Statistical Measures for the CAE-based Robustness Evaluation

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Conclusion

Today, stochastic calculations are more and more used in the virtual product development for the evaluation of the influence of input scattering on important result parameters. But this stochastic evaluation and calculation approach can also bring some uncertainties into the assessment of an engineering task. Beyond the reasons of deviation of the deterministic calculation results, statistical uncertainties in the estimation of statistical measures have to be considered. Thus, it is important to secure the reliability of the estimated statistical measure.

Crucial point of the reliability of statistical measures is a sufficient amount of random samples (calculations) for a secure determination of statistical parameters. In this regard, it is discussed how trustworthiness of correlation coefficients can be assessed with the help of confidence estimations. Thus, the Latin Hypercube Samplings need significantly less samples as the Monte Carlo Samplings regarding the confidence of the estimation. Another discussion point is how coefficients of determination can help to estimate how much of the variation of input parameters can be explained by the found correlations of input scattering.

Keywords: robustness evaluation, correlation analysis, coefficient of determination, confidence estimation, Latin Hypercube Sampling

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1 Introduction

In the virtual product development, more and more stochastic calculations are carried out for the evaluation of the influence of input scatters onto important response parameters. But this stochastic evaluation and calculation approach can also bring some uncertainties into the assessment of an engineering task. Beyond the reasons of deviation of the deterministic calculation results, like from modelling or approximation errors, also statistical uncertainties in the estimation of statistical measures have to be considered. Thus, it is important to secure the reliability of the estimated statistical measure.

The simplest statistic measure is the mean value of a response parameter and it builds bridges to common deterministic approaches. But when it comes to higher statistic measures for robustness analysis of system responses like variance, standard deviation, coefficients of correlation or variation, it is questionable how trustworthy the estimations of statistical measures of system responses are and in which order which measures have to be taken into consideration.

Key point of the reliability of statistic measures is a sufficient amount of samples (calculations) for a secure determination of statistic parameters. Numeric robustness analysis mainly examines the sensitivity of important system responses against input scatters. Therefore, mean values, coefficients of correlation and variation as well as coefficients of determination are utilized. This question can not be answered a priori, because for example for the determination of trustworthy correlation coefficients and coefficients of determination, the necessary amount of samples highly depends on the unknown character (dimension and nonlinearity) of the correlation. A conservative (too high) estimation of the sample size would often be impossible regarding the calculation time. Usually, as less as possible calculations should be necessary to estimate the statistic measure and it has to be secured to stay within statistic trustworthy bounds.

According to our experiences, it is important to adjust the amount of calculations to the correlation coefficients which are relevant for the task. Then, the statistic reliability should be secured by confidence estimation and the significance of identified correlations regarding the variation of response parameters should be examined with the help of coefficients of determination.

2 Important Measures of Mathematic Statistic for Robustness Analysis in Engineering Tasks

Mathematical statistic formulates statements about the features of a total quantity (population) based on knowledge about the features of a subset (samples) which are taken from a possible total quantity. The features can be random, quantitative (e.g. diameter of a wave) or qualitative (it functions or it does not).

The population is mathematically modified by the random variable x_i. In the quantitative case, x_i is usually the feature itself and in the qualitative case, the feature is defined by x_i (e.g. functions, if $x_i \geq 0$; disfunctions, if $x_i \leq 0$).

The sampling with the extent N is the random choice of N events from a population. Normally, the choice of samples is random and independent in mathematical statistics. In virtual created samples, this corresponds to the Monte Carlo Sampling.

Important features of random parameters can be estimated from concrete random samplings ($x_i^{(k)}$):

arithmetic mean value
$$\overline{x}_i = \frac{1}{N}\sum_{i=1}^{N} x_i^{(k)} \quad \text{(eq. 2-1)}$$

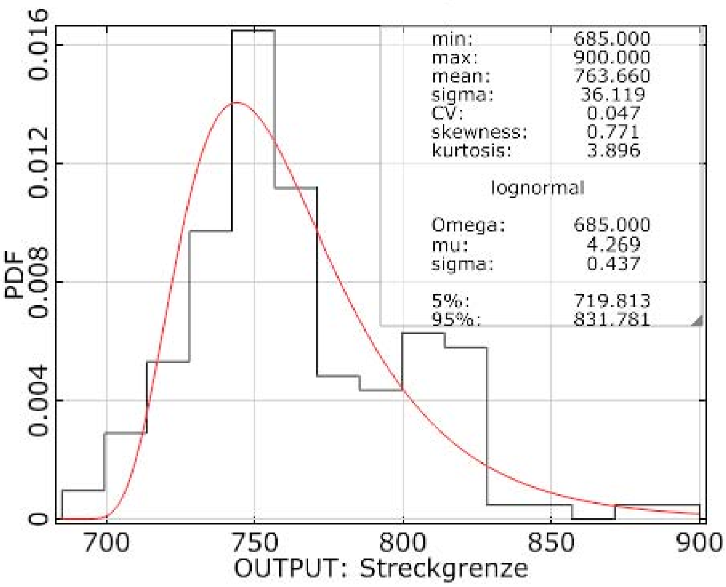
arithmetic variance
$$\sigma_{x_i}^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(x_i^{(k)} - \overline{x}_i\right)^2 \quad \text{(eq. 2-2)}$$

where σ corresponds to the standard deviation (medial quadratic deviation)

range of variation
$$R = x_{i-\max}^{(k)} - x_{i-\min}^{(k)} \quad \text{(eq. 2-3)}$$

coefficient of variation
$$COV_{x_i} = \frac{\sigma_{x_i}}{\overline{x}_i} \quad \text{(eq. 2-4)}$$

Main characteristic of a random parameter is its distribution or distribution function. To get a first idea about the distribution of a quantitative feature, histograms are created. These histograms are usually plotted as column of cumulative frequency of samples in a uniform interval arrangement of the random parameter range. Significance tests for different distribution hypothesis can be carried out for the assessment of which distribution hypothesis is suited for the description of the random variable. The distribution with the best fit can be chosen and be drawn into the histogram. Fractile values of the random response variable with their belonging probabilities can be estimated from the histograms or distribution functions. Because comparatively few samples are done in numeric robustness assessments, just the probabilities of relatively frequent events (> 1%) should be determined and valued. For a secure determination of small probabilities, methods of reliability analysis are recommended.



Picture 1 - histogram with the range of variation, mean value, standard deviation, coefficient of variation (CV) and fitted distribution function

Beyond statistical measures of single random input and response parameters, statistical measures about their correlation (especially between the input and response parameters) are very important for engineering tasks regarding sensitivity and robustness analysis. Therefore, regression and correlation analysis are carried out. The regression analysis deals with the functionality of the correlation and the correlation analysis ascertains the quantitative degree of the correlation.

3 Correlation Analysis

The degree of linear correlation between two coincidental events is indicated by the correlation coefficient ρ_{ij}.

$$\rho_{ij} = \frac{S_{ij}}{\sqrt{S_{ii} S_{jj}}} \qquad \text{(eq. 3-1)}$$

3.1 Linear Correlation Coefficients

The mostly used correlation estimation is based on a linear regression hypothesis. The linear correlation coefficient (Pearson Product Moment Correlation):

$$\begin{aligned} S_{ij} &= \sum_{k=1}^{N} \left(x_i^{(k)} - \bar{x}_i\right)\left(x_j^{(k)} - \bar{x}_j\right) \\ S_{ii} &= \sigma_{x_i}^2 (N-1) \qquad \text{(eq. 3-2)} \\ S_{jj} &= \sigma_{x_j}^2 (N-1) \end{aligned}$$

$$\rho_{ij} = \frac{1}{N-1} \frac{\sum_{k=1}^{N} \left(x_i^{(k)} - \bar{x}_i\right)\left(x_j^{(k)} - \bar{x}_j\right)}{\sigma_{x_i} \sigma_{x_j}} \qquad \text{(eq. 3-3)}$$

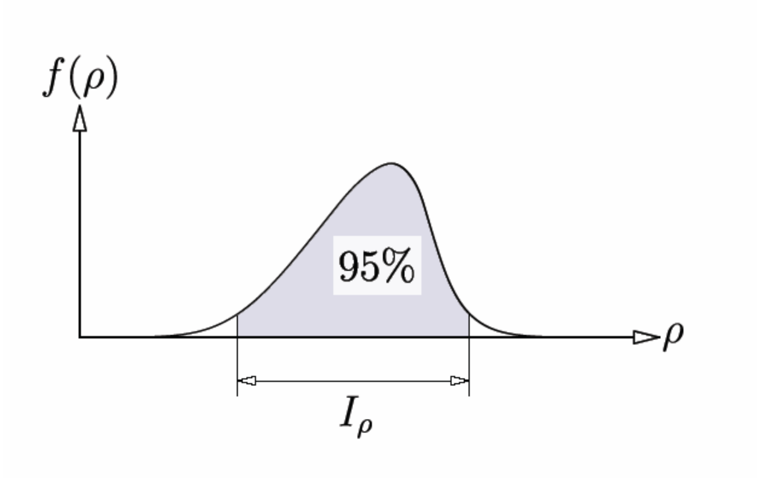
determines the direction and accordance of a line of best fit with the sample and it can have values between +1 and -1. There is a positive linear correlation for the correlation coefficient +1, both values together become smaller or bigger. If the correlation coefficient is -1, there is a negative correlation and if one value gets bigger, the other one gets smaller.

In the literature, correlations with a correlation coefficient > 0.80 or 0.70 are usually called strong correlations and correlations with a correlation coefficient < 0.50 weak correlations. But if a correlation coefficient is really significant, also depends on other existing correlations. There is no important linear connection for small correlation coefficients (< 0.30 or 0.20). In that case, it has to be examined, if there are really no connections or if some nonlinear correlations exist.

3.2 Confidence Estimation of linear Correlation Coefficients

All statistical measures stated before are point estimations in terms of mathematical statistics. They are characterized by estimations from different samples of the population which have different values. That is why these estimations can be useless, if nothing is known about the reliability of the estimation. Therefore, it is necessary to examine the accuracy and reliability of the estimation. These results can be received by estimations from confidence intervals. The correlation coefficients normally represent the basis of the sensitivity and robustness analysis. Thus, confidence estimations of linear correlation coefficients are discussed.

An interval ($I\rho$) is required to present the estimation parameter (ρ_{ij}) in such a way that it covers the unknown parameter with the probability ($1-\alpha$). The confidence level is defined with $\gamma = 1-\alpha$ and. The tolerable error probability is α which represents the probability that the estimated correlation coefficient is outside the confidence interval.

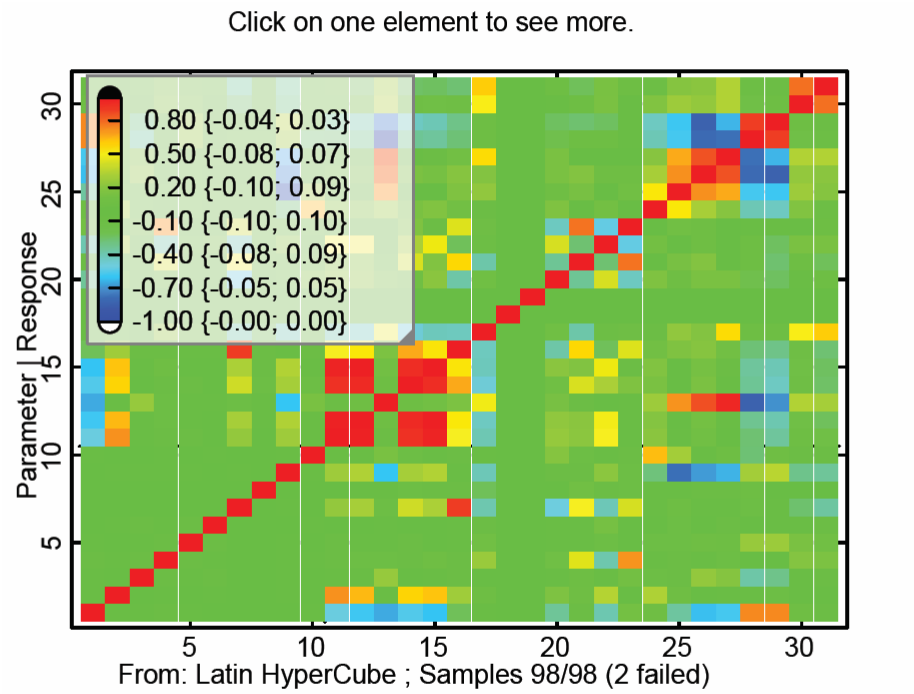


Picture 2 – confidence interval for correlation coefficients with an error probability of 5%

The correlation coefficients are projected into a normal distributed space by the Fischer-z transformation to estimate the confidence intervals. This is done, because the estimators of the linear correlation coefficients are not normally distributed. The confidence interval is given by:

$$\left[\tanh\left(z_{ij} - \frac{z_c}{\sqrt{N-3}}\right), \tanh\left(z_{ij} + \frac{z_c}{\sqrt{N-3}}\right)\right] \qquad \text{(eq. 3-4)}$$

The error probability should be valid for all correlation coefficients to be estimated $M = m\frac{(m-1)}{2}$ between m input and response parameters of the entire correlation matrix. The value z_c is determined with the help of Bonferroni corrected values of the confidence level $\alpha' = \frac{\alpha}{M}$. Thus, for a suitable confidence interval, there is a dependency between the required amount of samples (N) and the amount of input and response variables (m).



Picture 3 - matrix of linear correlations with confidence intervals

3.3 Influence of the Sampling Method on the Confidence Interval of Linear Correlation Coefficients

An appropriate amount of samples is necessary for the estimation of trustworthy correlation coefficients. The literature recommends minimal amounts of input parameters from $n+1$ up to n^2 for Monte Carlo Samplings. In contrast to the ‚observable' statistics, where normally Monte Carlo distributed samples are used, variance minimizing sampling methods can significantly increase the statistical safety of the estimation of correlation coefficients of virtual samples to be calculated. As a result, the influence of the Latin Hypercube Samplings onto confidence intervals has to be examined. In the following comparisons, the confidence intervals of the correlation coefficients are evaluated for an error probability of 5% (confidence level 95%) from Monte Carlo Samplings and Latin

Hypercube Samplings. Estimations are stated for confidence intervals which result from 1000 repetitions of samplings.

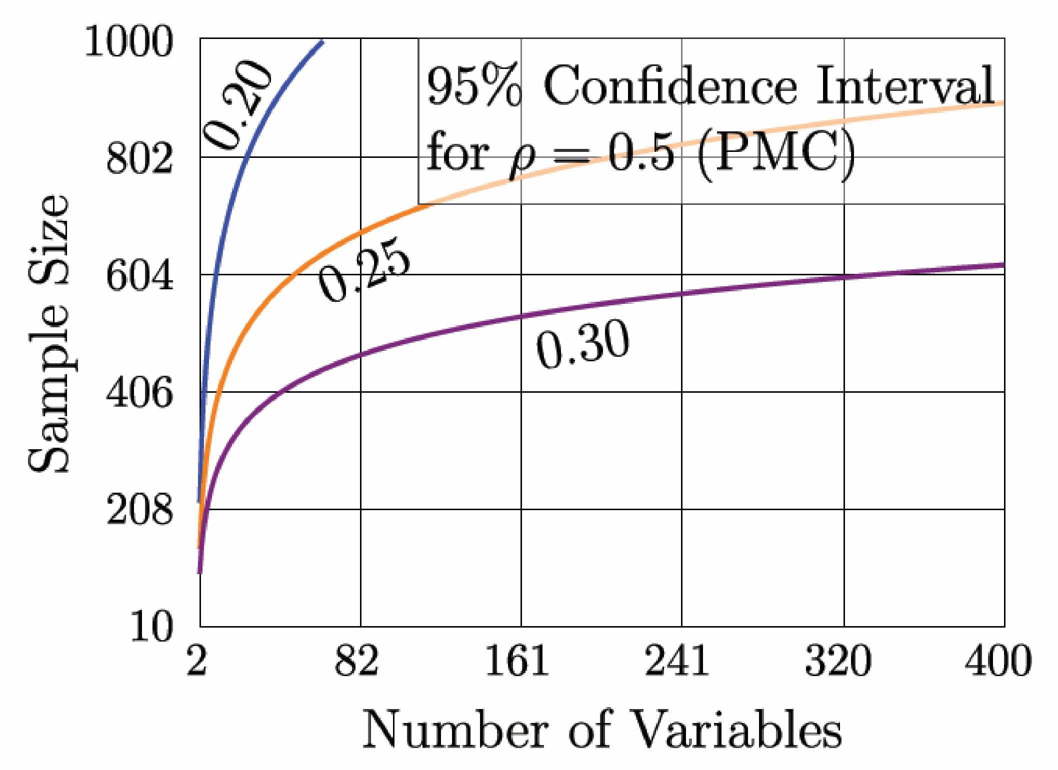
N	correlation coefficient ρ				
	0.0	0.3	0.5	0.7	0.9
10	1.261	1.231	1.054	0.757	0.299
30	0.712	0.682	0.557	0.381	0.149
100	0.409	0.374	0.306	0.199	0.079
300	0.230	0.209	0.170	0.116	0.045
1000	0.124	0.115	0.093	0.062	0.023

Table 1- confidence intervals for the estimation of a correlation coefficient (confidence level 95%) for Monte Carlo Sampling

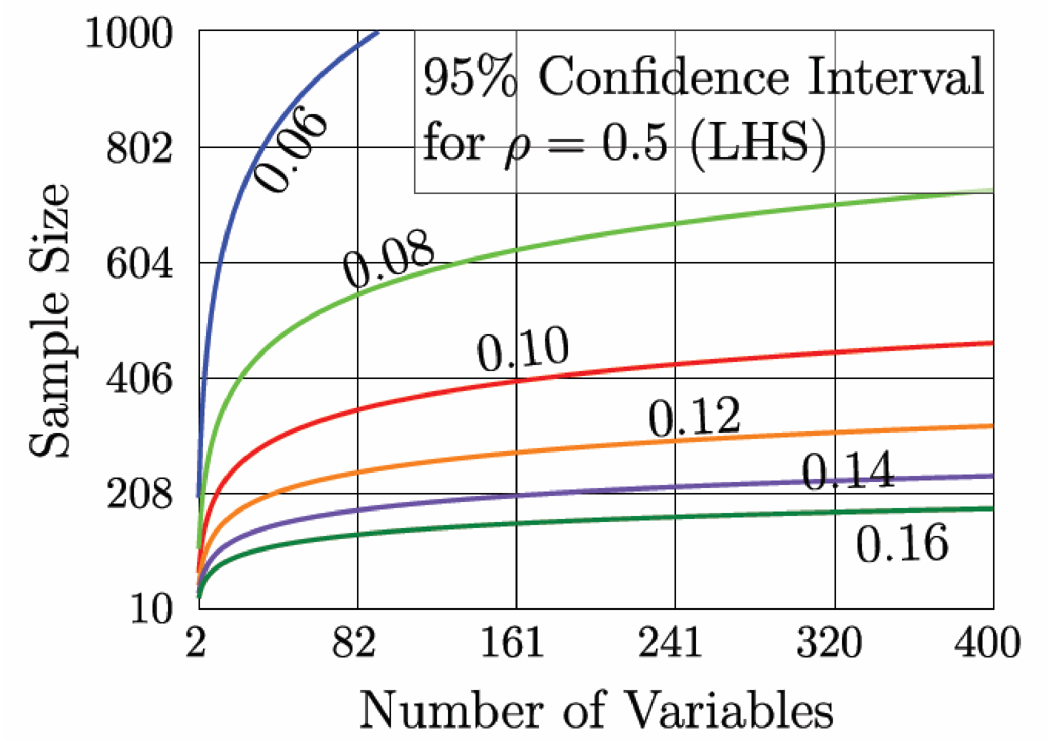
N	correlation coefficient ρ				
	0.0	0.3	0.5	0.7	0.9
10	0.420	0.382	0.260	0.158	0.035
30	0.197	0.194	0.139	0.073	0.018
100	0.111	0.101	0.071	0.042	0.009
300	0.065	0.057	0.042	0.024	0.006
1000	0.038	0.033	0.025	0.014	0.003

Table 2 – confidence intervals for the estimation of a correlation coefficient (confidence level 95%) for Latin Hypercube Sampling

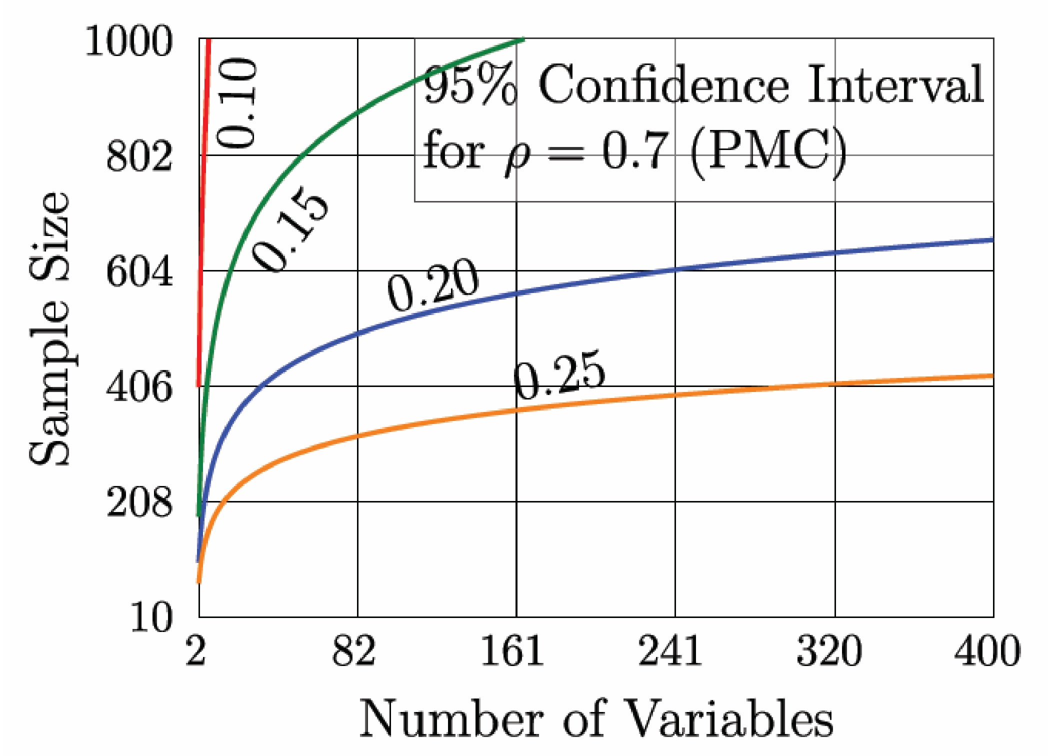
Table 1 and 2 show the dependency of confidence intervals of estimation of a correlation coefficient on the amount of samples. There is a significant improvement for the estimation of correlation coefficients, if the Latin Hypercube Sampling is used. For example, the estimation of the correlation coefficient 0.5 reaches a confidence interval of 0.093 by using Monte Carlo Sampling with 1000 samples and a confidence interval of 0.071 by using Latin Hypercube Sampling with just 100 samples. A Latin Hypercube Sampling with 1000 samples can accomplish a confidence interval of 0.025 and therefore it clearly creates a better estimation than the Monte Carlo Sampling. In summary, the Latin Hypercube Sampling requires a factor ~12 lower amount of samples to create similar confidence intervals like the Monte Carlo Sampling.



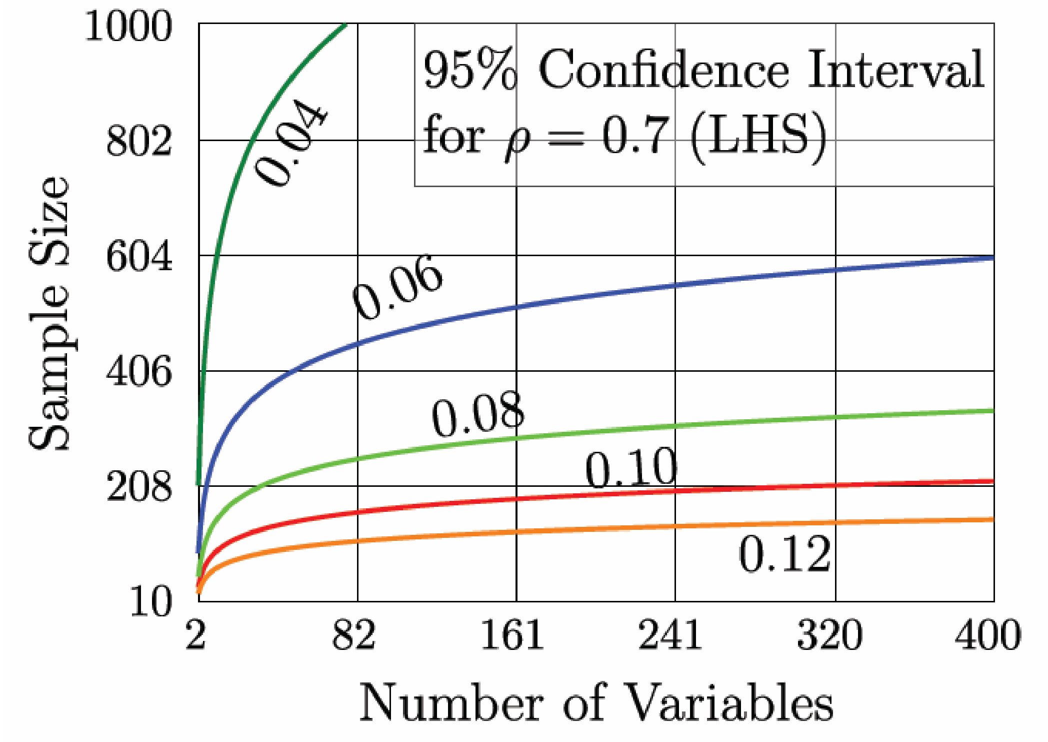
Picture 4 – confidence intervals (confidence level 95%) for m-correlation coefficients 0.5 Monte Carlo Sampling



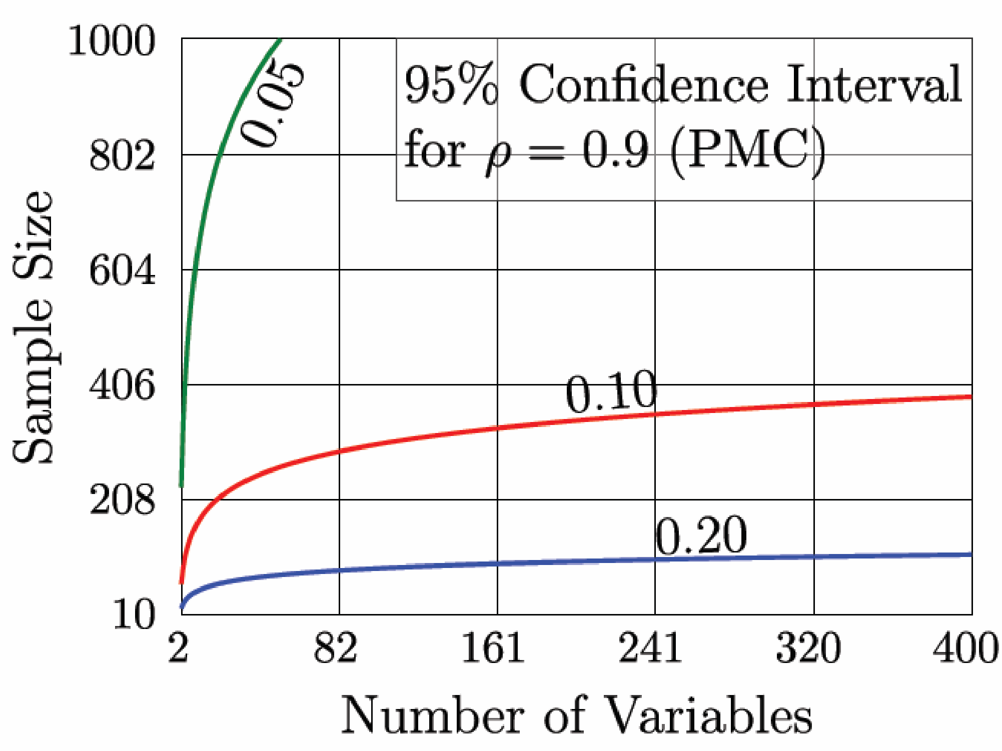
Picture 5 – confidence intervals (confidence level 95%) for m-correlation coefficients 0.5 Latin Hypercube Sampling



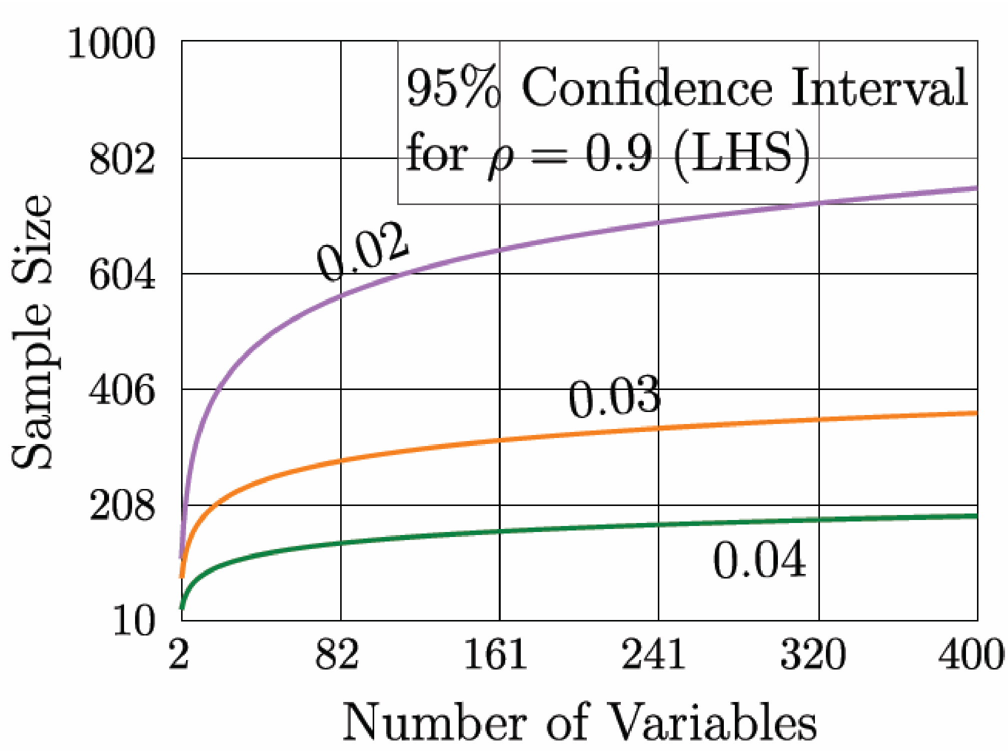
Picture 6 - – confidence intervals (confidence level 95%) m-correlation coefficient 0.7 Monte Carlo Sampling



Picture 7 - – confidence intervals (confidence level 95%) m-correlation coefficient 0.7 Latin Hypercube Sampling



Picture 8 - – confidence intervals (confidence level 95%) for m-correlations coefficients 0.9 Monte Carlo Sampling



Picture 9 - – confidence intervals (confidence level 95%) for m-correlation coefficients 0.9 Latin Hypercube Sampling

Pictures 4 and 9 show the dependency of the confidence intervals of the estimation of M correlation coefficients from m input and response parameters (number of variables) from the amount of samples (sample size). According to chapter 3.2, the confidence intervals were ascertained by Fischer's z-transformation and Bonferroni correction. The factor 12 was considered in the sample size between Monte Carlo Sampling and Latin Hypercube Sampling.

3.4 Coefficients of Determination

Confidence intervals of correlation coefficients indicate the reliability areas of the estimation. Regarding practical tasks, coefficients of determination are important criteria for the significance of the reliability analysis. The coefficient of determination is a quantitative measure about how much of the variation of a parameter can be explained by the correlation found to the input parameters. The coefficient of determination can have values between 0 and 1 or 0 up to 100%.

The coefficient of determination of a linear relation between two uncorrelated random variables is defined as the quadrate of the correlation coefficients.

$$R_{ij}^2 = \frac{S_{ij}^2}{S_{ii} S_{jj}} \qquad \text{(eq. 3-5)}$$

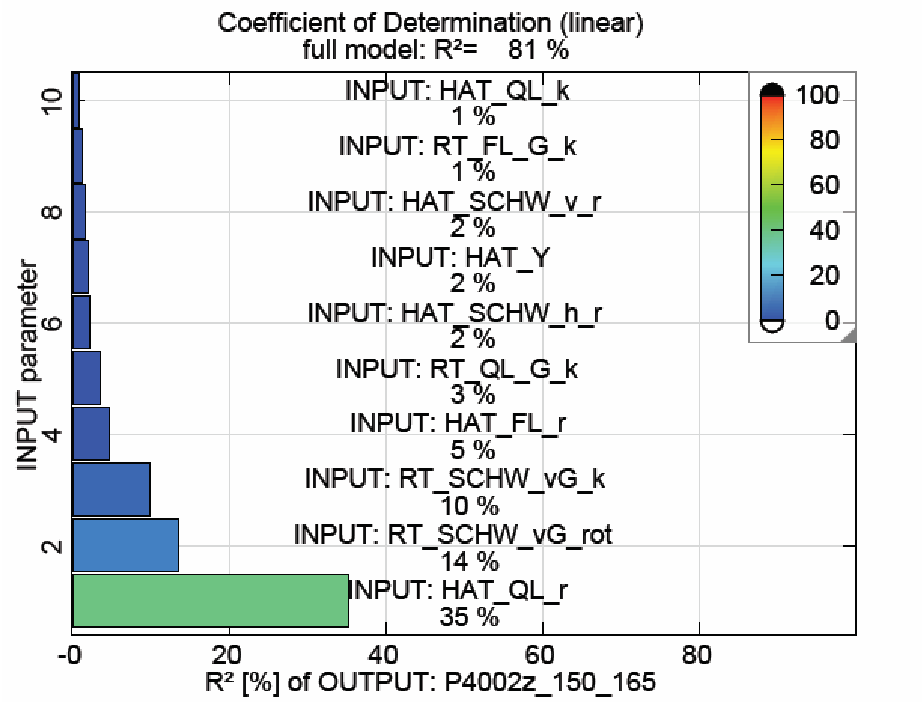
A more abstract determination (e. g. in optiSLang) of the coefficients of determination can be achieved with the help of the correlations of the observed response parameters z and the regression of fitted values $x_j = z^{(k)}(x_i)$.

If the coefficient of determination of an input parameter is determined by all n-input parameters, then a quantitative statement exists that indicates how much of the variation of the input parameters can be explained by the underlying regression hypothesis. In case of a significant deviation of 100% at linear regression hypothesis, either other important correlations exist (e.g quadratic correlations, clusters) or the estimation of the correlation coefficients is too imprecise or the variation of input parameters contains important noise. This noise can derive from the CAE calculation process or the extraction procedure of the response parameter.

Errors of the estimator at the estimation of coefficients of determination of multiple input parameters to a response parameter can sum up significantly, especially at small samples and low correlation coefficients. These correlation coefficients and attendant coefficients of determination of small correlation coefficients (e.g. < 0.3) show high statistical errors at small samples and therefore only increase the determination of a model seemingly. $adjusted\ R_j^{\,2}$ is used to verify this circumstance:

$$adjusted\ R_j^{\,2} = \sum_{i=1}^{n} \left(R_i^{\,2} - (1 - R_i^{\,2}) \right) \left(\frac{k-1}{n-k} \right) \qquad \text{eq. 3-6}$$

The significantly smaller $adjusted\ R_j^2$ than R_j^2 shows that numerous non-significant input parameters were not considered regarding the coefficient of determination. If the coefficients of correlation $R_j^2, adjusted\ R_j^2$ show huge differences, the estimation of the coefficients of determination is not trustworthy and should be repeated for a small set of significant input variables. The significance of input variables is ascertained by the size of the correlation coefficients.



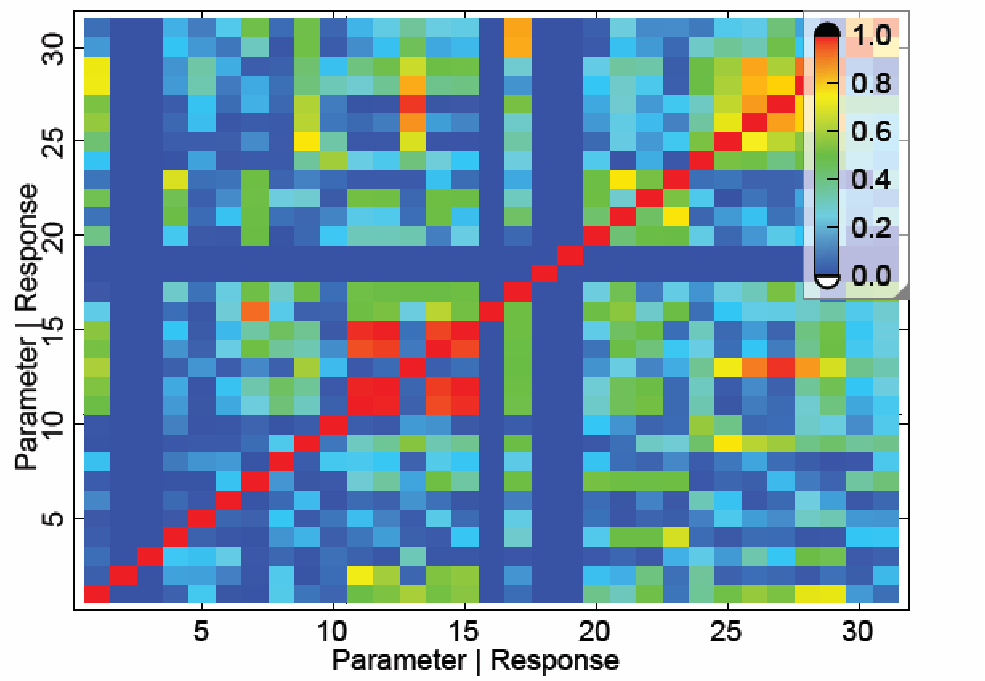
Picture 10 – Coefficients of determination of a response parameter regarding all inputs (full model) and regarding every single scattering input variable

3.5 Quadratic Correlation Coefficients

The literature often advises that the determination of small linear correlations is not an adequate reason for the assumption that no important connection exists between the variables. For example, if two variables are ideally quadratic correlated, then their linear correlation coefficient is 0.0 and their quadratic correlation coefficient is 1.0. That is why the correlation analysis in optiSLang was expanded to the quadratic regression hypothesis.
Quadratic correlation coefficients are normally identified by the quadratic regression of the response parameters x_j to the input parameters x_i.

$$x_j = A_i + B_i x_i + C_i x_i^2 = z(x_i) \qquad \text{eq. 3-7}$$

The regression coefficients A_i, B_i, C_i are normally ascertained by minimizing the error squares about the samples $x_i^{(k)}, x_j^{(k)}, k = 1...N$. The quadratic correlation coefficients result from the input of the fitted values $z^{(k)}$ at the place of $x_i^{(k)}$ and $x_j^{(k)}$ in equation 3.3. The values of the correlation coefficients regarding the quadratic function 3.7 contain a linear and a quadratic ratio and lie between 0.0 and 1.0. The coefficients of determination are determined analogue to the linear regression hypothesis from equation 3-6. The resulting matrix of the quadratic correlation coefficients is not symmetric, because the regression in equation 3-7 can not simple exchange the roles of x_i and x_j.



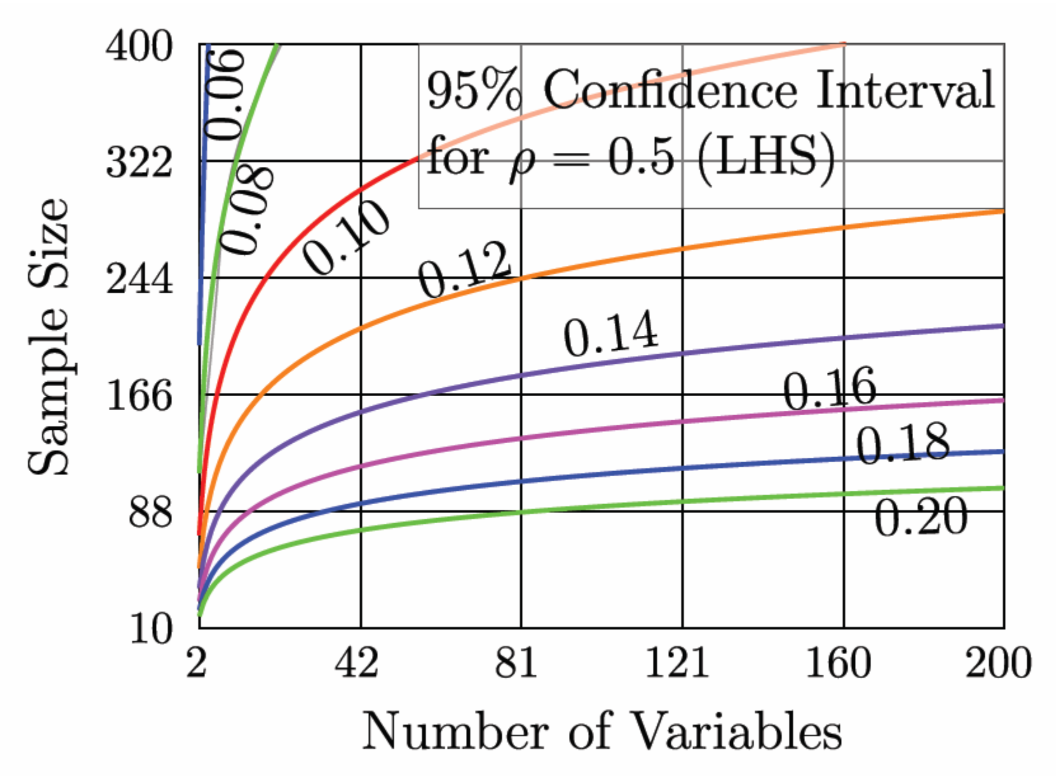
Picture 11 – matrix of quadratic correlations

4 Conclusion

From studies and previous experiences with numeric robustness evaluations, following recommendations can be drawn for practical tasks:

a) Use of a Hypercube Sampling

b) Determination of the amount of necessary calculations for the estimation of expected correlation coefficients with the desired confidence interval. If for example, linear correlation coefficients of 0.50 with a confidence interval 0.12 for a confidence level of 95% for all correlation coefficients are demanded, the necessary amount of samples can be estimated in consideration of the amount of input and response parameters from picture 12. Hence, 200 samples would be necessary for an amount of 40 input and response parameters and a correlation coefficient of 0.50 with 95% confidence within an error interval ±0.06 would be estimated.



Picture 12 – confidence intervals (confidence level 95%) for m-correlation coefficients 0.5 Latin Hypercube Sampling

c) After the calculations, the statistical measures can be taken into consideration in the following order:

a. Variation level and variation coefficient. If the variation level of the response parameters excesses allowed values or the variation coefficients of important response parameters are significantly higher than the variation coefficients of the input parameters related with these response parameters, then responsible input parameters should be identified via coefficients of determination and correlation coefficients.
b. Coefficients of determination of important response parameters of the linear correlation hypothesis. If there is a high (> 80 up to 100%) coefficient of determination ($R^2, adjusted\ R^2$), the variation of response parameters can be sufficiently explained by linear correlation. Correlations of important input parameters can be identified and related anthill plots can be checked regarding their plausibility.
c. If the coefficients of determination of linear correlation are smaller than 80%, the quadratic and linear correlation coefficients and coefficients of determination should be checked for these response parameters. Found significant quadratic correlations and their anthill plots should be tested concerning their plausibility.
d. If the variation of the response parameters can not be sufficiently explained by linear and quadratic correlation, all anthill plots of the input parameters to response parameters have to be checked for nonlinearities like clusters or bifurcations.
e. If no significant linear and quadratic correlations or nonlinearities can be found, other potential reasons have to be examined for the variation of response parameters. If small determinations of response parameters results from bifurcation problems of numeric noise, related physically scattered input parameters should be identified and integrated into the model. If then the determination of response parameters remains small, the construction should be designed more determined regarding the response parameter. If the variation of response parameters is highly influenced by approximation errors from CAE calculations or the extraction of response parameter creates scatters (e.g. via dependencies from time steps or filters) or small determinations result from inadequacies of the models, these deficiencies should be eliminated.

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