Constrained minimum energy designs

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Abstract

Space-filling designs are important in computer experiments, which are critical for building a cheap surrogate model that adequately approximates an expensive computer code. Many design construction techniques in the existing literature are only applicable for rectangular bounded space, but in real-world applications, the input space can often be non-rectangular because of constraints on the input variables. One solution to generate designs in a constrained space is to first generate uniformly distributed samples in the feasible region, and then use them as the candidate set to construct the designs. Sequentially constrained Monte Carlo (SCMC) is the state-of-the-art technique for candidate generation, but it still requires large number of constraint evaluations, which is problematic especially when the constraints are expensive to evaluate. Thus, to reduce constraint evaluations and improve efficiency, we propose the constrained minimum energy design (CoMinED) that utilizes recent advances in deterministic sampling methods. Extensive simulation results on 15 benchmark problems with dimensions ranging from 2 to 13 are provided for demonstrating the improved performance of CoMinED over the existing methods.

Keywords Computer experiment · Experimental design · Space-filling designs · Sequential Monte Carlo

1 Introduction

In deterministic computer experiments, we use computer codes to study the input/output relationship of some complex physical, economical, or engineering models, e.g., large eddy simulations for rocket engine injector design (Mak et al. 2018). However, computer simulations are often time-consuming. Thus, the first step is to build a computationally cheap surrogate model that approximates the expensive computer code using some offline simulation runs (Santner et al. 2018).

Space-filling designs are commonly used for constructing the experimental designs where we run the computer simulations. Since we do not have a priori information about the input/output relationship, it is important to have the design points well spread out across the entire design region \( \mathcal{X} \subseteq \mathbb{R}^p \). Minimax and maximin are the two popular space-filling measures proposed by Johnson et al. (1990). A minimax design aims to minimize the maximum distance from any point in \( \mathcal{X} \) to the closest design point, whereas a maximin design maximizes the minimum distance between any two design points. Due to computational tractability, the maximin measure is more commonly used in the literature, which is followed in this paper as well. However, maximin designs are often collapsing, that is, some design points share the same value in one-dimensional projections. Latin hypercube designs (LHD) are developed for having good projection of each factor (McKay et al. 1979), which can be further improved by integrating it with other space-filling criteria such as maximin (Morris and Mitchell 1995). However, maximin LHDs can only ensure good one-dimensional projection and full-dimensional space-fillingness. The maximum projection (MaxPro) designs (Joseph et al. 2015b), on the other hand, are able to achieve good space-filling properties on projections to all subsets of factors.

Most space-filling designs literature focus on bounded rectangular region \( \mathcal{X} = \prod_{d=1}^{p} [a_d, b_d] \subseteq \mathbb{R}^p \). However, in real-world applications such as the welded beam design problem (Dong et al. 2018) and the NASA speed reducer design...
problem (Liu et al. 2017), we frequently need to deal with non-rectangular bounded design space:

\[ \mathcal{X} = \left\{ x \in \prod_{d=1}^{p} [a_d, b_d] : g_k(x) \leq 0 \quad \forall k \right\}, \quad (1) \]

where \( \{g_k(x) \leq 0\}_{k=1}^{K} \) are arbitrary \( K \) inequality constraints. For simplicity, let us consider the bounded space of a unit hypercube, that is, \( a_d = 0, \ b_d = 1 \quad \forall d = 1, \ldots, p \). This is possible since we can always rescale the factors. Figure 1 shows a two-dimensional design space \( \mathcal{X} \) defined by the following three nonlinear inequality constraints,

\[
\begin{align*}
    g_1(x) &= x_1 - \sqrt{50(x_2 - 0.52)^2 + 2} + 1 \leq 0 \\
    g_2(x) &= \sqrt{120((x_2 - 0.48)^2 + 1) - 0.75 - x_1} \leq 0 \\
    g_3(x) &= 0.65^2 - x_1^2 - x_2^2 \leq 0
\end{align*}
\]

where \( 0 \leq x_i \leq 1 \quad (i = 1, 2) \).

The non-convex, non-rectangular shape makes it challenging to construct space-filling designs in \( \mathcal{X} \). Moreover, \( \mathcal{X} \) occupies only a very tiny fraction of \( [0, 1]^2 \). In this paper, we refer this fraction as the feasibility fraction.

Two primary approaches are proposed in the literature for constructing space-filling designs in non-rectangular design space. One approach is to directly employ general purpose constrained optimization techniques (Trosset 1999; Stinstra et al. 2003; Kang 2019). However, this approach can be computationally expensive and can be limited by the type of constraints and design properties (such as projections) it can handle. The alternative approach instead relies on a two-step process:

- **Candidate Generation**: generate a large set of uniformly distributed candidates in \( \mathcal{X} \).
- **Design Construction**: choose points from the set of candidates by a desired criterion.

The flexibility of choosing any design criterion aforementioned in the construction step easily allows for both space-filling and noncollapsing properties in the resulting designs, but how to efficiently generate good quality candidate points remains the key difficulty of this approach. The main objective of this paper is to propose a new efficient method to generate good quality candidate points that are suitable for constructing maximin designs.

Several candidates generation methods have been discussed in the literature. If the desired space \( \mathcal{X} \) is regularly shaped, e.g., simplex and circle, where the closed-form inverse Rosenblatt transform (Rosenblatt 1952) exists, we can obtain uniform samples in \( \mathcal{X} \) by applying the inverse transform on a set of low-discrepancy sequence in \([0, 1]^p\) (Fang and Wang 1994). However, we generally cannot compute the inverse Rosenblatt transform for arbitrary irregularly shaped space \( \mathcal{X} \). An alternative solution is to perform acceptance/rejection sampling on a large set of uniformly distributed points in \([0, 1]^p\), such as grid points (Pratola et al. 2017), Latin hypercube samples (Wu et al. 2019), and quasi-random points (Joseph 2016). For the design space \( \mathcal{X} \) considered in Fig. 1, given its small feasibility fraction of 0.53%, on average only 5 out of 1000 samples in the unit hypercube would land in the design space, indicating that the one-step acceptance/rejection approach can be highly inefficient. One remedy is to iterate between acceptance/rejection sampling and candidate augmentation (Draguljić et al. 2012). To benefit from simulated annealing (Kirkpatrick et al. 1983), the multi-step acceptance/rejection can be performed on a sequence of shrinking regions (Bect et al. 2017), and this idea is further improved using the probabilistic constraint, leading to the sequentially constrained Monte Carlo (SCMC) proposed by Golchi and Loeppky (2015) and Golchi and Campbell (2016). However, SCMC suffers the same issue of Monte Carlo sampling: many samples are repeated or are very close to each other, which add minimal value for the ultimate goal of constructing a maximin design. Moreover, by having the samples well spread out, fewer proposed samples are required to cover the entire design space, and thus fewer evaluations of the constraints, which is beneficial when the constraints are expensive to evaluate. Minimum energy design (MinED) is a state-of-the-art deterministic sampling method for simulating well-spaced samples for any distribution (Joseph et al. 2015a; Joseph et al. 2019). When the target distribution is uniform, the MinED is equivalent to the max-
mination design, showing its strong connection to the problem considered in this paper. Thus, by incorporating the probabilistic constraints from SCMC in MinED, we propose the constrained minimum energy design (CoMinED) as a more efficient approach for generating good-quality design candidate samples in arbitrarily constrained space.

The paper is organized as follows: Section 2 reviews the existing candidates generation algorithms. Section 3 discusses minimum energy design and proposes the constrained minimum energy design (CoMinED). Section 4 demonstrates the improvement of the proposed CoMinED with extensive simulation studies. We conclude the article with some remarks and future research directions in Sect. 5.

2 Existing algorithms

2.1 Candidate generation

2.1.1 Acceptance/rejection sampling

The simplest approach to generate candidates in any constrained space $X$ is to first simulate large set of uniformly distributed samples in a rectangular region that contains $X$, and then apply acceptance/rejection sampling based on the constraints to keep only the feasible samples. Figure 2 shows that only 14 out of the 2385 randomized Latin hypercube samples in $[0, 1]^2$ are feasible for the motivation problem in Fig. 1. The Latin hypercube samples are generated using R package lhs (Carnell 2020). Apart from the low percentage of feasible samples, we can see that these 14 points do not cover the feasible space uniformly well, showing that the one-step acceptance/rejection sampling performs poorly on constrained design problems with very small feasibility fraction. In fact, this issue becomes more serious in higher-dimensional problems.

The inefficiency of the one-step acceptance/rejection sampling results from wasting majority of resources exploring the unit hypercube rather than the target space $X$. Thus, a $T$-step acceptance/rejection sampling on a sequence of shrinking regions $[0, 1]^T = X_0 \supset X_1 \supset \cdots \supset X_T = X$ would allow for exploitation of the important region that is likely feasible. This is known as the subset simulation for estimating the probability of failure in reliability analysis (Bect et al. 2017). Consider a non-rectangular bounded design space that is defined by one inequality constraint, $X = \{ x \in [0, 1]^p : g(x) \leq 0 \}$. The subset simulation defines $\{ X_t \}_{t=0}^T$ by introducing a decreasing sequence of thresholds, $\infty = u_0 > u_1 > \cdots > u_T = 0$, such that $X_t = \{ x \in [0, 1]^p : g(x) \leq u_t \}$. The acceptance/rejection sampling is equivalent to sampling from a indicator function, so we can also view the subset simulation as sampling from the sequence of distributions $\{ \mathbb{1}_{X_t}(x) = \mathbb{1}(g(x) \leq u_t) \}_{t=0}^T$, and sequential Monte Carlo (SMC) sampling can be applied. The sampling step in SMC is usually by Markov chain Monte Carlo (MCMC; Robert and Casella 2013), but poor performances of MCMC on indicator function are observed in practice. One solution is to replace the hard constraint $g(x) \leq 0$ with a probabilistic constraint, leading to the sequentially constrained Monte Carlo (SCMC), which is discussed next.

2.1.2 Sequentially constrained Monte Carlo

For any inequality constraint $g(x) \leq 0$, Golchi and Loeppky (2015) proposed the following probabilistic relaxation using the probit function,

$$\rho_t(x) = \Phi(-\tau g(x)), \quad (5)$$

where $\Phi$ is the standard normal cumulative distribution function and $\tau \geq 0$ is the parameter that controls the rigidity of the constraint. We can see that the function $\rho_t$ assigns value close to 1 for $x$ that meets the constraint and value close to 0 otherwise. Moreover, in the limit,

$$\lim_{\tau \to \infty} \rho_t(x) = \lim_{\tau \to \infty} \Phi(-\tau g(x)) = 1(g(x) \leq 0). \quad (6)$$

The above can be generalized to multiple inequality constraints $\{g_k(x) \leq 0\}_{k=1}^K$ by

$$\rho_t(x) = \prod_{k=1}^K \Phi(-\tau g_k(x)). \quad (7)$$

This leads to the sequentially constrained Monte Carlo (SCMC) that replaces the sequence of indicator functions $\{ \mathbb{1}_{X_t} \}_{t=0}^T$ in the subset simulation by the sequence of probabilistic constraint functions $\{ \rho_t \}_{t=0}^T$ defined in (7) with an increasing sequence $0 = t_0 < t_1 < \cdots < t_T$ where $t_T$ is a large constant, e.g., $10^6$. However, in the SCMC algorithm of Golchi and Loeppky (2015), a pre-fixed normal distribution proposal is used in the Markov kernel of the MCMC step, but how to pick the scale of the normal proposal is difficult for high-dimensional problem with small feasible region. Thus, for a more robust comparison to our proposed approach, we improve the SCMC method by allowing adaptation of the Markov kernel. At each iteration, the scale (standard deviation) of the normal proposal is adapted to be the 75% quantile of the prior step samples’ distances to their closest neighbors divided by the square root of the problem dimension. This adaptive kernel shows robust performance for majority of the benchmark problems considered in this paper. Algorithm 1 details the adaptive SCMC algorithm for generating large
Algorithm 1 Adaptive Sequentially Constrained Monte Carlo (SCMC).

**Input:** (i) \{g_k(x) \leq 0\}_{k=1}^K, that define the design space \(X = \{x \in [0,1]^p : g_k(x) \leq 0 \ \forall k\}\), and (ii) the increasing sequence of rigidity parameter \(0 = \tau_0 < \tau_1 < \cdots < \tau_T\).

1: Simulate the initial \(M\) samples \(\{x_m^{(0)}\}_{m=1}^M\) from \([0,1]^p\).
2: for \(t = 1, \ldots, T\) do
3:   • **Weighting:** compute the importance weight,
4:   \[w_m^{(t)} = \frac{\rho_T(x_m^{(t-1)})}{\rho_{T-1}(x_m^{(t-1)})},\]
5:     \[\text{where } \rho(\cdot) \text{ is defined in } (7).\]
6:     Normalize the weight by \(\tilde{w}_m^{(t)} = w_m^{(t)}/\sum_{m=1}^{M} w_m^{(t)}\).
7:   • **Resample:** draw \(M\) samples \(\{y_m^{(t)}\}_{m=1}^M\) independently from \(\sum_{m=1}^{M} \tilde{w}_m^{(t)} \delta_{y_m^{(t)}}\) where \(\delta_x\) is the Dirac measure for any \(x \in X\).
8:   • **Sampling:** for \(m = 1, \ldots, M\), draw \(x_m^{(t)} \sim K^{\rho_T}(y_m^{(t)} \cdot , \cdot)\) where \(K^{\rho_T}(\cdot, \cdot)\) is a Markov kernel with target distribution \(\rho_T\) and adaptive scale
9:     \[\sigma_T = \left(75\% \text{ quantile of } \min_{j \neq m} |x_m^{(t-1)} - x_j^{(t-1)}|/\|x_m^{(t-1)} - y_m^{(t)}\|\right)/\sqrt{M}.\]
10: end for

**Output:** all particles \(\{x_m^{(T)}\}_{m=1}^M\) that are in \(X\).

2.2 Design construction

The ultimate goal is to construct an \(n\)-point design \(D_n = \{x_i \in X\}_{i=1}^n\) in \(X\) that achieves some good design properties. From the candidate generation step, we obtain a finite set of \(N\) (\(N \geq n\)) candidate points \(C_N = \{y_j \in X\}_{j=1}^N\) that are approximately uniformly distributed in \(X\). The next step is to find the \(n\) samples from the candidate set that maximize a desired design criterion \(\psi\), that is to solve

\[
\arg_{D_n \subseteq C_N} \max \psi(D_n).
\]
In the case of the maximin design, \( \psi(D_n) = \min_{x_i, x_j \in D_n, i \neq j} \| x_i - x_j \|_2 \) where \( \| \cdot \|_2 \) is the Euclidean distance. Many stochastic optimization algorithms have been developed to efficiently address the combinatorial optimization problem in (8), including local search, threshold accepting, simulated annealing (Morris and Mitchell 1995), enhanced stochastic evolutionary (Jin et al. 2003; Wu et al. 2019), etc. See Fang et al. (2005) Chapter 4 for a detailed review of the above methods. Though these methods could yield global optimum solution, they are computationally expensive when the number of candidate points is large. Alternatively, Kennard and Stone (1969) proposed a one-point-at-a-time greedy algorithm for solving (8). The idea is that by having an \( m \)-point design \( D_m (m < n) \), we generate the \( (m + 1) \)-th point by

\[
x_{m+1} = \arg \max_{x \in \mathcal{C}_n \setminus D_m} \psi(D_m \cup \{x\}).
\]

(9)

For the distance-based design criterion considered in this paper, the one-point-at-a-time greedy procedure generally require fewer number of pairwise distance computation than the stochastic optimization approaches in implementation, but it only provide a local optimum design. However, the one-point-at-a-time greedy procedure enjoys good empirical performance in practice, and it has been employed in the R package \texttt{mined} (Wang and Joseph 2019) for generating minimum energy design and the R package \texttt{MaxPro} (Ba and Joseph 2018) for design augmentation. Thus, we also use this greedy procedure in the constrained minimum energy design discussed in the next section.

3 Constrained minimum energy design

3.1 Minimum energy design

We begin by formally defining the minimum energy design (MinED).

**Definition 1** (Minimum Energy Design; Joseph et al. 2015a)

Let \( \pi \) be the target probability density function. An \( n \)-point minimum energy design of \( \pi \) is the optimal solution of

\[
\arg \min_{D_n \in \mathbb{D}_n} \sum_{x_i, x_j \in D_n, i \neq j} q(x_i)q(x_j) \| x_i - x_j \|_2^k,
\]

(10)

where \( \mathbb{D}_n = \{\{x_i\}_{i=1}^n : x_i \in \mathbb{R}^p\} \) is the set of all unordered \( n \)-tuple in \( \mathbb{R}^p \), \( q(\cdot) = 1/\pi^{1/(2p)}(\cdot) \) is the charge function and \( \| \cdot \|_2 \) is the Euclidean distance. Under the proposed charge function, the limiting distribution of the design points converges to \( \pi \).

Similar weighted space-filling design criterion is also considered in Borodachov et al. (2008) and Bowman and Woods (2013). However, the optimization problem in (10) is difficult to solve and numerically unstable. To circumvent this issue, Joseph et al (2019) recognize that (10) is closely related to

\[
\arg \min_{D_n \in \mathbb{D}_n} \left[ \sum_{x_i, x_j \in D_n, i \neq j} \left( \frac{q(x_i)q(x_j)}{\| x_i - x_j \|_2^k} \right) \right]^{1/k},
\]

(11)
for $k > 0$. As $k \to \infty$, the optimization problem becomes

$$\arg\min_{D_n \in \mathcal{D}_n} \max_{i \neq j} q(x_i)q(x_j) \frac{1}{\|x_i - x_j\|_2}.$$  \hspace{1cm} (12)

By substituting $q(\cdot) = 1/\pi^{1/(2p)}(\cdot)$ into (12), we obtain

$$\arg\min_{D_n \in \mathcal{D}_n} \max_{i \neq j} \frac{1}{\pi^{1/(2p)}(x_i)\pi^{1/(2p)}(x_j)}\|x_i - x_j\|_2$$

$$= \arg\max_{D_n \in \mathcal{D}_n} \min_{i \neq j} \frac{\pi^{1/(2p)}(x_i)\pi^{1/(2p)}(x_j)}{\|x_i - x_j\|_2}$$

$$= \arg\max_{D_n \in \mathcal{D}_n} \min_{i \neq j} \frac{1}{\|x_i - x_j\|_2} \log \gamma(x_i) + \frac{1}{2p} \log \gamma(x_j)$$

$$\text{where } \gamma \propto \pi \text{ is the unnormalized probability density function. Now, we only need to work with the log-unnormalized density, and therefore, the objective function is numerically more stable. Intuitively, (13) wants the design points to be as far apart as possible while are still placed in the high density regions. If we take } \pi = \text{Uniform}[0, 1]^p, \text{ then (13) reduces to}$$

$$\arg\max_{D_n \in \mathcal{D}_n} \min_{i \neq j} \|x_i - x_j\|_2.$$  \hspace{1cm} (14)

where $\mathcal{D}_n = \{\{x_i\}_{i=1}^n : x_i \in [0, 1]^p\}$ is the set of all unordered $n$-tuple in $[0, 1]^p$. (14) is the same optimization problem for the maximin design in the unit hypercube (Johnson et al. 1990). Joseph et al (2019) further propose a generalized distance,

$$\|u\|_s = \left(\frac{1}{p} \sum_{l=1}^p |u_l|^s\right)^{1/s}, \text{ } s > 0. \hspace{1cm} (15)$$

Under the distance measure defined in (15), the limiting distribution of the MinED points converge to $\pi$ for all $s > 0$. When $s \to 0$, the distance measure converge to $\|u\|_0 = \prod_{i=1}^p |u_i|^{1/p}$. If $\pi$ is the uniform distribution, MinED with $\|\cdot\|_0$ is the limiting case of the MaxPro design (Joseph et al 2019), showing that noncollapsing property can also be easily achieved by carefully choosing the distance measure.

### 3.2 Constrained minimum energy design

Now, consider the case that we need to generate MinED for $\gamma \propto \pi$, an unnormalized probability density function, in some non-rectangular bounded space $\mathcal{X} = \{x \in [0, 1]^p : g_k(x) \leq 0 \forall k = 1, \ldots, K\}$, then the optimization problem becomes

$$\arg\max_{D_n \in \mathcal{D}_n} \min_{i \neq j} \frac{1}{2p} \log \gamma(x_i) + \frac{1}{2p} \log \gamma(x_j)$$

$$+ \log \|x_i - x_j\|_s,$$

where $\mathcal{D}_n = \{\{x_i\}_{i=1}^n : x_i \in \mathcal{X}\}$ is the set of all unordered $n$-tuple in $\mathcal{X}$. However, constraint optimization is generally hard to solve, especially when some of the constraint functions are nonlinear. Similar to sequentially constrained Monte Carlo, we can simplify the optimization problem (16) by introducing the probabilistic relaxation $\rho_\tau$ defined in (7) for the inequality constraints $\{g_k\}_{k=1}^K$, leading to the constrained minimum energy design (CoMinED) defined below.

**Definition 2 (Constrained Minimum Energy Design)** Let $\gamma \propto \pi$ be the target unnormalized probability density function. An $n$-point minimum energy design of $\pi$ in any non-rectangular bounded space $\mathcal{X} = \{x \in [0, 1]^p : g_k(x) \leq 0 \forall k = 1, \ldots, K\}$ is the optimal solution of

$$\arg\max_{D_n \in \mathcal{D}_n} \min_{i \neq j} \frac{1}{2p} \log \tilde{\gamma}_\tau(x_i) + \frac{1}{2p} \log \tilde{\gamma}_\tau(x_j)$$

$$+ \log \|x_i - x_j\|_s,$$

where $\mathcal{D}_n = \{\{x_i\}_{i=1}^n : x_i \in [0, 1]^p\}$ is the set of all unordered $n$-tuple in unit hypercube, $\|\cdot\|_s$ is the distance measure function defined in (15), and

$$\tilde{\gamma}_\tau(\cdot) = \gamma(\cdot) \times \rho_\tau(\cdot) = \gamma(\cdot) \prod_{k=1}^K \Phi(-\tau g_k(\cdot)), \hspace{1cm} (18)$$

where $\tau$ controls the rigidity of the constraints. As $\tau \to \infty$, (17) is equivalent to (16) in the limit, and $\tau = 10^6$ is sufficient to achieve the limit numerically in practice, provided that the constraints are properly scaled, a point that we will discuss in detail in Sect. 4.

Although the CoMinED is applicable for any distribution $\pi$, in this paper, we mainly focus on $\pi = \text{Uniform}[0, 1]^p$ for a direct comparison to the existing methods for generating space-filling design in non-rectangular bounded regions. As pointed out in Joseph et al. (2015a); Joseph et al (2019) for MinED, solving the optimization directly using nonlinear programming solver is difficult and computationally expensive. The proposed remedy is to (i) generate the design from a set of candidate samples, and (ii) apply simulated annealing on $\tau$ by starting with an “easier” problem and slowly increasing the rigidity of the constraints, which is also employed in the sequentially constrained Monte Carlo. Suppose we do a $T$ step-simulated annealing, we need to
Algorithm 2 $n$-point Constrained Minimum Energy Design (CoMinED).

Input: (i) $\{g_t(x) \leq 0\}_{t=1}^T$ that define the design space $X = \{x \in [0, 1]^p : g_t(x) \leq 0 \ \forall k\}$, (ii) the increasing sequence of rigidity parameter $0 = t_0 < t_1 < \cdots < t_T = 10^6$, and (iii) the number of nearest neighbors $Q$ considered for candidate augmentation.

1: **Initialization**: simulate $N_1 > n$ (prime number) lattice points $\{y_j^{(1)}\}_{j=1}^{N_1}$ from $[0, 1]^p$ as the initial set of candidate samples $C^1$.

2: for $t = 1, \ldots, T$ do

3:  **Construction**: solve (17) with $\tau = t_1$ by one-point-at-a-time greedy algorithm (9) to obtain the CoMinED $D^t = \{x_i^t\}_{i=1}^n$, i.e., with $\{x_1^t, \ldots, x_m^t\}$, $x_{m+1}^t$ is given by

\[
x_{m+1}^t = \arg\max_{x \in C^t \setminus \{x_i^t\}_{i=1}^{m}} \min_{k=1}^{K} \frac{1}{2p} \log \Phi(-\tau g_k(x)) + \frac{1}{2p} \sum_{k=1}^{K} \log \Phi(-\tau g_k(x_i^t)) + \log \|x_i - x_j\|_p.
\]

4: if $t < T$ then

5:  **Augmentation**: augment the set of candidate samples $C^{t+1} = C^t \cup \tilde{C}^t$ where $\tilde{C}^t$ is the set of linear combinations of nearby points in $D^t$.

6: for $i = 1, \ldots, n$ do

7:  find the $Q$ nearest neighbors of $x_i$ in $D^t$.

8:  for each nearest neighbor $\tilde{x}_{i,q}$ ($q = 1, \ldots, Q$), compute the mid-point

\[
x_{i,q}^{(m)} = x_i + \frac{1}{2}(\tilde{x}_{i,q} - x_i) = \frac{x_i + \tilde{x}_{i,q}}{2}.
\]

9:  and the reflection mid-point

\[
x_{i,q}^{(r)} = x_i - \frac{1}{2}(\tilde{x}_{i,q} - x_i) = \frac{3x_i - \tilde{x}_{i,q}}{2}.
\]

10: Update $\tilde{C}^t = \tilde{C}^t \cup \{x_{i,q}^{(m)}, x_{i,q}^{(r)}\}$.

11: end for

12: Remove repeated points in $\tilde{C}^t$, and only keep points in $\tilde{C}^t$ that are not in $C^t$.

13: end if

14: end for

Output: (i) feasible candidate samples $\{y_i \in C^T : y_i \in X\}$ and (ii) the CoMinED $D^T$.

first define the increasing sequence of rigidity parameters $0 = t_0 < t_1 < \cdots < t_T = 10^6$. At each step, we generate the $n$-point intermediate CoMinED as follows. Let $\tau_t$ be the rigidity parameter, $C^t = \{y_j^t\}_{j=1}^{N_1}$ be the candidate samples, and $D^t = \{x_i^t\}_{i=1}^n \subseteq C^t$ be the CoMinED at the $t$-th step. To construct $D^{t+1}$, we first augment the candidate samples to $C^{t+1}$ by including the linear combinations of nearby points in $D^t$ which we call adaptive lattice grid refinement, and then apply the one-point-at-a-time greedy algorithm (9) to solve (17) with $\tau_{t+1}$ as the rigidity parameter. Algorithm 2 presents the detail procedures of generating CoMinED.

Now let us discuss the advantage of the proposed adaptive lattice grid refinement over the local maximin LHDs for candidate augmentation. In the MinED algorithm, Joseph et al. (2019) augment the candidate points by maximin LHDs in the local region of each MinED point, where the local region is defined as the hypercube inscribed in the ball with center being the MinED point and radius being the distance to its nearest neighbor in the design. The left panel of Fig. 4 shows the candidate augmentation by the local maximin LHDs. The initial set of points (red circles) are generated using “Lattice” function in R package mined (Wang and Joseph 2019) and maximin LHDs are generated using “maximinLHS” function in R package lhs (Carnell 2020). We see that (i) some of the augmented candidate samples are arbitrarily close because local regions are overlapping, and (ii) some regions are left unexplored since the proposed local hypercubes cannot fill the space fully. Given the aforementioned shortcoming of the local maximin LHDs, we propose the adaptive lattice grid refinement (ALGR) for a better “space-filling” candidate augmentation. The ALGR is based on the good rank-1 lattice rule (Nuyens and Cools 2006; Nuyens 2007), one popular type of quasi-Monte Carlo (QMC) methods. Different from other QMC samples such as Halton’ and Sobol’ points (Niederreiter 1992), lattice points possess a grid structure (see the red circles of Fig. 4) that make them advantageous for candidate augmentation. Under the grid structure, all lattice points share the same distance $\delta$ to their nearest neighbors. Augmenting the candidate samples by the mid-point (20) and reflection mid-point (21), we can ensure that the minimal interpoint spacing of the new candidate samples is $\delta/2$. If we do a $T$-step simulated annealing, then the minimum interpoint distance for the final set of candidates would be $\delta/2^T$, which agrees with the minimum interpoint distance constraints used in bridge design (Jones et al. 2015).

The right panel of Fig. 4 shows the candidate augmentation of the ALGR, which is better space-filling than the local maximin LHDs augmentation. Furthermore, the ALGR exhibits a good trade-off between exploration and exploitation. It starts
Fig. 4 One step candidate augmentation (in green diamonds) on 53 lattice points (in red circles) by 11 maximin LHDs in local regions (left panel) and adaptive lattice grid refinement (ALGR) considering 11 nearest neighbors (right panel). (Color figure online)

Fig. 5 Left panel shows 2,155 candidate samples from applying Algorithm 2 to generate \( n = 53 \) points CoMinED on the design space \( \mathcal{X} \) defined by (2) with \( Q = 5 \), \( N_1 = 263 \), \( T = 8 \), and \( \{\tau_t\}_{t=0}^8 = [0, e^1, e^2, e^3, e^4, e^6, e^7, 10^6] \). Red circles indicate the initial candidate set of 263 lattice points. Right panel shows the 915 feasible candidate samples. (Color figure online)

with a space-filling but sparse grid as the candidate set for good exploration of the whole hypercube. As the rigidity parameter \( \tau \) increases, the intermediate CoMinED would only occupy the key regions, leading to refinement of the lattice grid in those regions exclusively for exploitation, and that is why we call it the adaptive lattice grid refinement.

Figure 5 shows the candidate samples of applying Algorithm 2 to generate \( n = 53 \) points CoMinED with \( Q = 5 \) nearest neighbors and \( N_1 = 263 \) (the largest prime number that is less than \( Qn = 265 \)) lattice points as the initial candidate set in \( T = 8 \) steps. With 2,155 evaluations of the constraints, it yields 915 feasible samples that cover the design space uniformly well: almost no gap spotted visually in the right panel of Fig. 5, showing its significant improvement over one-step acceptance/rejection sampling on Latin hypercube samples (Fig. 2) and the adaptive sequentially constrained Monte Carlo approach (Fig. 3), which both conduct 2385 evaluations of the constraints to generate the feasible samples. See supplementary materials for the eight-step evolution of the CoMinED with ALGR augmentation and its comparison with local maximin LHDs augmentation.
Table 1 Basic information for the constraints of the benchmark problems

| Problem        | Dimension ($p$) | No. of LIC | No. of NIC | Feasibility Fraction |
|----------------|-----------------|------------|------------|----------------------|
| MOT (2)        | 2               | 0          | 3          | 0.0053               |
| G01 (Liu et al. 2017) | 13              | 9          | 0          | < 0.0001             |
| G04 (Liu et al. 2017) | 5               | 0          | 6          | 0.2696               |
| G06 (Liu et al. 2017) | 2               | 0          | 2          | 0.0001               |
| G07 (Liu et al. 2017) | 10              | 3          | 5          | < 0.0001             |
| G08 (Liu et al. 2017) | 2               | 0          | 2          | 0.0086               |
| G09 (Liu et al. 2017) | 7               | 0          | 4          | 0.0053               |
| G10 (Liu et al. 2017) | 8               | 3          | 3          | < 0.0001             |
| IBD (Wang 2003) | 4               | 0          | 3          | 0.0015               |
| PVD (Dong et al. 2018) | 4               | 3          | 1          | 0.4032               |
| SRD (Liu et al. 2017) | 7               | 0          | 11         | 0.0019               |
| TSD (Dong et al. 2018) | 3               | 1          | 3          | 0.0075               |
| TTD (Liu et al. 2017) | 2               | 0          | 3          | 0.2179               |
| WBD (Dong et al. 2018) | 4               | 1          | 5          | 0.0010               |
| SCBD (Dong et al. 2018) | 10              | 0          | 11         | 0.0005               |

LIC stands for linear inequality constraints and NIC stands for nonlinear inequality constraints. Feasibility fraction is estimated using $10^7$ Sobol’ points in $[0, 1]^p$.

4 Simulation results

In this section, we report the simulation results of applying CoMinED (Algorithm 2) and adaptive SCMC (Algorithm 1) to 15 benchmark problems with dimensions ranging from 2 to 13 that are popular in the constrained Bayesian optimization literature (Liu et al. 2017; Dong et al. 2018; Chaiyotha and Krityakierne 2020; Tao et al. 2020). Since the one-step acceptance/rejection sampling on Latin hypercube samples is at a clear disadvantage compared to both adaptive SCMC and CoMinED, we do not include the acceptance/rejection sampling simulation results in this section, but are provided in supplementary materials for the interested readers. Table 1 provides some basic information of the 15 problems, and their formulations are provided in supplementary materials. All problems are re-scaled to be in the unit hypercube, and the design measures are also compared under the scaling to $[0, 1]^p$.

Throughout the simulations, CoMinED is ran with $s = 2$ for the distance measure (15), the Euclidean distance. Also, we take $N_1$, the number of the initial candidate samples, to be the largest prime number that is less than the product of the number of CoMinED points $n$ and the number of neighbors to be considered for candidate augmentation $Q$.

4.1 Motivation example

Let us now consider the setting for the adaptive SCMC comparison. Given that we cannot control the total number of constraint evaluations in CoMinED as the repeated samples from augmentation are discarded, we choose the number of samples per iteration in adaptive SCMC to be

$$M = \max\left\{ nQ, \left\lceil \frac{NT}{T + 1} \right\rceil \right\},$$

such that (i) $M$ is larger than the number of initial samples of CoMinED ($N_1 < nQ$), and (ii) the total adaptive SCMC samples $M(T + 1)$ is larger than the total CoMinED samples $NT$. This puts CoMinED in a slightly disadvantageous position in the comparison for assuredly demonstrating its effectiveness over the adaptive SCMC.

Since CoMinED is a deterministic algorithm by the initial candidate of lattice points and the one-point-at-a-time greedy algorithm for designs construction, only one simulation run is performed. For the adaptive SCMC, 50 runs are used for the comparison. Source codes and tutorials can be found at https://github.com/BillHuang01/CoMinED.

Let us first consider the two-dimensional motivation example presented in Fig. 1 with constraints defined in (2). We compare the performance of CoMinED and adaptive SCMC on generating a 53-point design from their feasible candidate set under the following settings: CoMinED is ran with $Q = 5, 11, 17$, and the corresponding adaptive SCMC comparison is ran with $M$ computed by (22).
First, let us look at the quality of the feasible samples. Two metrics are considered for the evaluation. One is the feasible ratio, the percentage of total samples that are feasible. The larger the feasible ratio, the better the algorithm identifying the feasible region for exploitation. However, the feasible ratio alone could be misleading, as we can always restrict the sampling in an arbitrarily small ball around each feasible point, yielding many samples in the feasible region but also leaving unexplored gaps. For example, Fig. 3 shows that 50.5% (1205/2385) of the total adaptive SCMC samples are feasible, but it does not cover the feasible region well as the CoMinED does (Fig. 5), which has the feasible ratio of only 42.0%. Thus, the fill distance, the largest distance of any point in \( X \) to the closest feasible samples, is proposed as the other metric to assess how good the algorithm explores the feasible region completely. The smaller the fill distance the better. In simulation, the fill distance is approximated via \( 10^4 \) feasible samples from acceptance/rejection sampling on a very large set of Sobol’ points in unit hypercube. From Fig. 6, we can see that CoMinED exhibits significant improvement in the fill distance over the adaptive SCMC, though CoMinED has smaller feasible ratio. One intuitive explanation is that by the way of candidate augmentation, CoMinED only refines the lattice grid up to certain granularity such that further refinement would not yield candidate samples that add value to the final space-filling design construction, even though those samples are likely feasible. This shows that the CoMinED naturally comes with the heuristic for adaptive resource allocation between exploration and exploitation during candidate augmentation.

After getting the feasible candidate samples, the next step is to construct the desired \( n \)-point design using the candidate set. In this paper, we consider constructing both maximin and MaxPro designs by the one-point-at-a-time greedy algorithm. Given that the greedy approach likely results in local optimum, we allow for ten restarts to obtain the design with best measure. For maximin measure, the larger the better (Johnson et al. 1990); and for the MaxPro measure, the smaller the better (Joseph et al. 2015b). From Fig. 6, we can see that CoMinED outperforms adaptive SCMC on both maximin and MaxPro design construction using the candidate set, and the improvement is more significant when the total number of samples (i.e., constraints’ evaluations) is small. From both the candidates quality metrics (feasible ratio and fill distance) and the resulted design measures (maximin and MaxPro), additional samples bring minimal benefit for CoMinED as it already cover the feasible space well with \( Q = 5 \) presented in Fig. 5. Moreover, as \( Q \), the number of neighbors considered for candidate augmentation, increases, the total number of constraint evaluations also increases (2155 for \( Q = 5 \), 4951 for \( Q = 11 \), and 7689 for \( Q = 17 \)), and so does the computational time (2 seconds for \( Q = 5 \), 4 seconds for \( Q = 11 \), and 6 seconds for \( Q = 17 \)). Thus, the robust performance of CoMinED under small sample size (\( Q = 5 \)) makes it the favorable option especially when the constraints are expensive to evaluate.

In many real-world problems such as the welded beam design (WBD; Dong et al. 2018) problem, it is common that the constraints yield values in very different scales, as \( g_3 \) of WBD is in the scale of 10 s, but \( g_2 \) is in the scale of 10,000 s. It is natural to test out how CoMinED and adaptive SCMC perform under the aforementioned circumstance. Consider the
Fig. 7 Comparisons of the candidates quality and the resulted 53-point design from applying CoMinED (squares) and adaptive SCMC (violin plots over 50 runs) on the motivation problem (MOT-O, 2) and scaled motivation problem (MOT-S, 23). CoMinED is ran with $Q = 5, 11, 17$, and the corresponding adaptive SCMC comparison is ran with $M$ computed by (22). Results without (in blue) and with (in green) constraint value normalization are both presented. (Color figure online)

The blue squares and violin plots in Fig. 7 are the results from applying CoMinED and adaptive SCMC directly on the motivation problem (MOT-O, 2) and the scaled motivation problem (MOT-S, 23). Comparing the MOT-S and the MOT-O facet, we can see that both CoMinED (blue squares) and adaptive SCMC (blue violin plots) perform substantially worse on all evaluation metrics for the scaled problem. To overcome this deficiency, we propose constraint value normalization using the median absolute deviation (MAD) centered at zero. Suppose that we have evaluated the constraints on some samples $\{x_i\}_{i=1}^{N'}$, we replace the constraints $g_k$ in CoMinED and adaptive SCMC by

$$\tilde{g}_k(\cdot) = \frac{g_k(\cdot) - \text{Median}_{i=1:N'}(|g_k(x_i) - 0|)}{\sigma_k},$$

where $\sigma_k = \text{Median}_{i=1:N'}(|g_k(x_i) - 0|)$. The use of MAD instead of standard deviation is for robustness against large absolute constraint values. The green squares and violin plots in Fig. 7 shows the performance of CoMinED and adaptive SCMC with the constraint value normalization. Compared to the results without the constraint value normalization (blue squares and violin plots), substantial improvements are observed, especially on the scaled motivation example. Hence, for the rest of the simulations, we only compare CoMinED to adaptive SCMC after incorporating constraint value normalization.

scaled version of the motivation example (MOT-S) presented below:

$$g_1(x) = 10^{-1}(x_1 - \sqrt{50(x_2 - 0.52)^2 + 2} + 1) \leq 0$$
$$g_2(x) = \sqrt{120((x_2 - 0.48)^2 + 1)} - 0.75 - x_1 \leq 0$$
$$g_3(x) = 10^3(0.65^2 - x_1^2 - x_2^2) \leq 0$$

where $0 \leq x_i \leq 1$ ($i = 1, 2$).
Fig. 8 Comparisons of the candidates quality and the resulted 109-point design from applying CoMinED (squares) and adaptive SCMC (violin plots over 50 runs) on 14 benchmark problems. The problems are in ascending order by number of dimensions and descending order by the feasibility fraction. CoMinED is ran with $Q = 19$ for problems with dimension smaller than 10 and $Q = 27$ for problems with dimensions at least 10 (SCBD, G07, G01), and the corresponding adaptive SCMC comparison is ran with $M$ computed by (22). For each problem, the evaluation metrics are shifted such that the median of the adaptive SCMC results is 0 and rescaled such that the IQR of adaptive SCMC results is 1. Both metrics are truncated at $\pm 5$ for visualization purpose.

### 4.2 More benchmark problems

To further demonstrate the improvement of CoMinED, let us look at the simulation results on the 14 benchmark problems with dimensions ranging from 2 to 13, including seven real-world engineering problems. Top panels of Fig. 8 compare the quality of the candidate samples. Except for the two-dimensional problems (TTD, G08, G06), CoMinED shows strong improvement in the feasible sample ratio, especially on the high-dimensional problems. For example, 23.12% of the total CoMinED samples are feasible for problem G01, while adaptive SCMC only yields in average 0.78% feasible samples (see supplementary materials for the actual feasible ratio value). On the other hand, looking at the fill distance\(^1\), CoMinED outperforms the adaptive SCMC for all benchmark problems except G04, which is a five-dimensional problem with feasibility fraction of 27.0% (Table 1). Given that G04 is an “easy” problem, with more than 15,000 evaluations of the constraints (see supplementary materials), both CoMinED and adaptive SCMC should yield samples that cover the feasible region well. Next, let us look at the performance of the 109-point designs constructed from the feasible candidate samples. Similar to the motivation examples, we

\(^1\) Fill distance is again approximated by $10^4$ feasible samples by acceptance/rejection sampling on a larger set of Sobol’ points in unit hypercube. However, for problem G07, only $10^3$ samples are used since it is too expensive to generate more feasible samples by acceptance/rejection given its extremely small feasibility fraction (less than $1e^{-6}$).
allow for ten restarts of the one-point-at-a-time greedy algorithm to obtain the best design. From the bottom panels of Fig. 8, we can see that both maximin and MaxPro designs generated using the CoMinED candidates significantly outmatch the corresponding designs by the adaptive SCMC samples. In summary, from the extensive simulation results on the 14 benchmark problems, CoMinED is more robust than the adaptive SCMC for generating good space-filling design candidate points in arbitrary non-rectangular bounded design space, especially when the space is high dimensional and highly constrained.

5 Conclusion

This paper proposes the constrained minimum energy design (CoMinED; Algorithm 2) for constructing space-filling designs in any non-rectangular bounded space defined by inequality constraints. The key idea of the CoMinED is to employ the state-of-the-art deterministic sampling algorithm, minimum energy design (MinED), on the target distribution using the probabilistic constraints proposed in sequentially constrained Monte Carlo (SCMC). Different from the use of local maximin LHDs for candidate augmentation in the MinED algorithm, we propose the adaptive lattice grid refinement that would impose restriction on the minimal interpoint spacing for the candidate samples, making them more favorable as the candidate set for space-filling designs construction. The extensive simulations on the 15 benchmark problems with dimensions ranging from 2 to 13 demonstrate the significant improvement of CoMinED over adaptive SCMC, the best candidate generation approach we can find from the existing literature. CoMinED also enjoys from fewer number of constraint evaluations by avoiding the sampling of the arbitrarily close points that add minimal value for the space-filling designs construction. However, many real-world applications involve discrete variables, but CoMinED and adaptive SCMC can only handle continuous variables. One future research direction is to investigate how to construct constrained space-filling design on the set of mixed discrete and continuous variables. On the other hand, as some recent papers have proposed that “sampling can be faster than optimization” (Ma et al. 2019), another future research direction is to investigate how CoMinED might be useful for solving expensive constrained optimization problem.

Supplementary Information

Source codes are available at https://github.com/BillHuang01/CoMinED.

Supplementary Information

The online version contains supplementary material available at https://doi.org/10.1007/s11222-021-10054-2.

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Appendix

A Implementation details of the CoMinED algorithm

In this section, we discuss some implementation details of CoMinED (Algorithm 2) regarding the choice of parameters and ways to improve the computational efficiency. Let us assume that the number of design points \( n \) and the number of nearest neighbors considered in candidate augmentation \( Q \) are user-specific. For \( Q \), we suggest the use of any number between \( 2p + 1 \) and \( 3p + 1 \) depending on the available computational resource. One natural choice for \( N_{1} \), the number of initial lattice candidate points, is the greatest prime number that is smaller than \( Qn \). This approach is taken for all simulations ran in this paper. Next, let us discuss how to choose the increasing sequence of rigidity parameters \( \{\tau_{t}\}_{t=0}^{T} \) with \( \tau_{0} = 0 \) and \( \tau_{T} = 10^{6} \). In this paper, we use \( \{\tau_{t}\}_{t=0}^{8} = [0, e^{1}, e^{2}, e^{3}, e^{4}, e^{5}, e^{6}, e^{7}, 10^{6}] \) that shows robust performance on problems with dimensions ranging from 2 to 13. If the user wants to try different number of intermediate steps \( T \), one suggestion is to have them equally spaced in log-scale between \( e^{0} \) and \( e^{7} = 1096.6 \), i.e., \( \tau_{0} = 0 \),

\[
\tau_{t} = \exp \left\{ \frac{7}{T-1} t \right\} \quad \text{for} \quad t = 1, \ldots, T - 1,
\]

and \( \tau_{T} = 10^{6} \). Moreover, as pointed out by Golchi and Loeppky (2015), one adaptive approach to determine \( \tau_{t+1} \) from the existing samples is to ensure that the effective sample size does not fall below certain threshold when we transition from \( \tau_{t} \) to \( \tau_{t+1} \). Similar idea is also applicable for CoMinED.

Last, we address one computational burden of CoMinED resulted from the increasing number of candidate samples used at the one-point-at-a-time greedy algorithm in the intermediate designs construction step as the algorithm proceeds. Recall our goal is to solve

\[
D_{n}^* = \arg \max_{D_{n} \subseteq C} h(D_{n}),
\]
with
\[
 h(D_n) = \min_{x_i, x_j \in D_n} \frac{1}{2p} \log \rho_{\tau_i}(x_i) + \frac{1}{2p} \log \rho_{\tau_j}(x_j) + \log \|x_i - x_j\|_s,
\]

where \(\rho_{\tau_i}(\cdot) = \prod_{k=1}^{K} \Phi(-\tau_i g_k(\cdot))\) is the probabilistic constraints function and \(C^t\) is the \(t\)-th step \(N_t\)-point candidate set. One easy solution is to ignore samples in \(C^t\) that are not important, i.e., we only apply the greedy algorithm on \(\{y \in C^t : \log \rho_{\tau_i}(y) > \eta\}\) where \(\eta\) is some threshold indicating that whether a sample would have a impact on the solution of (26). For the distance measure \(s = 2\) considered in this paper, we know that the minimal interpoint distance of all candidate points is \(\delta_i = \delta/2^i\) where \(\delta\) is the minimal interpoint distance of the initial candidate set. Thus, \(\log \|x_i - x_j\|_2\) in (26) is lower bounded by \(\log \delta_i\). For notation simplicity, denote the log-likelihood value by \(v_i = \log \rho_{\tau_i}(x_i)\). Let \(D_n\) be the \(n\) samples from the candidate set \(C^t\) with the top log-likelihood value, and thus we have
\[
 h(D_n^*) \geq h(D_n) \geq \frac{1}{2p} v^{(n+1)} + \frac{1}{2p} v^{(n+1)} + \log \delta_t.
\]

To avoid numerical comparison issue caused by machine round-off, we use 2.5 instead of 2 in (29) in actual implementation.

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