coordinate system.
  - Radial coordinate reflects convergence performance
  - Angular coordinate reflects distribution of individuals
- Main contributions:
  - Mapping is consistent
    - Pareto dominance relationship, front shape and location, and the distribution of solutions is maintained
  - Allows for observation of the evolution process
    - Improvement of the approximation set can be tracked in location, range, and distribution as the population evolves
  - Decision-making is easy and effective
    - Solution quality and trade-offs can be observed from the plots
  - Scalable to any number of dimensions
    - High-dimensional objective spaces can be visualized, even with a large number of individuals on the front







- A new performance metric is proposed called *p*-metric that is based on the proposed visualization approach.
- Method:
  - For each direction vector *j*:
    - $r_{\min} = \min_{i=1:N_j} r_i$ , where  $N_j$  is the number of solutions associated with direction vector j and  $r_i$  is the radius value of solution i.

• 
$$d_j = \begin{cases} \frac{1}{r_{\min}}, & N_j > 0\\ 0, & N_j = 0 \end{cases}$$

- Compute performance score:
  - $S = \sum_{j=1:N} d_j$ , where *N* is the number of direction vectors.





### p-Metric Comparison



- All solutions except  $x_1$  in the approximate front 1 (blue) are dominated by at least one solution on the approximate front 2 (black).
  - Based on this property, the authors prefer front 2.
  - However, because  $x_1$  is so close to the true Pareto front, the IGD metric always assigns it as the closest point.
  - The *p*-Metric favors front 2 because it is well distributed with a solution for each direction vector and dominates most points on front 1.





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- All solutions except  $x_1$  in the approximate front 1 (blue) are dominated by a solution on the approximate front 2 (black).
  - Based on this property, the authors prefer front 2 (although  $x_1$  is close to the ideal point).
  - Front 1 encloses a larger area than front 2 so the hypervolume (S-metric) is larger for front 1.
  - The *p*-Metric favors front 2 because it is well distributed with a solution for each direction vector and dominates most points on front 1.





### *p*-Metric Comparison

- All solutions from approximate front 1 (blue) are focused in a single • neighborhood, as tends to happen in high-dimensional spaces.
- Approximate front 2 is well distributed, but farther from the ideal point.

  - Based on these properties, the authors prefer front 2. As with the previous examples, IGD and S-metric prefer front 1, even with extremely poor diversity.
  - The *p*-Metric favors front 2 because it is well-distributed, although somewhat farther from the ideal point than front 1.





### Experiments



- 5 MaOEAs are tested on 5-D and 10-D benchmark functions DTLZ1-DTLZ7.
- For each problem, the following parameters are used: •
  - Population size: 100

  - Stopping criteria: 10,000 generations Initial population: uniform random sampling Crossover: simulated binary crossover (SBX)  $p_c = 1$
  - Mutation: polynomial mutation  $p_m = \frac{1}{m}$
  - Number of decision variables (m):
    - 5-D DTI 71: 9
    - 10-D DTLZ1 & 5-D DTLZ2-DTLZ7: 14
    - 10-D DTLZ2-DTLZ7: 19
  - Number of direction vectors:
    - 126 for 5-D
    - 55 for 10-D
- Each algorithm is run 30 times to compute the average performance metric.





DTLZ1 has a linear Pareto front with a large number of local fronts.



- GrEA (blue) performs best and ε-MOEA (black) is worst.
- In 5-D DTLZ1, the MOEA/D front (magenta) is localized to the topright, behind the GrEA front (blue).
  - Despite poor diversity, MOEA/D still scores well with IGD and S-metrics.



5-D DTLZ1







### DTLZ2 has a single concave Pareto front.



- In 5-D DTLZ2, IGD shows that:
  - ε-MOEA (black) performs better than NSGA-III (yellow), but appears to have worse convergence.
  - MOEA/D (magenta) performs better than HypE (cyan), but has worse diversity.
- GrEA (blue) performs best, which is shown by the *p*-metric, but not by the S-metric.



5-D DTLZ2







DTLZ3 has a concave Pareto front and a large number of local Pareto fronts.







- GrEA (blue) performs best.
- Other algorithms can only converge to several different local Pareto fronts.

5-D DTLZ3







DTLZ4 has a single concave Pareto front with a non-uniform mapping from decision space to objective space to challenge solution diversity.



- GrEA (blue) continues to perform best.
- S-metric claims MOEA/D (magenta) and HypE (cyan) are best, despite poor diversity.
- In 10-D DTLZ4, IGD ranks ε-MOEA (black) above GrEA (blue) despite better convergence.
   In 10-D DTLZ4, S-
- In 10-D DTLZ4, Smetric ranks MOEA/D (magenta), HypE (cyan), and NSGA-III (yellow) above GrEA (blue) despite poor diversity.
- GrEA
   ↓ ε-MOEA
   NSGA-III
   ♦ MOEA/D
   ♦ HypE

5-D DTLZ4







DTLZ5 has a degenerated hypersurface as the Pareto front.



- In 10-D-DTLZ5, IGD ranks ε-MOEA (black) above NSGA-III (yellow), despite worse convergence.
- NSGA-III (yellow) and HypE (cyan) perform best on this problem.
- GrEA (blue) performs poorly on DTLZ5 with a degenerated hypersurface.
  - GrEA
    ★ ε-MOEA
    NSGA-III
    ♦ MOEA/D
    ➡ HypE

5-D DTLZ5







DTLZ6 has a large number of local Pareto fronts and disconnected Pareto-optimal regions.



- ε-MOEA (black) shows poor performance in DTLZ6.
- GrEA (blue) performs poorly in 10-D DTLZ6, but does well in 5-D DTLZ6.
- NSGA-III (yellow), HypE (cyan), and MOEA/D (magenta) perform best on high-dimensional disconnected problems.
- GrEA
   τ-MOEA
   NSGA-III
   MOEA/D
   HypE

5-D DTLZ6





DTLZ7 has a Pareto front at the intersection of a straight line and a hyperplane.

MaOP	Rank	<i>p</i> -metric	IGD	S-metric
DTLZ7	1	GrEA	GrEA	HypE
	2	HypE	HypE	GrEA
	3	NSGA-III	NSGA-III	MOEA/D
	4	MOEA/D	MOEA/D	ε-MOEA
	5	ε-MOEA	ε-MOEA	NSGA-III

MaOP	Rank	<i>p</i> -metric	IGD	S-metric
DTLZ7	1	HypE	GrEA	HypE
	2	GrEA	HypE	GrEA
	3	ε-MOEA	ε-MOEA	ε-MOEA
	4	MOEA/D	MOEA/D	MOEA/D
	5	NSGA-III	NSGA-III	NSGA-III



- None of the tested MaOEAs are effective at converging to the true Pareto front.
- A single metric alone cannot show this and some form of visualization is required to observe both convergence and diversity performance.



5-D DTLZ7





### Conclusion



- Visualization is an important tool for evaluating MaOEAs and MaOPs.
  - The proposed visualization approach maps a high-dimensional objective space into a 2D polar coordinate plot while preserving Pareto dominance, shape and location of the Pareto front, and population diversity.
  - The approach is scalable to a large number of dimensions and can display many individuals and fronts simultaneously.
- The proposed performance metric, *p*-Metric is wellsuited for high-dimensional MaOPs.
  - Convergence is measured by radial value.
  - Distribution is shown with angular coordinates.
  - Provides a comprehensive and consistent comparison among MaOEAs.