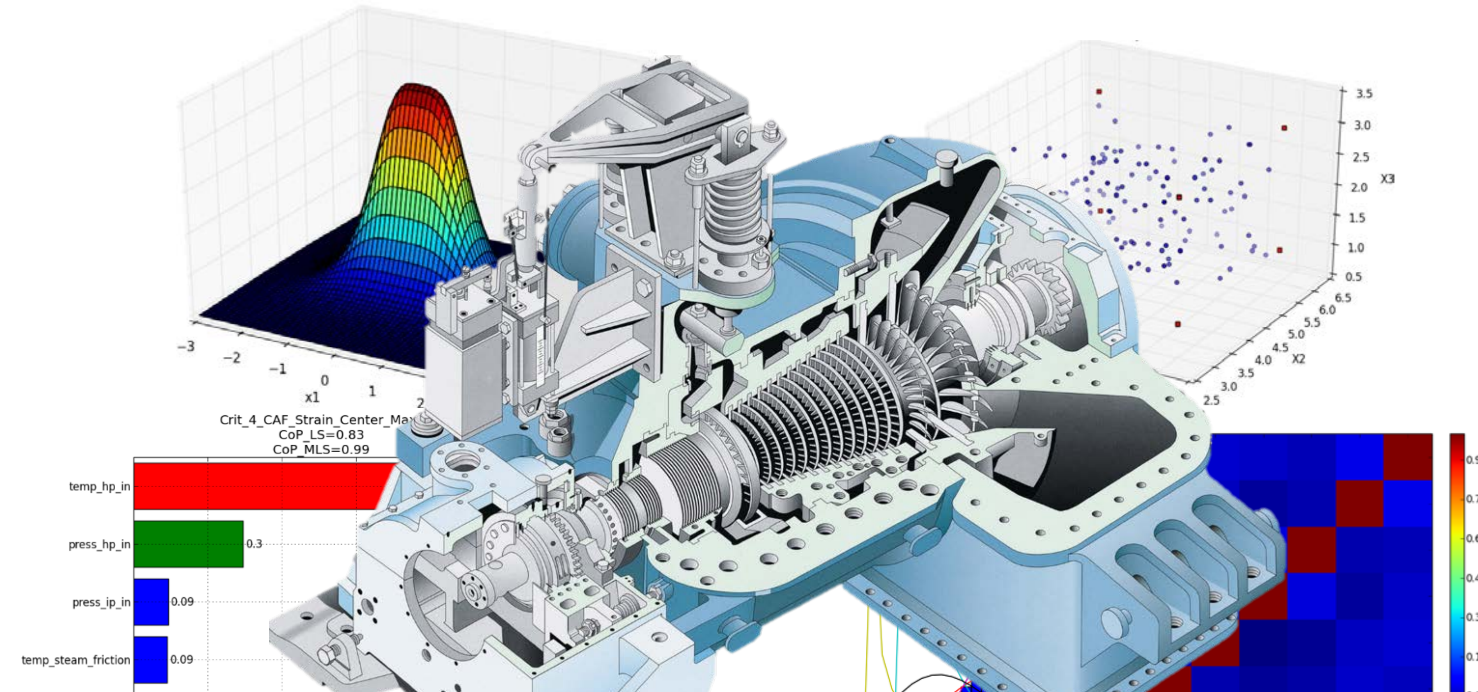


Anisotropic, hybrid meta models with maximized prognosis within multi-domain turbomachinery engineering

K.Cremanns, Prof. D. Roos
Institute of Modelling and High-Performance Computing,
Niederrhein University of Applied Sciences

P. Dumstorff
Siemens AG, Mülheim an der Ruhr

Outline

1. Introduction
   - Motivation

2. Process for optimized surrogates
   - Sampling
   - Variable selection
   - Surrogate creation

3. Examples
   - Benchmark results
   - Thermodynamic calculation of steam turbines
   - Notch factor calculation for rotor grooves
   - Labyrinth seal leakage in steam turbines
   - Zinc air battery optimization

4. Summary and outlook

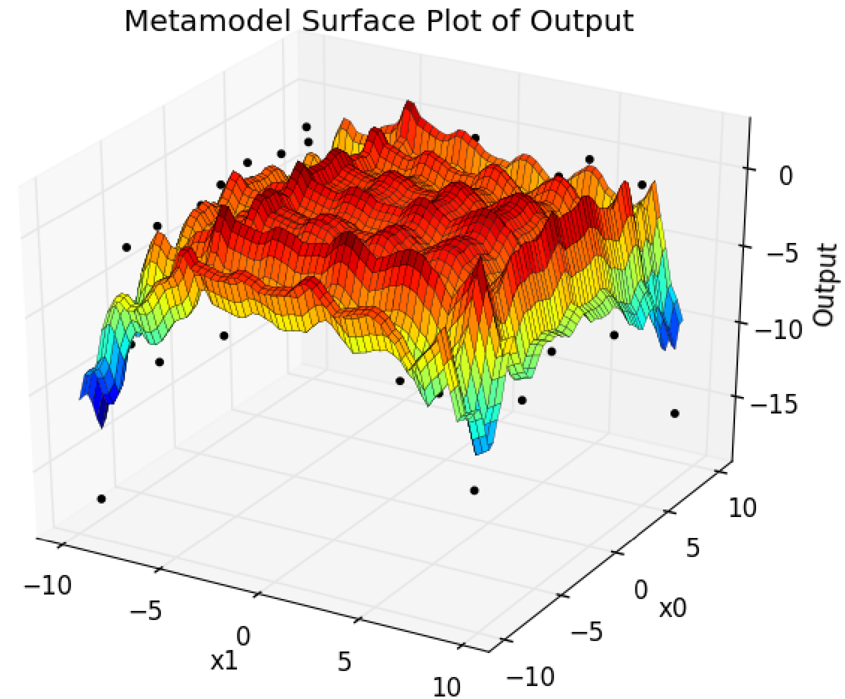
1. Introduction - Motivation

If your simulations or experiments are time and or resources expensive, …

- design optimization,
- robustness evaluation,
- design space exploration,
- sensitivity analysis,
- what-if analysis,
- …

becomes **impossible** since they require thousands or
even millions of simulation evaluations.

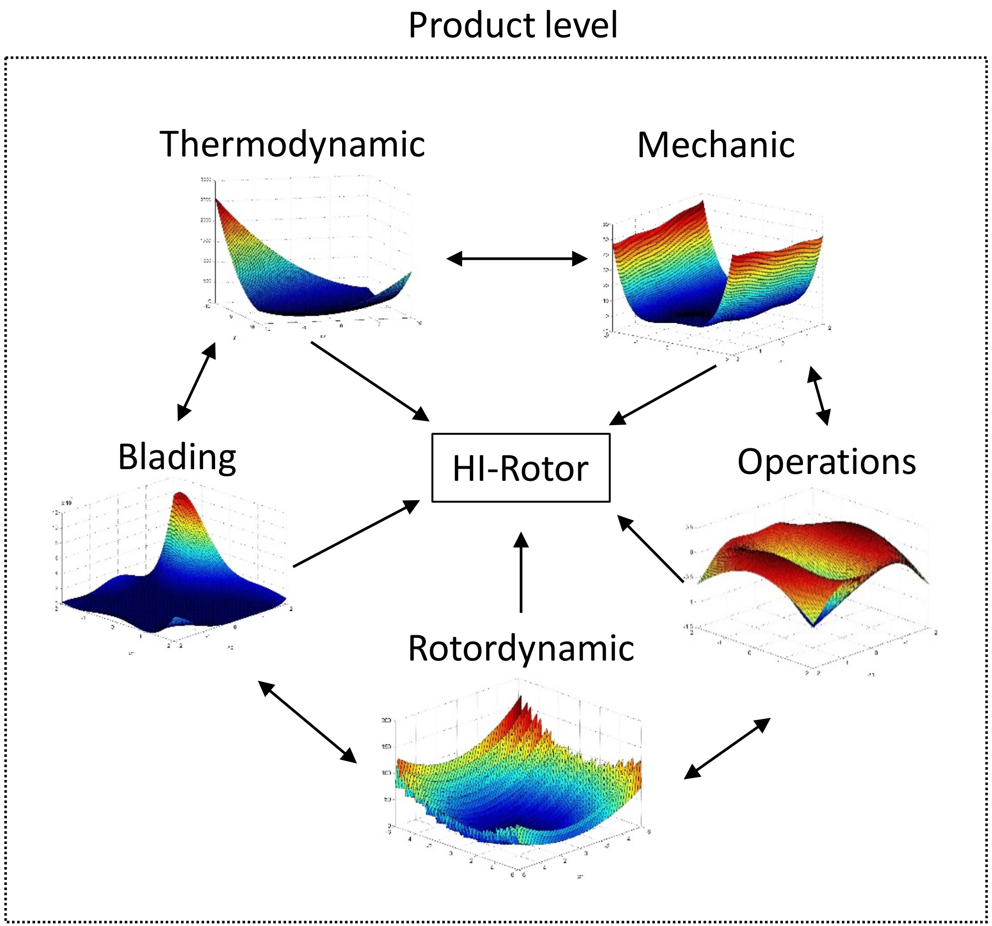
One way of alleviating this burden is by constructing approximation models, known as surrogate models, that mimic the behavior of the simulation model as closely as possible while being computationally cheap(er) to evaluate



1. Introduction - Motivation

Advantages:

- Fast and cheap model evaluations
- Connection of different simulations without consideration of interfaces
  −> Optimization on product level becomes easy
- Variance based sensitivity analysis gives information about input / output correlation
- Design optimization, robustness evaluation, design space exploration, sensitivity analysis, what-if analysis, … becomes **possible**



1. Introduction - Motivation

But which surrogate method is the right one for which problem?

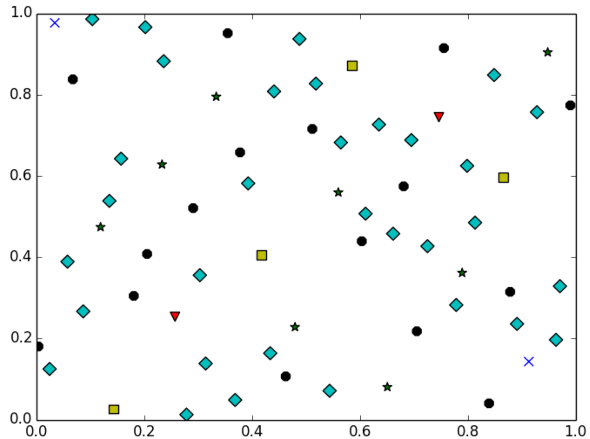
- The benchmark showed, that Kriging as interpolation method works on most problems really well. Especially the anisotropic version. Therefore it is also used in most commercial software tools [e.g. ASCMO, optiSLang, pSeven, iSight, Matlab (DACE/Toolbox)].
- The other methods showed nearly the same accuracy on the different problems.
- Moving least squares is a good method for regression and noisy practical problems (depending on the weighting function). A further development of this method to a anisotropic version (AMLS) [1] showed a further improvement for most applications.
- A combination of both method seems to be a good way to use the strength of both (regression and interpolation).
- An automatic self developed approach, which will select one of them or even a mixture is the „Optimal hybrid surrogate model“ (OHSM).

2. Process for optimized surrogates - Sampling

Input → Black Box

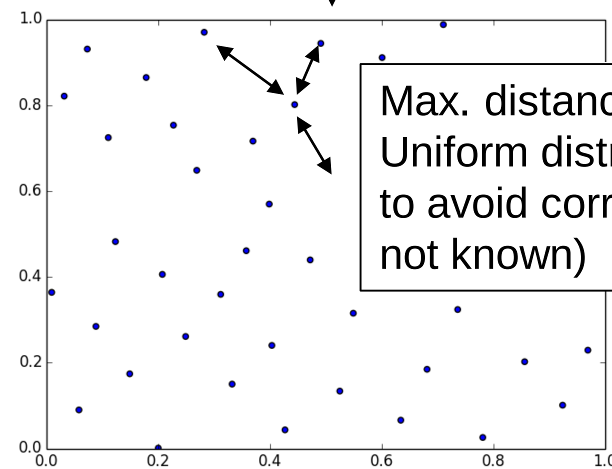
Simulations, Experiments → Output

- Unknown correlation between input and output
- Information through experiments are necessary
- Experiments are often time and resources expensive



Number of needed Samples?

Sequential Sampling



Max. distance
Uniform distribution
to avoid correlations (if not known)

Optimized experiment plans can save time and resources

2. Process for optimized surrogates - Surrogate creation

Examples of „A Metamodeling Method Using Dynamic Kriging and Sequential Sampling” L. Zhao, K. K. Choi and Ikjinn Lee, University of Iowa, 2010

1000 test points, Mean squared error as criteria

Example 1: $$f(x_1,x_2)=(4-2.1x_1^2+\frac{1}{3}x_1^4)x_1^2+x_1x_2+(-4+4x_2^2)x_2^2 \quad x_1\in[-3,3], x_2\in[-2,2]$$

Sample Size	UKG	BKG	PRS	RBF	SVR	DKG	OHSM
18	255,03	312,54	271,84	696,54	249,23	39,44	5,06e-22
19	231,77	301,66	249,47	684,71	223,31	11,53	
20	219,19	289,16	247,08	629,91	151,93	5,97	
21	196,29	278,34	132,94	601,13	157,93	4,81	
22	195,99	277,68	121,60	426,72	124,93	3,86	

UKG=Universal Kriging
BKG=Blind Kriging
PRS=Polynomial regression
RBF=Radial basis function
SVR=Support vector regression
DKG=Dynamic Kriging
OHSM=Optimal hybrid surrogate model

2. Process for optimized surrogates - Surrogate creation

Example 2:

$$f(x_1,x_2)=(x_2-\frac{5.1}{4\pi^2}x_1^2+\frac{5}{\pi}x_1-6)^2+10(1-\frac{1}{8\pi})\cos(x_1)+10 \quad x_1\in[-5,10],x_2\in[0,15]$$

Sample Size	UKG	BKG	PRS	RBF	SVR	DKG	OHSM
16	466,21	199,34	87,22	583,11	497,82	13,85	1,29
17	437,87	195,03	86,26	551,80	478,46	8,86	8e-21
18	237,93	71,87	75,73	550,38	465,66	1,94	
19	204,92	54,58	70,62	490,09	359,69	0,98	
20	200,48	16,90	66,17	529,19	348,85	0,39	1,64e-21

UKG=Universal Kriging
BKG=Blind Kriging
PRS=Polynomial regression
RBF=Radial basis function
SVR=Support vector regression
DKG=Dynamic Kriging
OHSM=Optimal hybrid surrogate model

2. Process for optimized surrogates - Surrogate creation

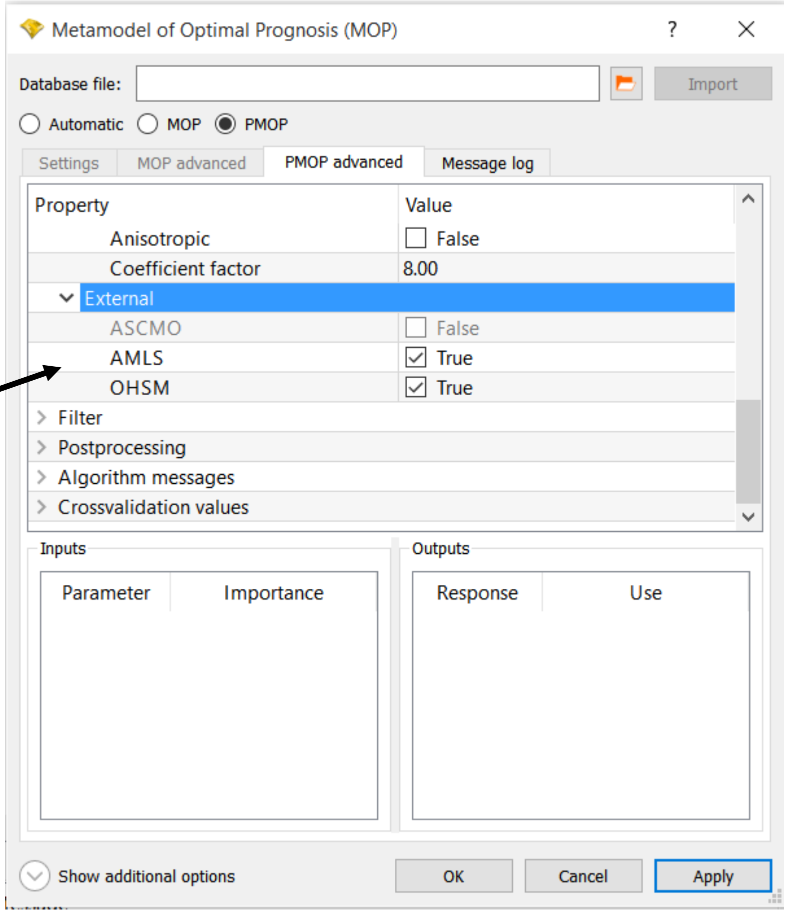
Summary:

1. Sensitivity analysis + variable selection.
2. …
3. Optimization of model parameters of Kriging and AMLS with cross validation (k-fold or leave one out) to avoid overfitting.

2. Process for optimized surrogates - Surrogate creation

Implementation:

- Complete process is implemented in pyhton 2.7.
- Data is loadable in python through .csv, .xls(x), .txt … so from every simulation / experiment.
- Interfaces for Matlab (Script)
- and optiSLang (new custom algorithm API). All optiSLang tools can be used together with these surrogate models, in the same way as usual.



3. Examples – Benchmark

Benchmark criteria:

Prognosis quality = $1 - \frac{\sum_{i=1}^{m}\left(y_i^0 - \tilde{y}_i^0\right)^2}{\sum_{i=1}^{m}\left(y_i^0 - E\left(y_i^0\right)\right)^2}$

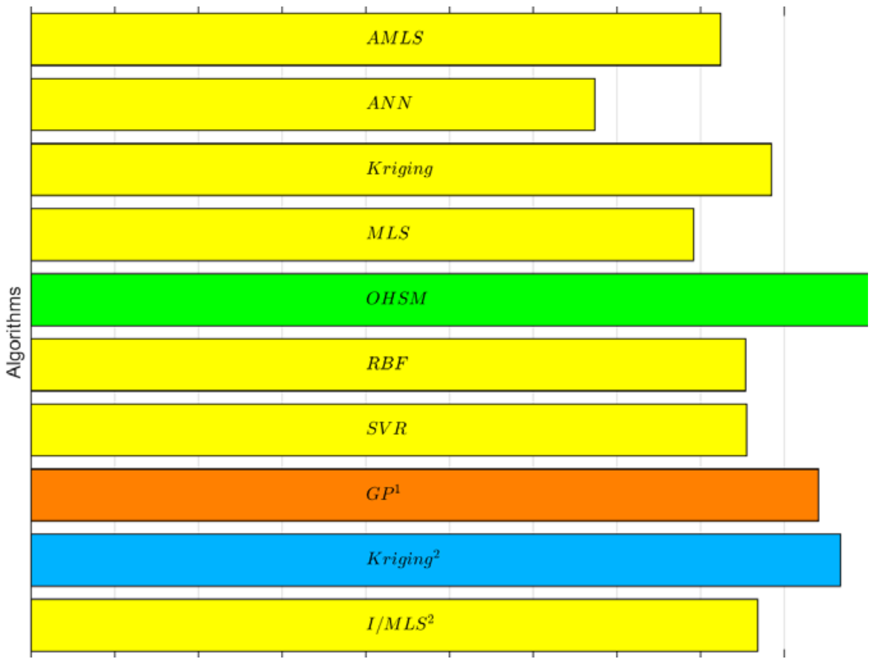
RMSE = $\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$

For testfunctions definition see [6]

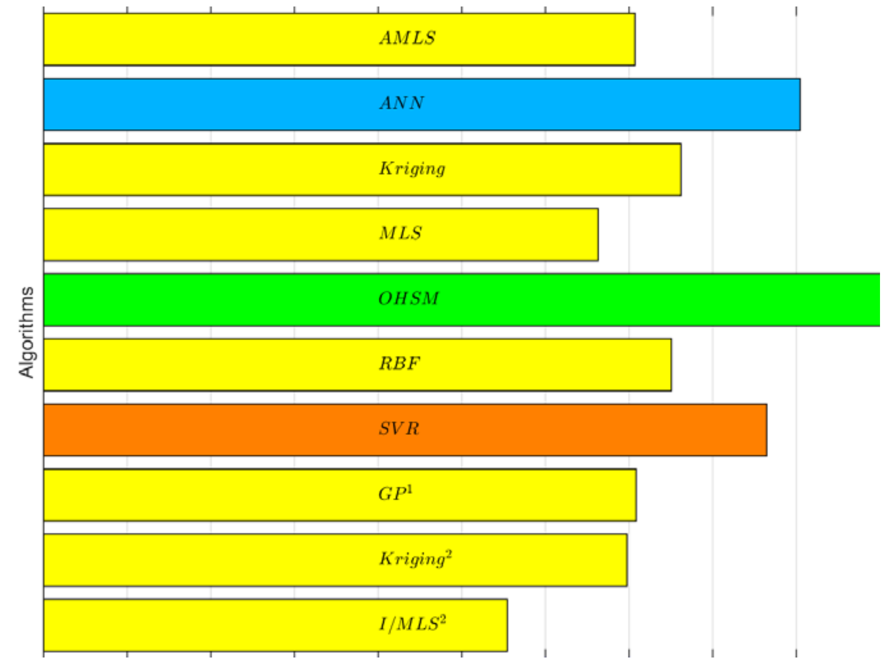
3. Examples – Benchmark

Inner region emphasized functions

Prognosis quality



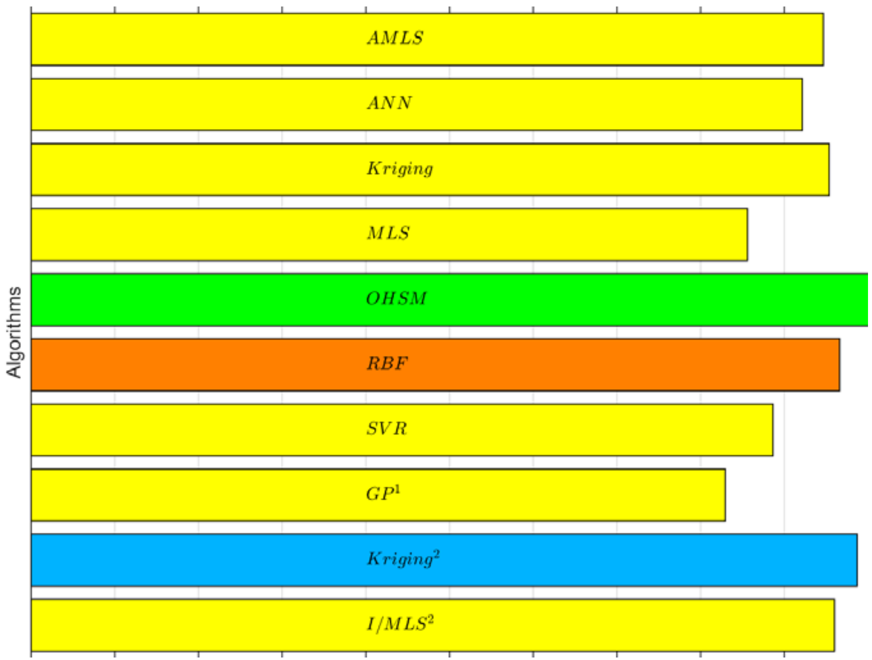
RMSE



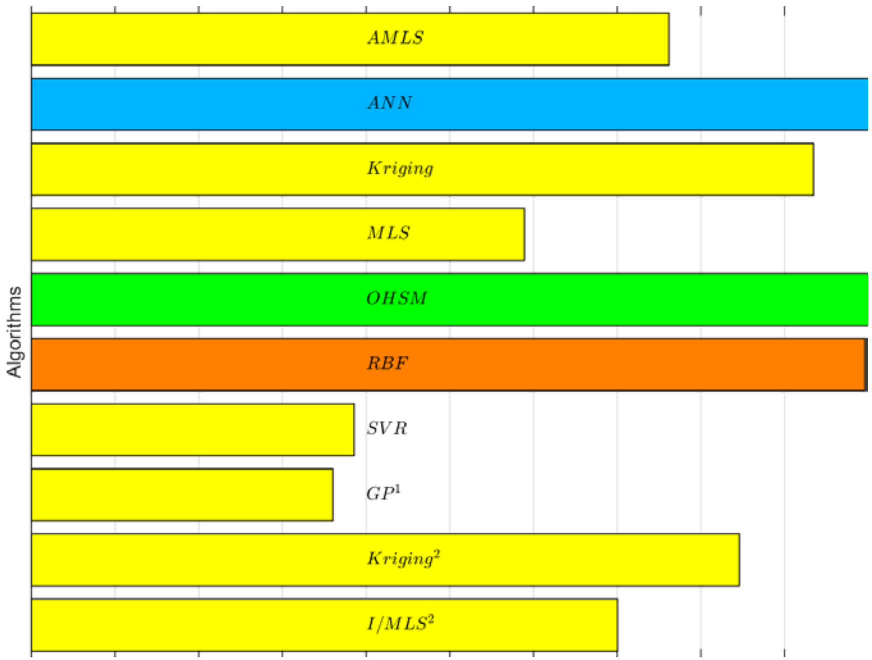
3. Examples – Benchmark

Outer region emphasized functions

Prognosis quality

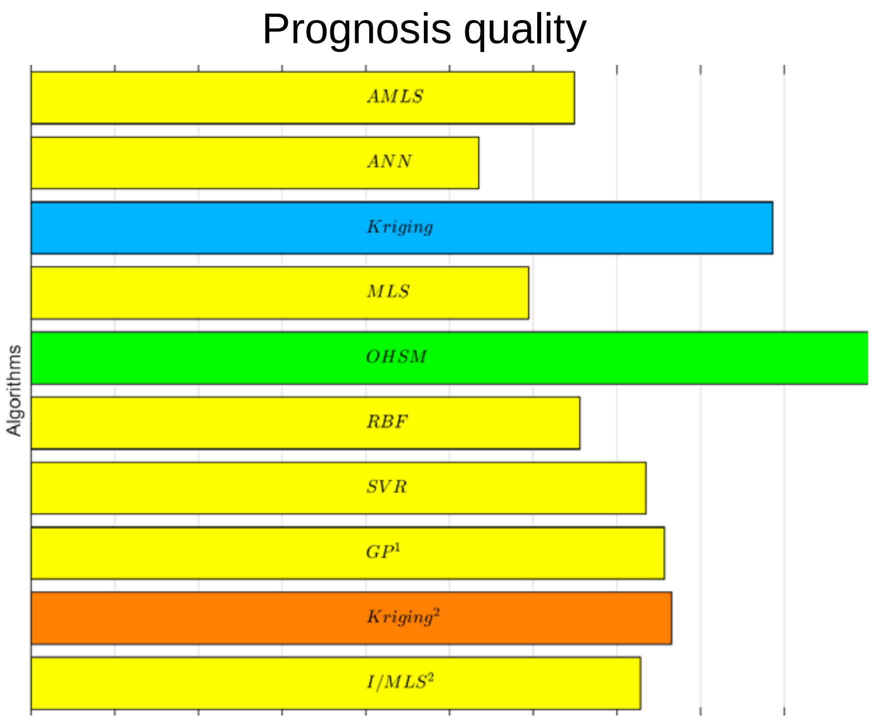


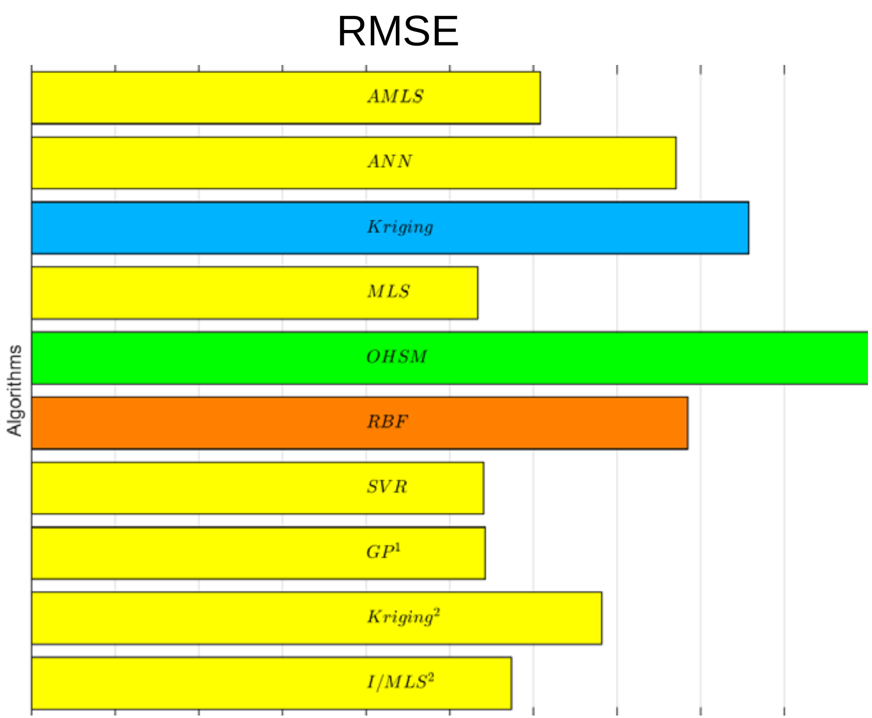
RMSE



3. Examples – Benchmark

Functions with high modality

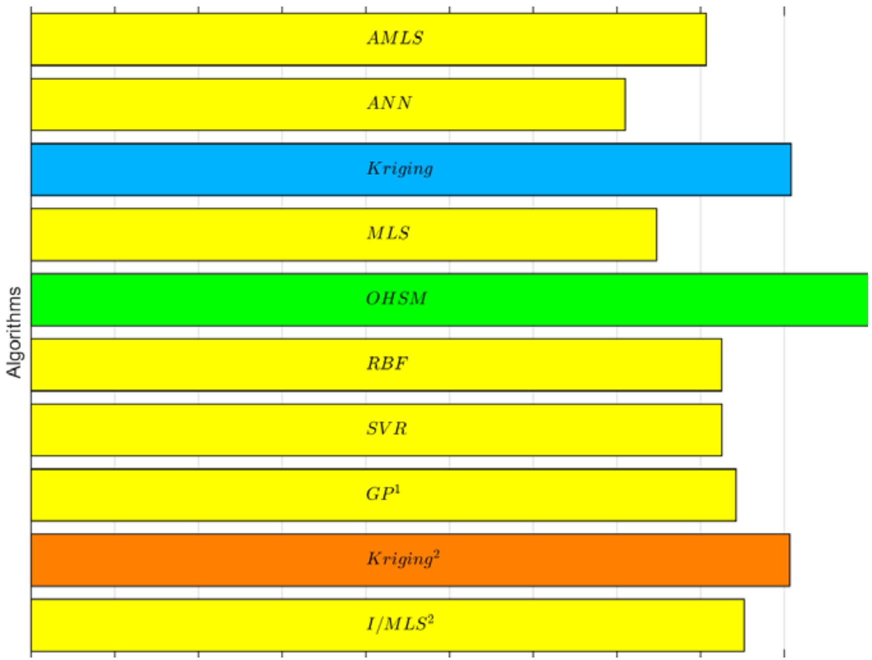




3. Examples – Benchmark

Total

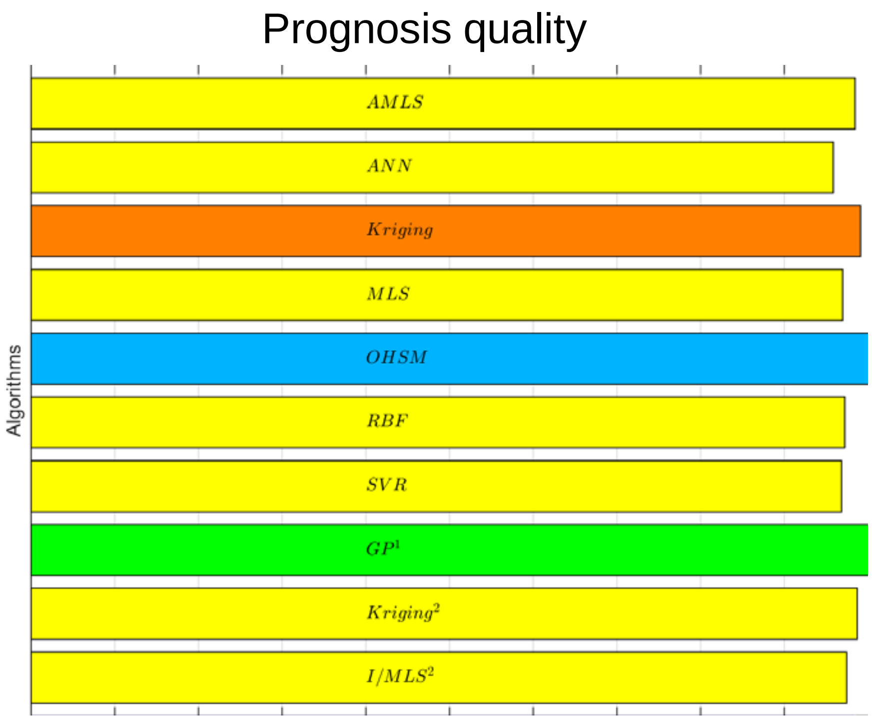
Prognosis quality

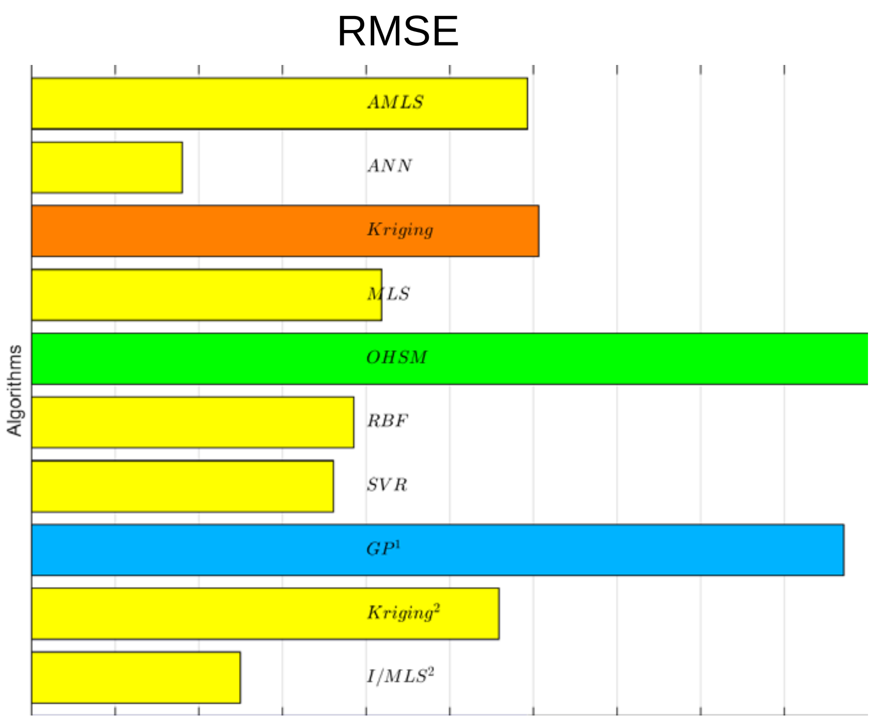


RMSE

3. Examples – Benchmark

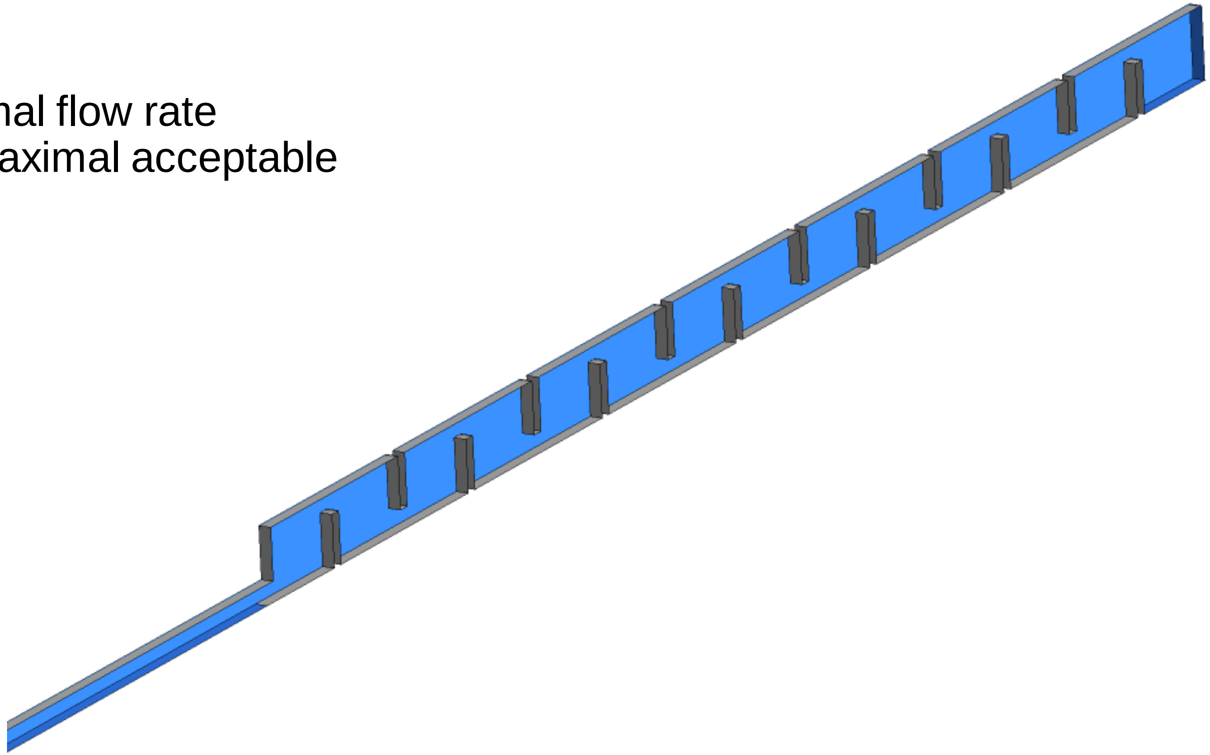
Mechanic example





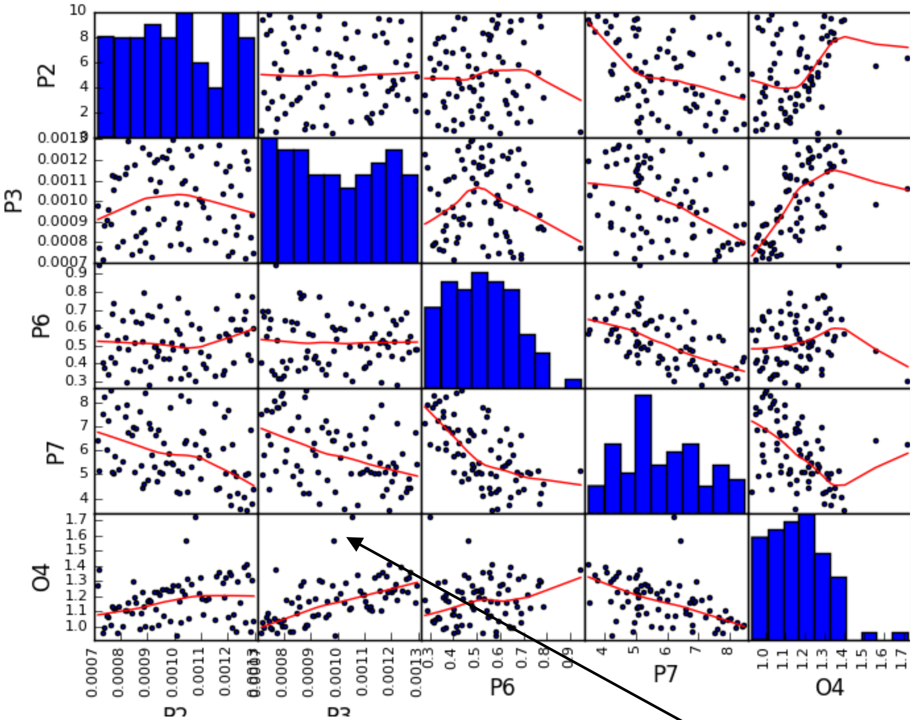
3. Examples - Labyrinth seal leakage in steam turbines

- 7 Input parameters.
- 4 Output parameters.
- 79 Samples.
- Optimization: minimal flow rate coefficient under maximal acceptable temperature rise

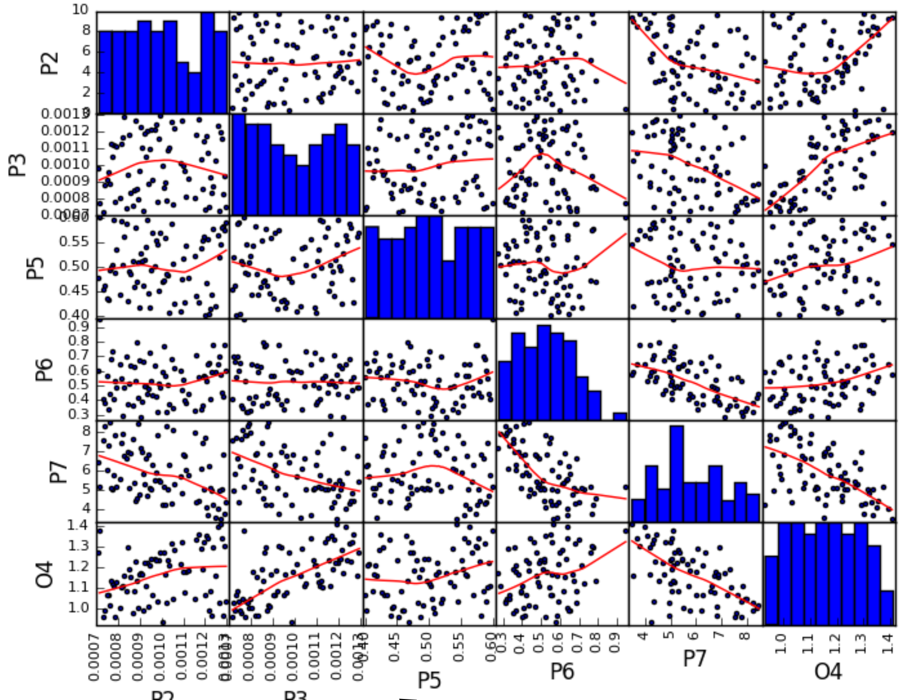


3. Examples - Labyrinth seal leakage in steam turbines

Prognosis quality = 0.59



Prognosis quality with LoF = 0.81

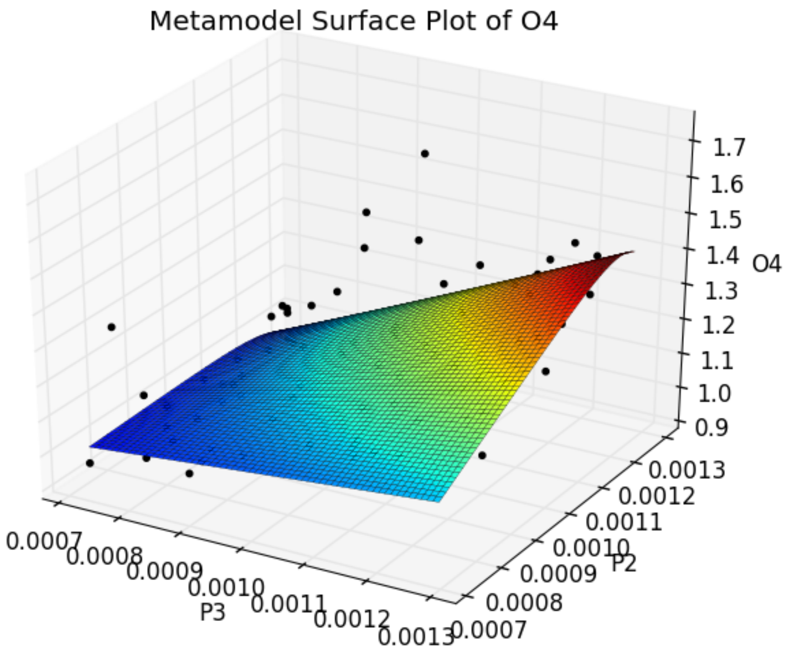


Detection of outliers

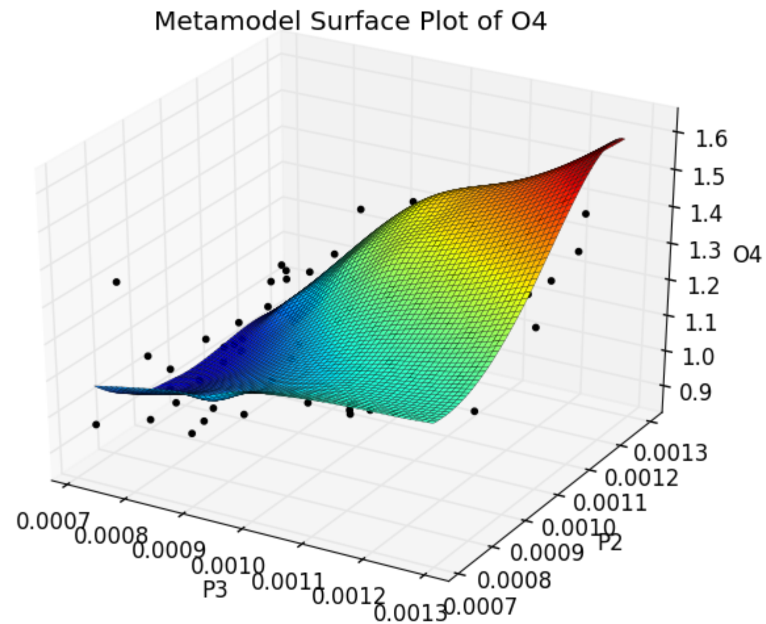
Leads to additional sensitive parameter

3. Examples - Labyrinth seal leakage in steam turbines

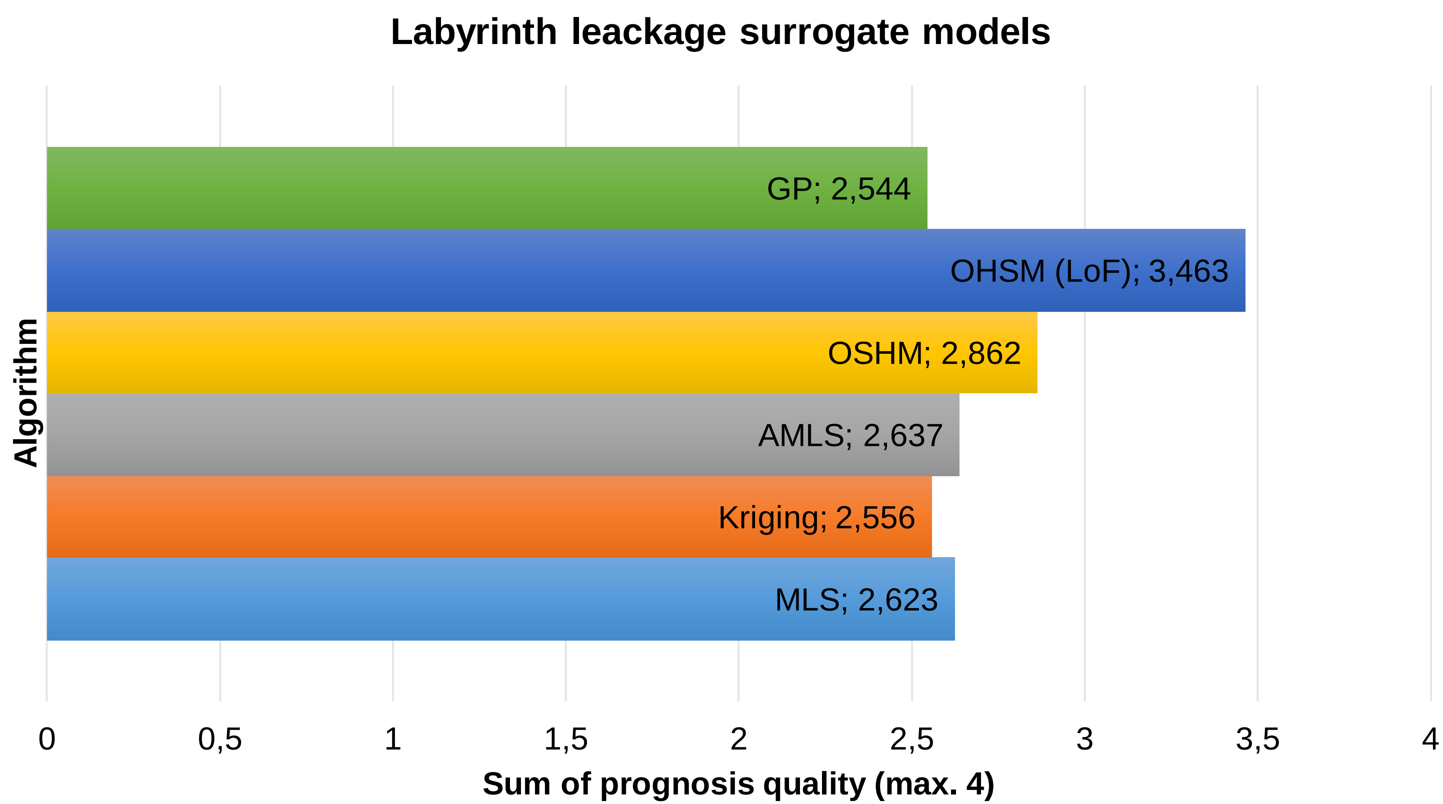
Prognosis quality = 0.59



Prognosis quality with LoF = 0.81



3. Examples - Labyrinth seal leakage in steam turbines

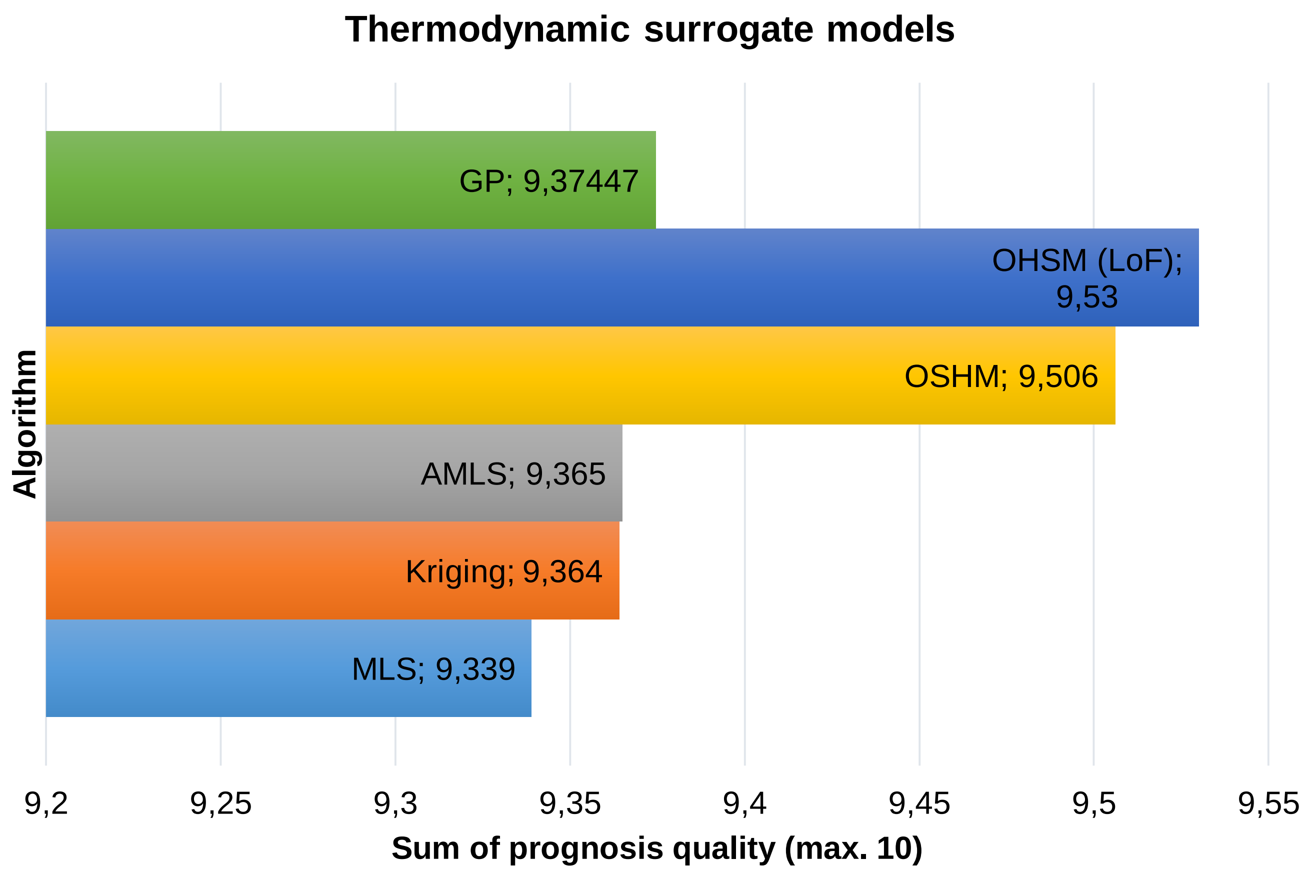


3. Examples - Thermodynamic calculation of steam turbines

Thermodynamic calculation of HP/IP/LP-turbines:

- 4 varied input parameters (temperatures and pressures).
- 10 Output parameters (efficiency, power, pressures, temperatures).
- 89 Samples.
- Internal solver create the geometry and blading depending on the constraints of temperature, pressure etc.

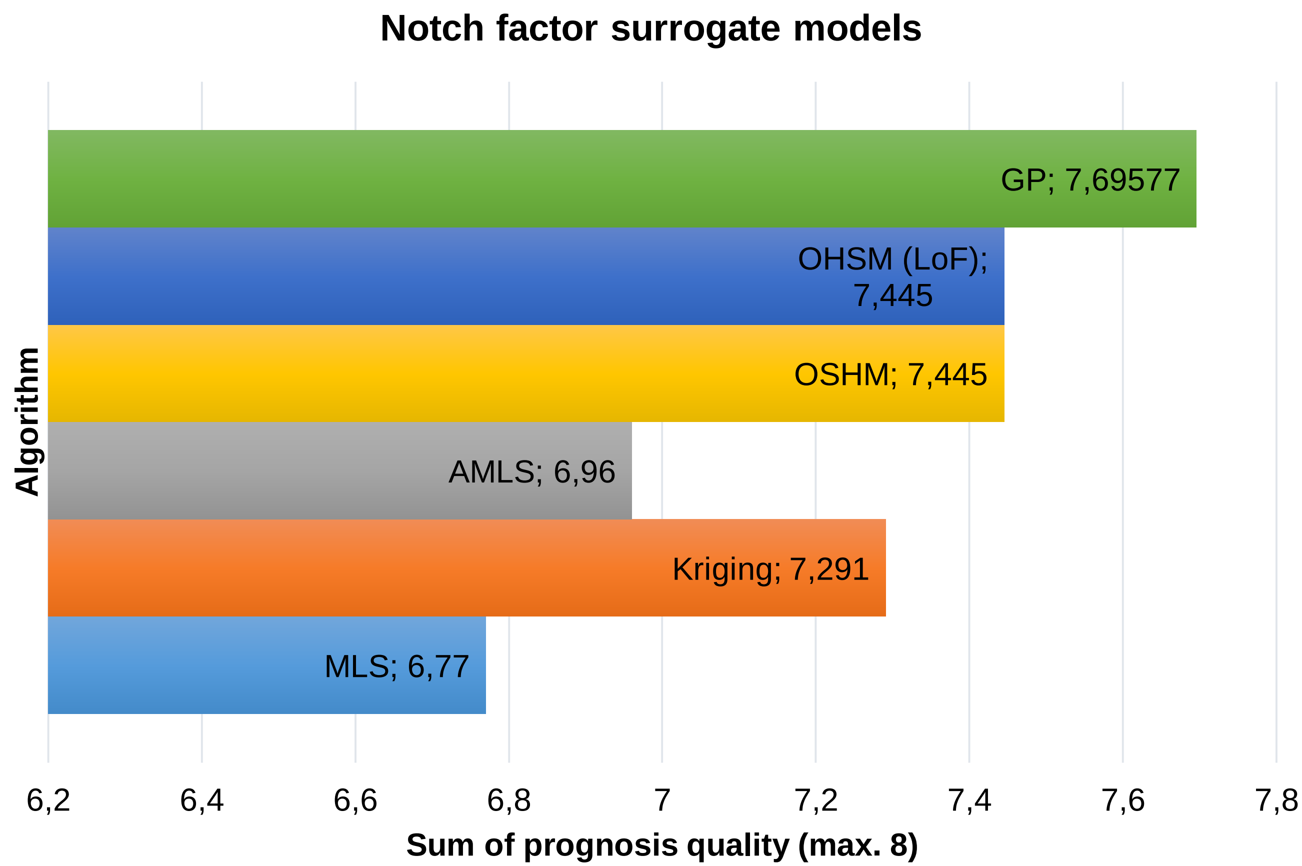
3. Examples - Thermodynamic calculation of steam turbines



3. Examples - Notch factor calculation for rotor grooves

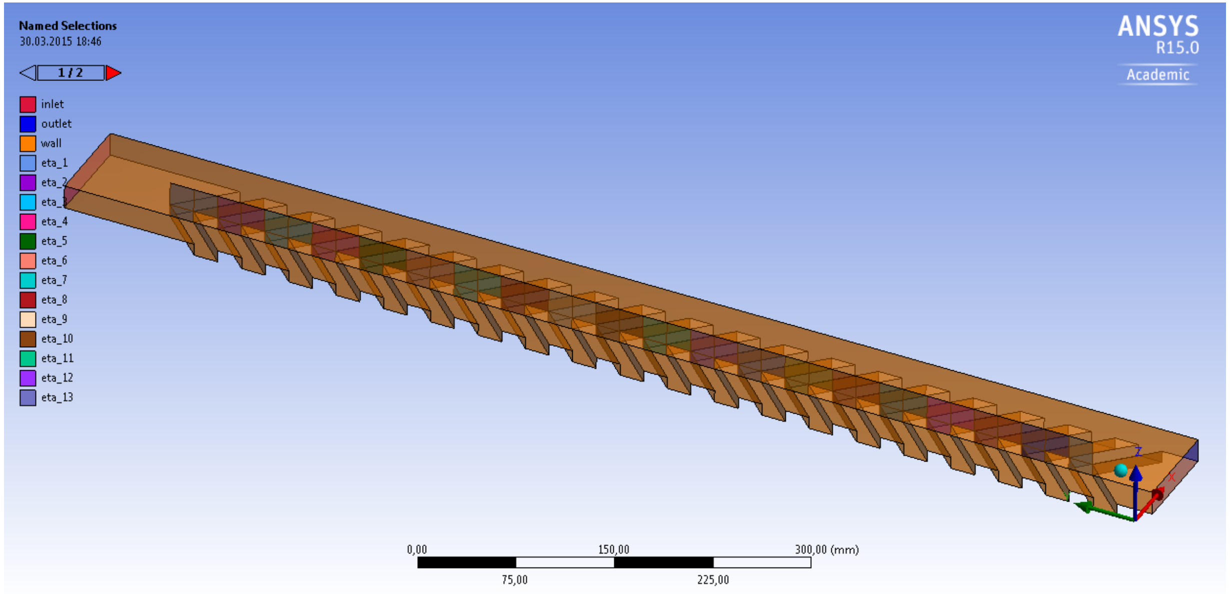
- 29 Input parameters (geometry).
- 8 Output parameters (notch factors of rotor grooves).
- 110 Samples.
- Notch factors optimization.
- Abaqus simulation.

3. Examples - Notch factor calculation for rotor grooves



3. Examples – Zinc air battery optimization

- 81 Input parameters (geometric)
- 61 Output parameters (efficiency, pressure)
- 96 Samples
- High transverse flow with minimal pressure lost



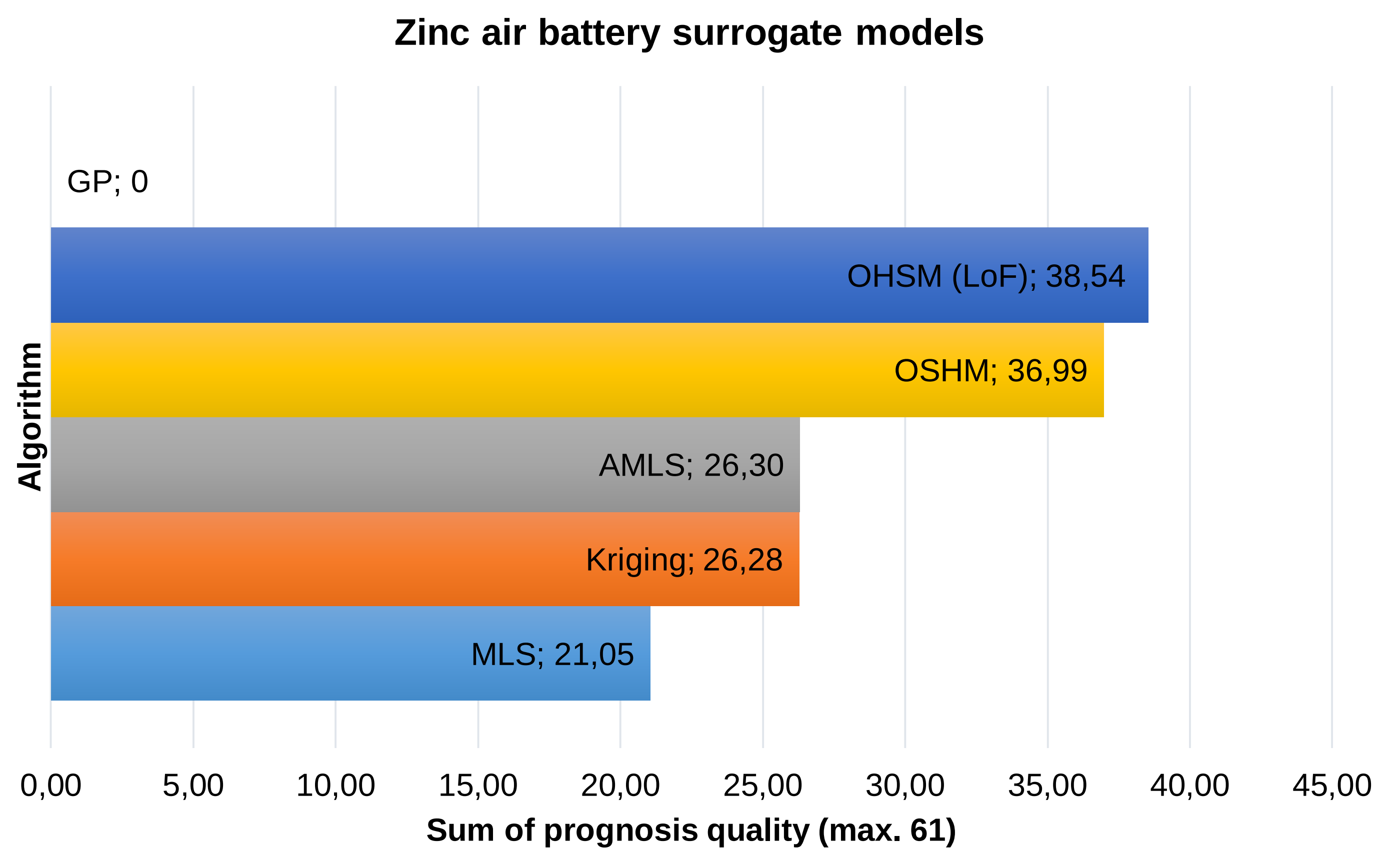
3. Examples – Zinc air battery optimization

Example outputs:

Output	MLS	Kriging	AMLS	GP	OHSM	OHSM (LoF)
g1_eta0x	0.26	0.33	0.55	0	0.75	0.82
g13_eta0x	0.40	0.40	0.56	0	0.79	0.78
average_etax0	0.29	0.39	0.37	0	0.55	0.71
g1_etax_abssum	0.24	0.39	0.52	0	0.50	0.67
g9_etax_abssum	0.38	0.41	0.30	0	0.62	0.72

Prognosis quality

3. Examples – Zinc air battery optimization



4. Summary and outlook

Summary:

- Overall process of:
  - Design of experiments
  - Sensitivity analysis and variable reduction.
  - Optimal hybrid surrogate model of self developed anisotropic moving least squares and anisotropic Kriging.
- Analytic benchmark results compared to most common surrogate methods.
- Comparison to commercial tools for practical examples.
- Fully implemented in python with interfaces to optiSLang and Matlab – easy to use.

4. Summary and outlook

Outlook:

- Further improvements of used methods (stability and speed).
- Implementation of further new features:
- Publications of the showed methods.

Literature

[1] K. Cremanns, D. Roos, “Requirements and new approaches of probabilistic optimal design from a practical point of view considering steam turbines”, Weimar optimization and stochastic days, 2014.

[6] C. Bogoclu, D.Roos, “A Benchmark of Contemporary Metamodeling Algorithms”, DPW8, Dresden, 2015.

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