Performance Study of Mode-Pursuing Sampling Method

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Abstract

Since the publication of our recently developed mode-pursing sampling (MPS) method, questions have been asked on its performance as compared with traditional global optimization methods such as genetic algorithm (GA), and when to use MPS as opposed to GA. This work aims to provide an answer to these questions. Similarities and distinctions between MPS and GA are presented. Then MPS and GA are compared via testing with benchmark functions and practical engineering design problems. These problems can be categorized from different perspectives such as dimensionality, continuous / discrete variables, or the amount of computational time for evaluating the objective function. It is found that both MPS and GA demonstrate great effectiveness in identifying the global optimum. In general, MPS needs much less function evaluations and iterations than GA, which makes MPS suitable for expensive functions. But GA is more efficient than MPS for inexpensive functions. In addition, MPS is limited by the computer memory when the total number of sample points reaches a certain extent. This work serves a purpose of positioning the new MPS in the context of direct optimization and provides guidelines for users of MPS. It is also anticipated that the similarities in concepts, distinctions in philosophy and methodology, and effectiveness as direct search methods for both MPS and GA will inspire the development of new direct optimization methods.

Keywords: Mode-Pursuing Sampling, Genetic Algorithm, Global Optimization

1. Introduction

Practical engineering design problems are usually highly nonlinear and involve many continuous and/or discrete variables. Often it is difficult to define a design problem or to express it as a mathematical model. In addition, the increasingly wide use of finite element analysis (FEA) and computational fluid dynamics (CFD) tools brings new challenges to optimization. FEA and CFD simulations involve a large number of simultaneous equations and therefore are considered computationally expensive and also "black-box"

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functions. The gradients computed from FEA and CFD, which require extra computing resources, are often not reliable (Haftka *et al.* 1998). Therefore, it is difficult to apply traditional gradient-based optimization methods on these black-box functions, thereby inhibiting solutions of many practical design problems. Metamodeling based design optimizations (MBDO) have emerged as a promising solution for the expensive black-box problems. Its essence is to use a computationally simpler model to approximate the original expensive black-box model. This approximation is realized by sampling in the design space and performing model fitting for a chosen metamodel type. The metamodel can then be optimized. Current research in MBDO focuses on developing better sampling methods, approximation models, or the whole global optimization strategy (Wang and Shan 2007). Recently, Wang *et al.* (2004) developed a new Mode Pursuing Sampling based global optimization (MPS) method for black-box functions. Its discrete variable version was in (Sharif *et al.* 2008). In several applications (Wang *et al.* 2004, Sharif *et al.* 2008, Liao and Wang 2008), the MPS was found to be effective and efficient.

Genetic Algorithm (GA), on the other hand, has been widely used in engineering for global optimization (Goldberg 1989). The development of Genetic Algorithms (GA) was inspired by the principles of genetics and evolution. GA employs the principal of "survival of the fittest" in its search process to generate and select chromosomes (design solutions) composed of genes (design variables). Chromosomes that are more adaptive to their environment (design objectives/constraints) are more likely to be chosen. Over a number of generations (iterations), desirable traits (design characteristics) will evolve and remain in the population (set of design solutions generated at each iteration). GA begins its search from a randomly generated population of design. Three operators are often used to propagate the populations from one generation to another to search for the optimum solution, namely, selection, crossover, and mutation. GA can be used for problems that are not well-defined, difficult to model mathematically, or black-box. It can also be used when the objective function is discontinuous, highly nonlinear, stochastic, or it has unreliable or undefined derivatives. The limitation of GA is that it usually demands a large number of function evaluations.

When analyzing the performance of MPS, it is found that there are many similarities between GA and MPS: (1) the initial population is randomly created in GA and the sampling points are randomly generated in MPS; (2) in GA, the chromosomes are chosen by a stochastic process and the probability of a chromosome to be selected is determined by its fitness value, while in MPS, the points are sampled according to a probability determined by its objective function value; (3) both GA and MPS are based on a set of solutions, or population, and render themselves well suited for parallel computation; (4) both methods use no gradient information and thus are called derivative-free methods, or direct methods.

The distinctions between GA and MPS are also manifold. First they are based on different philosophies. GA has its root in evolutionary processes, while MPS is based on "discriminative" sampling. Second, GA explores the space through operations of genes; it is intuitively a bottom-up approach from the perspective of exploring the entire design space. On the other hand, MPS is like a top-down approach as the entire space is explored at every iteration. Specific similarities and distinctions between the two methods are summarized in Table 1.

Table 1 Comparison of features of GA and MPS algorithms

		GA	**MPS**
Similarities	Mechanism	Generate more points around current best point; Uses probability in searching/sampling; Statistically cover the entire design space	
	Features	Random process; Derivative free; Population-based search	
	Capabilities	Perform a "global" optimization; Supporting parallel computation	
Distinctions	For discrete problem	Discrete in nature; Easily handle continuous problems	Needs different treatments for continuous and discrete problems
	Input parameters	Many parameters are set by the user, e.g. population size, reproduction operators, crossover probability, and mutation probability. The parameters are problem dependent and could be sensitive.	Fewer parameters need to be changed and not very sensitive.
	Efficiency	Normally a large number of function evaluations needed.	Developed specially for expensive functions to minimize the number of function evaluations
	Form of function values	Usually coded form of the function values rather than the actual values	Actual function values
	Robustness	Premature convergence may happen if the operators are not set properly.	For the problems with a large quantity of local optima, it may be trapped in a local optimum.

To better understand the performance and the problems that most amenable to MPS, this work studies the performance of MPS in parallel with GA. The selection GA is because of the similarities between the two algorithms and because GA is well-known and widely used by practitioners, which makes the performance study of MPS more relevant to real practice. The main purpose is thus to position MPS in the context of engineering global optimization in order to provide some guidelines for MPS users. The comparison between MPS and GA is thus not to determine which algorithm is the winner, but rather to shed lights on characteristics and performance behaviour of MPS in reference to GA.

2. Overview of MPS

MPS entails its continuous variable version, C-MPS (Wang *et al.* 2004), and its discrete variable version D-MPS (Sharif *et al*. 2008). This overview will focus on its original continuous-variable version, and provide a brief description of the new discrete-variable version.

2.1 Continuous-variable Mode-Pursuing Sampling (C-MPS) Method

The essence of MPS is the integration of metamodeling and a novel discriminative sampling method, which generates more sample points in the neighbourhood of the function mode (local optimal) and fewer points in other areas as guided by a special sampling guidance function.

Fundamental to MPS is the Fu and Wang's algorithm (Fu and Wang 2002), which is used to generate a sample of an asymptotic distribution of a given Probability Density Function (PDF). Given a *d*-dimensional PDF $g(x)$ with compact support $S(g) \subset \Re^d$, Fu and Wang's algorithm (Fu and Wang 2002) consists of three steps. In the first step, the discretization step, a discrete space $S_N(g)$ is generated consisting of N uniformly distributed base points in $S(g)$. Usually N is large and should be larger if the dimension of $g(x)$, d, is higher. These uniform base points may be generated using either deterministic or stochastic procedures. In the second step, the contourization step, the base points of $S_N(g)$ are grouped into K contours $\{E_1, E_2, \ldots, E_K\}$ with equal size according to the relative height of the function $g(x)$. For example, the first contour E_1 contains the $[N/K]$ points having the highest function values among all base points, whereas the last contour E_K contains the $[N/K]$ points having the lowest function values. Also in this step, a discrete distribution $\{P_1, P_2, \ldots, P_K\}$ over the K contours is constructed, which is proportional to the average function values of the contours. Finally, a sample is drawn from the set of all base points $S_N(g)$ according to the discrete distribution $\{P_1, P_2, \ldots, P_K\}$ and the discrete uniform distribution within each contour. As has been shown in the reference (Fu and Wang 2002), the sample drawn according to their algorithm is independent and has an asymptotic distribution $g(x)$. The approximation gets better for larger values of N and K.

For optimization, we wish to minimize an n-dimensional black-box function $f(x)$ over a compact set $S(f) \subset \Re^n$. Following the convention of engineering optimization, we refer to the minimum as the function mode. To simplify notation, assume that $S(f) = [a, b]^n$, where $-\infty < a < b < \infty$ are known, and

$f(x)$ is positive on $S(f)$ and continuous in a neighbourhood of the global minimum. In general, if $f(x)$ is negative for some $x \in S(f)$, then we can always add a positive number to $f(x)$, so that it becomes positive on $S(f)$. Note that minimizing $f(x)$ is equivalent to maximizing $-f(x)$. The MPS algorithm consists of the following four steps:

Step 1. Generate m initial points $x^{(1)}, x^{(2)}, ..., x^{(m)}$ that are uniformly distributed on $S(f)$ (m is usually small).

Step 2. Use the m function values $f(x^{(1)}), f(x^{(2)}),\ldots, f(x^{(m)})$ to fit a linear spline function

$$\hat{f}(x) = \sum_{i=1}^{m} \alpha_i \, \| x - x^{(i)} \|, \qquad \textbf{(1)}$$

such that $\hat{f}(x^{(i)}) = f(x^{(i)})$, $i = 1, 2,\ldots, m$, where $\| \bullet \|$ stands for the Euclidean norm.

Step 3. Define $g(x) = c_0 - \hat{f}(x)$, where c_0 is any constant such that $c_0 \geq \hat{f}(x)$, for all x in $S(f)$. Since $g(x)$ is nonnegative on $S(f)$, it can be viewed as a PDF, up to a normalizing constant, whose modes are located at those $x^{(i)}$'s where the function values are the lowest among $\{f(x^{(i)})\}$. Then apply the sampling algorithm of Fu and Wang [7] to draw a random sample $x^{(m+1)}, x^{(m+2)}, \ldots, x^{(2m)}$ from $S(f)$ according to $g(x)$. These sample points have the tendency to concentrate about the maximum of $g(x)$, which corresponds to the minimum of $\hat{f}(x)$.

Step 4. Combine the sample points obtained in Step 3 with the initial points in Step 1 to form the set $x^{(1)}, x^{(2)}, ..., x^{(2m)}$ and repeat Steps 2–3 until a certain stopping criterion is met.

For ease of understanding, the MPS method is illustrated with the well-known six-hump camel-back (SC) problem (Branin and Hoo 1972). The mathematical expression of SC is

$$f_{sc}(x) = 4x_1^2 - \frac{21}{10}x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4, \, (x_1, x_2) \in [-2,\ 2]^2 . \qquad \textbf{(2)}$$

A contour plot of the SC function is shown in Figure 1, where the H's represent local optima. H_2 and H_5 are two global optima at points (-0.090, 0.713) and (0.090, -0.713), respectively, with an equal function value $f_{\min} = -1.032$.

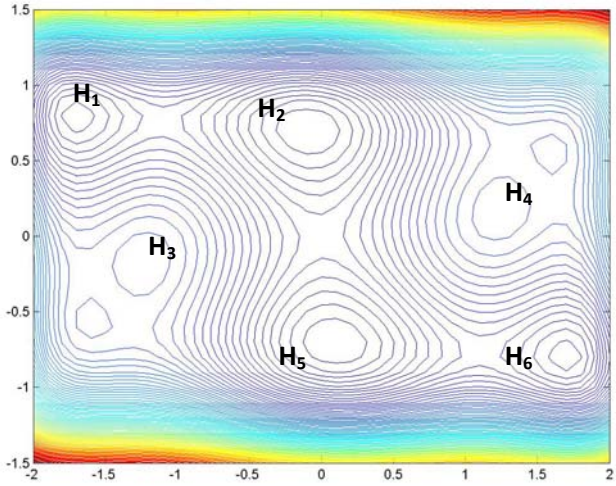


Figure 1 Contour plot of the SC function.

In the first step of the MPS algorithm, we start with $m = 6$ initial random points $x^{(1)}, x^{(2)}, \ldots, x^{(6)} \in [-2,\ 2]^2$. Then $\hat{f}(x)$ is computed by fitting Eq. 1 to $f(x^{(1)}), f(x^{(2)}), \ldots, f(x^{(6)})$. Further, the function $g(x)$ is obtained by using the maximum of $\{f(x^{(i)}),\ i=1,\ \ldots,\ 6\}$ as c_0.

Now Fu and Wang's algorithm is applied to draw a sample as follows. First, $N = 10^4$ uniformly distributed base points are generated to form $S_M(g)$, the discretized version of the sample space $[-2,\ 2]^2$. Note that the base points in $S_N(g)$ are cheap points, in contrast to the original $m = 6$ expensive points used to build $\hat{f}(x)$. Further, without loss of generality, suppose the points in $S_N(g)$ are sorted in ascending order of the values of function $\hat{f}(x)$. The sequence of corresponding function values of $\hat{f}(x)$ is plotted in Figure 2(a), whereas the function $g(x)$ is plotted in Figure 2(b).

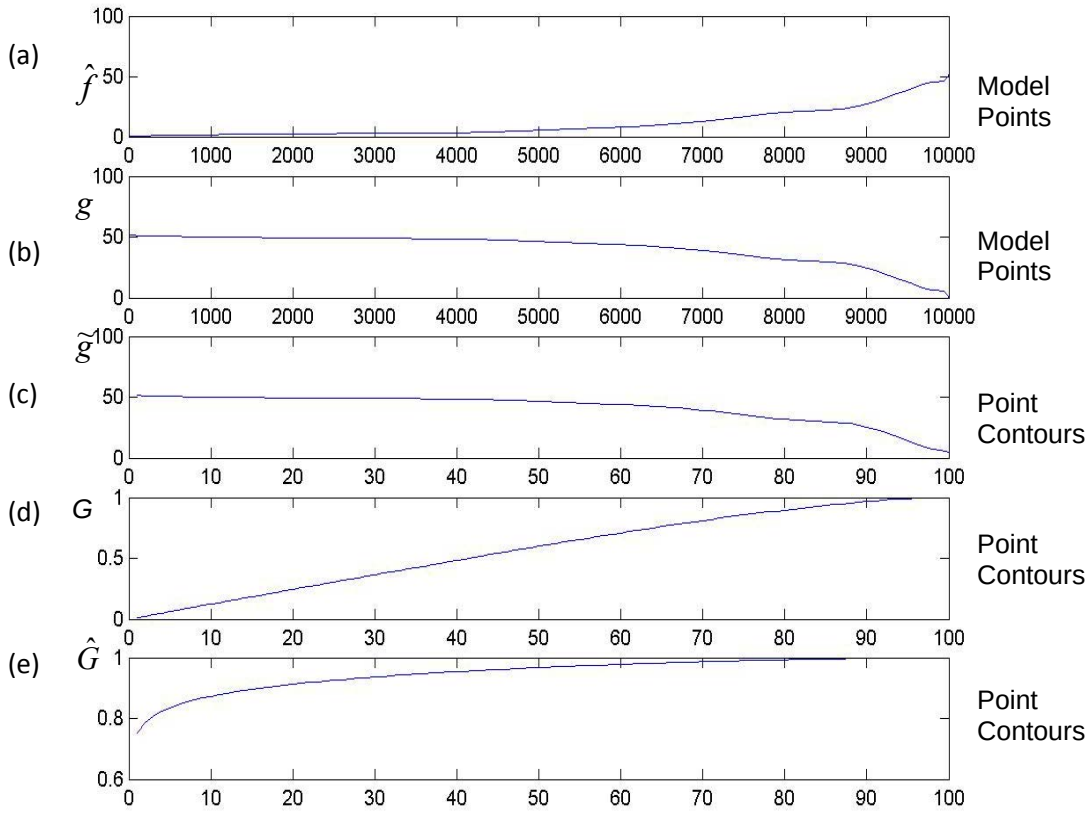


Figure 2 A screen shot of ranked point distribution of $\hat{f}$, g, $\tilde{g}$, G and $\hat{G}$ for the SC problem.

According to Fu and Wang's method (Fu and Wang 2002), the ordered 10^4 base points are grouped into $K = 10^2$ contours $\{E_1, E_2, \ldots, E_{100}\}$, with each having $N/K = 100$ points. For example, the first contour E_1 contains the 100 points at which the values of function $\hat{f}(x)$ are the lowest, whereas the last contour E_{100} contains the 100 points at which the values of $\hat{f}(x)$ are the highest. Let $\tilde{g}(i)$ be the average of $g(x)$ over E_i, $i = 1, 2, \ldots, 100$. The function $\tilde{g}(i)$, $i = 1, 2, \ldots, 100$ is plotted in Figure 2(c) and its cumulative distribution function $G(i)$ is displayed in Figure 2(d).

Finally, $m = 6$ contours are drawn with replacement according to distribution $\{G(i)\}$ and, if the contour E_i occurs $m_i > 0$ times in these draws, then m_i points are randomly drawn from E_i. All such points form the new sample $x^{(m+1)}, x^{(m+2)}, \ldots, x^{(2m)}$.

As one can see from Figure 2(d), the contours from E_{80}~E_{100} (corresponding to high $\hat{f}$ values) have lower selection probabilities for further sampling than other contours, since the G curve is relatively flat

in this area. However, such a probability for each contour is always larger than zero. On the other hand, it is generally desired to increase the probability of the first few contours as they correspond to low $\hat{f}$ values. To better control the sampling process, a speed control factor is introduced [3]. Figure 2(e) shows $\{\widehat{G}(i)\}$, which is obtained by applying the speed control factor to $\{G(i)\}$ in Figure 2(d). From Figure 2(e), one can see that the first few contours have high selection probabilities for next-step sampling, while the contours from E_{40} ~E_{100} have low probabilities. This curve shows an aggressive sampling step, as many more new sample points are close to the current minimum of $f(x)$ as compared to the sampling based on Figure 2(d).

The whole procedure is repeated eight times, so that a total of 48 sample points are generated. Figure 3 shows these 48 sample points, where the circles indicate attractive design points having a function value less than –0.5. Even with only 48 sample points, many attractive points have already shown up around H_2 and H_5. It can also be seen that points spread out in the design space with a high density around function mode H_2 (global minimum). In the mode-pursuing sampling step, every point has a positive probability of being drawn, so that the probability of excluding the global optimum is zero. As the iteration process continues, more and more sample points will be generated around the minimum of function $f(x)$.

2.2 Discrete-variable MPS (D-MPS)

D-MPS inherits the metamodeling and discriminative sampling ideas from C-MPS. For the discrete variable space, sample points are mapped from a continuous space to the discrete variable space. The main difference between C-MPS and D-MPS lies on their convergence strategies.

In C-MPS (Wang *et al.* 2004), a local quadratic metamodel is employed to adaptively identify a sub-area, with which a local optimization is called to search for the local optimum. For a discrete variable space, there lacks of a continuous sub-area to be approximated. Even if one could build a continuous function in a discrete space, the local optimum on a continuous function might not be a valid or optimal solution in the discrete space. Therefore the local quadratic metamodeling does not apply to discrete variable optimization problems.

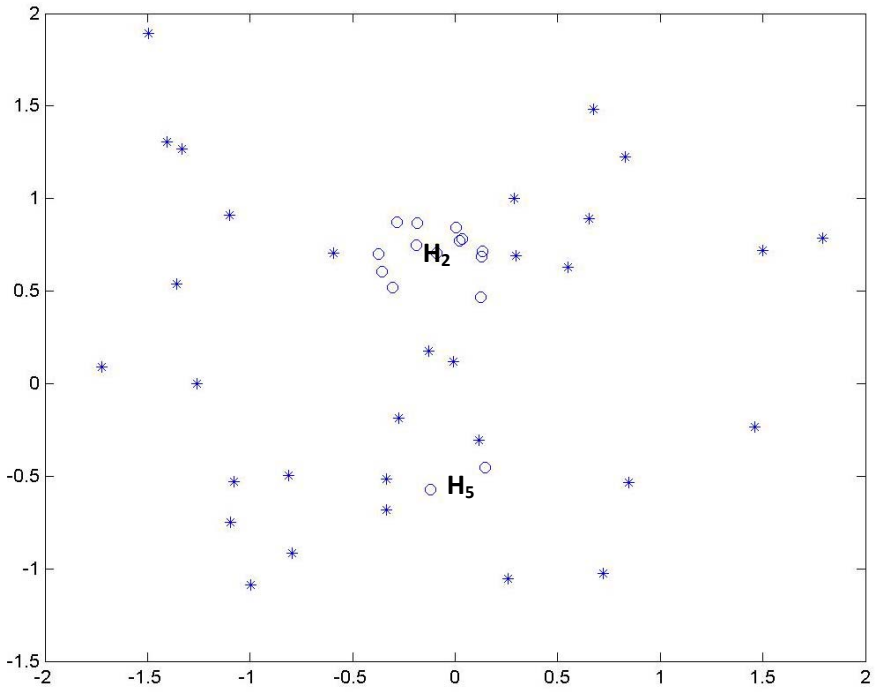


Figure 3 Sample points of the SC problem generated by the MPS method, where "o" indicates its function value less than –0.5; and H_2 and H_5 are the locations of two global optima.

For the discrete problems, a "Double Sphere" method is used. This method includes two areas (or "spheres") of dynamically changing radius. One sphere controls the "exploration," and the other controls "exploitation." Recall that the C-MPS is composed of three main steps, i.e., generating cheap points, approximation, and discriminative sampling. In D-MPS, these main steps will be performed on the domains provided by the double-sphere. For the objective function $f(x)$ on domain $S[f]$, the double-sphere strategy dynamically provides a domain $D_1 \cup D_2 \subset S[f]$; D_1 is the domain inside the smaller hyper-sphere; and D_2 is the domain between the smaller hyper-sphere and bigger hyper-sphere. The three main steps of D-MPS are performed on both D_1 and D_2. The discriminative sampling is performed independently in the two spheres until the optimum is found or the maximum number of iterations is reached. D-MPS thus does not call any existing local optimization routine and there is no local metamodeling. The optimum is found by sampling alone (Sharif *et al.* 2008).

3. Testing functions and problems

Given the focus on examining the performance of MPS, in this work a real-value GA is employed. The implementation from Ref. (Houck *et al.* 1995) is selected for a number of reasons. First, this implementation has commonly-used operators and it demonstrates good performance. Second, it is based on Matlab™, which renders a common basis for computational cost (CPU time) comparisons because MPS is also based on Matlab™. Last, since there exists a large number of GA implementations and algorithms, this work is not intended to draw any general conclusion in regard to GA as a whole. It is intended to obtain certain qualitative insights into MPS and provide guidelines to users of MPS, which should largely be insensitive to the choice of specific GA implementation.

The selected implementation (Houck *et al.* 1995) forces the design variable to only take values within its upper and lower bounds to ensure the feasibility of solutions. It uses three selection operators, namely, the normGeom selection (a ranking selection based on the normalized geometric distribution), the roulette selection (a traditional selection with the probability of surviving equal to the fitness of an individual over the sum of the fitness of all), and the tournament selection (choosing the winner of the tournaments as the new population). It also has three crossover operators, namely, the simple crossover, the heuristic crossover, and the arithmetic crossover. Finally, it uses four optional mutation operators, called the boundary mutation, multi-non-uniform mutation, non-uniform mutation, and uniform mutation. Details of these operators are in the reference (Houck *et al.* 1995). Two termination criteria are used in the GA implementation. The first is based on the maximum number of generations, which is suitable for problems without knowing the analytical optimum *a priori*. The second termination criterion occurs when the analytical optimum is reached. The GA optimization process will be terminated whenever one of these two criteria is met. For constrained optimization problems, the discard method was used in order to satisfy the constraints. Three constraint checks are performed on the initial population, with new children generated from crossover, as well as from mutation operations at each iteration. Any chromosome that does not pass the constraint check will be discarded from the population. For discrete variable problems, if all of the variables are integers, a simple rounding function is used to round a number to its closest integer. If the discrete variable values are picked from a set, for example, $x \in [16.2, 17.1, 18.5, 19.3]$, we first index the possible values, e.g., index = {1， 2，3，4}, and then generate a random number and round it to the closest index. For example, if index=3, then we use x=18.5. For mixed-variable problems, only the discrete variables are handled as described above.

Nine problems are tested for a performance comparison of the chosen GA implementation and MPS optimization algorithms. The characteristics of these problems are summarized in Table 2. In Table 2, only optimization problems with constraints other than bounds are referred as constrained problems.

Table 2 Characteristics of test functions and problems.

Function (*n*: number of variables)	**Characteristics**
Six-hump camel-back (SC) (*n*=2)	Multiple local optima
Corana (CO) function (*n*=2)	Flat bottom, multiple local optima
Hartman (HN) function (*n*=6)	Multiple local optima
Gear train (GT) problem (*n*=4)	Discrete, multiple local optima
A high dimensional function (F16) (*n*=16)	High dimension
Rosenbrock function (R10) (*n*=10)	Flat bottom, relatively high dimension, multiple local optima
Insulation layer (IL) design (*n*=2)	Constrained Engineering Problem
Pressure vessel (PV) design (*n*=4)	Constrained Engineering Problem
Fixture and joining position design (FJP) (*n*=4)	Constrained, expensive, black-box function

As one can see from Table 2, the test functions and problems present different challenges to the optimization algorithms. This section briefly describes each test problem.

- Six-hump camel-back (SC) problem

The SC problem is a well-known benchmark test problem. It appears early in Ref. (Branin and Hoo 1972) and it was used by many other researchers. The mathematical expression is shown in Eq. (2). The SC function has six local optima. A contour plot of the SC function is shown in Figure 1.

- The Corana (CO) function

The Corana function is a well known benchmark test function (Corana *et al.* 1987). It was also tested in Ref. (Humphrey and Wilson 2000). The Corana function is a paraboloid with axes parallel to the coordinate direction, except a set of open, disjoint, rectangular flat "pockets". Let the domain of the function $f(x)$ in an *n*-dimensional space be:

$$D_f \equiv \{x \in R^n : -a_i \le x_i \le a_i; a_i \in R_+^n, i = 1,2,.....n\}$$

Let D_m represent the set of "pockets" in D_f:

$$d_{k_1,.....,k_n} = \{x \in D_f : k_i s_i - t_i < x_i < k_i s_i + t_i; k_i \in Z; t_i, s_i \in R_+^n; t_i < \frac{s_i}{2}, i = 1,2,.....n\}$$

$$D_m = \bigcup_{k1,.....,kn} d_{k_1 \cdots, k_n} - d_{0,0,.....,0.}$$

The Corana function can then be defined as:

$$f(x) = \begin{cases} \sum_1^n d_i x_i^2, x \in D_f - D_m, d_i \in R_+^n \\ c_r \sum d_i z_i^2, x \in d_{k_1,....,k_n}, (k_1,....,k_n) \neq 0 \end{cases} \quad \textbf{(3)}$$

where $$z_i = \begin{cases} k_i s_i + t_i & , \quad k_i < 0 \\ 0 & , \quad k_i = 0 \\ k_i s_i - t_i & , \quad k_i > 0 \end{cases}$$

The parameters in this test are set to n=4, $a_i = 100, s_i = 0.2, t_i = 0.05, c_r = 0.15, d_i = e^{(i-1)}$. A less extreme weight d_i is used as compared to the standard representation, $10^{(i-1)}$. The searching space is $x_i \in$ [-100, 100]. The four-dimensional Corana function has its global minimum f^*=0 at x^*=(0, 0, 0, 0). A difficulty arises from the fact that the optimum is located in a deep valley, and several deep flat bottoms exist along the space. Figure 4 shows a 2-D Corana function in the range of [-0.5, 0.5].

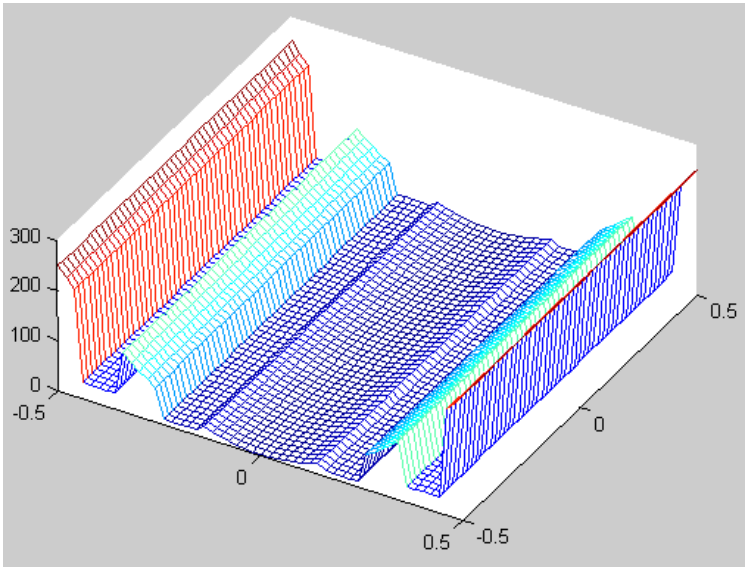


Figure 4 2-D corana function in [-0.5, 0.5]

- Hartman (HN) function

The Hartman function with n=6 was tested in Ref. [3]. It can be expressed as

$$f_{HN}(x) = -\sum_{i=1}^{4} c_i \exp\left[-\sum_{j=1}^{n} \alpha_{ij} (x_j - p_{ij})^2 \right], \; x_i \in [0,1], i = 1,...,n \quad \textbf{(4)}$$

where α_{ij} and p_{ij} are listed below.

i	α_{ij} , j=1,...,6						c_i
1	10	3	17	3.5	1.7	8	1
2	0.05	10	17	0.1	8	14	1.2
3	3	3.5	1.7	10	17	8	3
4	17	8	0.05	10	0.1	14	3.2

i	p_{ij}, j=1,...,6					
1	0.1312	0.1696	0.5569	0.0124	0.8283	0.5886
2	0.2329	0.4135	0.8307	0.3736	0.1004	0.9991
3	0.2348	0.1451	0.3522	0.2883	0.3047	0.6650
4	0.4047	0.8828	0.8732	0.5743	0.1091	0.0381

- Compound gear train (GT) design problem

This is a discrete variant problem involving a compound gear train design (Fu *et al.* 1991, Cai and Thierauf 1996), as shown in Figure 5. It is desired to produce a gear ratio as close as possible to 1/6.931. For each gear, the number of teeth must be an integer between 14 and 60. The integer design variables are the numbers of teeth, x=[T_d, T_b, T_a, T_f]^T=[x_1, x_2, x_3, x_4]^T. The optimization problem is formulated as:

$$\textbf{Minimize} \quad GT(X) = \left(\frac{1}{6.931} - \frac{x_1 x_2}{x_3 x_4} \right)^2 \quad \textbf{(5)}$$

Subject to

$$14 \le x_i \le 60, \quad i = 1,2,3,4$$

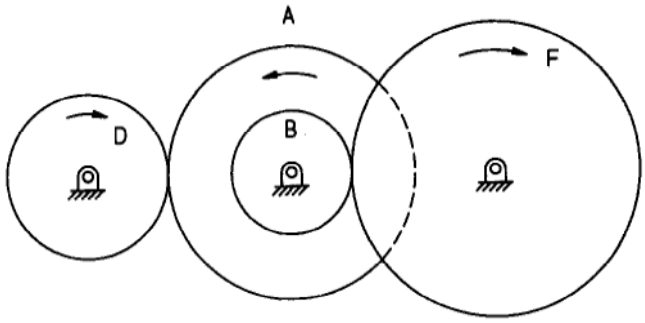


Figure 5 Compound gear train

- A function of 16 variables (F16)

This high dimensional problem was described in Ref. (Wang *et al.* 2004). It can be expressed by

$$f_{F16}(x) = \sum_{i=1}^{16}\sum_{j=1}^{16} a_{ij}(x_i^2 + x_i + 1)(x_j^2 + x_j + 1), \; i, j = 1, 2, \ldots, 16, \tag{6}$$

$$[a_{ij}]_{\text{row 1–8}} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \; [a_{ij}]_{\text{row 9–16}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

- Ten-dimensional Rosenbrock function (R10)

The Rosenbrock function is a widely used benchmark problem for testing optimization algorithms such as Refs. (Bouvry *et al.* 2000, Augugliaro *et al.* 2002). It can be expressed as

$$f_{RO}(x) = \sum_{i=1}^{n-1}(100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2) \tag{7}$$

The Rosenbrock function has its global minimum $f_{\min}$ =0 at x^*= (1,1…,1). While attempting to find a global minimum, a difficulty arises from the fact that the optimum is located in a deep parabolic valley with a flat bottom. In the present study, the 10-dimensional Rosenbrock function will be used as another high dimensional benchmark problem, in addition to F16. The searching range for each variable is [-5, 5].

- Two layer insulation design (IL) problem

This is a problem involving the design of a two-layer insulated steam pipe line, as shown in Figure 6. The objective is to design r_1 and r_2 to minimize the total cost per unit length of pipe ($/m) in one year of

operation. The total cost function includes the cost of heat loss, the cost of insulation materials, and the cost of fixed charges including interest and depreciation (with a rate of 15%). The parameters in the design are (1) Inner radius r_0= 273mm, (2) Steam temperature T_f= 400 deg. C, and the temperature of the ambient air T_a=25 deg. C, (3) The conductive resistance through the wall is neglected, (4) The convective heat transfer rate at the inner surface has h_f=55W/m^{2}K, (5) The first layer of insulation is rock wool, with a thermal conductivity k_1=0.06W/mK and thickness $\delta_1 = r_1 - r_0$, (6) The second insulation layer is calcium silicate with k_2=0.051W/mK and thickness of $\delta_2 = r_2 - r_1$, (7) The outside convective heat transfer coefficient is h_0=10W/m^{2}K, (8) The cost of heat is C_h=0.02\$/kWh; cost of rock wool, C_{i1}=146.7\$/m^3; cost of calcium silicate C_{i2}=336\$/m^3. The constraints are determined by the insulation requirement and other practical considerations, which are described in Ref. (Zaki and Al-Turki 2000).

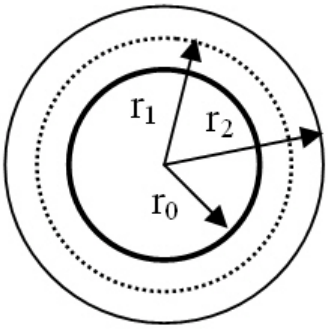


Figure 6 A steam pipe with two-layer insulation

The total cost per unit length of pipe can be expressed as:

Minimize

$$f_{IL}(r_1, r_2) = \tau C_h \frac{0.001(T_f - T_a)}{\frac{1}{2\pi r_0 h_f} + \frac{\ln(r_1/r_0)}{2\pi k_1} + \frac{\ln(r_2/r_1)}{2\pi k_2} + \frac{1}{2\pi r_2 h_o}} + f\pi\left[C_{i_1}(r_1^2 - r_0^2) + C_{i_2}(r_2^2 - r_1^2)\right] \quad \textbf{(8)}$$

Subject to:

$$38\text{mm} < \delta < 5r_0;\ r_1 > r_0\ ;\ r_2 > r_1;\ T_a + \frac{(T_f - T_a)}{\frac{1}{2\pi r_0 h_f} + \frac{\ln(r_1/r_0)}{2\pi k_1} + \frac{\ln(r_2/r_1)}{2\pi k_2} + \frac{1}{2\pi r_2 h_o}} \frac{1}{2\pi r_2 h_o} < 60 \quad \textbf{(9)}$$

The characteristic of this problem is its complexity in both the objective function and the last constraint. The optimum solution is f^*= 5.5362\$/m, at r_1=0.311m and r_2=0.349m.

- Pressure vessel design (PV) problem

The design of a pressure vessel was used as a test problem in Ref. (Wang *et al.* 2004) and it is shown in Figure 7. There are four design variables: radius, R, and length, L, of the cylindrical shell, shell thickness, T_s, and spherical head thickness, T_h, all of which are in inches. They have the following ranges of interest: $25 \le R \le 150$, $1.0 \le T_s \le 1.375$, $25 \le L \le 240$, and $0.625 \le T_h \le 1.0$.

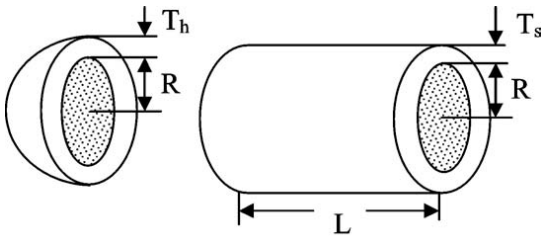


Figure 7 Pressure vessel (adapted from Ref. (Wang *et al.* 2004))

The design objective is to minimize the total system cost, which is a combination of welding, material and forming costs. The optimization model is then expressed as:

$$\textbf{Minimize} \quad f_{PV}(R, T_s, T_h, L) = 0.6224 T_s R L + 1.7781 T_h R^2 + 3.1661 T_s^2 L + 19.84 T_s^2 R \qquad \textbf{(10)}$$

$$\textbf{Subject to:} \quad Ts - 0.0193 \ge 0\,; \; Th - 0.00954 R \ge 0\,; \; \pi R^2 L + \frac{4}{3}\pi R^3 - 1.296E6 \ge 0 \qquad \textbf{(11)}$$

The optimum continuous solution is $f^* = 7006.8$, occurring at $R^*= 51.814$ in., $T_s = 1.0$ in., $L^*=84.579$in., and $T_h^*=0.625$in.

- Fixture and joining positions (FJP) optimization problem

Simultaneous optimization of fixture and joining positions for a non-rigid sheet metal assembly was studied by Liao and Wang (2008). This is a black-box function problem involving finite element analysis, which makes it computationally expensive. The optimization problem can be described as follows. In the presence of part variation and fixture variation, as well as the constrains from the assembly process and designed function requirements, find the best locations of fixtures and joining points so that the non-rigid sheet metal assembly can achieve the minimal assembly variation. An assembly of two identical flat sheet metal components by lap joints shown in Figure 8 is optimized. Assuming that these two components are manufactured under the same conditions, their fabrication variations are expected to be the same. The size of each flat sheet metal part is 100×100×1mm, with Young's modulus E = 2.62e+9 N/mm^2, and Poison's ratio v = 0.3. The finite element computational model of the assembly is created in ANSYS^{TM}. The

element type is SHELL63. The number of elements and the number of nodes are 1250 and 1352, respectively.

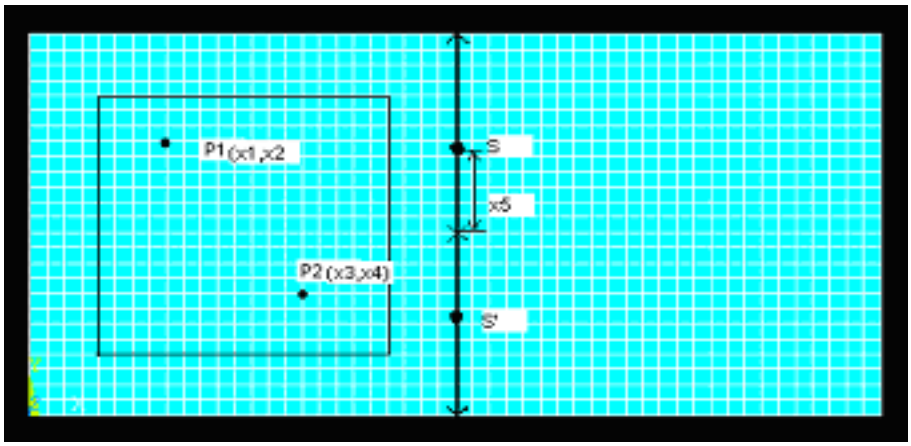


Figure 8 An assembly of two sheet metal parts

(note: The symbol 'p' indicates the fixture location and 's' indicates the joint positions)

The mathematical optimization model for this specific example can be written as follows,

$$\textbf{Minimize} \quad \Theta(x) = abs(U_z^1(x)) + abs(U_z^2(x)) \tag{12}$$

$$\textbf{Subject to} \quad (x_1\text{-}x_3)^2 + (x_2\text{-}x_4)^2 \geq 100;\ \ 20 \leq x_1, x_2, x_3, x_4 \leq 80;\ \ 10 \leq x_5 \leq 40 \tag{13}$$

where U is the deformation of critical points in an assembly. It is obtained by modeling the assembly deformation using the finite element analysis through ANSYS™. In this study, ANSYS™ and Matlab™ are integrated to implement the optimization on a FEA process for both MPS and GA.

4. Results and discussions

4.1 Performance criteria

Two main performance criteria are used to evaluate the two algorithms, namely effectiveness and efficiency. The effectiveness includes the robustness of the algorithm and the accuracy of the identified global optimum. For robustness, 10 independent runs are carried out for each problem and each algorithm, except for the expensive FJP problem, where only 5 runs are performed. The range of variation and median value of the optima are recorded and compared against the analytical or known optimum. If the known solution of a problem is not zero, the accuracy of an algorithm is quantified by

$$Q_{sol} = 1 - \left| \frac{solution - known\ \ solution}{known\ \ solution} \right| \tag{14}$$

If the known solution is zero, the deviation of the solution from zero is examined. When there is no analytical or known optimum, the optima found by GA and MPS are compared by the values. The second criterion for comparison is efficiency. In this study, the efficiency of an algorithm in solving a problem is evaluated by the number of iterations, *nit*, and number of function evaluations, *nfe*, as well as the CPU time required to solve the problem. Again, the average (arithmetic mean) and median values of these values in 10 (or 5) runs are used.

4.2 Effects of tuning parameters

As discussed previously, there are several optimization operators to be set in the GA program. In testing the same problems, these factors were found to have significant effects on the efficiency. Figure 9 shows the variation of GA performance under different crossover rates, *Pc*, when solving the SC function (with a population size of 100 and a mutation rate of *Pm*=0.01). A general trend can be observed in Figure 9, whereby increasing *Pc* implies that the number of function evaluations, *nfe*, increases and the number of iterations, *nit*, decreases, while the computation time remains at a similar level. With a small *Pc*, the GA needs more generations to establish the optimum, therefore more iterations are needed. When *Pc* is set to be very large, *nfe* increases sharply because almost all parents are replaced and few good solutions are inherited.

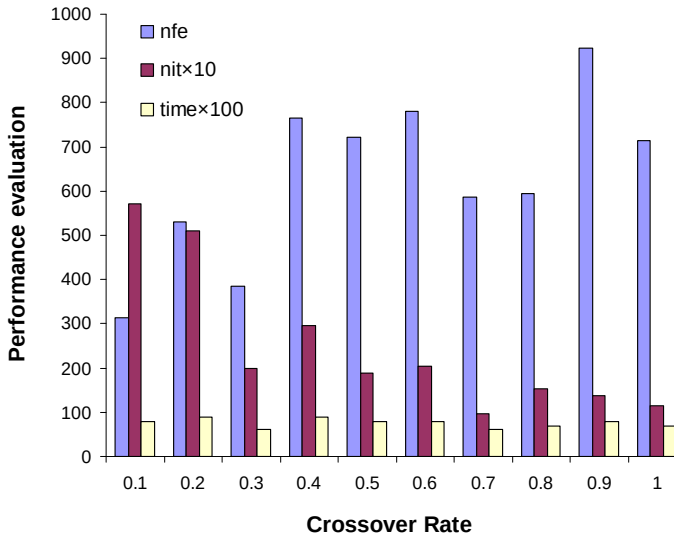


Figure 9 Performance evaluation with different crossover rates in solving the SC problem.

Similarly, the effect of mutation rate, *Pm*, on GA's performance in solving the SC problem (with a population size of 100 and crossover rate of *Pc*=0.6) is studied. It is observed that the minimum of *nfe* occurs at *Pm*=0.1 and *nfe* increases with *Pm*>0.1.

In the MPS program, there is a tuneable parameter (difference coefficient, *k*), which was also found to have noticeable effect on performance of the MPS. The difference coefficient, *k*, (denoted as c_d in Ref. [3]) is used for a convergence check in a quadratic model detection. A smaller difference coefficient makes the MPS have a more accurate solution, but it may cause more computational expense, as shown in Table 3. By examining the MPS performance in several problems in this study, it is found that *k*=0.01 is a good choice for most problems. However, for the discrete GT problem and the R10 problem, a larger coefficient (*k* > 0.5) must be used to establish an acceptable solution.

Table 3 Efficiency of MPS with different *k* values on the SC and PV problems

SC problem

Coefficient, *k*	Average CPU time (s)	average of *nit*	Average of *nfe*
0.001	15.3531	17.9	67.1
0.01	4.6312	9.6	34.7
0.1	3.5311	6.9	27.8

PV problem

Coefficient, *k*	Average CPU time (s)	Average of *nit*	Average of *nfe*
0.001	46.6891	8.8	51.8
0.01	26.2938	5.2	37.2
0.1	31.2279	5.8	39.9

Both the random characteristic and the effects of their tuning parameters necessitate the method of using results of multiple runs in this comparison study. Specifically for the comparison in this work, we used crossover rates of 0.6 or 0.7, mutation rates of 0.05 or 0.1 for GA. For MPS, we used the difference coefficient of 0.01 for most problems but a coefficient larger than 0.5 for the GT problem and the R10

problem. For both MPS and GA, different combinations of parameters for a problem are first tested; and the set of parameters that yields the best solution is then used for comparison. Hence for each test problem, the best results of GA are compared with the best results of MPS.

4.3 Effectiveness comparison of GA and MPS

For those problems with known optima of non-zero (SC, HN, F16, IL, PV), the qualities of the solutions (using the median solution) are compared based on Eq. (14). The results are shown in Figure 10. It can be seen that for all these five problems, both GA and MPS methods can find solutions of high quality close to 100%. Only a lower quality of 98.7% was obtained by GA on the HN problem.

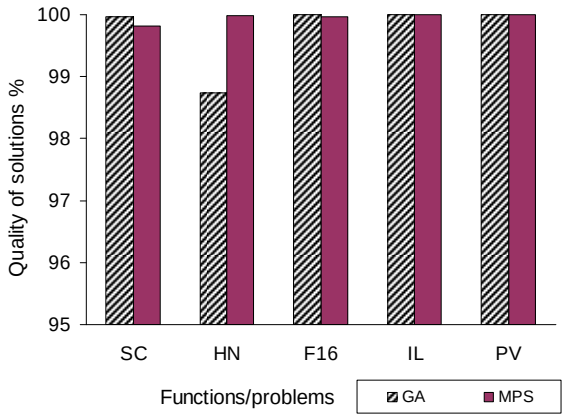


Figure 10 Mean quality ratings of solutions obtained by GA and MPS for 5 testing problems.

The two algorithms, however, show great differences in solving the other problems. For the CO problem (analytical optimum of zero), GA finds very good solutions ranging from 0 to 0.003, while MPS only finds solutions from 34.25 to 5,337.44. For the ten-dimensional R10 function (analytical optimum of zero), GA also outperforms MPS. The solutions obtained by GA range from 0 to 0.013, while those obtained by MPS range from 73.92 to 128.79. It was found in solving the R10 function MPS reaches the computer memory limit when the number of function evaluations reaches about 2,500. This is because all of the 2500 points participate in the construction of the metamodel defined by Eq. (1). GA, on the other hand, can afford around 3,000,000 function evaluations. In a later comparison, we let both GA and MPS run for 2,500 points and found that the results are similar with those of the MPS, as shown in Table 4.

Table 4 Comparison of effectiveness of GA and MPS for R10 and CO problems (*: solutions of GA for 2500 *nfe*'s)

Function	N	Space	Minimum			
			GA		MPS	
			Range of variation	Median	Range of variation	Median
CO	4	[-100,100]	[0.000, 0.003]	0	[34.256, 5337.445]	306.019
R10	10	[-5,5]	[0, 0.013]	0.003	[73.926, 128.794]	118.341
			[63.641,207.665]*	130.889*		

A particular interest in this study is to compare the effectiveness of GA and MPS in solving discrete problems. In this study, a well known gear train (GT) problem is solved and the solutions are compared. Table 5(a) shows the solutions of the GT problem with different optimization algorithms. The MPS outperforms most of the other approaches, including GA. Table 5(b) shows the solutions with 10 runs of both GA and MPS. The MPS outperforms GA for the discrete problem.

Table 5 Solutions of the gear train design problem

(a) Best results

Approach	Optimization solution	$GT_{\min}$
PFA [11]	14,29,47,59	4.5×10^{-6}
2-ES [12]	18,15,32,58	1.4×10^{-6}
GA	20,20,47,59	9.75×10^{-10}
MPS	16, 19, 43,49	2.7×10^{-12}

(b) Solutions of 10 runs

Solutions / Algorithm	Range of variation	Median	Average
GA	$[9.745\times10^{-10}, 1.683\times10^{-6}]$	4.615×10^{-9}	4.033×10^{-7}
MPS	$[2.701\times10^{-12}, 1.827\times10^{-8}]$	5.544×10^{-10}	$2.423e\times10^{-9}$

Another particular problem, the FJP problem, also deserves more explanation. It is an expensive black-box function problem which involves finite element analysis (FEA). When testing this problem with GA, the maximum number of generations is set as 60; population size is 100 with the normGeomSelect parameter, as well as the 3 crossover (Pc=0.7) and 4 mutation methods (Pm=0.1) as described in Section 2. For MPS, k=0.01. The results are shown in Table 5. Both GA and MPS give good solutions in all five independent runs. But MPS provides a wider range of variation of the solutions and it gives a better optimum of 0.1515.

Table 6 Comparison of optimal solutions of the FJP problem by GA and MPS

(a) With 5 runs

Solutions / Algorithm	Range of variation	Median	Average
GA	[0.2177, 0.3451]	0.2468	0.2714
MPS	[0.1515, 0.4104]	0.2187	0.2453

(b) Best results

Algorithm	Optimization solution	Θ_{min}
MPS	P1= (75.153,31.709), P2= (68.117, 59.831), S= 37.473	0.1515
GA	P1= (63.944, 65.459), P2= (20.043, 27.741), S=18.297	0.2177

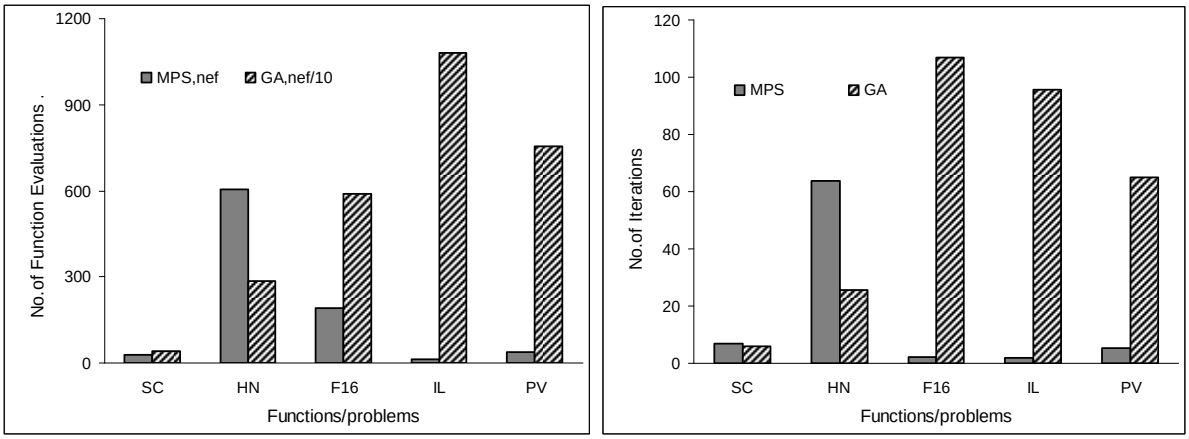
4.4 Efficiency comparison of GA and MPS

The efficiencies are compared in Figure 11 in terms of the number of function evaluations, the number of iterations, and CPU times used to solve the problems. The number of function evaluations and iterations needed by GA are dramatically larger than those needed by MPS for most problems, except the HN problem. In Figure 11 (a), note that the *nfe* of GA is scaled by 0.1 for better illustration. It can also be found that GA needs more function evaluations and iterations for high dimensional problems and complex design problems, such as the F16, PV and IL problems. The lower *nfe* of MPS occurs because of

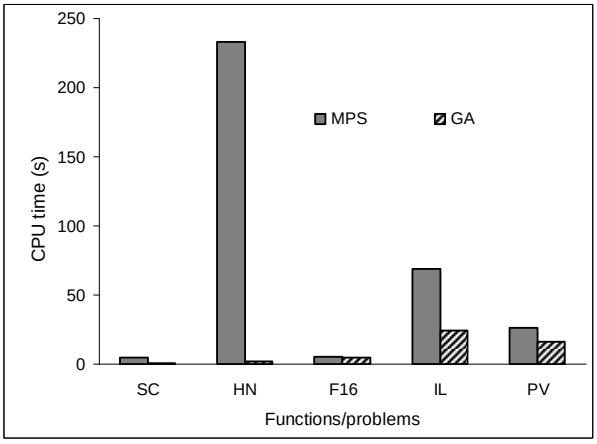
its discriminative sampling and metamodeling formulation in the algorithms. Only the expensive points are calculated using the objective function, while the cheap points are calculated using an approximate linear spline function or quadratic function. Since only several expensive points are generated in MPS, *nfe* is very low. However, for GA, each individual in the population is calculated using the objective function, so *nfe* is very high.

As for the CPU time used for solving the problems, MPS method uses more CPU time than GA in all of the five problems, especially the HN problem, where MPS spends 100 times more CPU time than the GA, as shown in Figure 11 (c). The reason is that MPS needs to generate ten thousand points per iteration, and calculate the function value of each point from the metamodel, thereby leading to a large computing load and high CPU time. But this has not been counted as a function evaluation since the fundamental assumption of MPS is that the objective function evaluation is at least one magnitude more expensive than evaluation with a metamodel in MPS.

For the other functions / problems, the computational expenses by GA and MPS are listed in Table 7. Generally GA performs better than MPS on the high dimensional problems with inexpensive functions. The efficiency advantage of MPS shows in the expensive function problem, the FJP problem, in which MPS uses only half of the computational efforts of GA and finds better solutions.



(a) (b)



(c)

Figure 11 Computational expenses of MPS and GA for the solution of five testing problems (a) numbers of function evaluations (b) numbers of iterations and (c) CPU times

Table 7 Efficiency of the GA and MPS algorithms in some optimization problems

Function or Problem	Number of function evaluations, *nfe*				Number of iterations, *nit*				CPU time(s)			
	GA		MPS		GA		MPS		GA		MPS	
	Average	Median	Average	Median	Average	Median	Average	Median	Average	Median	Average	Median
SC	418.8	408	27.8	27	5.9	6	6.9	7	0.5	0.5	4.6	3.9
HN	2837.1	2193.5	603.4	535	25.7	23.5	63.9	56.5	1.9	1.5	232.8	79.9
F16	5887	5889	191.8	163	106.8	107.5	2.2	4	4.5	4.5	5.1	3.9
IL	10821.2	10812.2	12.7	13	95.7	97	2	2	24.3	24.2	68.6	68.7
PV	7566	4643.5	37.2	34	65.1	39.5	5.2	4.5	16.1	10.1	26.3	23.3
CO	2854.7	2807.5	20.3	19	65.2	65.5	1.2	1	2.5	2.5	1.0	0.6
GT	291.7	283	1610	2000	4.5	4.5	402	500	0.5	0.5	3847.6	4846.3
R10	2928774.5	2928511	2231	2434	4963.8	4972.5	158.5	173	1648.9	1652.4	23830.9	26043.7
FJP	3421	3752	1371	1591	37	42	234.8	291	27595.9	11766.5	12393.2	4864.5

5. Summary and Remarks

This paper studies the performance of mode-pursuing sampling (MPS) method, in reference to widely used Genetic Algorithm (GA). Based on qualitative analysis of MPS and GA and quantitative comparisons on test problems, the following observations are made:

1. MPS can robustly and accurately identify the global optimum for a majority of test problems, including both continuous and discrete variable problems. It meets its limitation, however, when the number of function evaluations required for convergence is larger than a certain value that exceeds the computer memory. From this regard, MPS is best suited for low dimensional problems and high dimensional problems with simple functions. For high-dimensional complex or expensive functions, large-memory computers are needed or a better memory-management strategy needs to be developed for MPS.
2. MPS is recommended for global optimization of expensive functions. MPS is developed for expensive functions and it therefore does not bear advantages over GA for global optimization on inexpensive functions.
3. The difference coefficient, k, is a sensitive parameter for MPS. It is recommended to set k=0.01 if the user has no *a priori* knowledge of the optimization problem.
4. Common features of MPS and GA, such as the group-based (or population-based) sampling and selective generation of new samples may be found in other recognized global optimization methods, e.g. simulated annealing, ant colony optimization, particle swamp optimization, etc. The unique philosophy behind MPS, namely, the top-down exploration and discriminative sampling, may inspire the development of future algorithms.

Future research on MPS is to enhance its capability for high dimensional problems. One possible method is to employ a more economical metamodeling method to avoid using all of the evaluated points in model fitting while still providing an overall guide for discriminative sampling.

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