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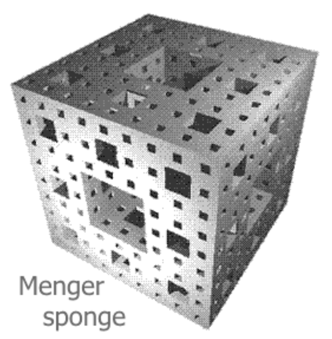
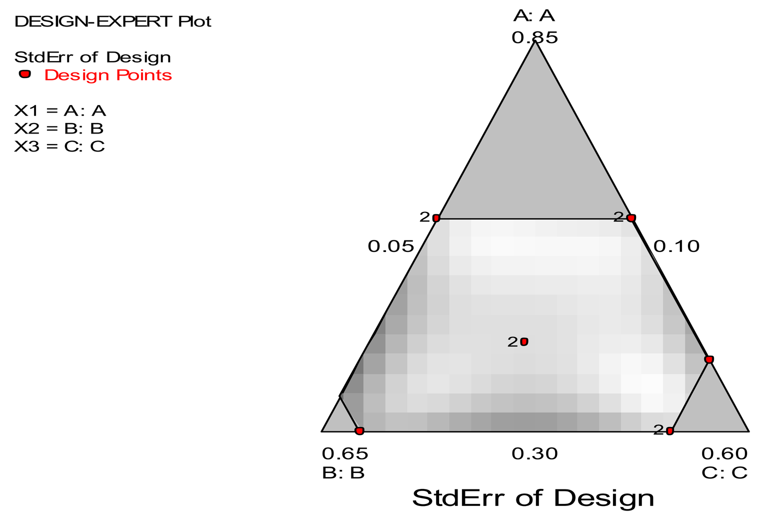
Coordinate-Exchange Simulated Annealing Algorithm for Constrained Optimal Design

Lulu Kang, Department of Applied Mathematics, Illinois Institute of Technology, Chicago, IL



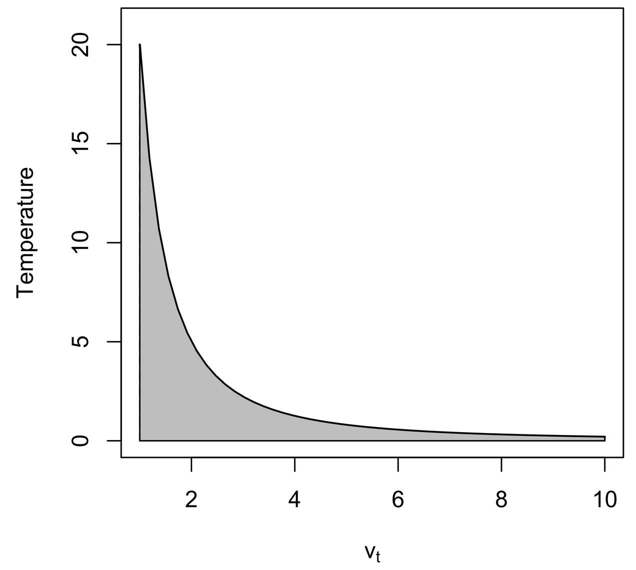
Motivations

- **Physical Experiments: mixture experiments. (Cornell, 2002)**



Linear Constraints only!

- **Computer Experiments**



More Complex Constraints!

E.g. Nonlinear Constrain for the Mathematical Model for the Low Pressure Chamber.

Literature on Constrained DOE

- **Physical Experiments:**
  - **Mainly are mixture experiments (Cornell 2002)**
  - **Montgomery et al. (2002): bond strength of adhesive**
  - **Hung et al. (2010) and Hung (2011)**

All methods are for linear constraints only!

- **Computer Experiments:**
  - **Sasena et al. (2002): applied optimization**
  - **Trosset (1999) and Stinstra et al (2003)**
  - **Draguljie, Dean, and Santner (2012)**

Can work for nonlinear Constraints. But need advanced NLP solver!

Can work for nonlinear Constraints. But need to generate huge candidate set!

Not accessible or Inefficient!

Coordinate-Exchange Algorithm

- Finding the *optimal* coordinate is a one-dimension optimization problem, *easier and less computational!*
- *No sophisticated NLP solvers are needed.*
- *Coordinate-exchange method can handle broader range of constraints.*
  - Fix all the other p-1 dimensional variable value and vary only one variable value.
  - If the p-dimensional constraints are convex, then the projected one-dimension feasible region becomes a single-interval set.
  - If the p-dimensional design space are non-convex or disconnected, then the one-dimension feasible region contains multiple intervals.
- *Exchanging one coordinate of the design leads to less computation in updating the objective function.*

Simulated Annealing (SA) Algorithm

- Randomize the selection of coordinate $D_{i,j}$ to exchange.
- Always accept improvement, but also accept the setback with a probability.
- Simulate the metal cooling process, in order to avoid local optimum.
- Initial temperature T_0: large, specified according to the setting of the design.
- Rate of temperature decreasing β between [0.96, 0.99].

Coordinate-Exchange SA Algorithm

D: the design matrix of size n-by-d; Ω is the d-dimension constrained space; $\boldsymbol{x}_i$ is the design point in Ω; ψ(.) is design criterion.

Set the tuning parameters of SA algorithm T_0, β, and $T\varepsilon$. Construct the initial design *D*.

⇩

Compute the row deletion function $d_r(\boldsymbol{x}_i)$ for each row $\boldsymbol{x}_i$ and column deletion function $d_c(X_j)$ for each column X_j. Random choose the row i^* and column j^* with probabilities proportional to $d_r(\boldsymbol{x}_i)$ and $d_c(X_j)$.

⇩

Denote the delta function $\Delta(x_{i^*,j^*}, x)$ as the measurement of improvement of the design criterion by exchanging the coordinate x_{i^*,j^*} with another value x. Solve the optimization problem:

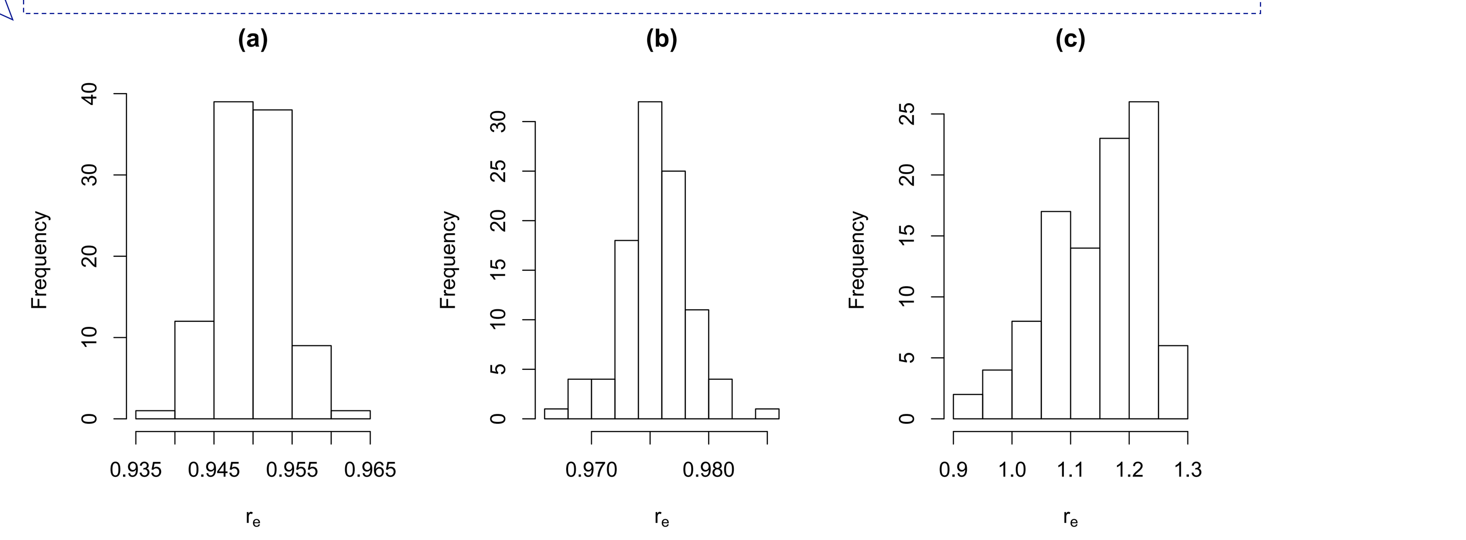
$$\text{Min or Max } \Delta(x_{i^*,j^*}, x) \text{ s.t. } x \text{ in } \Omega_{j^*}(\boldsymbol{x}_{i^*}),$$

where $\Omega_{j^*}(\boldsymbol{x}_{i^*})$ is the projected constraints for $\boldsymbol{x}=\boldsymbol{x}_{i^*}$. Deonte the optimal solution as x^*.

Exchange the optimal solution x^* with x_{i^*,j^*} according to the probability $\pi=\min\{1, \exp(-\Delta(x_{i^*,j^*}, x)/T\}$. Then update all the deletion functions and design matrix. Update the temperature $T \leftarrow T\beta$.

⇧

Iterate Step 1-3 until $T<T\varepsilon$. Return the current design D as the optimal design with the optimal criterion ψ(D).



Histogram of efficiencies of optimal designs returned by proposed method w.r.t. the ones returned by JMP. (a) D-optimal (b) A-optimal (c) ϕ_p space filling design. (with box constraints only!).

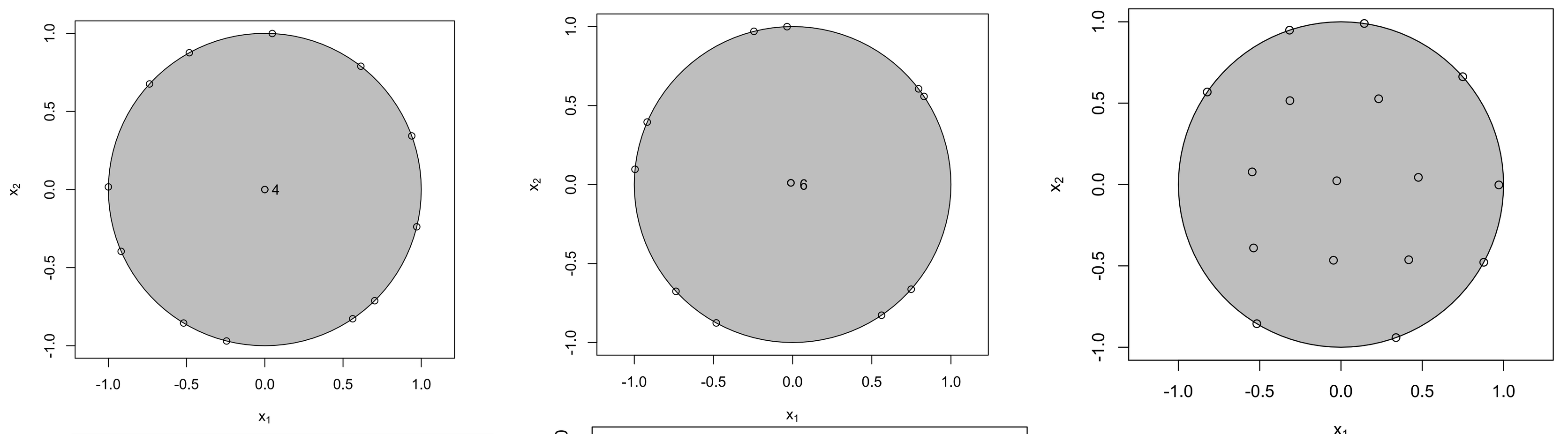
Three design-criterion

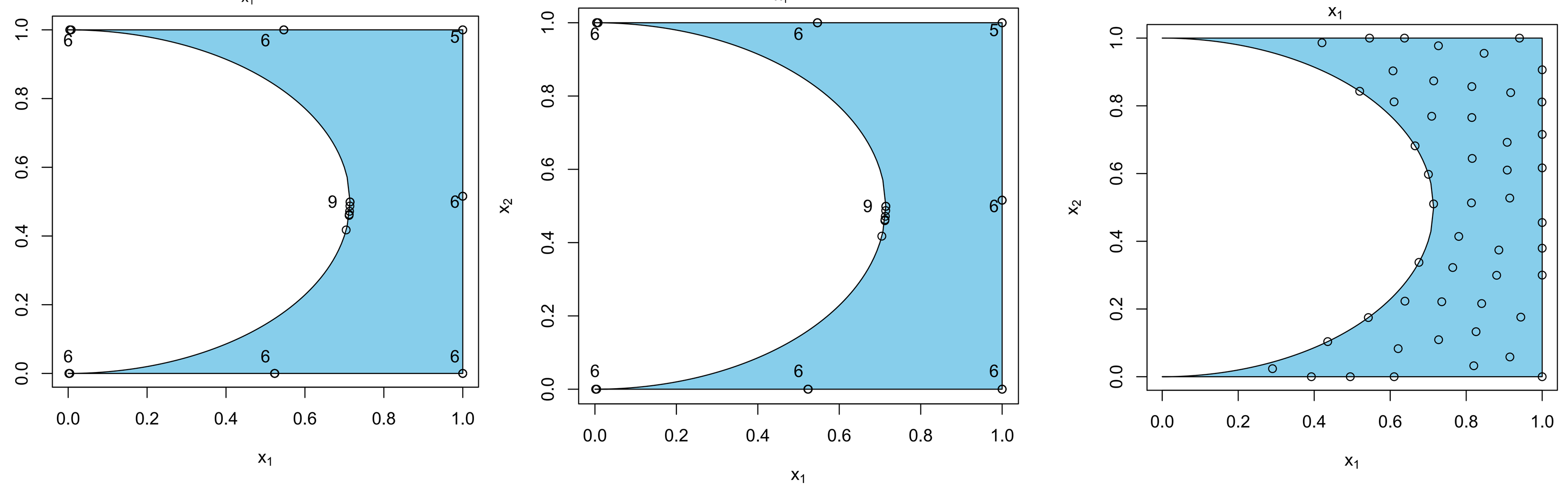
- D-optimal: $\psi(D)=\det(\boldsymbol{F}^T\boldsymbol{F})$
- Linear-optimal: $\psi(D)=\mathrm{tr}(M(\boldsymbol{F}^T\boldsymbol{F})^{-1})$
- ϕ_p space filling: $\psi(D)=\phi_p(D)=\left(\sum_{i,j=1}^{n} d(\mathbf{x}_i,\mathbf{x}_j)^{-p}\right)^{1/p}$

Need to derive the delta function, deletion functions, and updating formula for different criteria.

Examples

- **Convex Constraint:** $x_1^2+x_2^2 \leq 1$
- **Non-convex Constraint:** $(0.7x_1)^2+(x_2-0.5)^2 \geq 0.25$





D-optimal A-optimal Space Filling