presented at the 17th Weimar Optimization and Stochastic Days 2020 |
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Recent Developments in Metamodeling, Optimization and Uncertainty Quantification

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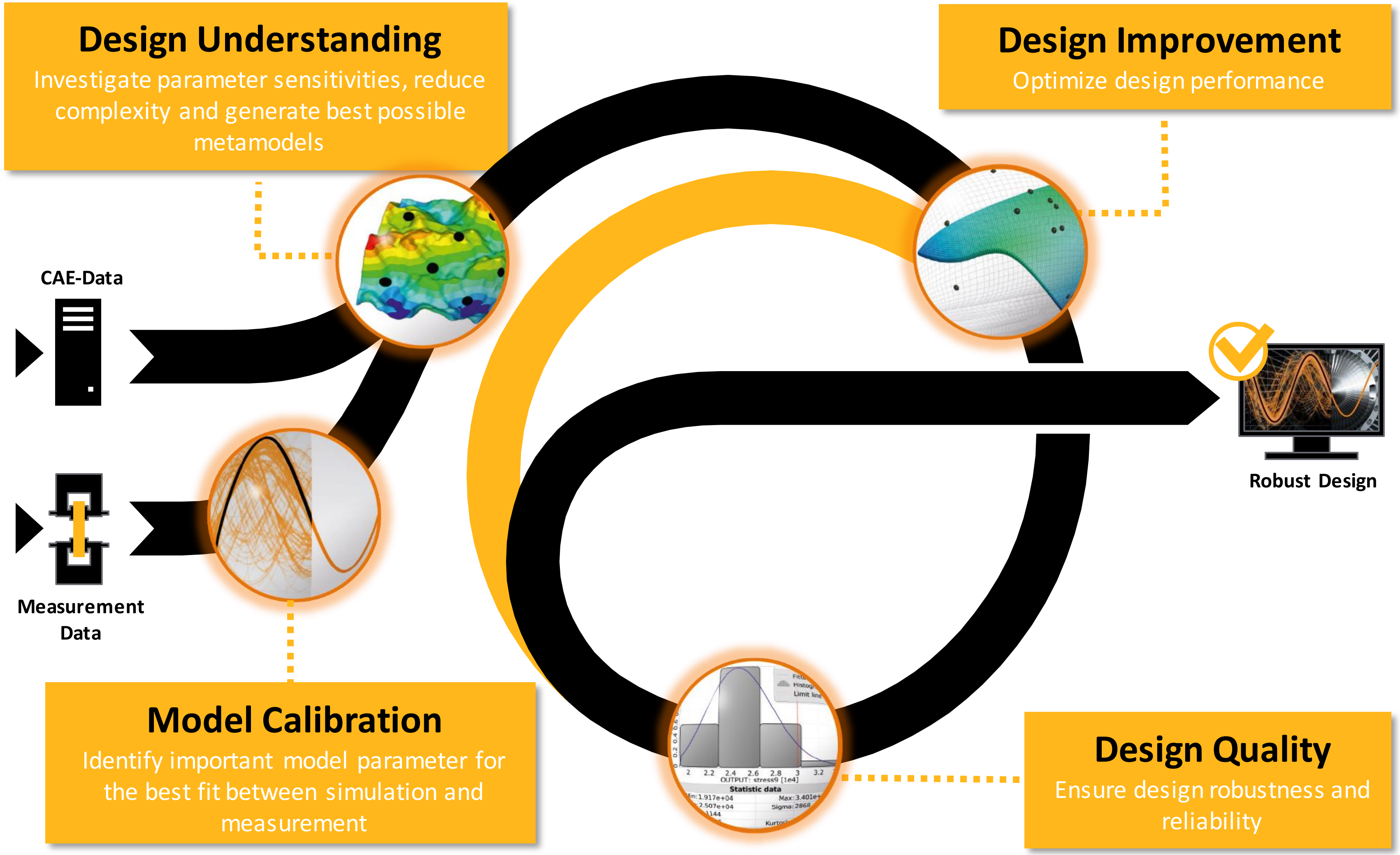
WOST 2020

Introduction Ansys optiSLang

Power of variation analysis - Best Practice Guideline for Virtual Product Development

- **Fit/calibrate** simulation and measurement data for model qualification
- **Understand your design** via optiSLang sensitivity module
  - Which parameters influence what?
  - Which constraints and goal conflicts I need to address?
  - Can I calibrate to measurements?
- Powerful metamodeling module
- Find the **best design** based on your goals and limitations
- Powerful **Robustness/Reliability**
- Enables customer to address Robust Design Optimization (RDO), Uncertainty Quantification (UQ), Design for Six Sigma (DfSS)



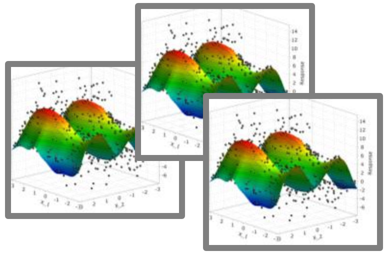
Sensitivity Analysis with Metamodel of Optimal Prognosis

Dynardo's metamodels: MOP – Metamodel of Optimal Prognosis

MOP for scalar values:

- Objective measure of prognosis quality = **CoP**
- Determination of **relevant parameter subspace**
- Determination of **optimal approximation model**
- Approximation of solver output by fast surrogate model **without over-fitting**
- Evaluation of **variable sensitivities**

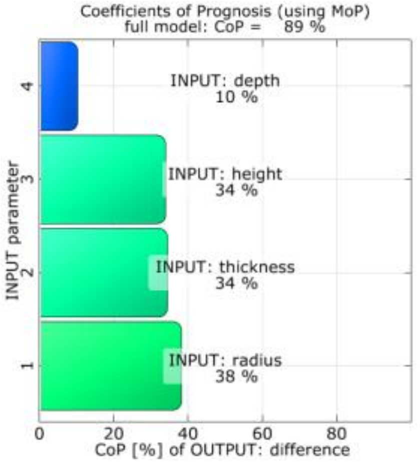
investigate response by response based on LHS sampling

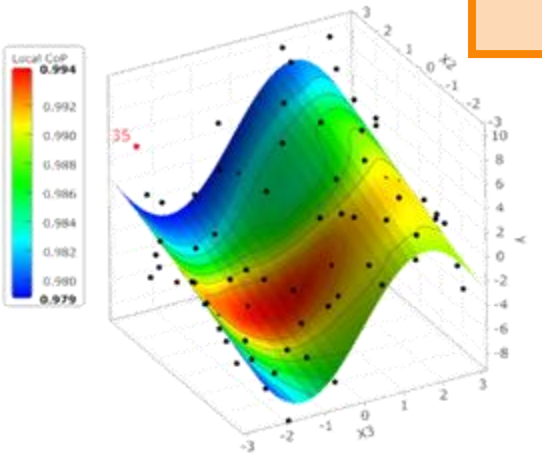


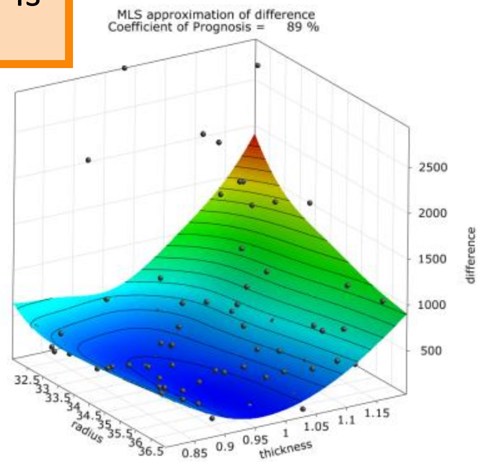
generate competing meta-models

calculate forecast quality using **CoP** (**C**oefficient **o**f **P**rognosis)

The winner is … **MOP**







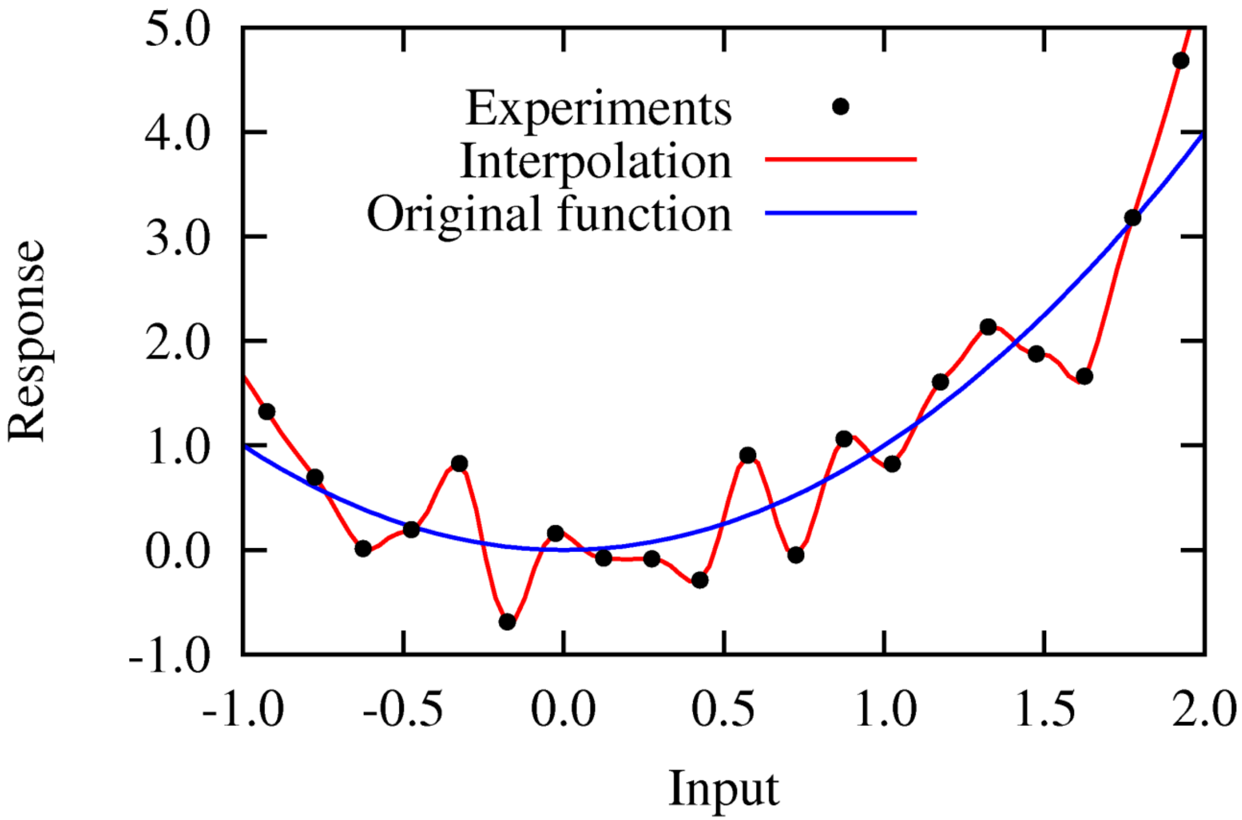
Measure Goodness of Fit = Coefficient of Determination (CoD)

- Coefficient of Determination quantifies merely the Goodness of Fit.
- Interpolation models (e.g. MLS, Kriging) can reach CoD of 1.00
- **But perfect fit does not mean perfect forecast quality!**

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

$$SS_E = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

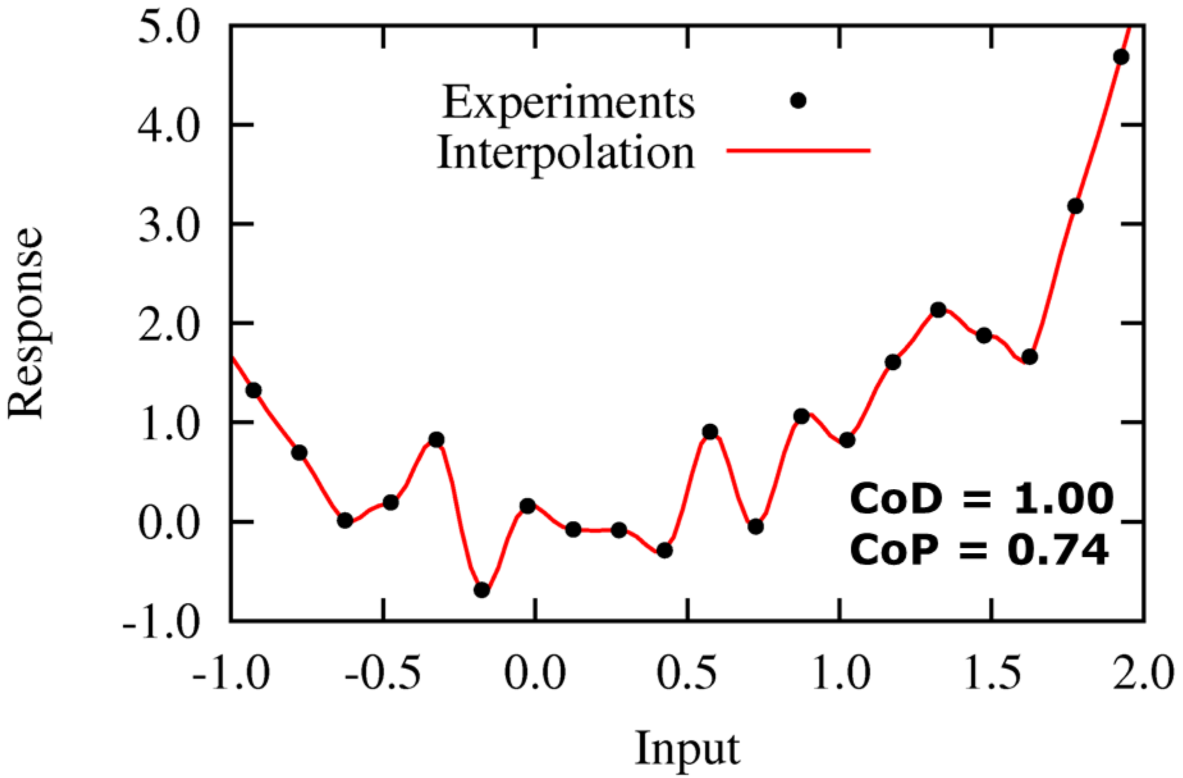
$$SS_T = \sum_{i=1}^{N} (y_i - \mu_Y)^2$$



Measure forecast quality = Coefficient of Prognosis (CoP)

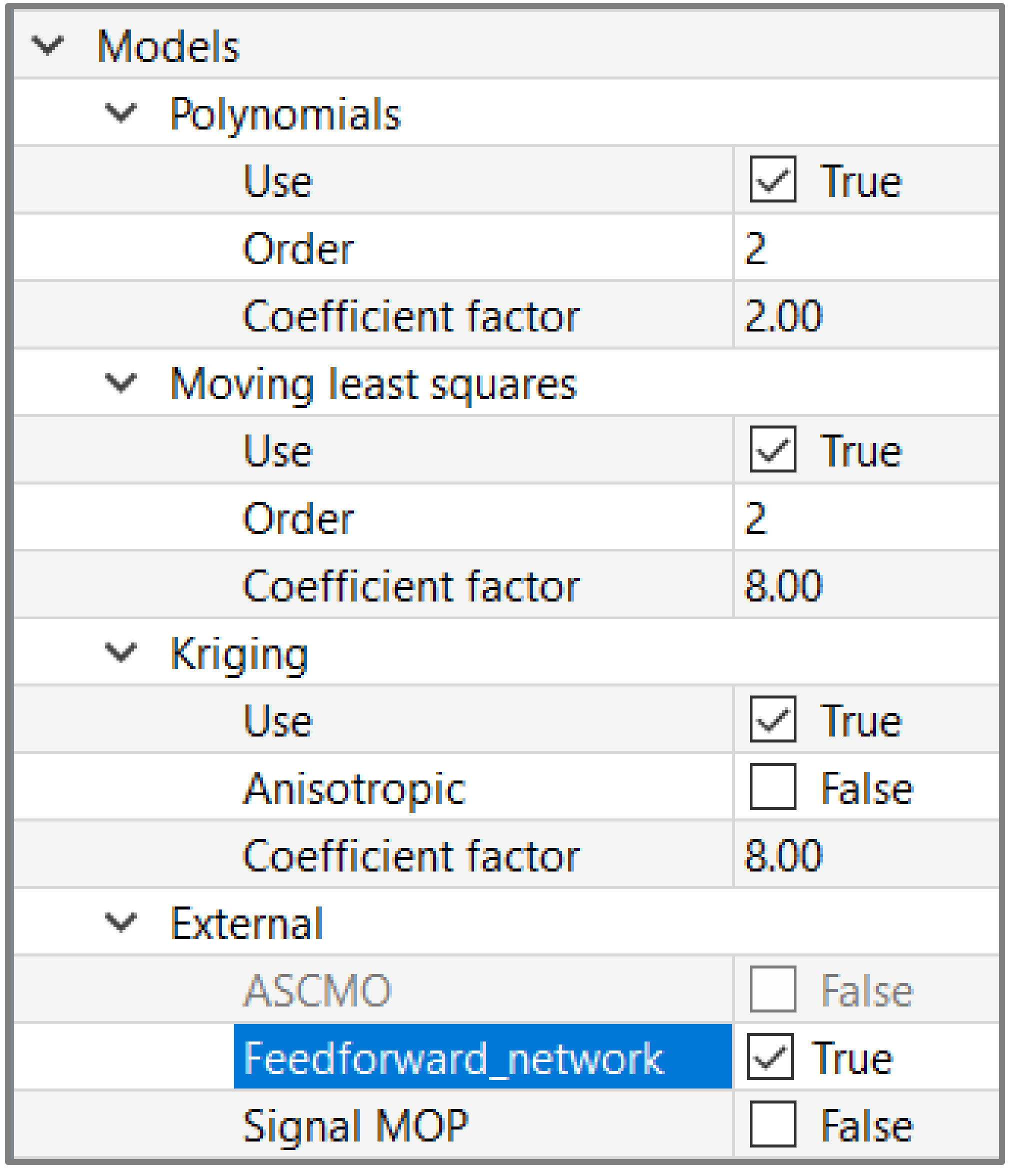
- Coefficient of Prognosis sums up the errors from both cross validation cases:
- **CoP is an objective measure of forecast quality.**

$$CoP = 1 - \frac{SS_E^{Prediction}}{SS_T}$$



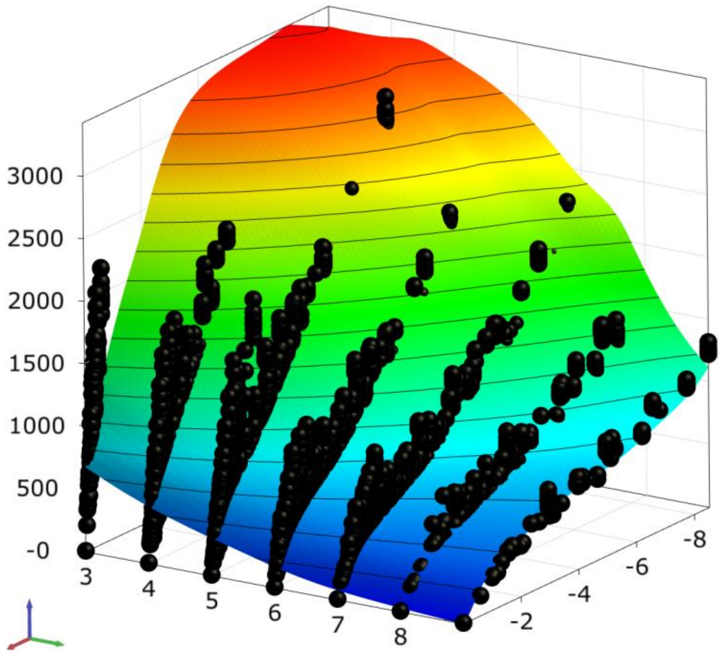
Approximation Models

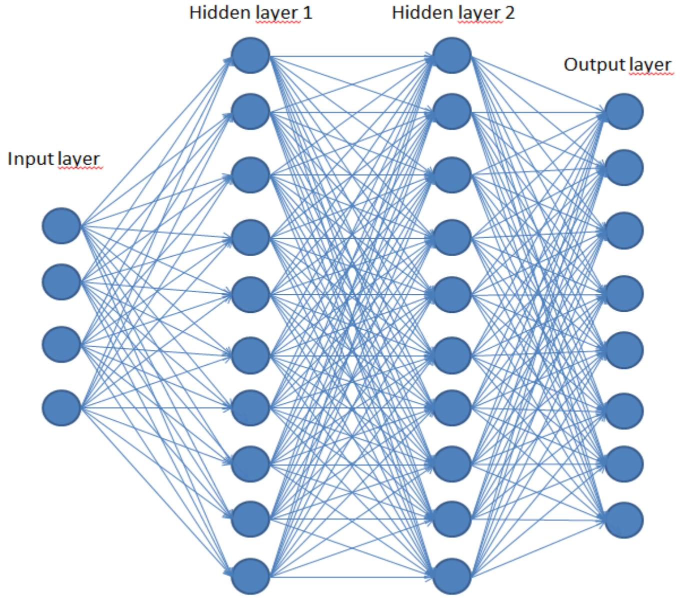
- **Polynomials - Linear Regression**
  - Linear & quadratic with/without mixed terms
- **Moving Least Squares**
  - Linear and quadratic basis
  - Exponential or regularized kernel
- **Kriging**
  - Isotropic & anisotropic kernel
- **Externals**
  - ASCMO
  - Neural networks (Tensorflow)
  - DX meta models (GARS, Support Vector Regression)



Deep Learning Extension

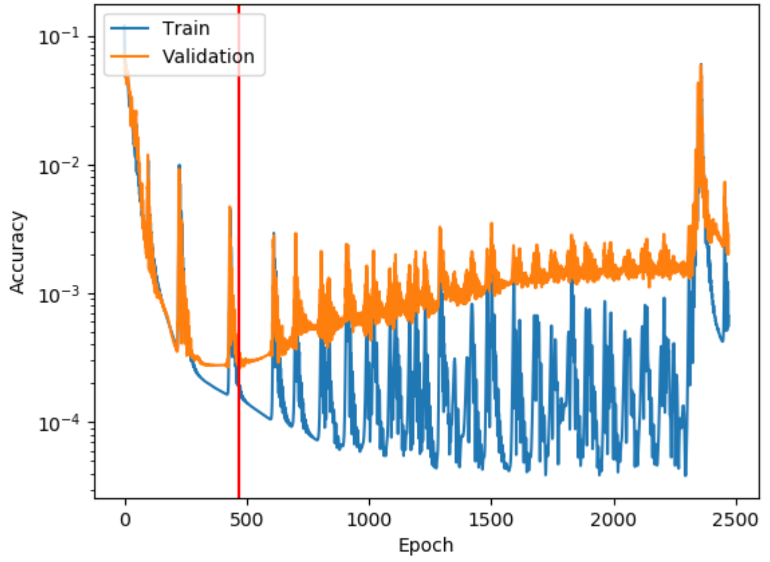
- Automatic configuration of neurons and layers
- Cross validation to estimate Coefficient of Prognosis
- Available as external python environment
- Neural networks are treated as one of a library of approximation models
- Competition is done in the MOP framework based on the CoP



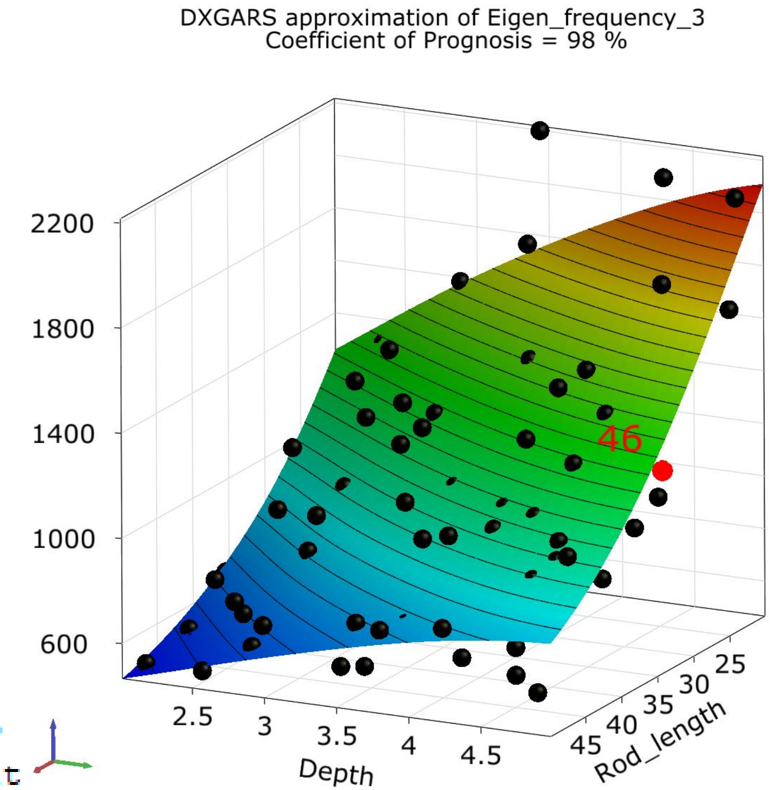


Deep Learning

K + TensorFlow



Integration of DX meta-models (2020 R2)



- Implementation of Python wrapper within custom surrogate
- Cross validation estimates have been verified
- ➢ DX models can be considered in the MOP competition

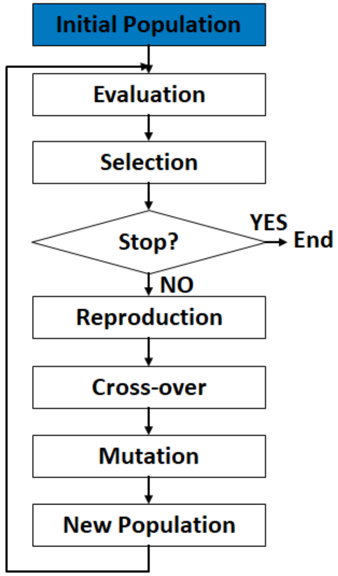
Response	CoD adjusted	CoP	Model
Eigen_frequency_1	0.841747	0.836	Linear Regression of order 1 (no
Eigen_frequency_1	0.955115	0.945973	Linear Regression of order 1 (wit
Eigen_frequency_1	0.984982	0.983589	Linear Regression of order 2 (with mixed terms, BoxCox)
Eigen_frequency_1	0.998362	0.973476	Moving Least Squares of order 1 (e
Eigen_frequency_1	0.999582	0.979185	Moving Least Squares of order 2 (e
Eigen_frequency_1	0.997524	0.988275	Kriging (isotropic kernel, BoxCox)
Eigen_frequency_1	0.998804	0.987579	Kriging (anisotropic kernel)
Eigen_frequency_1	1	0.980692	DXGARS
Eigen_frequency_1	1	0.980452	DXKriging
Eigen_frequency_1	1	0.921952	DXNPR
Eigen_frequency_1	0.998672	0.991904	Feedforward_network

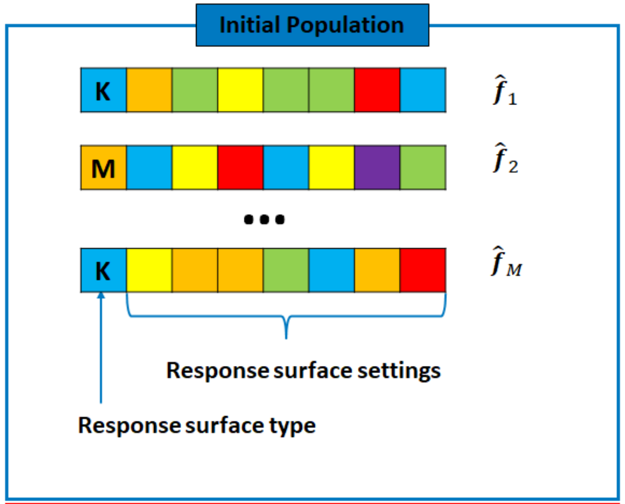
External	
ASCMO	False
DXGARS	True
DXKriging	True
DXNPR	True
DXPoly	False
Feedforward_network	False

DX Genetic Aggregation Response Surface (GARS)

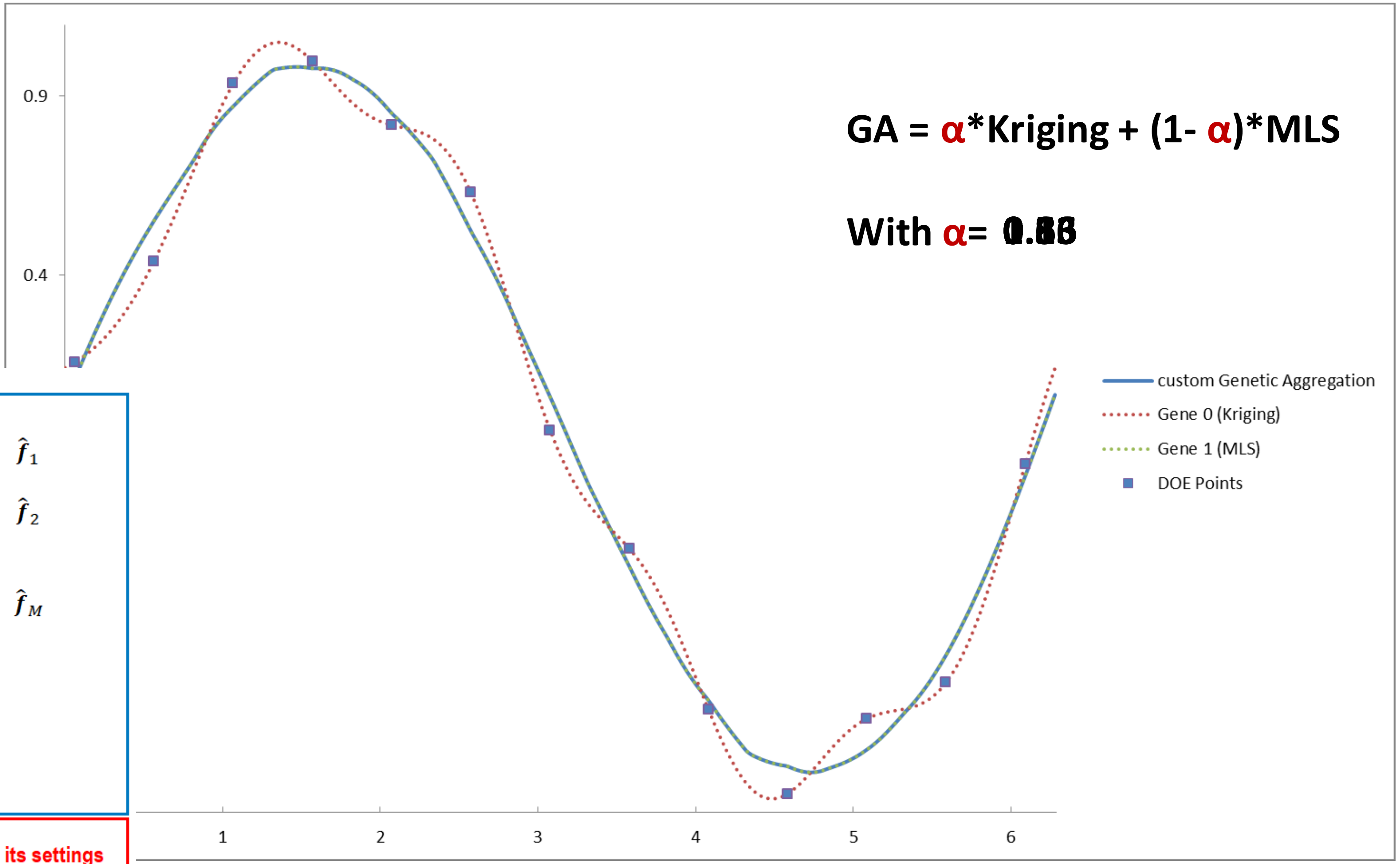
GA = α*Kriging + (1- α)*MLS

With α= [illegible]





1 individual = 1 Response Surface type with its settings



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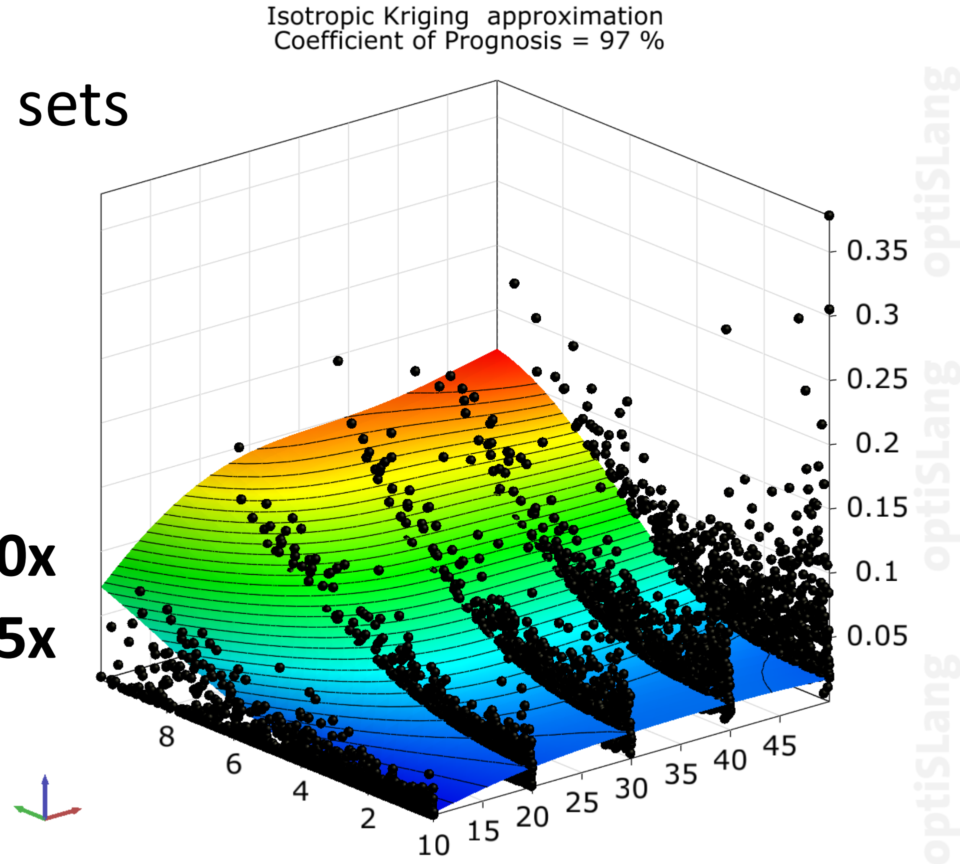
MOP Solver Performance (2020 R2)

➢ Significant improved performance for large data sets



Customer example 1

6000 data points, 7 inputs, 5 outputs

-	Load file	10 min -> 3 sec	**Speedup 200x**
-	Solve design	25 sec -> 0,2 s	**Speedup 125x**

Customer example 2

1500 data points, 22 inputs, 47 outputs

-	Load file	15 min -> 1 min	**Speedup 15x**
-	Solve design	20 sec -> 1,5 s	**Speedup 15x**

Single- and Multi-Objective Optimization

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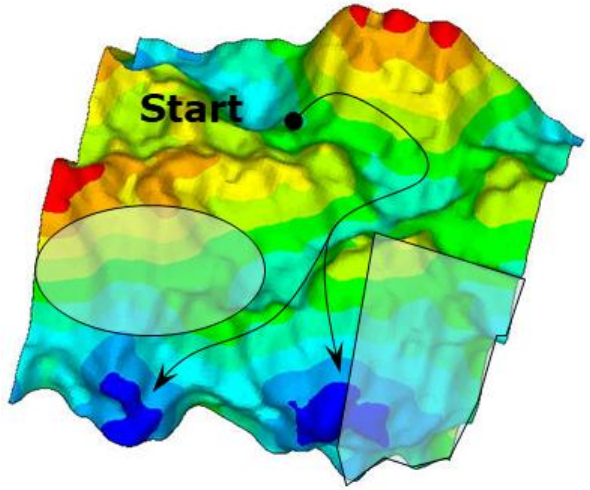
optiSLang Optimization Algorithms

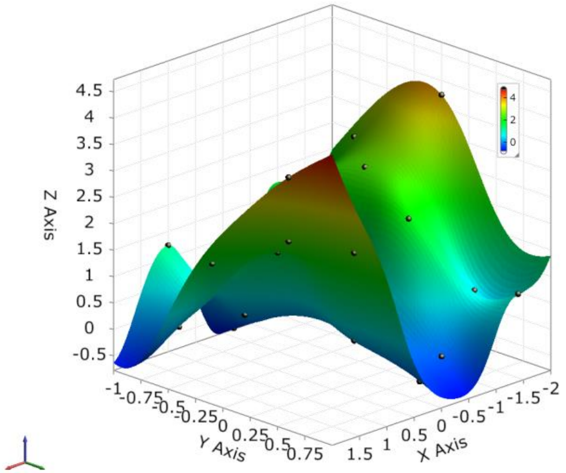
Gradient-Based Methods

- Clear favorite if objective function smooth and without local minima
- Repeated local search as strategy when there are few local minima



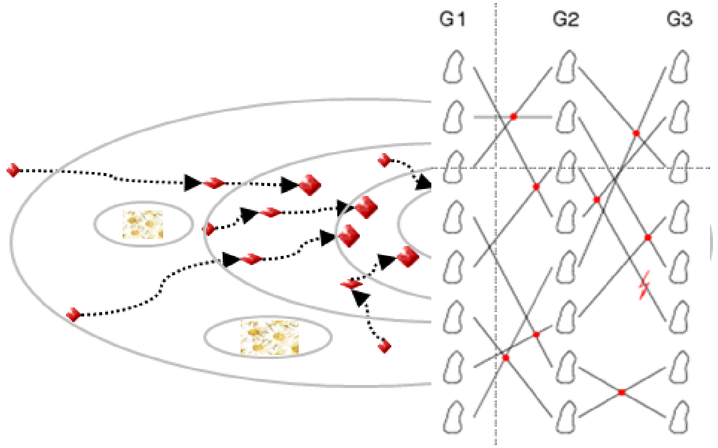
Adaptive Response Surface Method

- ARSM is the default choice
- Balance between robustness and efficiency
- Best if dimension<20



Nature-Inspired Optimization

- Recommended for global search
- Widest applicability (binary or discrete parameters, …)
- Realize optimization potential also in challenging situations



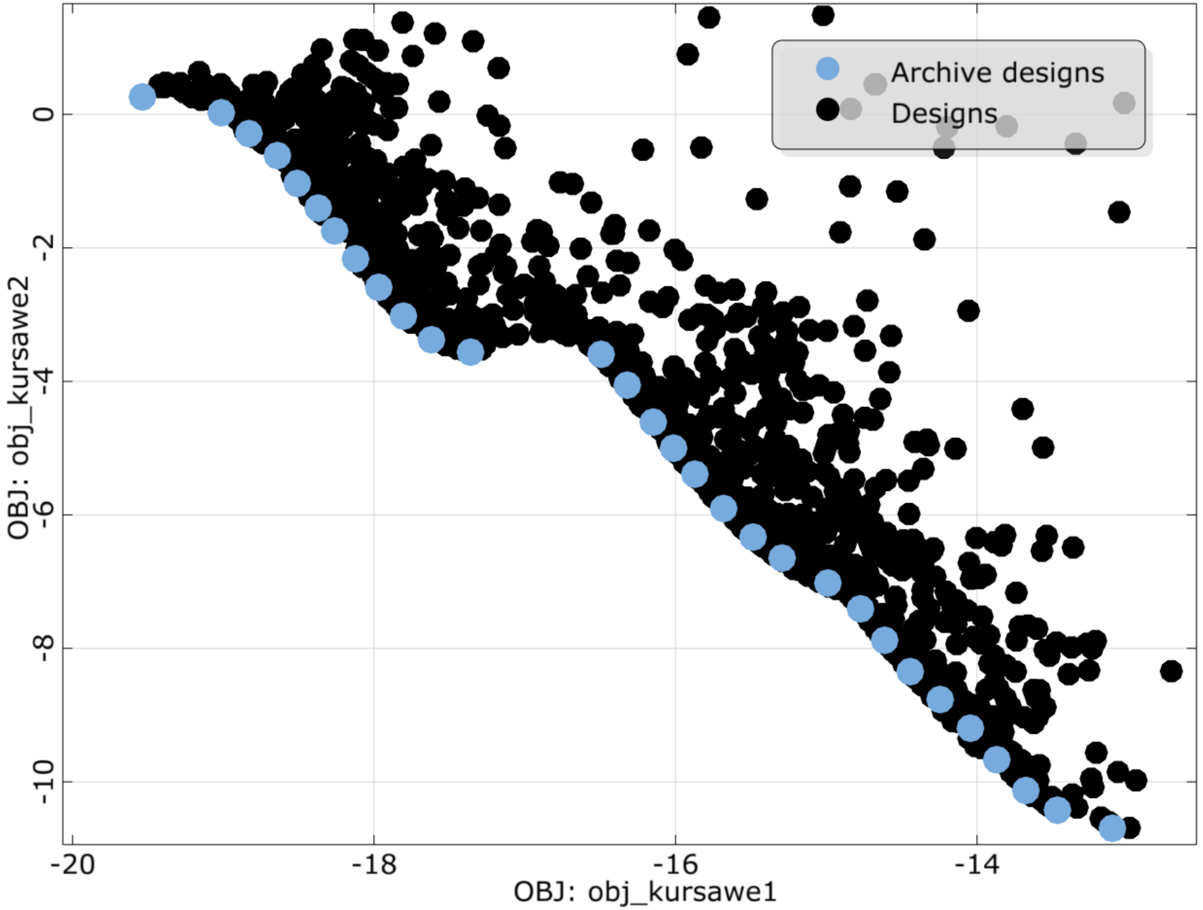
Nature Inspired Optimization – Next Generation (2020 R2)

Algorithms

- Evolutionary Algorithm
- Particle Swarm Optimization
- Stochastic Design Improvement
- Covariance Matrix Adaptation (2021 R1)

Fitness evaluation

- Penalty with **automatic scaling**
- Rank order approach for **large number of constraints**
- **Space-filling Pareto front** or weighted sum for multi-objective



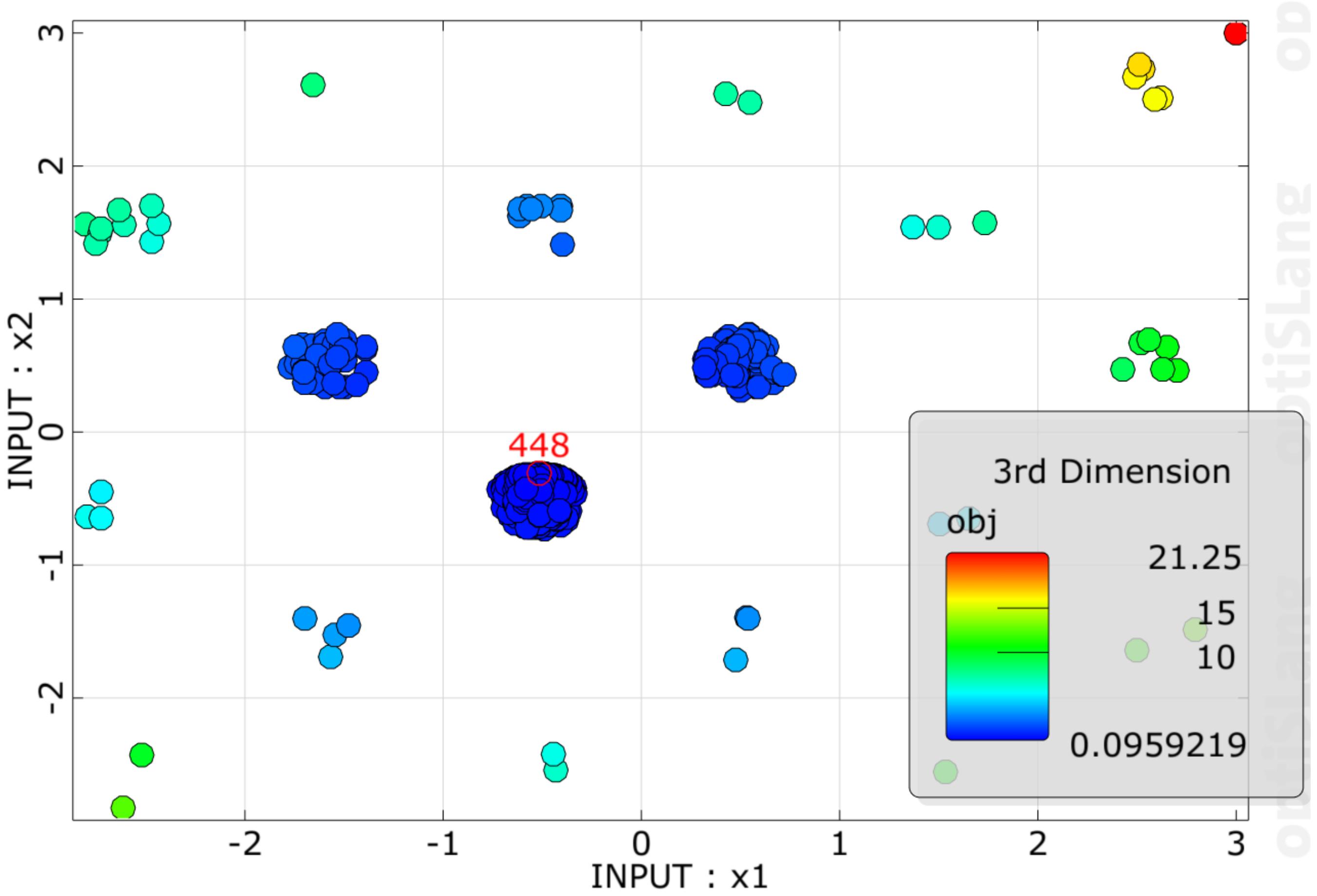
Nature Inspired Optimization – Next Generation (2020 R2)

Offspring generation

- **Avoid duplicated designs**
- **Consider input constraints**

- Classical crossover & mutation operators for EA

- Passive congregation (grouping behavior) and fly-back for PSO

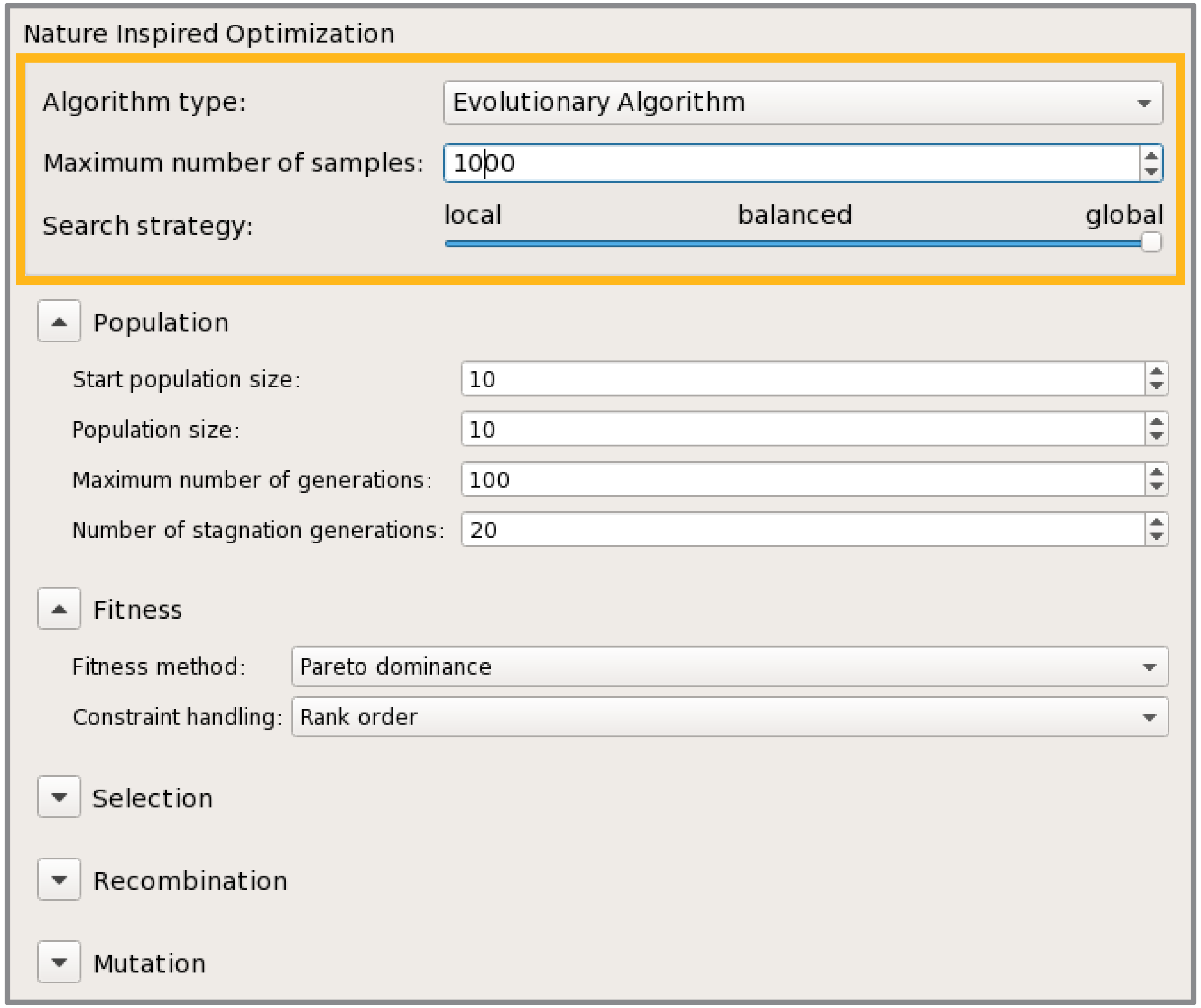


Nature Inspired Optimization – Next Generation (2020 R2)

Simplified settings

- **Definition of algorithm**
- **Number of designs**
- **Search strategy**

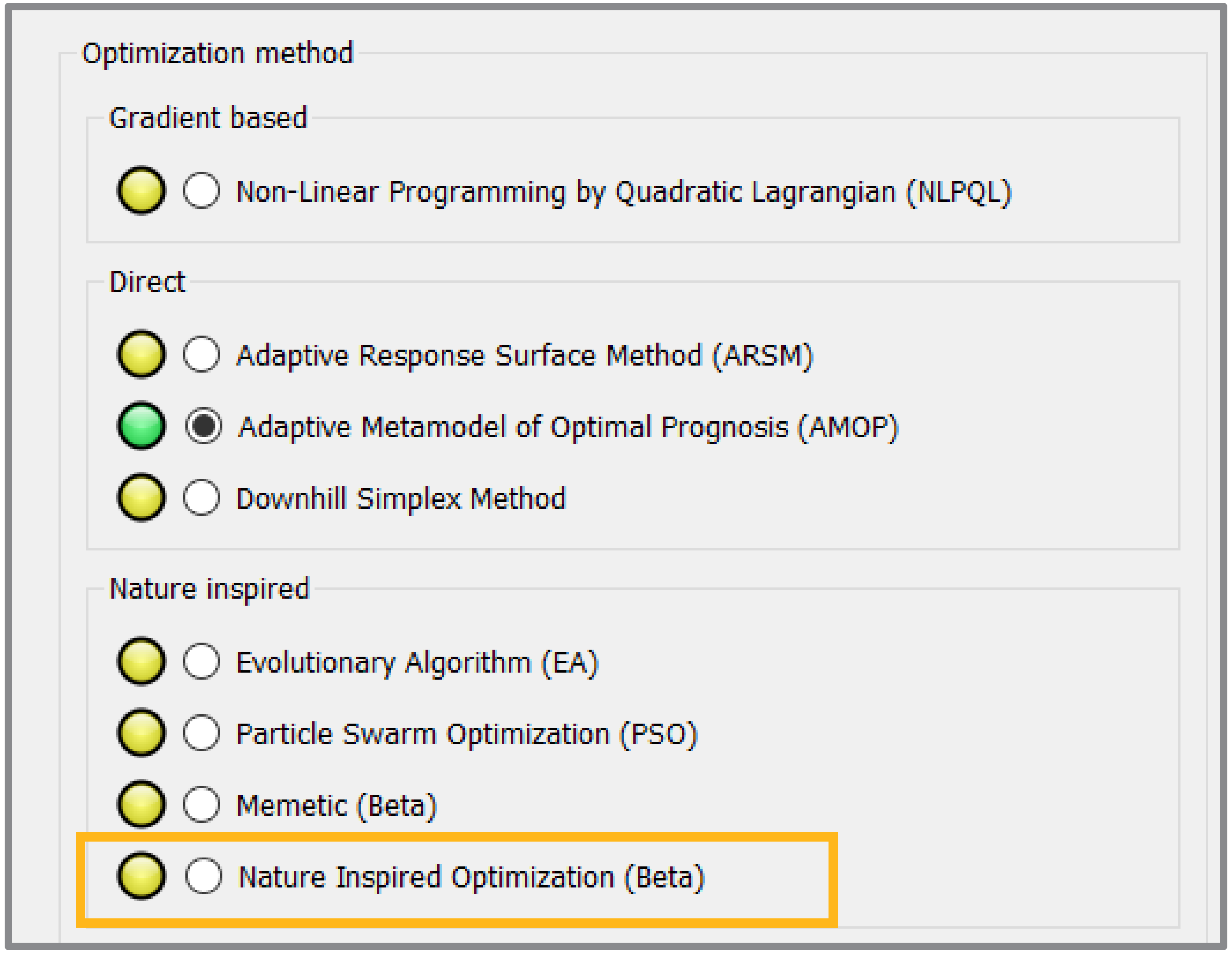
- Specific settings for EA, PSO operators are derived depending on number of inputs and optimization criteria



Nature Inspired Optimization – Next Generation (2020 R2)

Wizards

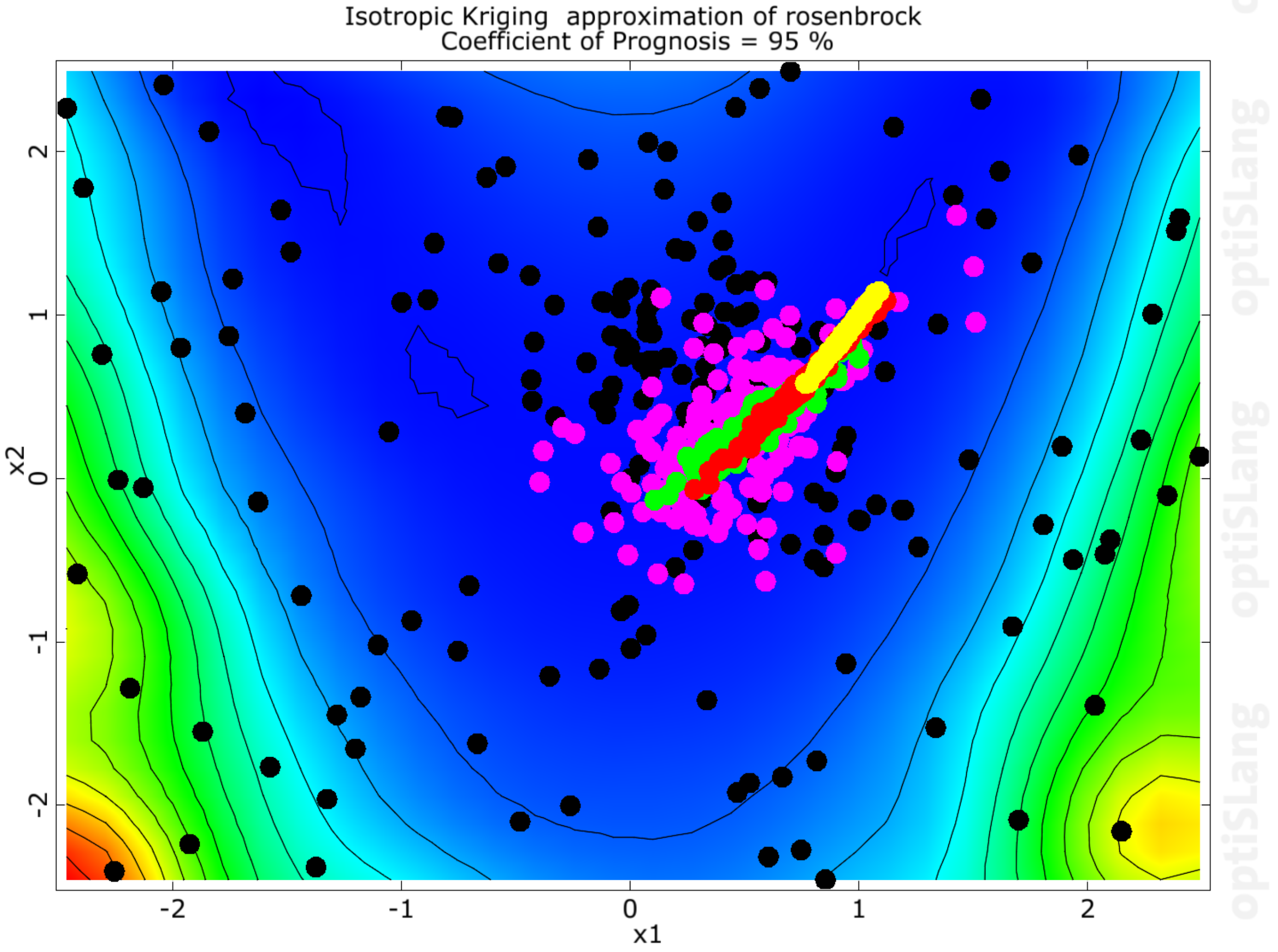
- Available in optimization wizard as beta feature in 2020 R2
- Replacing classical EA and PSO in 2021 R1



Nature Inspired Optimization – Next Generation

Outlook 2021 R1 - Covariance Matrix Adaptation

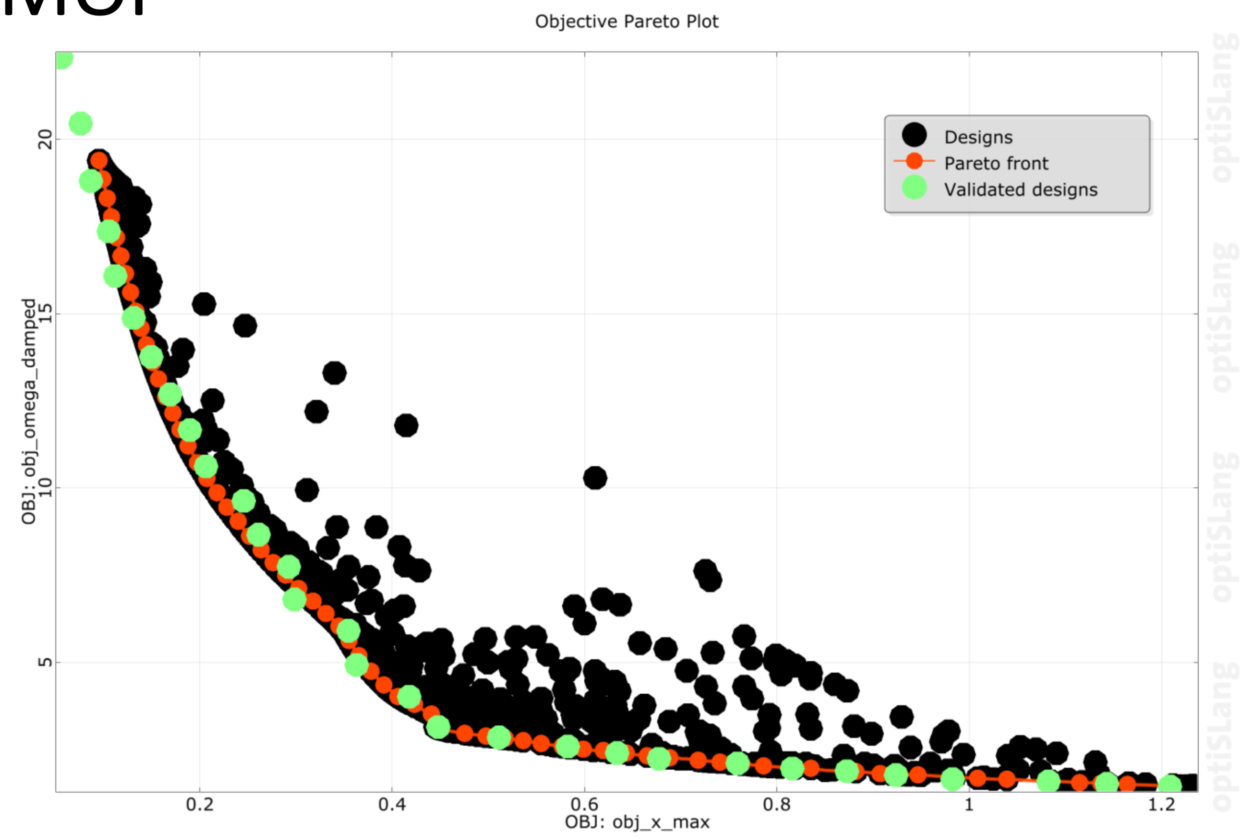
- Automatic adjustment of sampling/mutation density to objective and constraints

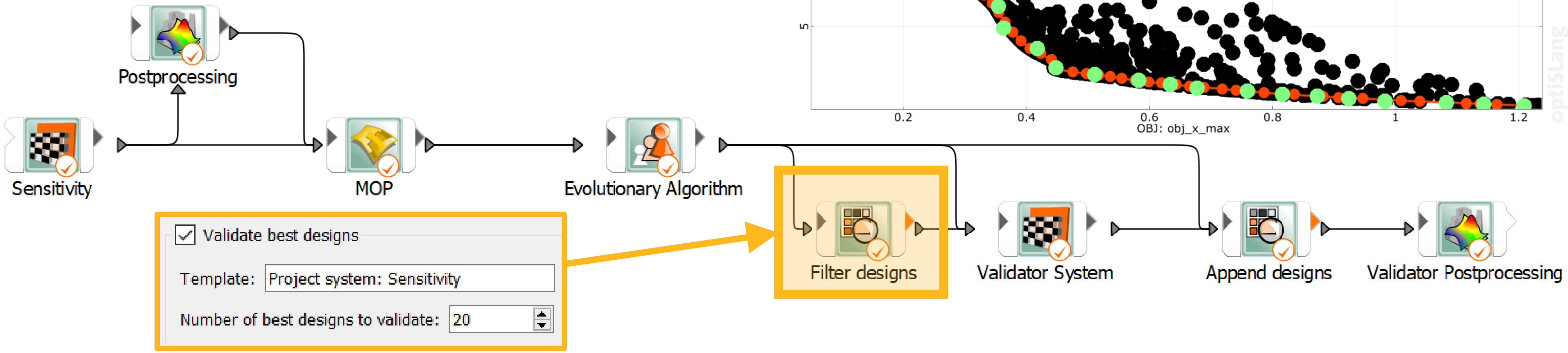


Multi-objective Optimization on MOP

Validation of Pareto frontier

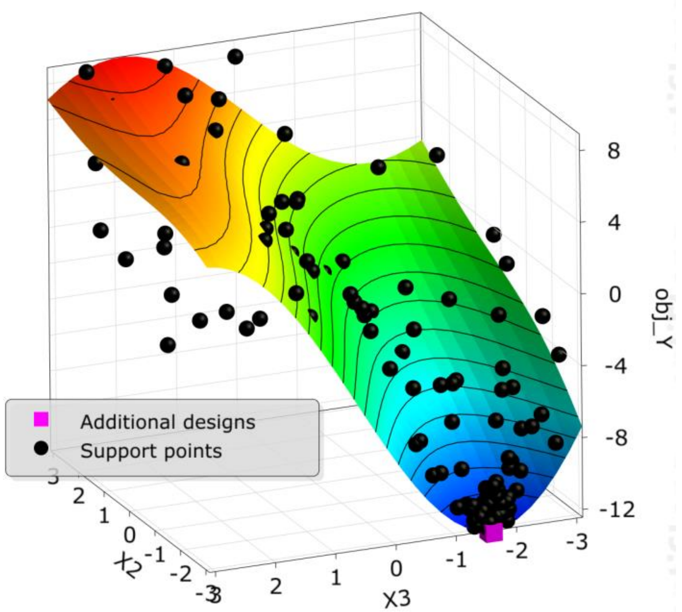
- Space-filling criterion to filter subset of well distributed Pareto optimal designs for validation

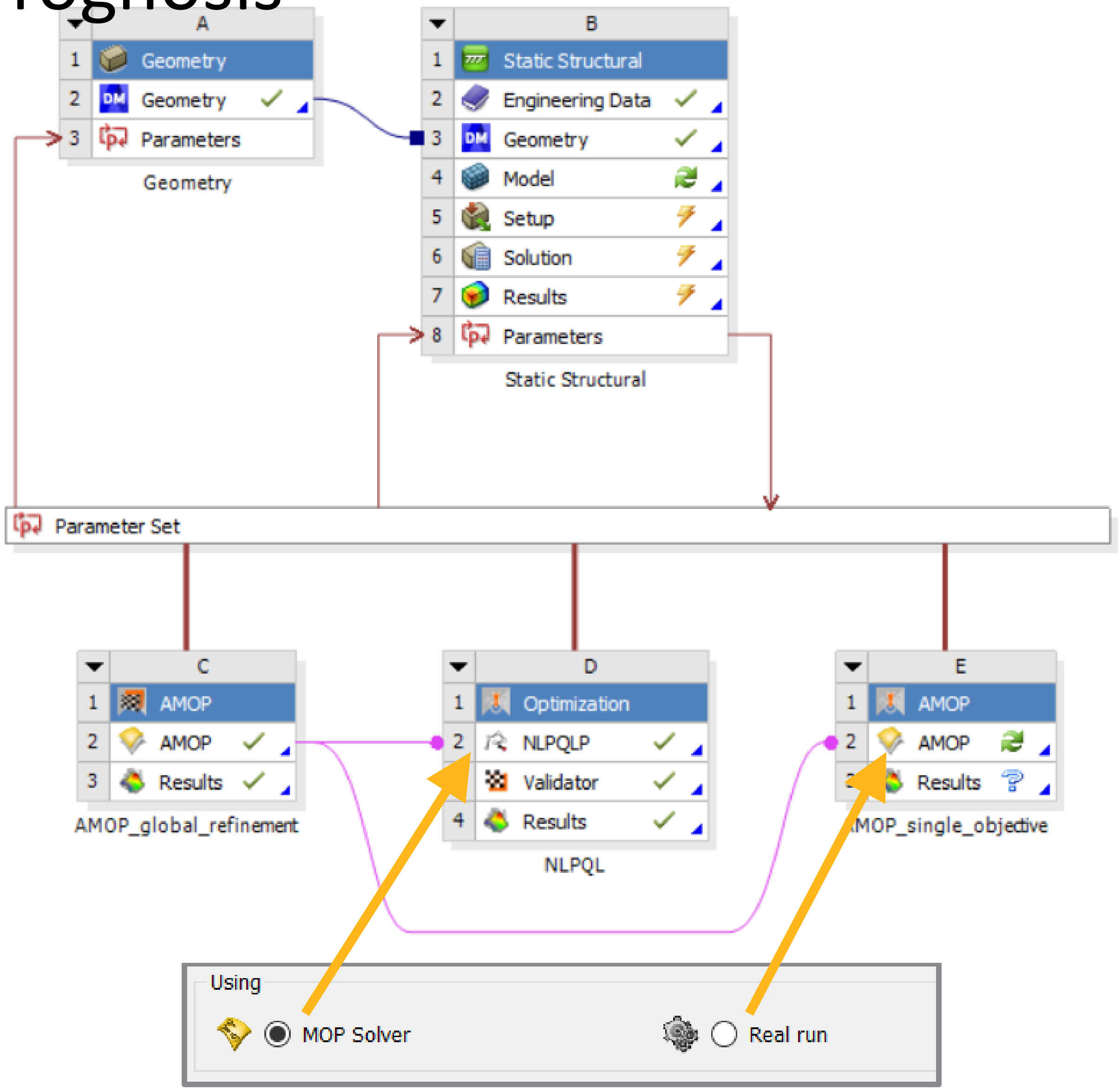




Adaptive Metamodel of Optimal Prognosis

- **2020 R2: Full featured availability in ANSYS Workbench extension**
- Optimization on Adaptive MOP meta-model as well as local refinement of existing meta-model by additional solver runs is possible

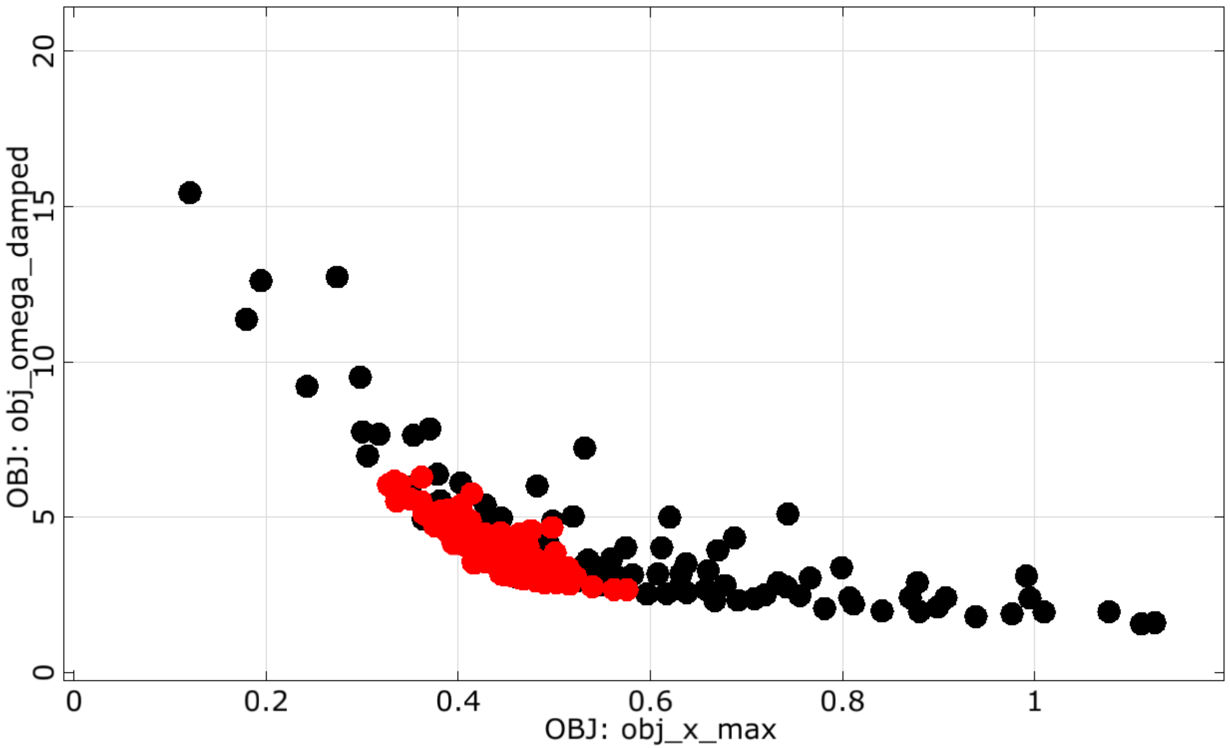




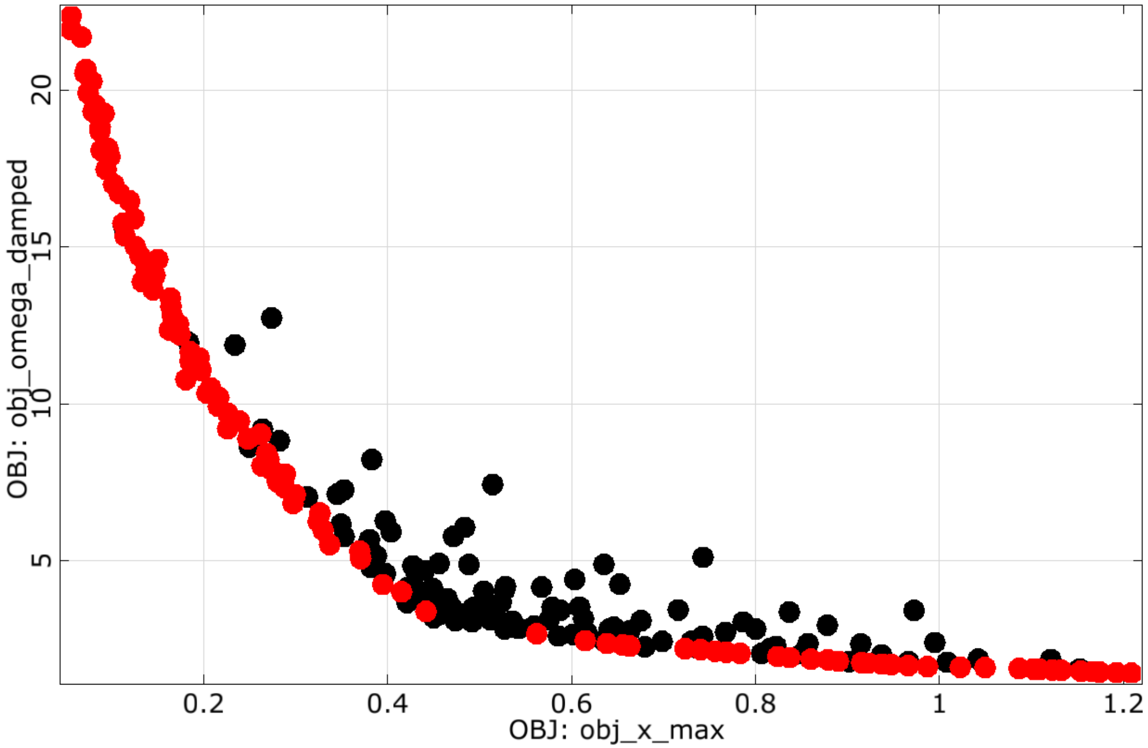
Adaptive Metamodel of Optimal Prognosis

Outlook 2021 R1: Extension of multi-objective refinement strategies

Expected improvement = Best compromise



Space-filling Pareto Optimality = Maximum spread of frontier



Uncertainty Quantification, Robustness and Reliability Analysis

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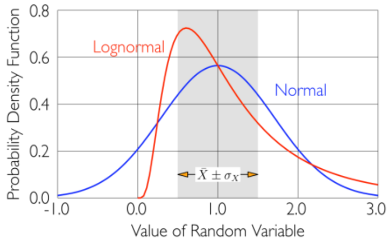
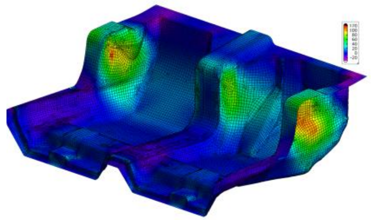
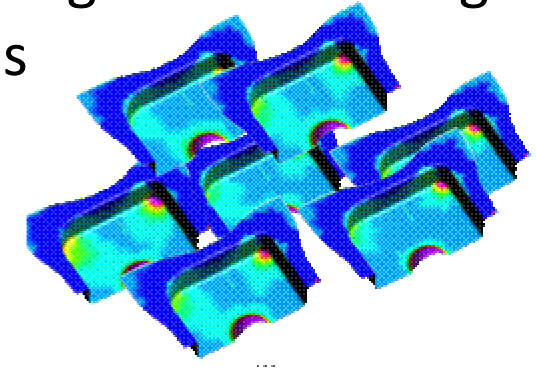
Variance based Robustness Analysis

1) Define the robustness space using scatter range, distribution and correlation

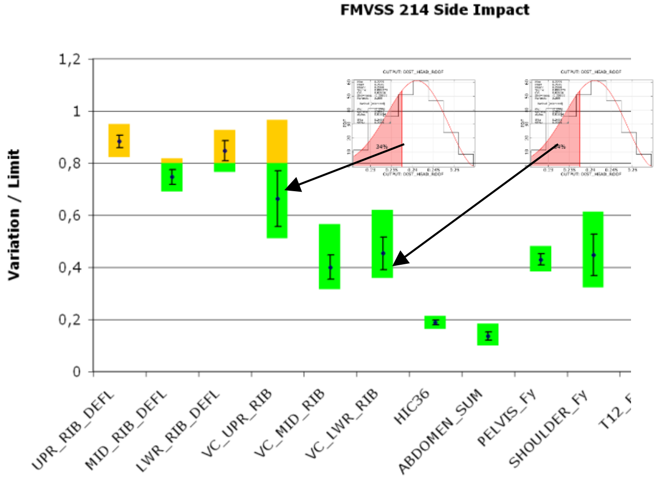




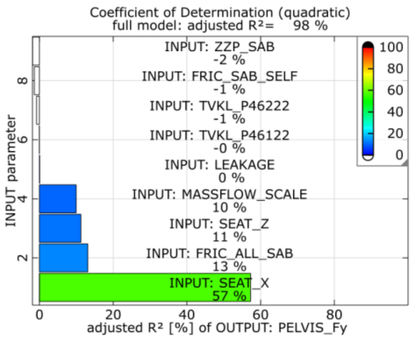
2) Scan the robustness space by producing and evaluating *n* designs



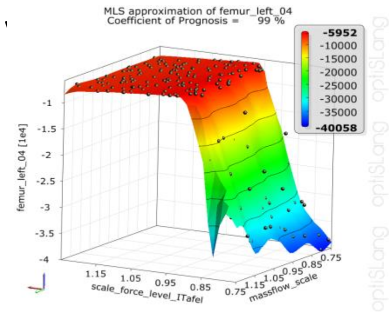
3) Check the variation



4) Check the explainability of the model



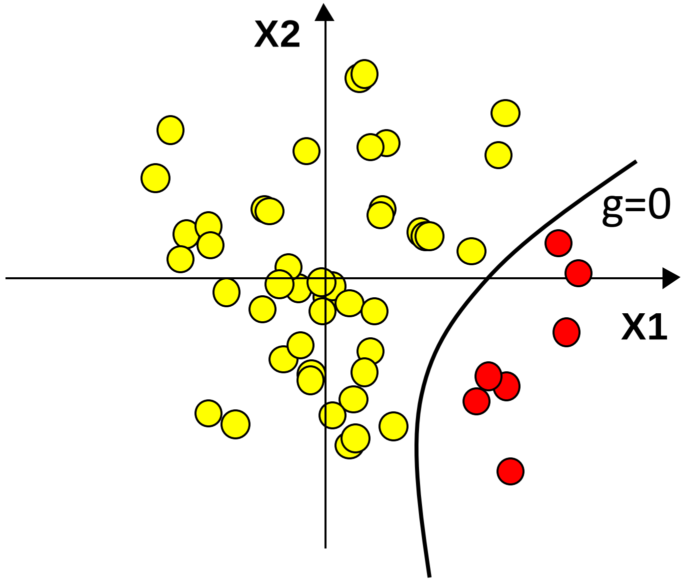
5) Identify the most important scattering



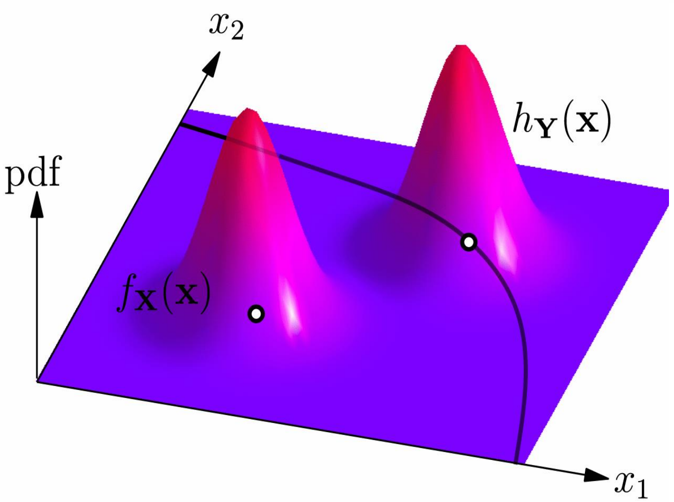
Reliability based Robustness Analysis

- ➢ Quantify rare event probabilities with minimum effort and maximum confidence

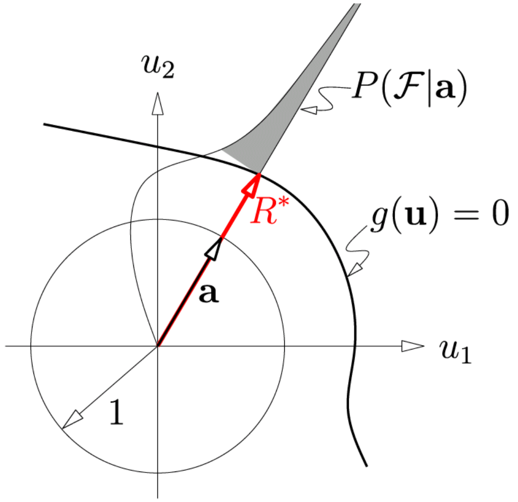
Monte Carlo Sampling



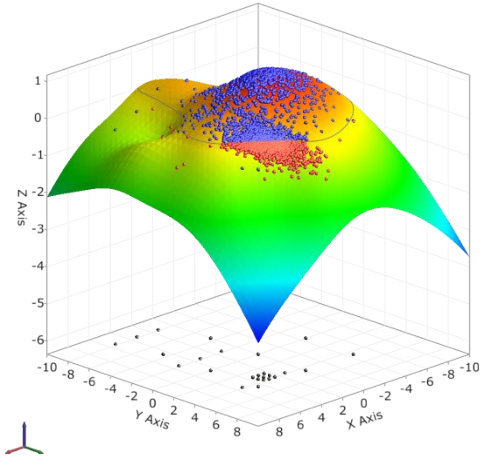
Importance Sampling



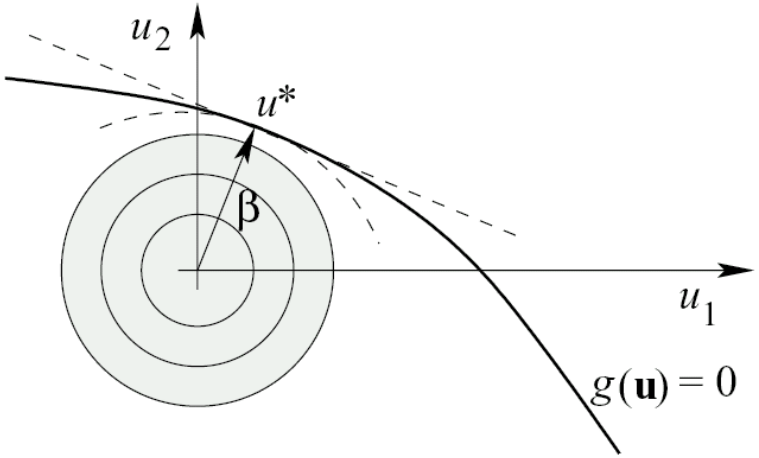
Directional Sampling



Adaptive RSM



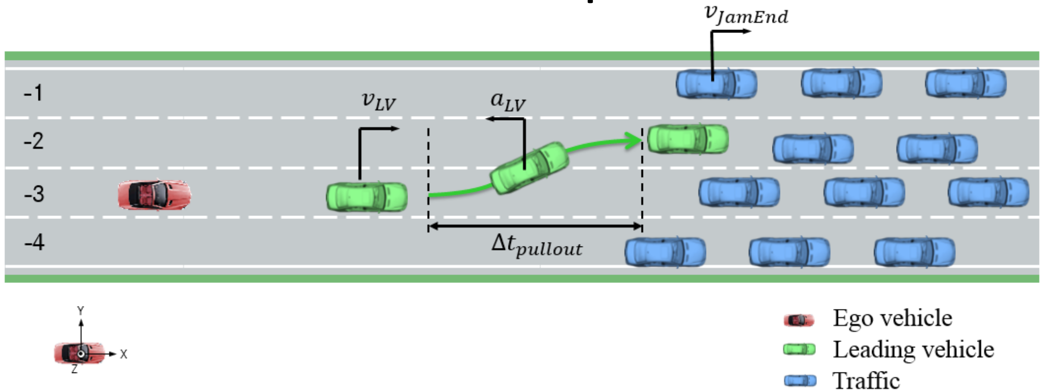
First Order Reliability Method



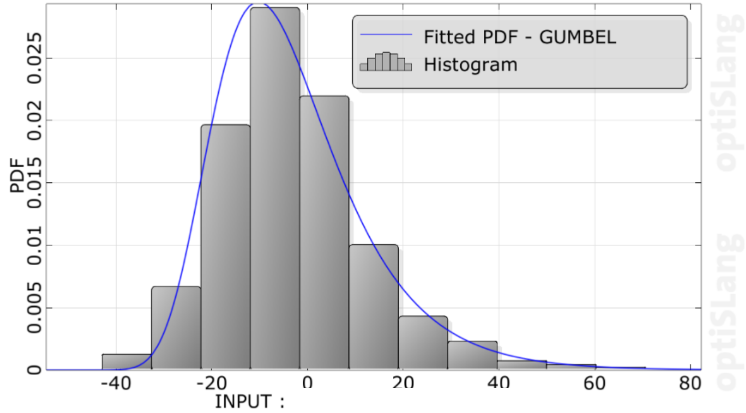
Reliability Analysis of Automated Driver Assistance Systems

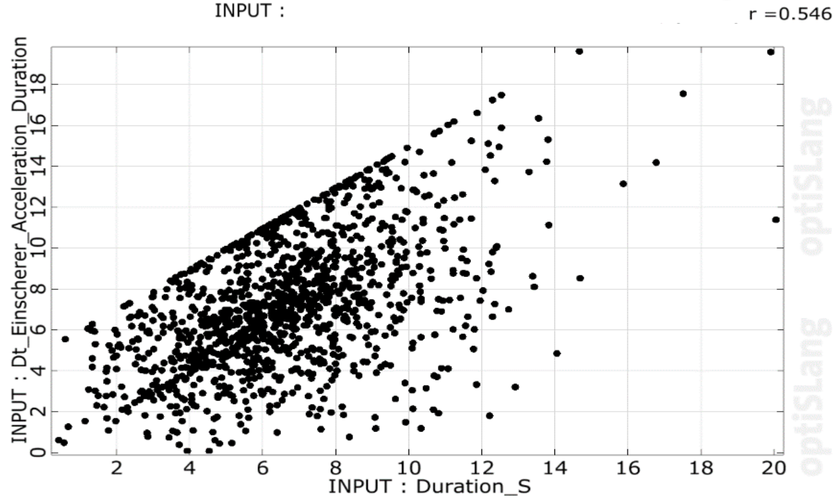
Scenario Definition & Parameterization

1. Define scenario parametric

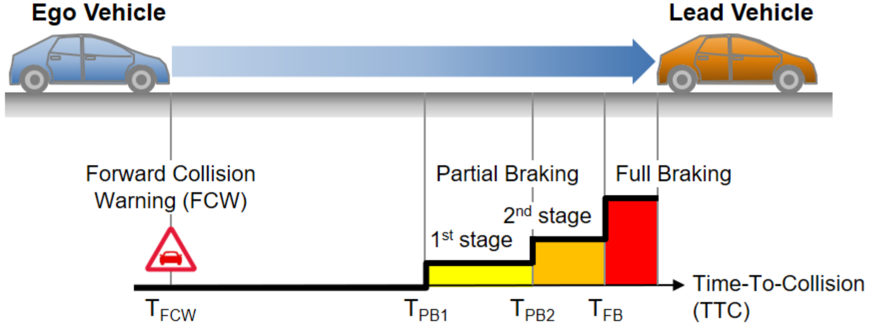


2. Derive parameter scatter and correlation from data





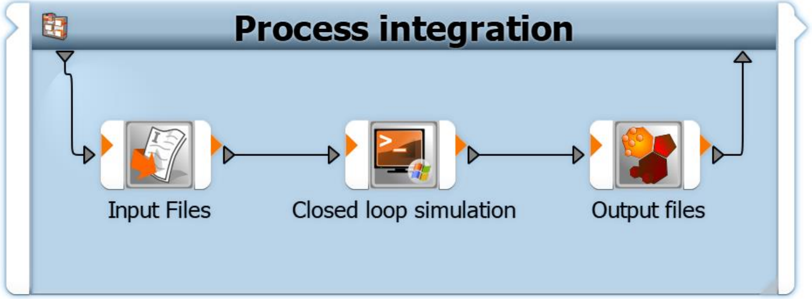
3. Define criticality by means of available KPIs



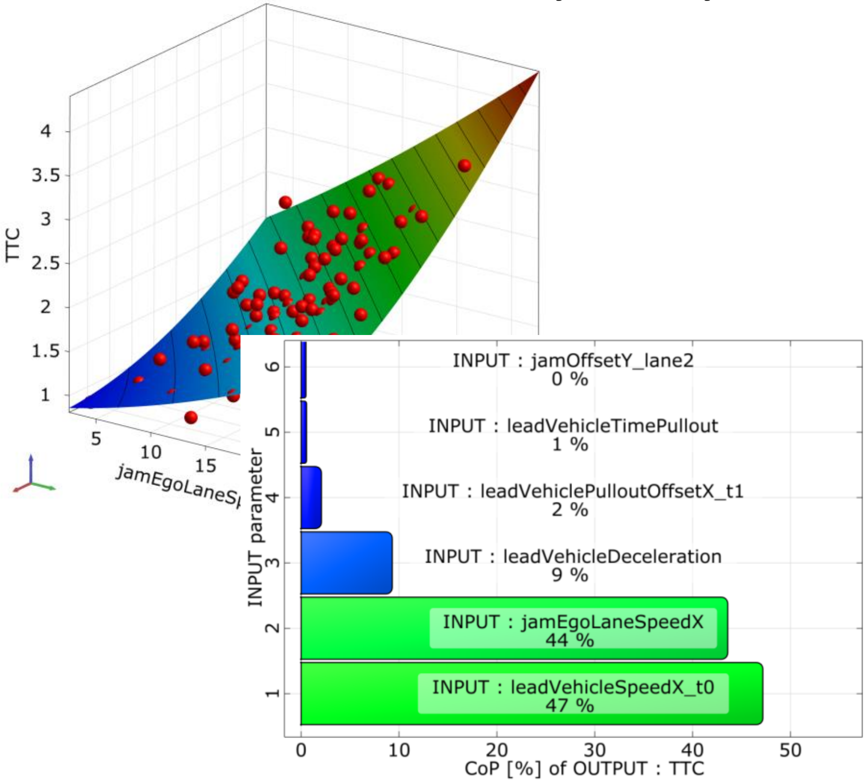
Reliability Analysis of Automated Driver Assistance Systems

Scenario Variation & Safety Assessment

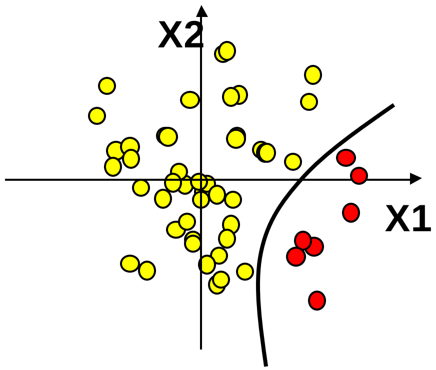
4. Integrate closed loop simulation
in automated workflow

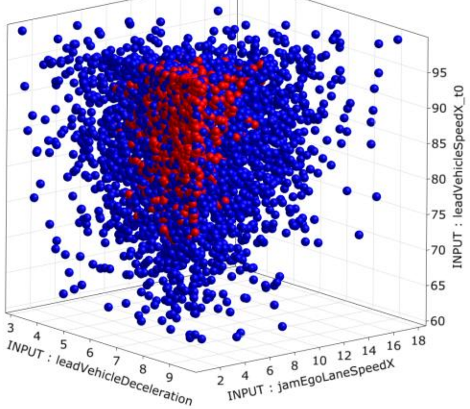


5. Get parameter importance by
robustness/sensitivity analysis



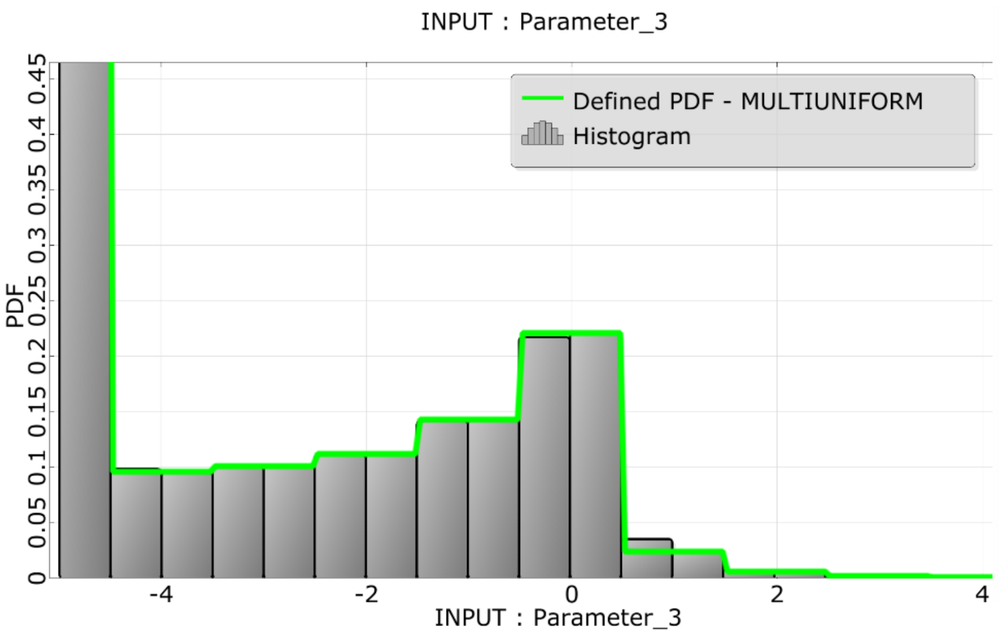
6. Estimate failure probability
of critical states by reliability analysis

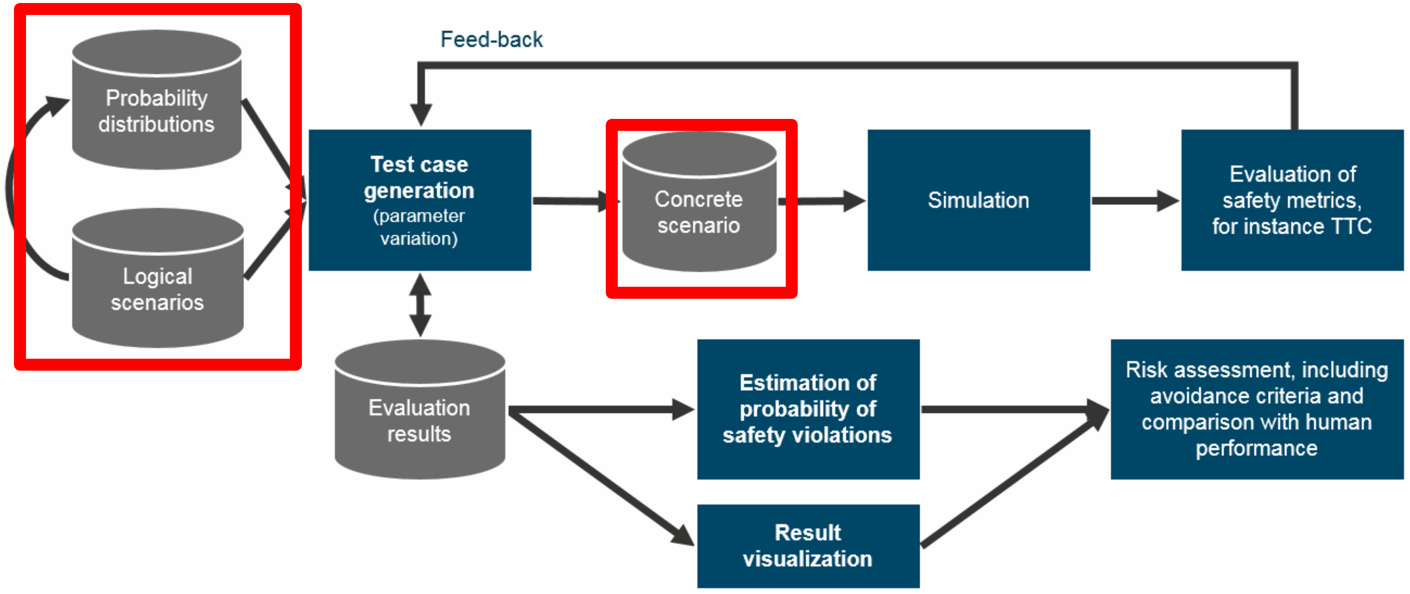




Data-based Fitting of Random Distribution Functions

- Automatic fitting of distribution parameters based directly on data for multi-uniform distribution
- High flexibility to represent multi-modal data
- ➢ Enables **data-based scenario variation** in verification of **ADAS** systems





Questions ?

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