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A novel model-based multiobjective evolutionary algorithm

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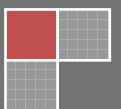
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ABSTRACT

As is known that the Pareto set of a continuous multi-objective optimization problem with m objective functions is a piecewise continuous $(m-1)$ -dimensional manifold in the decision space under some mild conditions. However, how to utilize the regularity to design multi-objective optimization algorithms has become the research focus. In this paper, based on this regularity, a model-based multi-objective evolutionary algorithm with regression analysis (MMEA-RA) is put forward to solve continuous multi-objective optimization problems with variable linkages. In the algorithm, the optimization problem is modelled as a promising area in the decision space by a probability distribution, and the centroid of the probability distribution is $(m-1)$ -dimensional piecewise continuous manifold. The least squares method is used to construct such a model. A selection strategy based the non-dominated sorting is used to choose the individuals to the next generation. The new algorithm is tested and compared with NSGA-II and RM-MEDA. The result shows that MMEA-RA outperforms RM-MEDA and NSGA-II on the test instances with variable linkages. At the same time, MMEA-RA has higher efficiency than the other two algorithm. A few shortcomings of MMEA-RA have also been identified and discussed in this paper.

KEYWORDS

Multi-objective evolutionary algorithm; Least squares method; Performance metric; Model-based algorithm; Regression analysis.



INTRODUCTION

Evolutionary algorithm has become an increasingly popular design and optimization tool in the last few years^[1]. Although there have been a lot of researches about evolutionary algorithm, there are still many new areas needed to be explored with sufficient depth. One of them is how to use the evolutionary algorithm to solve multi-objective optimization problems. The first implementation of a multi-objective evolutionary algorithm dates back to the mid-1980s^[2]. Since then, many researchers have done a considerable amount of works in the area, which is known as multi-objective evolutionary algorithm (MOEA).

Because of the ability to deal with a set of possible solutions simultaneously, evolutionary algorithm seems particularly suitable to solve multi-objective optimization problems. The ability enables it possible to search several members of the Pareto optimal set in a single run of the algorithm^[3]. Obviously, evolutionary algorithm is more effective than the traditional mathematical programming methods in solving multi-objective optimization problem because the traditional methods need to perform a series of separate runs^[4].

In 2005, Zhou et al. proposed to extract regularity patterns of the Pareto set by using local principal component analysis (PCA)^[5]. They had also studied two naive hybrid MOEAs. In the two MOEAs, some trial solutions were generated by traditional genetic operators and others by sampling from probability models based on regularity patterns in 2006^[6].

In 2007, Zhang et al. conducted a further and thorough investigation along their previous works^[5] and^[6]. They proposed a regularity model-based multi-objective estimation of distribution algorithm and named it as RM-MEDA^[7]. At each generation, the proposed algorithm models a promising area in the decision space by a probability distribution whose centroid is a $(m-1)$ -dimensional piecewise continuous manifold. The local principal component analysis algorithm is used to build such a model. Systematic experiments have shown that RM-MEDA outperforms some other algorithms on a set of test instances with variable linkages.

In 2008, Zhou et al proposed a probabilistic model based multi-objective evolutionary algorithm to approximate PS and PF (Pareto front) for a MOP in this class simultaneously, and named the algorithm as MMEA^[8]. They proposed two typical classes of continuous MOPs as follows. One class is that PS and PF are of the same dimensionality while the other one is that PF is a $(m-1)$ -dimensional continuous manifold and PS is a continuous manifold with a higher dimensionality. There is a class of MOPs, in which the dimensionalities of PS and PF are different so that a good approximation to PF might not approximate PS very well. MMEA could promote the population diversity both in the decision spaces and in the objective spaces.

Modeling method is a crucial part for MOEA because it determines the performance of the algorithms. Zhang et al. built such a model by local principal component analysis (PCA) algorithm^[7]. The test results show that the method has great performance over some instances with linkage variables. However, there are still some shortcomings about the method. The first shortcoming is that RM-MEDA needs extra CPU time for running local PCA at each generation. The second one is that the model is just linear fitting for all types of PS, including the one with nonlinear linkage variables, which enables that the result may be not accurate.

In the paper we proposed a model-based multi-objective evolutionary algorithm with regression analysis, which is named as MMEA-RA. In MMEA-RA, a new modeling method based on regression analysis is put forwards. In the method, least squares method (LSM) is used to fit a 1-dimensional manifold in high-dimensional space. Because least squares can fit any type of curves through its model, the shortcomings of RM-MEDA can be avoided, especially for the instances with non-linkage variables.

The rest of this paper is organized as follows. After defining the continuous multi-objective optimization problem in section algorithm model, the new model of multi-objective evolutionary algorithm based on regression analysis is put forwards in section algorithm model. Then, a description of the test cases for MMEA-RA follows in section result and discuss. After presenting the results of the tests, the performance of MMEA-RA is analyzed and some conclusions are given in section conclusion.

ALGORITHM MODEL

In this paper, we consider the following continuous multi-objective optimization problem (continuous MOP):

$$\min F(x) = (f_1(x), f_2(x), \dots, f_m(x))^T \quad (1)$$

s. t. $x \in X$

Where $X \subset R^n$ is the decision space and $x = (x_1, \dots, x_n)^T$ is the decision variable vector. $F: X \rightarrow R^m$ consists of m real-valued continuous objective functions $f_i(x)$ ($i = 1, \dots, m$). R^m is the objective space.

Let $a = (a_1, \dots, a_n)^T \in R^n$ and $b = (b_1, \dots, b_n)^T \in R^n$ are two vectors, a is said to dominate b , denoted by $a < b$, if $a_i \leq b_i$ for all $i = 1, \dots, n$, and $a \neq b$. A point $x^* \in X$ is called (globally) Pareto optimal if there is no $x \in X$ such that $F(x) < F(x^*)$. The set of all Pareto optimal points, denoted by PS, is called the Pareto set. The set of all Pareto objective vectors, $PF = \{y \in R^m \mid y = F(x), x \in PS\}$, is called the Pareto front^[10].

Under certain smoothness assumptions, it can be induced from the Karush-Kuhn-Tucker condition that the PS of a continuous MOP defines a piecewise continuous $(m-1)$ -dimensional manifold in the decision space^[9]. Therefore, the PS of a continuous bi-objective optimization problem is a piecewise continuous curve in R^2 .

The population in the decision space in a MOEA for (1) will hopefully approximate the PS and is uniformly scattered around the PS as the search goes on. Therefore, we can envisage the points in the population as independent observations of a random vector $\xi \in R^n$ whose centroid is the PS of (1). Since the PS is a $(m-1)$ -dimensional piecewise continuous manifold, ξ can be naturally described by

$$\xi = \zeta + \varepsilon \tag{2}$$

Where ζ is uniformly distributed over a piecewise continuous $(m-1)$ -dimensional manifold, and ε is an n -dimensional zero-mean noise vector. Figure 1 illustrates the basic idea.

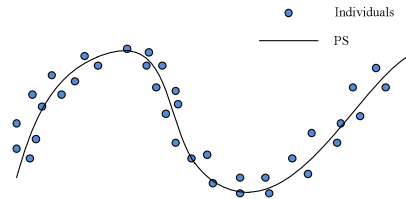


Figure 1 : Individual solutions should be scattered around the PS in the decision space in a successful MOEA

Fitting the expression (2) to the points in $Pop(t)$ is highly related to principal curve analysis, which aims at finding a central curve of a set of points in R^n ^[10]. However, most current algorithms for principal curve analysis are rather expensive due to the intrinsic complexity of their models. RM-MEDA uses the $(m-1)$ -dimensional local principal component analysis (PCA) algorithm^[11], it is less complex compared with most algorithms for principal curve analysis. However, it needs much more CPU time compared with the traditional evolutionary algorithms which adopt genetic recombination operators such as crossover and mutation. Moreover, the PS can be not exactly described by local PCA because it only uses linear curves to approximate the model at one cluster of the $Pop(t)$.

In this implementation, we do not make use of clustering method in the modeling process. We try to find the principal curve of the whole points in $Pop(t)$, not just the local part of them. As is known, least squares approach is a simple and effective method for linear curve fitting and nonlinear curve fitting, such as polynomial or exponential curve fitting. Then we consider whether this technique could be made use of to describe the expression (2).

For the sake of simplicity, it could be assumed that the centroid of ξ is a manifold ψ in the formula (2), ζ is uniformly distributed on ψ . ψ is a $(m-1)$ -dimensional hyper-rectangle. Particularly, in the case of two objectives, ψ is a curve segment in R^2 . A line in 3-dimensional space can be expressed as

$$\begin{cases} x = az + c \\ y = bz + d \end{cases} \tag{3}$$

where a, b, c and d are the coefficients of the expression.

The geometric meaning of the expression (3) is that a 3-dimensional line l can be seen as the intersecting line of two planes $m_1: x = az + c$ and $m_2: y = bz + d$. Figure 2 illustrates this meaning. The expression $x = az + c$ can be seen as the projection of the line l in the xOz plane, and $y = bz + d$ is the one in the yOz plane. As a 3-dimensional line can be expressed by the intersecting of 2 planes, then a n -dimensional line can be expressed as the intersecting of $(n-1)$ planes as (4).

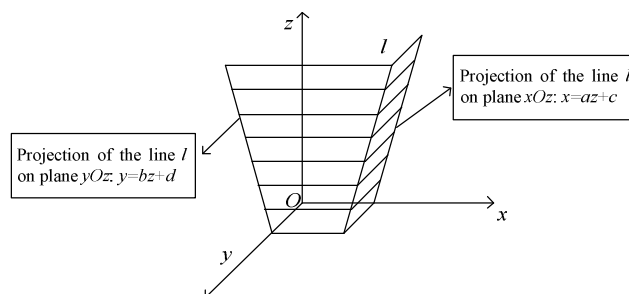


Figure 2 : Illustration of the geometric meaning of the expression (3)

$$\begin{cases} x_2 = a_1 + b_1x_1 \\ x_3 = a_2 + b_2x_1 \\ \vdots \\ x_n = a_{n-1} + b_{n-1}x_1 \end{cases} \tag{4}$$

Expression $x_i = a_{i-1} + b_{i-1}x_1$ can be regarded as the projection of the n -dimensional line in x_iOx_1 plane.

By the expression (4), we further conclude that a n -dimensional curve can be regarded as the intersecting of $(n-1)$ surface, the expression (5) shows this idea.

$$\begin{cases} x_2 = a_{1,0} + a_{1,1}x_1 + a_{1,2}x_1^2 + \dots + a_{1,p}x_1^p \\ x_3 = a_{2,0} + a_{2,1}x_1 + a_{2,2}x_1^2 + \dots + a_{2,p}x_1^p \\ \vdots \\ x_n = a_{n-1,0} + a_{n-1,1}x_1 + a_{n-1,2}x_1^2 + \dots + a_{n-1,p}x_1^p \end{cases} \tag{5}$$

Expression $x_j = a_{j-1,0} + a_{j-1,1}x_1 + a_{j-1,2}x_1^2 + \dots + a_{j-1,p}x_1^p$ can be regarded as the approximate projection of the n -dimensional curve in x_jOx_1 surface. Each expression is a p -order polynomial. (x_1, \dots, x_n) is a point on the n -dimensional curve. Then the thing that we need to do is to find out all the coefficients $a_{i,j}$, which could make the curve fit the population in the decision space well, and here we used least squares approach method to help us finding out the best coefficients.

Least squares approach is mainly used to fit the curve, that is to say, to capture the trend of the data by assigning a single function across the entire range. Figure 3 shows the idea. In Figure 3, Figure 3(a) looks linear in trend, so we can fit the curve by choosing a general form of the straight line $f(x) = ax + b$, and then the goal is to identify the coefficients a and b such that $f(x)$ fits the data well, the method to identify the two coefficients is called as linear regression. Figure 3(b) looks nonlinear, we use higher polynomial $f(x) = ax^2 + bx + c$, and the goal is to find out the coefficients a, b and c such that $f(x)$ fits the data well. It is called as nonlinear regression compared with linear regression. In fact, there are a lots of functions with different shapes that depend on the coefficients. The methods to find out the best coefficients are just called as regression analysis (RA).



Figure 3: Illustration of the least squares approach

Consider the general form for a polynomial with order j

$$f(x) = a_0 + a_1x + a_2x^2 + \dots + a_jx^j = \sum_{k=0}^j a_kx^k \tag{6}$$

How can we choose the coefficients that best fits the curve to the data? The idea of least squares approach is to find a curve that gives minimum error between data y and the fitting curve $f(x)$. As is shown in the Figure 4, we can firstly add up the length of all the solid and dashed vertical lines, then pick curve with minimum total error. The general expression for any error using the least squares approach is

$$err = \sum_{i=1}^n (d_i)^2 = (y_1 - f(x_1))^2 + (y_2 - f(x_2))^2 + \dots + (y_n - f(x_n))^2 \tag{7}$$

For the expression (7), we want to minimize the error err . Replace $f(x)$ in the expression (7) with the expression (6), then have (8)

$$err = \sum_{i=1}^n (y_i - \sum_{k=0}^j a_kx_i^k)^2 \tag{8}$$

where n is the number of data points given, i is the current data points being summed, j is the polynomial order. To find the best line means to minimize the square of the distance error between line and data points. Find the set of coefficients a_0, a_1, \dots, a_j , that is to say, to minimize the expression (8).

In Figure 4, there are four data points and two fitting curves $f_1(x)$ and $f_2(x)$. Obviously, $f_1(x)$ is better than $f_2(x)$ because there is smaller error between the four points and the fitting curve $f_1(x)$.

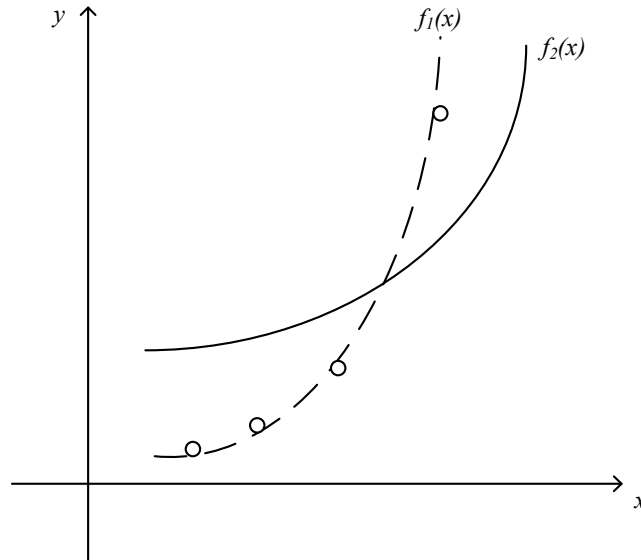


Figure 4 : Four data points and two different curves

To minimize the expression (8), take the derivative with respect to each coefficient a_k for $k = 0, 1, \dots, j$, set each to zero.

$$\begin{cases} \frac{\partial err}{\partial a_0} = -2 \sum_{i=1}^n \left(y_i - \sum_{k=0}^i a_k x^k \right) = 0 \\ \frac{\partial err}{\partial a_1} = -2 \sum_{i=1}^n \left(y_i - \sum_{k=0}^i a_k x^k \right) x = 0 \\ \vdots \\ \frac{\partial err}{\partial a_j} = -2 \sum_{i=1}^n \left(y_i - \sum_{k=0}^i a_k x^k \right) x^j = 0 \end{cases}$$

Re-write these $j+1$ equations, and put into matrix form

$$\begin{pmatrix} n \sum x_i & \sum x_i^2 & \dots & \sum x_i^j \\ \sum x_i & \sum x_i^2 & \sum x_i^3 & \dots & \sum x_i^{j+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum x_i^j & \sum x_i^{j+1} & \sum x_i^{j+2} & \dots & \sum x_i^{j+j} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_j \end{pmatrix} = \begin{pmatrix} \sum y_i \\ \sum x_i y_i \\ \vdots \\ \sum x_i^j y_i \end{pmatrix} \tag{9}$$

The coefficients a_k for $k=0, 1, \dots, j$ can be solved by matrix computation.

With the above work, we can describe the 1-dimensional manifold ψ as (10):

$$\psi = \{x = (x_1, \dots, x_n) \in R^n \mid x_i = \sum_{j=0}^p a_{i-1,j} x_1^j, a_1 - 0.25(b_1 - a_1) \leq x_1 \leq b_1 + 0.25(b_1 - a_1), i = 2, \dots, n\} \tag{10}$$

Where p is the polynomial order, a_1 and b_1 are the minimum and maximum value on x_1 :

$$a_1 = \min_{1 \leq j \leq N} x_1^j \tag{11}$$

$$b_1 = \max_{1 \leq j \leq N} x_1^j \tag{12}$$

In order to approximate the PS better, ψ is extended by 50% along x_1 . Figure 5 shows this idea. In Figure 5, ψ' could not approximate the PS very well, but its extension ψ can provide a better approximation.

When we find out the coefficients $a_{i,j}$ ($i=1, \dots, n-1, j=0, \dots, p$) based on least square approach above, we could get ζ in the expression (2). ζ is generated over ψ uniformly and randomly.

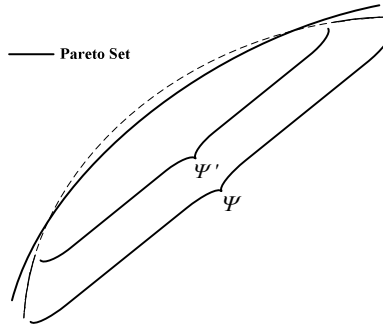


Figure 5 : Illustration of extension

In the expression (2), ε is a n -dimensional zero-mean noise vector, it is designed as the following description.

$$\varepsilon = (\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n) \quad (13)$$

Where ε_i is a random number between (-noise, noise). The noise is changed from big to small as the generation goes on because big noise can accelerate the convergence of the population in the early generation and small noise can maintain the accuracy of the population in the end. The expression (14) shows the implementation.

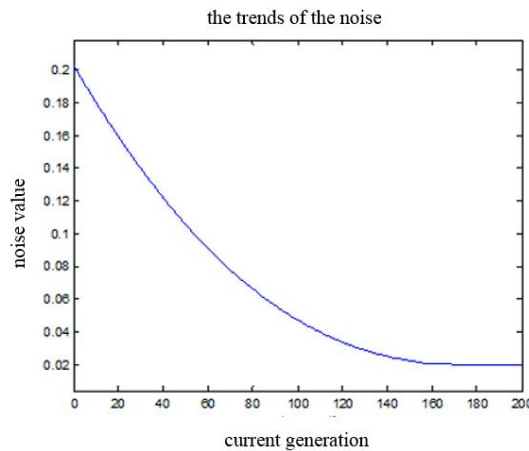


Figure 6 : The trends of the noise

$$noise = F_0 * 10^{e^{(1 - \frac{maxGen}{maxGen+1-curGen})}} \quad (14)$$

Where maxGen is the max generation of the algorithm and is set to be 200, curGen is the current generation. F0 is set to be 0.2 when the algorithm begins. Then the noise is changed from 0.2 to 0.02. The trends of the noise can be seen in Figure 6. As is shown in Figure 6, the noise decreases as the generation increases, and it will be stable after the 160th generation.

RESULT AND DISSCUSS

In this paper, the performance metric used to evaluate the solutions is the convergence metric, which is also the common performance metric in multi-objective optimization algorithm. The metric γ measures that the solutions will be convergent to a known set of Pareto-optimal solutions. We find a set of 500 uniformly solutions from the true Pareto-optimal front in the objective space. And then to compute the minimum Euclidean distance of each solution from chosen solutions on the Pareto-optimal front. The average of theses distances is used as the metric γ .

There are three algorithms employed to solve the test instance for a comparison. These three algorithms are RM-MEDA, NSGA-II and MMEA-RA, while MMEA-RA is the new algorithm proposed in this paper. The three algorithms are implemented by C++. The machine used in the test is Core 2 Duo (2.4GHz, 2.00GB RAM). The experiment setting is as follows.

The number of new trial solutions generated at each generation is set to be 100 for all tests.

The number of decision variables is set to be 30 for all tests.

Parameter setting in RM-MEDA: The number of cluster K is set to be 5 in local PCA algorithm.

Parameter setting in MMEA-RA: The order is set to 2.

We run each algorithm independently 10 times for the test instance. The algorithms stop after a given number of generations. The maximal number of generations in three algorithm is 1000.

TABLE 1 gives the test instance^[7]. In the test instance, the feasible decision space is a hyper-rectangle. There are nonlinear variable linkages in the test case. Furthermore, the test instance have many local Pareto fronts since its $g(x)$ has many locally minimal points. It also has some characteristics such as concave PF, nonlinear variable linkage, multimodal with Griewank function. If an element of solution x , sampled from MMEA-RA or RM-MEDA, is out of the boundary, we simply reset its value to a randomly selected value inside the boundary.

TABLE 1 : Test instance

Test case	Variables	Objectives
T1	$[0,1]^n \times [0,10]^{n-1}$	$f_1(x) = x_1$
		$f_2(x) = g(x)[1 - \sqrt{\frac{f_1(x)}{g(x)}}]$
		$g(x) = \frac{1}{4000} \sum_{i=2}^n (x_i^2 - x_1)^2 - \prod_{i=2}^n \cos\left(\frac{x_i^2 - x_1}{\sqrt{i-1}}\right) + 2$

The evolution of the average γ -metric of the non-dominated solutions for the test case is shown in Figure 7. It should be noted that the solutions of all three algorithms are stable when the iteration generation is more than 300. After the solutions are stable, the convergence values of the three algorithms are small than 0.1. Because we adopt the average of the minimum Euclidean distance of each solution from chosen solutions as the metric γ , the smaller the convergence values, the better the convergence metric. As is shown by Figure7, among the three algorithms, MEMA-RA has best convergence performance, NSGA-II and RM-MEDA follows.

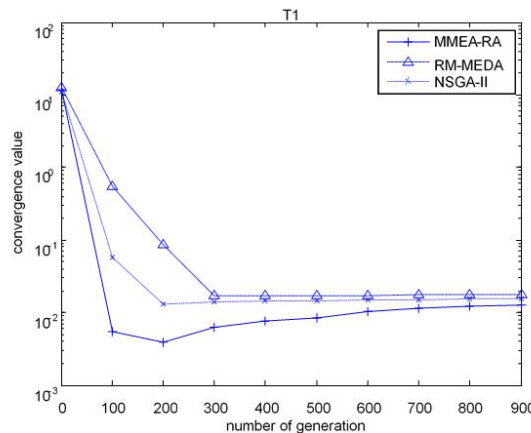


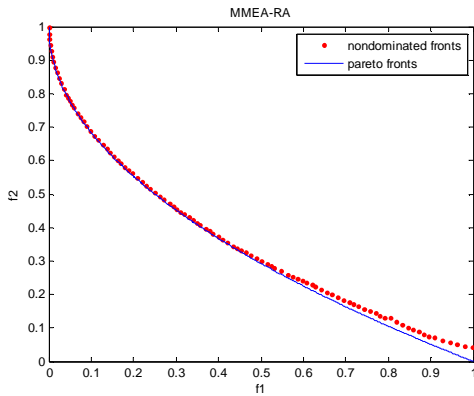
Figure 7 : The evolution of the average γ -metric of the nondominated solutions in three algorithms for T1

Figure 8 shows the final non-dominated solutions and fronts obtained by MMEA-RA on the test case. Figure 8(a) is the result with the lowest γ -metric obtained in 10 runs while Figure 8(b) is all the 10 fronts in 10 runs. It can be seen that the non-dominated fronts with the lowest γ -metric is very close to the Pareto front, especially when f_1 tends to 0 and f_2 tends to 1. It can also be noted that the non-dominated solutions in every run have some small fluctuations around the Pareto front.

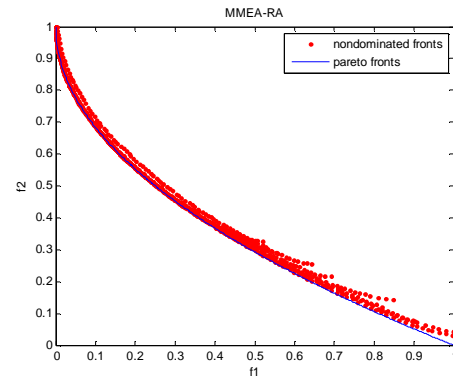
The final non-dominated solutions and fronts obtained by RM-MEDA on the test case are shown in Figure 9. Similarly, Figure 9(a) is the result with the lowest γ -metric obtained in 10 runs while Figure 9(b) gives all the 10 fronts in 10 runs. Similar to Figure8, the non-dominated solution (s) in Figure9(a) and Fib.9(b) are marked as the red. The pareto fronts are marked as the blue. The pareto fronts are given in Figure9(a) and Figure9(b) only for comparing the quality of the non-dominated solutions. It can be seen that the non-dominated front with the lowest γ -metric is very consistent with the Pareto front although there are some differences between them. Specially, it should be noted that all results in 10 runs from RM-MEDA match the Pareto front better than MMEA-RA. But it also should be noted that there is an isolated point in the non-dominated solutions for all 10 runs in Figure 9(b), maybe because RM-MEDA falls into a local minimum and could not jump out.

The final non-dominated solutions and fronts obtained by NSGA-II on the test case are shown in Figure 10. Again, Figure 10(a) means the result with the lowest γ -metric obtained in 10 runs and Figure 10(b) means all 10 fronts in 10 runs. As is shown in Figure 10(a), the non-dominated front with the lowest γ -metric is close to the Pareto front, but different to the result obtained by MMEA-RA. The non-dominated front with the lowest γ -metric in NSGA-II does not tend to the Pareto

front very close. It does also not match the Pareto front as good as the result obtained by RE-MEDA. Similarly, the non-dominated solutions in every run have some small fluctuations around the Pareto front.

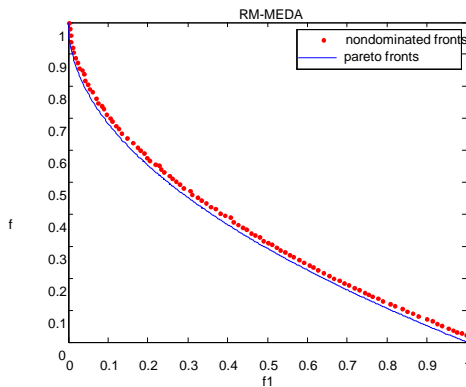


(a) the result with the lowest γ -metric

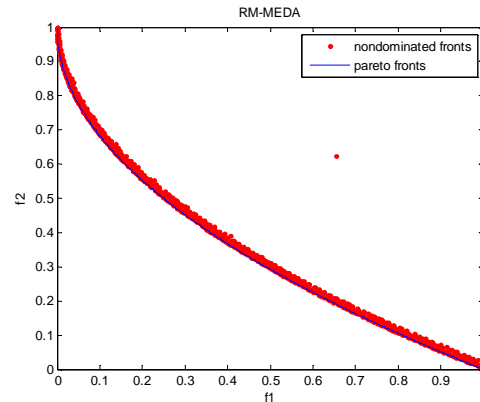


(b) all the 10 fronts in 10 runs

Figure 8 : The final non-dominated solutions and fronts found by MMEA-RA

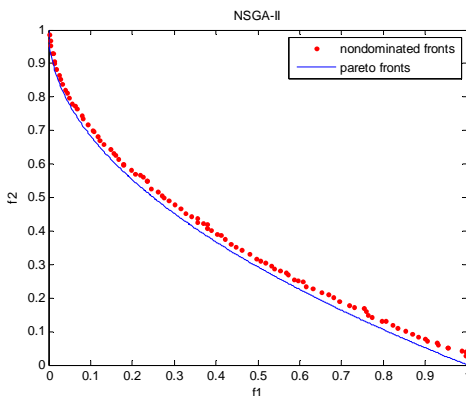


(a) The result with the lowest γ -metric

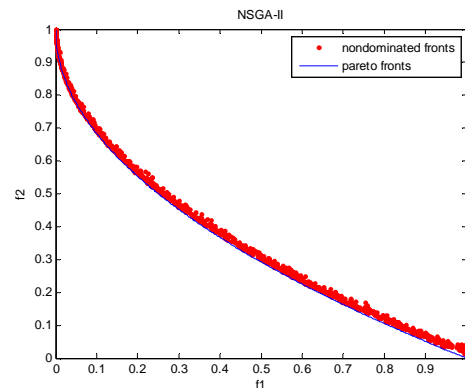


(b) all the 10 fronts in 10 runs

Figure 9 : The final non-dominated solutions and fronts found by RE-MEDA



(a) The result with the lowest γ -metric



(b) all the 10 fronts in 10 runs

Figure 10 : The final non-dominated solutions and fronts found by NSGA-II

The running time of the three algorithms are given in TABLE 2. From the point of the running time, as is shown in TABLE 2, among the three algorithms, NSGA-II is best, then MMEA-RA follows, and RM-MEDA is worst. This result is consistent with the main idea of the three algorithms. In RM-MEDA, local principal component analysis (PCA) is used to construct the model, and it need extra CPU time for running local PCA at each generation. In MMEA-RA, the least squares

method is used to construct the model, and it is easy to running the least squares by matrix computation. MMEA-RA is slower than NSGA-II because the selection in MMEA-RA is based on NSGA-II.

TABLE 2 : The compare of the running time (Unit:ms)

	NSGA-II	RM-MEDA	MEMA-RA
The running time	79.368	127.543	92.771

Obviously, it can be seen that the non-dominated front with the lowest γ -metric obtained by MMEA-RA is closest to the Pareto front in the three algorithms, which shows MMEA-RA is suitable to solve the problem with some characteristics such as concave PF, nonlinear variable linkage, multimodal with Griewank function. In contrast, the results in 10 runs from RM-MEDA mostly match the Pareto front, which shows the performance of RM-MEDA is good in common.

CONCLUSIONS

In this paper, a model-based multi-objective evolutionary algorithm based on regression analysis (MMEA-RA) is put forward to solve continuous multi-objective optimization problems with variable linkages. MMEA-RA models a promising area whose centroid is a complete and continuous curve described by the expression (8). Because of this feature, MMEA-RA does not need to cluster the population. The least squares approach is simple yet enough to describe the nonlinear principal curve using the polynomial model.

The less CPU time of MMEA-RA does not come without a price. MMEA-RA samples points uniformly around the PS in the decision variable space, and the centroid of the model is not piecewise but complete curve. This makes it very difficult for MMEA-RA to approximate the whole PF. The experimental results also reveal that MMEA-RA may fail in test instances with many local Pareto fronts.

The future research topics along this line should include the following points.

- (1) Designing an accurate model to describe the decision space. As the case of 3 objectives, the PS is a surface, so the expression (8) cannot solve the problems with 3 objectives right now.
- (2) Combining MMEA-RA with traditional genetic algorithms using operators such as crossover and mutation for accelerating the convergence of the algorithm.
- (3) Improving the method to calculate random noise value to make the final population more convergent.
- (4) Considering the distribution of the solutions in the objective space when sampling solutions from the models to improve the performance of MMEA-RA on the instance.
- (5) Incorporating effective global search techniques for scalar optimization into MMEA-RA in order to improve its ability for global search.

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