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GAUSSIAN MIXTURE MODEL-BASED RANDOM SEARCH FOR CONTINUOUS OPTIMIZATION VIA SIMULATION

Wenjie Sun
Zhaolin Hu

School of Economics and Management
Tongji University
Shanghai 200092, CHINA

L. Jeff Hong

Department of Management Sciences
City University of Hong Kong
Kowloon, Hong Kong, CHINA

ABSTRACT

This paper studies integrated random search algorithms for continuous optimization-via-simulation (COvS) problems. We first tailor the Gaussian process-based search (GPS) algorithm to handle COvS problems. We then analyze the potential sampling issue of the GPS algorithm and propose to construct a desirable Gaussian mixture model (GMM) which is amenable for efficient sampling and at the same time also maintains the desirable property of exploitation and exploration trade-off. Then, we propose a Gaussian mixture model-based random search (GMRS) algorithm. We build global convergence of both the tailored GPS algorithm and the GMRS algorithm for COvS problems. Finally, we carry out some numerical studies to illustrate the performance of the GMRS algorithm.

1 INTRODUCTION

Random search algorithms are widely implemented approaches to optimization-via-simulation (OvS) problems. Depending on the attributes of decision variables, OvS problems can be roughly classified as discrete OvS (DOvS) where the decision variables take discrete values and continuous OvS (COvS) where the decision variables take continuous values. In the literature, there have been numerous random search algorithms developed for DOvS problems. These algorithms could typically be divided into locally convergent algorithms and globally convergent algorithms. Based on their approaches to handling the exploitation and exploration trade-off in the random search, globally convergent random search algorithms can be divided into four classes – exploitation based, exploration-based, combined, and integrated. Exploitation-based algorithms, e.g., COMPASS (Hong and Nelson 2006) and stochastic ruler (Yan and Mukai 1992), mainly focus on local search around current optimal solutions while exploration-based ones, e.g., the random search of Andradóttir (1996), spend their search efforts on unexplored regions. As the adaptive methods, combined and integrated algorithms have been the main pursuit in the recent study. For a thorough introduction of OvS algorithms, readers are referred to, e.g., Andradóttir (1995), Hong and Nelson (2006), Andradóttir and Prudius (2009), and Sun et al. (2014).

There have also been various random search algorithms for COvS. The classical literature concerning COvS is mainly about pure random search, e.g., Marti (1982) and Yakowitz and Lugosi (1990). More recent studies focus on developing adaptive random search algorithms. Hu et al. (2007) proposed an algorithm called model reference adaptive search (MRAS) for deterministic continuous problems. Hu et al. (2008) further extended the approach to stochastic settings and proposed the stochastic MRAS (SMRAS) algorithm. MRAS and SMRAS are representatives of integrated random search algorithms. Andradóttir and Prudius (2010) studied the COvS problems and proposed an approach called adaptive random search with resampling (ASR). The ASR approach can be viewed as a combined random search algorithm. In Andradóttir and Prudius (2010), the authors provided a framework for developing various

combined procedures for COvS. Besides these approaches, there are also a class of approaches termed as Bayesian optimization. Bayesian optimization approaches usually target for optimization problems where it is very expensive (or time-consuming) to evaluate the objective function. The approaches then aim to design some procedure based on Bayesian update of certain surrogate model to find a good solution using as few function evaluations as possible. Readers are referred to, e.g., Jones et al. (1998), Scott et al. (2011), Wu and Frazier (2016) and Wang et al. (2016) for a thorough investigation. The problem settings in the Bayesian optimization approaches are different from the settings we consider in this paper. For the OvS problems we consider, the computational effort typically could afford thousands to even millions of function evaluations.

Depending on the search mechanism, OvS algorithms are also often divided into instance-based algorithms and model-based algorithms, see, e.g., Zlochin et al. (2004). In instance-based algorithms, the evolution of the solution depends directly on the previously visited solutions. In model-based algorithms, the evolution of the solution relies on some sampling distribution that often integrates the surface information. MRAS (SMRAS) of Hu et al. (2007; 2008) and GPS of Sun et al. (2014) are typical model-based methods. In this paper, we focus on COvS and propose to develop alternative model-based procedures. We start from the work of Sun et al. (2014). Sun et al. (2014) proposed to balance exploitation and exploration using a Gaussian process-based random search (GPS). The GPS algorithm of Sun et al. (2014) is developed for DOvS. It is clear that in terms of COvS problems, the global convergence of those random search algorithms for DOvS problems is often difficult to be extended. A key reason behind is that the global convergence for DOvS is typically based on the very assumption that the noise involved in simulation can be reduced by repeatedly sampling the same feasible solution, which, however, is impossible for COvS problems where the feasible region is continuous (uncountable). Andradóttir and Prudius (2010) conducted some novel analysis for their ASR algorithm and built the convergence for this algorithm. In this paper, we overcome this challenge by developing a new estimation scheme based on which we build the global convergence of a new GPS algorithm for COvS problems. Our estimation scheme is motivated by Andradóttir and Prudius (2010). However, our approach is more flexible as a generalization of Andradóttir and Prudius (2010). For instance, in our approach, more variety of concentration inequalities can be taken into consideration, which leads to a more flexible estimation scheme. Due to the flexibility, we show that alternative convergent conditions can be developed by our method.

The fast constructed Gaussian process in the GPS algorithm can be used to collect information about the unknown response surface as an efficient metamodel approach of simulation output performance measures. This makes the sampling distribution in GPS capable of balancing the exploitation and exploration trade-off during the search. However, because the sampling distribution is constructed from a metamodel, it is still complicated. This raises an issue about sampling. This issue motivates us to develop some alternative sampling distribution that is also capable of balancing the exploitation and exploration trade-off and is more tractable for sampling. In this paper, we choose to use the Gaussian mixture models (GMM). The main reasons why we choose GMM as the sampling distribution are as follows:

- Almost any continuous density function can be approximated with arbitrary accuracy by using a sufficient number of Gaussians, and by adjusting their means and covariances and the component proportions (Bishop 2006).
- COvS problems are typically nonconvex and multimodal where there may exist a number of local optima. The density of GMM is multimodal. This structure enables GMM to capture the structure of multimodal OvS problems.
- Sampling from a GMM is essentially as easy as sampling from a Gaussian distribution.

However, a crude GMM is far from being desirable due to the lack of knowledge about the unknown response surface of the targeted simulation output. In this paper, we propose to project the sampling distribution of the GPS algorithm onto GMM, based on some statistical distances (divergences). We expect that the resulting GMM can also possess desirable properties of exploitation and exploration trade-off by

learning from the sampling distribution of the GPS algorithm. To conduct the projection, we choose to use some expectation-maximization (EM) algorithm. The EM algorithm (Dempster et al. 1977; McLachlan and Peel 2000) is a classical approach to finding maximum likelihood estimator (MLE) for GMM. Nevertheless, the conventional EM algorithm is developed to solve maximum likelihood estimation (MLE) while, in our work, the projection problem is formulated as a weighted MLE (WMLE) problem. Therefore, in this paper, we develop a Monte Carlo EM (MCEM) algorithm to solve this problem.

The rest of this paper is organized as follows. In §2, we tailor the GPS algorithm for COvS problems. In §3, we first discuss the expected properties of a desirable GMM and then discuss how to construct the GMM. Consequently, we give a detailed illustration of the Gaussian mixture model-based random search (GMRS) algorithm, and build the convergence of the algorithm. In §4, several numerical examples are studied. The paper is concluded in §5.

2 GPS ALGORITHM FOR COVS PROBLEMS

Throughout this paper, we consider the following COvS problem

$$\sup_{x\in\Theta\subseteq\Re^d} h(x) = \mathrm{E}(H(x,\xi)) \tag{1}$$

where Θ is a nonempty compact subset of $\Re^d$ and the vector ξ represents the random input which is assumed to follow a certain distribution. The expectation in (1) is taken with respect to (w.r.t.) the distribution. The closed form of $h(x)$ is unavailable to us but the value of $H(x,\xi)$ can be obtained by running simulation experiments. Let h^* be the optimal value of (1). We assume that $h^* < \infty$. Our goal is to pursue the decision vector x that maximizes the expected performance of the target system.

In order to balance exploitation and exploration in DOvS problems, Sun et al. (2014) proposed a fast approximation of Gaussian process as follows:

$$Y(x) = M(x) + \lambda^T(x)(\bar{h}(x) - \mathbb{M}) + \lambda^T\xi \tag{2}$$

where $M(x)$ is a stationary Gaussian process with mean 0 and covariance function $\sigma^2\gamma(\cdot,\cdot)$, $\mathbb{M} = (M(x_1),\cdots,M(x_m))^T$, $\lambda(\cdot)$ are weight functions and ξ is an m-dimensional random vector following a multivariate normal distribution with mean 0 and covariance matrix

$$\Sigma_\xi = diag\left\{\frac{\sigma^2(x_1)}{n_1},\cdots,\frac{\sigma^2(x_m)}{n_m}\right\}.$$

In addition, both correlation function $\gamma(\cdot,\cdot)$ and weight functions $\lambda(\cdot)$ satisfy certain conditions (see, e.g., Sun et al. 2014). The model (2) can be viewed as a metamodel of the original objective function $h(x)$. It not only captures the continuity and uncertainty of $h(x)$ but also incorporates the information from past observations. Then based on this model, Sun et al. (2014) put forward a Gaussian process-based search (GPS) with the following sampling distribution

$$f(x) = \frac{P^*\{Y(x) > c\}}{\int_\Theta P^*\{Y(x) > c\}\nu(dx)}$$

where $P^*\{Y(x) > c\}$ is the conditional probability of the improvement over current best value c, "$*$" refers to all available information and ν is the Lebesgue measure defined on Θ.

The GPS algorithm in Sun et al. (2014) is developed for DOvS. However, this procedure can be easily adapted for COvS. In this section we briefly summarize the main steps of the GPS algorithm for COvS problems with a more generalized simulation-allocation rule (SAR). In the discussion below we first assume that a SAR is given. Let Θ_k be the set of visited solutions by the end of iteration k. Accordingly, the number of visited solutions by the end of iteration k is denoted by $|\Theta_k|$ where $|\cdot|$ is a counting measure.

Let $N_k(x)$ be the number of observations at solution x until iteration k. Then $N_k(x) = \sum_{i=1}^{k} a_k(x)$ where $a_k(x)$ is the number of observations allocated to solution x by the SAR at iteration k. Let $\hat{h}_k(x)$ denote the sample mean of the random output $H(x)$ by iteration k. Then $\hat{h}_k(x) = \frac{1}{N_k(x)} \sum_{i=1}^{N_k(x)} H_i(x)$. By Proposition 1 in Sun et al. (2014), the calculation of $\mathrm{Var}^*[Y(x)]$ involves the value of $\mathrm{Var}[H(x,\xi)]$ which can be substituted by its sample counterpart $\hat{\sigma}^2(x)$. Different from the setting in Sun et al. (2014), here we impose that for all $x \in \Theta_k$, $N_k(x) \geq N_k$ where $\{N_k\}$ is a sequence monotonically increases to $+\infty$ as $k \to \infty$. Let $\mathscr{F}_k$ be a filtration, an increasing sequence σ-field, containing the history generated by the algorithm until iteration k. We modify the GPS in Sun et al. (2014) and propose the following algorithm.

GPS-COvS Algorithm

Step 0. Set iteration count $k = 0$ and construct the set of starting points Θ_0 by uniformly sampling from Θ. For all $x \in \Theta_0$, calculate $\hat{h}_0(x)$ and sample variance $\hat{\sigma}_0^2(x)$. In order to prevent $\hat{\sigma}_0^2(x)$ from being zero, if $\hat{\sigma}_0^2(x) < \sigma_0^2$, set $\hat{\sigma}_0^2(x) = \sigma_0^2$. To avoid $\hat{h}_0(x)$ deviating far away from $h(x)$, we set an artificial lower bound $\underline{M}$ which is an extremely small number. If $\hat{h}_0(x) < \underline{M}$, set $\hat{h}_0(x) = \underline{M}$. Let $\hat{x}_0^* = \underset{x \in \Theta_0}{\operatorname{argmax}} \{\hat{h}_0(x)\}$ and break the tie arbitrarily if it exists, and let $\hat{h}_0^* = \max_{x \in \Theta_0} \{\hat{h}_0(x)\}$.

Step 1. Set $k = k+1$. Construct the following sampling distribution based on history $\mathscr{F}_{k-1} \triangleq \sigma\left(\left\{\Theta_{k-1}, \{\hat{h}_{k-1}(x) | x \in \Theta_{k-1}\}, \{N_{k-1}(x) | x \in \Theta_{k-1}\}, \{\hat{\sigma}_{k-1}^2(x) | x \in \Theta_{k-1}\}\right\}\right)$,

$$f_k(x) = \frac{P\{Y_{k-1}(x) > \hat{h}_{k-1}^* | \mathscr{F}_{k-1}\}}{\int_\Theta P\{Y_{k-1}(x) > \hat{h}_{k-1}^* | \mathscr{F}_{k-1}\} \nu(dx)}.$$

Step 2. Generate independent and identically distributed (i.i.d.) sample $x_1^k, \cdots, x_s^k$ from distribution $f_k(x)$. Let $S_k = \{x_1^k, \cdots, x_s^k\}$ and $\Theta_k = \Theta_{k-1} \bigcup S_k$.

Step 3. For all $x \in \Theta_k$, determine $a_k(x)$ according to the SAR, update N_k and $N_k(x)$ and compute $\hat{h}_k(x)$. If $\hat{\sigma}_k^2(x) < \sigma_k^2$, set $\hat{\sigma}_k^2(x) = \sigma_k^2$. If $\hat{h}_k(x) < \underline{M}$, set $\hat{h}_k(x) = \underline{M}$.

Step 4. Let $x_k^* = \underset{x \in \Theta_k}{\operatorname{argmax}} \{\hat{h}_k(x)\}$. Check whether the stopping criterion is satisfied. If not, return to Step 1.

The convergence of the GPS-COvS algorithm and the discussion of the detailed conditions that a SAR should satisfy is deferred to next section.

3 GMM-BASED RANDOM SEARCH FOR COVS PROBLEMS

It is well known that sampling distribution plays a fundamental role in integrated random search algorithms. Both the GPS algorithm and the SMRAS algorithm of Hu et al. (2008) aim to construct desirable sampling distributions. In this section, we first briefly compare how the two algorithms construct the sampling distributions. Based on this, we then introduce our main algorithm that relies on a different sampling distribution.

SMRAS proposes to construct some reference distribution that could evolve itself. However, the reference distribution is typically difficult to sample from. SMRAS then proposes to project the reference distribution onto some exponential family, e.g., the multivariate normal distribution. The projected distribution is taken as the sampling distribution. Typically it is easy to sample from the projected distribution. Furthermore, it is expected that the projected distribution could sufficiently approximate the reference distribution. Therefore, it can be interpreted that SMRAS tries to make a balance between learning the response surface and the sampling tractability. As introduced above, GPS proposes to use some Gaussian process (a metamodel) to learn the response surface of the targeted system. Based on the metamodel, the GPS algorithm then proposes to construct some sampling distribution that balances the exploitation and exploration trade-off. Since the sampling distribution in GPS relies on the metamodel, rather than the original response surface,

it is more tractable than the reference distribution in SMRAS. However, sampling from the sampling distribution in GPS is more difficult than from the projected distribution (e.g., the multivariate normal distribution) in SMRAS. In Sun et al. (2014), alternative sampling methods like the acceptance-rejection sampling procedure and the Markov chain coordinate sampling are designed. In this paper, we propose to design some sampling distribution that is able to balance the exploitation and exploration trade-off whereas at the same time is easy to sampling from. To achieve the goals, we resort to the well known Gaussian mixture model.

3.1 Construction of Desirable Gaussian Mixture Models

Gaussian mixture models have been used widely in various areas. For instance, in statistical learning, GMM is often used for clustering (McNicholas 2016). The density of a GMM is simply a weighted sum of several normal densities, which takes the following expression

$$g_\theta(x) = \sum_{j=1}^{K} \pi_j \mathcal{N}(x|\mu_j, \Sigma_j),$$

where each component $\mathcal{N}(x|\mu_j, \Sigma_j)$ is a (multivariate) normal density function with mean vector μ_j and covariance matrix Σ_j, and the component proportions $\pi_j \geq 0, j = 1, \ldots, K$ satisfy $\sum_{j=1}^{K} \pi_j = 1$. Throughout this paper, we denote by θ the parameters $\pi_j, \mu_j, \Sigma_j, j = 1, \ldots, K$.

We use an example to motivate our idea of using GMM. Consider a well known multimodal function called Griewank function, with a surface shown in Figure 1 (a). Intuitively, the surface is similar to the surface of the probability density function of a GMM shown in Figure 1 (b).

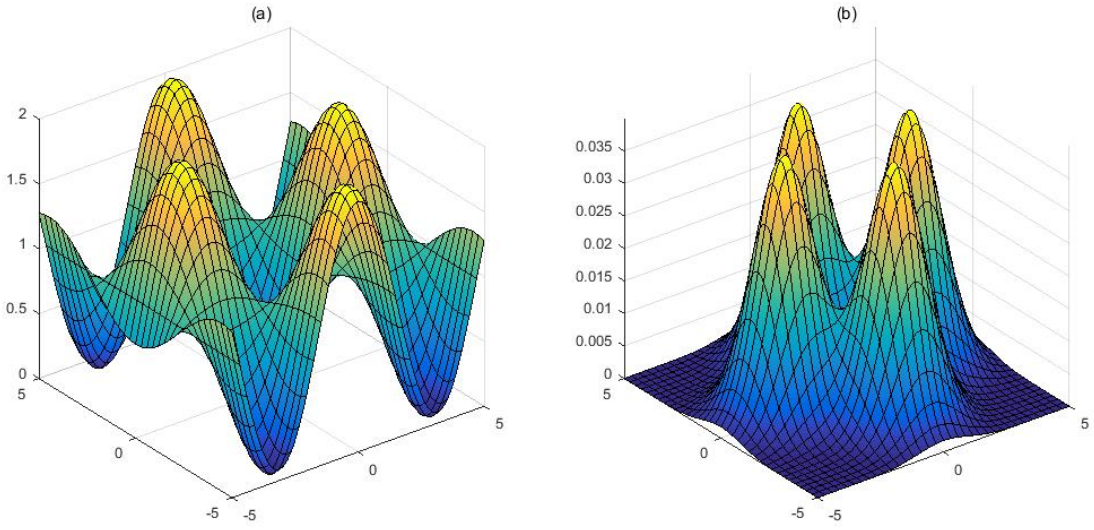

Figure 1: (a) Surface plot of Griewank function; (b) Surface plot of probability density function (PDF) of GMM.

Note that if we use some unimodal density function, e.g., a multivariate normal density, to approximate the multimodal surface, we may not obtain a good approximation. Compared with a single Gaussian distribution, which belongs to the exponential family used by Hu et al. (2007; 2008), GMM can better approximate the reference distribution in terms of minimized KL-divergence.

Despite the similar multimodality shown in Figure 1, there are substantial difference between the two different surfaces in Figure 1. In Figure 2 we plot the contour for the two surfaces.

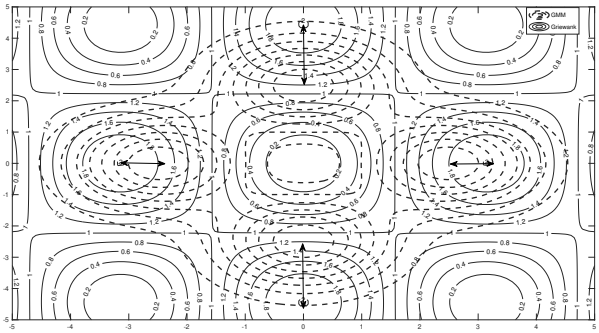

Figure 2: Contour plot of Griewank function and PDF of GMM.

From Figure 2 we can see that there is discrepancy between the (near) optima of Griewank function and mean value of various Gaussian components of GMM. Therefore, to obtain better approximations, we need to modify the parameters of the GMM.

In OvS problems, it may be difficult to directly construct a GMM from the original problem because the objective function is unknown. In this paper, we adopt a two-stage approach. In the first stage, we propose to use some sampling distribution as in GPS or some reference distribution as in SMRAS to learn the surface of the true response. In the second stage, we propose to use some GMM to approximate the sampling (or reference) distribution. To obtain a good approximation, we choose to project the sampling (reference) distribution onto the family of GMM.

In what follows we focus our analysis on the sampling distribution f_k of GPS. The analysis for the reference distribution of SMRAS could be left as the future research.

Consider the sampling distribution $\{f_k(\cdot)\}$, which is constructed as in Step 1 of GPS-COvS Algorithm. We project it onto the parameterized GMMs $\{g_\theta(\cdot), \theta \in \mathbb{S}\}$ by minimizing the following Kullback-Leibler (KL) divergence

$$\underset{\theta \in \mathbb{S}}{\text{minimize}} \; D(f_k \| g_\theta), \tag{3}$$

where

$$D(f_k \| g_\theta) = \mathrm{E}_{g_\theta}\left[\frac{f_k(X)}{g_\theta(X)} \ln \frac{f_k(X)}{g_\theta(X)}\right] = \mathrm{E}_{f_k}\left[\ln \frac{f_k(X)}{g_\theta(X)}\right]$$

denotes the KL divergence from $f_k(\cdot)$ to $g_\theta(\cdot)$. The notation $\mathrm{E}_f[\cdot]$ denotes that the expectation is taken w.r.t. a distribution $f(\cdot)$. Note that the KL divergence is an instance of the ϕ-divergence family (Pardo 2006). To conduct the projection, we can use different ϕ-divergences. This provides more freedom for the algorithm design of our approach. In this paper, we choose the commonly used KL divergence and leave the analysis for alternative ϕ-divergences as the future study.

When the sampling distribution $f_k(\cdot)$ is fixed at certain iteration k, the term $\mathrm{E}_{f_k}[\ln f_k(X)]$ is independent of θ. Thus Problem (3) can be formulated equivalently as follows:

$$\underset{\theta \in \mathbb{S}}{\text{maximize}} \quad \mathrm{E}_{f_k}\left[\ln \sum_{j=1}^{K} \pi_j \mathcal{N}(X|\mu_j, \Sigma_j)\right]. \tag{4}$$

Suppose $\{x_1,\cdots,x_n\}$ is a set of i.i.d. sample generated from $f_k(\cdot)$. We can obtain the following sample counterpart of Problem (4):

$$\underset{\theta\in\mathbb{S}}{\text{maximize}} \quad \frac{1}{n}\sum_{i=1}^{n}\ln\sum_{j=1}^{K}\pi_j\mathscr{N}(x_i|\,\mu_j,\Sigma_j). \tag{5}$$

Problem (5) is similar to the maximum likelihood estimation (MLE) of GMM (Bishop 2006). MLE can be solved by classical EM algorithms (Bishop 2006). However, there is a fundamental difference between (5) and the conventional MLE due to the very fact that the sample in MLE is collected from the true GMM which is to be determined, while the sample in Problem (5) is simulated from $f_k(\cdot)$. Therefore, Problem (5) could be more properly referred to as the quasi-maximum likelihood estimation (White 1998) involving the misspecified model.

However, as we have discussed above, sampling from the distribution $f_k(\cdot)$ is itself an issue for the implementation of GPS. To overcome this difficulty, we propose to use a change of measure technique. In the following analysis, we let g_{θ_k} denote the optimal projected GMM at iteration k. Suppose at iteration k we have obtained the projected distribution $g_{\theta_{k-1}}$ of the previous iteration. Then, by implementing the change of measure technique and plugging in the expression of $f_k(\cdot)$, we have Problem (4) is equivalent to the following problem

$$\underset{\theta\in\mathbb{S}}{\text{maximize}} \quad \mathrm{E}_{g_{\theta_{k-1}}}\left[\frac{P\{Y_{k-1}(X)>\hat{h}^*_{k-1}|\mathscr{F}_{k-1}\}\ln g_\theta(X)}{g_{\theta_{k-1}}(X)}\right],$$

where the conditional probability $P\{Y_{k-1}(X)>\hat{h}^*_{k-1}|\mathscr{F}_{k-1}\}=\Phi\left(\frac{\mathrm{E}[Y_{k-1}(X)|\mathscr{F}_{k-1}]-\hat{h}^*_{k-1}}{\mathrm{Var}[Y_{k-1}(X)|\mathscr{F}_{k-1}]}\right)$ with $\Phi(\cdot)$ being the standard normal distribution function. Then, following the same reasoning line as in the conventional EM algorithm, we suggest determining the parameters of the GMM $g_{\theta_k}(\cdot)$ using the following equations:

$$\pi_j^k=\frac{\sum_{i=1}^n\gamma_{ij}w(x_i)}{\sum_{j=1}^K\sum_{i=1}^n\gamma_{ij}w(x_i)},\quad j=1,\cdots,K, \tag{6}$$

$$\mu_j^k=\frac{\sum_{i=1}^n\gamma_{ij}w(x_i)x_i}{\sum_{i=1}^n\gamma_{ij}w(x_i)},\quad j=1,\cdots,K, \tag{7}$$

$$\Sigma_j^k=\frac{\sum_{i=1}^n||x_i-\mu_j^k||^2\gamma_{ij}w(x_i)}{\sum_{i=1}^n\gamma_{ij}w(x_i)}\mathbf{I},\quad j=1,\cdots,K, \tag{8}$$

where

$$\gamma_{ij}=\frac{\pi_j^k\mathscr{N}(x_i|\,\mu_j^k,\Sigma_j^k)}{\sum_{j=1}^K\pi_j^k\mathscr{N}(x_i|\,\mu_j^k,\Sigma_j^k)},\quad j=1,\cdots,K, \tag{9}$$

$$w(x_i)=\frac{P\{Y_{k-1}(x_i)>\hat{h}^*_{k-1}|\mathscr{F}_{k-1}\}}{\sum_{j=1}^K\pi_j^{k-1}\mathscr{N}(x_i|\,\mu_j^{k-1},\Sigma_j^{k-1})},\quad j=1,\cdots,K,$$

with $\{x_1,\cdots,x_n\}$ being a set of i.i.d. sample generated from $g_{\theta_{k-1}}(\cdot)$.

Remark 1 In (6)-(8) we only consider the GMM with a diagonal covariance type given by $\sigma_j\mathbf{I}$ where $\mathbf{I}$ is the identity matrix and σ_j is a variance parameter of the component j. Therefore, the total number of parameters increases linearly with the dimension of each component in GMM.

Note that from (6)-(8) we could not directly derive the parameters because the right hand sides of (6)-(8) also contain $\pi_j^k,\mu_j^k,\Sigma_j^k$. Then, we put forward the following Monte Carlo EM (MCEM) algorithm that relies on the parameter updating rule (6)-(8).

Monte Carlo EM Algorithm (MCEM)

Step 1. Initialize μ_j^k, Σ_j^k and π_j^k based on the sample generated by $g_{\theta_{k-1}}(\cdot)$. Set $\varepsilon_0 \in (0,1)$.
Step 2. E Step. Compute γ_{ij} according to Equation (9).
Step 3. M Step. Re-estimate μ_j^k, Σ_j^k and π_j^k according to Equations (6), (7) and (8). If there exists $j \in \{1,\cdots,K\}$ such that $\pi_j^k < \varepsilon_0$, set $K = K-1$. Set a small positive number σ_0^2. For all $\{\Sigma_j^k\}_{j=1}^K$, set $\Sigma_j^k := \Sigma_j^k + \sigma_0^2\mathbf{I}$.
Step 4. Check whether the stopping criterion is satisfied. If not, return to Step 2.

In Step 3 of MCEM, the components providing insufficient contribution (with the component proportion lower than ε_0) to explaining the data should be pruned. Therefore, even with an initially large K, surplus components can be effectively removed over iterations. In the algorithm, a very small positive number σ_0^2 called regularization value is added to the diagonal of each covariance matrix so that the matrix will not be ill-conditioned.

3.2 Algorithm Description

Now we propose a new integrated random search algorithm that is based on GMM. The main notations of this algorithm are the same as the ones of the GPS-COvS algorithm proposed in Section 2. The procedures of the algorithm are illustrated as follows:

GMM-Based Random Search Algorithm (GMRS)

Step 0. Set iteration count $k = 0$ and construct the set of starting points Θ_0 by uniformly sampling from Θ. For all $x \in \Theta$, calculate $\hat{h}_0(x)$ and sample variance $\hat{\sigma}_0^2(x)$. If $\hat{\sigma}_0^2(x) < \sigma_0^2$, set $\hat{\sigma}_0^2(x) = \sigma_0^2$; and if $\hat{h}_0(x) < \underline{M}$, set $\hat{h}_0(x) = \underline{M}$. Let $\hat{x}_0^* = \underset{x\in\Theta_0}{\operatorname{argmax}}\{\hat{h}_0(x)\}$ and break the tie arbitrarily if it exists, and let $\hat{h}_0^* = \max\limits_{x\in\Theta_0}\{\hat{h}_0(x)\}$. Set component number $K = K_0$, $Kmax$, $Kmin$ and $\alpha > 1$.
Step 1. Set $k = k+1$. Update the parameters $\theta_k = \{\pi_j^k, \mu_j^k, \Sigma_j^k\}_{j=1}^m$ of desirable GMM $g_{\theta_k}(\cdot)$ using the MCEM algorithm based on history $\mathscr{F}_{k-1}$.
Step 2. Generate i.i.d. samples $x_1^k,\cdots,x_s^k$ from $g_{\theta_k}(\cdot)$. Let $S_k = \{x_1^k,\cdots,x_s^k\}$ and $\Theta_k = \Theta_{k-1}\bigcup S_k$.
Step 3. For all $x \in \Theta_k$, determine $a_k(x)$ according to the SAR, update N_k and $N_k(x)$ such that $N_k(x) \geq N_k$ and compute $\hat{h}_k(x)$. If $\hat{\sigma}_k^2(x) < \sigma_0^2$, set $\hat{\sigma}_k^2(x) = \sigma_0^2$; and if $\hat{h}_k(x) < \underline{M}$, set $\hat{h}_k(x) = \underline{M}$. Update the metamodel (2) based on history $\mathscr{F}_k$.
Step 4. Let $\hat{x}_k^* = \underset{x\in\Theta_k}{\operatorname{argmax}}\{\hat{h}_k(x)\}$ and break the tie arbitrarily if it exists, and let $\hat{h}_k^* = \max\limits_{x\in\Theta_k}\{\hat{h}_k(x)\}$. If $P\{Y_k(\hat{x}_k^*) > \hat{h}_{k-1}^*\} < \delta$ and $K \leq Kmax$, or if $K < Kmin$, set $K := \lceil \alpha K \rceil$. Check whether the stopping criterion is satisfied. If not, return to Step 1.

At Step 4, the number component is increased by the factor α if no significant improvement is made according to a prescribed accuracy δ. Therefore, the exploration capability of the algorithm can be enhanced with increasing components. In addition, if the component number is so large that overfitting problem is incurred, surplus components providing insufficient contribution for explaining data will be automatically removed from the GMM as in Step 3 of the MCEM algorithm. As a whole, the component number of GMM adaptively changes in GMRS.

3.3 Convergence

We have described in detail both the GPS-COvS algorithm and the GMRS algorithm. In this subsection, we briefly discuss the convergence of the algorithms and the conditions that ensure the convergence. First, we make the following assumptions for Problem (1).

Assumption 1 For each $\varepsilon > 0$, $\nu(\Theta_\varepsilon) > 0$ where $\Theta_\varepsilon = \{x \in \Theta | h(x) \geq h^* - \varepsilon\}$, $h^* = \max_{x\in\Theta} h(x)$ and $\nu(\cdot)$ is the Lebsegue measure defined on Θ.

This assumption ensures that the probability of points in any neighbourhood of the optimal solution being sampled will be positive. It is a conventional assumption for COvS, see, e.g., Hu et al. (2007). Next, we make the following assumption about the estimation scheme that is motivated by Andradóttir and Prudius (2010).

Assumption 2 For each $x \in \Theta_k$, let $\{H_i(x)\}_{i=1}^{\infty}$ be the i.i.d. observations of $H(x,\xi)$. For each $\varepsilon > 0$, there exists $N(\varepsilon)$ such that for $N_k(x) > N(\varepsilon)$,

$$P\left\{\left|\frac{1}{N_k(x)}\sum_{i=1}^{N_k(x)} H_i(x) - h(x)\right| \geq \varepsilon\right\} \leq \lambda(N_k(x),\varepsilon),$$

where $\sum_{k=1}^{\infty} |\Theta_k| \sum_{N_k(x)\geq N_k} \lambda(N_k(x),\varepsilon) < \infty$.

This assumption can be satisfied by many different kinds of concentration inequalities and simulation-allocation rule (SAR). Here we consider some realization of Assumption 2 as follow.

Suppose the condition holds: There exists a constant $l \in \mathbb{N}^+ \setminus \{0,1\}$, and a constant R which may depend on l, such that $\mathrm{E}\left[(H(x)-h(x))^{2l}\right] \leq R$ for all $x \in \Theta$. Then, by Markov's inequality and Lemma 1 of Andradóttir and Prudius (2010), for each $\varepsilon > 0$, there exists $C(\varepsilon)$ such that for all $n \in \mathbb{N}^+$ and for all $x \in \Theta$,

$$P\left\{\left|\frac{1}{n}\sum_{i=1}^{n} H_i(x) - h(x)\right| \geq \varepsilon\right\} \leq \frac{C(\varepsilon)}{n^l}.$$

Letting $\lambda(N_k(x),\varepsilon) = \frac{C(\varepsilon)}{(N_k(x))^l}$, $N_k = C_1 k^c + C_2$ $(C_1 > 0, c > 0, C_2 > 1)$ and $|\Theta_k| = sk (s > 0)$, if $c(l-1) > 2$, we have

$$\begin{aligned}
\sum_{k=1}^{\infty} |\Theta_k| \sum_{N_k(x)\geq N_k} \lambda(N_k(x),\varepsilon) &= s\sum_{k=1}^{\infty} k \sum_{N_k(x)=C_1k^c+C_2}^{\infty} \frac{C(\varepsilon)}{N_k(x)^l} \\
&\leq \frac{s}{l-1}\sum_{k=1}^{\infty} k \int_{C_1k^c}^{\infty} \frac{1}{t^l} dt \\
&\leq \frac{sC_1^{1-l}}{l-1}\sum_{k=1}^{\infty} \frac{1}{k^{c(l-1)-1}} < \infty.
\end{aligned}$$

Thus Assumption 2 is satisfied.

In the GPS-COvS algorithm and the GMRS algorithm introduced above, we suppose that some SAR is given. To ensure the convergence of the algorithms, we require that the SAR satisfies Assumption 2.

The following theorem builds the convergence of the GPS-COvS algorithm.

Theorem 1 Suppose that GPS-COvS is used to solve Problem (1) and Assumptions 1 and 2 are satisfied. Then, $\hat{h}_k^* \to h^*$ w.p.1 as $k \to \infty$.

The sketch of proof: It suffices to show that, for each $\varepsilon > 0$, $P\{|\hat{h}_k^* - h^*| > \varepsilon \quad i.o.\} = 0$. Then, because

$$P\{|\hat{h}_k^* - h^*| > \varepsilon \quad i.o.\} \leq P\{\hat{h}_k^* < h^* - \varepsilon \quad i.o.\} + P\{\hat{h}_k^* > h^* + \varepsilon \quad i.o.\},$$

the key point here is to prove $P\{\hat{h}_k^* < h^* - \varepsilon \quad i.o.\} = 0$ and $P\{\hat{h}_k^* > h^* + \varepsilon \quad i.o.\} = 0$, which concludes the proof. □

For the GMRS algorithm, we have the following theorem about its convergence.

Theorem 2 Suppose that GMRS is used to solve Problem (1) and Assumptions 1 and 2 are satisfied. Then $\hat{h}_k^* \to h^*$ w.p.1 as $k \to \infty$.

The sketch of proof: Similar to the proof of Theorem 1. □

4 NUMERICAL ILLUSTRATION

In this section, we implement our approach to solve two test problems. We first consider the following classical function optimization problem with multiple local optima:

$$\underset{(x_1,x_2)\in[0,100]\times[0,100]}{\text{maximize}} \quad h(x_1,x_2) = \mathrm{E}[H(x_1,x_2,\xi)], \tag{10}$$

where $H(x_1,x_2,\xi) = 10\times(F(x_1)+F(x_2))+\mathcal{N}(0,1^2)$ with $F(x)$ given by

$$F(x) = \frac{\sin^6(0.05\pi x)}{2^{2(\frac{x-10}{80})^2}}.$$

A DOvS counterpart of Problem (10) is also used in Sun et al. (2014) as a test problem. The global optimum of Problem (10) is $h(10,10) = 20$. In the experiments, we set $N_k = \lceil C_1 k^c + C_2 \rceil (C_1 > 0, c > 0, C_2 > 1)$ and $|\Theta_k| = sk(s > 0)$, and set the main parameters of GMRS as follows: $s = 100$, $C_1 = 0.1$, $C_2 = 5$, $c = 0.5$, $\varepsilon_0 = 1/s$, $\delta = 0.2$, $\sigma_0^2 = 0.1$, $K_0 = 2$, $Kmax = 10$, $Kmin = 2$ and $\alpha = 1.03$. The remaining parameter setting about the construction of the metamodel (2) follows the one in Sun et al. (2014). The left panel of Figure 3 shows the performance of 30 independent simulation runs of GMRS. We also compare the performance of GMRS with that of SMRAS. The parameter settings of SMRAS are suggested in Hu et al. (2008). On the right panel of Figure 3, we plot the average performances of 30 independent simulation runs for the two algorithms. From the figure, we can see GMRS has a competitive performance.

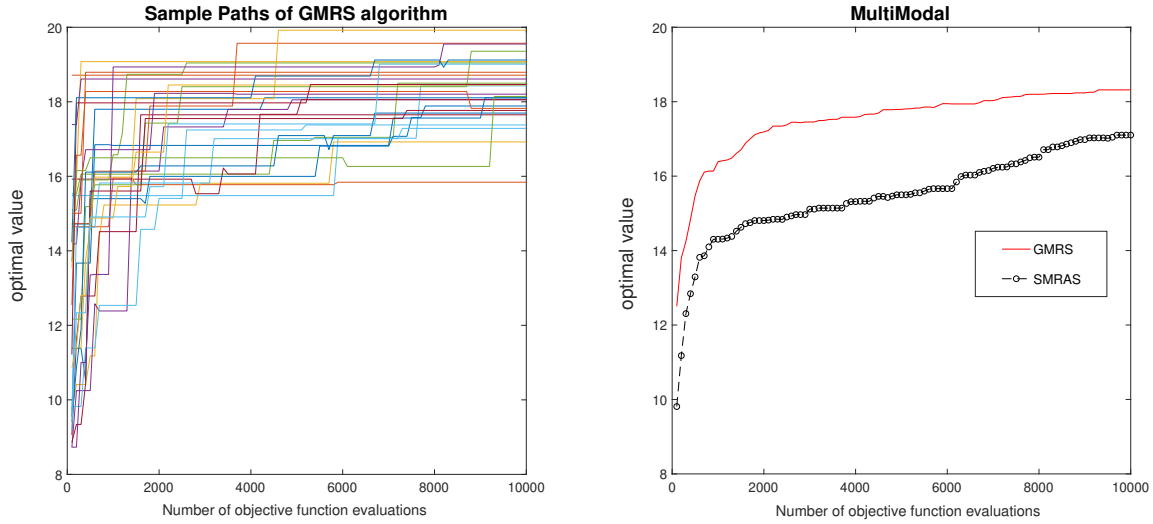

Figure 3: Empirical Performance of GMRS and SMRAS for Problem (10).

We next consider the following optimization problem:

$$\underset{x\in[-500,500]^d}{\text{minimize}} \quad h(x) = \mathrm{E}[H(x,\xi)], \tag{11}$$

where

$$H(x,\xi) = 418.9829d - \sum_{i=1}^{d} x_i \sin(\sqrt{|x_i|}) + \mathcal{N}(0,5^2).$$

The objective function h is called a Schwefel function. We set the dimension d of the decision vector x to be 20. Thus Problem (11) is a high dimensional optimization problem with multiple local optima. With the parameter settings the same as for preceding example. We run GMRS and SMRAS on the problem. In Figure 4, we plot the average performances of 30 independent simulation runs for the algorithms.

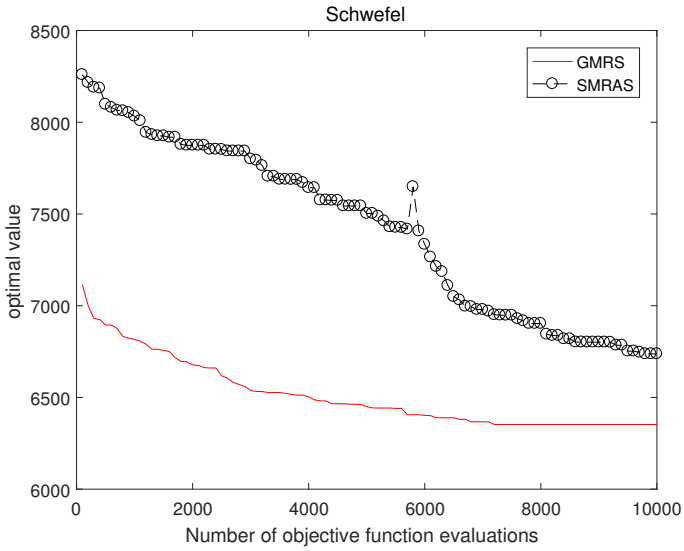

Figure 4: Empirical Performance of GMRS and SMRAS for Problem (11).

The result again shows the potential of our GMRS algorithm. Note that in both test problems, the objective functions are multimodal. The preliminary experiments suggest that the GMRS algorithm could be an attractive approach for this class of problems. To make further comparisons for the algorithms, more thorough numerical study is necessary.

5 CONCLUSIONS

In this paper, we have proposed a novel COvS algorithm called Gaussian mixture model-based random search based on the construction of desirable GMM that can automatically balance exploitation and exploration. We have tested the proposed algorithm on two test problems. As the future study, we will further enhance our algorithm by designing some more efficient SAR.

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AUTHOR BIOGRAPHIES

WENJIE SUN is a master student in the School of Economics and Management at Tongji University. He is working on simulation optimization and stochastic optimization. His email address is r13381638770@sina.com.

ZHAOLIN HU is a professor in the School of Economics and Management at Tongji University. His current research interests include simulation theory and practice, stochastic optimization, statistical learning, and risk management. His email address is russell@tongji.edu.cn.

L. JEFF HONG is a chair professor of Management Sciences in the College of Business at the City University of Hong Kong. His research interests include stochastic simulation, stochastic optimization, and financial risk management. He is currently an area editor for simulation department of Operations Research and associate editor of Management Science. His email address is jeffhong@cityu.edu.hk.