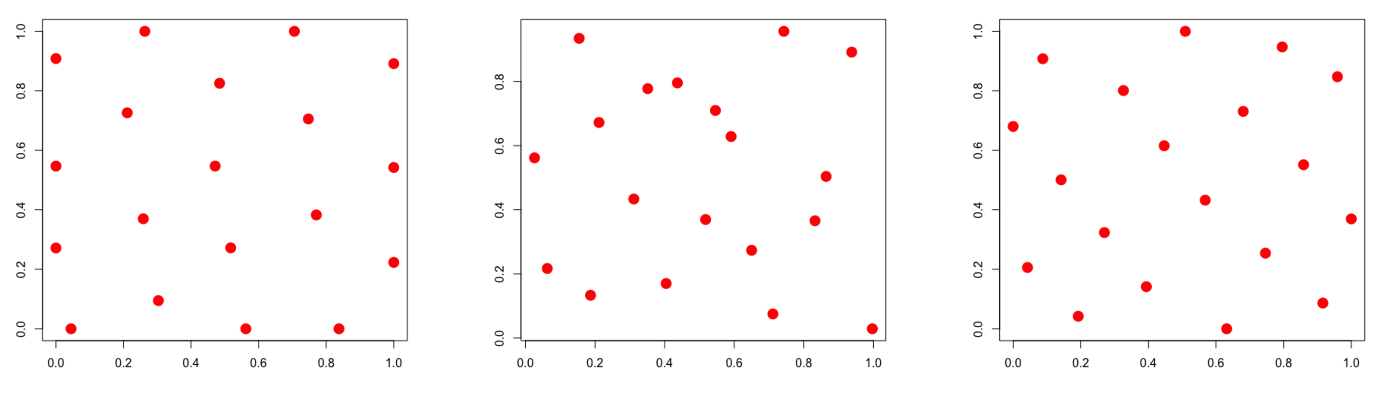
Constrained Minimum Energy Designs

Chaofan Huang [1] V. Roshan Joseph [1] Douglas M. Ray [2]

[1]Gerogia Institue of Technology [2]US Army - CCDC Armaments Center

Space-Filling Designs



(a) Maximin (b) Maximin LHD (c) MaxPro

- Most of the space-filling designs focus on unit hypercube $\mathcal{X} = [0,1]^p$.
- Many real world problems deal with non-rectangular bounded design space

$$\mathcal{X} = \left\{x \in [0,1]^p : g_k(x) \leq 0 \; \forall k = 1, \dots, K\right\},$$

where the rectangular shape is jeopardized by the K inequality constraints.
- How can we construct space-filling design in the constrained region?

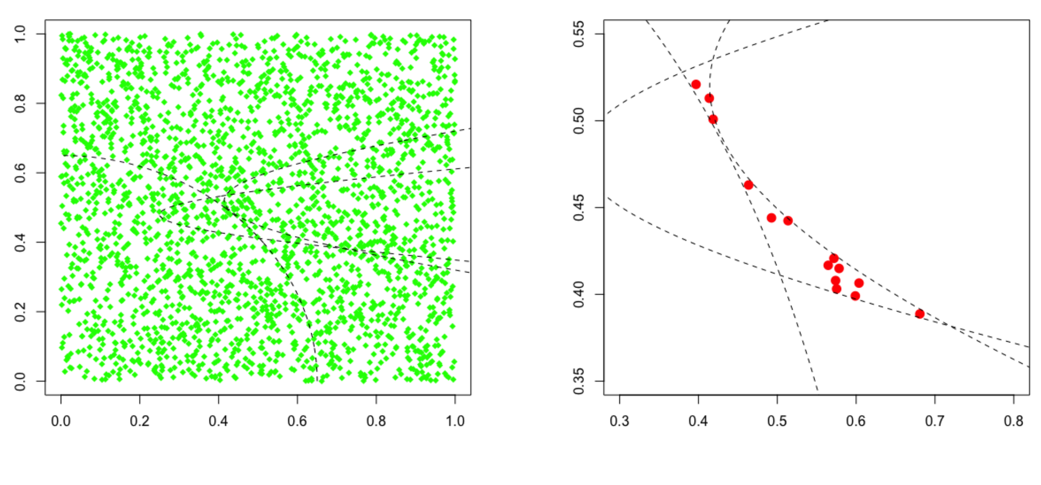
Constrained Space-Filling Designs

- General purpose constrained optimization techniques: **Expensive!**
- Alternative two-step approach:
  - **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 key difficulty is to efficiently simulate good quality candidate points.

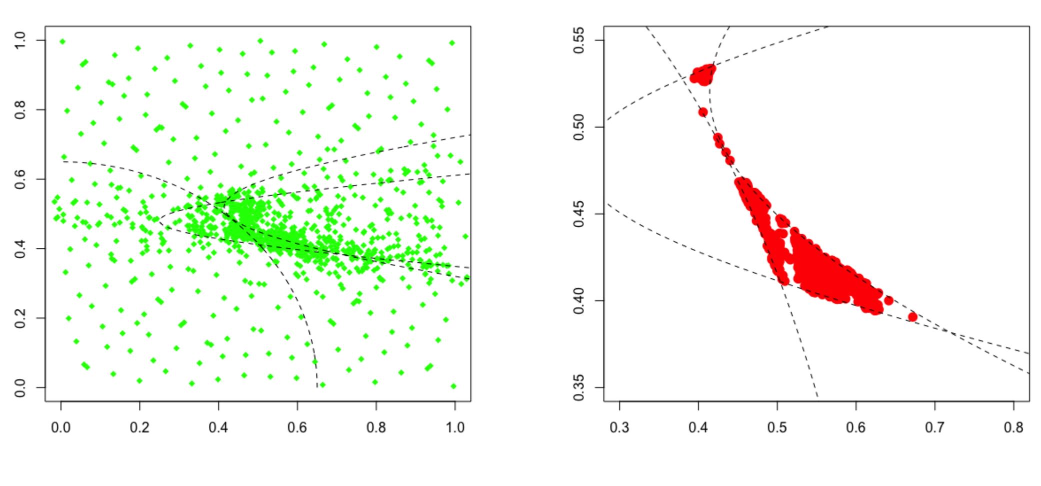
Existing Candidate Generation Methods

- Acceptance/rejection sampling on Latin hypercube designs (LHDs).



(a) 2,385 LHD samples (b) 14 feasible samples

- Sequentially constrained Monte Carlo (SCMC) with kernel adaptation.



(a) 2,385 SCMC samples (b) 1,205 feasible samples

Probabilistic Relaxation of Constratint

- Introduced in SCMC to relax constriant $g(x) \leq 0$ via probit function,

$$\rho_\tau = \Phi(-\tau g(x)) ,$$

where Φ is the standard normal c.d.f. and τ is the *rigidity* parameter.
- When $\tau = 0$, we have the uniform distribution. When $\tau \to \infty$, we have

$$\lim_{\tau \to \infty} \rho_\tau(x) = \lim_{\tau \to \infty} \Phi(-\tau g(x)) = \mathbb{1}(g(x) \leq 0) .$$

- The generalization to multiple constraints $\{g_k(x) \leq 0\}_{k=1}^K$ is straightfoward,

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

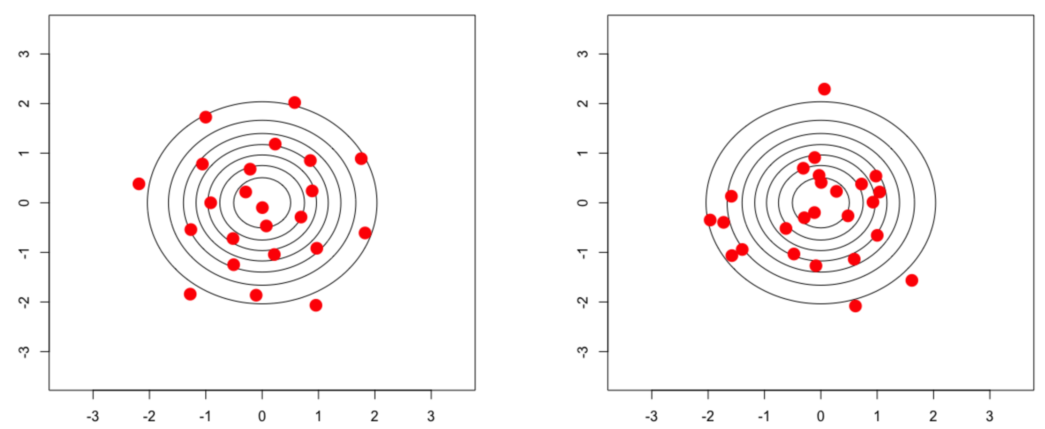
- This allows for a sequential approach by starting with an easy problem ($\tau = 0$) and slowly increasing τ to a large number, e.g. 10^6, to achieve the space-filling design in the desired constrained region.

Minimum Energy Designs

- Minimum energy designs (MinED) finds the design that minimizes the total potential energy with respect to any distribution π. Its design criterion is

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

where $\gamma \propto \pi$ is the unnormalized p.d.f. When $\pi = \text{Uniform}[0,1]^p$, it reduces to a maximin design in the unit hypercube.



(a) MinED (b) Monte Carlo

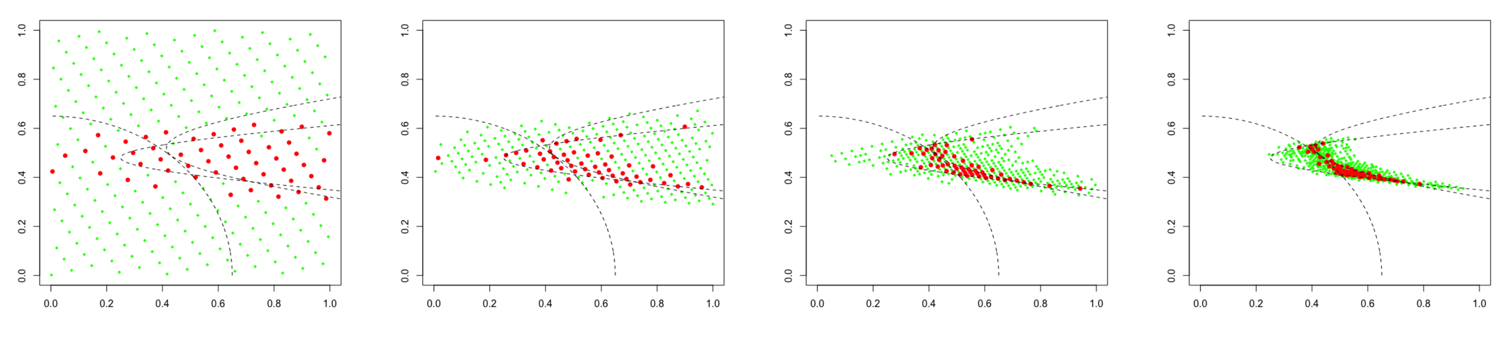
Constrained Minimum Energy Designs

- Constrained minimum energy designs (CoMinED) with respect to π and the non-rectangular bounded space $\mathcal{X} = \{x \in [0,1]^p : g_k(x) \leq 0 \; \forall k = 1, \dots, K\}$ is the optimal solution of

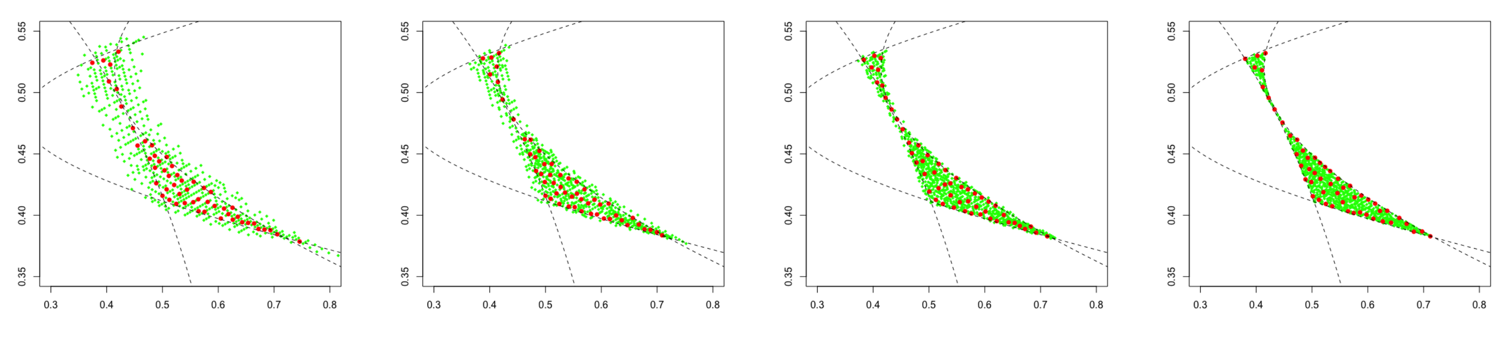
$$\arg\max_{\mathcal{D}_n} \min_{\substack{x_i, x_j \in \mathcal{D}_n \\ i \neq j}} \frac{1}{2p} \log \tilde{\gamma}_\tau(x_i) + \frac{1}{2p} \log \tilde{\gamma}_\tau(x_j) + \log \|x_i - x_j\|_2 ,$$

where $\tilde{\gamma}_\tau(\cdot) = \gamma(\cdot) \times \rho_\tau(\cdot) = \gamma(\cdot) \prod_{k=1}^K \Phi(-\tau g_k(\cdot))$ and $\gamma \propto \pi$.
- We focus on $\pi = \text{Uniform}[0,1]^p$ for the comparison with existing methods.
- The algorithm iterates between (i) the intermediate design construction with respect to the increasing τ_t and (ii) the candidate samples augmentation to exploit the important region indicated by the intermediate design.

Evolution of CoMinED



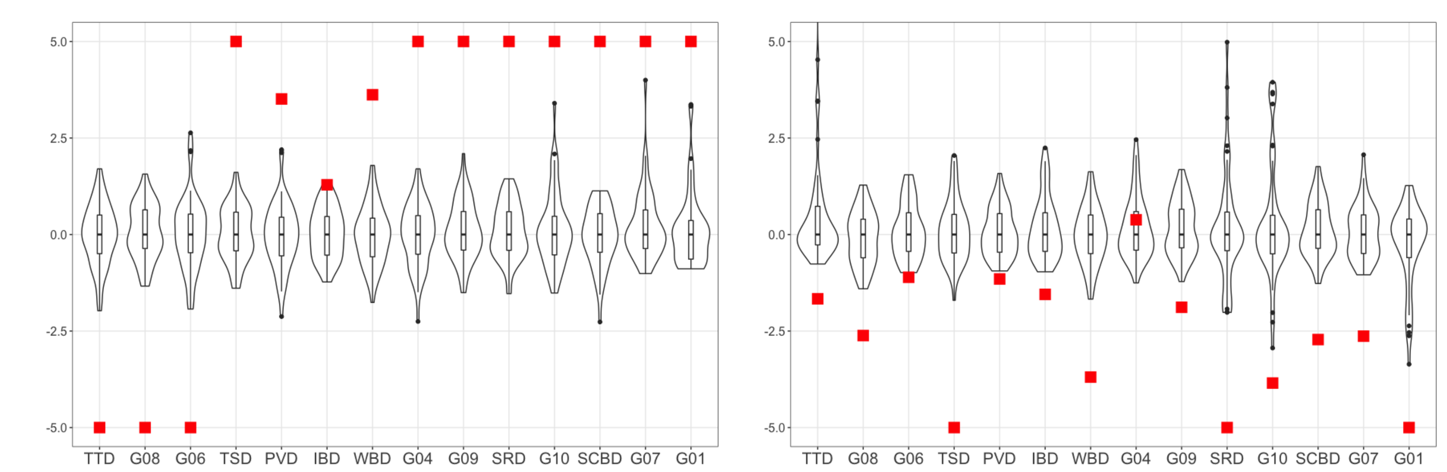
(a) $\tau_1 = e^1$ (b) $\tau_2 = e^2$ (c) $\tau_3 = e^3$ (d) $\tau_4 = e^4$



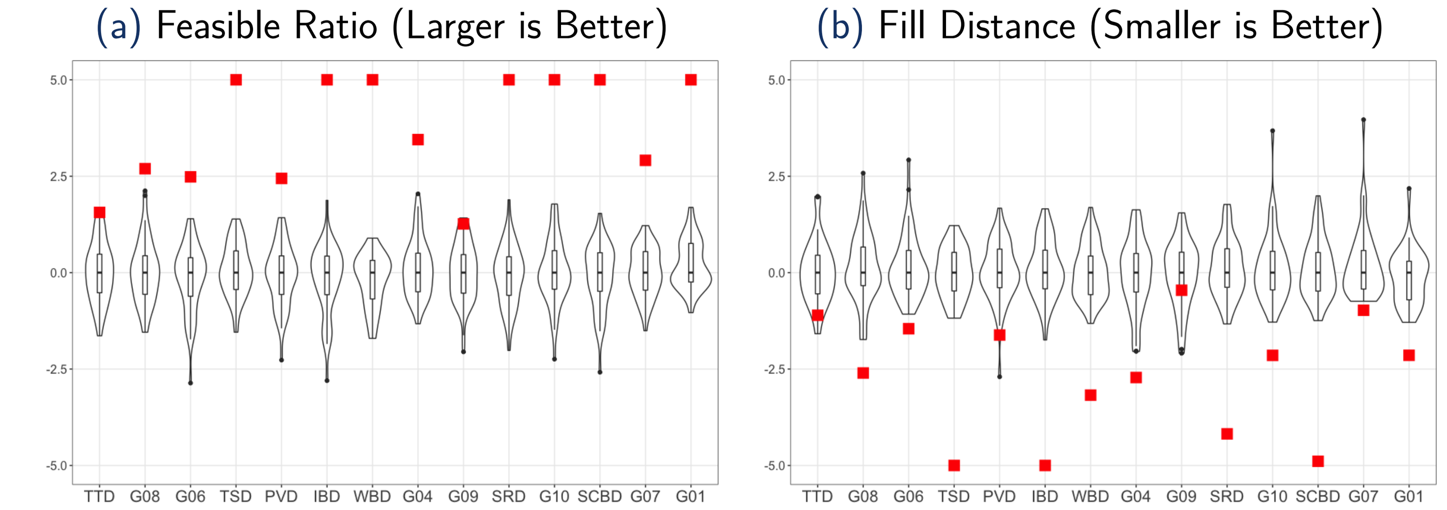
(e) $\tau_5 = e^5$ (f) $\tau_6 = e^6$ (g) $\tau_7 = e^7$ (h) $\tau_8 = e^8$

- Total of 2,155 evaluations of the constraints, 915 feasible samples.

Numerical Results



(a) Feasible Ratio (Larger is Better) (b) Fill Distance (Smaller is Better)



(c) Maximin (Larger is Better) (d) MaxPro (Smaller is Better)

Figure: 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 (2 - 13) and descending order by the feasibility ratio (11 out of 14 are less than 0.01 with the smallest being 1e-6).

References

[1] Joseph, V. R., Gul, E., and Ba, S. (2015), "Maximum projection designs for computer experiments," *Biometrika*, 102.2, pp. 371-380.

[2] Golchi, S. and Campbell D. A. (2016), "Sequentially constrained Monte Carlo," *Computational Statistics & Data Analysis*, 97, 98-113.

[3] Joseph, V. R., Wang, D., Gu, L., Lyu, S., and Tuo, R. (2019), "Deterministic sampling of expensive posteriors using minimum energy designs,", *Technometrics*, 61, 297-308.