

Surrogate Optimization: Space-Filling Designs

BIOE 498/598 PJ

Spring 2021

From local to global optimization

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- ▶ It's possible a better operating condition exists far away.
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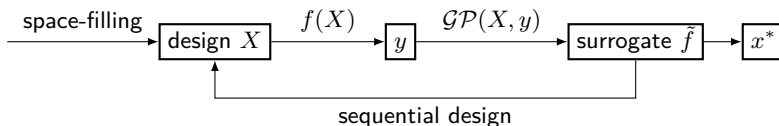
Method	Search	# of samples	Sampling
Steepest Ascent/RSM	local	10–100's	very expensive, noisy
Surrogate Optimization	global	100–1000's	moderately expensive
Reinforcement Learning	global	10,000+	very inexpensive

Surrogate Optimization

- ▶ Assume we are trying to optimize a function f that is **expensive** to evaluate.
- ▶ Instead, we use evaluations of f to build a surrogate model \tilde{f} that is **cheap** to evaluate.
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Why use surrogates?

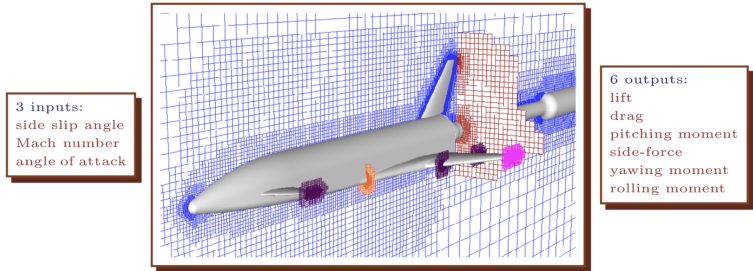


FIGURE 2.1: Drawing of the LGBB computational fluid dynamics computer model simulation. Adapted from Rogers et al. (2003); used with permission from the authors.

Surrogate optimization by many names

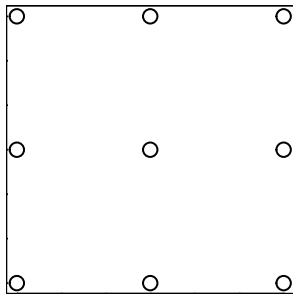
- ▶ **Computer experiments, emulation, or metamodeling** based on historical usage.
- ▶ **Kriging** from geostatistics (refers to prediction with GPR).
- ▶ **Nonparametric Bayesian optimization** to impress your manager.
- ▶ **Sequential design** in the DOE field.
- ▶ **Active learning** in the ML field.

Today: Space-Filling Designs

- ▶ Global optimization requires data from every part of the design space.
- ▶ We want to cover as much of the space as possible with the fewest number of points.
- ▶ **Space-Filling Designs** spread samples over a multidimensional space $[0, 1]^k$.
 - ▶ Other design spaces can be rescaled to match this hypercube.
- ▶ Later we will use the surrogate to *intelligently* augment the initial design.

How about evenly-spaced designs (grids)?

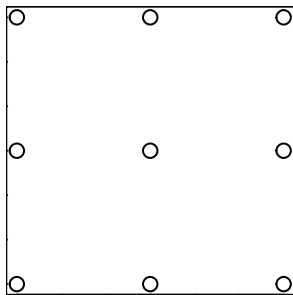
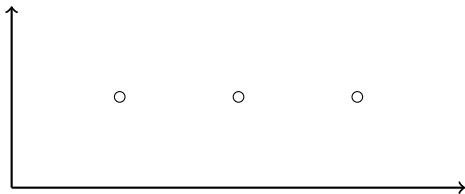
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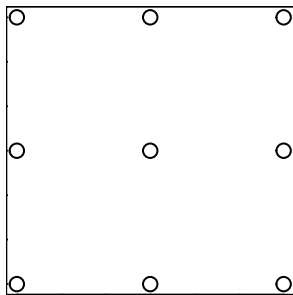
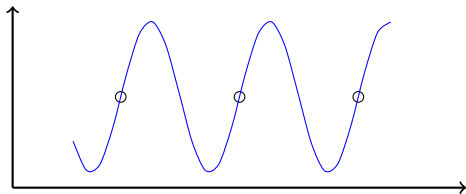
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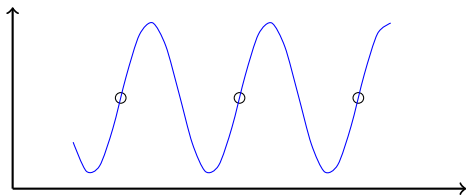
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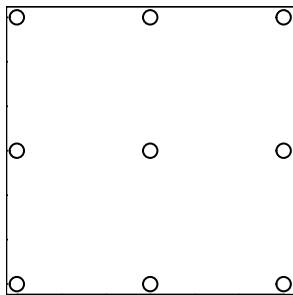
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2. Regular designs have poor **projection spacing**. This is a problem because of effect sparsity!

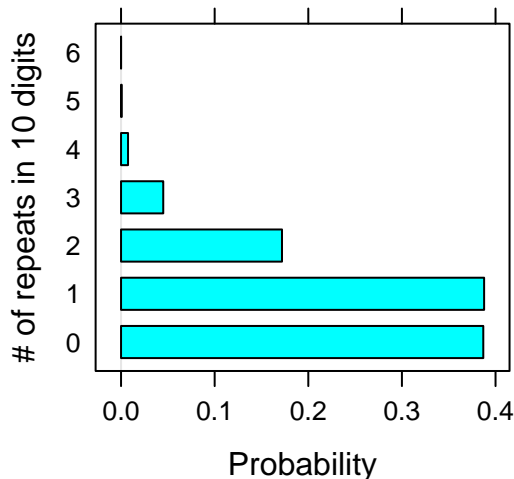


Why not random locations?

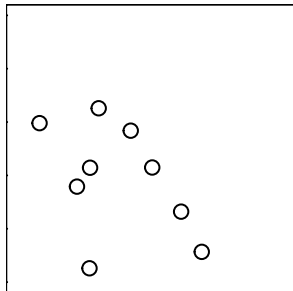
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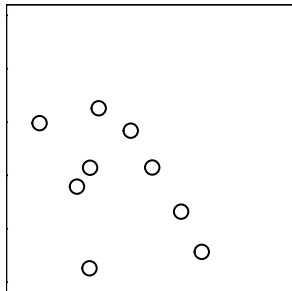
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We need a **Space-Filling Design** that

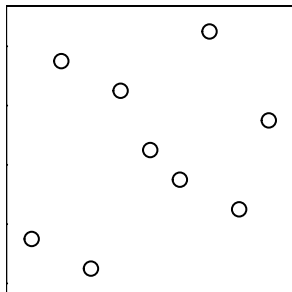
1. Places points semi-randomly to avoid aliasing
2. Avoids "clumps" of points
3. Projects well onto lower dimensions



Latin Hypercube Designs

A Latin Hypercube Design (LHD) is a semi-random design that guarantees uniform projection.

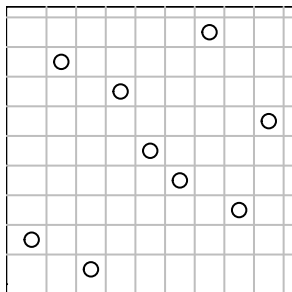
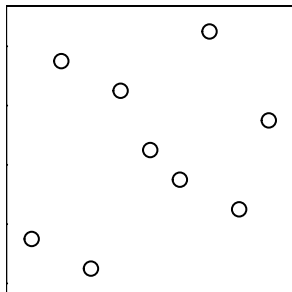
- ▶ Each dimension is divided into n intervals.
- ▶ Points are placed randomly, but only one point is allowed in each interval along each dimension.
- ▶ Points can be placed in the center or a random position in each "square".
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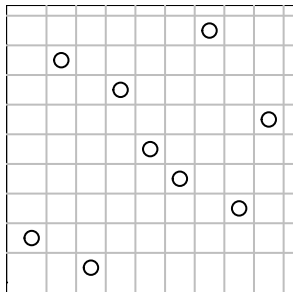
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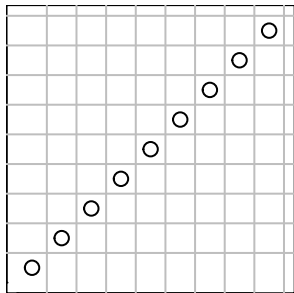
Building a LHD

1. The interval along the first dimension is simply $1 \dots n$; there is no need to randomize.
2. For each subsequent dimension, select a random permutation of $\{1 \dots n\}$

x_1	x_2
1	2
2	8
3	1
4	7
5	5
6	4
7	9
8	3
9	6

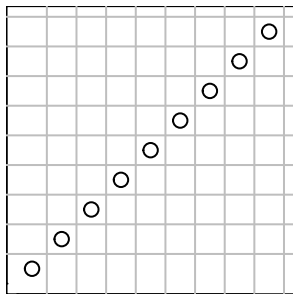


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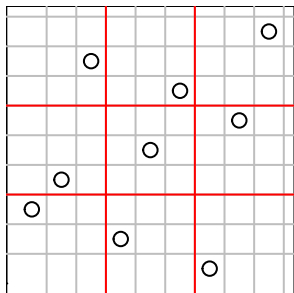


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One alternative is an Orthogonal Array LHD.

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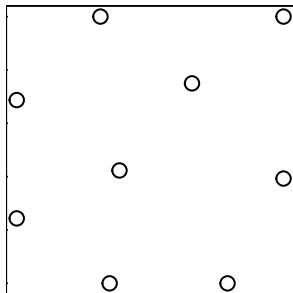
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Computationally, we begin with a random set of n points and iteratively move points until a local optimum is found.

The maximin package

The maximin package creates sequential space-filling designs.

```
X1 <- maximin::maximin(  
  n=9, p=2, T=100)
```

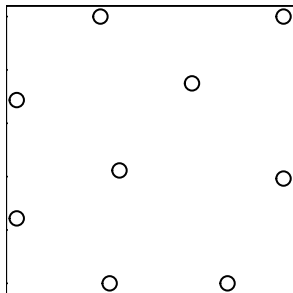


n=number of samples, p=number of dimensions, T=number of iterations for the optimizer.

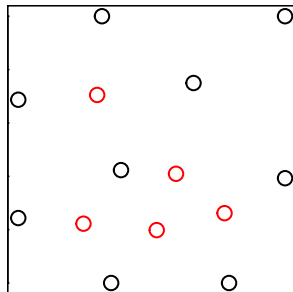
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```
X1 <- maximin::maximin(  
  n=5, p=2, T=100,  
  Xorig=X1$Xf)
```



n=number of samples, p=number of dimensions, T=number of iterations for the optimizer.

Summary

- ▶ Surrogate optimization begins with a space-filling design.
- ▶ Grid and random designs are not good.
- ▶ LHD and Maximin designs spread points globally and project well to lower dimensions.
- ▶ **Next time:** Building a surrogate model from an initial space-filling design.