MaxPro Designs for Computer Experiments

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(joint work with Shan Ba and Evren Gul)

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Georgia Tech College of Engineering
H. Milton Stewart School of
Industrial and Systems Engineering

Outline

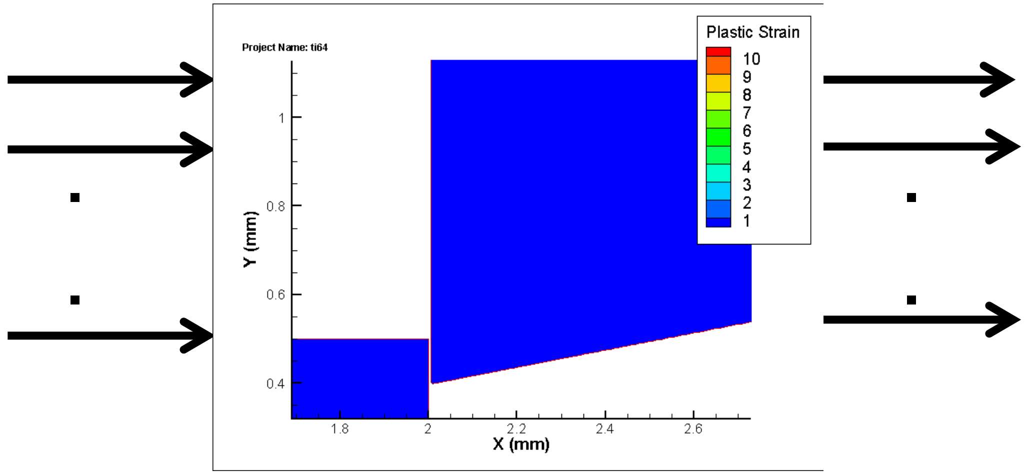
- Introduction
- Space-filling design
  - Minimax, maximin, LHD
  - MaxPro
- Qualitative factors
- R package: MaxPro

Introduction

Joseph, V. R. (2016). “Space-Filling Designs for Computer Experiments: A Review,” (with discussions and rejoinder), *Quality Engineering*, 28, 28-44.

Computer experiments

inputs

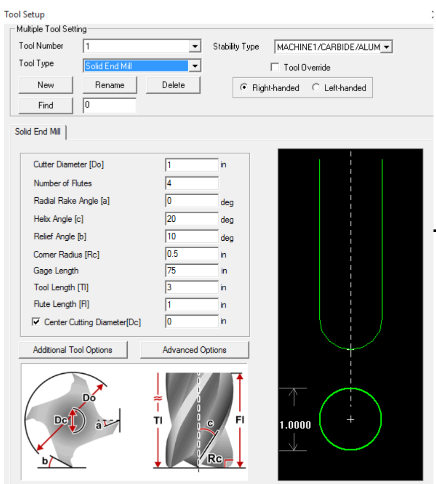


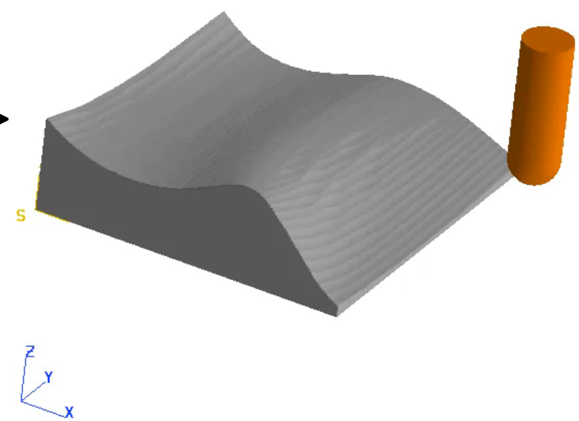
outputs

- Expensive black-box code
- Deterministic outputs
- Complex relationships

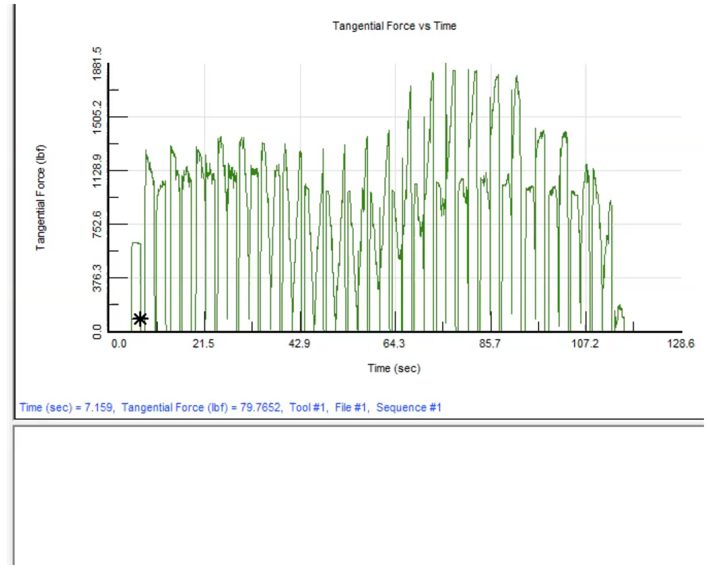
An Example: machining simulation

Inputs



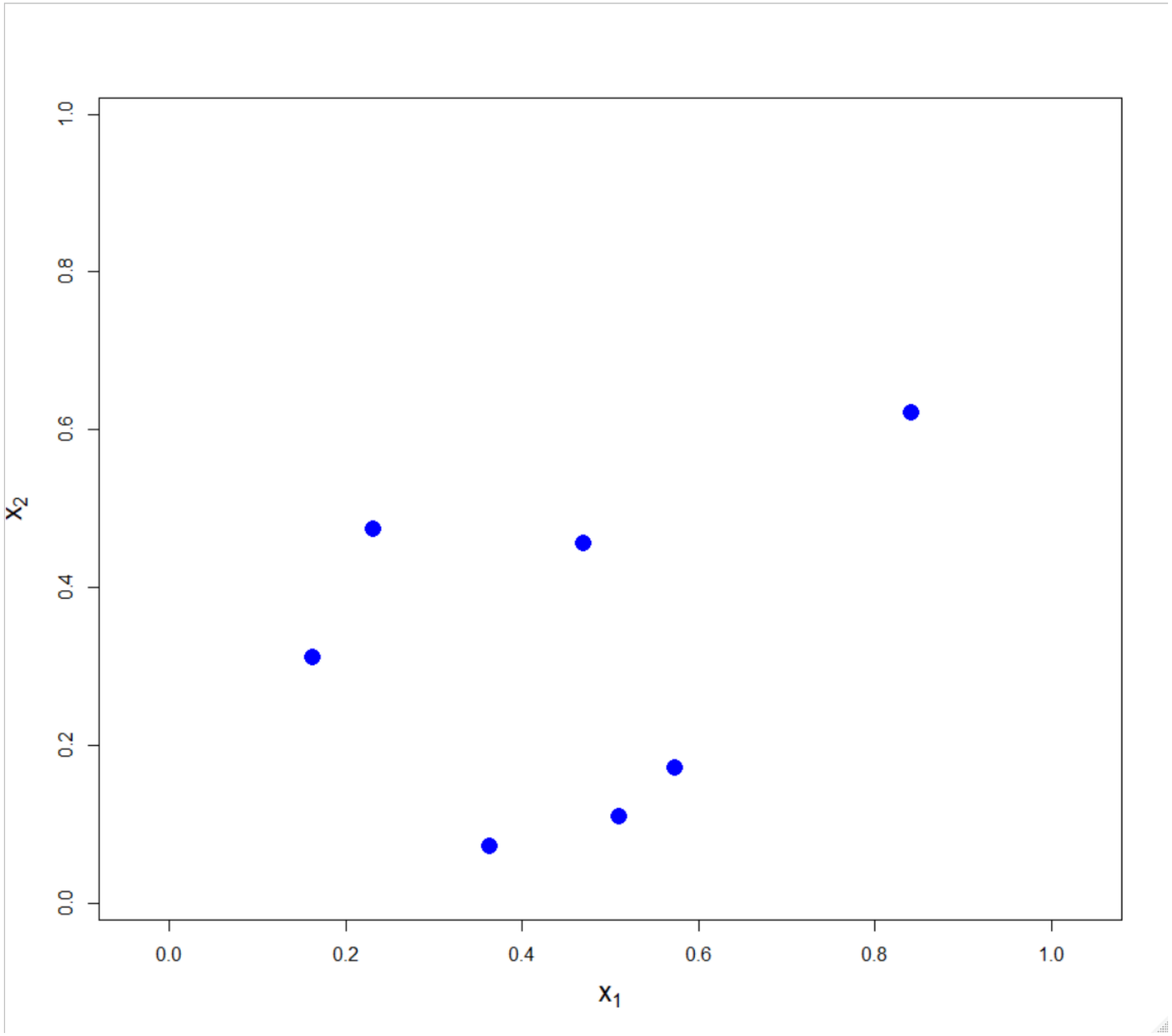


Output

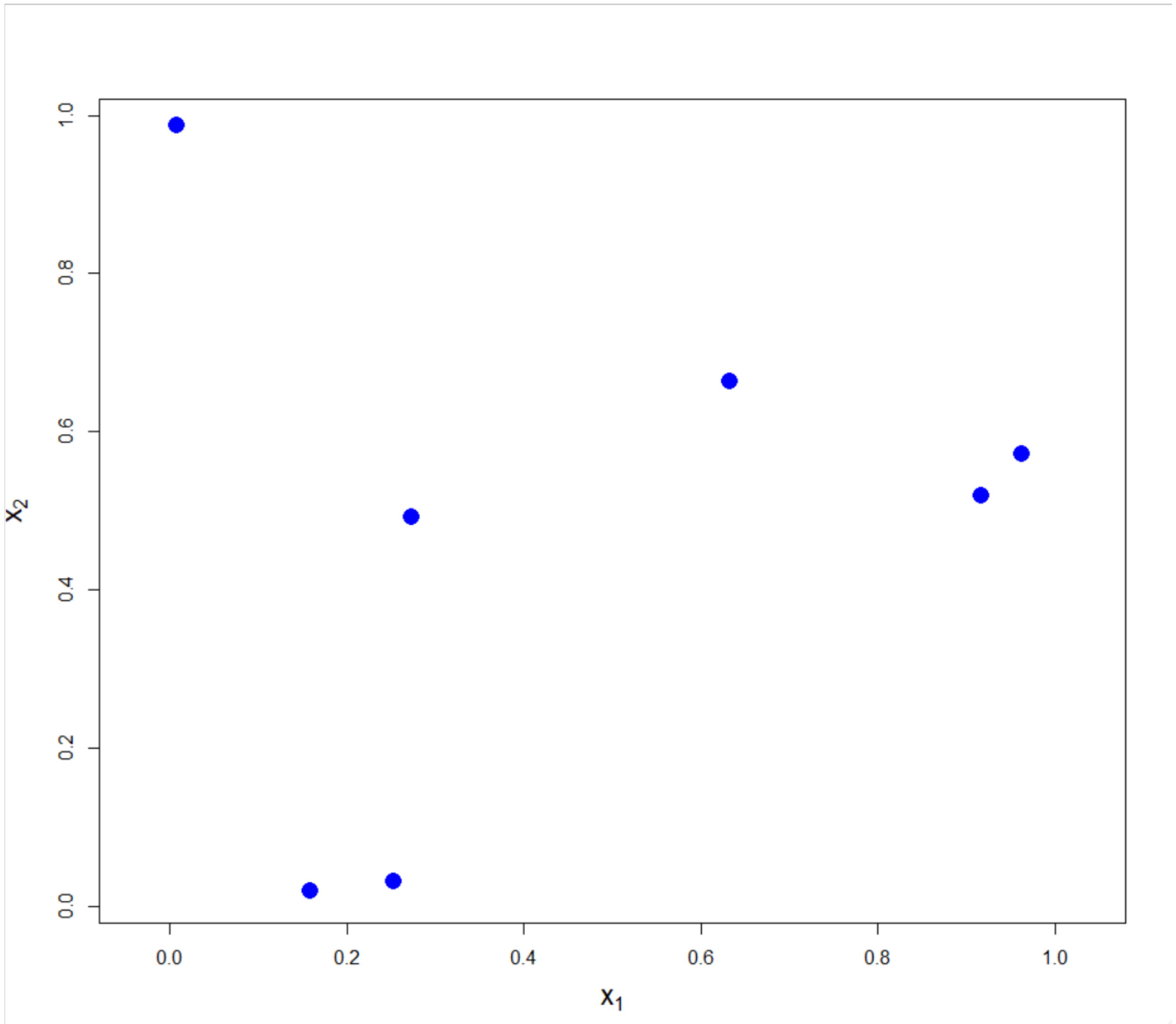


Gul, E., Joseph, V. R., Yan, H., and Melkote, S. N. (2018). “Uncertainty Quantification in Machining Simulations Using In Situ Emulator,” *Journal of Quality Technology*, 50, 253-261.

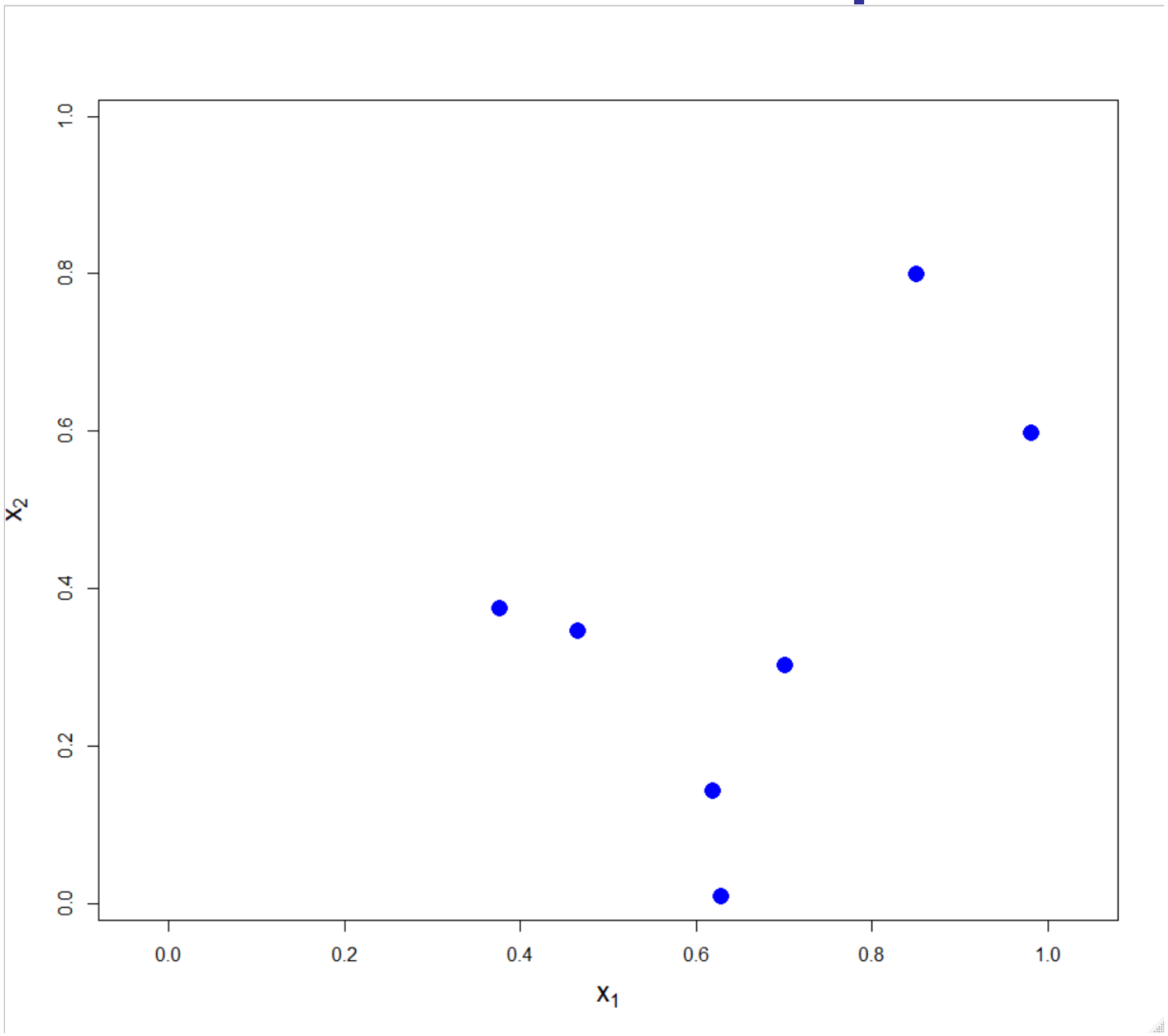
Random Sample



Random Sample



Random Sample



Space-Filling Designs

- Definition:

  designs that fill the space!

- What is the meaning of filling the space?
  - Maximin distance
  - Minimax distance
  - Uniform

Minimax design

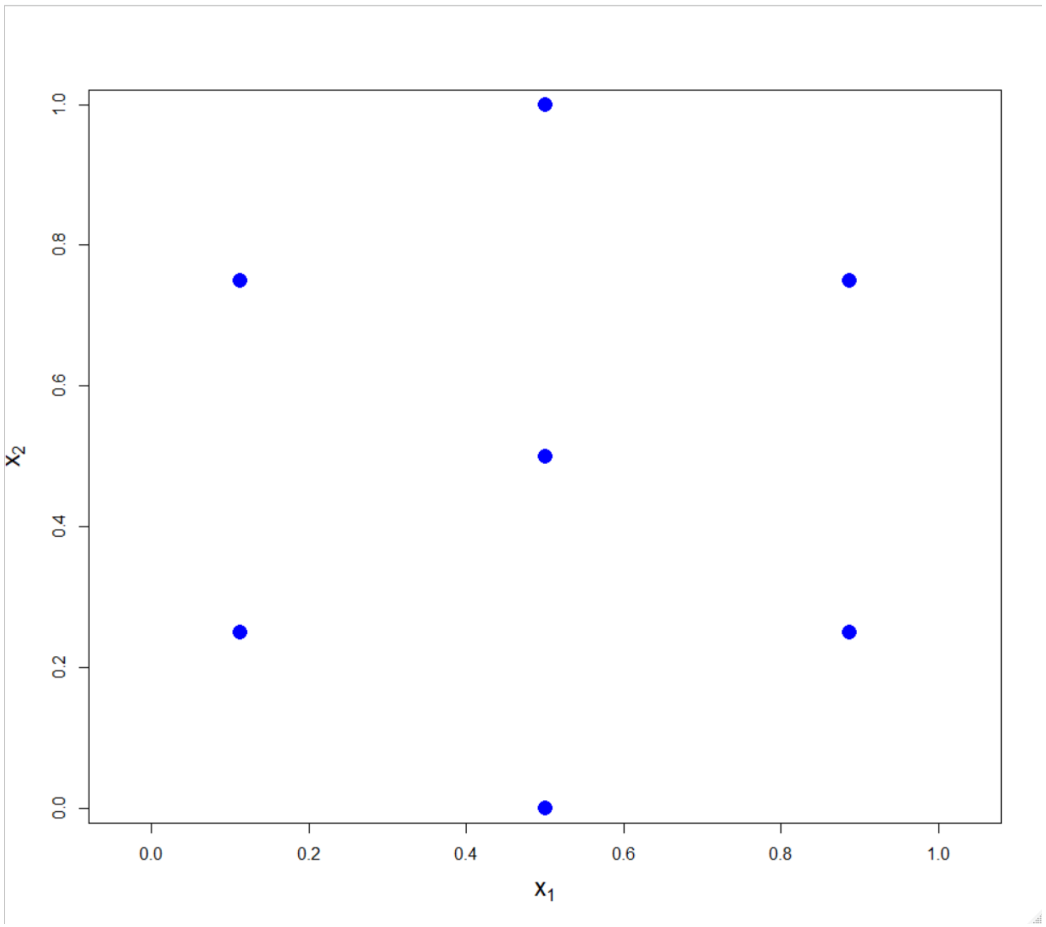
$$D = \{x_1, x_2, \ldots, x_n\} \qquad x_i \in \mathcal{X} = [0,1]^p$$

- Johnson, Moore, and Ylvisaker (1991)

$$\min_{D} \max_{x \in \mathcal{X}} d(x, D),$$

where $d(x, D) = \min_{x_i \in D} d(x, x_i)$.

Minimax design



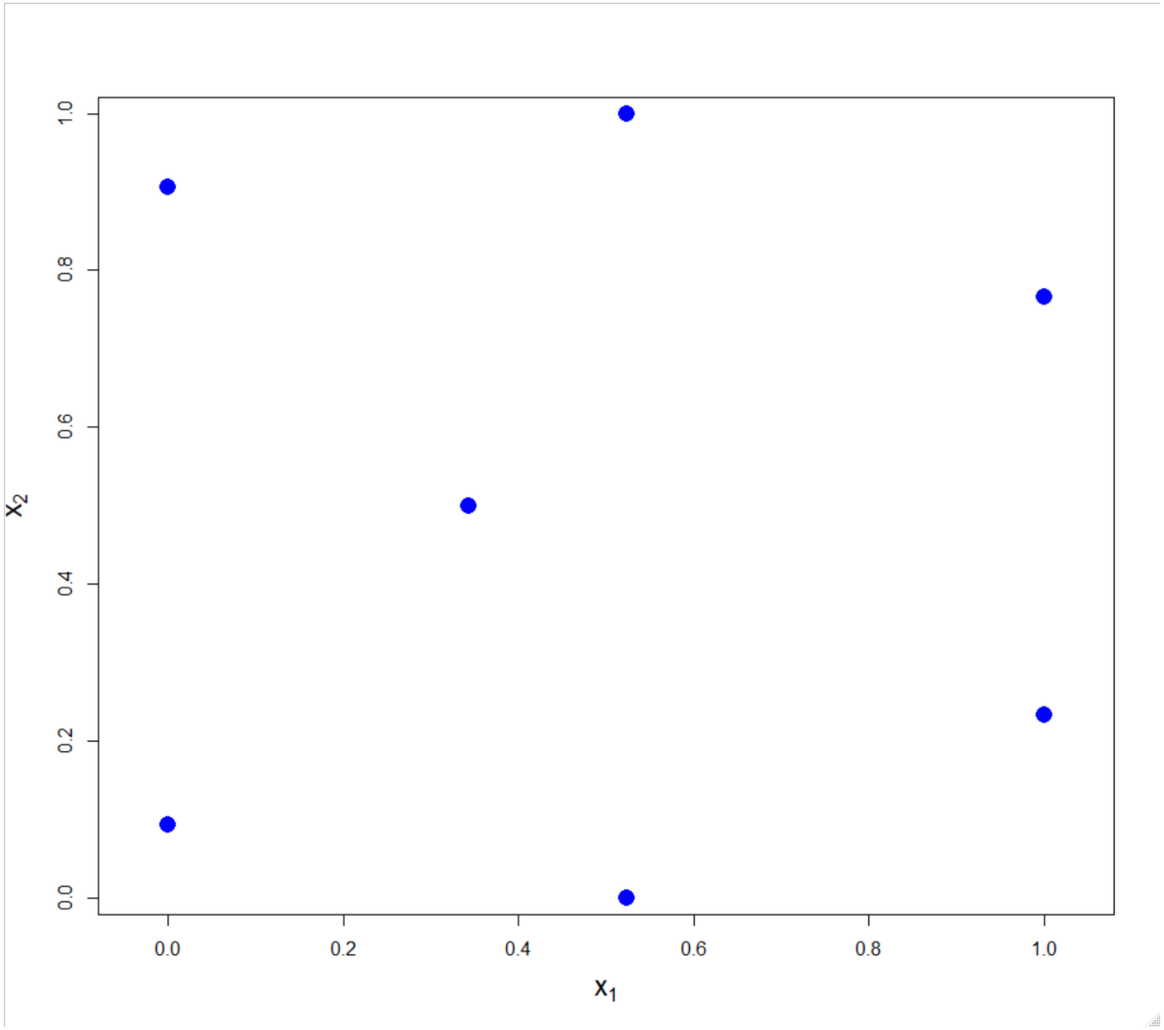
Mak, S. and Joseph, V. R. (2018). "Minimax and Minimax Projection Designs Using Clustering," *Journal of Computational and Graphical Statistics*, 27, 166-178.

Maximin design

- Johnson, Moore, and Ylvisaker (1991)

$$\max_{D} \min_{\boldsymbol{x}_i, \boldsymbol{x}_j \in D} d(\boldsymbol{x}_i, \boldsymbol{x}_j),$$

Maximin design



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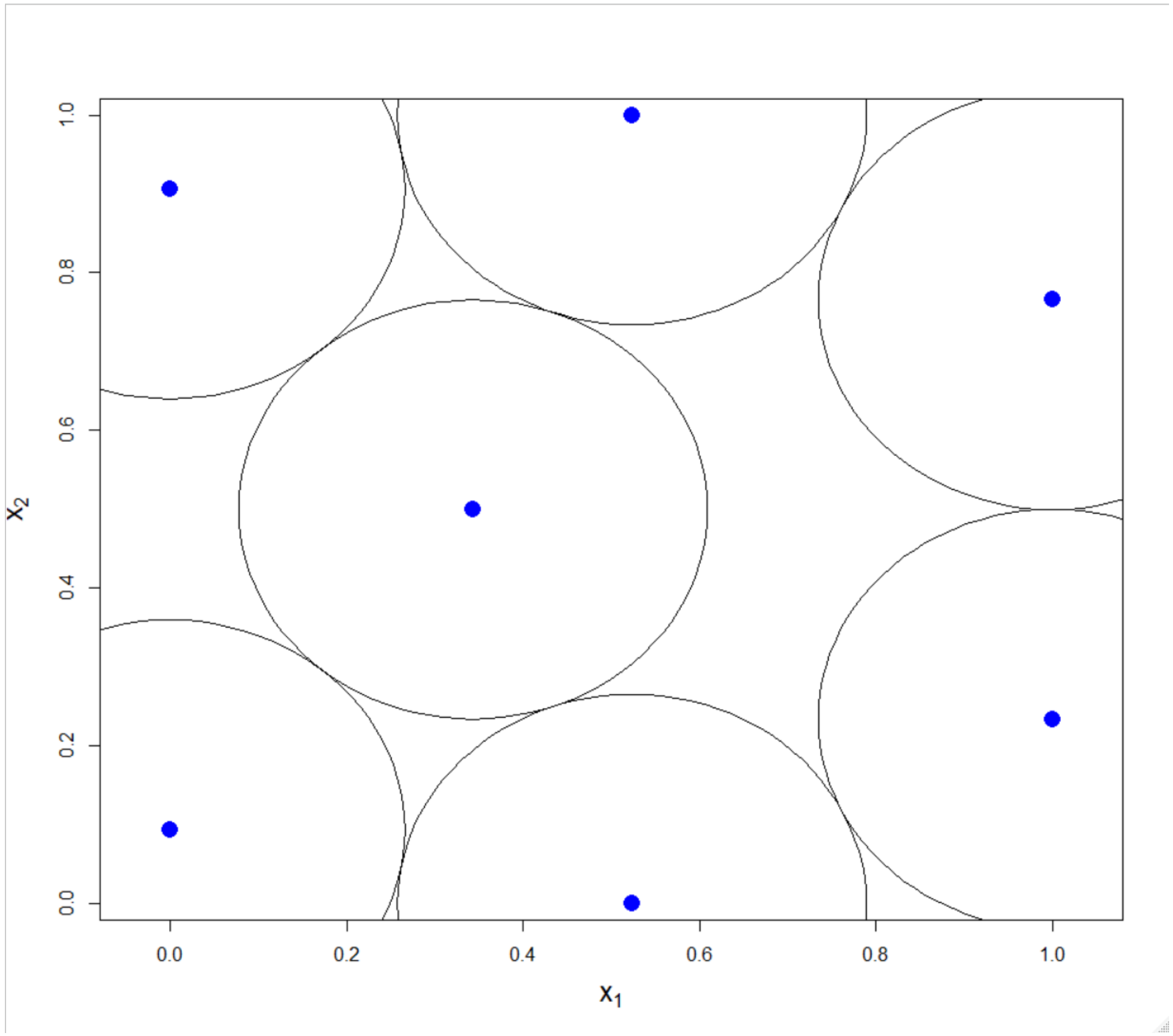
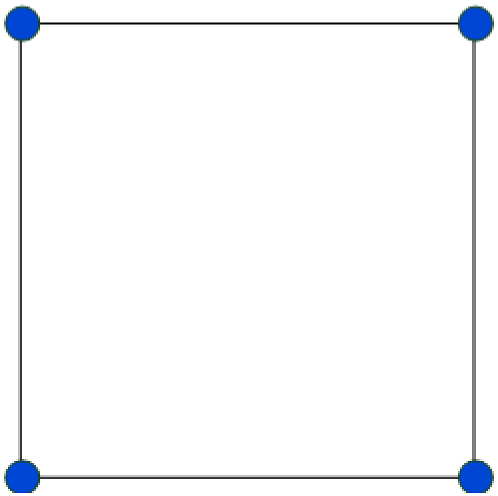
Maximin design or Sphere Packing Designs

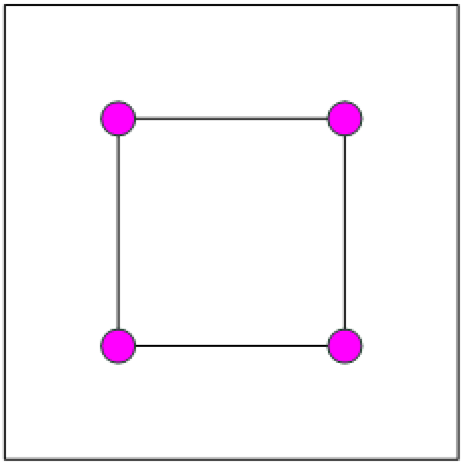


Issues with Maximin and Minimax Designs

Maximin design



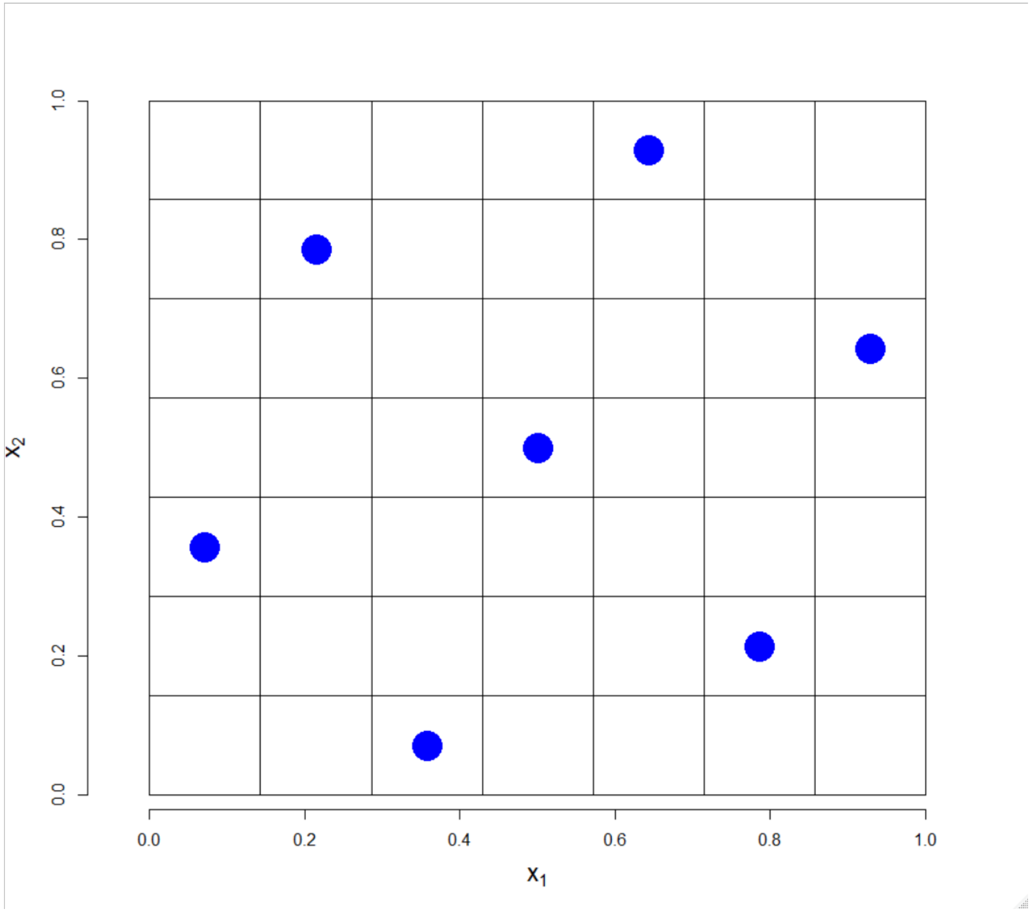
minimax design



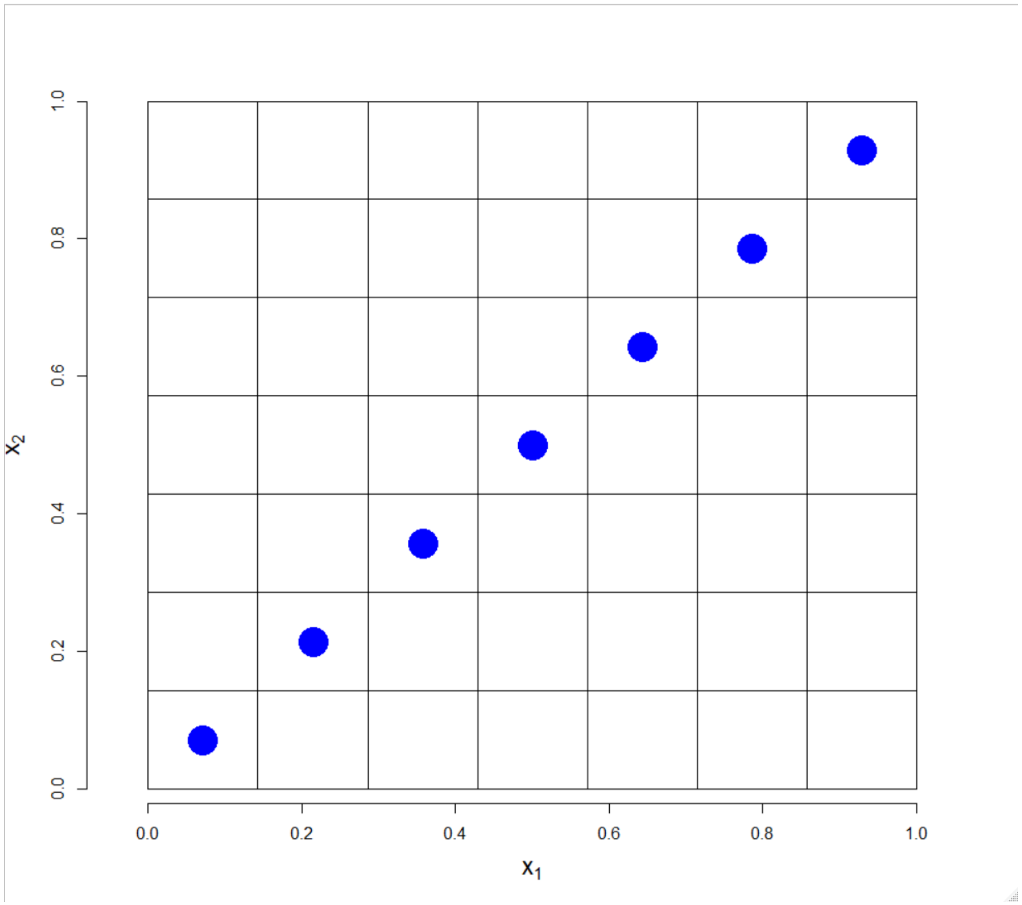
Poor projections!

Latin hypercube design

- McKay, Conover, Beckman (1979)



Latin hypercube design



Not good!

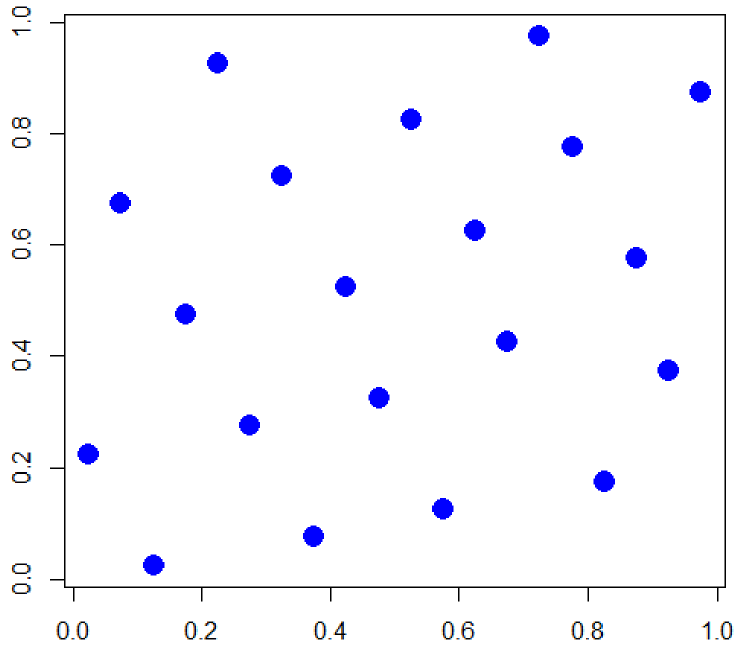
Maximin Latin hypercube design

- Morris and Mitchell (1995): Maximin design within the class of Latin hypercube designs $\mathcal{L}$.

$$\min_{\boldsymbol{D}\in\mathcal{L}} \left\{ \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{1}{d^k(\boldsymbol{x}_i, \boldsymbol{x}_j)} \right\}^{1/k}$$

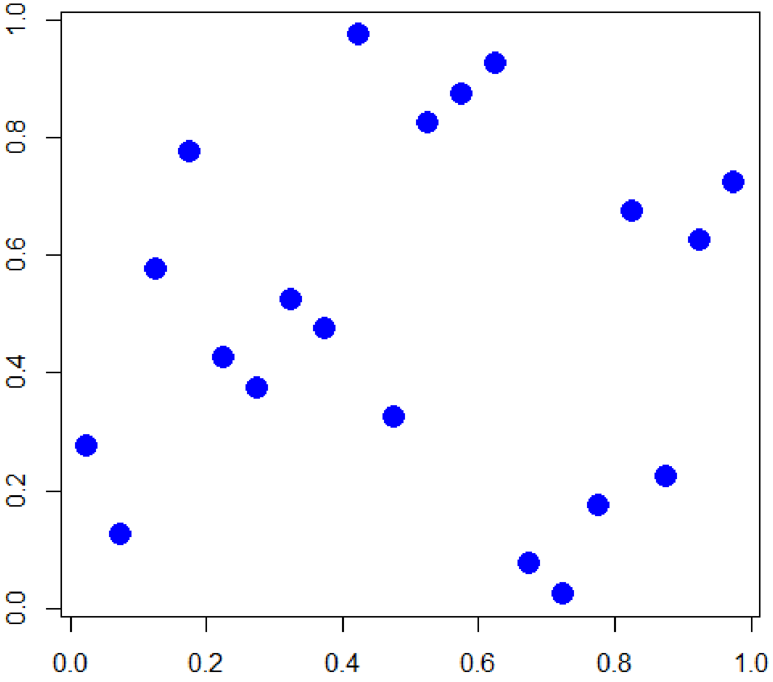
MmLHD

- MmLHD (20,2)



MmLHD

- A two-dimensional projection of MmLHD (20,10)



MmLHD

$$\min_{D \in \mathcal{L}} \left\{ \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{1}{d^k(\boldsymbol{x}_i, \boldsymbol{x}_j)} \right\}^{1/k}$$

- Ensures good space-filling in *p* dimensions and uniform one-dimensional projections, but their projections in 2,…,*p*-1 dimensions can be poor.

Improvements to MmLHD

- Draguljic, Santner, Dean (2012)

$$\min_D \left[\frac{1}{\binom{n}{2} \sum_{q \in J} \binom{p}{q}} \sum_{q \in J} \sum_{r=1}^{\binom{p}{q}} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left\{ \frac{q^{1/2}}{d_{qr}(x_i, x_j)} \right\}^k \right]^{1/k}$$

- Criterion is computationally expensive.

Maximum Projection (MaxPro) criterion

- Weighted Euclidean distance:

Let $0 \leq \theta_i \leq 1$

$$d(\boldsymbol{x}_i, \boldsymbol{x}_j; \boldsymbol{\theta}) = \left(\sum_{l=1}^{p} \theta_l (x_{il} - x_{jl})^2 \right)^{\frac{1}{2}}.$$

- Modify the Morris-Mitchell criterion to

$$\min_{\boldsymbol{D}} \phi_k(\boldsymbol{D}; \boldsymbol{\theta}) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{1}{d^k(\boldsymbol{x}_i, \boldsymbol{x}_j; \boldsymbol{\theta})}$$

Joseph, V. R., Gul, E., and Ba, S. (2015). “Maximum Projection Designs for Computer Experiments,” *Biometrika*, 102, 371-380.

Bayesian criterion

- We don't know about θ before the experiment!
- Prior:

$$p(\boldsymbol{\theta}) = \frac{1}{(p-1)!}, \text{ for } \boldsymbol{\theta} \in S_{p-1},$$

where $S_{p-1} = \{\boldsymbol{\theta} : \theta_1, \theta_2, \ldots, \theta_{p-1} \geq 0, \sum_{i=1}^{p-1} \theta_i \leq 1\}$.

- Then, the criterion becomes

$$\min_{\boldsymbol{D}} \mathbb{E}(\phi_k(\boldsymbol{D}; \boldsymbol{\theta})) = \int_{S_{p-1}} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{1}{d^k(\boldsymbol{x}_i, \boldsymbol{x}_j; \boldsymbol{\theta})} p(\boldsymbol{\theta}) d\boldsymbol{\theta}.$$

MaxPro criterion

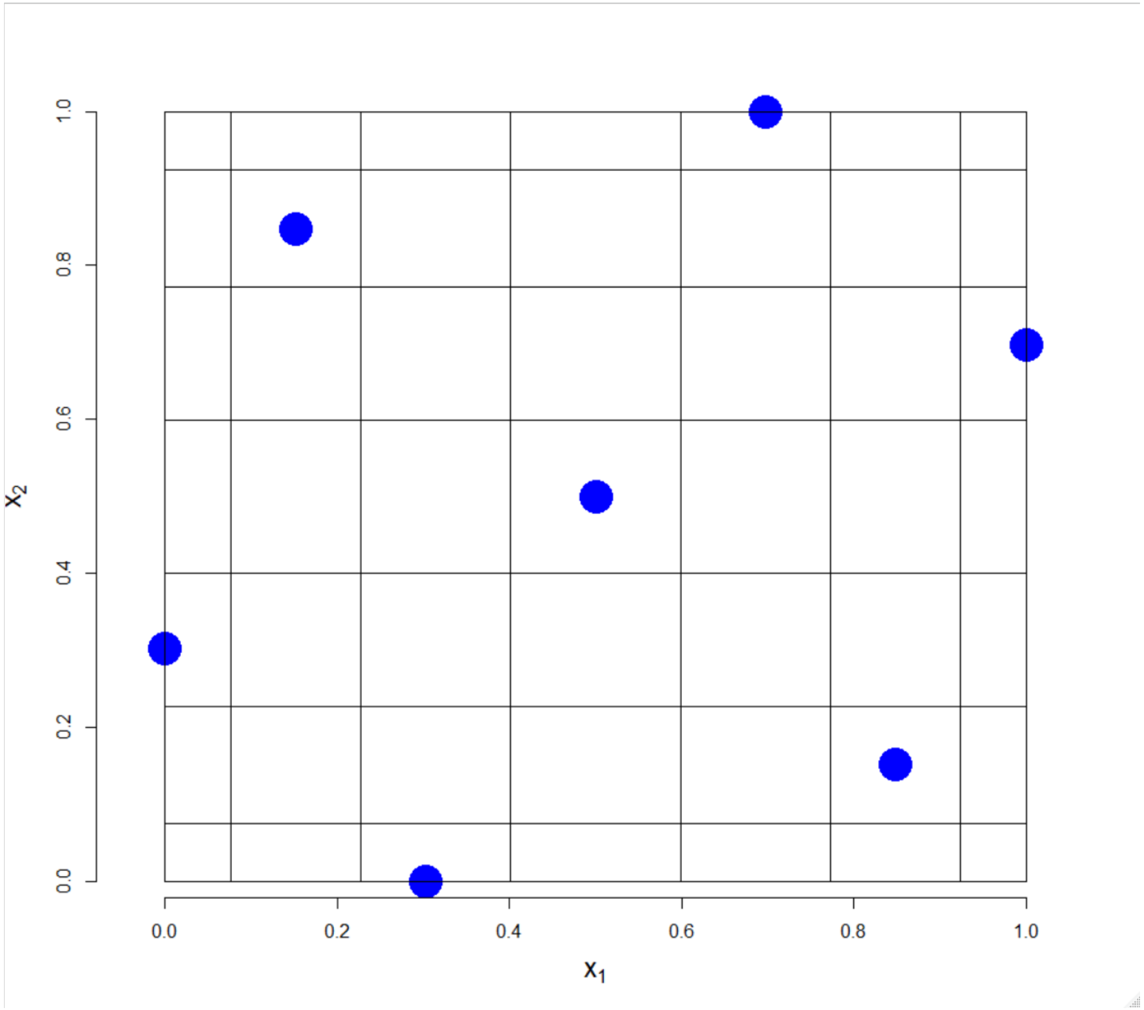
$$\text{If } k = 2p, \text{ then}$$

$$\mathbb{E}(\phi_k(\boldsymbol{D};\boldsymbol{\theta})) = \frac{1}{[(p-1)!]^2} \sum_{i=1}^{n-1} \sum_{j=1+1}^{n} \frac{1}{\prod_{l=1}^{p} (x_{il} - x_{jl})^2}.$$

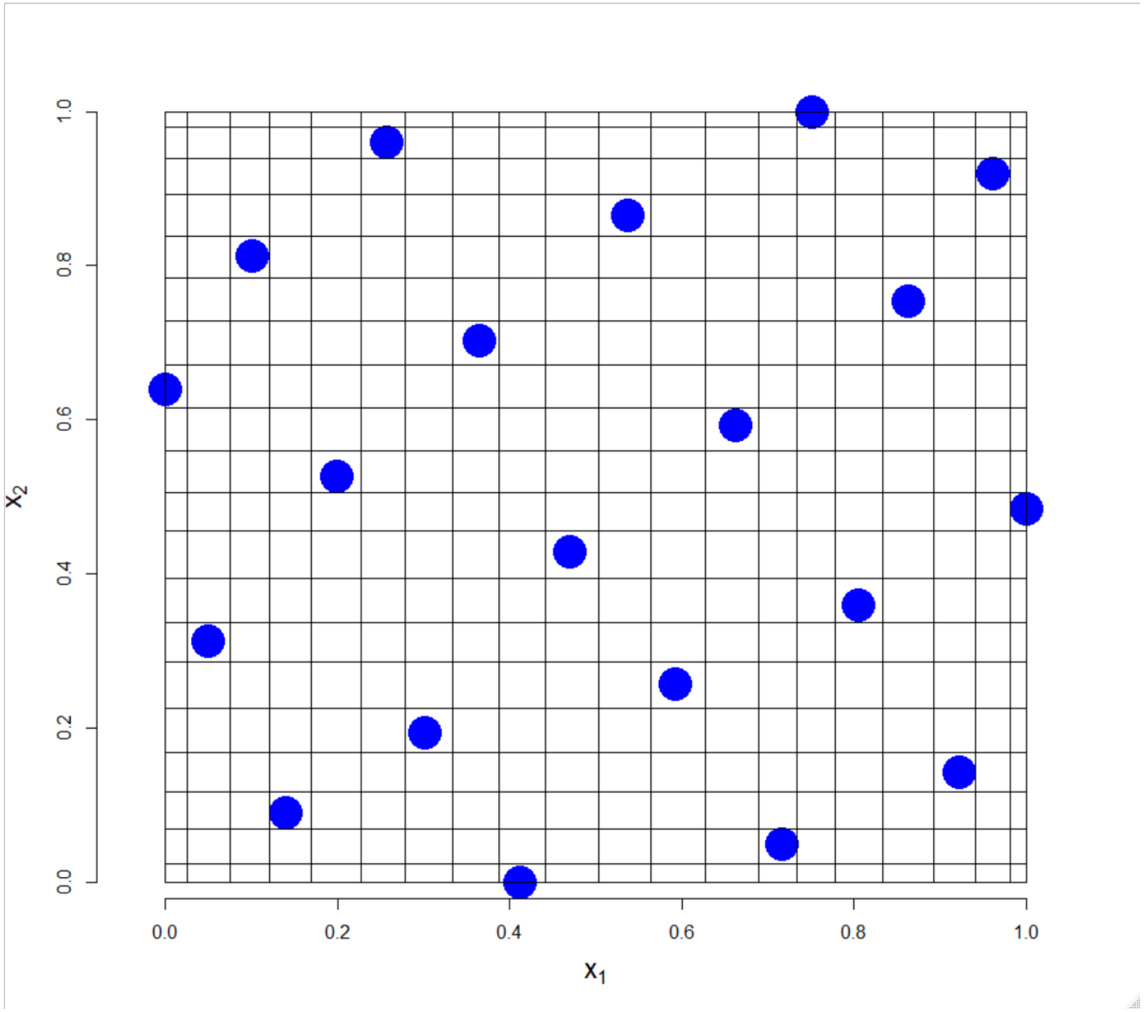
- MaxPro criterion:

$$\psi(\boldsymbol{D}) = \left(\frac{1}{\binom{n}{2}} \sum_{i=1}^{n-1} \sum_{j=1+1}^{n} \frac{1}{\prod_{l=1}^{p} (x_{il} - x_{jl})^2} \right)^{1/p}.$$

Example



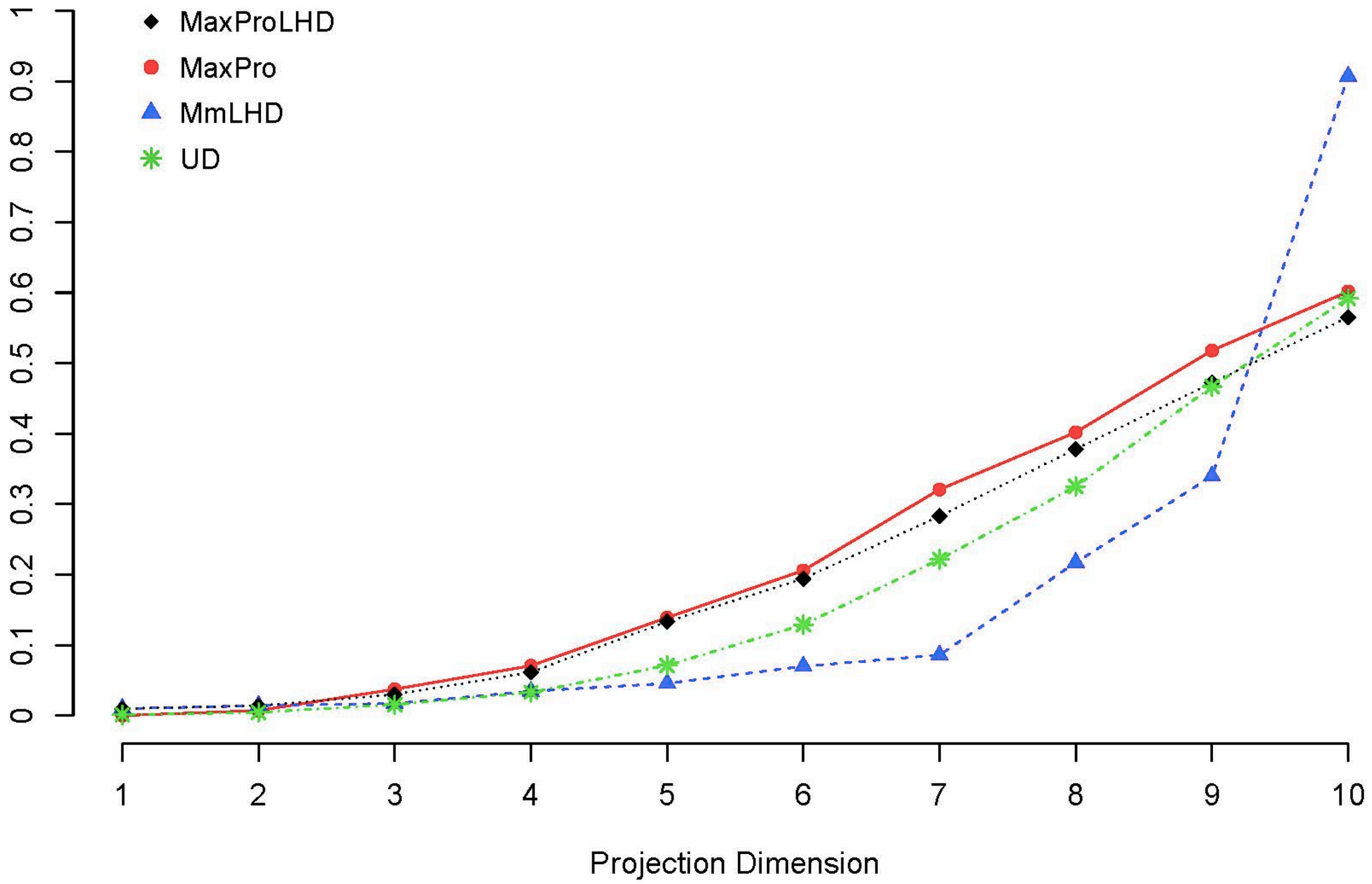
Example



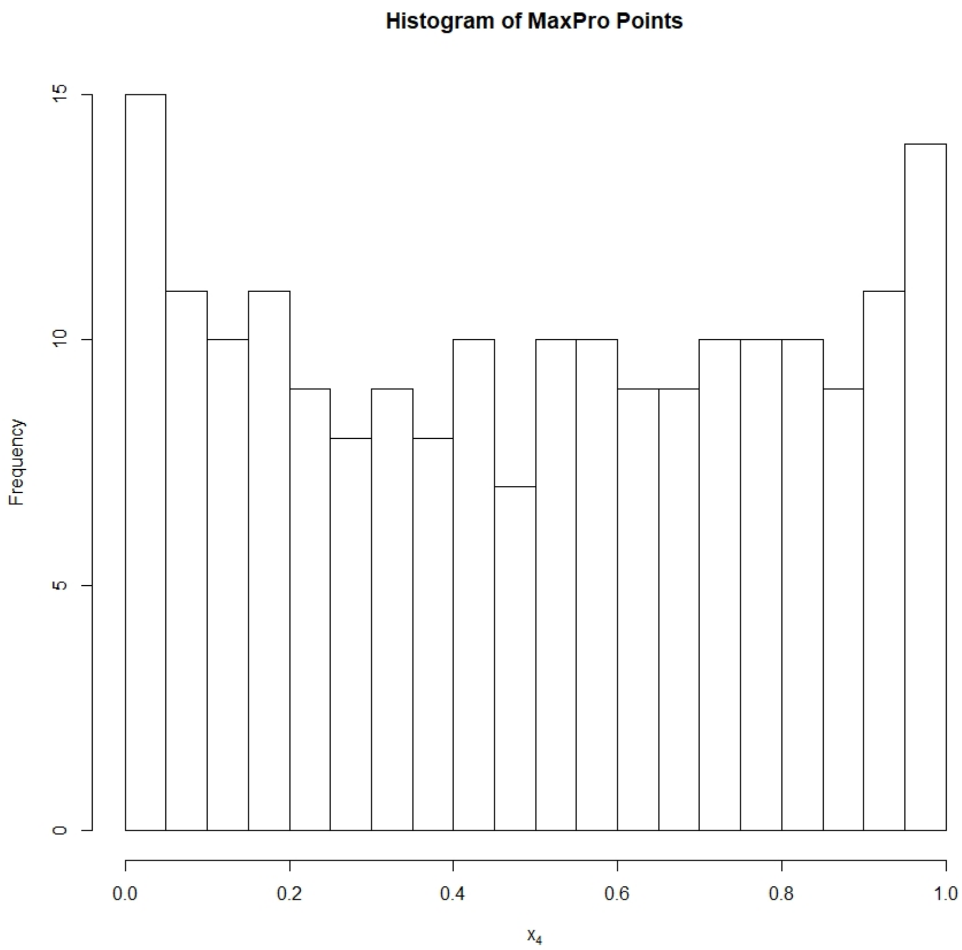
LHD property

- for any l, if $x_{il} = x_{jl}$ for $i \neq j$, then $\psi(\boldsymbol{D}) = \infty$.
- MaxPro design must have *n* distinct levels for each factor.
- LHD requirement is automatically enforced in the criterion!

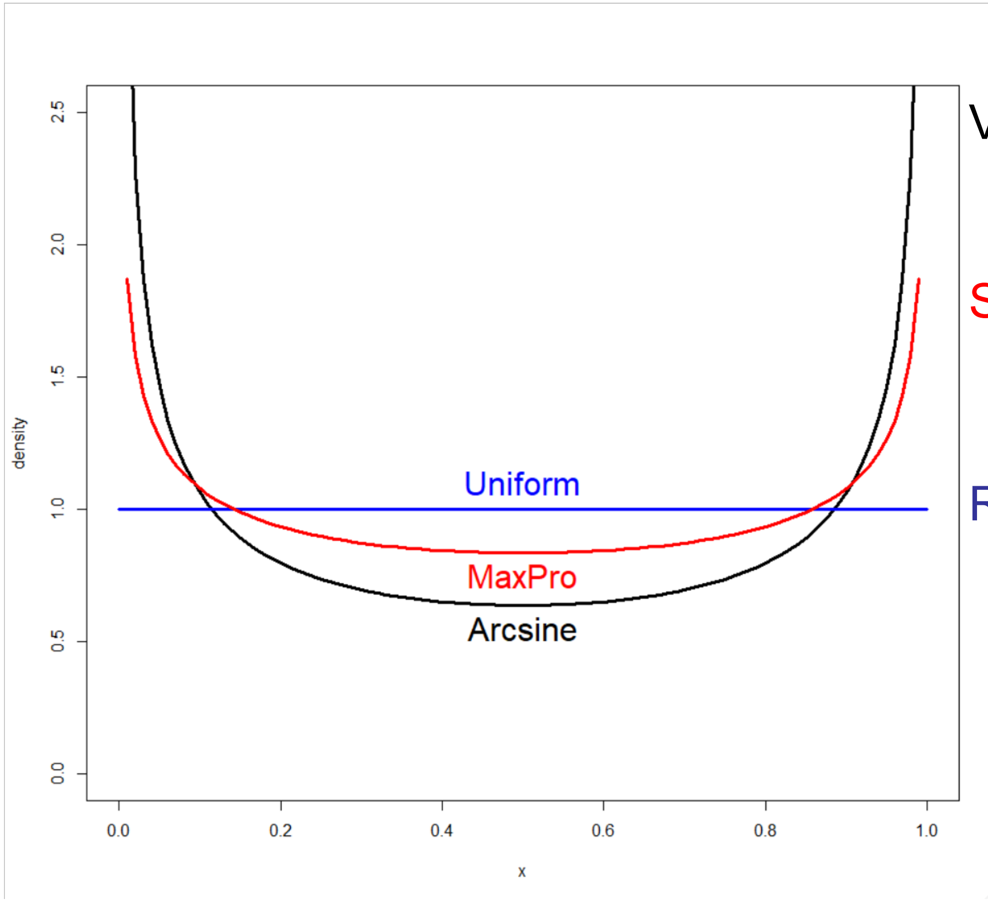
Minimum distance (larger-the-better)



Distribution of MaxPro Points



Distribution of MaxPro Points



Very smooth surfaces

Smooth surfaces

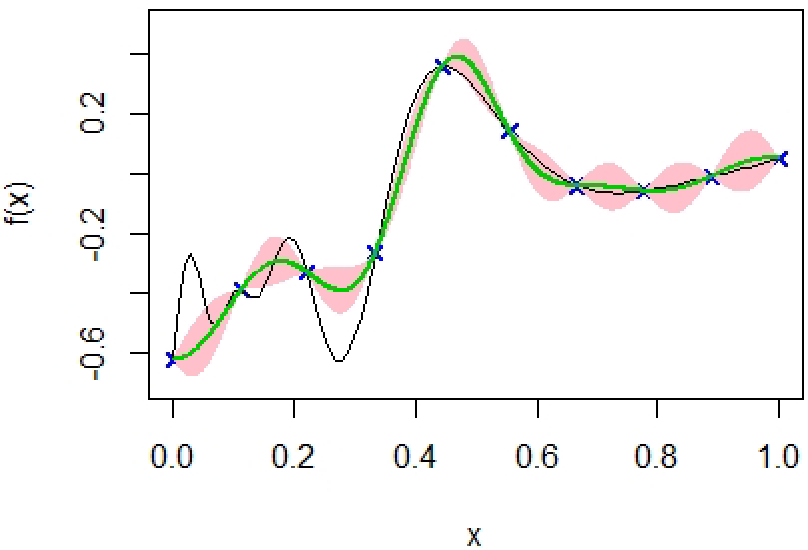
Rough surfaces

Dette, H., and Pepelyshev, A. (2010), Generalized Latin Hypercube Design for Computer Experiments," *Technometrics*, 52, 421-429.

Gaussian Process Modeling

$$Y(\boldsymbol{x}) \sim GP(\mu, \sigma^2 R(.))$$

$$R(\boldsymbol{x}_i - \boldsymbol{x}_j; \boldsymbol{\alpha}) = e^{-\sum_{l=1}^{p} \alpha_l (x_{il} - x_{jl})^2}$$



An optimality result

- Noninformative Prior:

$$p(\boldsymbol{\alpha}) \propto 1, \quad \text{for} \quad \boldsymbol{\alpha} \in \mathbb{R}_{+}^{p}.$$

- A MaxPro design minimizes

$$\mathbb{E}\{\sum_{i=1}^{n}\sum_{j\neq i}\boldsymbol{R}_{ij}\}$$

Proof:
$$\mathbb{E}(\sum_{i=1}^{n}\sum_{j\neq i}\boldsymbol{R}_{ij}^{\gamma}) = \sum_{i=1}^{n}\sum_{j\neq i}\mathbb{E}\left\{\prod_{l=1}^{p} e^{-\gamma\alpha_l(x_{il}-x_{jl})^2}\right\}$$
$$= \sum_{i=1}^{n}\sum_{j\neq i}\left\{\prod_{l=1}^{p}\int_0^{\infty} e^{-\gamma\alpha_l(x_{il}-x_{jl})^2}\, d\alpha_l\right\}$$
$$= \frac{1}{\gamma^p}\sum_{i=1}^{n}\sum_{j\neq i}\frac{1}{\prod_{l=1}^{p}(x_{il}-x_{jl})^2},$$

Another Justification

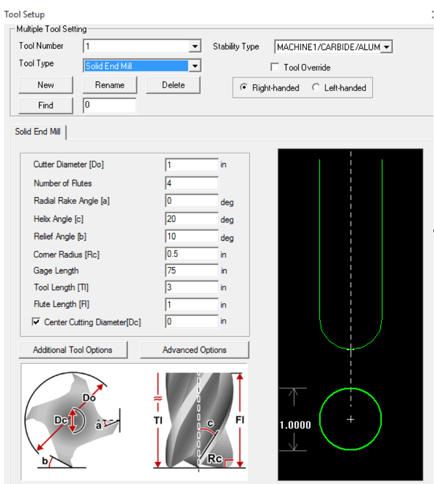
$$d_s(\boldsymbol{u}, \boldsymbol{v}) = \left(\frac{1}{p} \sum_{l=1}^{p} |u_l - v_l|^s \right)^{1/s}$$

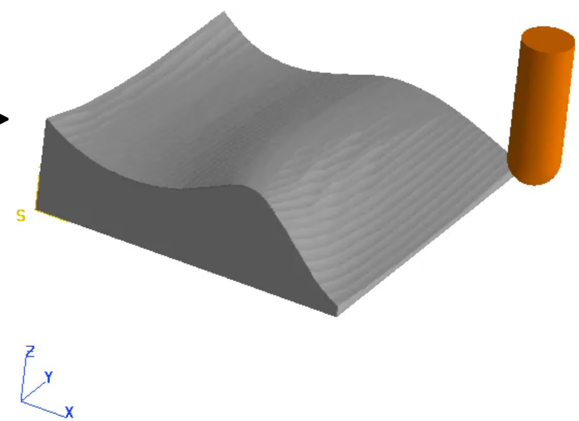
$$\lim_{s \to 0} d_s(\boldsymbol{u}, \boldsymbol{v}) = \left(\prod_{l=1}^{p} |u_l - v_l| \right)^{1/p}$$

Joseph, V. R., Wang, D., Gu, L., Lv, S., and Tuo, R. (2019). "Deterministic Sampling of Expensive Posteriors Using Minimum Energy Designs". *Technometrics*, 61, 297-308.

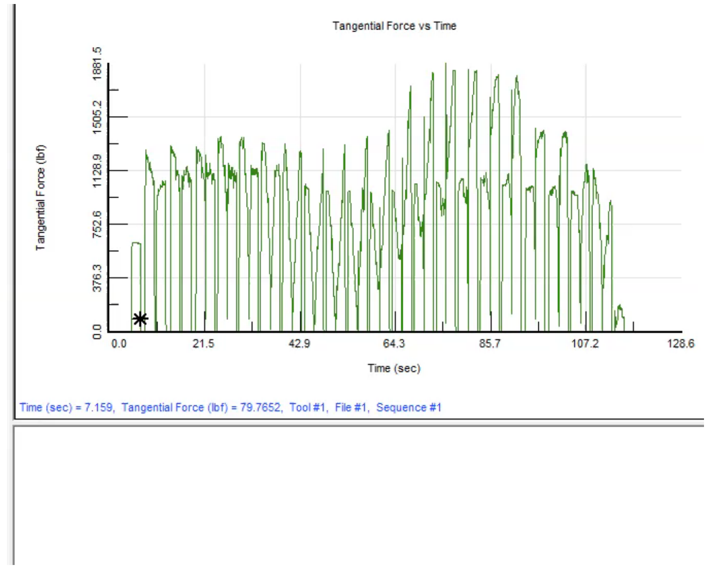
Qualitative Factors

Inputs





Output



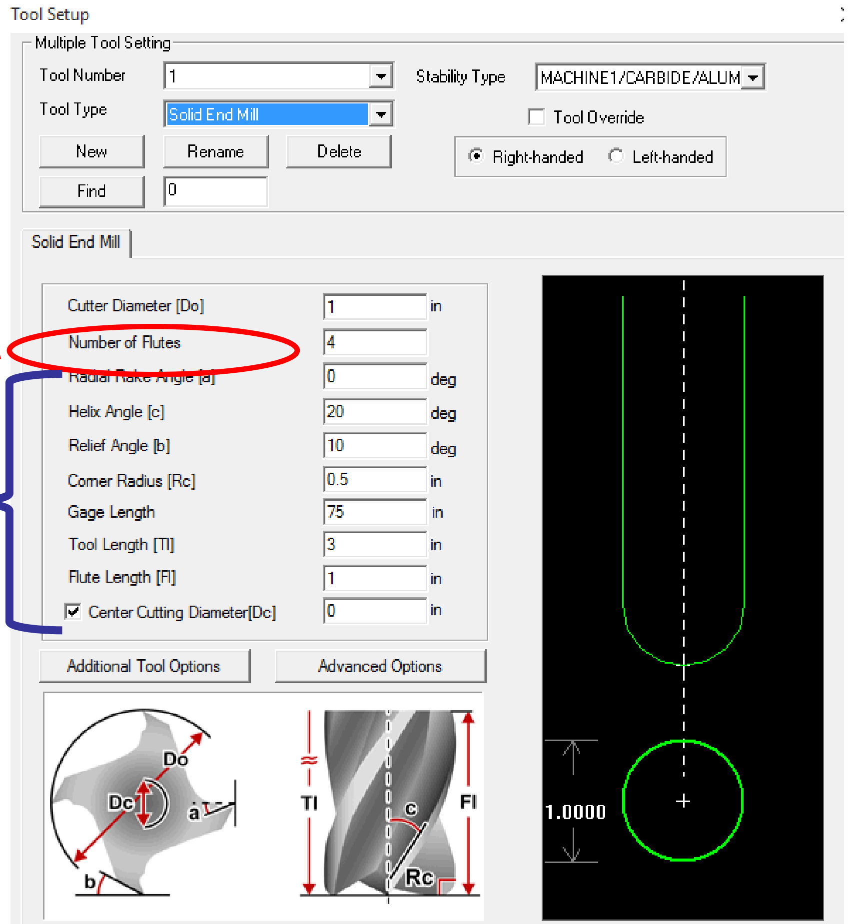
Joseph, V. R., Gul, E., and Ba, S. (2020), "Designing computer experiments with multiple type of factors: The MaxPro approach," *Journal of Quality Technology*, 52, 343-354.

Qualitative Factors

Quantitative factors

Discrete-numeric

Continuous



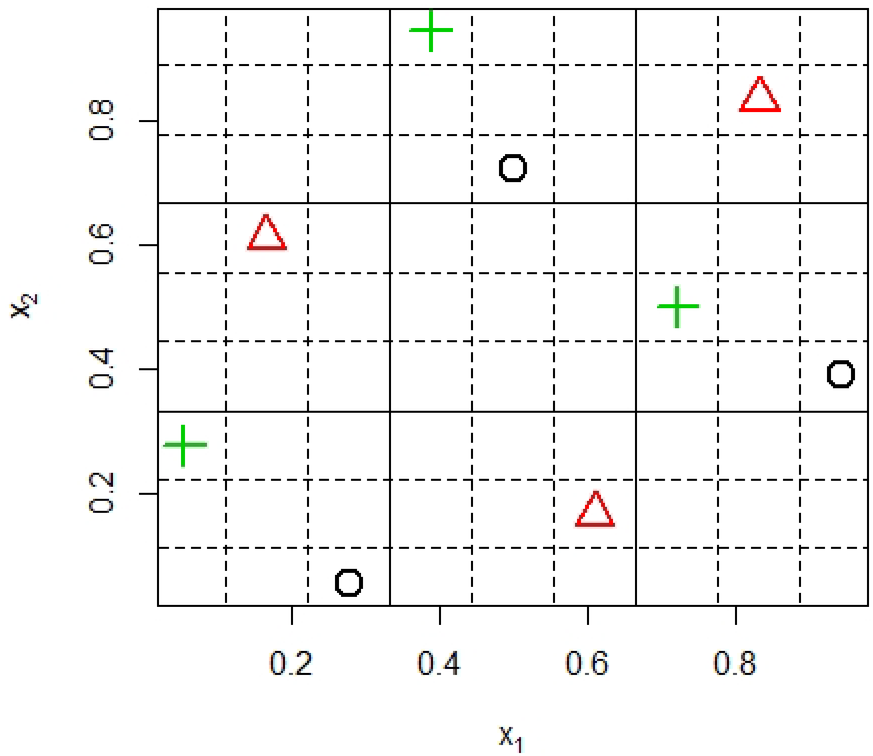
Qualitative factors

Tool material: Ti-6Al-4V, Ti-6Al-6V-2Sn,…-> **Nominal**

Condition of tool: Excellent, very good, good,…-> **Ordinal**

Continuous and Nominal factors

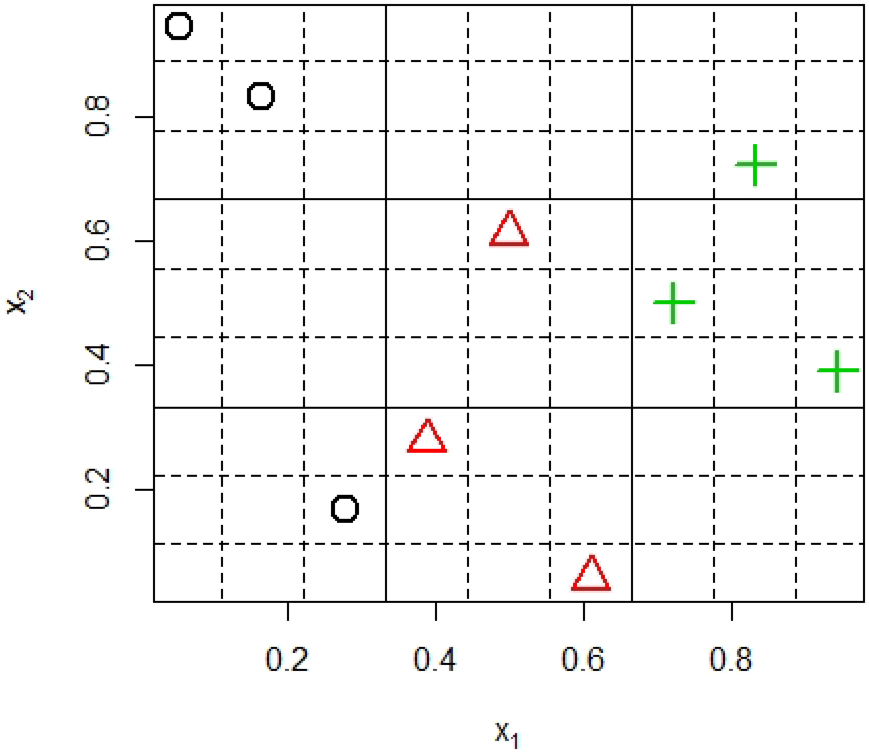
- Sliced LHD (Qian 2012)
- Example: 2 continuous, 1 nominal at 3 levels



SLHD with 3 slices!

Continuous and Nominal factors

- Sliced LHD (Qian 2012)
- Example: 2 continuous, 1 nominal at 3 levels



Not an SLHD!

MaxPro Designs

- A MaxPro design minimizes

$$\mathbb{E}\{\sum_{i=1}^{n} \sum_{j \neq i} \boldsymbol{R}_{ij}(\boldsymbol{\alpha})\}$$

- So we only need to choose appropriate correlation functions for the different types of factors!

MaxPro Designs

- Correlation function (continuous and discrete numeric factors are scaled in 0 to1)

$$\exp\left\{-\sum_{l=1}^{p_1}\alpha_l|x_{il}-x_{jl}|-\sum_{k=1}^{p_2}\beta_k|u_{ik}-u_{jk}|-\sum_{h=1}^{p_3}\gamma_h I(v_{ih}\neq v_{jh})\right\}$$

MaxPro Designs

- We can't use noninformative prior for discrete numeric and nominal factors.
- Informative prior:

$$\alpha_l \sim^{iid} Gamma(2, \bar{\alpha}_l), l = 1, \ldots, p_1,$$

$$\beta_k \sim^{iid} Gamma(2, \bar{\beta}_k), k = 1, \ldots, p_2,$$

$$\gamma_h \sim^{iid} Gamma(2, \bar{\gamma}_h), h = 1, \ldots, p_3.$$

MaxPro Designs

$$\mathbb{E}\{\sum_{i=1}^{n}\sum_{j\neq i}\boldsymbol{R}_{ij}(\boldsymbol{\alpha},\boldsymbol{\beta},\boldsymbol{\gamma})\}$$

$$= \int\int\int \sum_{i=1}^{n}\sum_{j\neq i} R(\boldsymbol{w}_i - \boldsymbol{w}_j; \boldsymbol{\alpha},\boldsymbol{\beta},\boldsymbol{\gamma}) \prod_{l=1}^{p_1} \bar{\alpha}_l^2 \alpha_l e^{-\bar{\alpha}_l \alpha_l} \prod_{k=1}^{p_2} \bar{\beta}_k^2 \beta_k e^{-\bar{\beta}_k \beta_k} \prod_{h=1}^{p_3} \bar{\gamma}_h^2 \gamma_h e^{-\bar{\gamma}_h \gamma_h} \, d\boldsymbol{\alpha}\, d\boldsymbol{\beta}\, d\boldsymbol{\gamma}$$

$$= \sum_{i=1}^{n}\sum_{j\neq i}\prod_{l=1}^{p_1}\int \bar{\alpha}_l^2 \alpha_l e^{-\{|x_{il}-x_{jl}|+\bar{\alpha}_l\}\alpha_l} d\alpha_l \prod_{k=1}^{p_2}\int \bar{\beta}_k^2 \beta_k e^{-\{|u_{ik}-u_{jk}|+\bar{\beta}_k\}\beta_k} d\beta_k \prod_{h=1}^{p_3}\int \bar{\gamma}_h^2 \gamma_h e^{-\{I(v_{ih}\neq v_{jh})+\bar{\gamma}_h\}\gamma_h} d\gamma_h$$

$$= \sum_{i=1}^{n}\sum_{j\neq i}\prod_{l=1}^{p_1}\frac{\bar{\alpha}_l^2}{\{|x_{il}-x_{jl}|+\bar{\alpha}_l\}^2}\prod_{k=1}^{p_2}\frac{\bar{\beta}_k^2}{\{|u_{ik}-u_{jk}|+\bar{\beta}_k\}^2}\prod_{h=1}^{p_3}\frac{\bar{\gamma}_h^2}{\{I(v_{ih}\neq v_{jh})+\bar{\gamma}_h\}^2}.$$

MaxPro criterion

- Minimize

$$\frac{1}{\binom{n}{2}} \sum_{i=1}^{n} \sum_{j \neq i} \frac{1}{\prod_{l=1}^{p_1} \{|x_{il} - x_{jl}| + \bar{\alpha}_l\}^2 \prod_{k=1}^{p_2} \{|u_{ik} - u_{jk}| + \bar{\beta}_k\}^2 \prod_{h=1}^{p_3} \{I(v_{ih} \neq v_{jh}) + \bar{\gamma}_h\}^2}$$

- $\bar{\alpha}_l = 0, \bar{\beta}_k = 1/m_k, \bar{\gamma}_h = 1/L_h$

Number of levels

Solid End Milling

- Three Continuous: rake angle, relief angle, and helix angle
- One discrete numeric: number of flutes
- Two nominal factors

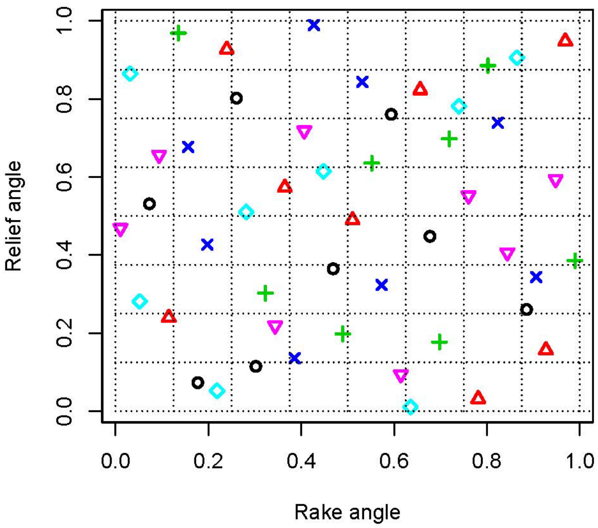
Level	Titanium Alloy	Tool Path Optimization
1	Ti-6AI-4V	None
2	Ti-6AI-2Sn-4Zr-6Mo	In-Cut
3	Ti-6AI-2Sn-4Zr-2Mo	Air-Cut
4	Ti-6AI-6V-2Sn	Both
5	Ti-4AI-4Mo-2Sn	
6	Ti-10V-2Fe-3AI	

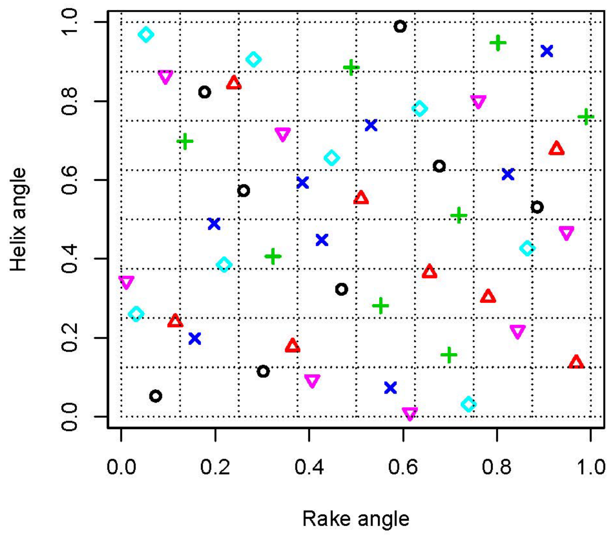
Solid End Milling

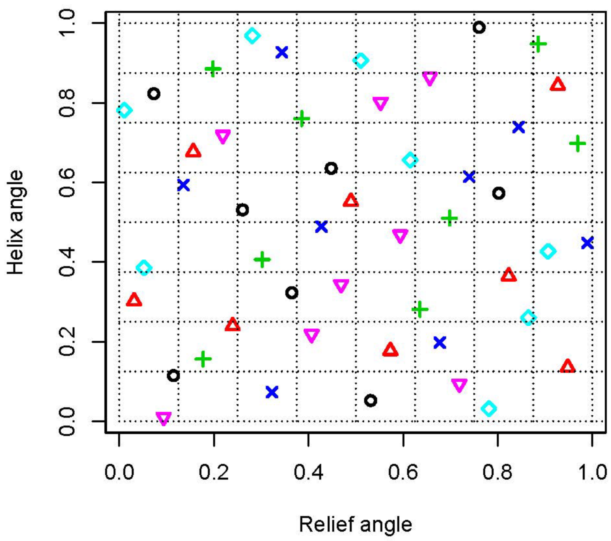
- Run size $n = 48$
- SLHD with 5 points in each slice would require 360 runs!

Solid End Milling

Six symbols for six levels of Titanium alloy

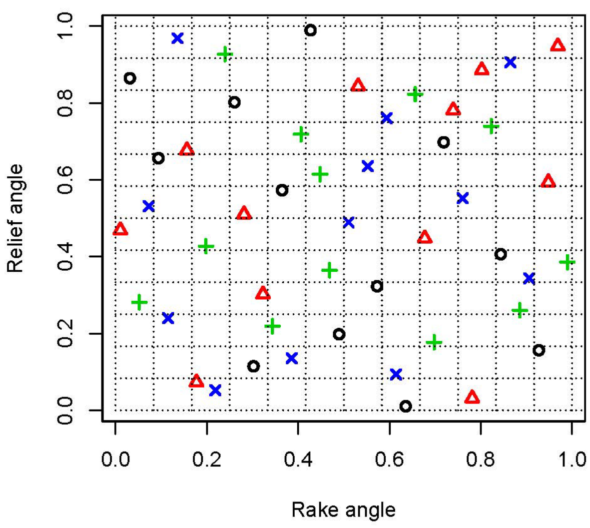


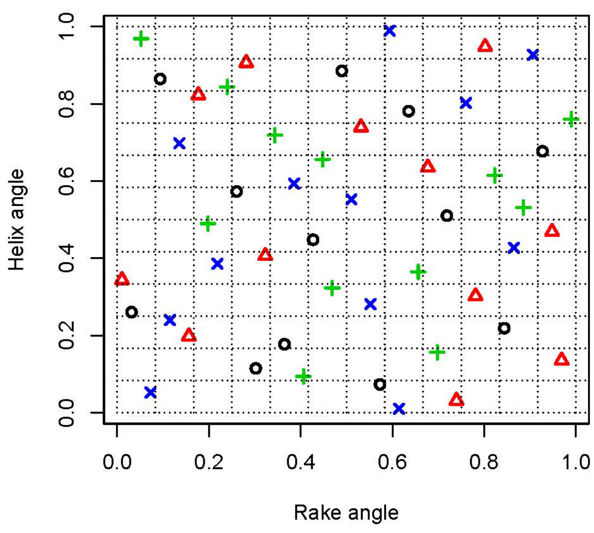


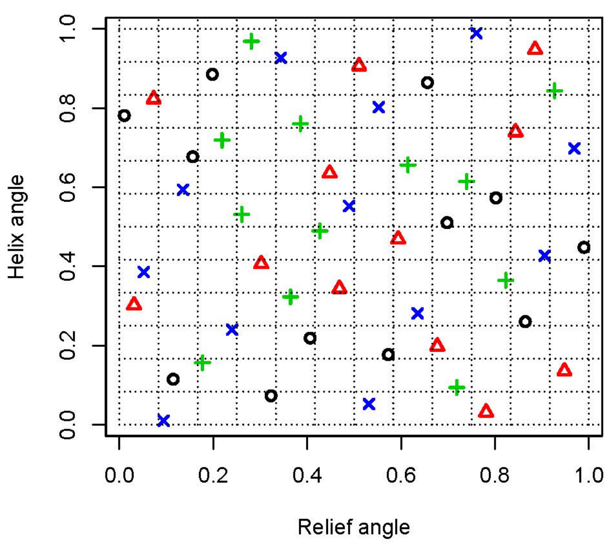


Solid End Milling

Four symbols for four levels of tool path optimization

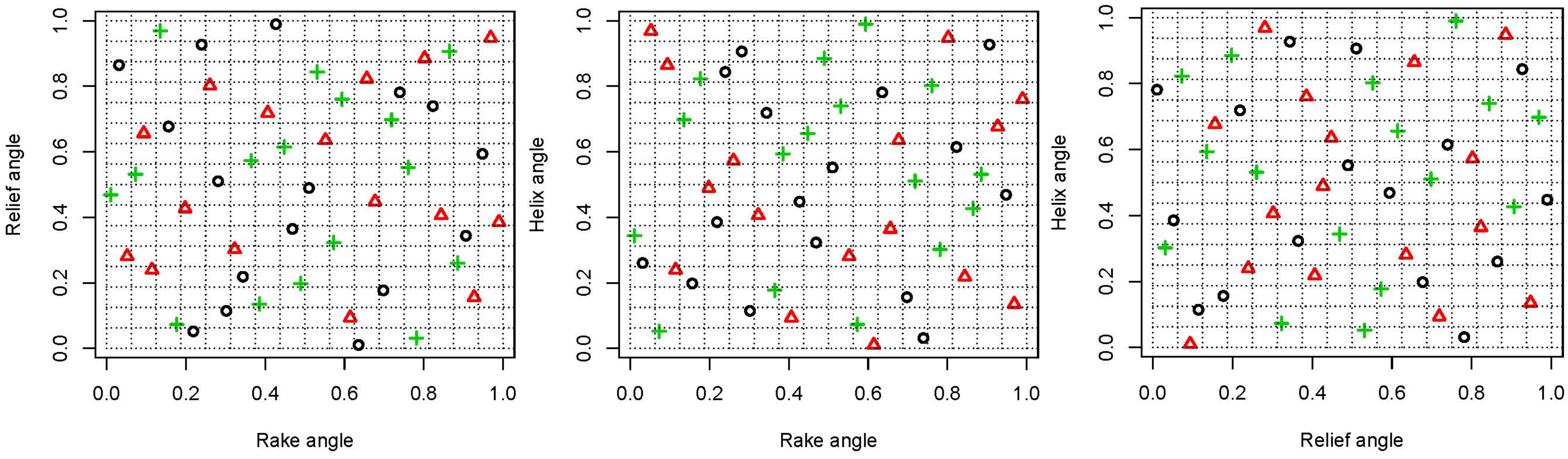






Solid End Milling

Three symbols for three levels of number of flutes

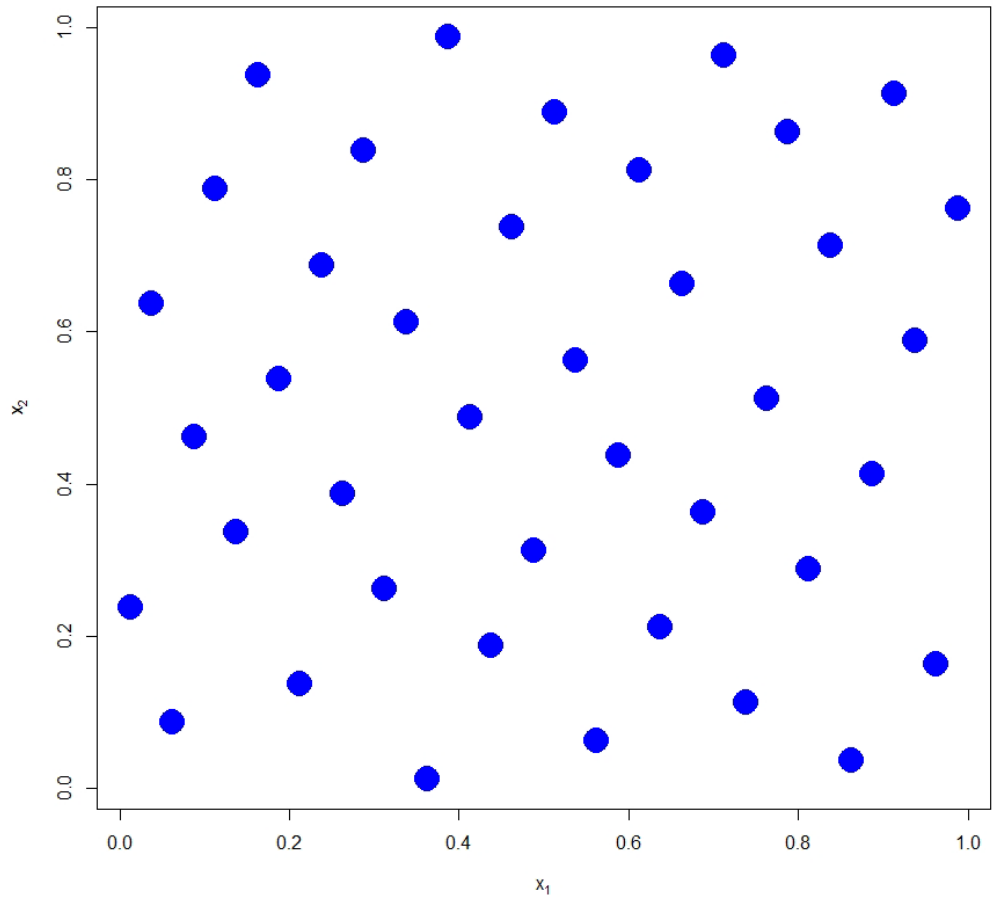


R Package: MaxPro

Ba, S. and Joseph, V. R. (2018). “MaxPro: Maximum Projection Designs”. R 4.1-2.

MaxProLHD

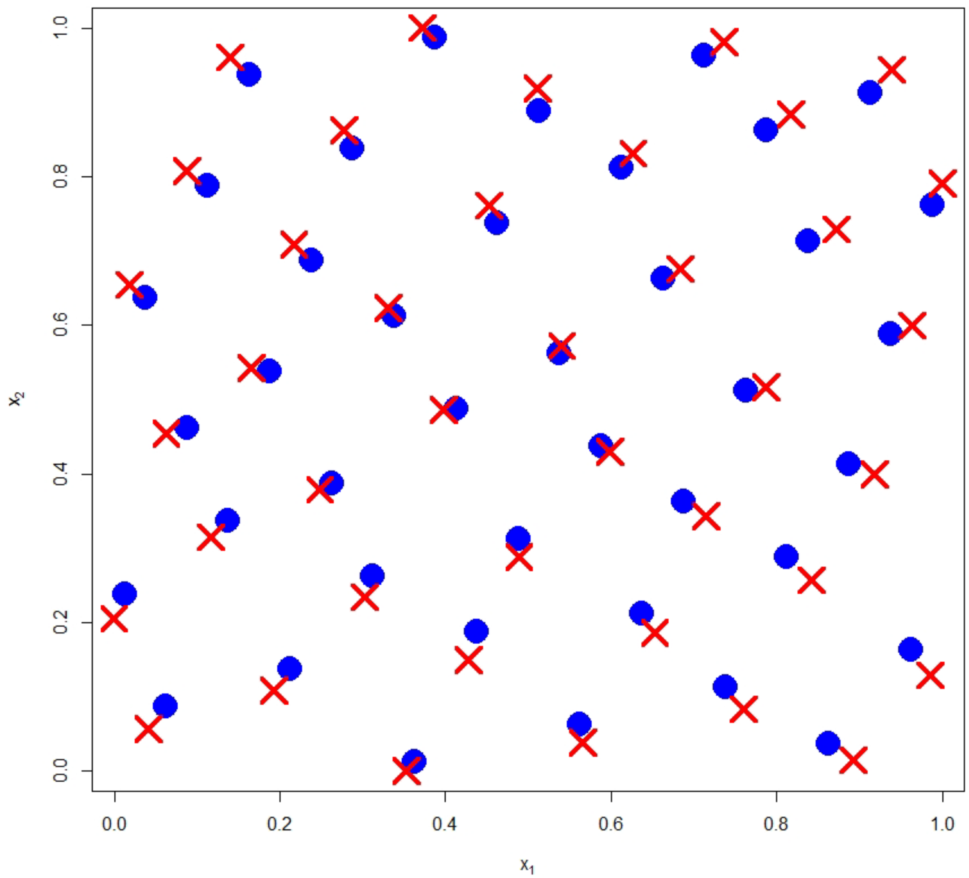
```
> D=MaxProLHD(n=40,p=2)$Design
```



Exchange algorithm

MaxPro

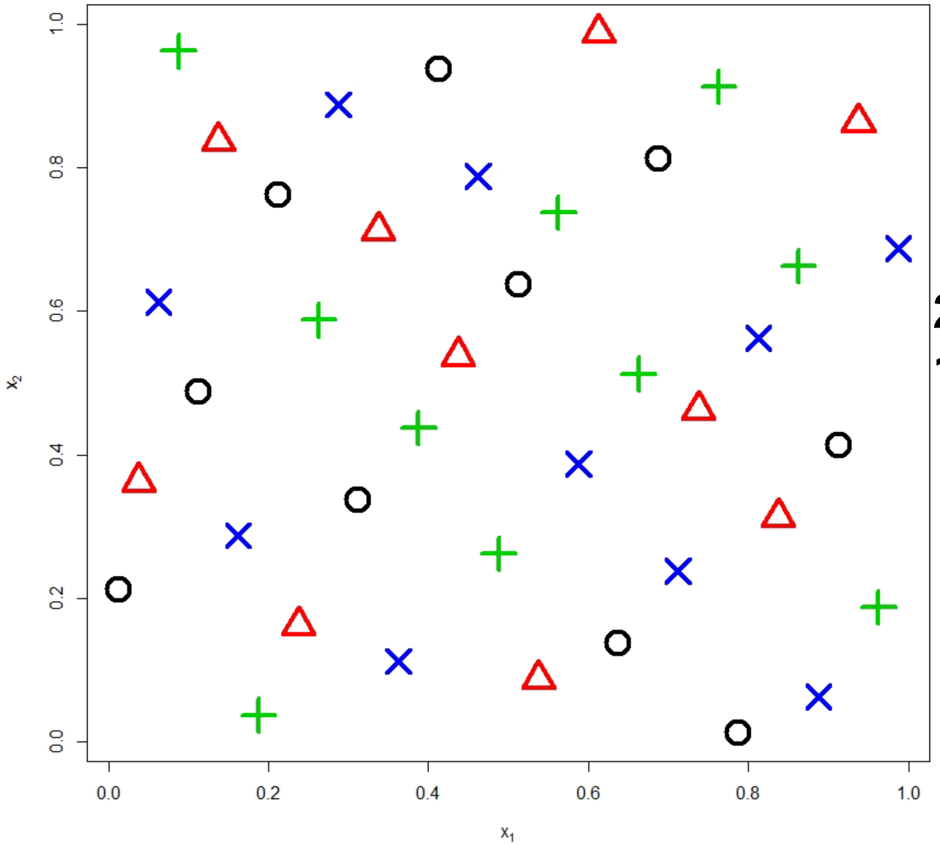
```
> D2=MaxPro(InitialDesign = D)$Design
```



Local optimization

MaxProQQ

```
> n=40
> D1=MaxProLHD(n=40,p=2)$Design
> D2=rep(1:4,10)
> D=MaxProQQ(InitialDesign = cbind(D1,D2),p_nom = 1)$Design
```



2 Continuous
1 Nominal (4 levels)

MaxProAugment

- One-at-a-time greedy procedure:

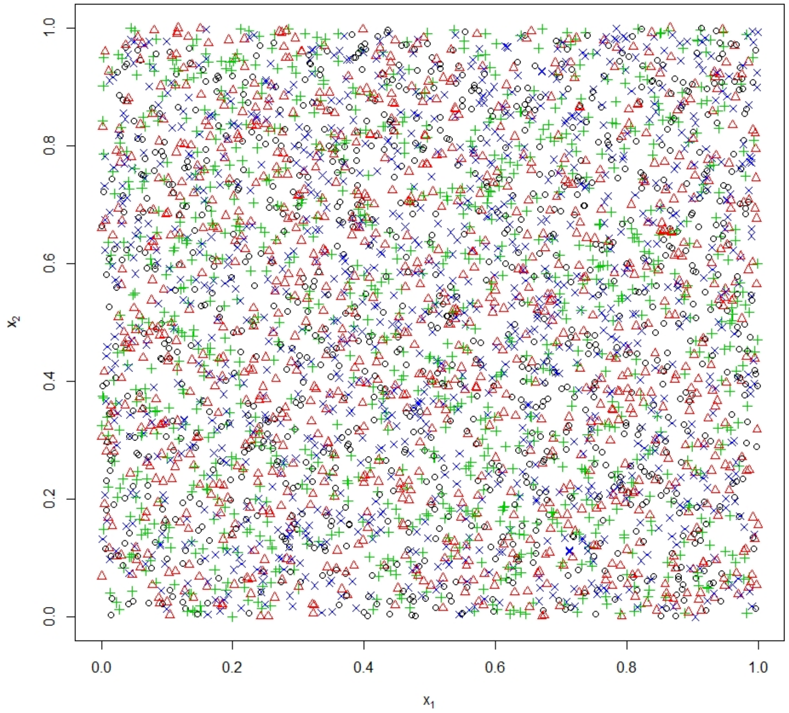
$$\mathbf{x}_{n+1} = \min_{\mathbf{u}\in\mathcal{C}} \sum_{i=1}^{n} \frac{1}{\prod_{l=1}^{p} |u_l - x_{il}|^2}.$$

Joseph, V. R. (2016), “Rejoinder,” *Quality Engineering*, 28, 42-44.

Non-Adaptive Sequential Designs

- Need a candidate set

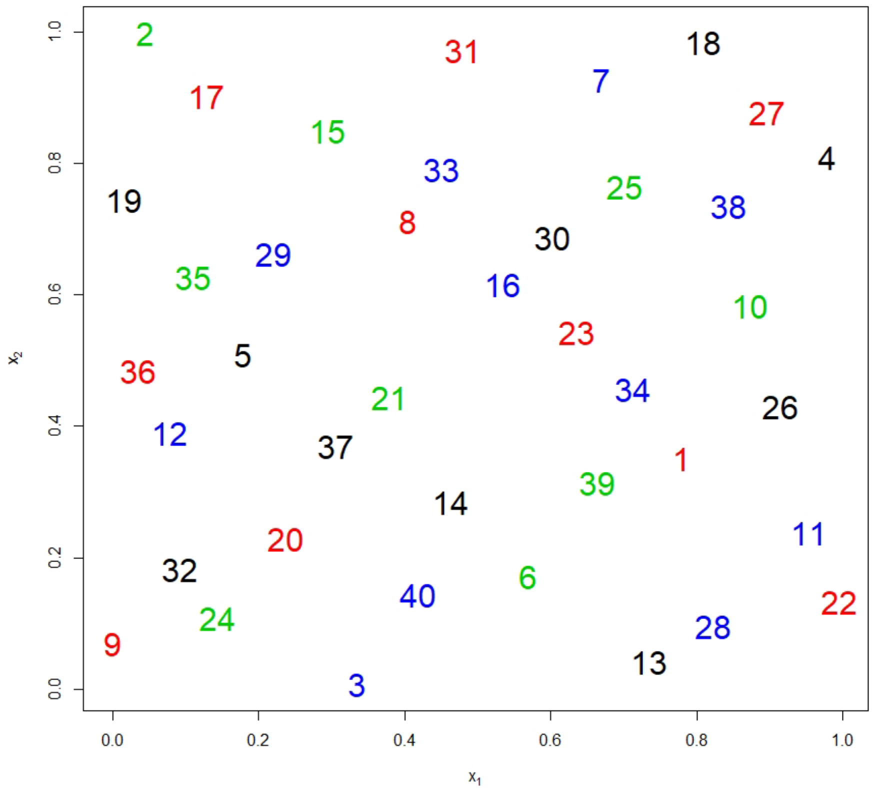
```
> n=40
> cand=CandPoints(100*n,p_cont = 2,l_nom = 4)
```



2 Continuous
1 Nominal (4 levels)

Non-Adaptive Sequential Designs

```
> st=matrix(cand[1,],nrow = 1)
> D=MaxProAugment(st,CandDesign = cand, nNew = n-1,p_nom = 1,l_nom=4)$Design
```



2 Continuous
1 Nominal (4 levels)

```
> table(D[,3])
 1  2  3  4
10 10  9 11
```

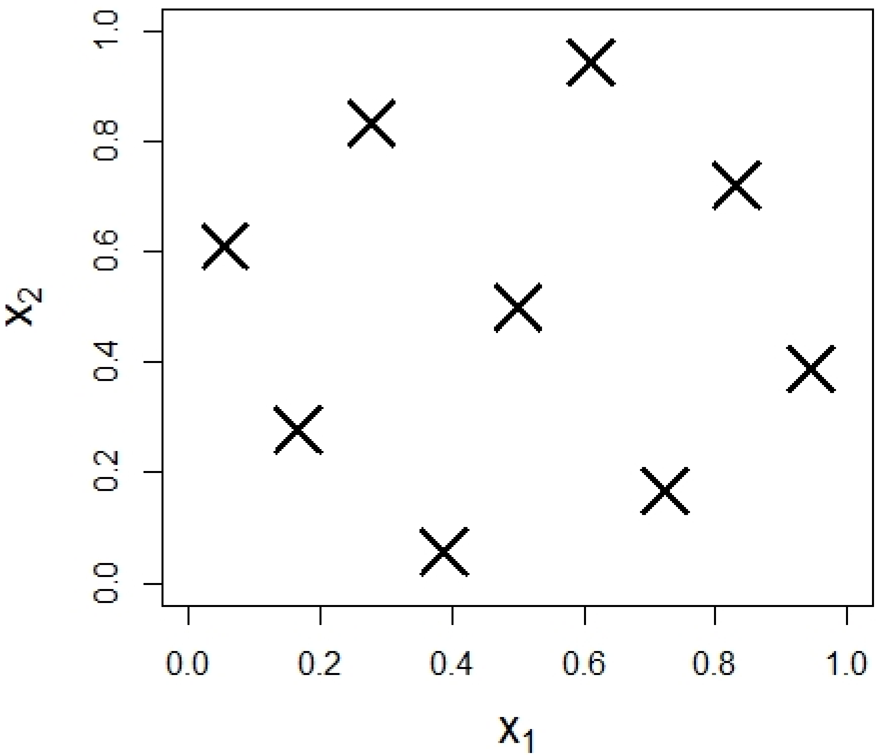
Constrained Regions

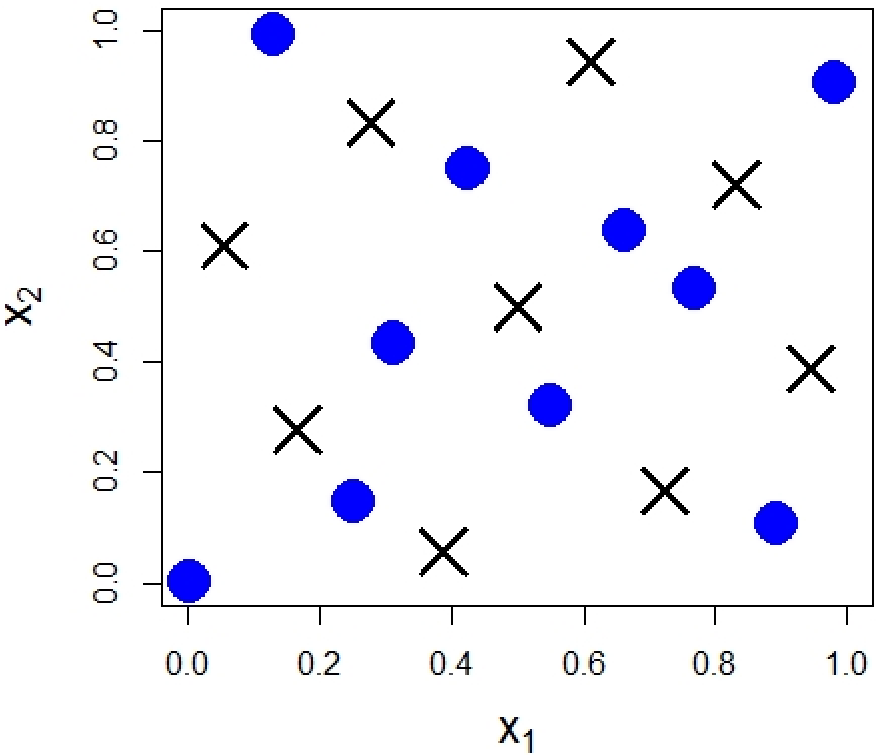
```
> D=MaxProAugment(st,CAND,nNew=29)$Design
```

Huang, C., Josep … *s and Computing*, to appear.

Validation experiments

```
> D=MaxProAugment(exist,CAND,nNew = 10)$Design[-(1:9),]
```





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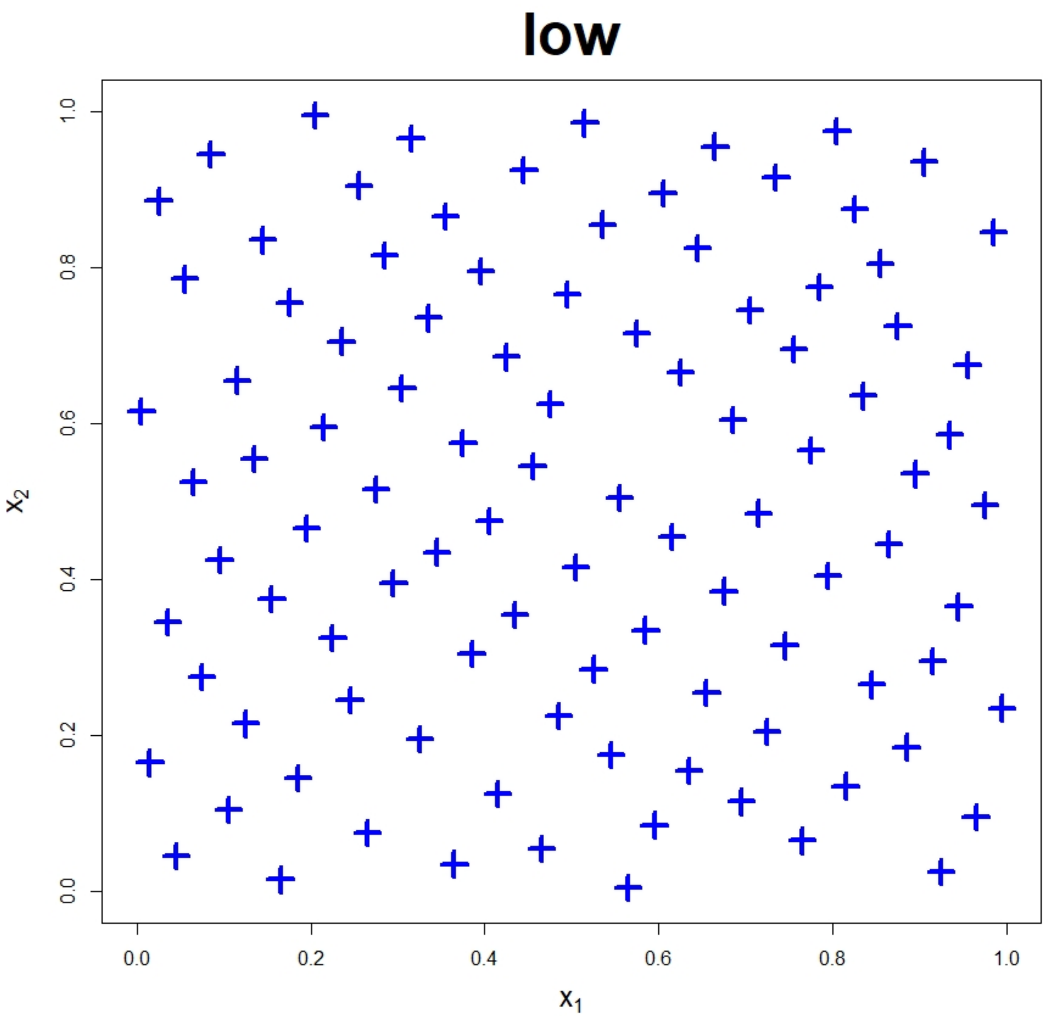
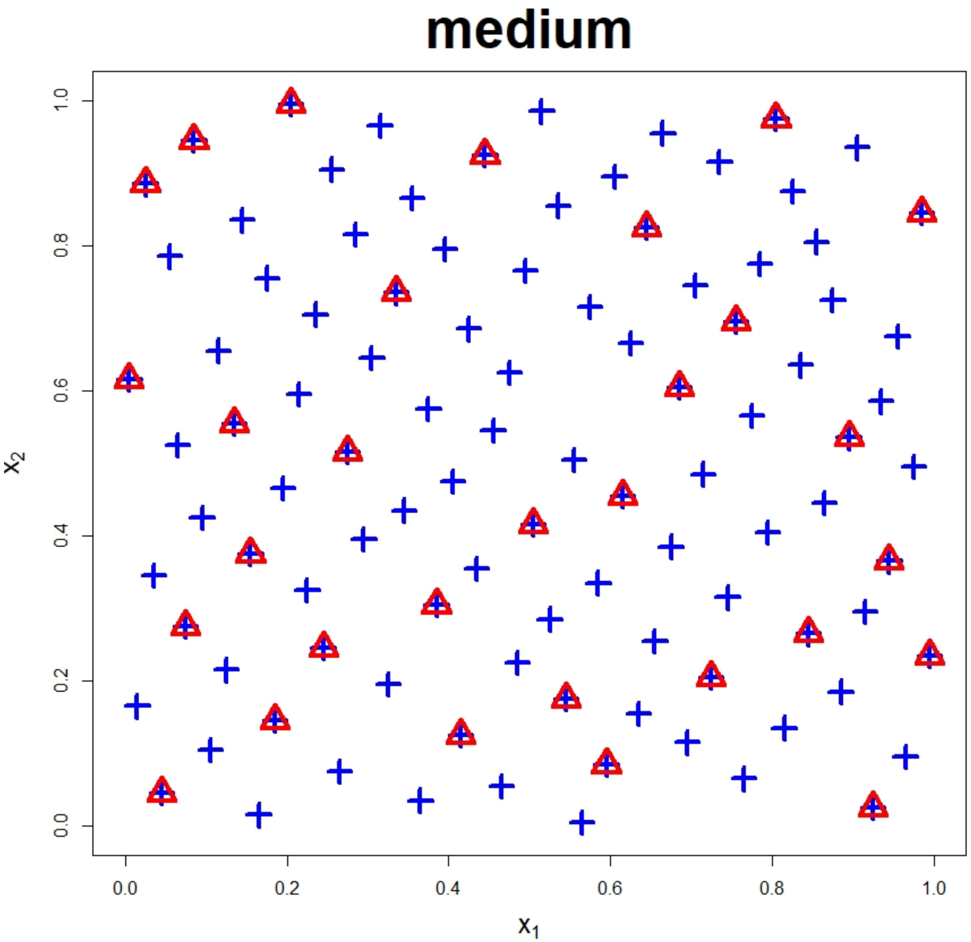
Nested Designs

```
> D3=MaxProLHD(n3,p)$Design
```



Nested Designs

```
> st=D3[sample(1:n3,1),]
> D2=MaxProAugment(st,D3,n2-1)$Design
```



Nested Designs

```
> st=D2[sample(1:n2,1),]
> D1=MaxProAugment(st,D2,n1-1)$Design
```