Design of computer experiments

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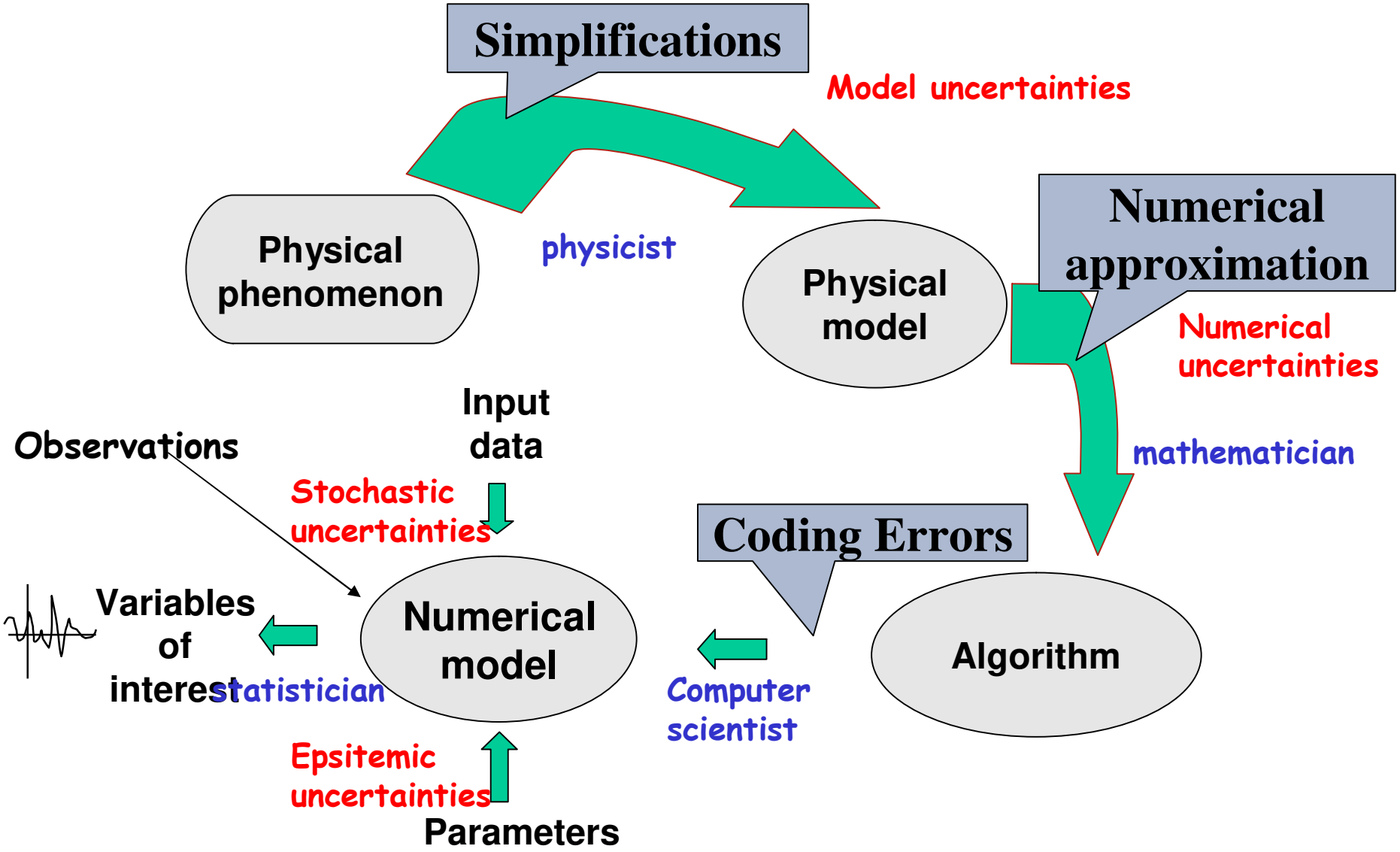
07/07/2014

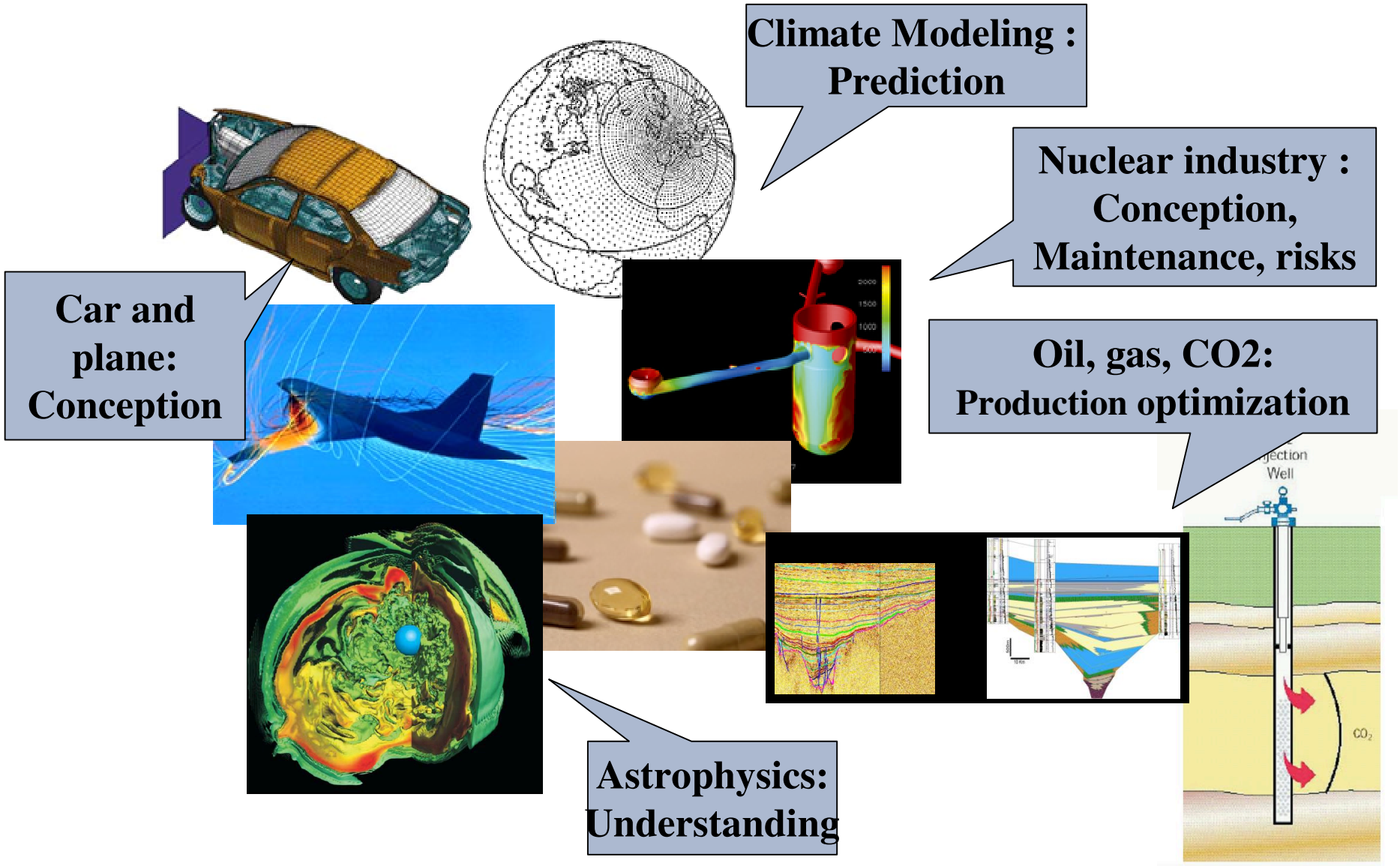
Starting point: uncertainties everywhere in the modeling chain !

Main problem: credibility of predictions



Similar safety and uncertainty issues in CS&E and Nature sciences

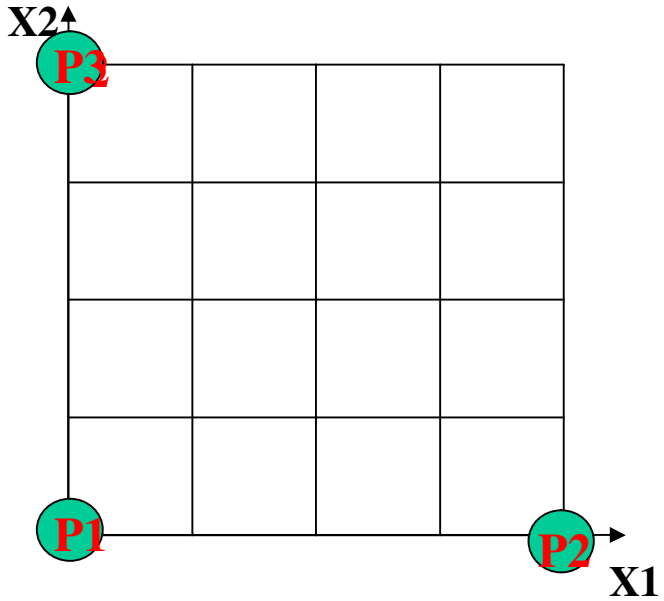
CS&E : Computational Science & Engineering



Main stakes of uncertainty management

- **Modeling phase:**
  - Improve the model
  - Explore the best as possible different input combinations
  - Identify the predominant inputs and phenomena in order to priorize R&D
- **Validation phase:**
  - Reduce prediction uncertainties
  - Calibrate the model parameters
- **Practical use of a model:**
  - **Safety studies:** assess a risk of failure (rare events)
  - **Conception studies:** optimize system performances and robustness

Typical engineering practice : One-At-a-Time (OAT) design



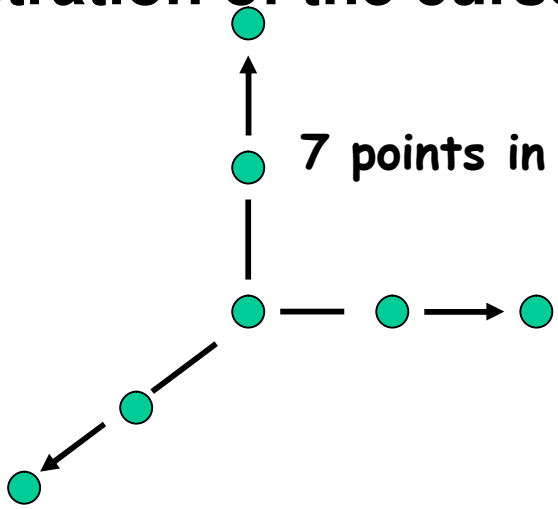
<u>Main remarks :</u>

OAT brings some information, but potentially wrong

Exploration is poor: Non monotonicity ? Discontinuity ? Interaction ?

Leave large unexplored zones of the domain (curse of dimensionality)

Illustration of the curse of dimensionality

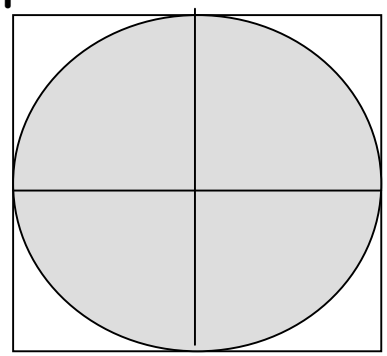


7 points in a 3D space

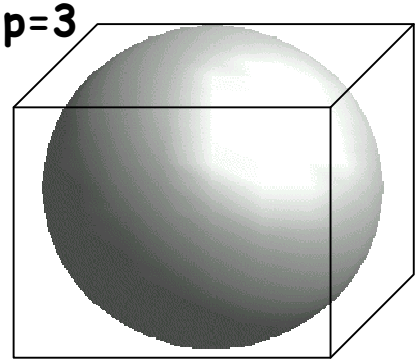
Bad space covering

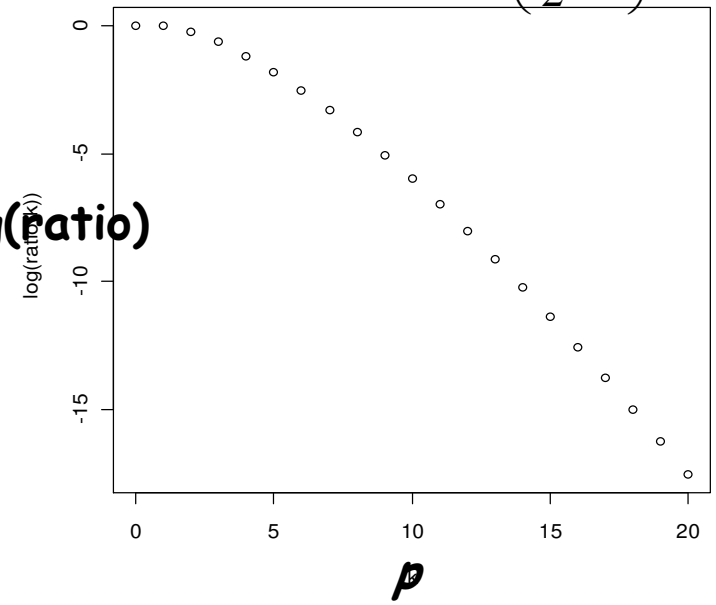
$$\text{vol. sphere}\,(r=0.5) = \frac{\pi^{p/2}}{\Gamma\left(\frac{p}{2}+1\right)}\left(\frac{1}{2}\right)^p$$

p=2



p=3





Surf. circle / Surf. square ~ 3/4

Vol. sphere / Vol. cube ~ 1/2

p=10 → Ratio ~ 0.0025

hypercube volume >> (included and tangent) hypersphere volume

For large dimensions, all the points will be in the corner of the hypercube

Model exploration goal

GOAL : explore as best as possible the behaviour of the code

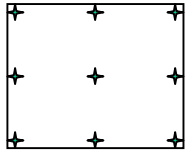
Put some points in the whole input space in order to « maximize » the amount of information on the model output

Contrary to an uncertainty propagation step, it depends on *p*

Regular mesh with n levels → $N = n^p$ simulations

Ex: $p = 2$, $n = 3$ → $N = 9$

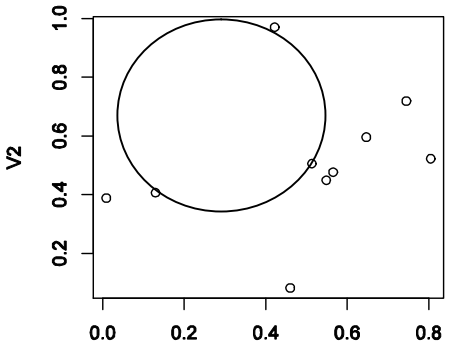
$p = 10$, $n = 3$ → $N = 59049$



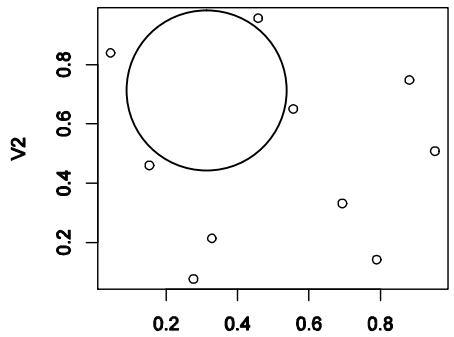
To minimize N, needs to have some techniques ensuring good « coverage » of the input space

Simple random sampling (Monte Carlo) does not ensure this

Ex: $p = 2$
$N = 10$



Monte Carlo



Optimized design

Exploration in physical experimentation

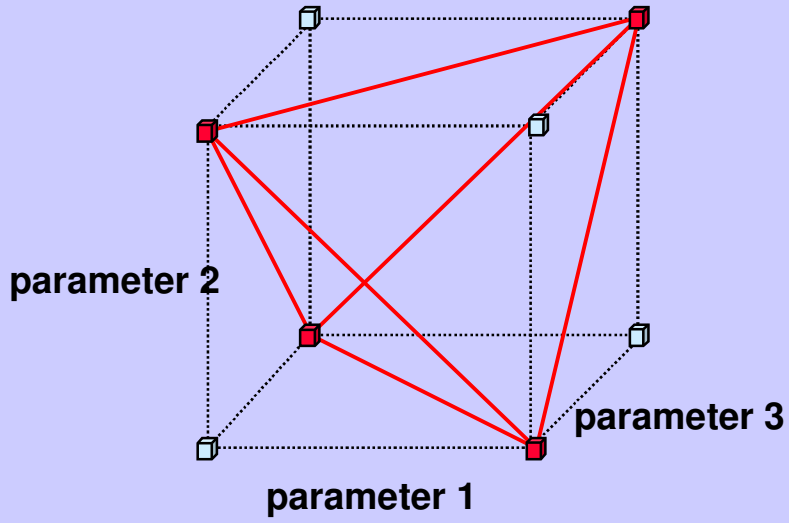
Design of experiments develops strategies to define experiments in order to obtain the required information as efficiently as possible

Designs for real experiments

Estimate parameters of linear regression with a minimal number of points

Examples :

- Full factorial design 2^3
- Fractional factorial design 2^{3-1}



Biblio : Fisher (1917), Box et Wilson (1954), Taguchi (1960), Mitchell (1958), ŭ

Designs for numerical experiments

Characteristics

Deterministic experiments (no error),

Large number of input variables,

Large range of input variation domain,

Multiple output variables,

Strong interactions between inputs,

High non linearity in the model

→ space filling designs (uniform coverage in the input space)

Biblio : Kleijnen (1970), McKay (1979), Morris (1995), Sacks (1989), ŭ

PLAN

ð **Part 1 : Factorial designs**

- Full factorial design
- Fractional factorial design
- Resolution

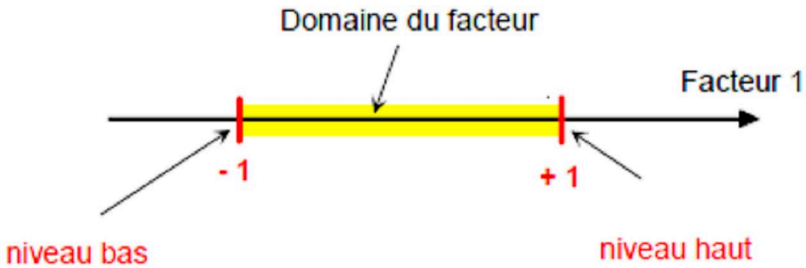
ð **Part 2 : Designs for numerical experiments**

- Properties
- Low discrepancy sequence
- Latin Hypercube sampling (LHS)

PART 1 : FACTORIAL DESIGNS

Full factorial design

- **Hypothèses :**
  - ***p* inputs (« factors »)**
  - **2 levels per factor**



- **Full factorial design**
  - **Orthogonality principle**

    Variation of each factor when the others are are succesively fixed at their 2 possible values

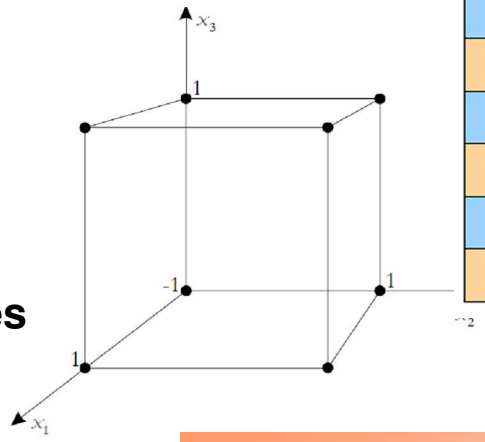
    ⇒ 2^p experiments.

  - **For continuous or dicrete factors**

  - **Problem: Number of experiments becomes too large when *p* or the number of levels increase.**

Ex : p=10 factors at 2 levels ⇒ 1024 experiments

X_1	X_2	X_3
–1	–1	–1
1	–1	–1
–1	1	–1
1	1	–1
–1	–1	1
1	–1	1
–1	1	1
1	1	1



Factorial design at 2 levels for *p* = 3 factors

PART 1 : FACTORIAL DESIGNS

Full factorial design

Exploitation of a factorial design

- realisation of the experiments

- exploitation => computation of coefficients b_{ij} => construction of a simplified model

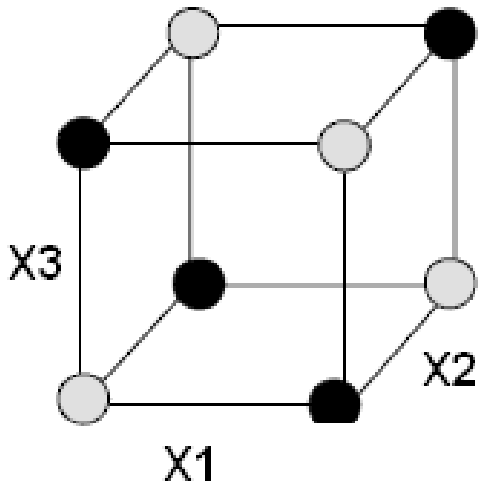
$$Y = Cste + \sum_{i} b_i X_i + \sum_{i<j} b_{ij} X_i X_j + \sum_{i<j<k} b_{ijk} X_i X_j X_k + \ldots$$

Response **Main effects** **Interactions of order 2**

PART 1 : FACTORIAL DESIGNS

Fractional factorial design

- **Study of all the factors with a reduced number of experiments**
- **Fraction of a full design**
  - ⇒ 2^{p-q} **experiments**
- **Selection of this fraction ?**
  - ⇒ **Choice of an alias structure**
  - ⇒ **determine which effects are confused**



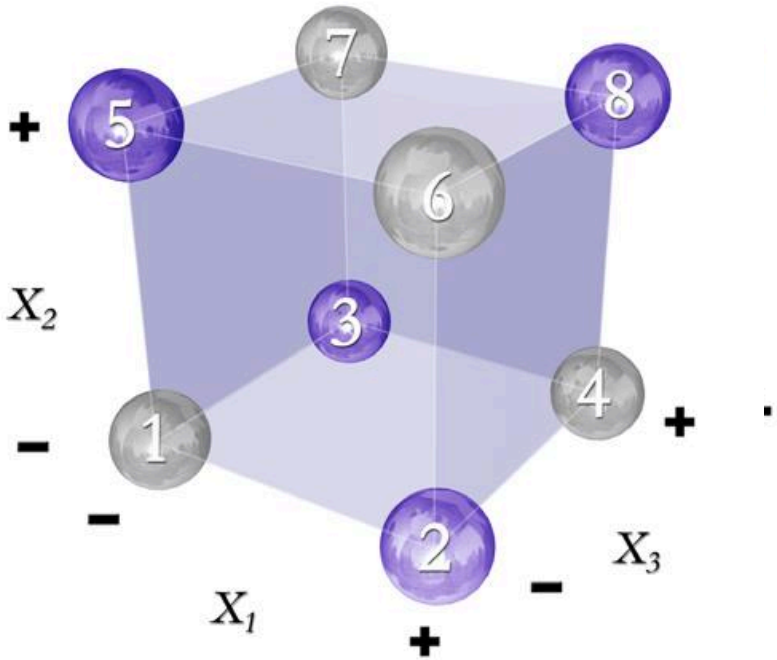
Full factorial design 2^3 decomposed in 2 fractional factorial designs 2^{3-1} (black and white)

$$Y = Cste + \sum_i b_i X_i + \sum_{i<j} b_{ij} X_i X_j + \sum_{i<j<k} b_{ijk} X_i X_j X_k + \ldots$$

Response **Main effects** **Interactions of order 2**

ILLUSTRATION

Fractional factorial designs



X_1	X_2	X_3
+	−	−
−	−	+
−	+	−
+	+	+

Well-balanced design

All the factors (and interactions) are produced at their low and high levels the same number of times.
The columns are orthogonals.
→ Good statistical properties

PART 1 : FACTORIAL DESIGNS

Fractional factorial design

Example of a fractional factorial design for p = 5 factors and q = 2

- **design with 2^{5-2} = 8 experiments:**
  - Full design at 3 factors for (X_1, X_2, X_3)
  - Effects of X_4 confused with interaction X_1X_2
  - Effects of X_5 confused with interaction X_1X_3

    $\Rightarrow$ 3 alias of 1
    - $X_1 X_2X_4 = 1$
    - $X_1 X_3X_5 = 1$
    - $X_2X_3X_4X_5 = 1$

- **Resolution R :**

  R = minimal number of elements of the alias of 1

  = cardinal of the smallest alias generator

  Example : R = III

A design of resolution R does not confound the effects of order s1 and s2 with s1 + s2 < R

X_1	X_2	X_3	$X_4 = X_1 X_2$	$X_5 = X_1 X_3$
–1	–1	–1	1	1
1	–1	–1	–1	–1
–1	1	–1	–1	1
1	1	–1	1	–1
–1	–1	1	1	–1
1	–1	1	–1	1
–1	1	1	–1	–1
1	1	1	1	1

Fractional factorial design 2^{5-2}

PART 1 : FACTORIAL DESIGNS

Resolution of a fractional factorial design

- **Résolution III :** all the main effects are not confused

- **Resolution IV :** a main effect cannot be confused with an interaction, but 2 interactions can be confused

- **Resolution V :** we can pose a model with the effects and interactions of order 2 without confusion

		nb of variables								
		3	4	5	6	7	8	9	10	11
nb of runs	4									
	8									
	16									
	32									
	64									
	128									

R3 R4 R5

Resolution V is considered as sufficient in most of the applications

resolution III is considered as a minimal property

PLAN

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  - Resolution

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  - Low discrepancy sequence
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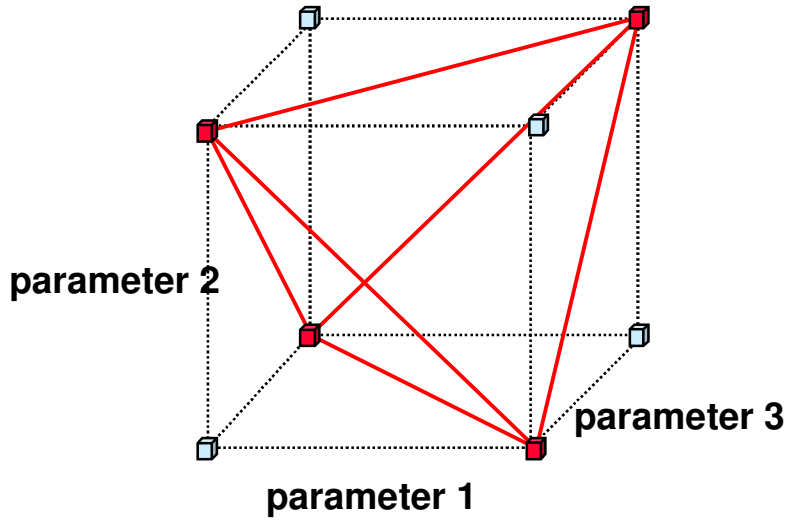

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Objectives

When the objectives is to discover what happens inside the model and when no model computations have been realized, we want to respect the two following constraints:

- To spread the points over the input space in order to capture non linearities of the model output,

- To ensure that this input space coverage is robust with respect to dimension reduction.

Therefore, we look some design which insures the « best coverage » of the input space

<u>Main question:</u>

- How to define this « best » ?

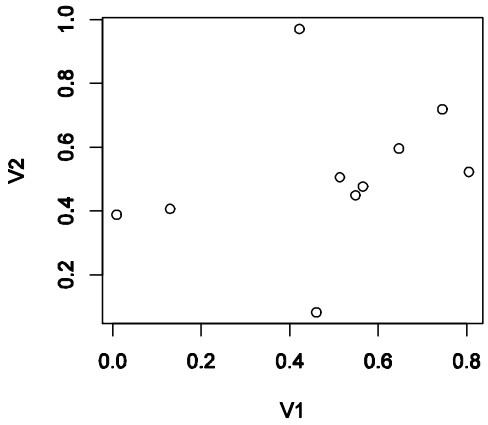
Space filling designs

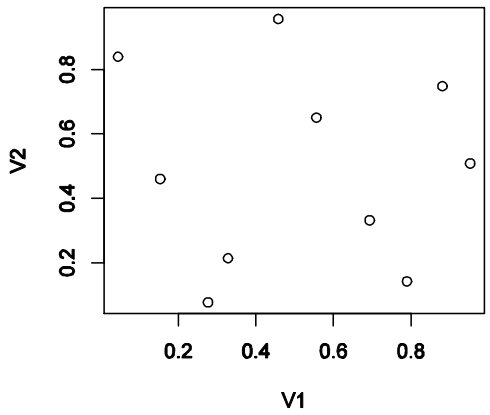
Sparsity of the space of the input variables in high dimension

The learning design choice is made in order to have an optimal coverage of the input domain

The space filling designs are good candidates.

Simple Random Sample (SRS)





Space Filling Design (SFD)

<u>Example:</u> Sobol sequence

<u>Two possible criteria:</u>

1. Distance criteria between the points: minimax, maximin, …
2. Uniformity criteria of the design (discrepancy measures)

Geometrical criteria (1/2)

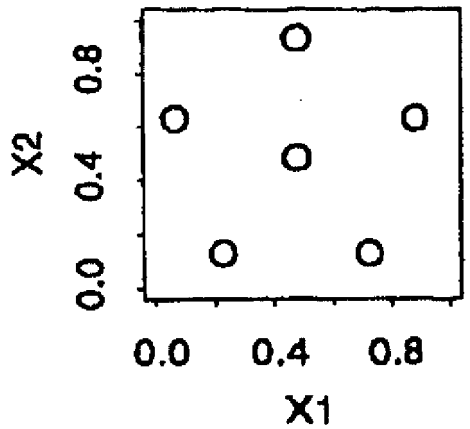
- Minimax design D_{MI}: Minimize the maximal distance between one point of the domain and one point of the design

$$\min_{D} \max_{x} d(x, D) = \max_{x} d(x, D_{MI})$$

[Johnson et al. 1990]
[Koehler & Owen 1996]

$$\text{where } d(x, D) = \min_{x^{(0)} \in D} d(x, x^{(0)})$$

All points in $[0,1]^p$ are not too far from a design point



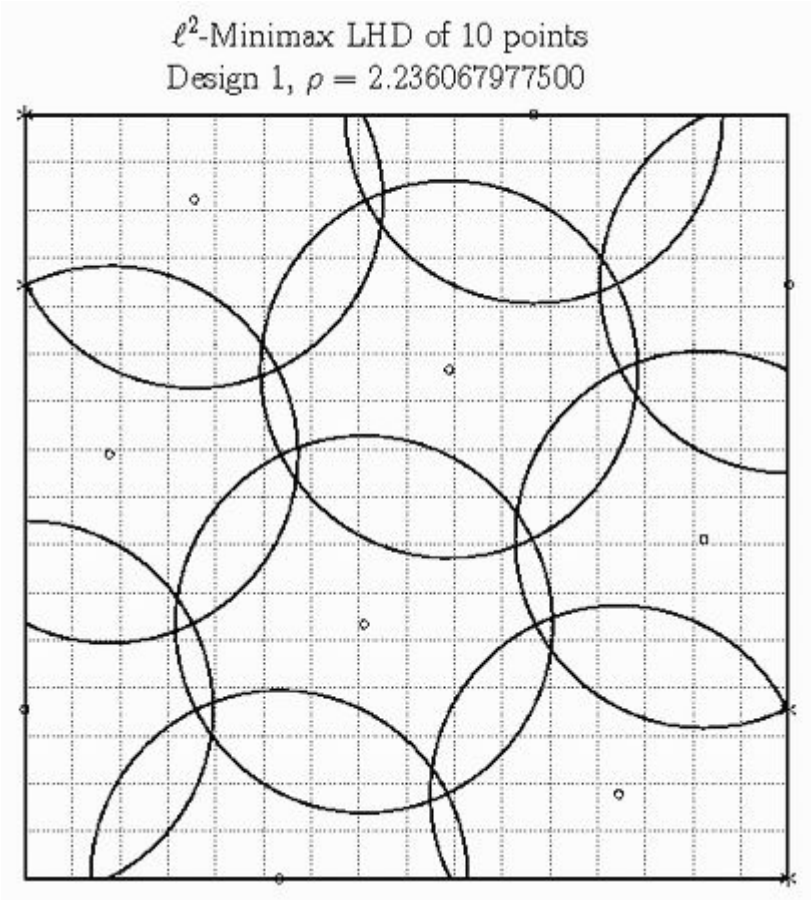
(a) Minimax

=> One of the best design, but too expensive to find D_{MI}

Minimax design

ðp = 1 ; X_i = (2i-1)/(2N) ; ϕ_{mM} = 1 / 2N

ðp > 1 : sphere recovering



[www.spacefillingdesigns.nl]

Geometrical criteria (2/2)

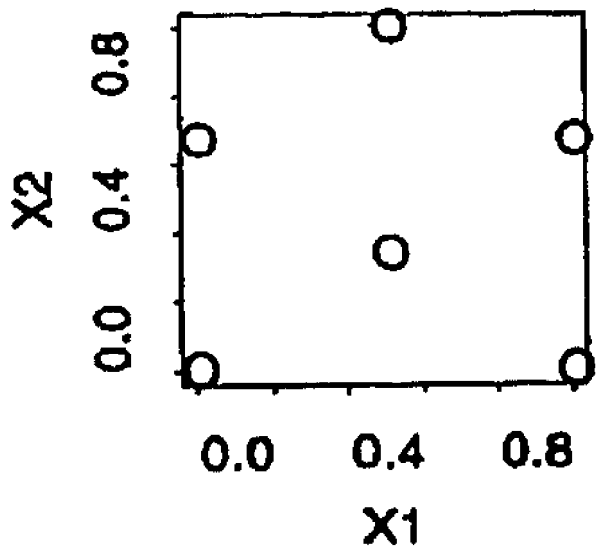
- Mindist distance: $\phi(\Xi^N) = \min_{x^{(1)},x^{(2)} \in \Xi^N} d(x^{(1)}, x^{(2)})$ (L_2 norm for example)

➡ Maximin design Ξ^N_{Mm} :

maximize minimal distance between two points of the design

$$\max_{\Xi^N} \min_{x^{(1)},x^{(2)} \in \Xi^N} d(x^{(1)}, x^{(2)}) = \min_{x^{(1)},x^{(2)} \in \Xi^N_{\mathrm{Mm}}} d(x^{(1)}, x^{(2)})$$

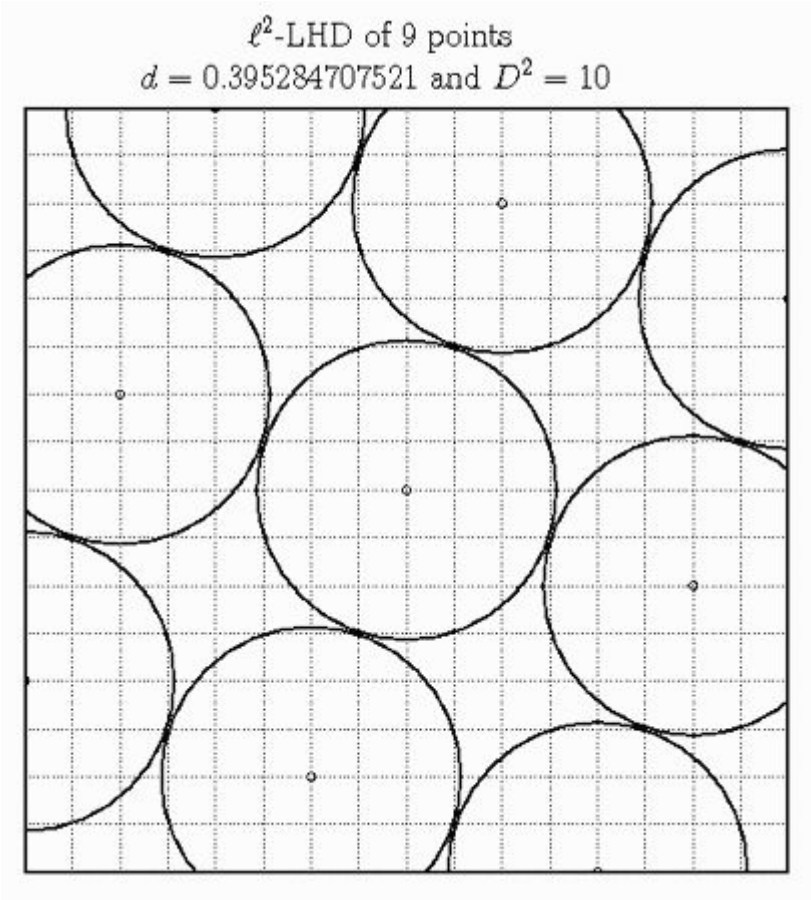
- ŭ



Maximin design

ðp = 1 ; X_i = (i-1)/(N-1) ; ϕ_{mM} = 1 / (N-1)

ðp > 1 : sphere packing



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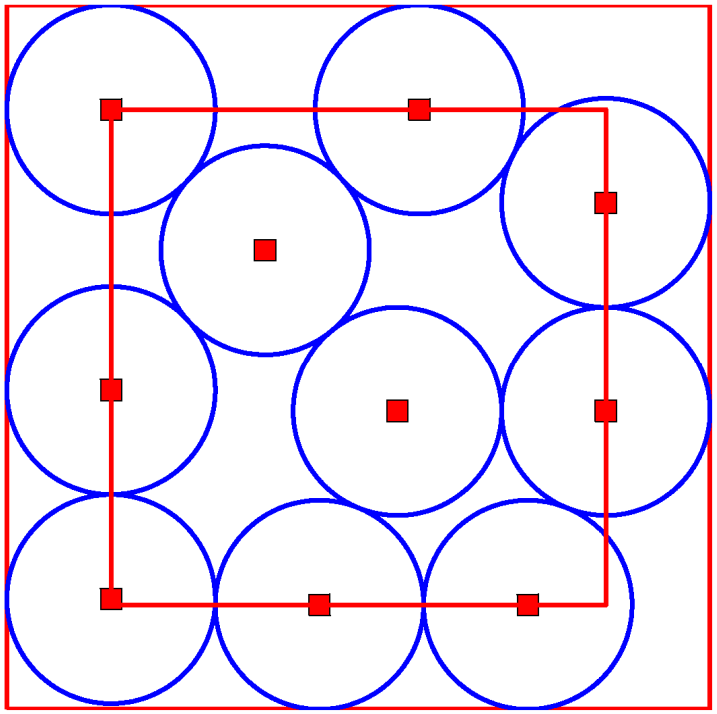
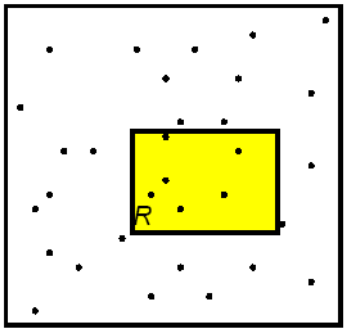


[www.packomania.com]

Space filling measure of a design: the discrepancy

Measure of the maximal deviation between the distribution of the sample's points to an uniform distribution



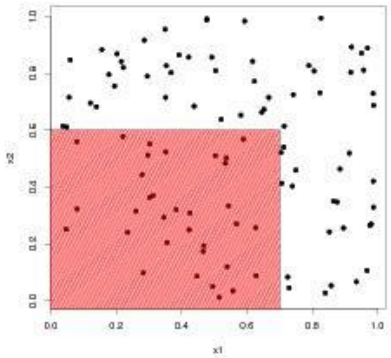
$\Rightarrow$ Measure of deviation from the uniformity

<u>Geometrical interpretation:</u>

Comparison between the volume of intervals and the number points within these intervals

$$Q(t) \in [0,1[^p \,, Q(t) = [0, t_1[\times[0, t_2[\times \ldots \times[0, t_p[$$

$$\mathrm{disc}(D) = \sup_{Q(t)\in[0,1[^p} \left| \frac{N_{Q(t)}}{N} - \prod_{i=1}^{p} t_i \right|$$



Lower the discrepancy is, the more the points of the design D fill the all space

Link with the integration problem

$$I = \int_{[0,1[^p} f(x)dx$$

$$\text{Monte Carlo}: I_N^{\text{MC}} = \frac{1}{N}\sum_{i=1}^{N} f(x^{(i)})$$

$$\text{with } \left(x^{(i)}\right)_{i=1\ldots N} \text{ a sequence of random points in } [0,1[^p$$

$$\mathrm{E}\left(I_N^{\text{MC}}\right) = I \;;\; \mathrm{Var}\left(I_N^{\text{MC}}\right) = \frac{\mathrm{Var}(N)}{N} \Rightarrow \varepsilon = O\left(\frac{1}{\sqrt{N}}\right)$$

General property (**Koksma-Hlawka inequality):** $\varepsilon \leq V(f) \times \mathrm{disc}(D)$

With a low discrepancy sequence *D* (quasi Monte Carlo sequence) :

$$\varepsilon = O\left(\frac{(\ln N)^p}{N}\right)$$

Well-known choice: Sobol' sequence

L_2 discrepancy

Several definitions, depending on considered norms and intervals

$$D^*\left(\Xi^N\right) = \sup_{\mathbf{t}\in[0,1[^p} \left| \frac{1}{N}\sum_{i=1}^{N} 1_{\mathbf{x}^{(i)}\in Q(\mathbf{t})} - \text{Volume}(Q(\mathbf{t})) \right|$$

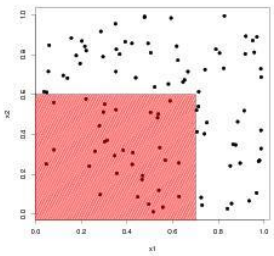
Choice allowing computations : L^2 discrepancy ***[Hickernell 1998]***

L^2 discrepancy at origin : $D_2^*\left(\Xi^N\right) = \left[\int_{[0,1[^p} \left[\frac{1}{N}\sum_{i=1}^{N} 1_{\mathbf{x}^{(i)}\in Q(\mathbf{t})} - \text{Volume}(Q(\mathbf{t})) \right]^2 d\mathbf{t} \right]^{1/2}$

<u>Missing property:</u> taking into account uniformity of the point projections On lower-dimensional subspaces of [0,1[^{p}

=> Modified L_2 discrepancies

$$D_2\left(\Xi^N\right) = \left[\sum_{u\neq\emptyset} \int_{C^u} \left[\frac{1}{N}\sum_{i=1}^{N} 1_{\mathbf{x}_u^{(i)}\in Q_u(\mathbf{t})} - \text{Volume}(Q_u(\mathbf{t})) \right]^2 d\mathbf{t} \right]$$

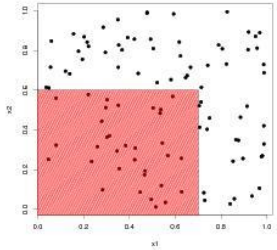


with $u \subset \{1,\ldots,p\}$

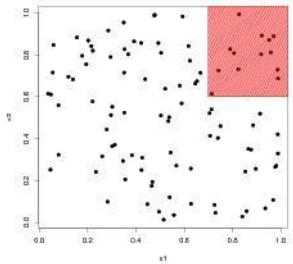
and $Q_u(\mathbf{t}) =$ projection of $Q(\mathbf{t})$ on C^u (unit cube of coordinates in u)

Discrepancy computation in practice

- **Modified L_2-discrepancy** (intervals with minimal boundary 0)

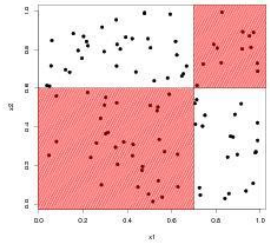


- **Centered L_2-discrepancy** (intervals with boundary one vertex of the unit cube)



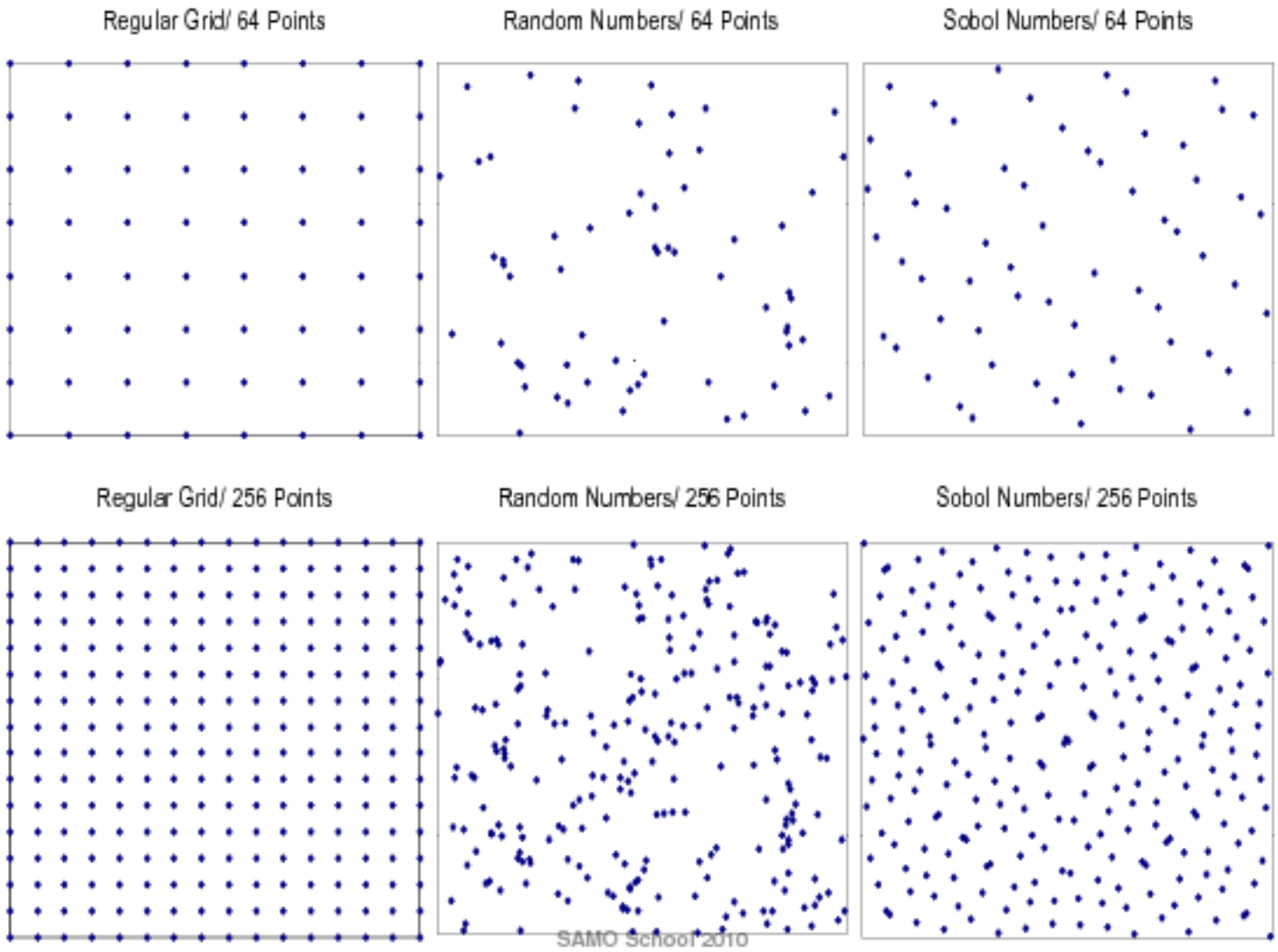
$$\mathrm{disc}_2(D) = \left(\frac{13}{12}\right)^p - \frac{2}{N}\sum_{i=1}^{N}\prod_{k=1}^{p}\left(1+\frac{1}{2}\left|x_k^{(i)}-\frac{1}{2}\right|-\frac{1}{2}\left|x_k^{(i)}-\frac{1}{2}\right|^2\right)$$
$$+\frac{1}{N^2}\sum_{i,j=1}^{N}\prod_{k=1}^{p}\left(1+\frac{1}{2}\left|x_k^{(i)}-\frac{1}{2}\right|+\frac{1}{2}\left|x_k^{(j)}-\frac{1}{2}\right|-\frac{1}{2}\left|x_k^{(i)}-x_k^{(j)}\right|\right)$$

- **Symetric L_2-discrepancy** (intervals with boundary one « even » vertex of the unit cube)



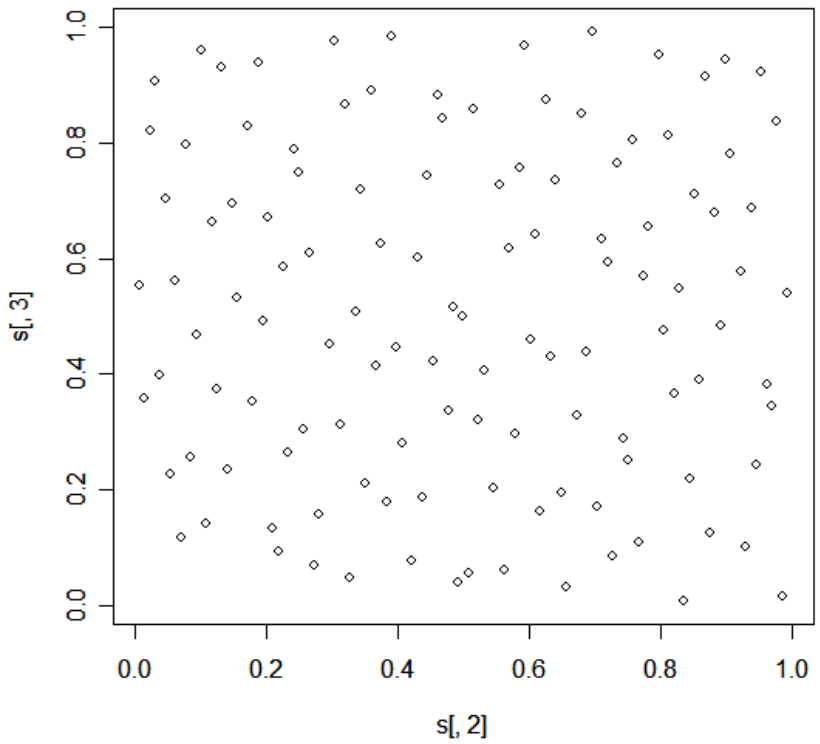
Sobol ˘sequence vs. Random sample vs. regular grid

[From: Kucherenko, 2010]

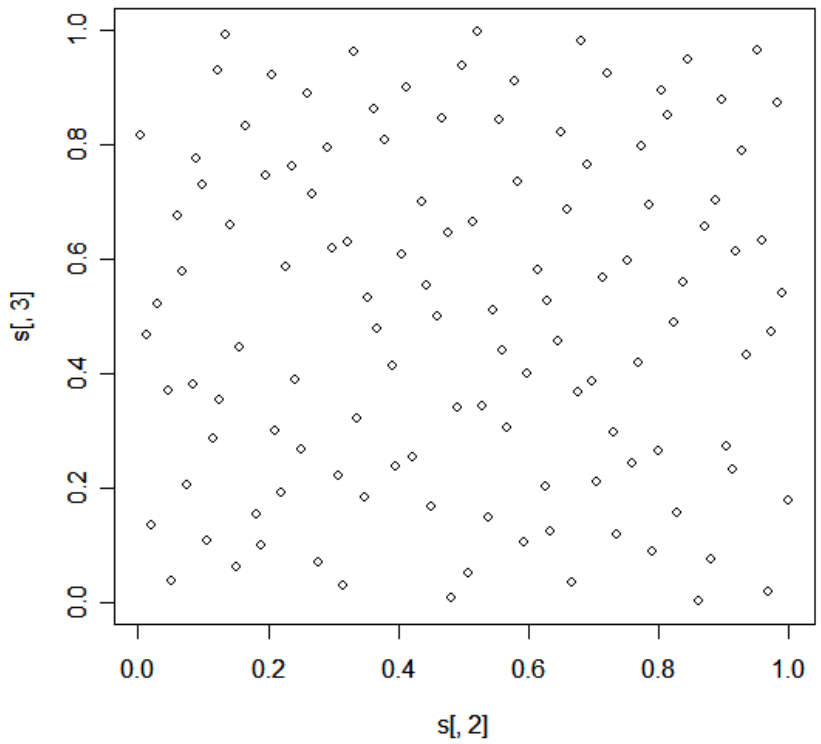


Example - N = 150 - Dimension = 8

Sobol

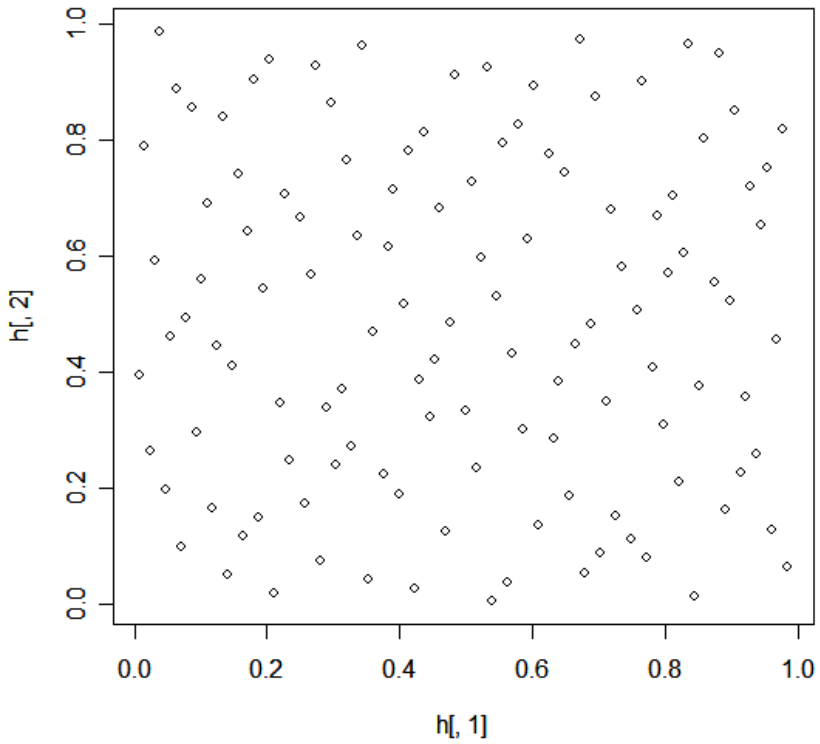


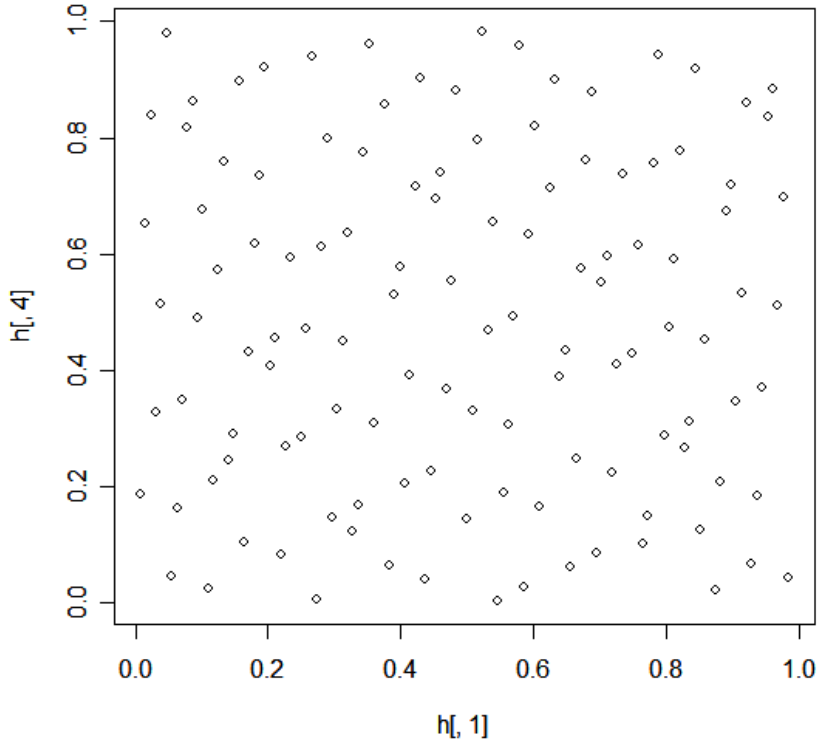
Sobol scrambling Owen



Example - N = 150 - Dimension = 8

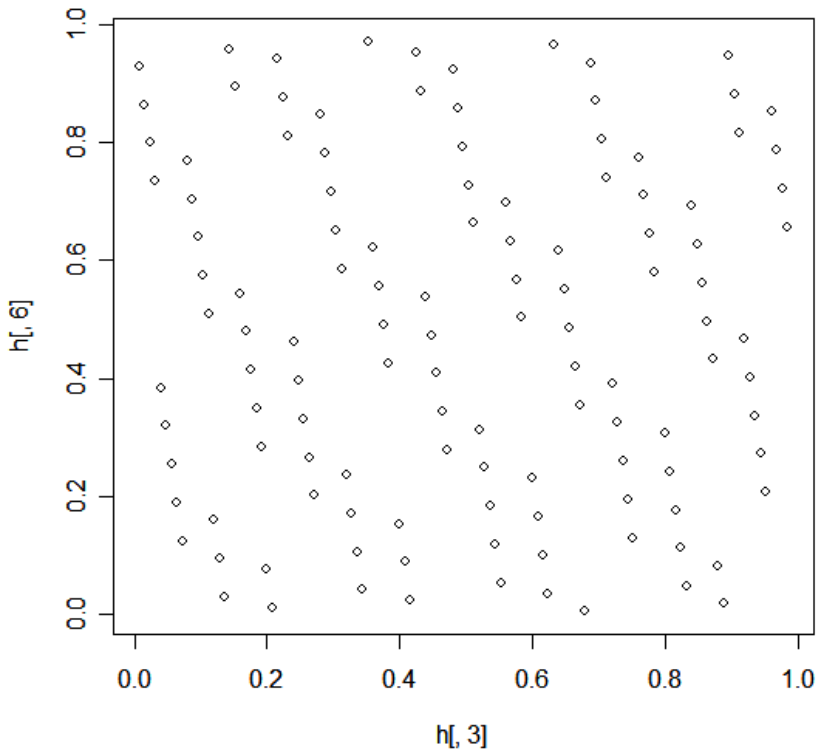
Halton

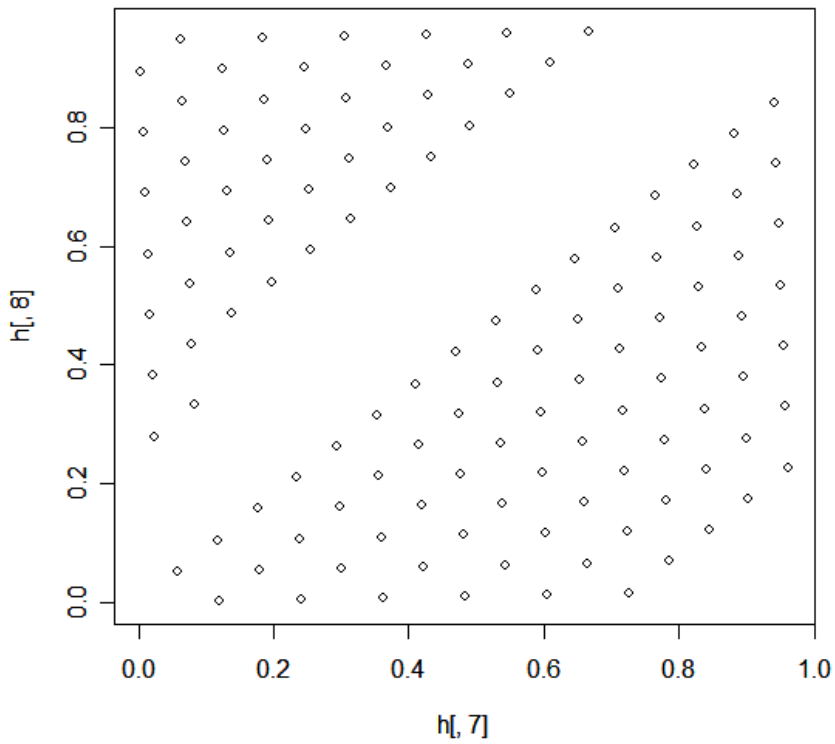




Pathologies on 2D projections

Halton

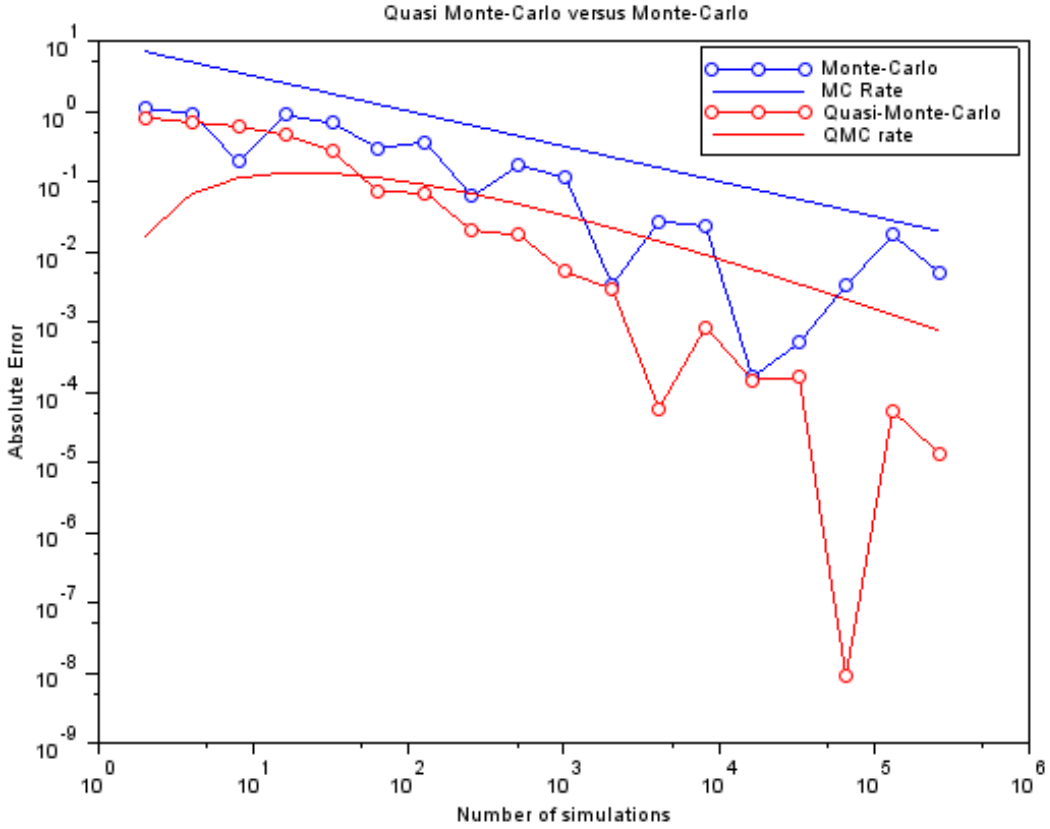




Tests: low-discrepancy sequences vs. Monte Carlo

For integration: convergence often close to 1/N for p < 40.

Example: Ishigami function, dimension $p = 3$

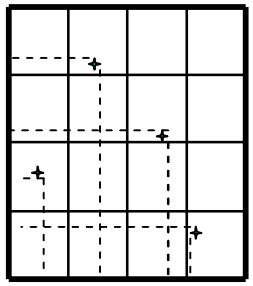


Important property: robustness in terms of subprojections

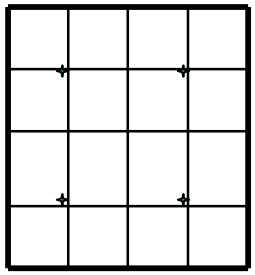
Most of the times, the function $f(\mathbf{X})$ has low <u>effective dimensions:</u>
- in the truncation sense (p_1 = number of influent inputs) $\Rightarrow$ $\boldsymbol{p_1} << \boldsymbol{p}$
- in the superposition sense (p_2 = higher order of influent interaction) $\Rightarrow$ $\boldsymbol{p_2} << \boldsymbol{p}$

Then, we need SFD which keeps their space-filling properties in low-dimensional subspaces (by importance: in dimensions p'=1, then p'=2, ...)

ð $p' = 1 \Rightarrow$ LHS ensures good 1D projection properties



good



bad

ð $p' \geq 2$
In their definition, the modified L^2-discrepancy criteria take into account subprojections

In contrary design points distance criteria are not robust at all

Latin Hypercube Sample (LHS)

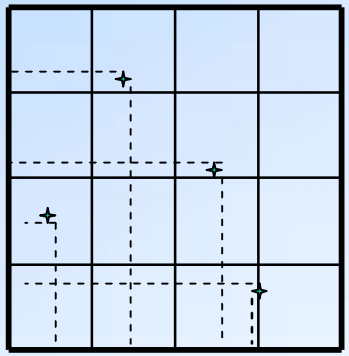
[McKay et al. 1979]

Most often, only a small number of variables are influent

Property: Uniform projections on margins

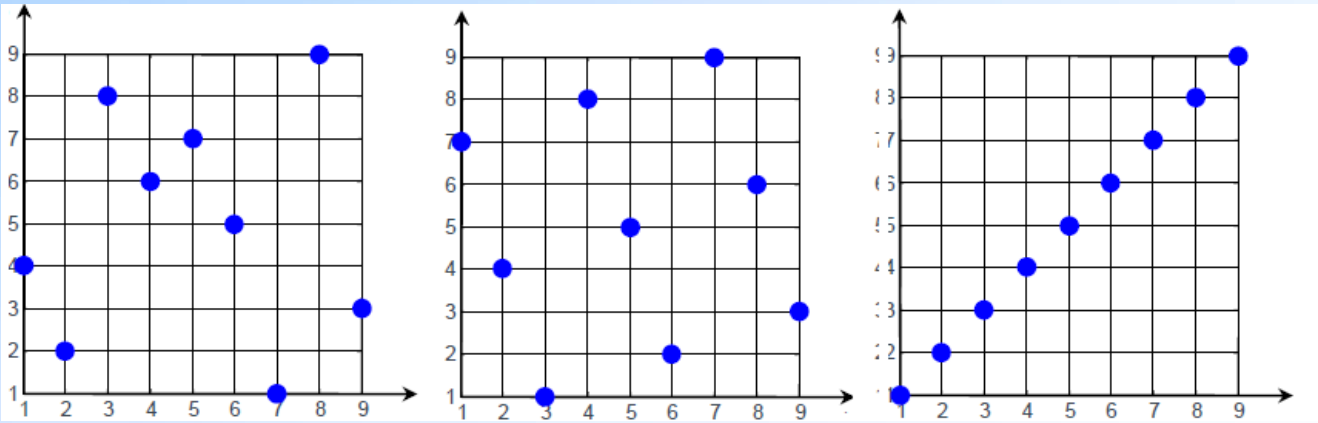
Principle: p variables, N points $\Rightarrow$ $LHS(p,N)$

Divide each dimension in N intervals
Take one point in each stratum



Exemple : p =2, N =4

Each level is taken only one time by each variable
$\Rightarrow$ Each column of the design is a permutation of { 1,2,..,N}

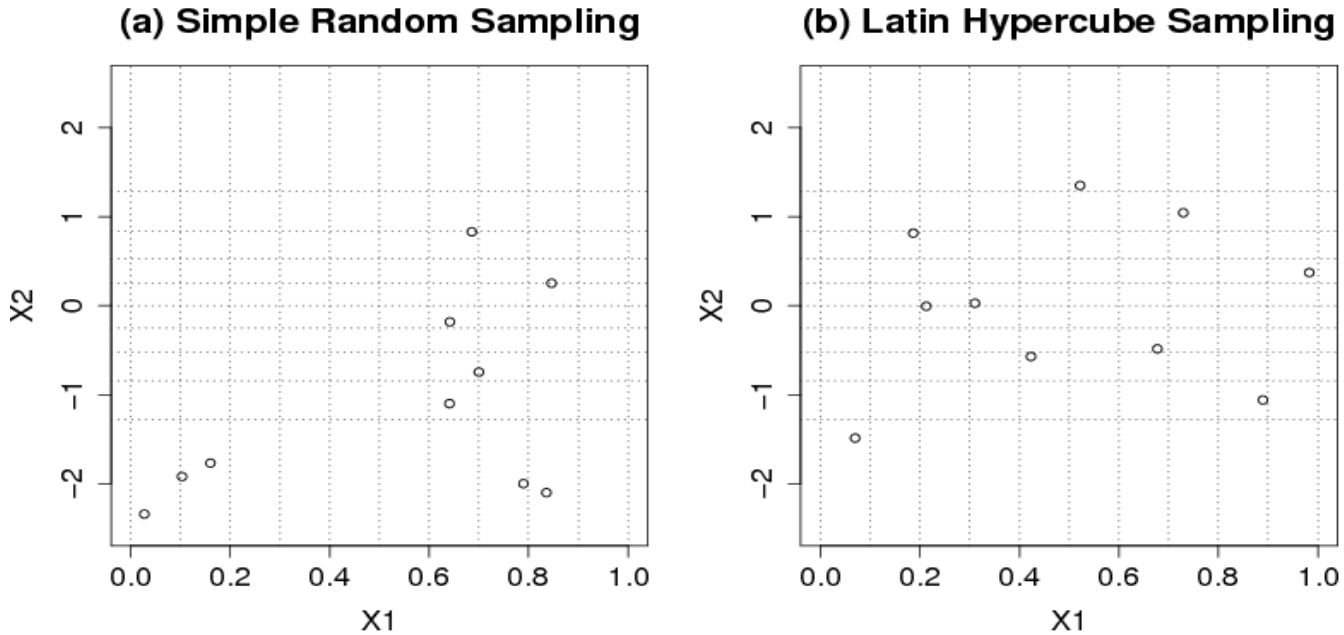


Algorithm of LHS(*p*,*N*) ¯ Stein method

```
  ran = matrix(runif(N*p),nrow=N,ncol=p) #tirage de N x p valeurs selon loi
U[0,1]
  x = matrix(0,nrow=N,ncol=p)            # construction de la matrice x


  for (i in 1:p) {
        idx = sample(1:N) #vecteur de permutations des entiers
{1,2,…,N}
        P = (idx-ran[,i]) / N    # vecteur de probabilités
        x[,i] <- quantile_selon_la_loi (P)  }
```

<u>Example :</u> p =2, N =10, X_1 ~ U[0,1], X_2 ~ N(0,1)



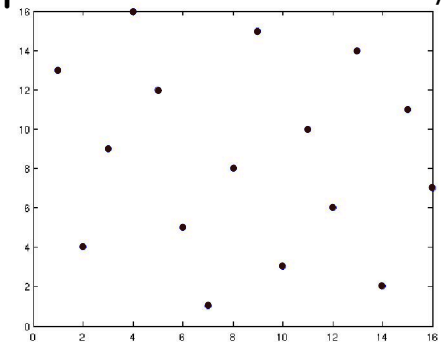
Optimisation of LHS => Space-filling LHS

[Park 1993; Morris & Mitchell 1995]

<u>Simple method:</u> produce a large number (for ex 1000) of different LHS. Then, choose the best with respect to a criterion $\phi(.)$ (« space filling »)

Example : LHS(2,16)

Maximin criterion

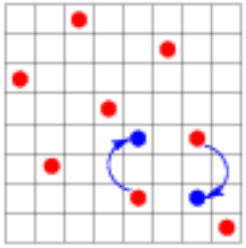


BUT: the number of LHS is huge : $(N!)^p$

<u>Methods via optimization algo</u> (ex: minimisation of $\phi(.)$ via simulated annealing) :

1. Initialisation of a design Ξ (LHS initial) and a temperature T

2. While $T > 0$:
   1. Produce a neighbor Ξ_{new} of Ξ (permutation of 2 components in a column)
   2. replace Ξ by Ξ_{new} with proba $\min\left(\exp\left[-\frac{\phi(\Xi_{new})-\phi(\Xi)}{T}\right],1\right)$
   3. decrease T

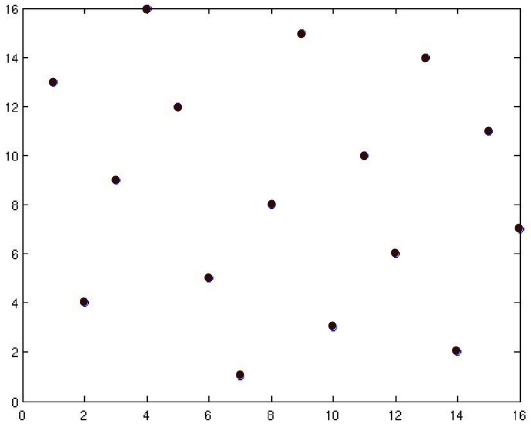


3. Stop criterion => Ξ is the optimal solution

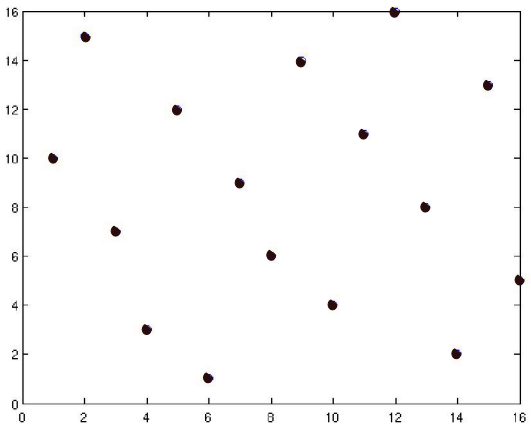
Examples of optimized LHS

Joining the two properties (space filling and LHS)

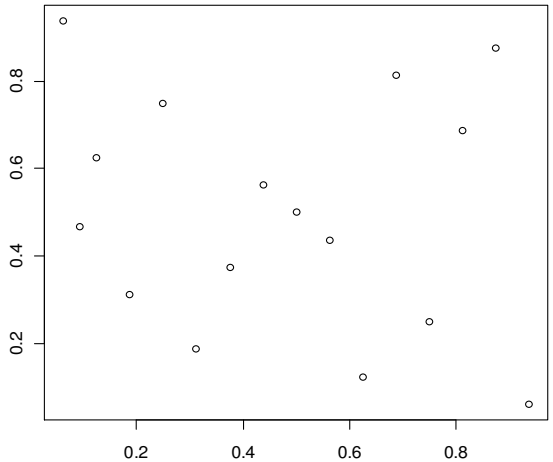
Example: $p = 2$ – $N = 16$



Maximin LHS



Low wrap-around discrepancy LHS



For comparison: Sobol sequence

Summary on the design of numerical experiments

Goal: Sample a high dimensional space in an « optimal » manner (obtain the maximum of information on the behaviour of the output $Z / \mathbf{X} \in \mathbb{R}^p$)

<u>Problem:</u> a pure random sample (Monte Carlo) badly fills the space

1. « Space filling » designs are good candidates:

- Based on a distance criterion between points (minimax, maximin, …)

- Based on a citerion of uniform distribution of the points <u>(discrepancy)</u>

2. Property of uniform projections on margins can be obtained via the Latin hypercube designs (LHS)

3. It is possible to couple 1 and 2

Synthesis on the properties of space filling designs

	Patterns, alignment	Sequentiality	Dimension reduction
Monte Carlo	No	Yes	Yes
Faure, Halton, Sobol	Yes, in high dim.	Yes	Yes, but pathologies
LHS à discrép centrée faible	No	No	Yes
LHS maximin	Yes	No	No

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