

Generation of deviated geometry based on manufacturing process simulations

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Abstract

Every process underlies fluctuations of input and ambient parameters. In manufacturing processes, these fluctuations manifest i.a. in geometric deviations of manufactured workpieces which in turn hugely decrease the function and quality of technical products. Therefore, these deviations have to be limited by geometric tolerances. In this regard, tolerance simulations aim at determining and quantifying the effects of deviations on the product quality. However, in order to obtain resilient predictions about the impacts of process fluctuations on the quality of technical products realistic samples of deviated geometries have to be available which reflect the observable geometric manufacturing deviations. The proposed approach employs methods from computer vision and regression analysis for generating realistic geometry samples based on a limited set of observations, e.g. gathered from manufacturing process simulations or measurements, considering manufacturing process parameters. An exemplary application using the software "Statistics on Structure" (SoS) and "optiSLang" by dynardo GmbH is given.

Keywords: SoS, optiSLang, Manufacturing Process Simulation, Computer Aided Tolerancing.

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1 Geometric Deviations and Computer Aided Tolerancing

Geometric deviations, that means deviations from the nominal geometry, are observable on every manufactured workpiece. They ground on the axiom of manufacturing imprecision and measurement uncertainty and are consequences of process parameter fluctuations DIN EN ISO (2009); Zhang et al. (2011). The observable geometric deviations can be classified into lay, waviness and roughness Weckenmann et al. (2001); Verein Deutscher Ingenieure (1991) and have effects on the subsequent steps of the product lifecycle such as the assembly and use. The aim of computer aided tolerancing is predicting and quantifying these effects on the product quality and the functional behaviour early in product development and ensuring the product function by limiting geometric deviations through geometric tolerances.

2 Modelling Geometric Deviations in Tolerance Simulations

As mentioned earlier, geometric deviations can be classified into lay, waviness and roughness. Beside this classification, geometric deviations can be distinguished as systematic and random deviations Zhang (2011); Henke et al. (1999); Desta et al. (2003). This classification is based on the experience that in many manufacturing processes similar geometric deviations can be observed on every part whereas some geometric deviations can be observed only on a few workpieces. The systematic deviations are deterministic, predictable and reproducible Zhang (2011) and may be depending on the manufacturing process e.g. products of clamping errors or the machine behaviour. In contrast to that, random deviations arise from fluctuations of the production process such as tool wear, varying material properties or fluctuations in environmental parameters (temperature, humidity, et cetera) Zhang (2011).

Tolerance simulations aim at predicting the effects of these various deviations on the product behaviour during use. In order to obtain realistic results, it is crucial that the input geometries for these simulations show geometric deviations which are close to reality.

Basically, one idea for obtaining these geometry samples is to generate them based on the nominal part geometry employing adequate mathematical modelling techniques. In this context, the use of modern parametric CAD-system functionalities Weber et al. (1998), the application of Bézier-curves, splines und NURBS Stoll et al. (2010); Stoll (2006), the modelling of systematic deviations by quadric surfaces and random deviations by various sampling methods Zhang et al. (2011) as well as the adoption of random fields Bayer et al. (2009); Choi et al. (2007); Bucher (2009); Schleich et al. (2012a,b) can be mentioned. On the other hand, deviated geometries can be obtained by measuring real prototypes or from manufacturing process simulations. However, this approach is quite costly and time-expensive which typically leads to small data sets with few observations. Thus, in the following an approach is proposed which aims at generating new geometry sample shapes based on a limited training set taking manufacturing process parameters into consideration which may be used in stochastic geometry-based tolerance simulations.

3 Mathematical Background

For the sake of comprehension and completeness, this section introduces a few mathematical concepts which build the background for the following sections.

3.1 Principal Component Analysis

The principal component analysis (PCA), also known as Karhunen-Loève-Transform, is a well known method in statistics and data mining. It was invented by PEARSON Pearson (1901) in 1901 and is commonly used nowadays in many different applications Kruger et al. (2008). There is given only a brief introduction to PCA since a lot of literature around this topic can be found. For instance Jolliffe (2002) can give deeper insights.

PCA is a technique to reduce large data sets and to express the gathered information by a smaller number of principal components Jolliffe (2002). These components are uncorrelated (orthogonal) and "are ordered so that the first few retain most of the variation present in all of the original variables" Jolliffe (2002).

Finding a matrix $X \in \mathbb{R}^{n \times p}$ of *n* samples of a *p*-element vector x of random variables where the (i, j)th entry x_{ij} is the *i*th observation of the *j*th variable. Let $\overline{X} \in \mathbb{R}^{n \times p}$ be the so-called mean matrix where each entry in the *j*th column is:

$$\overline{x}_j = \frac{1}{n} \sum_{i=1}^n x_{ij}, \quad j = 1, 2, \dots, p$$

the mean of the jth variable. Then:

$$S = \frac{1}{n-1} (X - \overline{X})' (X - \overline{X})$$

is the covariance matrix of the samples. Let \boldsymbol{a}_k be an eigenvector of \boldsymbol{S} corresponding to its kth largest eigenvalue l_k . Then the kth sample principal component (PC) is $\boldsymbol{a}'_k \boldsymbol{x}$ for $k = 1, 2, \ldots, p$. $\tilde{z}_{ik} = \boldsymbol{a}'_k \boldsymbol{x}_i$ is the score for the *i*th observation on the kth PC for $i = 1, 2, \ldots, n$ and $k = 1, 2, \ldots, p$ Jolliffe (2002).

The matrix of PC scores can also be defined as:

$$Z = (X - \overline{X})A$$

where $\boldsymbol{A} \in \mathbb{R}^{p \times p}$ is the orthogonal matrix whose kth column is \boldsymbol{a}_k .

To achieve data reduction the number m of computed largest eigenvalues and corresponding eigenvectors should be smaller than the dimension of \boldsymbol{x} , so $m \ll p$.

The original sample set X can then be approximated by:

where:

$$ilde{oldsymbol{X}} = \overline{oldsymbol{X}} + (oldsymbol{Z} \cdot oldsymbol{A}').$$

If a_k is normalized, i.e. has unit length $(a'_k a_k = 1)$, then $var(\tilde{z}_k) = l_k$, that means that l_k is the variance of \tilde{z}_k . Therefore, it is simple to determine the percentage of the total variability explained by each principal component and the cumulative percentage of total variation explained by a subset m of principal components t_m Jolliffe (2002):

$$t_m = 100 \cdot \frac{\sum_{k=1}^m l_k}{\sum_{k=1}^p l_k}.$$

As mentioned before, PCA received a lot of attention in many research areas. Nevertheless, it may lead to unsatisfying results for data which is non-linearly correlated, since it "only projects the samples onto an optimal linear subspace" Ma and Zabaras (2011). There are also approaches to overcome this problem, which should be used to deal with non-linear relations in the sample space. "Work on nonlinear PCA, or NLPCA, can be divided into the utilization of autoassociative neural networks, principal curves and manifolds, kernel approaches or the combination of these approaches" Kruger et al. (2008). KRUGER et al. Kruger et al. (2008) analysed these approaches with respect to computational issues and their generalization of linear PCA. It can be found that principal curves and autoassociative neural networks are quite computationally demanding for larger data sets and do not adhere to the variance maximization criterion of the linear PCA Kruger et al. (2008). For example Kruger et al. (2008), Ma and Zabaras (2011) and Schölkopf et al. (1998) can give further insights.

3.2 Kernel Density Estimation

The Kernel Density Estimation (KDE), also known as the Parzen–Rosenblatt window method, is a method for estimating the underlying probability density function from N independent and identically distributed (i.i.d.) samples Parzen (1962). The probability density function of an unknown multivariate distribution is approximated by:

$$\hat{f}(x;K,h,d) = \frac{1}{Nh^d} \sum_{n=1}^N K\left(\frac{x-x_n}{h}\right) \tag{1}$$

where d is the dimension of the data, x_n are the samples for n = 1, 2, ..., N, h is the bandwith and $K(u) \ge 0$ a kernel function Matuszyk et al. (2010).

However, the choice of the kernel function K does not have a big influence on the results obtained by the KDE, but there are general rules for the choice of the value of h. For practical use of the KDE most numerical software systems offer functions for the kernel density estimation which compute the value of h as a function of the sample points N Matuszyk et al. (2010); Parzen (1962); The MathWorks (2010).

3.3 Statistical Shape Analysis

Statistical Shape Analysis (SSA) is very common in fields of computer vision and medical image interpretation Cootes et al. (2004), but can also be used in engineering applications. The field of SSA involves various methods to "measure, describe and compare the shape of objects" Dryden and Mardia (1999). Particularly, these methods focus on the analysis of objects, which can be described "by key points called landmarks" Dryden and Mardia (1999). Main goals are "to estimate population average shapes, to estimate the structure of population variability and to carry out inference on population quantities" Dryden and Mardia (1999).

The main goal in computer vision and medical image interpretation is image understanding Cootes et al. (2004). Therefore, SSA is used to develop Statistical Shape Models (SSMs), which enable machine vision "not only to recover image structure but also to know what it represents" Cootes et al. (2004). For this purpose, new unknown shapes are compared to a training set (i.e. a shape population). In contrast to that, in this work SSA and SSMs are used to create and simulate new shapes based on observations.

The procedure of SSA can be summarized as follows Zhang (2011); Stegmann and Gomez (2002):

1. Acquire a training set of n observations:

In the following applications the training set is gathered from manufacturing process simulations or measurement data.

2. Determine the correspondence between the training set:

This means, that landmarks have to be set or similar methods have to be used to express the correspondence between the training set. In general, this task is not easy, but for the applications presented in this work we use a quite forward approach. Cootes et al. (2004); Dryden and Mardia (1999); Niu et al. (2007) can give further detail.

3. Align the training set:

If the shapes differ in terms of rotation, scale and location, these differences need to be corrected. For example Procrustes Analysis, Generalized Procrustes Analysis and Tangent Space Projection are methods which can be used for this purpose Stegmann and Gomez (2002). Due to the structure of the training sets used in the context of this work, no alignment operations are necessary.

4. Establish a Statistical Shape Model: Some common SSMs are presented in the following subsections.

3.3.1 Univariate Shape Model

The univariate shape model represents the deviation of a shape with an univariate distribution for each point Zhang (2011); Matuszyk et al. (2010), which implies that the points are assumed to be statistically independent Matuszyk et al. (2010). Each distribution describes the deviation of a point in the direction of its normal Zhang (2011). Usually the underlying distribution for each point is assumed to be a Gaussian distribution.

This idea is quite simple but involves also some difficulties and limitations. Since the model consists of the information about the distribution of *each* point, the data can become confusing and "distilling important information from such a large set of descriptive statistics and developing an intuitive understanding of dimensional variation in the manufactured assembly" Matuszyk et al. (2010) can become very difficult. Though, the main problem is that in reality the deviations of the points are not statistically independent. Therefore, the univariate model tends to generate implausible shapes and likely overrates the variation of points close to each other Matuszyk et al. (2010).

3.3.2 Point Distribution Model

The point distribution model (PDM) was developed by COOTES et al. Cootes and Taylor (1992); Cootes et al. (1995); Cootes and Taylor (1997) and was originally designed for pattern recognition in computer vision Matuszyk et al. (2010). It has been extended by many researchers during the last 15 years and adopted to various fields besides computer vision Matuszyk et al. (2010). The basic idea behind the PDM is to express each shape as a combination of the mean shape \overline{X} , wich can be computed easily by:

$$\overline{\boldsymbol{X}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{X}_{i}$$

and the variation of the shape around the mean along the main modes:

$$\boldsymbol{X}_i \approx \overline{\boldsymbol{X}} + \boldsymbol{\Phi} \boldsymbol{b}_i.$$
 (2)

The main modes of variation are identified by applying a principal component analysis to the data. The scores \boldsymbol{b} of the mean modes are then described by estimating a multivariate Gaussian distribution Cootes et al. (2004); Matuszyk et al. (2010).

3.3.3 Kernel Density Estimate/Point Distribution Model

The Kernel Density Estimate/Point Distribution Model (KDE/PDM) introduced by MA-TUSZYK et al. Matuszyk et al. (2010) is based on the PDM. It enhances this model by applying a kernel density estimation to describe the distribution of the scores \boldsymbol{b} . Therefore, the assumption of a multivariate Gaussian distribution of the scores is lapsed. This results in a more precise description of the underlying main modes of variation and therefore in a better understanding and generation of random shapes based on the samples.

3.3.4 Kernel Principal Component Analysis/Kernel Density Estimate/Point Distribution Model

Another approach to deal with non-linearly correlated input data is to set up a point distribution model employing the kernel principal component analysis (KPCA) to estimate the main modes of variation Φ . The distribution of the scores b can then, similarly to the KDE/PDM, be estimated by a kernel density estimation. Since this model is similar to the PDM, but makes use of the KPCA and the KDE, it is referred to as KPCA/KDE/PDM.

In contrast to the PDM based on the linear PCA, the pre-images of the reconstructed data have to be found. Therefore, the KPCA/KDE/PDM is more computationally demanding than the KDE/PDM.

4 Representation and Generation of deviated Geometry

4.1 Procedure for the Representation and Generation of deviated Geometry

The highlighted SSMs, especial the point distribution models (PDM, KDE/PDM, KP-CA/KDE/PDM), can be employed for representing deviated sample shapes in the training set as well as for generating new samples based thereon. For this purpose, firstly all steps of the SSA as mentioned in the preceding section 3.3 have to be passed. After applying the linear or a nonlinear PCA to the training set the training set can be represented as:

$$X \approx \overline{X} + \Phi b,$$
 (3)

where each shape in the training set is expressed as a combination of the mean shape \overline{X} and the variation of each shape around this mean shape along the main modes of variation Φ . The scores **b** can then be found as random variables whose distribution can be estimated via a multivariate Gaussian distribution (PDM), a kernel density estimate (KDE/PDM, KPCA/KDE/PDM) or a polynomial chaos expansion (PCE). The generation of new samples from these distributions can then be performed by the inverse

transform method, i. e. samples are drawn from a standard uniform distribution and then put in the estimated inverse cumulative distribution function.

The overall procedure of generating new sample shapes can be summarized as follows (see also Figure 1):

- Drawing of samples from the estimated score distributions.
- Generation of new sample shapes following equation (2).



Figure 1: Generation of new sample shapes by the KDE/PDM

4.2 Consideration of Process Parameters

If the sample shapes in the training set stem from stochastic manufacturing process simulations, i. e. simulations with varying process parameter combinations or other parameters which have an influence on the shape of the samples (e. g. forces in structural finite element analysis), then the principal component scores b can be estimated from these parameters by employing meta models instead of estimating the score distributions by the KDE. In this case, the generation of new shapes starts with the drawing of samples from the parameter distributions. From these samples the resulting principal component scores are then calculated via the meta models. These scores in turn are then analogically to the mentioned KDE/PDM approach transformed by equation (2) in order to obtain new sample shapes which correlate to the sampled values for the process parameters. The procedure is illustrated in Figure 2.

In case of employing regression models for the estimation of the principal component scores from the manufacturing process parameters, the explanatory power of these regression models can be determined by the coefficient of determination R^2 , where R_k^2 depicts the coefficient of determination of the regression model for the *k*th principal component ϕ_k in the following. By weighting these coefficients with the portion of explained variability of each principal component and summing over all considered principal components, a prediction about the explanatory power of the whole approach can be derived:

$$R_w^2 = \sum_{i=1}^m R_i^2 \cdot \frac{\lambda_i}{\sum_{j=1}^p \lambda_j}.$$
(4)



Figure 2: Generation of new sample shapes according to the KDE/PDM considering the manufacturing process parameters

This metric R_w^2 is depicted as weighted Coefficient of Determination (wCoD) in the following. If other meta models than regression models are used for predicting the principal component scores from the process parameters then this idea can also be applied to the coefficient of prognosis CoP Most and Will (2008) and the weighted Coefficient of Prognosis can be obtained.

4.3 Training Set Size

As mentioned earlier, the training set of sample shapes is usually obtained from costly and time-expensive manufacturing process simulations or measurements. Thus, it may be relevant to know if the training set reflects the variability of the basic population or if the adding of new observations to the training set would lead to a better reflection of the populations variability.

For this purpose, it is advisable to plot the variability in the training set t_m stepwise for m = 1, 2, ..., N. If it can be seen that the variability stagnates of even decreases then it can be assumed that the adding of new observations to the training set will not introduce new variability and that therefore the training set size seems sufficient.

4.4 Subsumption

The proposed approach helps reducing the number of required manufacturing process simulations for generating a sufficient number of deviated geometry samples based on the process parameters. Therefore, it can be described as a meta modelling technique on geometry level since it aims at establishing an approximative relationship between the inputs (the manufacturing process parameters) and the resulting output geometry.

Of course, when considering the process parameters it is important to provide a sufficient quality of prognosis of the established meta models for ensuring an adequate quality of prognosis of the whole approach. The weighted Coefficient of Determination is a good basis for the evaluation of the explanatory power of the method.

The dynardo software product "Statistics on Structure" is a tool which allows visualizing the geometry samples as well as reducing the dimension of the underlying random field. This corresponds to the principal component analysis, that means that SoS allows for evaluating the principal components as well as the principal component scores.

	Cooling Time	Cooling Temp.	Injection Rate	Melting Temp.	Dwell Press.	Dwell Time	Density	Melt-Flow -Rate
$\mathcal{N}(\cdot, \cdot)$	[s]	$[^{\circ}C]$	$[cm^3/s]$	$[^{\circ}C]$	[MPa]	[s]	$[g/cm^{3}]$	[g/10min]
μ	10.0000	26.0000	24.8000	230.0000	25.0000	3.0000	0.9289	35.0000
σ	0.0600	0.6000	0.2300	1.5000	0.3000	0.0300	0.0030	0.5000

Table 1: Varied Process Parameters in the Molding Simulation



Figure 3: Variability in the Training Set

Thereafter, the obtained results can be imported and processed in optiSLang. This allows a simple and fast possibility for deriving the structural fluctuations of part geometry from the process parameters. The proposed approach was implemented in MATLAB but, however, it can also be performed in SoS and optiSLang in practical use.

5 Case Study – Molding Process Simulation

5.1 Introduction and Analysis of the Training Set

The reference part of the case study is a flat plate with a change in the wall thickness manufactured from a molding process from polypropylene. A stochastic manufacturing process simulation using Autodesk Simulation MoldFlow with 68 runs were performed, where eight process parameters were varied according a latin hypercube design plan (see Table 1). Figure 3 illustrates the variability in the result geometries of the training set with regard to the position of the element midpoints.

Employing SoS, the first four Eigenshapes of the structure were determined and plotted (see Figure 4) and the portion of variability explained by each principal component as well as their cumulative portion of explained variability were computed (see Figure 5). It can be seen, that the first principal component explains more than 98% of the geometric variability present in the training set.

Thereafter, for every principal component a regression model between the principal component score and the manufacturing process parameters was established. The coefficient of determination of the regression models is shown in Figure 6.

It can be seen, that especial the regression models for rear principal components have only weak explanatory power. However, since the first principal component already explains 98% of the variability in the training set, the corresponding regression model of this first principal component has the main effect on the power of this approach in this case. By weighting the coefficient of determination of each regression model with the portion of explained variability of the corresponding principal component, the weighted Coefficient of Determination can be derived, which results in case of ten considered principal



Figure 4: First four Eigenshapes of the reference Part



Figure 5: Explained Variability with respect to the number of considered PCs



Figure 6: Coefficient of Determination of the established Regression Models



Figure 7: Variability in the Training Subset against the number of considered Observations

components in this case study to:

$$R_w^2 = \sum_{i=1}^{10} R_i^2 \cdot \frac{\lambda_i}{\sum_{j=1}^p \lambda_j} = 98.0245.\%$$

It may be inferred that the generation of new geometry sample shapes based on the linking of meta models and the principal component analysis seems promising in this example.

For eventually clarifying if new observations should be added to the training set, the variability in the training set is stepwise plotted against the number of considered observations (see Figure 7). A plateau and even a slightly decreasing trend can be observed for the number of considered observations greater than 60. This implies a sufficient number of observations in the training set since it can be expected that the adding of new observations to the training set will not introduce new variability.

5.2 Generation of new Geometry Sample Shapes

The generation of new geometry sample shapes based on the given training set and the linking between the regression models and the principal component analysis can be performed as illustrated in Figure 2. First of all, new manufacturing process parameter combinations are sampled which serve as input parameters for the regression models. The so computed principal component scores are then put in equation (2) and new geometry sample shapes can be obtained.

For the reference part a geometry sample was generated for a process parameter combination which was also simulated in MoldFlow. Figure 8 shows the difference of the deviations of the element midpoints between the proposed approach and the simulation.

The difference with regard to the element midpoint deviations between simulation and the proposed approach lie in a range of $[-8.23 \cdot 10^{-4}; 2.79 \cdot 10^{-4}]$, which is about 8% in relation to the largest midpoint deviation in the data set.

Figure 9 shows the variation of the element midpoint deviations. A good accordance can be seen compared to the observed variation in the training set (see Figure 3) which implies that the generated geometry sample shapes reflect the observed variability in the training set quite well. Thus, the proposed approach seems to give good results for the



Figure 8: Difference of Element Midpoints between the proposed Approach and the Simulation



Figure 9: Variability in the generated Geometry Sample Shapes

generation of deviated geometry based on manufacturing process simulations and can therefore be used in tolerance simulations.

5.3 Analysis of Sensitivity with Respect to the Manufacturing Process Parameters

Based on the obtained information about the relationship between manufacturing process parameters and the principal component scores conclusions about the influence of the process parameters on the geometric deviations of the structure can be derived. Since, in this example the first principal component accounts for more than 98% of the variability in the training set it seems adequate to focus only on this first pc in the analysis of sensitivity. For this purpose, the principal component scores of the first PC were determined in SoS and afterwards exported to an optiSLang result file. In optiSLang the Coefficient of Importance for every manufacturing process parameter with respect to the scores of the first principal component were evaluated (see Figure 10).

Obviously, the melting temperature has the main influence on the scores of the first principal component and therefore for the geometric deviations of the reference part.

Based on the proposed approach for the generation of deviated geometry the effects of fluctuating process parameters on the geometric deviations of the part can be demonstrated. For this purpose, based on the assumptions about the distributions of the manufacturing process parameters (see Table 1) random samples of the manufacturing process parameters were drawn where only one parameter was varied at a time. From these samples new geometries were generated. The standard deviations of the element midpoint deviations are shown in Figure 11.

It can be seen that the variation of the melting temperature has the major effect on the geometric deviations. Furthermore, a quite good impression of the effects of manufacturing process parameter variations on the geometric deviations can be obtained.



Figure 10: Coefficient of Importance of the Manufacturing Process Parameters for the first Principal Component Scores

6 Conclusion and Outlook

Fluctuations of manufacturing process parameters have considerable effects on the origin of geometric deviations which hugely decrease the quality and function of technical products. Therefore, product developers try to predict these effects by the use of 3D tolerance simulations and to ensure the product function by specifying geometric tolerances. For performing these simulations, it is necessary to generate realistic part geometries which reflect the observable geometric deviations.

The proposed approach aims at generating deviated geometry sample shapes based on a limited training set of observations. In contrast to existing approaches which generate these geometry samples randomly the proposed method considers knowledge about manufacturing process parameters and links the geometric deviations to these process parameters. Thereby, geometric sample shapes can be generated from a given parameter combination.

The approach was illustrated in a simple case study of a molding part. Important steps of the procedure were performed employing SoS and optiSLang by dynardo. The application to more complex structures and processes, the transfer to other fields of robust design (e.g. structural finite element analysis) as well as improving the combination of existing software tools are ongoing research topics.

Acknowledgements

The authors thank the dynardo GmbH for their support and the provision of optiSLang and Statistics on Structure for research.



Figure 11: Effects of the Variation of Manufacturing Process Parameters on the Standard Deviation of the Element Midpoint Deviation

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