PSEA

A Pareto Set Estimation Algorithm for Multi-objective Optimisation

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March 10, 2014

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Introduction

Multi-objective optimisation problems

Many real-world optimisation applications involve more than one optimisation criteria (objectives) which are in conflict with each other. Such kind of problems, called multiobjective optimisation problems (MOPs), can be described as follows:

$$\begin{aligned} \min \quad & F(\vec{x}) = (f_1(\vec{x}), f_2(\vec{x}), ..., f_m(\vec{x})) \\ \text{s.t.} \quad & \vec{x} \in X \end{aligned} \tag{1}$$

where $X \subset \mathbb{R}^n$ is the decision space and $F \subset \mathbb{R}^m$ is the objective space which consists of m different objective functions $f_i(\vec{x})$ $(i = 1, 2, 3, ..., m)$.

Pareto set

Since the objectives are contradictory with each other, in general, no one single solution is able to optimize all objectives at the same time.

Instead of one solution, there exist a set of solutions (*Pareto set*, denoted as *PS*) which trade off between different objectives.

Correspondingly, the set containing solutions in the objective space is called a *Pareto front*, denoted as *PF*.

Pareto dominance

The Pareto set is defined based on the relationship called *Pareto dominance*, where the definition is as follows:
A solution $\vec{x}^*$ is said to dominate another solution $\vec{x}$ (denoted as $\vec{x}^* \succ \vec{x}$) iff

$$\begin{cases} \forall i \in 1,2,3,...,m : f_i(\vec{x}^*) \leq f_i(\vec{x}) \\ \exists j \in 1,2,3,...,m : f_j(\vec{x}^*) < f_j(\vec{x}) \end{cases} \tag{2}$$

Non-dominated solutions

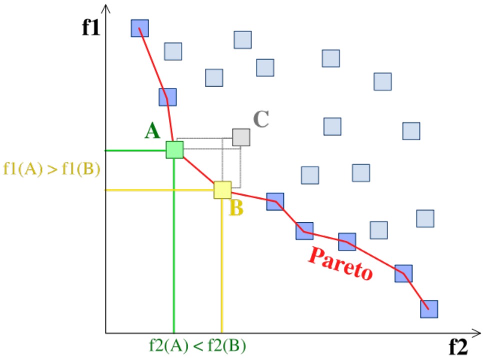

Figure : A and B are non-dominated solutions, and they both dominate solution C.

Traditional methods to solve MOPs

1. Non-dominated sorting based method (NSGA-II)
2. Weighted-aggregation based method (MOEA/D)
3. Indicator based method (Hypervolume)

Estimation of distribution algorithms (EDAs)

- Estimation of Distribution Algorithms (EDAs) are optimisation methods that guide the stochastic search by training and sampling *probabilistic models* of promising candidate solutions.
- Although EDAs belong to the class of Evolutionary Algorithms (EAs), a significant difference is that EAs make use of a group of pre-defined stochastic operators (e.g., crossover and mutation) whilst the EDAs are based on explicit probability distribution models.

Advantages of EDAs

1. Ability to sample solutions
2. Ability to capture the geometric structure of a Pareto front.

The proposed algorithm

Motivation

Normally, although a continuous *PF* / *PS* contains **infinite** number of points, most traditional multi-objective evolutionary algorithms are only able to estimate the *PF* / *PS* with **limited** number of solutions which may not be interested by the decision maker.
In order to sample solutions arbitrarily according to **user preference**, the Pareto set estimation algorithm (PSEA) is proposed.

Basic idea

Firstly, models representing the structure of a *PF* are directly built in the objective space F; and thereafter, in order to obtain the corresponding solutions in *PS*, the inverse projections from the objective space F to the decision space X are modeled as well.

In the current work, we start from *2-objective* MOPs and then the algorithm can be extended for 3-objective MOPs or even more.

Framework

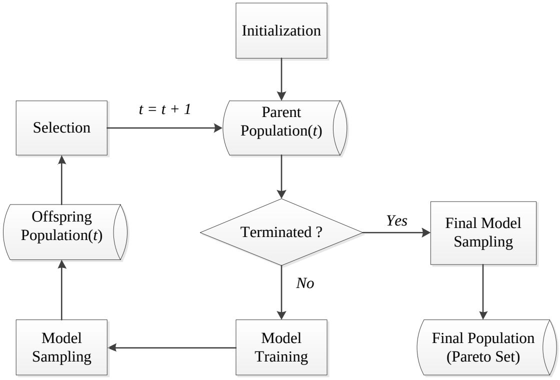

Figure : The framework of the proposed PSEA.

2-objective Pareto front presentation

In 2-objective MOPs, a continuous *PF* is normally a smooth curve (either convex or concave), which can be achieved by adopting *polynomial regression*.

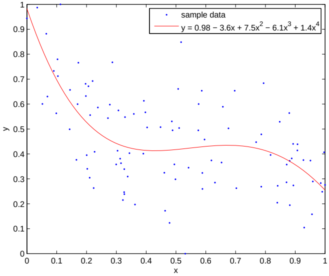

Figure : An example of the polynomial regression.

Projections from PF to PS

For 2-objective MOPs, although PF is only 2-dimensional, the dimensionality of PS can be much higher, which is determined by the decision variables. Therefore, the projection relationship from PF to PS is a *two-to-many* projection, which is not easy to model directly.

Projections from PF to PS

A *decomposition* method is adopted to transform the *two-to-many* projections to a group of *one-to-one* projections, based on the following theorem:
Under certain smoothness assumptions, induced from the Karush-Kuhn-Tucker condition, both the *PS* and the *PF* are $(m-1)$-D manifolds in the decision space and objective space respectively, where m is the number of objectives.

Projections from PF to PS

Each of the projection relationship can be represented by a unique polynomial regression model.

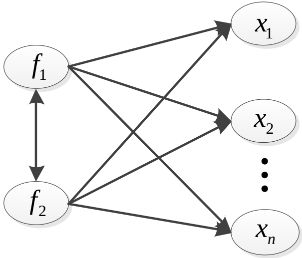

Figure : Decomposition of the projection from *PF* to *PS*.

Model sampling

Normally, a group of well selected sampling data is able to represent a promising distribution of candidate solutions, thus providing an effective guideline for the future model training.

Model sampling

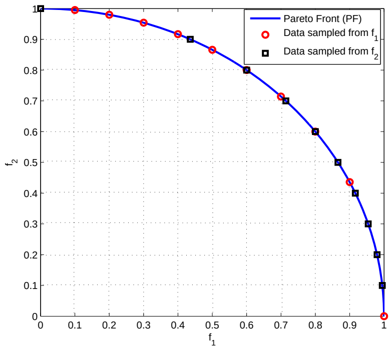

Figure : An example of data sampling. The total number of sampled solutions is 20, i.e., 10 data points are sampled from each objective, respectively.

Experimental results

Benchmark test problems

The widely used ZDT test suit and DTLZ test suit are applied in the experiments.

Sampling ability

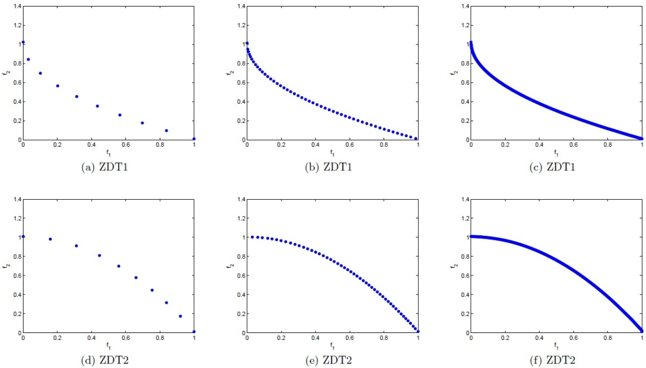

Figure : The sampling results of the final PF obtained by PSEA. A number of 10, 50, 500 solutions are tested.

Numerical measurements

A convergence measurement (Generational Distance, GD) and a spreading measurement (Δ) are used respectively to evaluate the quality of the solutions obtained by PSEA, in comparison with NSGA-II and MOEA/D, which are two widely reported multi-objective evolutionary algorithms.

Numerical comparisons (GD)

Function	PSEA	NSGA-II	MOEA/D
ZDT1	8.67E-03 3.92E-08	**9.28E-04** 3.37E-11	7.21E-02 1.05E-03
ZDT2	7.94E-03 2.87E-07	**6.80E-04** 1.45E-07	2.61E-03 4.86E-07
ZDT3	8.68E-03 1.67E-07	**1.05E-03** 5.96E-10	2.52E-02 1.76E-04
ZDT4	**9.58E-04** 2.14E-09	5.56E-03 1.32E-06	5.78E-01 2.96E-02
ZDT6	1.69E-01 1.97E-02	**6.14E-03** 5.27E-08	1.36E-01 1.27E-02
DTLZ1	9.74E+00 8.77E+00	9.75E-01 1.05E-01	**5.51E-01** 8.14E-02
DTLZ2	**4.39E-04** 7.09E-11	1.93E-03 3.05E-07	1.68E-03 1.34E-08
DTLZ3	2.02E+02 2.56E+02	**5.02E+01** 9.13E+01	1.12E+02 4.47E+00
DTLZ4	2.08E-03 1.28E-09	1.35E-03 1.12E-08	**9.53E-04** 2.58E-06
DTLZ5	**4.61E-04** 1.84E-09	1.93E-03 3.05E-07	1.51E+00 8.25E-05
DTLZ6	**6.15E-04** 1.20E-10	2.77E+00 1.64E-02	5.90E+00 1.78E-03

Numerical comparisons (Δ)

Funcion	PSEA	NSGA-II	MOEA/D
ZDT1	**7.11E-02** 2.69E-04	6.02E-01 4.27E-04	9.64E-01 2.04E-03
ZDT2	**5.83E-02** 2.84E-04	5.99E-01 4.41E-05	9.77E-01 2.25E-03
ZDT3	**7.89E-01** 3.15E-04	9.04E-01 1.46E-04	1.11E+00 6.20E-04
ZDT4	**7.59E-02** 4.15E-04	9.16E-01 1.57E-02	1.14E+00 2.02E-03
ZDT6	1.05E+00 2.68E-02	**6.05E-01** 3.90E-04	8.49E-01 4.98E-04
DTLZ1	**4.58E-01** 1.90E-01	7.41E-01 4.88E-03	1.78E+00 2.08E-02
DTLZ2	**9.51E-02** 1.62E-06	6.01E-01 6.18E-04	4.58E-01 7.85E-05
DTLZ3	7.82E-01 4.50E-03	**6.34E-01** 1.46E-02	1.46E+00 4.28E-03
DTLZ4	7.17E-01 8.53E-05	**6.04E-01** 6.24E-04	1.11E+00 2.74E-02
DTLZ5	**9.23E-02** 1.86E-05	6.36E-01 5.64E-04	4.69E-01 7.77E-03
DTLZ6	**8.94E-02** 4.35E-06	7.05E-01 6.83E-03	6.50E-01 9.73E-03

A Pareto front

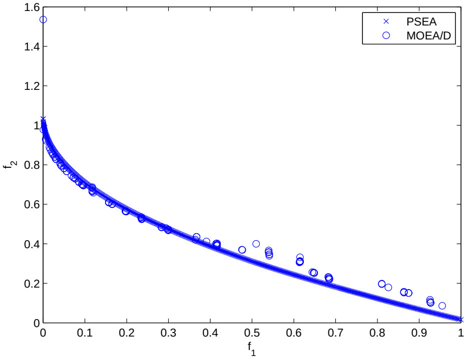

Figure : The Pareto fronts of ZDT1 obtained by the proposed PSEA and MOEA/D, respectively.

Summary and future work

The proposed 2-objective PSEA

As a very preliminary work, although the current PSEA is only able to solve 2-objective MOPs so far, it has already shown promising potentials which has distinguished itself from most existing MOEAs: once the model training is completed, with the trained model, the decision maker is able to sample arbitrary solutions according to his/her preference.

Extension from 2-objective to *m*-objective

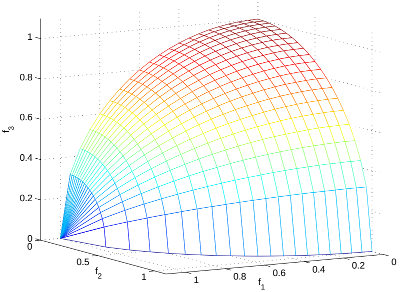

Figure : *Divide-and-conquer* methodology can be adopted to recursively transform a *m*-objective PF (hyper-surface) to a group of 2-objective PFs (curves).

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