

# Surrogate-based multi-objective stator optimization using variation of complex free-form surfaces

K. Cremanns, A. Graßmann, D. Roos<sup>1</sup>, C. Fütterer, J. Palluch<sup>2</sup>

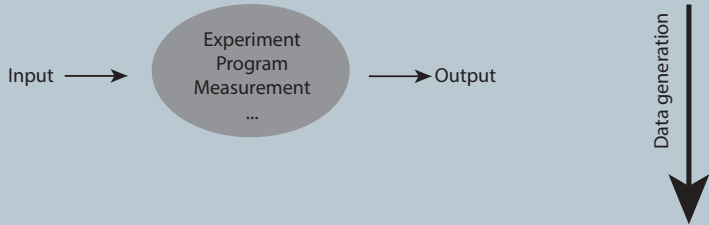
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# Outline

- 1 Introduction to machine learning
  - Key concepts of supervised machine learning
  - Technical applications areas
- 2 Creation of supervised machine learning models
  - Sampling, outlier and variable selection
  - Deep Gaussian covariance networks
  - Model validation
- 3 TU-Berlin stator optimization
  - Parametric CAD model and CFD setup
  - Optimization
  - Results

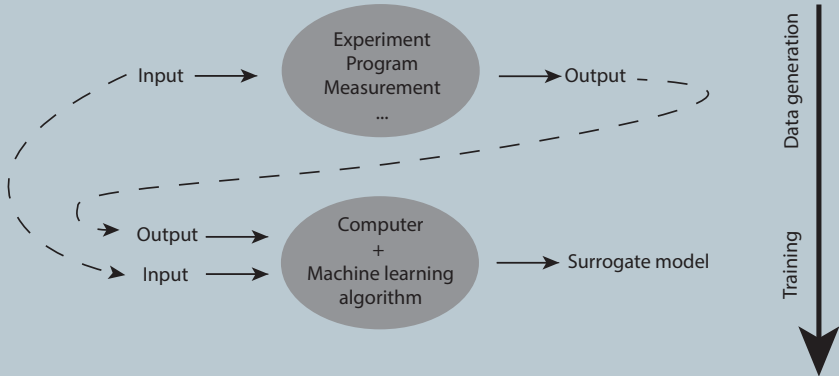
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# Definition of machine learning (supervised)

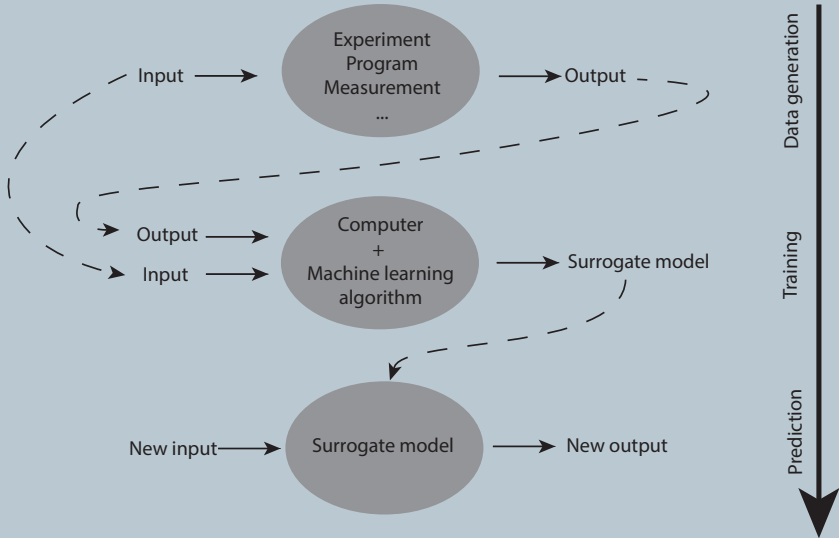




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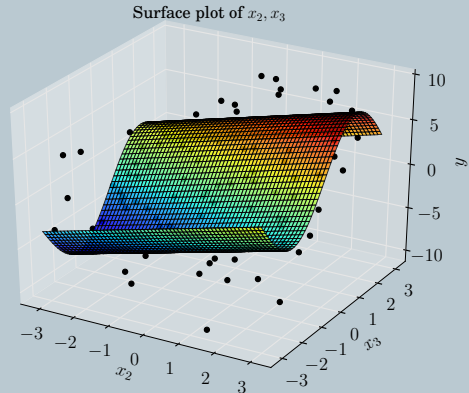


# Definition of machine learning (supervised)



# Advantages

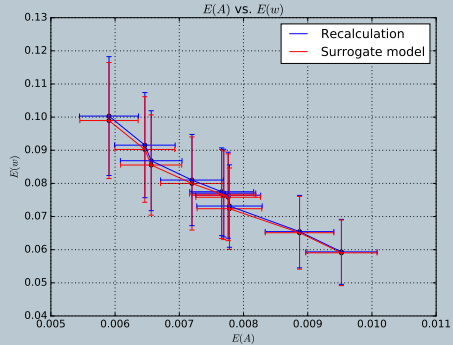
- Fast and cheap model evaluations
- Deeper knowledge of your data (sensitivity analysis)
- Connection of tools without interface problems
- Forecast the future (time dependent problems)
- Expensive design optimization, robustness evaluation, ... becomes possible



# Examples of machine learning

In the field of mechanical engineering:

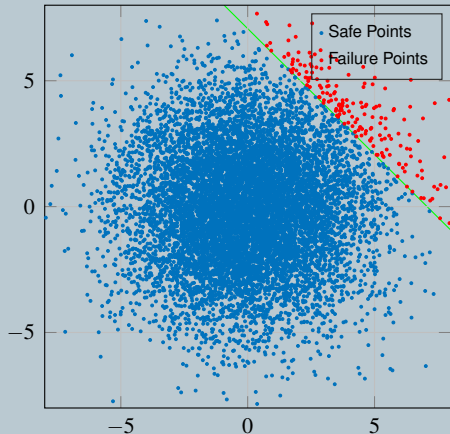
- (Robust) Design optimization



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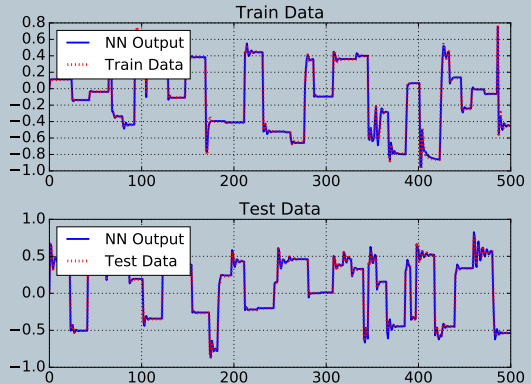
- (Robust) Design optimization
- Robustness / reliability analysis



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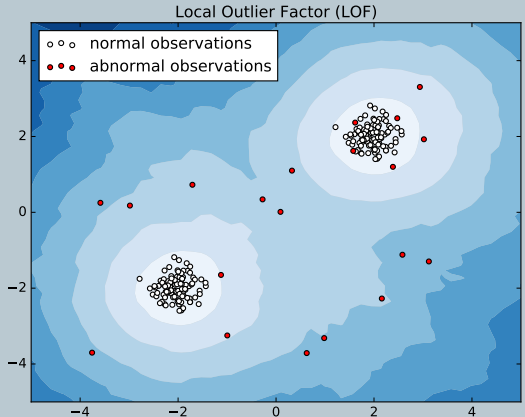
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- Robustness / reliability analysis
- Time series forecasting



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In the field of mechanical engineering:

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- Classification / anomaly detection



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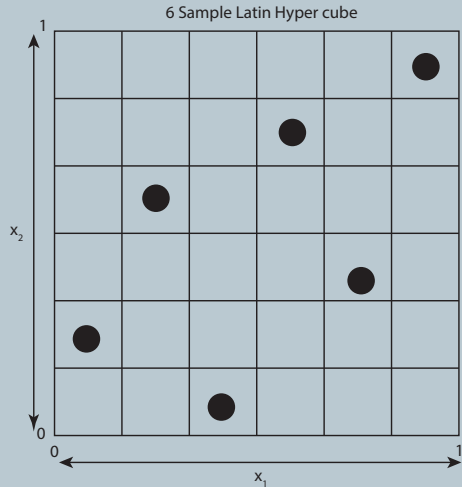
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- Time series forecasting
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- ...



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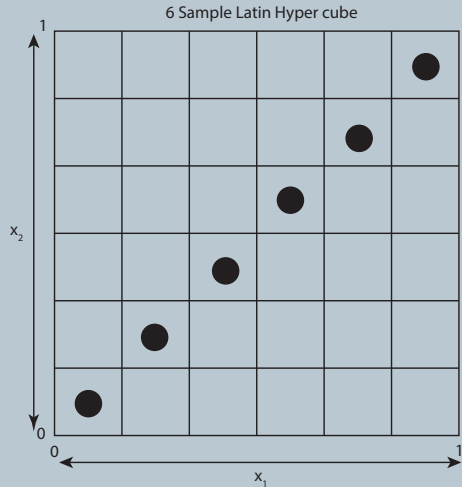
# Design of Experiment - Latin hypercube sampling

- Latin Hypercube sampling (LHS) is one of the most used sampling methods for design plans...

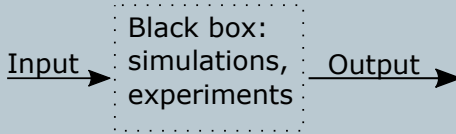


# Design of Experiment - Latin hypercube sampling

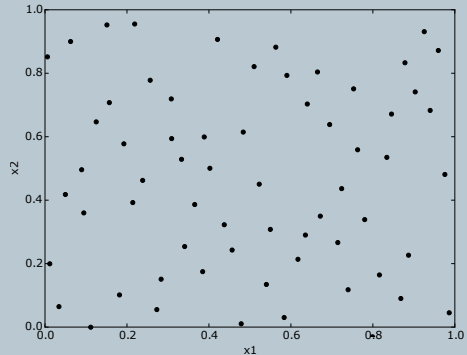
- Latin Hypercube sampling (LHS) is one of the most used sampling methods for design plans...
- but it can also be very useless if it is not optimized



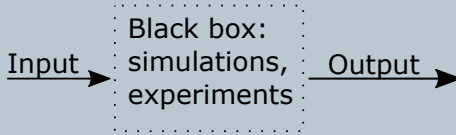
# Optimized Latin hypercube sampling



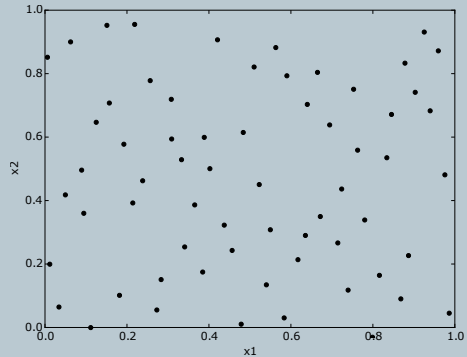
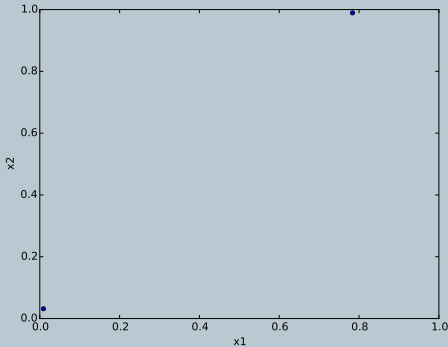
- Space filling
- No unwanted correlation
- One shot / Sequential



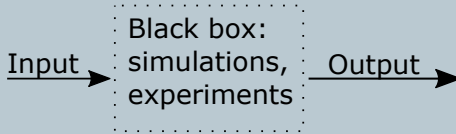
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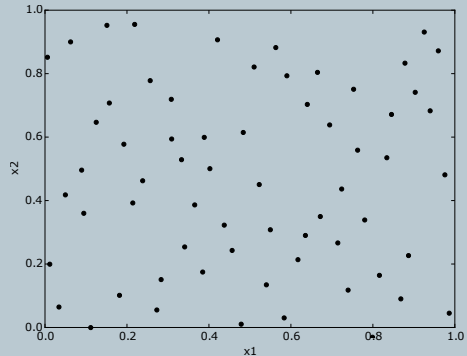
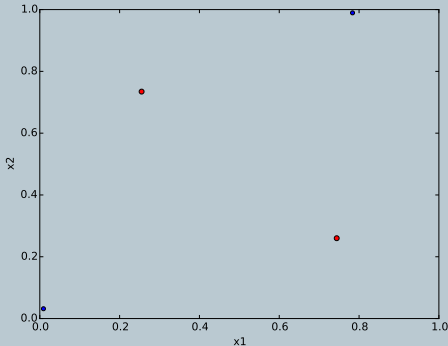
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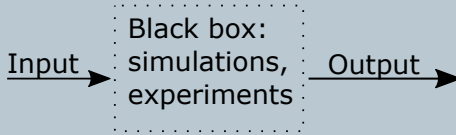
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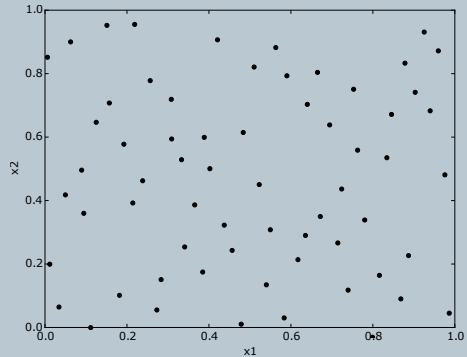
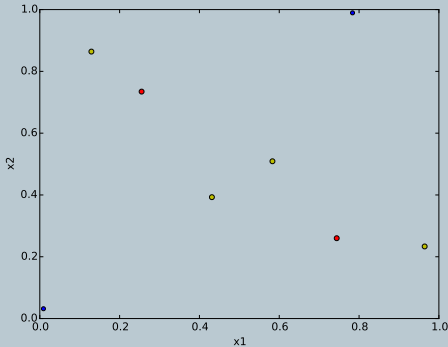
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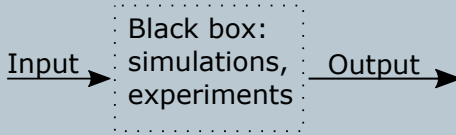
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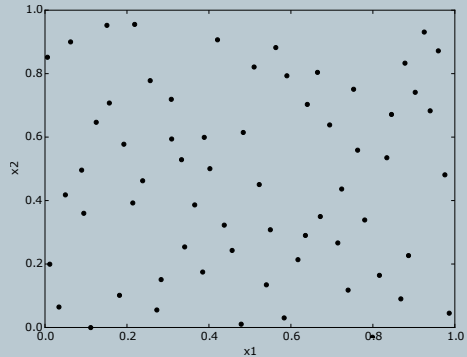
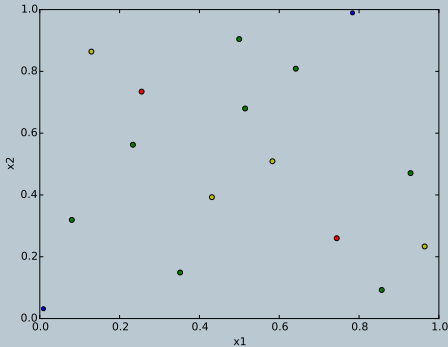
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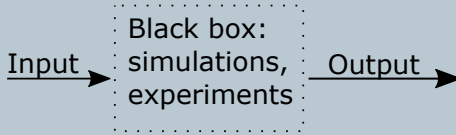


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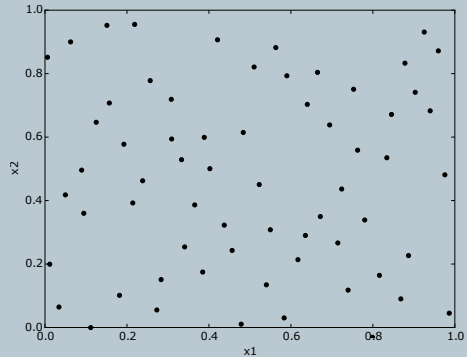
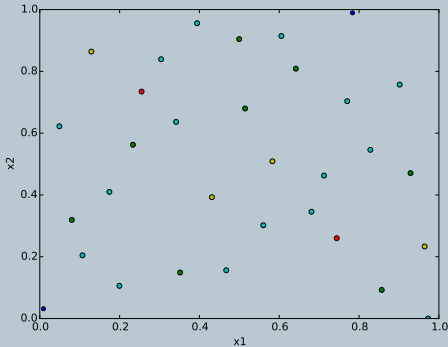




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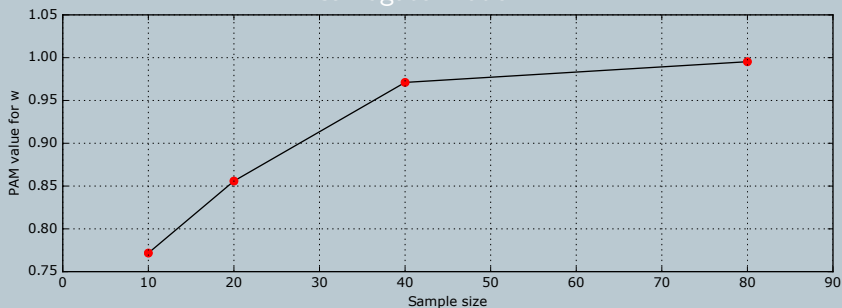


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# Stepwise convergence check

Sequential sampling can be used for convergence check of surrogate model

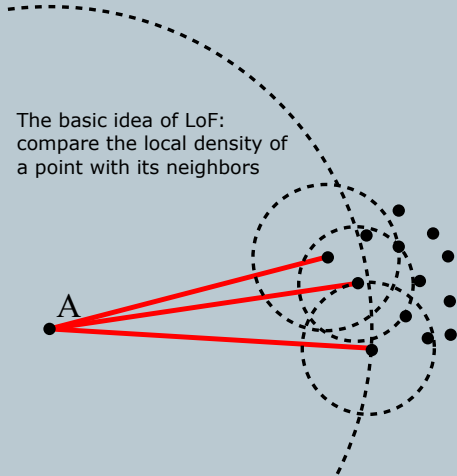


No wasted samples

# Automatic outlier detection

- Local outlier factor (LoF).  
Density based outlier detection.
- It detects outliers in data with areas of different density.
- Just one outlier can have a huge impact on the prognosis quality.
- Searches for each output individually for outliers.
- $\text{LoF} \gg 1$  outlier.

The basic idea of LoF:  
compare the local density of  
a point with its neighbors



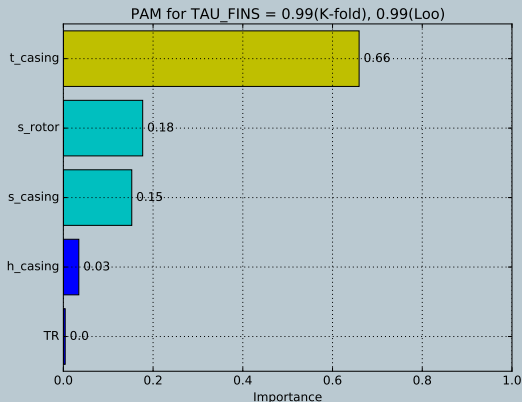
# Variance based sensitivity analysis

First order:

- $S_i = \frac{V_i}{Var(y)}$

Total order:

- $S_{T_i} = \frac{E_{x \sim i}(Var_{x_i}(y|x \sim i))}{Var(y)}$
- Sum of  $S_{T_i} > 1$  if interaction effects between  $x, y$  are present.
- Non-linear, non-monotonic, multivariate sensitivities.
- Useful for root cause analysis



# Deep Gaussian covariance networks - Advantages

- Any training samples size is possible **even on** low hardware resources, **since flexible batch training can be used.**

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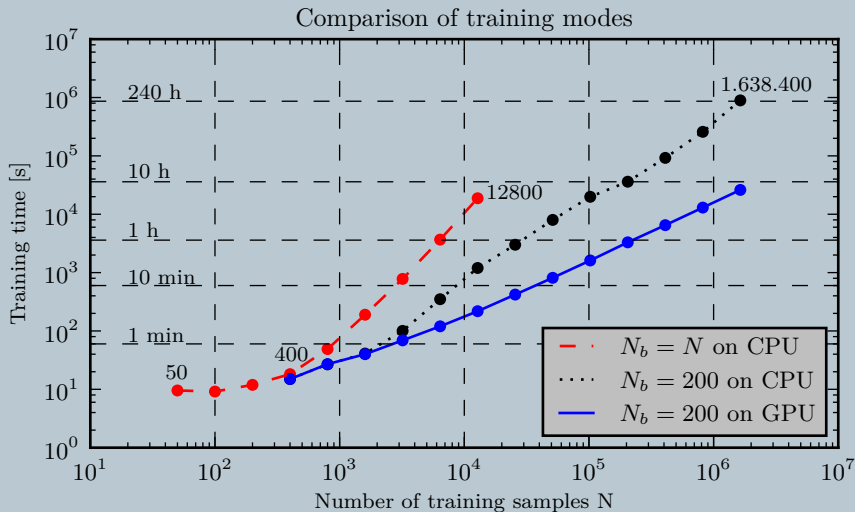
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- Multiple different Gaussian process covariance functions are used and trained simultaneously. So complex problems can be predicted even better.

## Training time comparison (1/2)

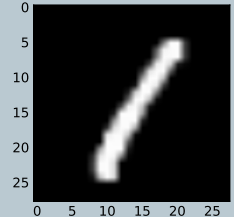
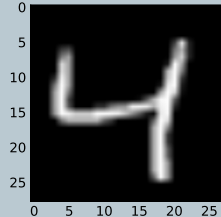
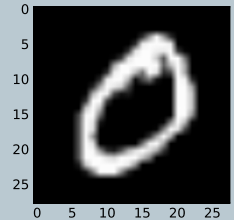
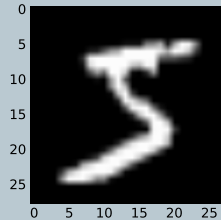
- Test function with 100 input parameters and 1 output.
- Training is based on 100 epochs (reasonable good model in most cases).
- Training samples  $N$  range from 50 to 1.638.400 (doubling).
- 13.360 trainable hyperparameters.
- 3 training modes are compared:
  - Batch size =  $N$  on CPU
  - Batch size = 200 on CPU
  - Batch size = 200 on GPU
- Training on a HPC (distributed learning) would also be possible.
- Used CPU: Intel Core i7 3770 2 cores at 3.50 GHz.
- Used GPU: Nvidia Quadro 4000 256 Cuda cores (7 years old)  
modern GPU have 3840 Cuda cores.

# Training time comparison (2/2)



## Example - Classification MNIST data set (1/2)

- 60.000 training and 10.000 test points of handwritten digits
- Each data point is defined by an 28X28 pixel image (784 parameters)
- Corresponding number represented by a 10 element vector (0,1,2,3,4,5,6,7,8,9)

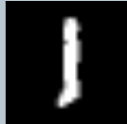


## Example - Classification MNIST data set (2/2)

Predicted: 6



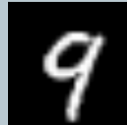
Predicted: 1



Predicted: 7



Predicted: 9



Predicted: 5



Predicted: 3



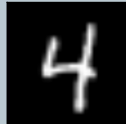
Predicted: 0



Predicted: 9



Predicted: 4



- Training time  $\sim 10$  min
- Error rate  $\sim 5\%$

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- The framework also includes a calculation mode for sequential dependent problems.

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- In this case the framework even learns the hyper parameters not only dependent on  $X$  but also over the time  $t$ .



# Validation methods

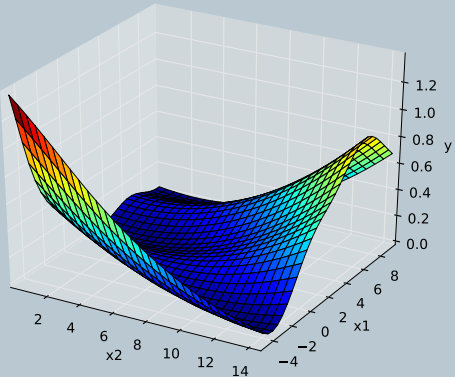
- To estimate the prognosis quality of the surrogate model,  $R_{pred}^2$  calculated via cross validation:

$$R_{pred}^2 = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - E(y_i))^2}$$

- Predicted vs. observed plot.
- Visual check of the model for example surface plot.
- Prediction of further test data.
- Uncertainty estimation of the prediction.

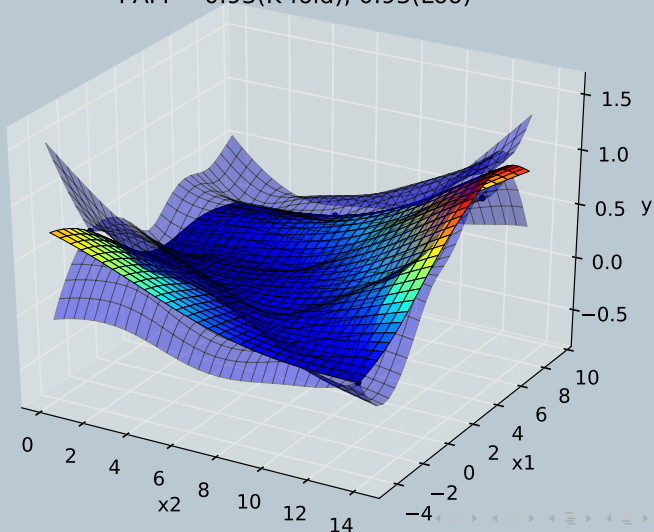
# Confidence intervals

- The framework provides the opportunity to give the confidence interval of its prediction.
- Model uncertainties can be visualized.
- Useful for sampling adaption strategies and surrogate based robust / reliability analysis.
- Example: Branin function



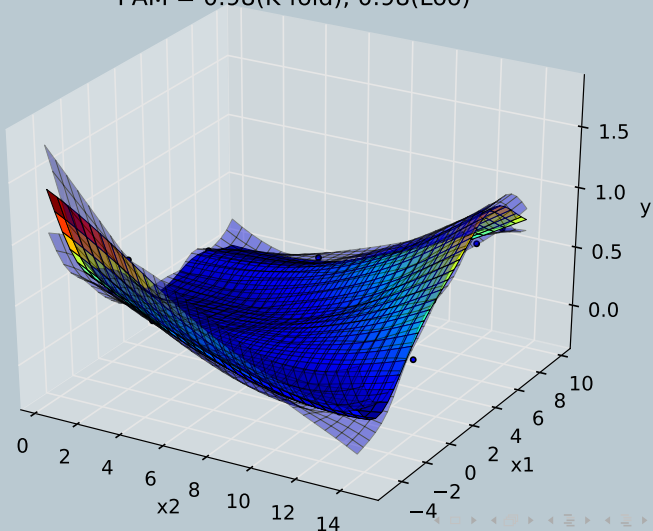
# 16 samples with 95% confidence intervals (1/3)

Metamodel Surface Plot of  $y$   
PAM = 0.93(K-fold), 0.93(Loo)



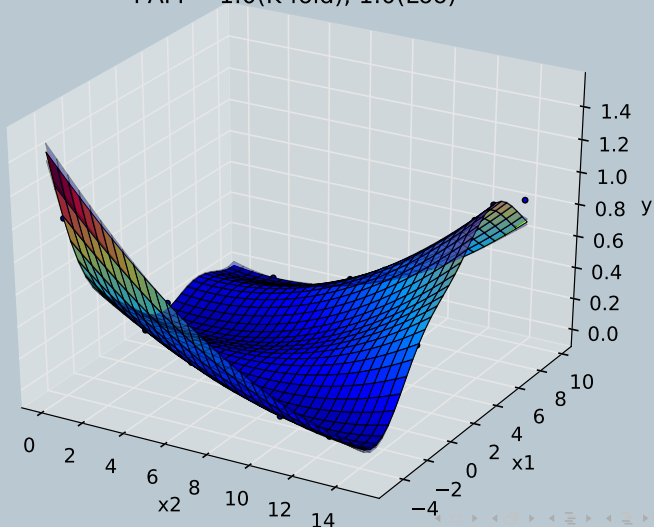
## 32 samples with 95% confidence intervals (2/3)

Metamodel Surface Plot of  $y$   
PAM = 0.98(K-fold), 0.98(Loo)



## 64 samples with 95% confidence intervals (3/3)

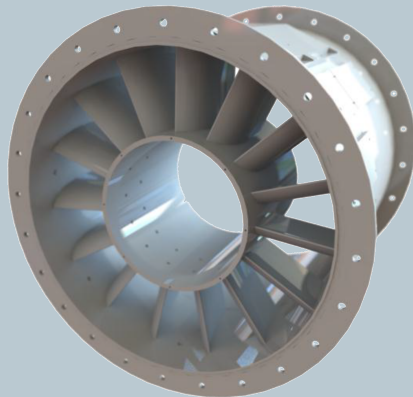
Metamodel Surface Plot of  $y$   
PAM = 1.0(K-fold), 1.0(Loo)



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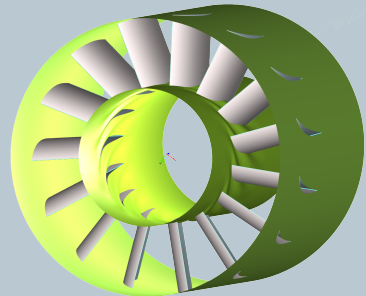
# Application

- The "TurboLab Stator" is a stator in a measurement rig at the TU Berlin.
- An initial stator geometry has been designed based on a representative stator geometry.
- The task is to reduce the total pressure loss and to minimize the flow angle deviation at the outlet over an incidence range.
- 3 operation points (inlet flow angle varies  $\pm 5^\circ$ ).



# Parametric model

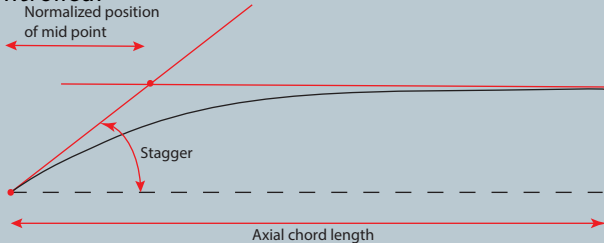
- CAD tool CAESES.
- Overall 73 input parameters:
  - 5 profile sections.
  - 28 main parameters (stagger angle, camberline, thickness).
  - 6 stacking parameters.
  - 31 tuning parameters (thickness tuning).
  - 8 endwall contouring parameters (amplitude, position).





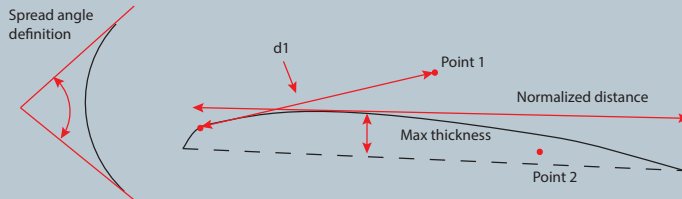
# Main parameters - Camberline / Stagger angle

- NURBS curve connects three points.
- Weight of the second point can be controlled.



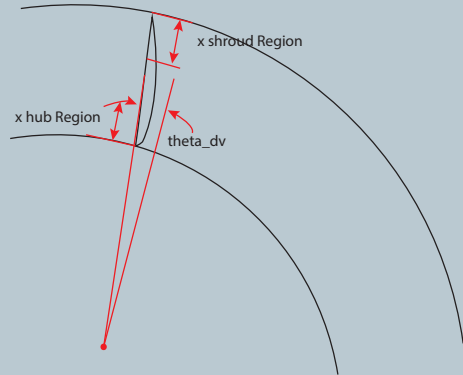
# Main parameters - Thickness

- LE, TE is given by radius , ellipse factor and spread angle.
- With LE angle the point 1 is created.
- With TE angle and the parameter TE Shape point 2 is created.
- NURBS curve connects LE with TE including point 1 and point 2.
- Distance d1 to point 1 is optimized internally to get a maximum thickness.



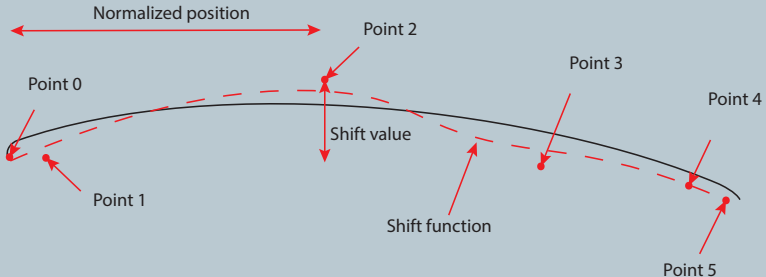
# Stacking parameters

- Stacking axis is controlled by 4 points, which can be varied by its:
  - theta angle.
  - the distance of the mid points from inner and outer radii.



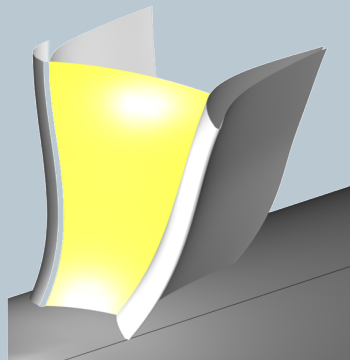
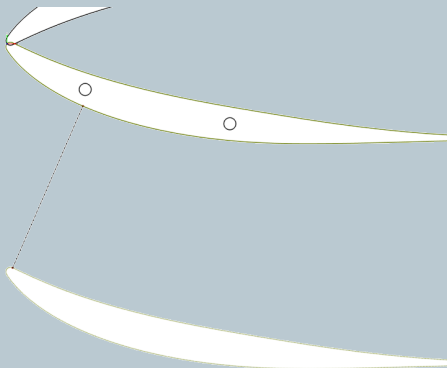
# Tuning parameters

- Shift function can shift the thickness distribution in x and y direction.



# Throat optimization

- In order to place the throat at the leading edge of the profile, the spread angle of the leading edge is optimized internally.



# Endwall contouring - Trigonometric approach

- Crosssection of endwall for one blade passage is represented by sine function, controlled by:
  - Frequency.
  - Amplitude.
  - Phase shift.
- Functions control how these parameters change in streamwise direction.

# CFD setup / Constraints

- CFX solver.
- Meshing in ICEM.
- Spalart-Allmaras turbulence model.
- Scalable wall function.
- 3 operation points with  $37^\circ$ ,  $42^\circ$ ,  $47^\circ$  inlet whirl angle.
- Specific heat coefficient of 1.4.
- Inlet total pressure: 102713.0 Pa.
- Inlet total temperature: 294.314 K.
- Inlet pitch angle:  $0^\circ$ .
- Inlet turbulence intensity: 4%.
- Outlet massflow of 9.0 kg/s (full annulus).

# Process chain



- Creates geometry
- Export .ttin file for ICEM
- Controls DoE work-flow
- Check manufacturing constraints.

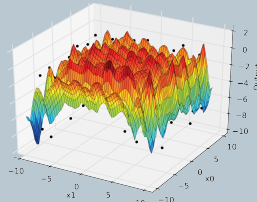
Design



- ICEM creates mesh
- 3 load cases in CFX
- Calculate objectives

Data for  
surrogate model

Input



Output

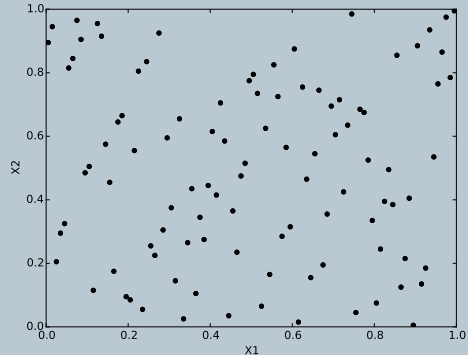
Optimal design

Optimizer

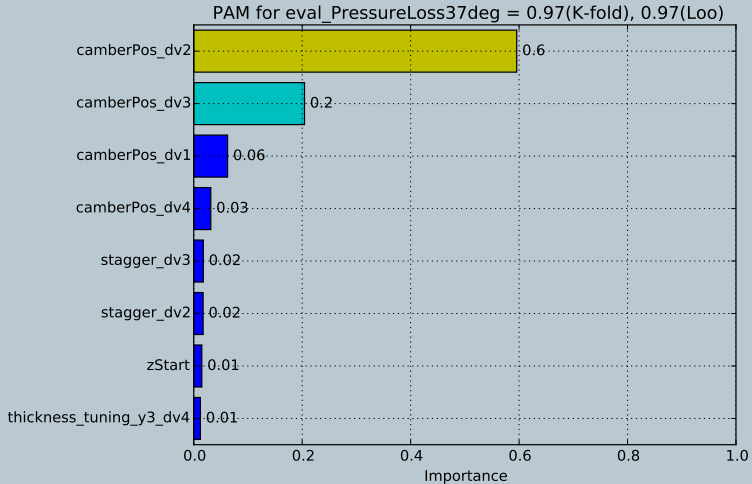


# Design of experiment

- Pre studies within CAESES to check geometry stability (no calculations on CFX).
- Starting around  $\pm 20\%$  of the initial blade geometry for the parameters (if possible).
- Final DoE with overall 80 designs (73 input parameters) calculations with optimized LHS.

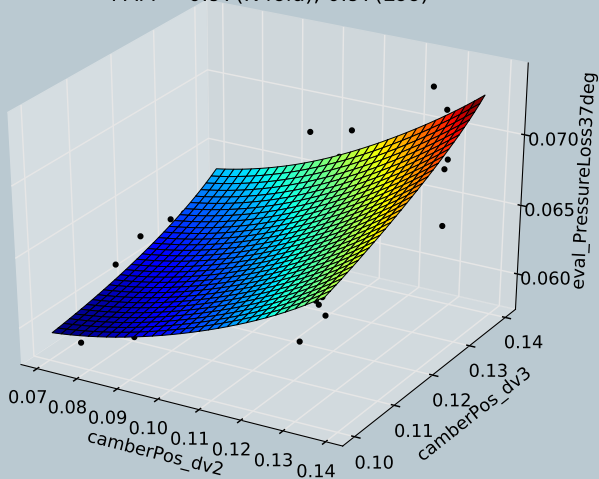


# Sensitivity - pressure loss 37°



# Sensitivity - pressure loss $37^\circ$

Metamodel Surface Plot of eval\_PressureLoss37deg  
PAM = 0.97(K-fold), 0.97(Loo)



# Optimization objective

Two optimization criteria, leading to a multi-objective optimization problem. In addition three operating points have to be considered:

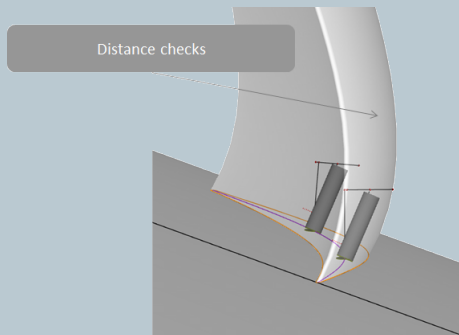
- Minimize the total pressure loss between inlet and outlet under the constraint of keeping the mass flow at  $9.0 \pm 0.1$  kg/s (full annulus). The total pressure loss is defined as
$$loss = \frac{p_{total_{in}} - p_{total_{out}}}{p_{total_{in}} - p_{static_{in}}}.$$
- Minimize the flow angle deviation at the CFD outlet from the axial direction.
- The inlet whirl angle is allowed to vary by  $\pm 5^\circ$ . Thus three operating points have to be considered.

# Optimization constraints - Manufacturing constraints

- The number of blades is fixed to  $n = 15$ .
- The axial chord of the blade has to be kept constant.
- The minimum value for leading and trailing edge radius is 1mm.
- The two holes for the fixture in the middle of the blade have a radius of 2.5 mm and a depth of 20 mm. The blade thickness at these positions has to accommodate a cylinder of material with a radius of 5 mm and a depth of 20mm. The two holes have to be at least 60mm apart from each other.
- The blade has to be mountable on a plate of dimensions 200mm x 80 mm.
- The reduction of radius due to the hub contouring has to be  $\leq 5\text{mm}$  and the increase of the radius due to the hub contouring has to stay below 10mm.

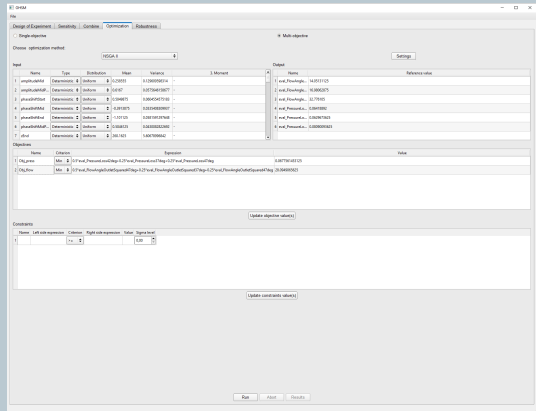
## Constraints - Drilling clearances - drilling angle

- After the position is obtained, the drilling angle will be optimized, to avoid an intersection of the drilling with the blade surface.
- Drilling angle is the difference angle to the normal, applied around the z-axis.

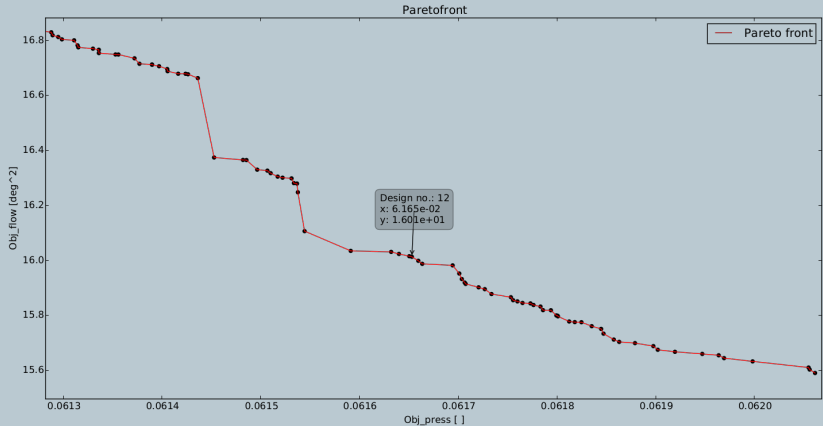


# Optimization on surrogate model

- NSGA II optimization algorithm.
- 300 generations, with 50 population size.
- 15000 overall design evaluations on surrogate model.
- 5 minutes on surrogate model against 625 days on CFX (32 cores per operation point).



# Multi-objective Pareto-front





# Results

## Recalculation chosen design

	Design point 42°	Off-design 37°	Off-design 47°
Total pressure loss (%)	6.09/6.16	5.95/6.13	7.05/7.39
Rel. error (%)	1.15	3.02	4.82
Exit whirl angle ( $deg^2$ )	14.98/15.44	12.63/12.95	27.28/27.78
Rel. error (%)	3.07	2.53	1.83

## Baseline vs. optimum objective function results

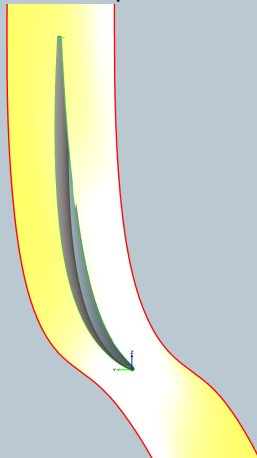
	Design point 42°	Off-design 37°	Off-design 47°
Improvement TPL(%)	5.23	2.85	5.98
Improvement EWA(%)	30.57	19.31	28.27

# Comparison: blade geometry - hub

Baseline



Optimum

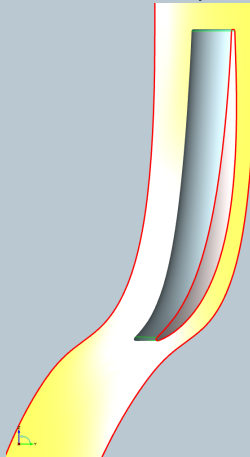


# Comparison: blade geometry - shroud

Baseline

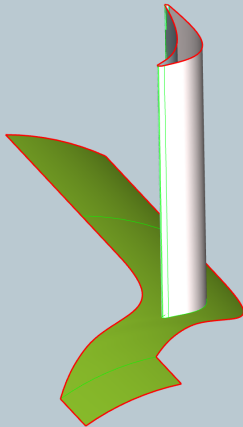


Optimum

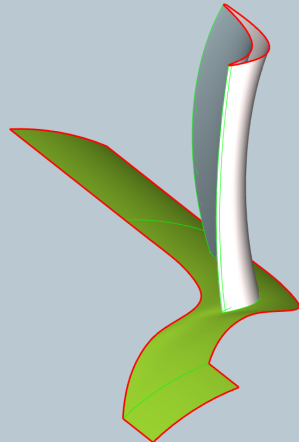


# Comparison: blade geometry - front

Baseline

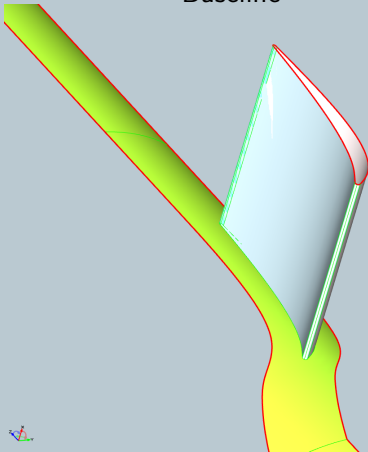


Optimum

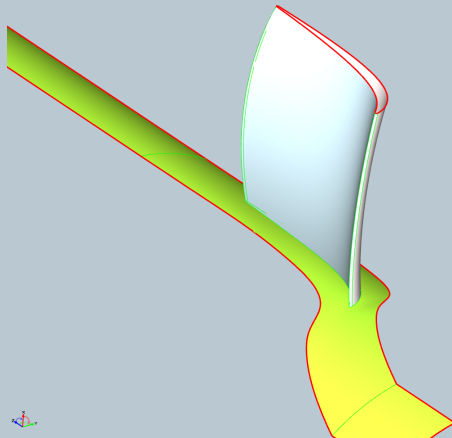


# Comparison: blade geometry -side

Baseline

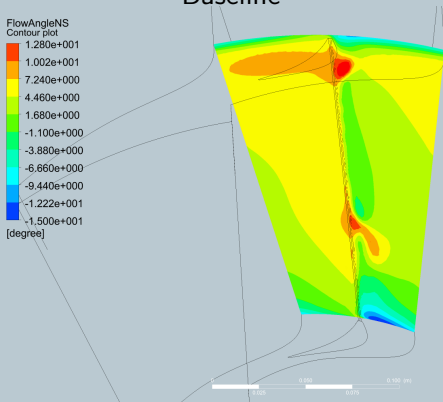


Optimum

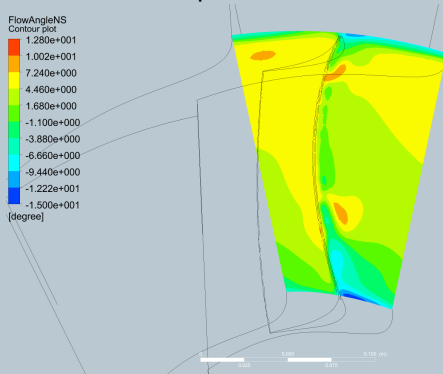


# Comparison: 2D field axial flow angle

Baseline



Optimum



# Summary

- Deep Gaussian covariance networks are capable to handle different type of problems with arbitrary size of data, with fast training times and high prognosis quality.
- Automatic variable selection and deeper knowledge of your data through sensitivity analysis.
- Multi-objective optimization application TU-Berlin stator with only 80 designs for 73 input parameters and 3 operation points.
- Good accuracy of surrogate model and efficient improvement for both objective functions of 4.86% for the pressure loss and 27.85% for the axial flow deviation.

