Space-Filling Designs for Computer Experiments

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Supported by ARO W911NF-14-1-0024

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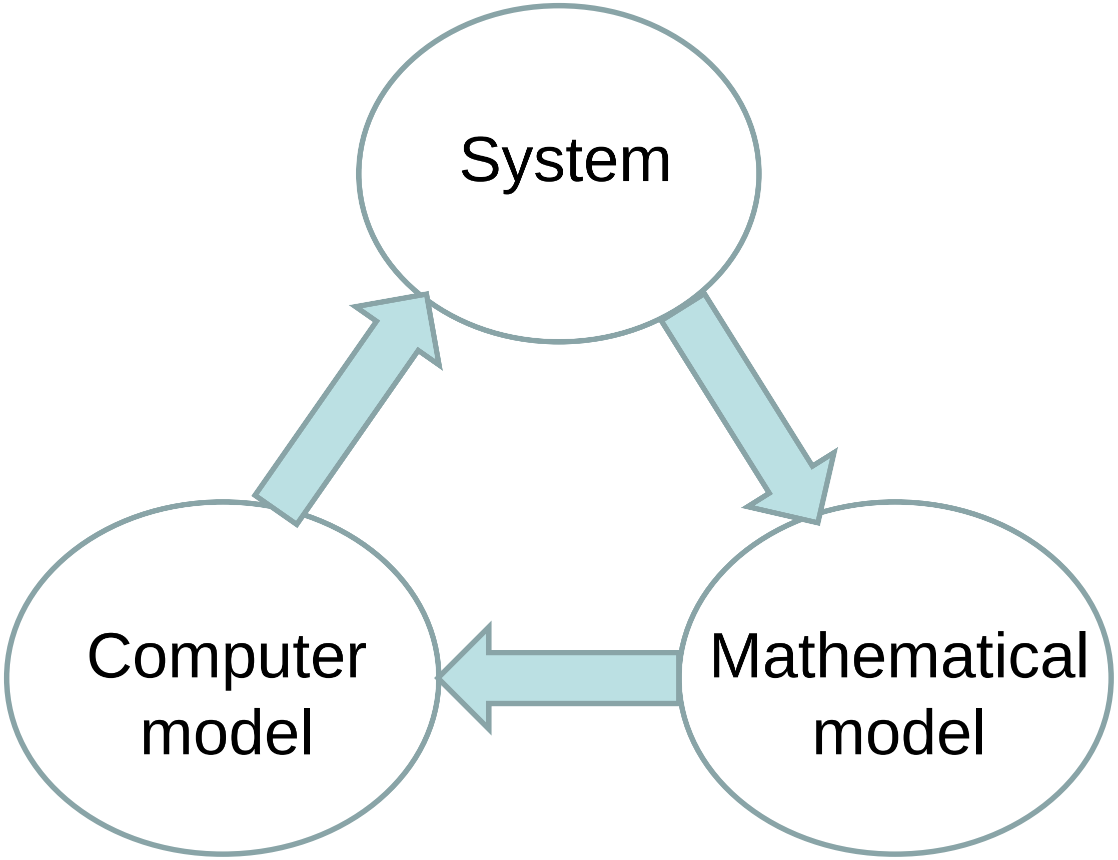
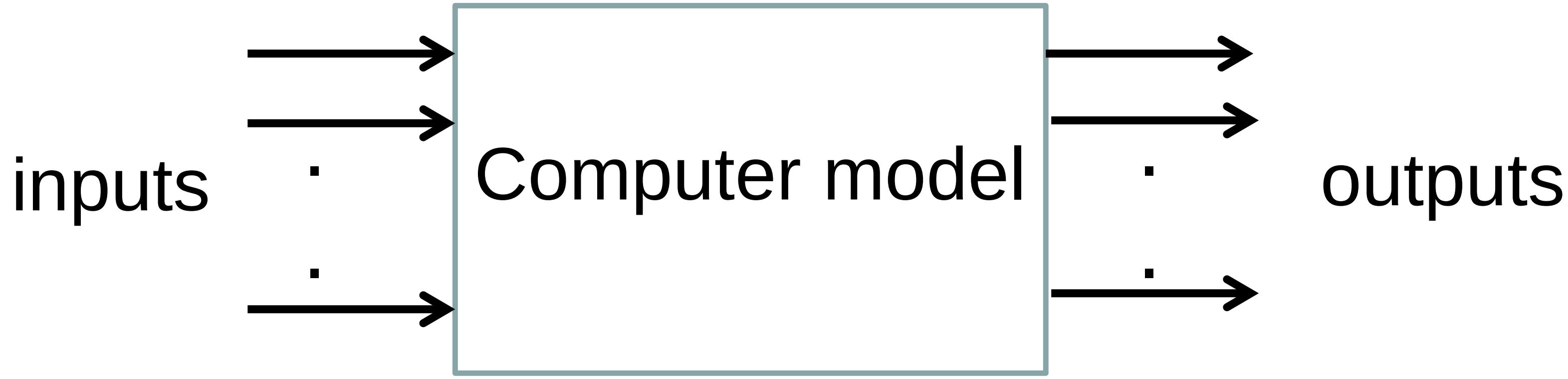
Computer model

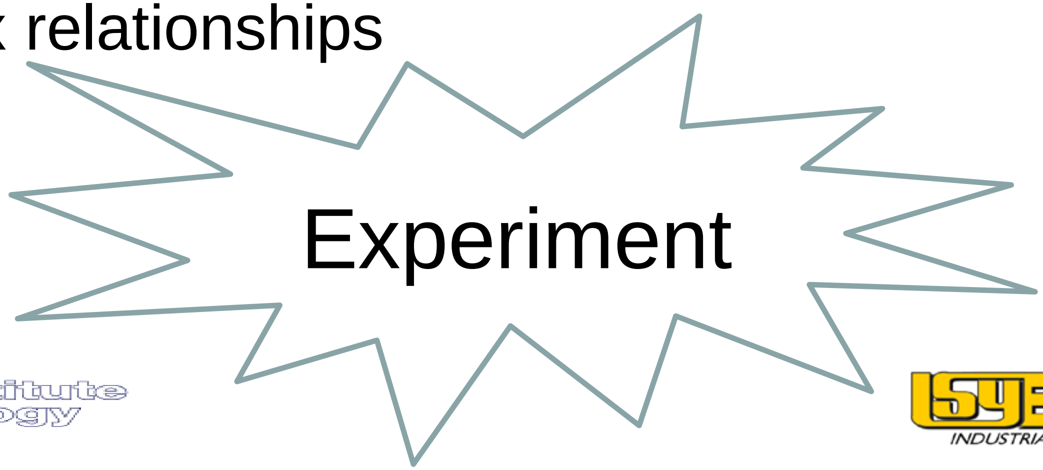


- Computer model is a numerical implementation of the mathematical model.

Computer experiments



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

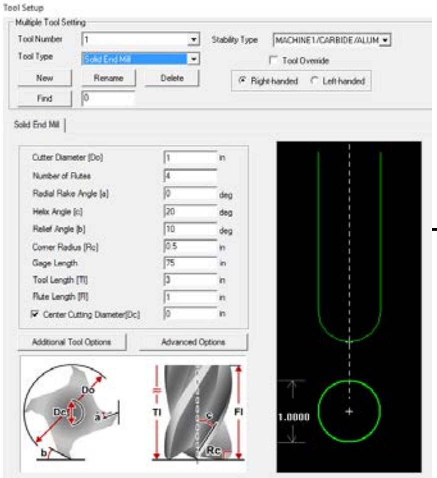


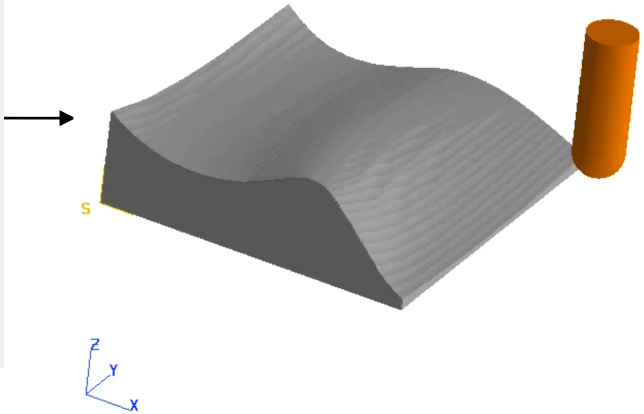
Applications

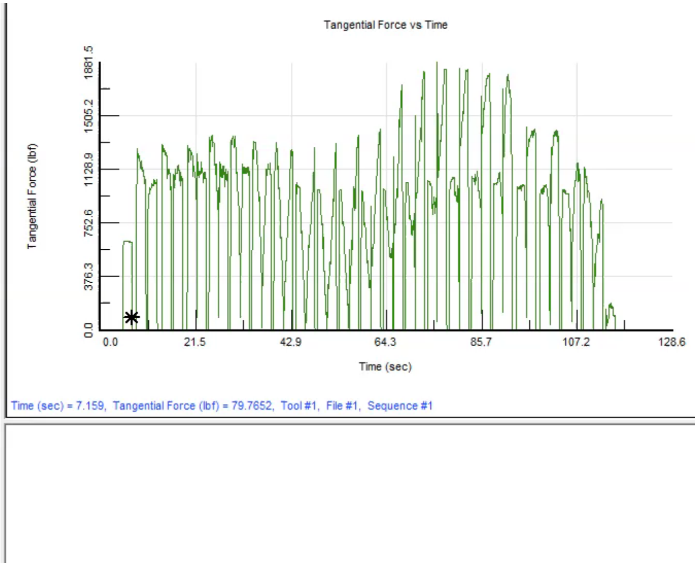
- Approximation
- Sensitivity analysis
- Calibration
- Optimization
- Uncertainty quantification

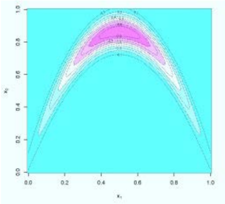
Uncertainty Quantification

Uncertainty sources



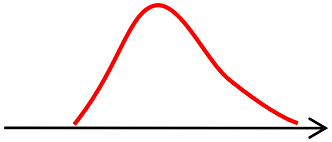






Input

Propagation of uncertainty



Output

Gul, E., Joseph, V. R., Yan, H., and Melkote, S. N. (2015). "Uncertainty Quantification in Machining Simulations Using In Situ Emulator," Under Review.

Review of Space-Filling Designs

- No need to worry about
  - Replication
  - Randomization
  - Blocking
- What type of designs?
  - Fractional factorial designs, orthogonal arrays,…? No, use space-filling designs!

Space-Filling Designs

- Definition:

  designs that fill the space!

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

Maximin distance design

- Johnson, Moore, and Ylvisaker (1991)

$$\mathcal{X} = [0,1]^p$$

$$\boldsymbol{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\} \quad \boldsymbol{x}_i \in \mathcal{X}$$

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

where $d(\boldsymbol{x}_i, \boldsymbol{x}_j)$ is the Euclidean distance between the points $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$.

Minimax distance design

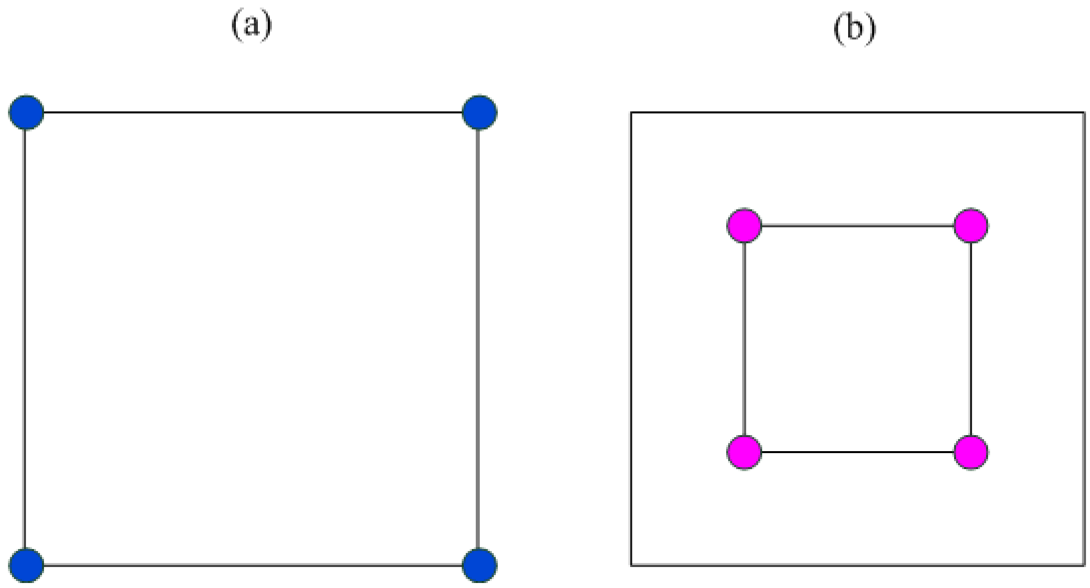
- Johnson, Moore, and Ylvisaker (1991)

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

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

Examples of Maximin and Minimax Designs

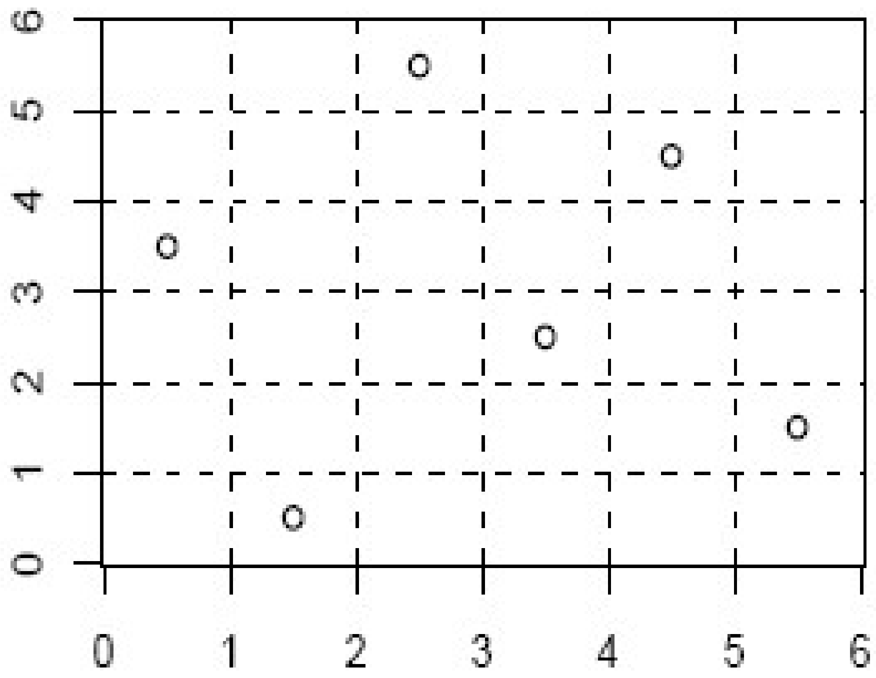
Consider the simple case of four-run design in two factors (n=4, p=2).



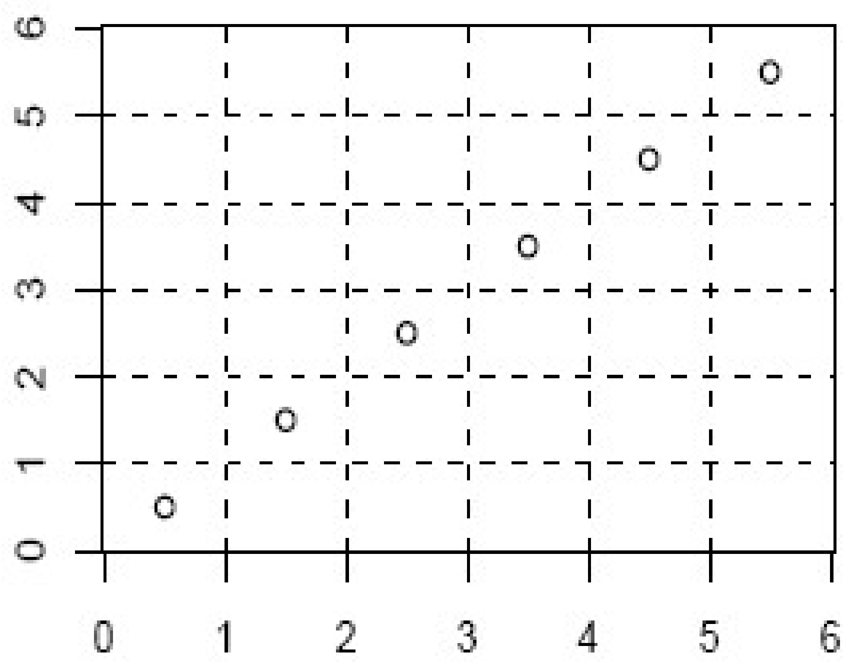
Maximin distance design. Minimax distance design.

Latin hypercube design

- McKay, Conover, Beckman (1979)



Latin hypercube design



Maximin Latin hypercube design

- Morris and Mitchell (1995): Maximin distance design within the class of Latin hypercube designs.

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

where *D* is an LHD.

Uniform design

- Fang (1980)

$$\min_{\boldsymbol{D}} \int_{\mathcal{X}} \{F_n(\boldsymbol{x}) - F(\boldsymbol{x})\}^2 d\boldsymbol{x},$$

$$F_n(\boldsymbol{x}) = \frac{1}{n} \sum_{i=1}^{n} I(\boldsymbol{x}_i \le \boldsymbol{x}).$$

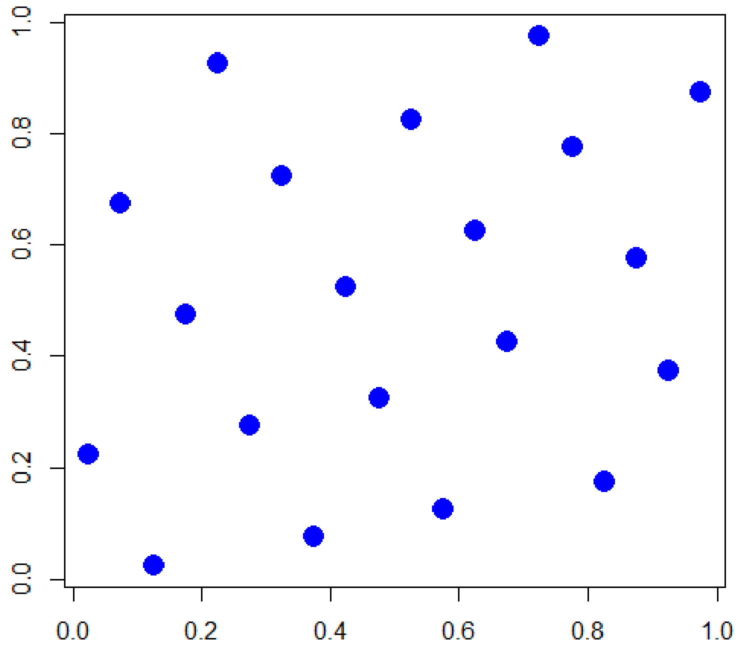
- Good for approximating integrals by sample averages.

Maximum Projection Designs

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

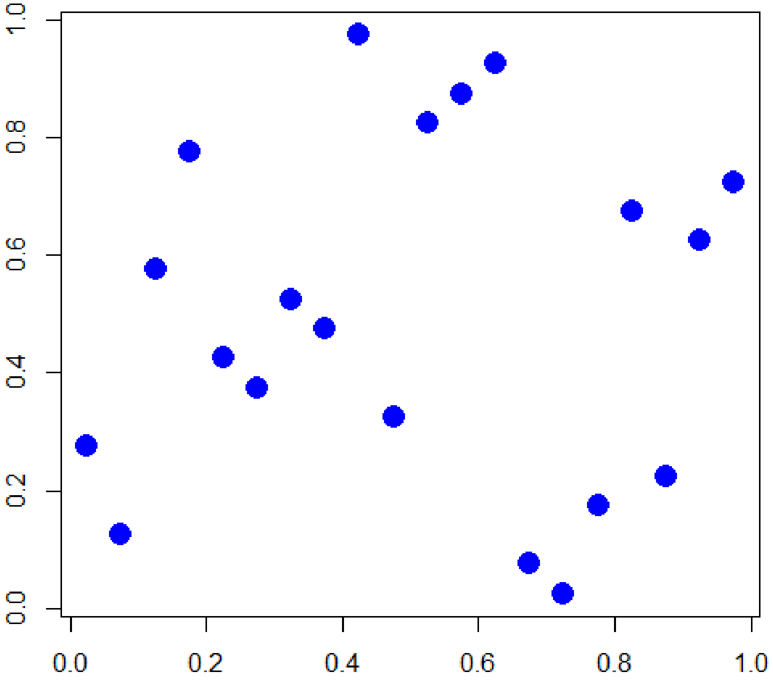
MmLHD

- 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.

Uniform Design

- Hickernell (1998) proposed CL_2 criterion that ensures projections to all subspaces.

$$\min_{\boldsymbol{D}} \quad \left(\frac{13}{12}\right)^p - \frac{2}{n}\sum_{l=1}^{n}\prod_{j=1}^{p}\left[1+\frac{1}{2}|x_{lj}-.5|-\frac{1}{2}|x_{lj}-.5|^2\right]$$
$$+\frac{1}{n^2}\sum_{l=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{p}\left[1+\frac{1}{2}|x_{li}-.5|+\frac{1}{2}|x_{ji}-.5|-\frac{1}{2}|x_{li}-x_{ji}|\right]$$

- But is uniformity important in computer experiments?

Generalized LHD

- Dette and Pepelyshev (2010): placing more points in the boundaries than around the center can minimize the prediction errors from GP modeling.

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

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

where $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_{p-1})'$ and $\theta_p = 1 - \sum_{i=1}^{p-1} \theta_i$.

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

Theorem 1 *If $k = 2p$, then under the prior in (7)*

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

- MaxPro criterion:

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

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!

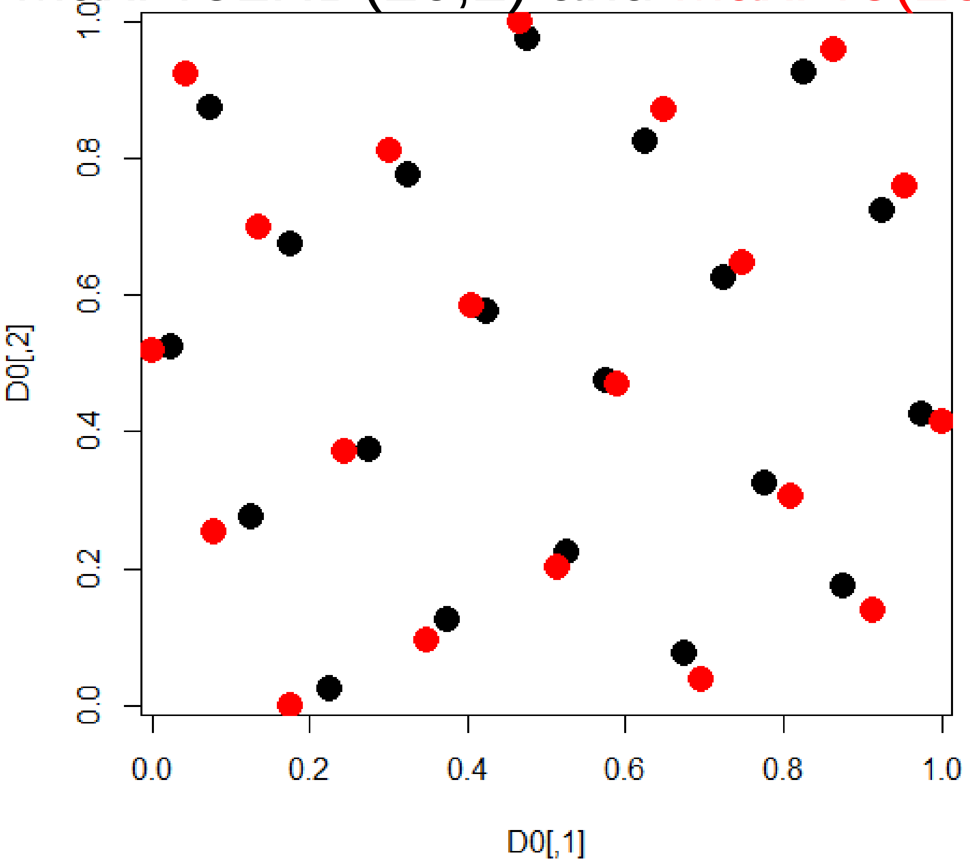
Design construction algorithm

- Minimizing MaxPro objective function is not easy!
  - *np* number of variables
  - many local minima

R Package: MaxPro
JMP 12 (under FFF)

Examples

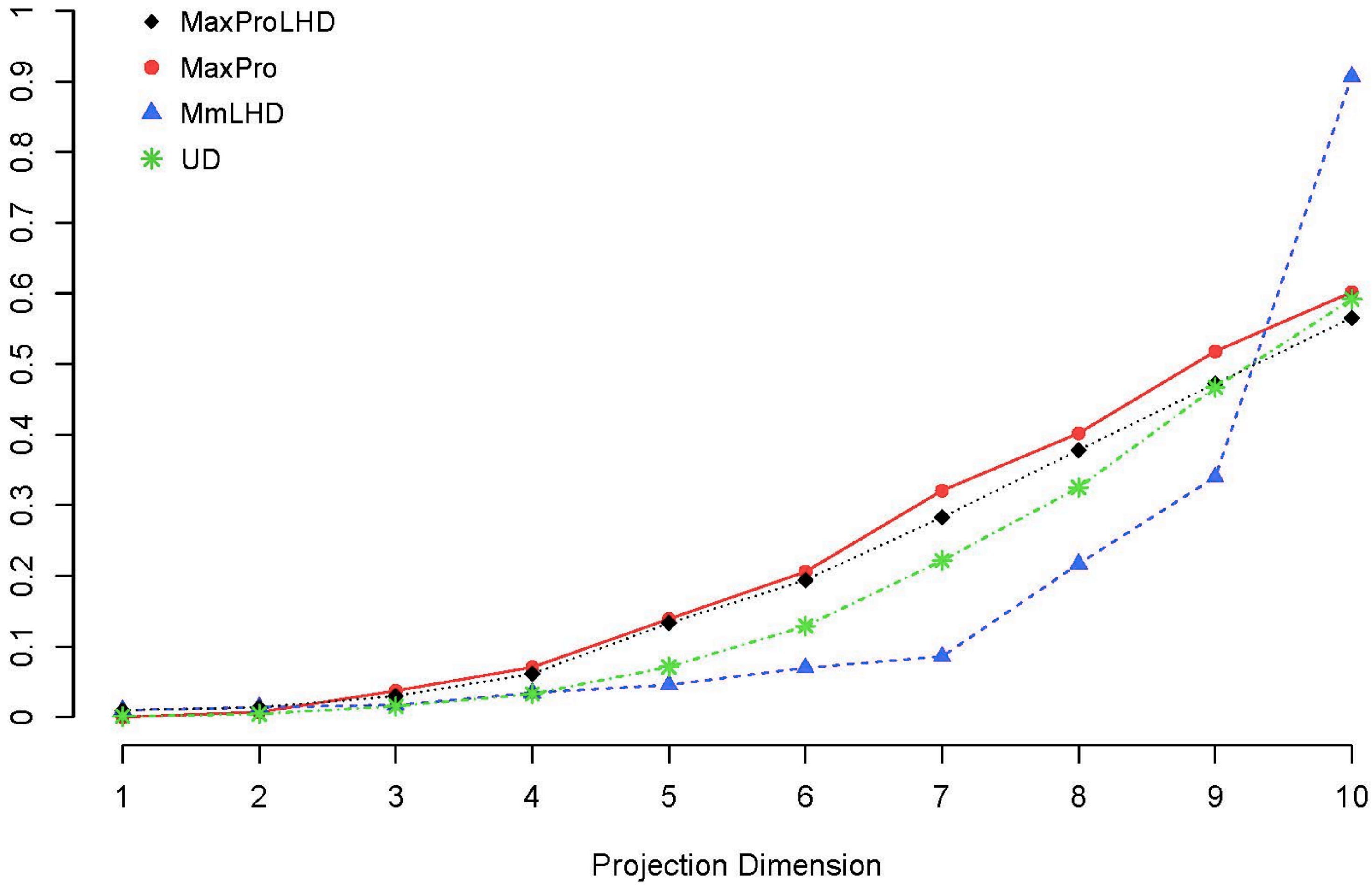
MaxProLHD(20,2) and MaxPro(20,2)



Numerical comparisons

- n=100, p=10
- Designs:
  - MaxPro
  - MaxProLHD
  - MmLHD
  - UD
  - GLHD
- Criteria:
  - Maximin
  - miniMax
  - CL_2

Minimum distance (larger-the-better)



GP-based criteria

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

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

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An optimality result

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

Theorem 2 *For the Gaussian correlation function and the noninformative prior for* $\boldsymbol{\alpha}$ *in (14), MaxPro designs minimize*

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

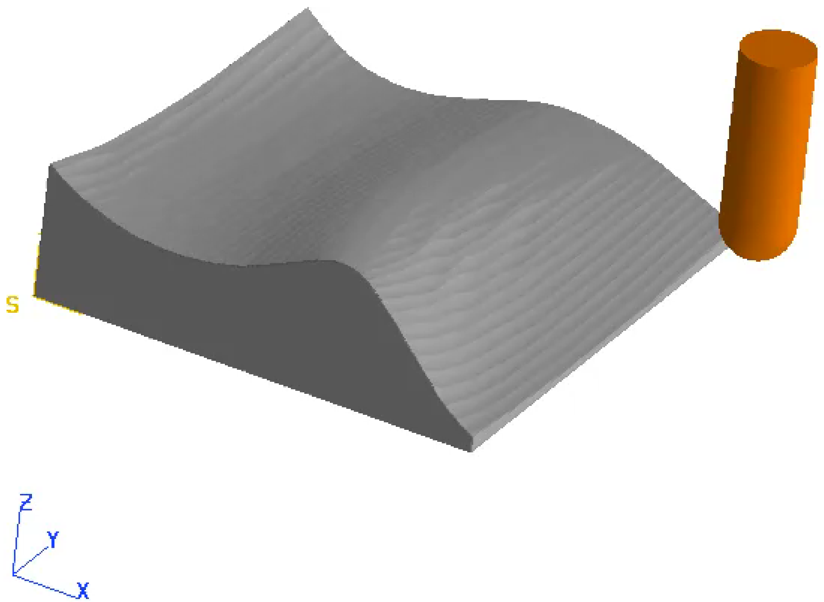
for any $\gamma > 0$.

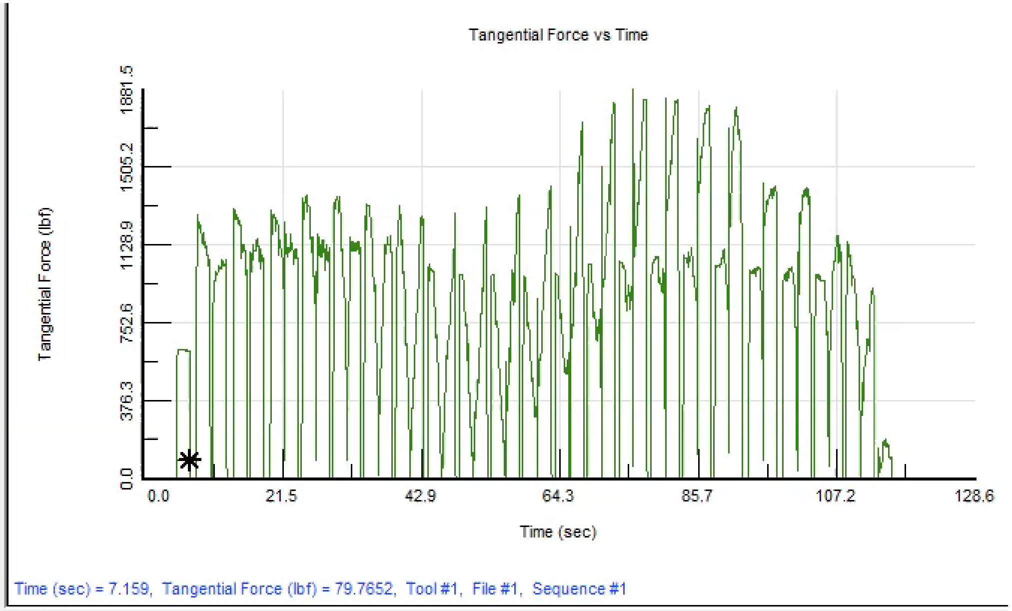
- MaxPro design is good in terms of Entropy, condition number, prediction variance, etc.

Applications

Solid End Milling Process

- Simulation on computer model of Production Module software

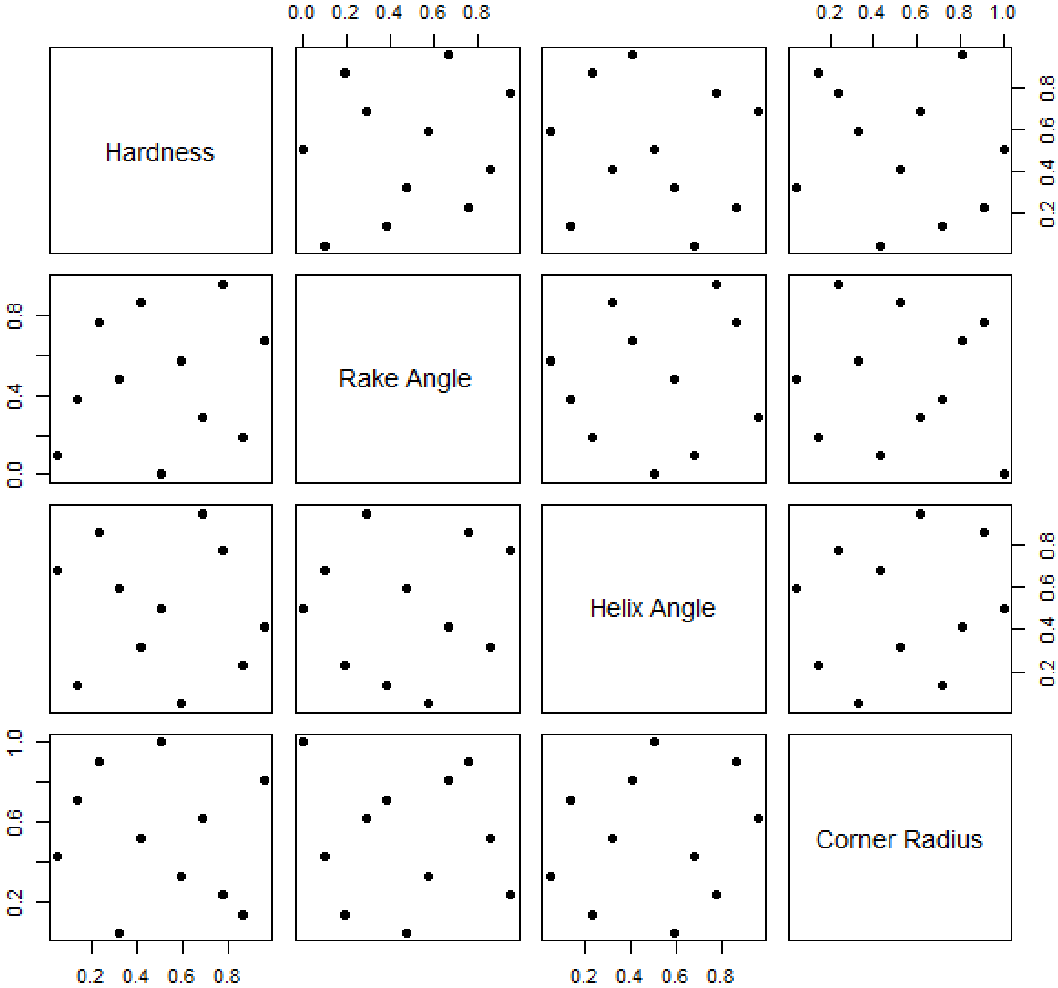




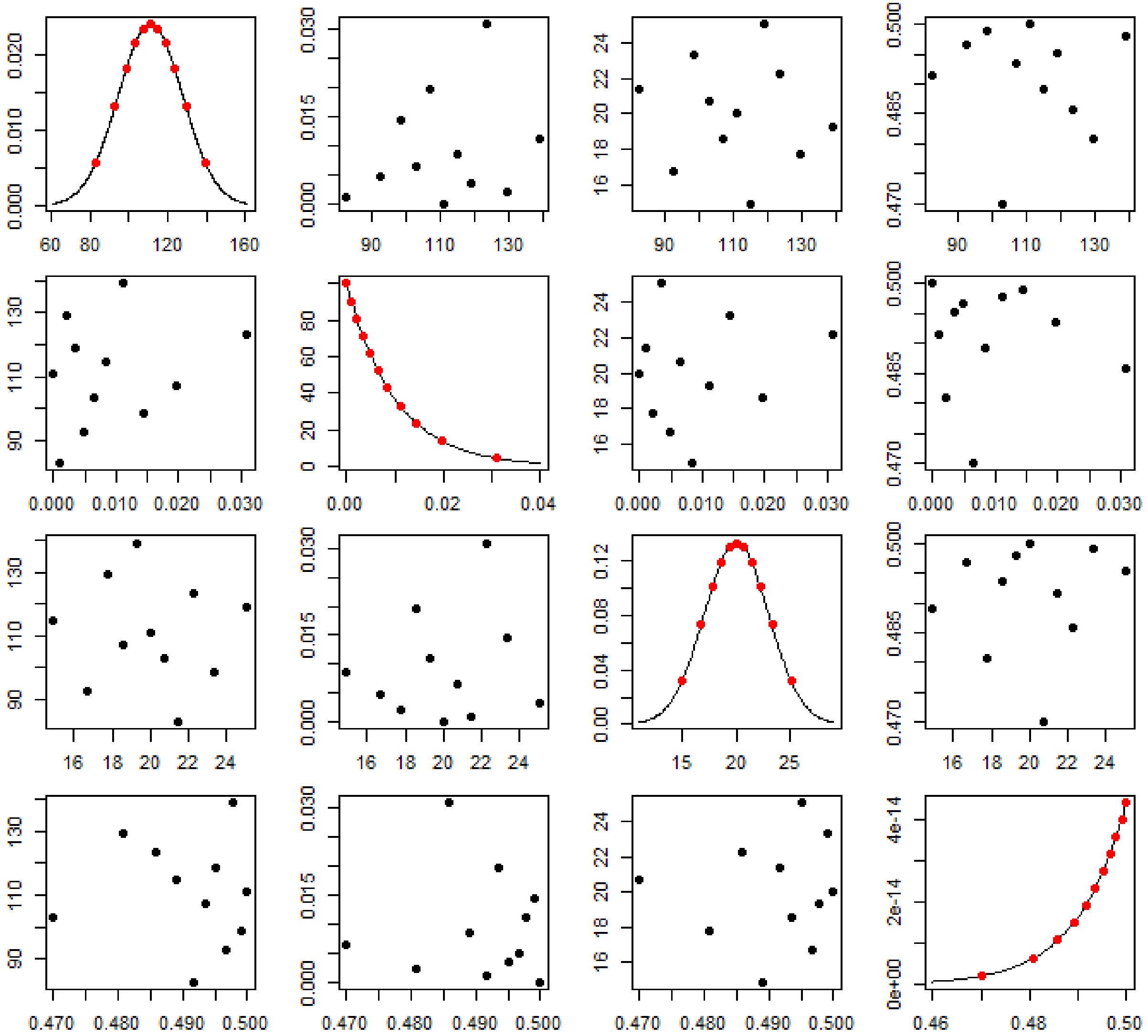
UQ for Solid End Milling

Parameter	Nominal Setting	Probability Dist.
Hardness	111 Bhn	$N(111, (111*0.15)^2)$
Rake Angle	0 deg	$Exp(\lambda=100)$
Helix Angle	20 deg	$N(20, (20*0.15)^2)$
Corner Radius	0.50 mm	$Beta(\alpha=50, \beta=1)/2$

MaxPro LHD


Hardness
Rake Angle
Helix Angle
Corner Radius
0.0 0.2 0.4 0.6 0.8
0.2 0.4 0.6 0.8 1.0

After Inverse probability transform



In-Situ Emulator

$$\hat{f}(\boldsymbol{u}, t) = exp\{\log f(\boldsymbol{u_0}, t) + \hat{\delta}_t(\boldsymbol{u})\}$$

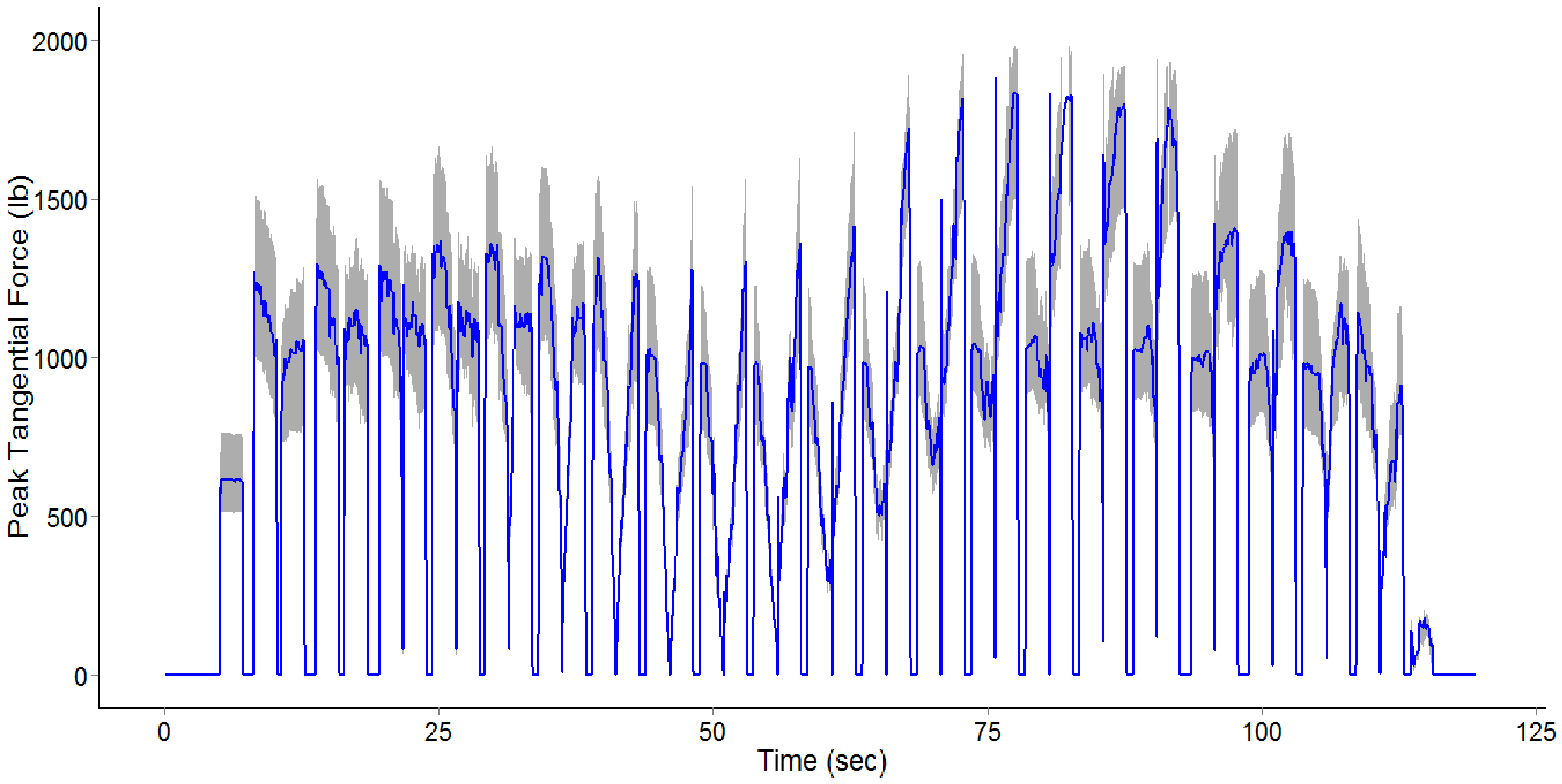
$$\hat{\delta}_t(\boldsymbol{u}) = \boldsymbol{r}(\boldsymbol{u})'\boldsymbol{R}^{-1}(\boldsymbol{w}_t - \boldsymbol{w}_{0,t})$$

where

$$R_t(\boldsymbol{u}_i - \boldsymbol{u}_i) = R_{t,\boldsymbol{u}}(\boldsymbol{u}_i - \boldsymbol{u}_j) - R_{t,\boldsymbol{u}}(\boldsymbol{u}_i - \boldsymbol{u}_0) - R_{t,\boldsymbol{u}}(\boldsymbol{u}_j - \boldsymbol{u}_0) + 1,$$

$$R_{t,\boldsymbol{u}}(\boldsymbol{u}_i - \boldsymbol{u}_j) = \exp\left\{-\sum_{k=1}^{p} \theta_{t,k}\left(u_{ik} - u_{jk}\right)^2\right\}.$$

Output with 95% confidence region



Computational time

	UD (n=2000)	In-Situ Emulator
Curve cutting	1 day	8 mins
5-axis cutting	9 days	1 hour

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References

- V. Roshan Joseph (2016). “Space-Filling Designs for Computer Experiments: A Review,” (with discussions and rejoinder), *Quality Engineering*, 28, 28-44.
- V. Roshan Joseph, Gul, E., and Ba, S. (2015). “Maximum Projection Designs for Computer Experiments,” *Biometrika*, 102, 371-380.
- Gul, E., V. Roshan Joseph, Yan, H., and Melkote, S. N. “Uncertainty Quantification in Machining Simulations Using In Situ Emulator,” Under review.

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