Design and Analysis of Computer Experiments for Bulk Acoustic Wave filters:

Comparison of several types of Designs and Comparison of Kriging vs Pseudo-Cubic Thin-Plate Type Spline as Metamodel

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Outlines

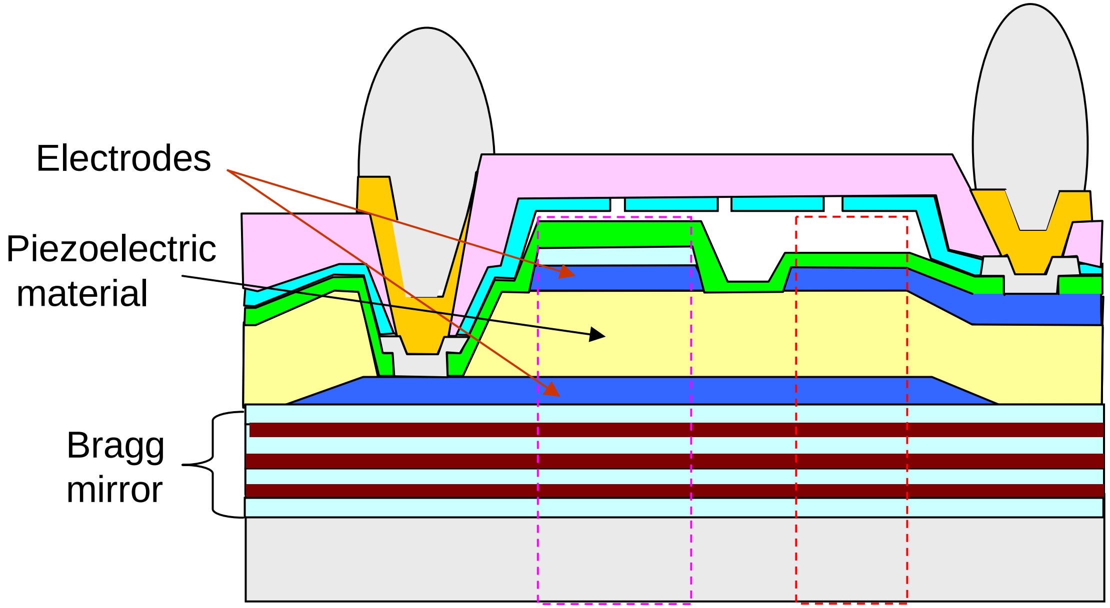
- What is a BAW ?
- 3 different designs
- 2 test sets
- 3 different types of metamodels
- Comparisons
- Conclusion

What is a BAW? (1/2)

- BAW = Bulk Acoustic Wave filter

Objective: 80 000 BAW per wafer

- Must transmit only a small frequency band of an electric signal, in the GHz range.
- Convert electrical energy into mechanical energy, and conversely.



The electric incoming signal generates mechanical (acoustic) waves in the piezoelectric material.

These acoustic waves propagate vertically.

The acoustic waves generate electric signal at the outcoming electrodes.

This process is efficient if and only if there is mechanical resonance at the appropriate frequency.

Use of the mechanical resonance of a piezoelectric layer to obtain an electrical resonance

What is a BAW? (2/2)

- Present in most of radio transmitters, including cellular phones.
  - ✓ *Technologically, it's a film (1µm) of piezoelectric material sandwiched between electrodes.*
  - ✓ *Charge and passivation layers above the film*
  - ✓ *Bragg mirror below the film*
- In our model, it is characterized by a 10 layer device
  - ✓ *10 independent variables*
  - ✓ *deviation from nominal thickness divided by process dispersion*
  - ✓ *Range : [-3 ; 3] or [-4 ; 4]*

Which responses ?

What is a BAW?
3 DOE
2 test sets
3 metamodels
Comparison
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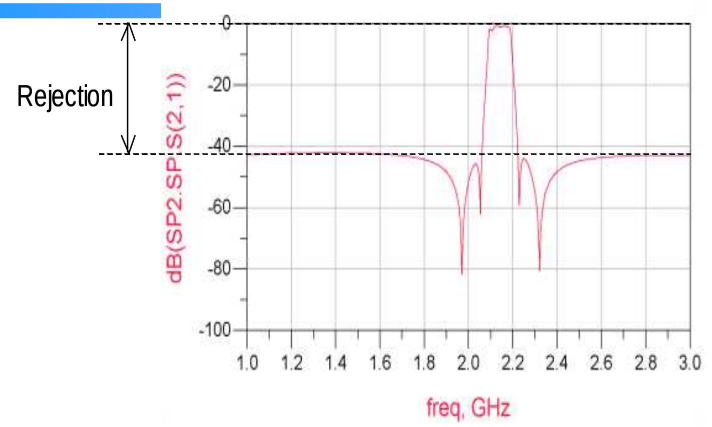
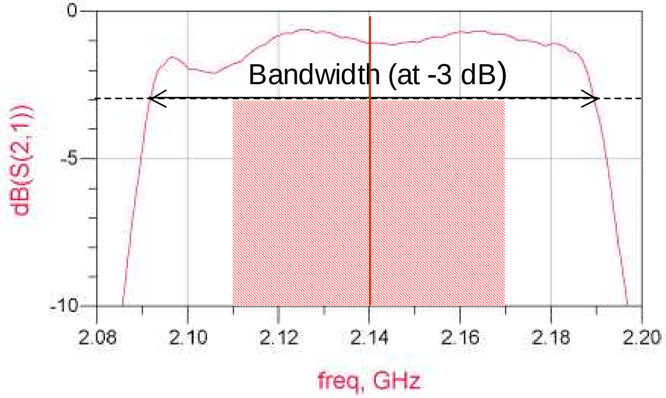
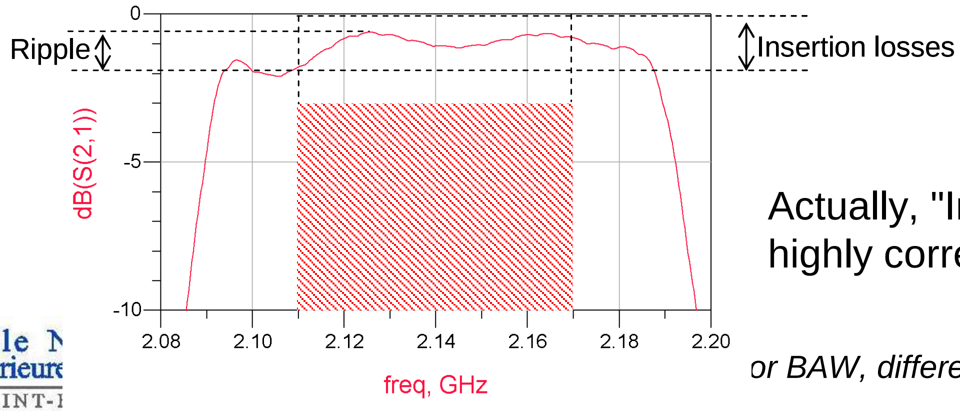


Rejection



Bandwidth

Centre frequency



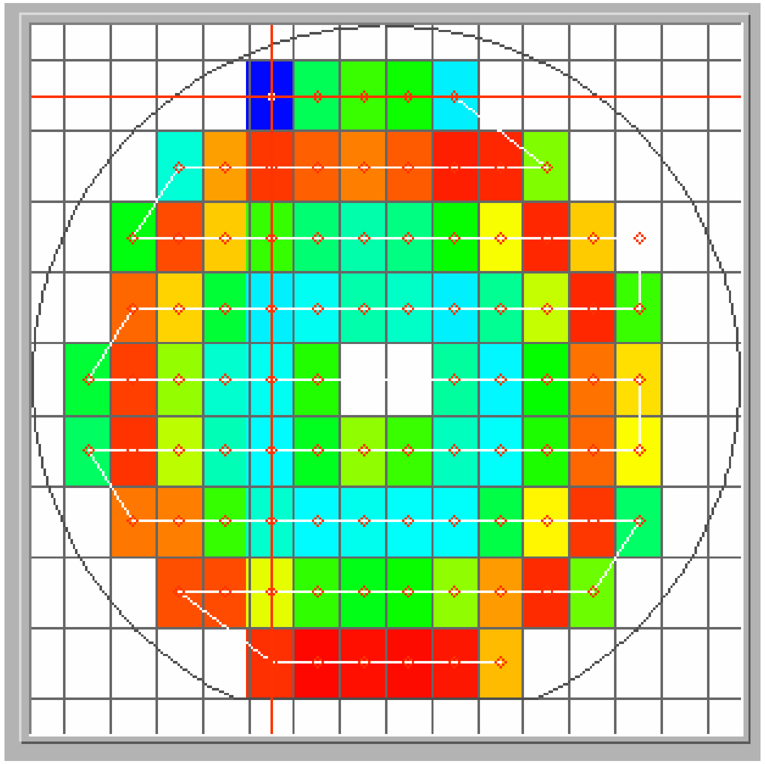
Insertion losses

Ripple

Actually, "Insertion losses" and "Ripple" are very highly correlated and we use only "Ripple"

Why do we need a metamodel ?

- Estimation of **fabrication yield**, in industrial context, using a Monte Carlo approach and thresholds on each response.
- A simulator exists, but far too time consuming for Monte-Carlo use.
- Total thickness variance has two components:



- ✓ *position dependent on the wafer*
- ✓ *at the same location, wafer to wafer*

Cartography of the mean thickness of the piezoelectric layer on a wafer.

(*red: too thick* *blue : too thin*)

We need a fast running reliable metamodel for each response.

Outlines

What is
a BAW?

3 DOE

2 test
sets

3
metamodels

Comparison

Conclusion

- What is a BAW ?
- 3 different designs of 1003 simulations each
  1. Interweaving of different classical sub DOE
  2. MaxiMin Latin Hypercube Sampling
  3. Halton's sequence
  - ✓ Continuous transformation for the two space filling designs
- 2 test sets
- 3 different types of metamodels
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Interweaving of different classical sub DOE

- Arbitrary combination of DOE that are classical for true experiments

  1. *central point*
  2. *2^(10-3) at scale 0.75*
  3. *2^(10-3) at scale 1.50, foldover of the previous one*
  4. *2^(10-3) at scale 2.25, with different alias generator*
  5. *2^(10-3) at scale 3.00, foldover of the previous one*
  6. *10 series of star points with pitch 0.25 (all factors at 0.0 except one)*
  7. *Box-Behnken at scale 1.5*
  8. *5 series of 2^(5-1) at scale 1.00 for the 5 first factors except the j th at scale 2.5 (j from 1 to 5), the five last (Bragg mirror) at 0.0*

- Total : 1003 points

- This DOE emphasizes the most external regions

use of Design Expert

Two space filling Designs, 1003 points each

- Maximin Latin Hypercube Sampling (LHS)
  - *Maximization of the minimum distance between sampling points.*
  - *using the "lhsdesign" of the statistics toolbox of Matlab*

- Halton's low discrepancy sequence
  - *Generalization of the Van der Corput design*
  - *using R software*

- Usual advantages of space filling designs
  - ✓ *Projection in any subspace (straight line, plane, …) has no multiple points.*
  - ✓ *well adapted for perfectly repetitive simulations (no white noise)*

Continuous transformation for space filling designs

- What is a BAW?
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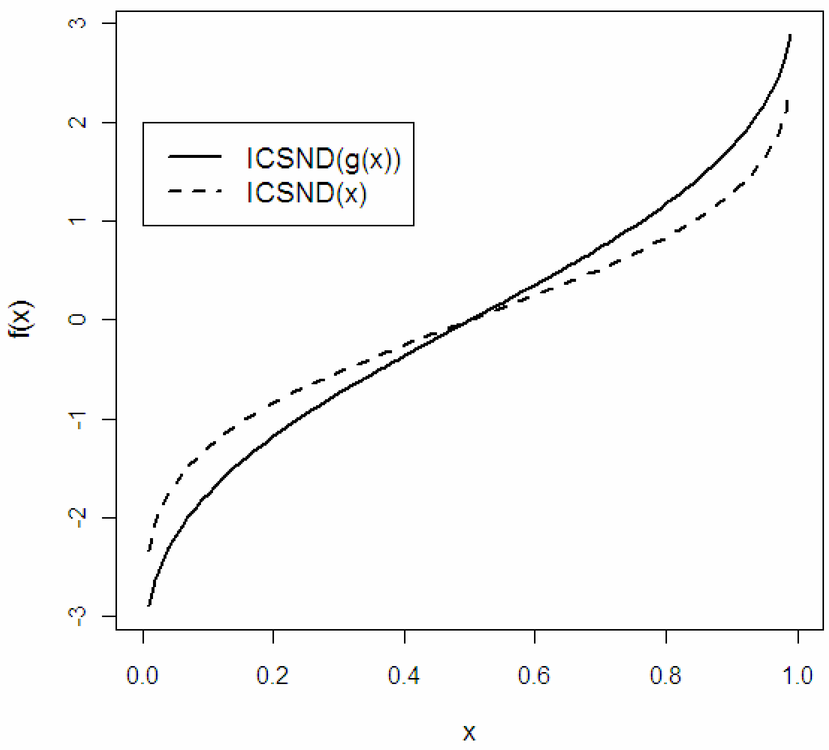
- The 2 space filling designs was obtained on $[0 ; 1]^{10}$ but we want to use them on $[-4 ; 4]^{10}$
- We wish to get locally accurate metamodels in the center of the domain (most probable region)
- Naturally, use of the Inverse Cumulative Standard Normal Distribution (ICSND(x))
- In fact, we wanted to reduce the concentration of points in the central region : Use of ICSND(g(x))



Outlines

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- **2 test sets**
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Two test sets of 500 points each.

- What is a BAW?
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➢ Quality of prediction tested using two test sets, each one of 500 random points:

1. *Normally distributed in R^{10}*
2. *Uniformly distributed in $[-3 ; 3]^{10}$*

➢ The 1st set focus on the most probable region

➢ The 2nd set focus on the full range of interest

Outlines

- What is a BAW ?
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- 3 different types of metamodels
  - ✓ Ordinary kriging
  - ✓ Universal kriging
  - ✓ Pseudo-cubic thin-plate type interpolating spline
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Ordinary and Universal Kriging

- Well Known in literature[1] Probabilistic Bayesian interpretation[2]
- Gaussian process $E[y(x)] = f(x).\beta$ and $Cov[Y(x^{(1)}),Y(x^{(2)})] = k(x^{(1)},x^{(2)})$
- Gaussian kernel with process variance σ and range parameters θ

$$k(x^{(1)},x^{(2)}) = \sigma^2 \exp\left(-\sum_{i=1}^{d}\left(\frac{(x_i^{(1)} - x_i^{(2)})}{\theta_i}\right)^2\right)$$

- Ordinary kriging : f(x)=1
- Universal kriging : f(x): 1 ; $x^{(j)}$, j=1, … ,10
- Usual way to determine θ , β and σ with the maximum of likelihood
- Nuggets are sometime necessary to stabilize.
- Mean and standard deviation available in any points.

[1] :T. J. Santner, B. J. Williams, W. I. Notz, *The Design and Analysis of Computer Experiments,* Springer, 2003
[2] C. Helbert, D. Dupuy and L. Carraro, "*Assessment of uncertainty in computer experiments: from universal kriging to bayesian kriging*", Applied Stochastic Models in Business and Industry, 25, 2009, 99-113.

Pseudo-cubic Thin-plate type Spline

- Proposed by Duchon[1]. May be smoothing or **interpolating**.
- Minimization of total energy: $E_{total} = E_c(f) + \rho * \underbrace{\sum_{i=1}^{n} \omega_i \left(y_i - f(t_i)\right)^2}$

Curvature energy

Inverse of smoothing parameter. Infinite for interpolating spline

residual variance, null for interpolating spline

$$E_c(f) = \int_{R^d} \sum_{k=1}^{d} \sum_{p=1}^{d} \left[Four\left(\frac{\partial^2 f}{\partial t_k \partial t_p}\right)(u) \right]^2 \|u\|^{d-1} du_1\, du_2 \,....\, du_d$$

- Solution: $f(t) = \sum_{i=1}^{n} \lambda_i\, H(t, t_i) + \sum_{k=1}^{d} \alpha_k t^{(k)} + \alpha_o$

Radial basis function

Software "Plaque" from CEA

[1]: J. Duchon, "*Splines minimizing rotation-invariant semi-norms in Sobolev space*", Lecture Notes in Mathematics, vol 571, pp85-100, 1977

Pseudo-cubic Thin-plate type interpolating Spline

$$H(t,t_i) = \left(\sum_{k=1}^{d} dil_k^2 \left(\frac{t^{(k)} - t_i^{(k)}}{\sigma_k} \right)^2 \right)^{3/2}$$

σ_k : standard deviation of the k^{th} variable
dil_k : scale dilatation for the kth variable

For given scale dilatation dil_k , the coefficients λ_i and α_j are solutions of a n+d+1 symmetric linear system:

$$\begin{cases} \sum_{j=1}^{n} \lambda_j H(t_i,t_j) + \cancel{\dfrac{\lambda_i}{\rho\,\omega_i}} + \sum_{k=1}^{d} \alpha_k \dfrac{dil_k}{\sigma_k} t_i^{(k)} + \alpha_o = y_i & \text{for } i=1, \ldots, n \\ \sum_{j=1}^{n} \lambda_j \dfrac{dil_k}{\sigma_k} t_j^{(k)} = 0 & \text{for } k=1, \ldots , d \\ \sum_{j=1}^{n} \lambda_j = 0 & \end{cases}$$

this term disappears for interpolating spline

Software "Plaque" from CEA

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Pseudo-cubic Thin-plate type interpolating Spline

What is a BAW?

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3 metamodels

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Choice of the scale dilatations dil_k ?

- ✓ Inspired by BootStrap
  - *Random partition into Q subsets (typically q = 10 to 20)*
  - *For each subset, the spline is computed without the points of this subset and used only on these points.*
  - *Mean square difference between predicted and actual values for the Q subsets.*
  - *Iterative process on dil_k to minimize this mean square difference.*

- ✓ Convergence enhancement:
  - *Use of dimensionless factor* $t^{+(k)} = \dfrac{dil_k}{\sigma_k} t^{(k)}$
  - *Mean square second dimensionless derivatives tends to be the same value, whatever the factor k:*

$$\sum_{i=1}^{n} \left(\frac{\partial^2 f}{\partial t^{+(k)\,2}} (t_i) \right)^2$$

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Kriging and pseudo-cubic spline

What is a BAW?
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- Both are based on radial basis function.
- Both are usable in any dimension, without severe constraints on the localization of sampling points.
- Kriging : **statistic approach**, probabilistic Bayesian interpretation[1]
- Spline : **energetic approach**, minimization of a curvature energy
- Uncertainty of a prediction: **Kriging: yes** **Spline: no**
- To build the metamodel (choice of θ or dil_k):
  - ✓ *iterative process with resolution of a linear system (roughly the same size) at each iteration.*
  - ✓ *Numerical stability: seems better for spline than kriging*
- CPU time to use the metamodel : similar for kriging and spline

[1] C. Helbert, D. Dupuy and L. Carraro, "*Assessment of uncertainty in computer experiments: from universal kriging to bayesian kriging*", Applied Stochastic Models in Business and Industry, 25, 2009, 99-113.

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- What is a BAW ?
- 3 different designs
- 2 test sets
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- Comparisons
  - ✓ Principles of the comparison
  - ✓ Comparison of the Designs of Experiments
  - ✓ Comparison of the types of metamodels
  - ✓ Confidence interval and yield estimation
- Conclusion

Principles of the comparisons

What is a BAW?
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- For numerous combinations of :

  { DOE ; response ; type of metamodel ; test set }

- Estimation of the Mean Square Error (MSE) :

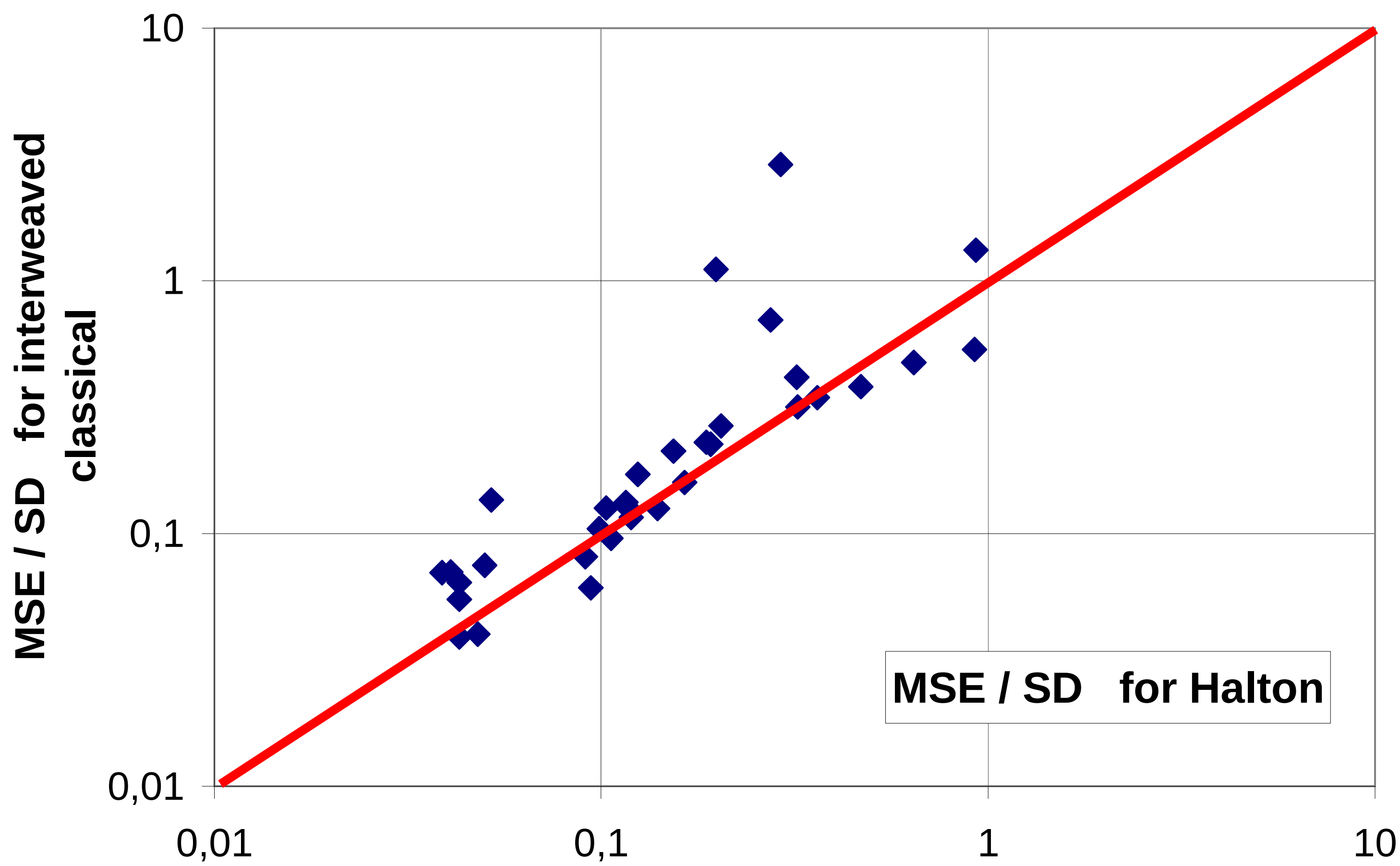
$$MSE = \sqrt{\frac{\sum_{i=1}^{m} (y_i - f(t_i))^2}{m}}$$

- Comparison with the Standard Deviation (SD) of this response for this test set:

$$SD = \sqrt{\frac{\sum_{i=1}^{m} (y_i - \bar{y})^2}{m}}$$

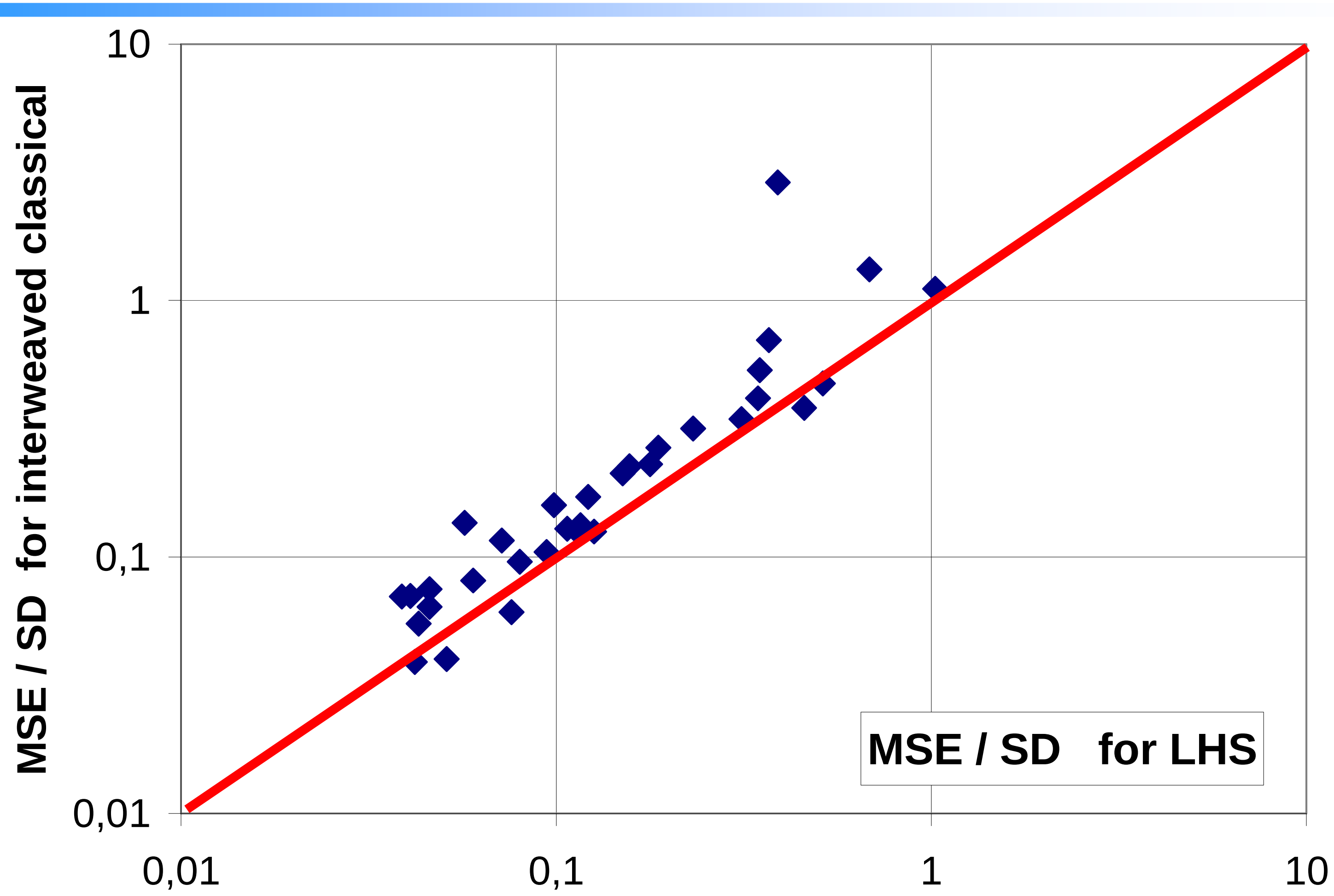
- Use of ratio MSE/SD to quantify the prediction quality

Comparison of the Designs of Experiments



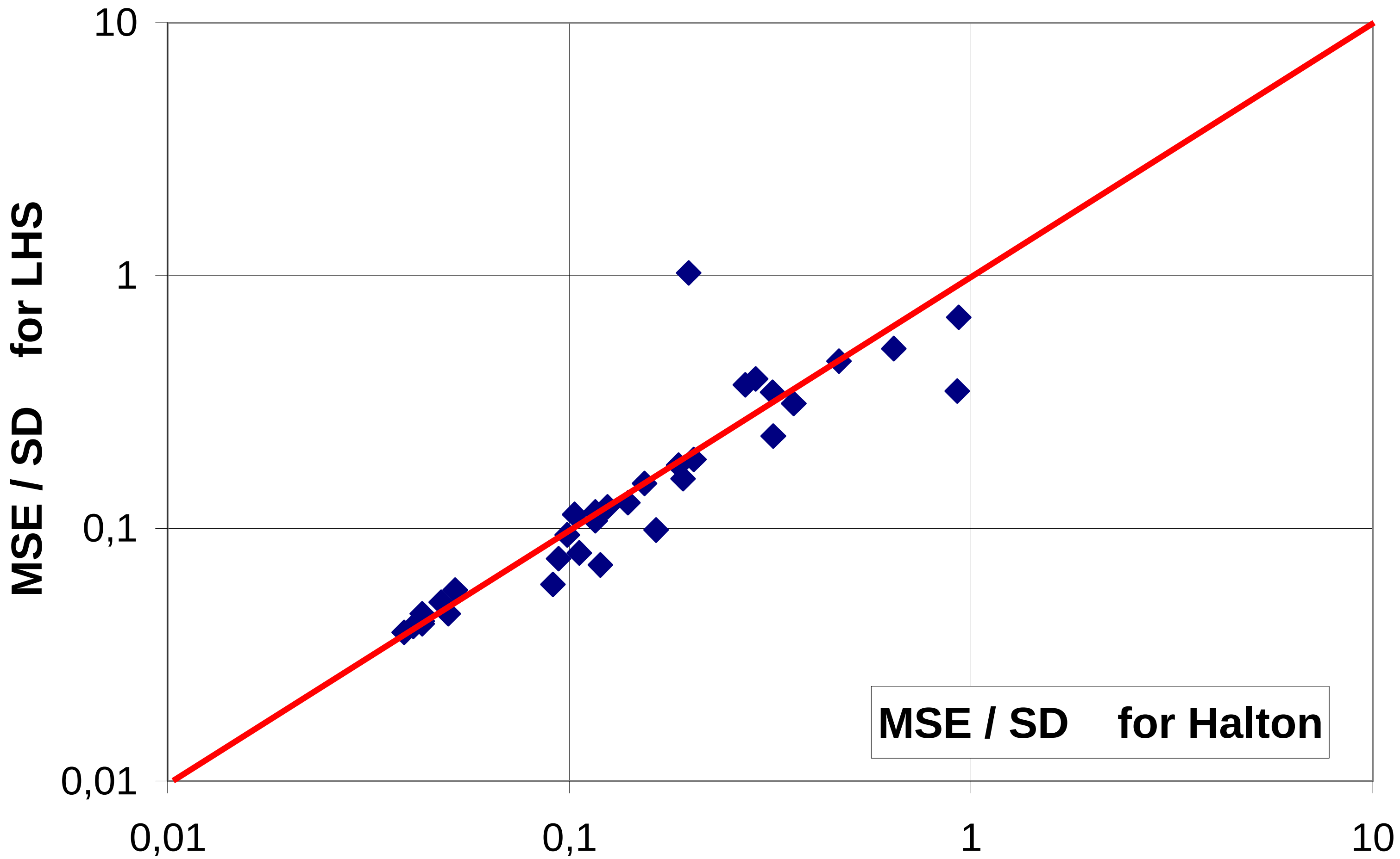
Halton's sequence usually better than Interweaved classical DOE

Comparison of the Designs of Experiments



Maximin LHS usually better than Interweaved classical DOE

Comparison of the Designs of Experiments



Maximin LHS usually better than Halton's sequence

Comparison of the Designs of Experiments

Usually:

MaxiMin LHS better than Halton's sequence

Halton's sequence better than "Interweaved Classical DOE"

In our specific industrial case, with 1003 simulations in a 10 dimension space

Comparison of the types of metamodels

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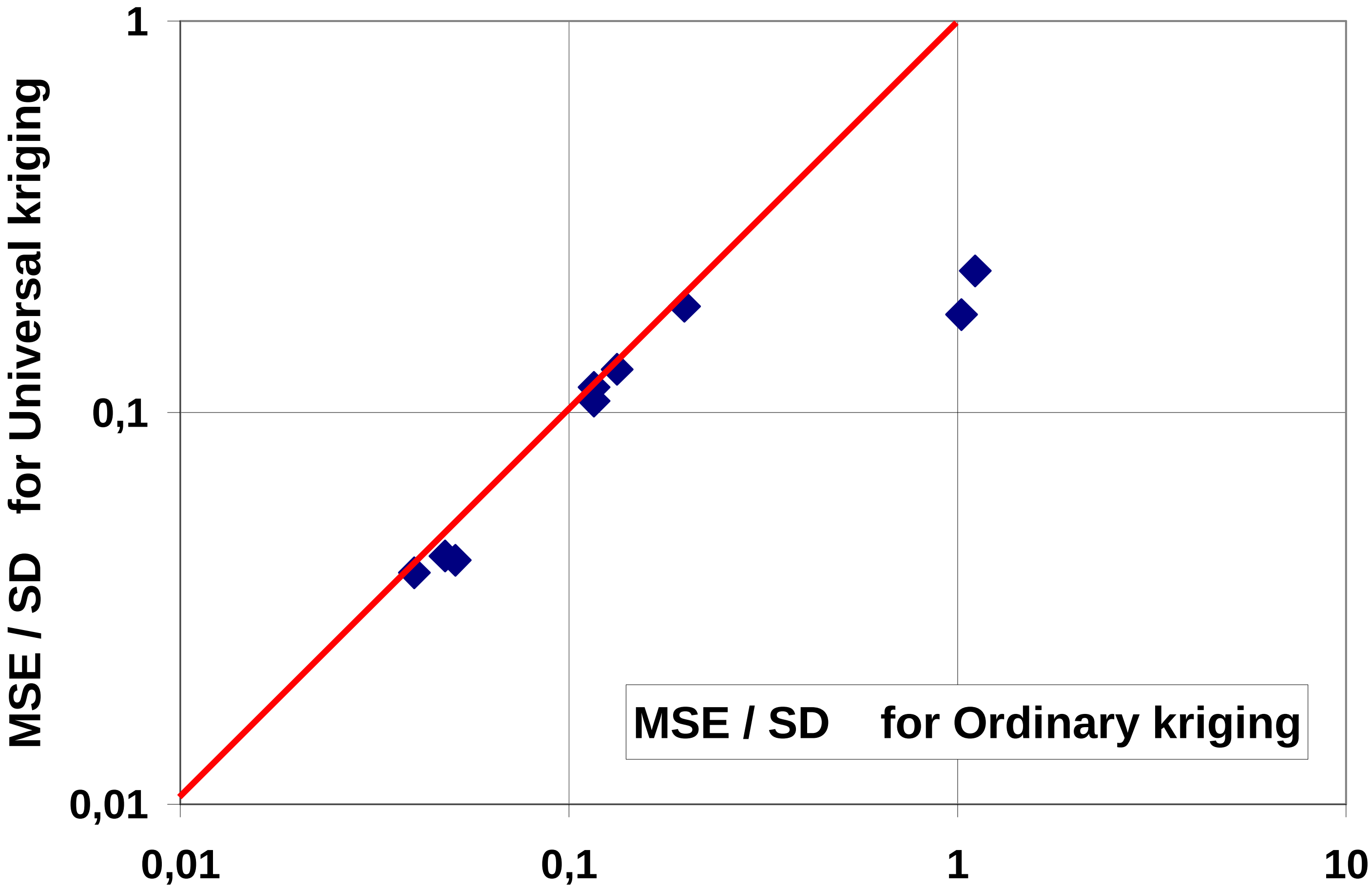
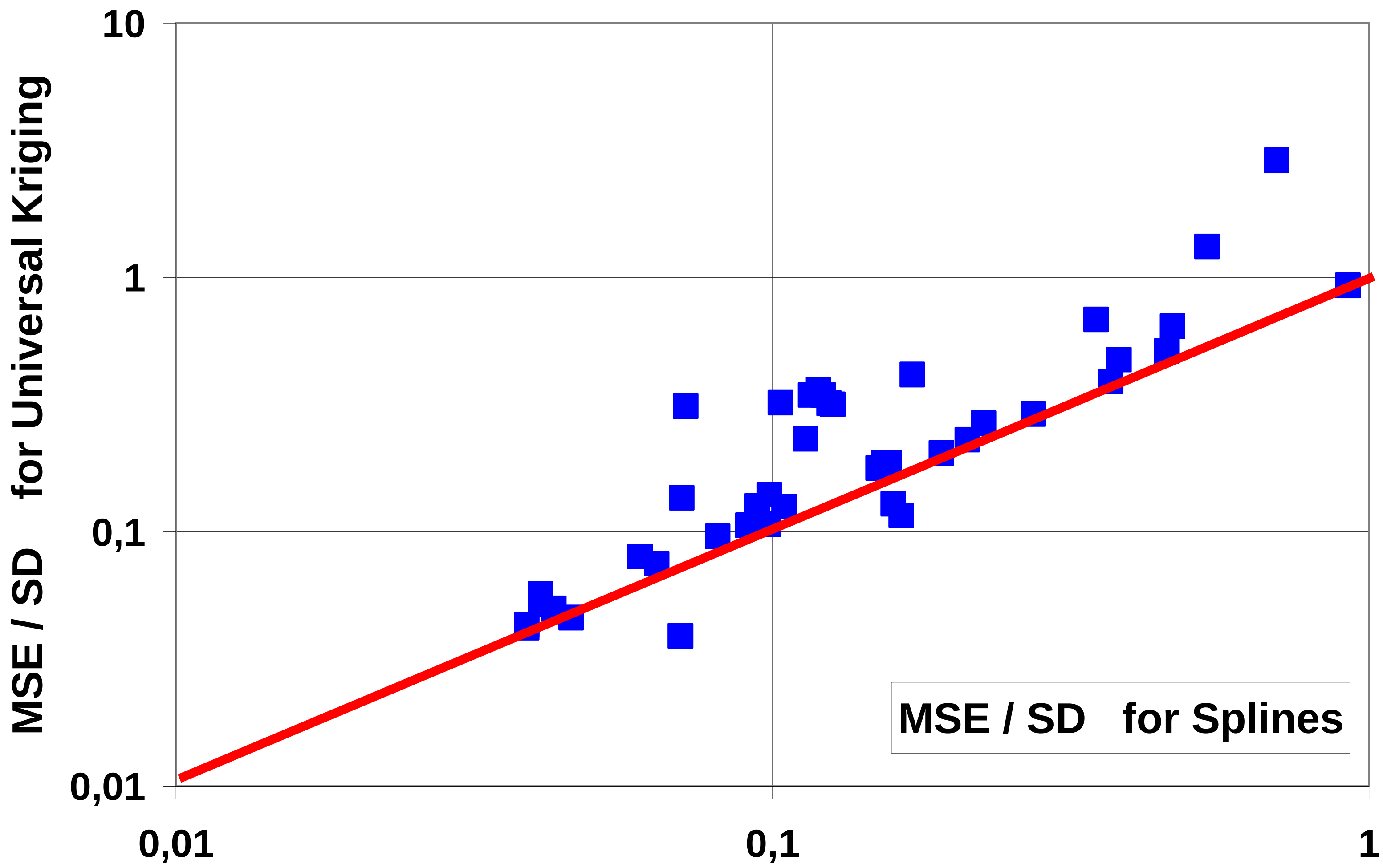


Universal kriging always better than Ordinary kriging

Comparison of the types of metamodels



Pseudo-cubic Splines usually better than Universal kriging

Comparison of the types of metamodels

What is a BAW?

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Conclusion

Pseudo-cubic thin-plate type spline usually better than Universal kriging

Universal kriging always better than ordinary kriging

In our specific industrial case, with 1003 simulations in a 10 dimension space

Confidence interval and yield estimation

What is a BAW?

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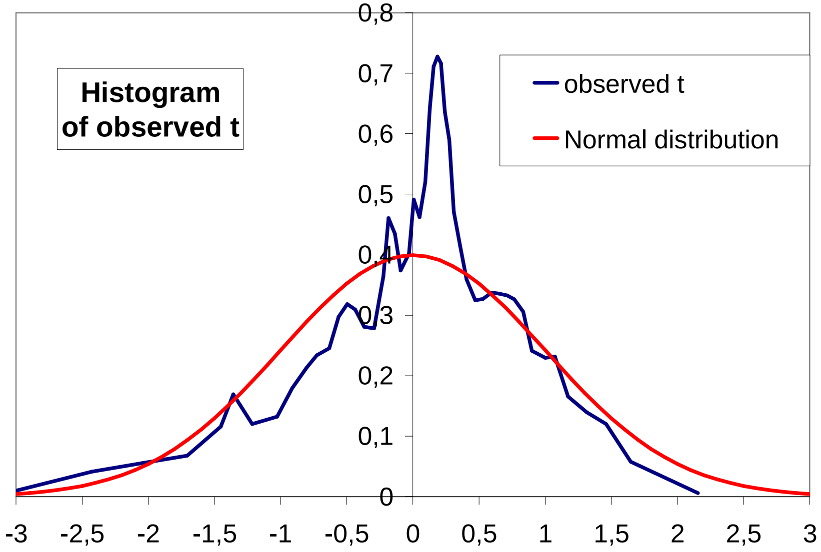
Confidence interval around the mean value: a real advantage for the kriging!

Tested over the two test set with universal kriging, "adaptation" and Maximin LHS

kriging   true value

$$t_i = \frac{f(x_i) - y_i}{e_i}$$

uncertainty



Yield estimation using Monte-Carlo estimation.

Acceptation criteria of type $R_k < T_k$ or $R_k > T_k$: the quantity $t_k(x) = \dfrac{R_k(x) - T_k}{e_k(x)}$ is transformed into a probability p_k of acceptation for this response via the cumulative distribution function of a normal distribution.

The yield is estimated by $$yield = \frac{1}{N}\sum_{i=1}^{N}\left(\prod_{k=1}^{P} p_k(x_i)\right)$$

Probability of acceptation of this particular point

Summation over N Monte Carlo points

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Summary and Conclusion

For our industrial case (10 factors, 1003 simulations) :

- ✓ Space filling designs, especially Maximin LHS, are usually better than Classical DOE

- ✓ Advantage of the pseudo-cubic thin-plate type spline:
  - *Usually more precise on independent test sets*
  - *Often numerically more stable*

- ✓ Advantage of the universal kriging (better than ordinary kriging):
  - *Estimation of the uncertainty, useful for yield estimations.*

Needs for estimation of uncertainty of interpolating spline!

Questions ?