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Lectures

Recent advances in Metamodel of Optimal Prognosis

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presented at the Weimar Optimization and Stochastic Days 2010
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Recent advances in Meta-model of Optimal Prognosis

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Abstract

In real case applications within the virtual prototyping process, it is not always possible to reduce the complexity of the physical models and to obtain numerical models which can be solved quickly. Usually, every single numerical simulation takes hours or even days. Although the progresses in numerical methods and high performance computing, in such cases, it is not possible to explore various model configurations, hence efficient surrogate models are required.

Generally the available meta-model techniques show several advantages and disadvantages depending on the investigated problem. In this paper we present an automatic approach for the selection of the optimal suitable meta-model for the actual problem. Together with an automatic reduction of the variable space using advanced filter techniques an efficient approximation is enabled also for high dimensional problems.

Keywords: surrogate models, meta-modeling, regression analysis, optimal prognosis, variable reduction

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1 Introduction

Meta-modeling is one of the most popular strategy for design exploration within nonlinear optimization and stochastic analysis (see e.g. Booker et al. (1999); Giunta and Watson (1998); Simpson et al. (2003)). Moreover, the engineer has to calculate the general trend of physical phenomena or would like to re-use design experience on different projects. Due to the inherent complexity of many engineering problems it is quite alluring to approximate the problem and to solve other design configurations in a smooth sub-domain by applying a surrogate model (Sacks et al. (1989); Simpson et al. (2001)). Starting from a reduced number of simulations, a surrogate model of the original physical problem can be used to perform various possible design configurations without computing any further analyzes. In one of our previous publications (Roos et al. (2007)) we investigated several meta-model types and variable reduction techniques by means of several examples. In this previous paper we summarized that no universal approach exists and the optimal filter configurations can not be chosen generally. Therefor we developed an automatic approach for this purpose based on a library of available meta-models and tools for variable reduction. This approach serve us based on a new measure for the approximation quality the Meta-model of Optimal Prognosis. This optimal meta-model serves the best compromise between available information (samples) and model representation in terms of considered input variables.

This paper is constructed as follows: first we present the meta-model approaches which are used later in our investigations. Then we investigate different measures which are used to assess the prognosis quality of the approximation model. In the fourth section we present our procedure to estimate global parameter sensitivities in the reduced parameter space of the optimal meta-model. Finally we present the framework of the meta-model selection and its implementation in optiSLang.

2 Meta-model approaches

2.1 Polynomial regression

A commonly used approximation method is polynomial regression, where the model response is generally approximated by a polynomial basis function

$$\begin{aligned}\mathbf{p}^T(\mathbf{x}) = \big[1\ x_1\ x_2\ x_3\ \ldots\ x_1^2\ x_2^2\ x_3^2\ \ldots \\ \ldots\ x_1x_2\ x_1x_3\ \ldots\ x_2x_3\ \ldots\big]\end{aligned} \tag{1}$$

of linear or quadratic order with or without linear coupling terms. The model output y_j for a given sample $\mathbf{x}_j$ of the input parameters $\mathbf{X}$ can be formulated as the sum of the approximated value $\hat{y}_j$ and an error term ϵ_j

$$y(\mathbf{x}_j) = \hat{y}_j(\mathbf{x}_j) + \epsilon_j = \mathbf{p}^T(\mathbf{x}_j)\boldsymbol{\beta} + \epsilon_j, \tag{2}$$

where $\boldsymbol{\beta}$ is a vector containing the unknown regression coefficients. These coefficients are generally estimated from a given set of sampled support points by assuming independent errors with equal variance at each point. By using a matrix notation the resulting least squares solution reads

$$\hat{\boldsymbol{\beta}} = (\mathbf{P}^T\mathbf{P})^{-1}\mathbf{P}^T\mathbf{y} \tag{3}$$

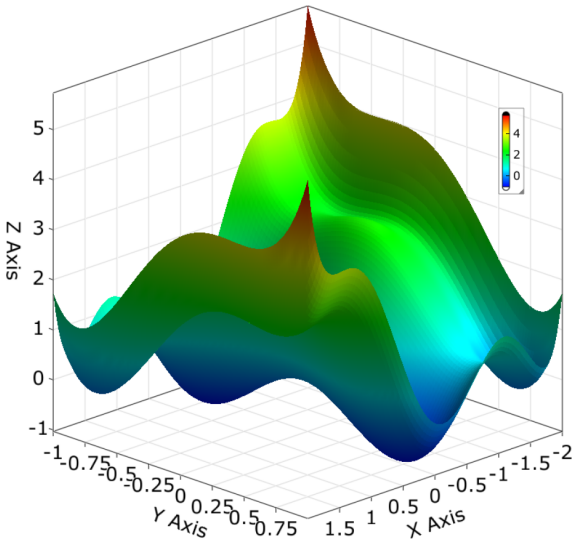


Figure 1: Original model response function $z(x, y)$

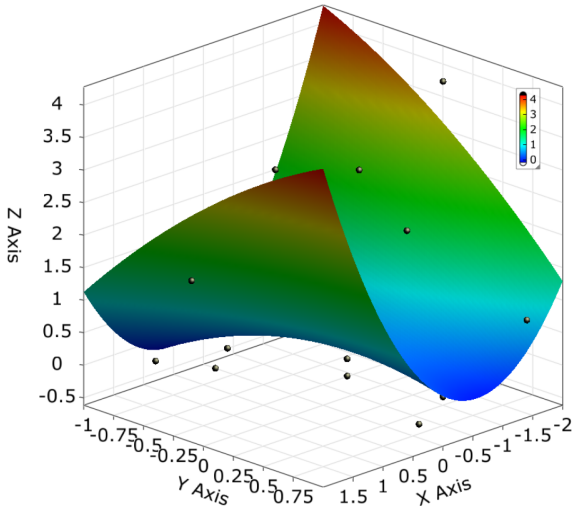


Figure 2: Polynomial least square approximation with quadratic basis

where $\mathbf{P}$ is a matrix containing the basis polynomials of the support point samples.

Since in the MOP approach the original parameter space is reduced to a much smaller subspace of important variables, small artificial noise has to be smoothed by the approximation method. Polynomial regression is very suitable for this purpose. Nevertheless, only global linear or quadratic function can be represented. For more complex coherence between model input and output local regression methods have to be used instead of global polynomial regression.

2.2 Moving Least Squares approximation

In the Moving Least Squares approximation a local character of the regression is obtained by introducing position depending radial weighting functions. MLS approximation can be understood as an extension of the polynomial regression. Similarly the basis function can contain every type of function, but generally only linear and quadratic terms are used. This basis function can be represented exactly by obtaining the best local fit for the actual interpolation point. The approximation function is defined as

$$\hat{y}(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{a}(\mathbf{x}) \tag{4}$$

with changing ("moving") coefficients $\mathbf{a}(\mathbf{x})$ in contrast to the global coefficients of the polynomial regression. The final approximation function reads

$$\hat{y}(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})(\mathbf{P}^T\mathbf{W}(\mathbf{x})\mathbf{P})^{-1}\mathbf{P}^T\mathbf{W}(\mathbf{x})\mathbf{y} \tag{5}$$

where the diagonal matrix $\mathbf{W}(\mathbf{x})$ contains the weighting function values corresponding to each support point. Distance depending weighting functions $w = w(\|\mathbf{x} - \mathbf{x}_i\|)$ have been introduced. Mostly the well known Gaussian weighting function is used

$$w_{exp}(\|\mathbf{x} - \mathbf{x}_i\|) = exp\left(-\frac{\|\mathbf{x} - \mathbf{x}_i\|^2}{\alpha^2 D^2}\right) \tag{6}$$

where the definition of the influence radius D influences directly the approximation error. A suitable choice of this quantity enables an efficient smoothing of noisy data as shown in Figure 3. In our work the influence radius D is chosen automatically.

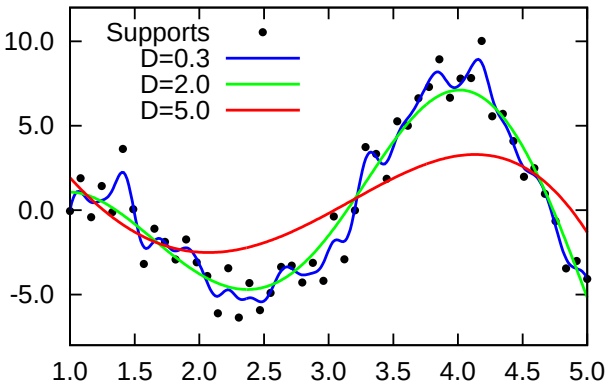


Figure 3: Classical MLS approximation depending on the influence radius D

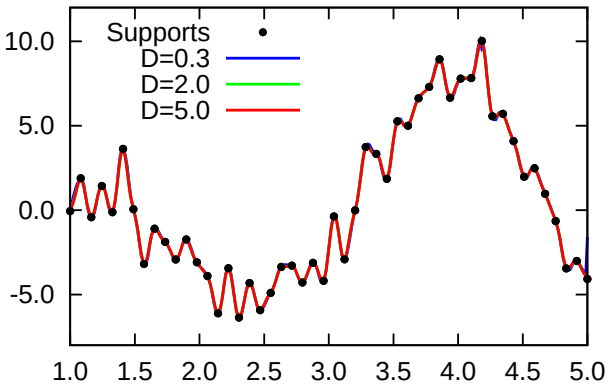


Figure 4: Interpolating MLS approximation with regularized weighting

In an earlier publication Roos et al. (2007) a regularized weighting function was presented which enables the fulfillment of the MLS interpolation condition with high accuracy. This approach is very suitable for problems where an interpolating meta-model is required. For problems of noisy input data the noise is represented by the approximation function as shown in Figure 4 and thus the classical MLS approach with exponential weighting function is more suitable. Due to the reduction of the variable space in the MOP approach, the occurring artificial noise would be represented if the interpolating MLS approach would be used. For this reason we recommend only the use of the classical MLS method inside of the MOP framework.

The main advantage of the MLS approach compared to the polynomial regression is the possibility to represent arbitrary complex nonlinear (but still continuous) functions. By increasing the number of support points the approximation function will always converge to the exact formulation. Furthermore, the MLS approximation requires no computational demanding training algorithm as Kriging or neural networks. This is a very important property required to accelerate the MOP algorithm.

3 Adequacy of the regression model

3.1 Coefficient of determination

In order to verify the approximation model, the Coefficient of determination CoD has been introduced

$$CoD = 1 - \frac{\sum_{j=1}^{n}(y_j - \hat{y}_j)^2}{\sum_{j=1}^{n}(y_j - \bar{y})^2}. \tag{7}$$

For polynomial regression models the coefficient of determination can be alternatively calculated as

$$CoD = \frac{\sum_{j=1}^{n}(\hat{y}_j - \bar{y})^2}{\sum_{j=1}^{n}(y_j - \bar{y})^2}, \text{ or } CoD = \rho^2_{\mathbf{y}\hat{\mathbf{y}}}. \tag{8}$$

For a perfect representation of the support point values this measure is equal to one. This can be the case if the approximation can represent the model perfectly or if the degree of the basis polynomial is equivalent to the number of support points. In order to penalize the second case the adjusted coefficient of determination was introduced

$$CoD_{adj} = 1 - \frac{n-1}{n-p}(1 - R^2), \tag{9}$$

where p is the number of coefficients used in the regression model. In Figure 5 the

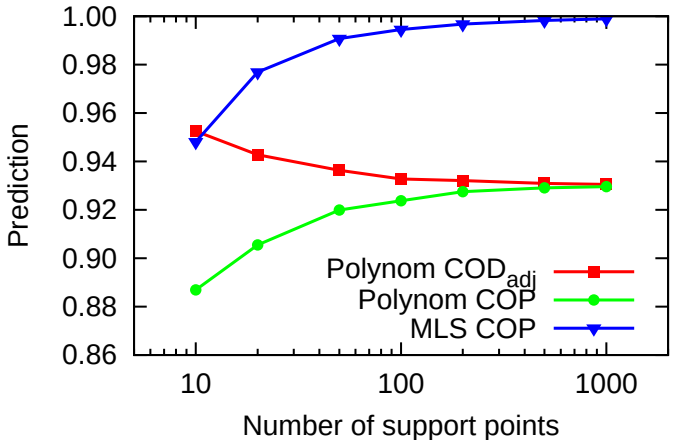


Figure 5: Convergence of coefficient of determination and the coefficient of prognosis depending on the number of support points of a linear polynomial and MLS approximation of a coupled nonlinear two-dimensional model

convergence of the CoD_{adj} is shown for a linear approximation of a two-dimensional quadratic model ($Y = 2X_1 + 4X_2 + 0.5X_1^2 + X_1X_2$) with standard normally distributed input variables. The figure indicates, that for small numbers of support points the CoD_{adj} is to optimistic and gives an overestimate of the approximation quality.

3.2 Coefficient of prognosis

In order to improve our quality measure we introduce the Coefficient of prognosis based on cross validation. In the cross validation procedure the set of support points is mapped to q subsets. Then the surrogate model is built up by removing subset i from the support points and approximating the subset model output $\tilde{y}_j$ using the remaining point set.

The Coefficient of prognosis is now formulated with respect to the general definition of the CoD according to Eq. 7. In contrast to the polynomial CoD in Eq. 7, this value can be slightly negative if the variance of the residuals is larger as the variance of the response itself. However, this case indicates that the meta-model as not suitable for the approximation. Other formulations for the CoP as the squared linear correlation coefficient between the approximated and true model outputs are not suitable for all meta-model types. In Figure 5 the CoP values are shown for the simple example using polynomial regression and MLS approximation. The figure indicates, that the CoP values are not to optimistic for small sample numbers as the CoD values.

The evaluation of the cross validation subsets, which are usually between 5 and 10 sets, causes additional numerical effort in order to calculate the CoP. Nevertheless, for

polynomial regression and Moving Least Squares, this additional effort is still quite small since no complex training algorithm is required. For other meta-modeling approaches as neural networks, Kriging and even Support Vector Regression, the time consuming training algorithm has to be performed for every subset combination, which makes an application inside of the MOP framework not very attractive.

In an earlier implementation Most and Will (2008) we used a splitting of the original data in test and training points to calculate the coefficient of prognosis. There, we could observe a strong dependence of the CoP estimates an the way how the samples were split, although the approximation was almost identical. This is shown in Figure 6. With the application of the cross validation procedure this problem could be solved and much more reliable estimates of the CoP could be obtained as shown in Figure 7.

4 Sensitivity of input parameters

4.1 Coefficient of Importance

Generally the coefficient of determination CoD is interpreted as the fraction of the variance of the true model represented by the approximation model. This can be used to estimate the Coefficient of Importance based on the regression model

$$CoI_i = CoD_{\mathbf{X}} - CoD_{\mathbf{X}_{\sim i}}, \tag{10}$$

where $CoD_{\mathbf{X}}$ is obtained using the complete parameter set to build up the regression model and $CoD_{\mathbf{X}_{\sim i}}$ originates from a regression model with the reduced parameter set $\mathbf{X}_{\sim i}$.

4.2 Coefficient of Prognosis for single variables

Analogous to the coefficient of importance, the CoP for single variables can be defined as the difference between the full and the reduced approximation model. In Figure 8 these values are shown in comparison to the CoI values using polynomials and also using MLS approximation for the two-dimensional quadratic model. The figure indicates a strong overestimation of the influence of the single variables for the MLS approximation if the number of supports is small.

For this reason total effect sensitivity indices are used instead. For our purpose these indices are directly evaluated on the regression model using the standard estimators with a large number of samples. The resulting estimates of the indices are finally scaled with the CoP of the regression model. In Figure 8 the estimated total sensitivity indices are shown additionally which converge significantly faster than the estimates using the reduction approach. For purely additive models the single variable indices sum up to the total CoP of the regression model. If coupling terms are present in the approximation, their sum is larger than the total CoP.

In Figure 9 the estimated sensitivity indices are given for the well known Ishigami function. The figure indicates a very good agreement with the analytical values. As discussed above, the data splitting CoP may strongly depend on the splitting fractions. In this example the CoP values are to optimistic for a small amount of test samples. This is not the case if cross validation is applied where the sensitivity indices are more reliable.

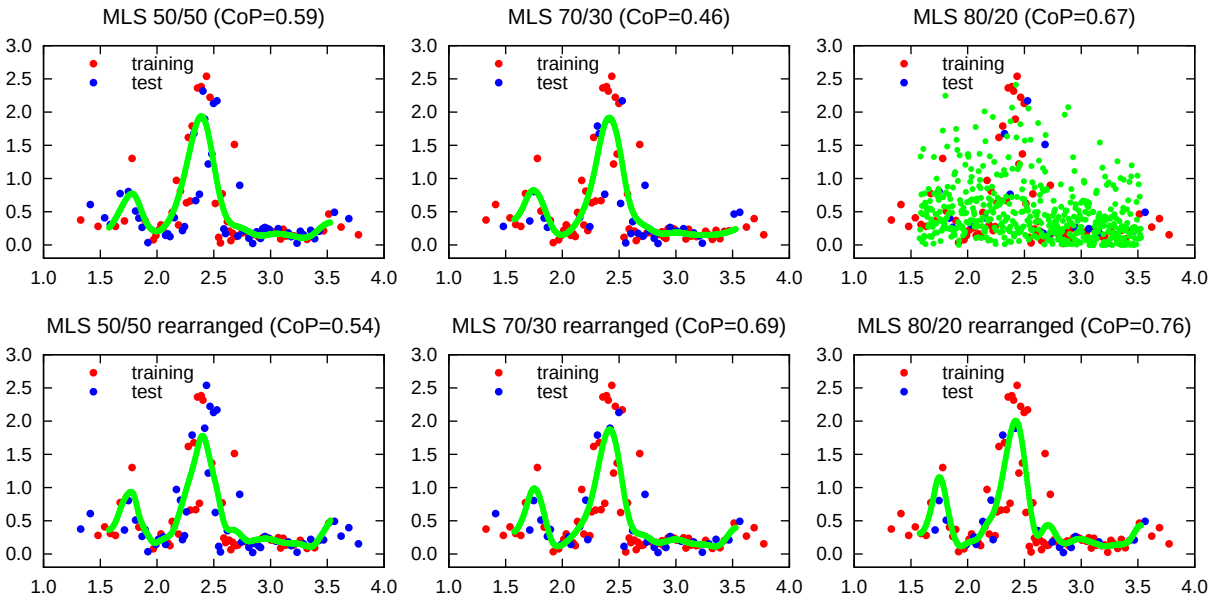


Figure 6: Approximation with corresponding CoP values using data splitting

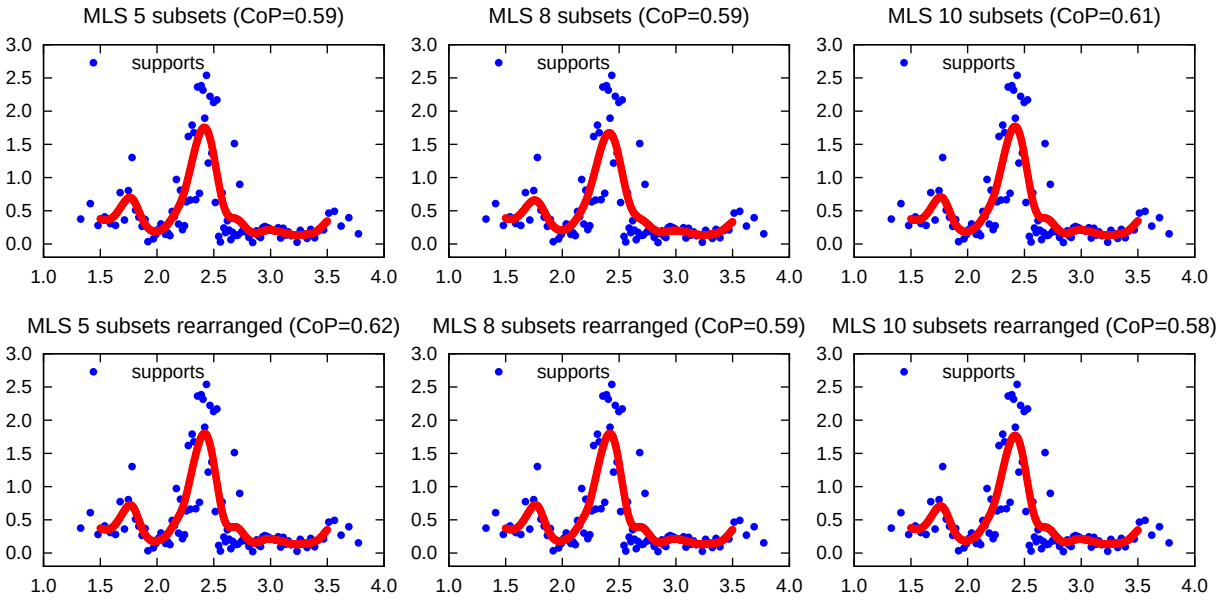


Figure 7: Approximation with corresponding CoP values using cross validation

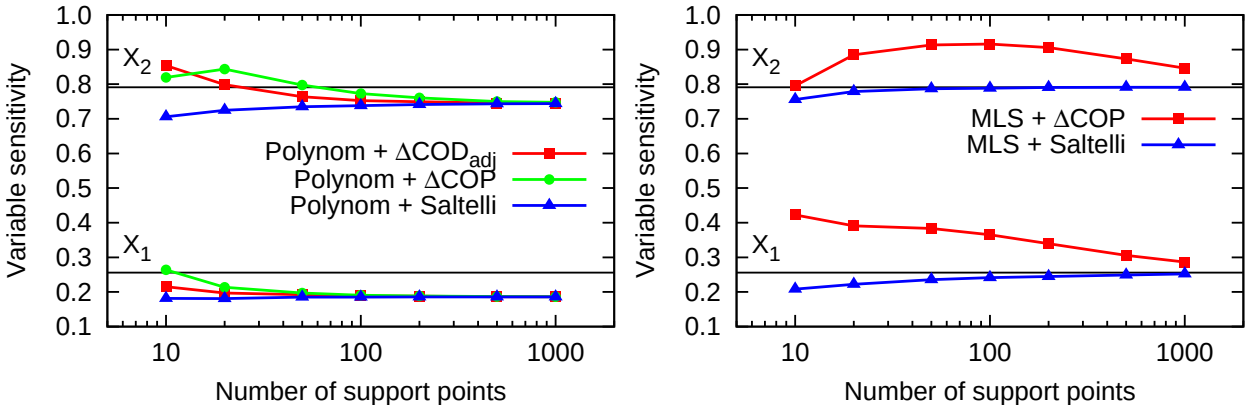


Figure 8: Convergence of the sensitivity indices for the nonlinear two-dimensional model

5 MOP framework

5.1 Significance filter

The coefficients of correlation ρ_{ik} are calculated from all pairwise combinations of both input variables and response according to:

$$\rho_{ij} = \frac{1}{n-1} \quad \frac{\sum_{k=1}^{N} \left(x_i^{(k)} - \mu_{x_i}\right)\left(x_j^{(k)} - \mu_{x_j}\right)}{\sigma_{x_i}\sigma_{x_j}}. \tag{11}$$

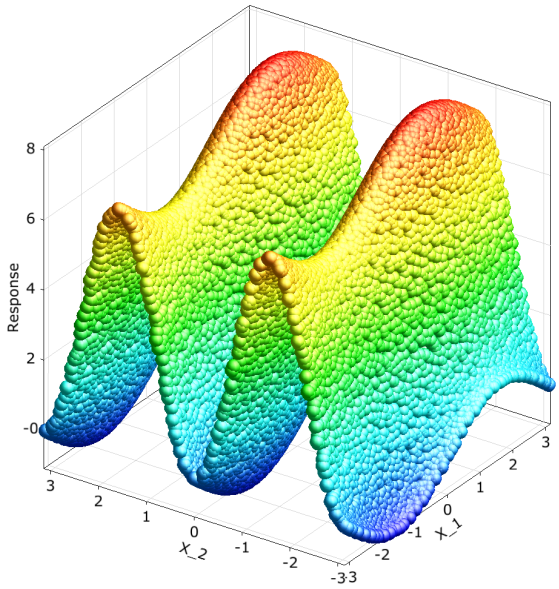
The quantity ρ_{ij}, called the linear correlation coefficient, measures the strength and the direction of a linear relationship between two variables. All pairwise combinations (i, j) can be assembled into a correlation matrix as shown in Figure 10.

The computed correlation coefficients between the input variables vary from the assumed values depending on the sample size. This deviation is used to judge in a first step, which variables are significant concerning there influence on the output variables. We define an error quantile which is chosen between 90% and 99% and compute the corresponding correlation error in the input-input correlations. This is done for linear and quadratic correlations simultaneously. Based on these quantile values we assume only these input variables to be significant concerning an output variable if there correlation values are above the given error values. For the most practical cases this leads to a reduced number of input variables which is shown in Figure 10. All values in gray are assumed to be insignificant.

5.2 Importance filter

Generally the remaining variable set still contains variables which are not needed for an approximation. With the importance filter we identify the important variables for the approximation model as described as follows: Based on a polynomial regression using the remaining variables of the significance filter we estimate the quality of the model representation by the coefficient of determination (CoD). Based on a given value of the minimum required coefficient of importance CoI_{min} only the variables having

$$CoI_i \geq CoI_{min} \tag{12}$$



	Analytical	Splitting 50/50	Splitting 70/30	Splitting 80/20	Cross validation
CoP	-	0.95	0.98	0.99	0.96
CoP_1	0.56	0.57	0.61	0.61	0.58
CoP_2	0.44	0.38	0.39	0.40	0.40
CoP_3	0.24	0.27	0.26	0.26	0.25

Figure 9: Ishigami test function and calculated sensitivity indices using 500 samples with data splitting and cross validation

are considered in the final approximation. Generally the value CoI_{min} is taken between 1% and 9%.

5.3 Determination of the optimal meta-model

Based on the definition of the coefficient of prognosis we can derive the optimal meta-model with corresponding variable space as follows: For each meta-model type we investigate all possible significance and filter configurations by varying the significance quantile from 99% down to a given minimal value. Then a polynomial regression is built up and the coefficients of importance are calculated for each variable. The threshold CoI_{min} is varied from 0.01 to a given value and based on the remaining variables the meta-model is built up and the coefficient of prognosis is computed. The configuration with the maximum CoP based on cross validation is finally taken as optimal meta-model with corresponding variable space for each approximated response quantity.

Finally a certain reduction of the best CoP by a given ΔCoP around 3% is allowed in order reduced further the number of input variables and even the complexity of the meta-model. This means, that if for example MLS approximations gives the best CoP of 85%, but polynomial regression with the same number of inputs leads to 83%, polynomial regression, which is the simpler model, is preferred. This helps the designer to explain the response variation with a minimum number of inputs while keeping the approximation model as simple as possible.

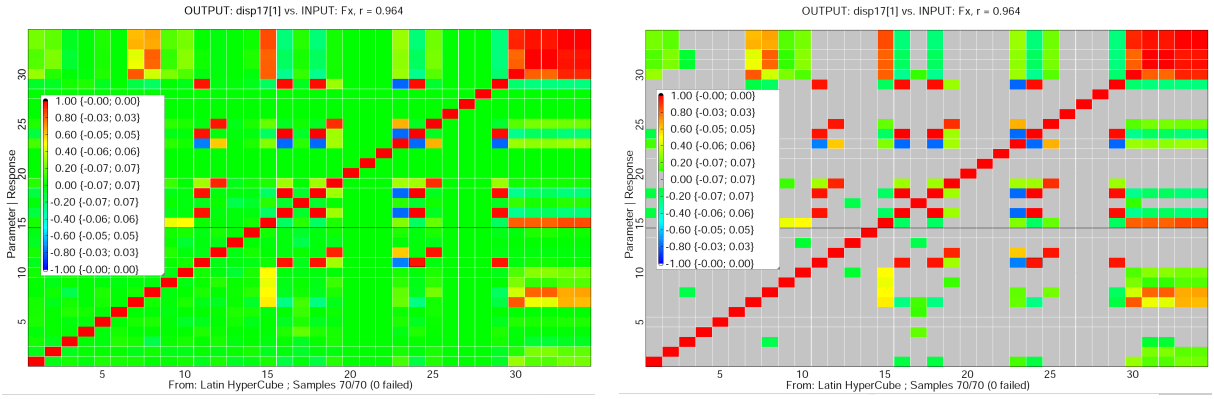


Figure 10: Full linear correlation matrix and reduced matrix considering the most significance linear correlation coefficients

5.4 Implementation of CoP/MOP in optiSLang

Since version 3.1 the CoP/MOP approach is included in the commercial software optiSLang DYN (2009). There is a flow created which can evaluate CoP/MOP for any set of samples or test data. The user can choose cross validation or data splitting, the different filter settings and can force to reduce (Delta CoP) the number of important variables in the final MOP model.

Since it is available in optiSLang the generation of the meta-model of optimized prognosis and the calculation of coefficient of prognosis was successfully applied at several problem types. The following example shows a noise non-linear problem having 8 optimization variables and 200 samples. Running traditional correlation analysis using Spearman ranked data two important variables could be identified and a CoI of 73% (Fig. 11) for the full model was measured. Running CoP/MOP we also find the two important variables, but with very good representation of the nonlinear response function we can achieve a CoP of 99% (Fig. 11,12).

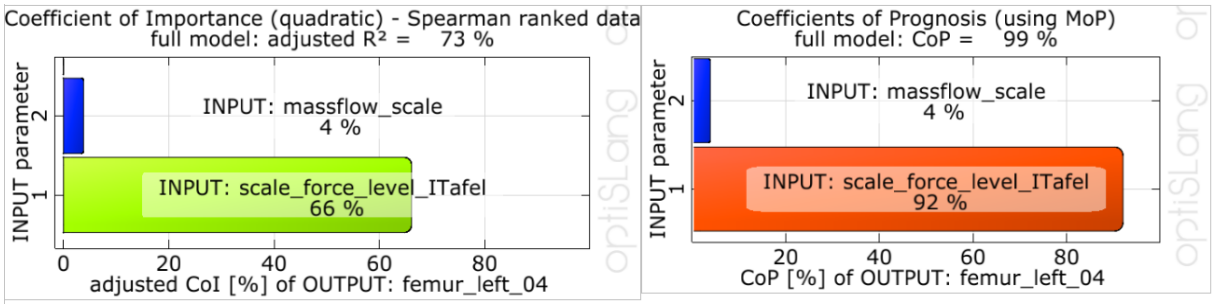


Figure 11: Left: Coefficient of Importance using traditional correlation analysis, right: Coefficient of Prognosis using CoP/MOP approach

From our experience so far we can state and recommend:

- Compare CoI of correlation analysis and CoP, the differences between the two should be verified.
- Check plausibility and prognosis quality by plotting the MOP with the two most important input variables.

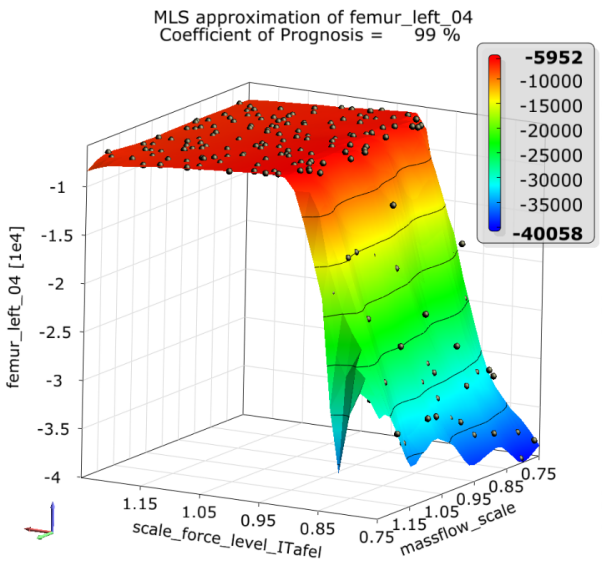


Figure 12: Visualization of the MOP approximation in the subspace of the two most important variables

- If the MOP approach can reduce the set of important to a very small number (< 5), very good representation of nonlinearities are achieved even with small number of samples (50).
- If the MOP approach cannot reduce the set of important input parameters smaller than $10 \ldots 20$, the sample set must be large to represent non-linear correlation.
- The CoP measure of the full model is more reliable than the CoI measure of the full model.

6 Conclusion

In this paper we presented an approach for an automatic selection of the optimal meta-model for a specific problem. We introduced the coefficient of prognosis which enables an objective assessment of the meta-model prognosis based on cross validation. The approach can identify the required variables efficiently and the obtained optimal meta-model can be used afterwards for an optimization. We could show that cross validation gives more reliable estimates of the CoP for small samples sizes than sample splitting with only minimal additional numerical costs for polynomials and MLS. Furthermore, Saltelli's approach for sensitivity analysis combined with MOP could improve the accuracy of the variable indices significantly.

In our future work we will address the following improvements:

- Consideration of dependent inputs in the sensitivity measures.
- Development of filter procedures for the detection of coupling terms.
- Bootstrapping of the CoP in order to assess its estimation quality depending on the number of samples.

After generation of MOP the next step will be to use the MOP for optimization purpose within optiSLang. Then a black box algorithm combining high end sensitivity study and optimization will be available for medium and high dimensional non linear problems.

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