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AN INTEGRATED SURROGATE MODELING APPROACH FOR MATERIALS AND PROCESS DESIGN

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Abstract

In order to describe continuous optimization tasks for the efficient design of materials and production processes from a reasonable data sample size, we propose an integrated surrogate modeling approach. We show the proof of concept by application to a draw bending simulation that describes the relation between the process parameters and the spring-back as the process result. The introduced concept can also be directly applied to experimental data while taking into account the process noise as uncertainty (e.g. for process control). The integrated approach combines three components: Design of Experiments, surrogate process modeling (based on function approximation by regression, e.g. Artificial Neural Networks) and optimization of process or material parameters. The identified parameters enable to rapidly find the optimal operating conditions for real experiments or to constrain them for further detailed simulation studies. Future work involves applications to more complex experiments or simulations to efficiently determine the optimal process or material parameters by sparse and adaptive data samples.

Introduction

Process and materials design requires a high effort when all possible parameter combinations have to be executed (high complexity). Instead, a systematic procedure such as Design of Experiments (DoE) is needed to select a reasonable number of runs from experiments or simulations in order to gain the most information for a selected sample size. Hence, the effort of material and personnel cost in case of experiments as well as computational cost in case of simulations can be reduced. However, the selected data sample only represents discrete candidates and the optimal solution might lie somewhere in between. Surrogate models created from the data sample allow continuous and fast predictions that span the entire search space (by interpolation). The optimal material or process parameters can be determined with respect to a desired result using the surrogate process model. With our proposed integrated surrogate modeling approach, we concentrate on solving continuous optimization tasks from a reasonable data sample size.

Our previous work deals with statistical process control in deep drawing. The force as a time-dependent parameter for the sheet metal forming process is optimized to reach a given final stress state in the sheet under consideration of uncertainty during processing (overview [1], control details [2]). We have generated the underlying data sample from basic deep drawing simulations superimposed by artificially created, normally distributed process noise. Since the data sampling does not induce high computational cost in this

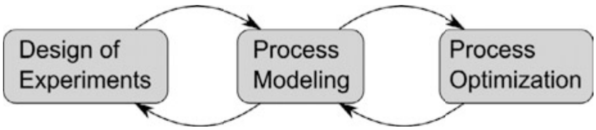

Figure 1: Integrated approach for rapid prototyping with interconnected components

particular case, we have created an extensive sample (with all parameter combinations) to establish the process model in a next step.

In contrast to conventional DoE, Sequential DoE is not limited to a data sample size that is fixed in advance. Instead, Sequential DoE enables the adaption of the data sample during processing taking into account already existing information. [3] points out the application of Sequential DoE with generalized linear models. [4] compares different sequential design methods for global surrogate modeling on a real-world electronics problem. [5] builds a surrogate model by adaptive sampling. These three Sequential DoE approaches have in common that the data sampling and modeling is interconnected and adaptive which is a big advantage for complex tasks that are difficult or even impossible to handle with conventional DoE.

In this paper, we do not focus on process models and control, but on connecting DoE, process modeling and process optimization to realize rapid prototyping for materials and process design on the one hand, and to handle more complex tasks with Sequential DoE and adaptive learning models on the other hand. We exemplify the introduced concept with data from a draw bending simulation.

Integrated Surrogate Modeling Approach

Our integrated surrogate modeling approach combines three components as depicted in Figure 1. The single components are exchangeable (e.g. different designs or model types) and the integrated procedure enables a forward and backward adaption of the individual components. This enables rapid prototyping for materials and process design as described hereinafter. A data sample is created by DoE from simulations or experiments. The data serves as a base for surrogate modeling to describe the relation between process parameters (input) and result (output). The established process model allows to determine the optimal parameters with respect to a desired result (process optimization).

Design of Experiments

Design of Experiments [6] allows to plan runs of simulations or experiments to gain the most information about a process with reasonable effort. Additional runs are required to quantify the uncertainty in real experiments compared to deterministic simulations. It is possible to determine the sample size beforehand if the variance in the process is known. Instead of using a fixed sample size, the data sample can be adapted by Sequential DoE such that individual runs are added incrementally until a stopping criterion is reached (e.g. based on the distance of parameter combinations).

Process Modeling

The relation between process input and output can be described with surrogate models [7] based on function approximation by regression. There exist linear regression models such as Partial Least Squares Regression (PLS) [8]. PLS combines regression with dimension reduction by decreasing the dimensionality of the input and output space, and at the same time, maximizing the covariance between the reduced quantities. This procedure is suitable for models with many input and output dimensions, since the complexity (in terms of model degrees of freedom) is decreased by dimension reduction. However, PLS does not consider nonlinearities that can on the other hand be addressed with Artificial Neural Networks (ANNs) [9]. A typical feed-forward ANN consists of three interconnected layers: input, hidden and output. The input nodes are connected with the hidden nodes which are again connected with the output nodes. The connections are associated with weight factors. In the hidden and output layer, for each node, the sum of all incoming connections multiplied with the connection weights is calculated and subject to an activation function (hidden layer: hyperbolic tangent or linear, output layer: linear). The training of an ANN involves the adjustment of the connection weights such that its prediction approximates the output from the given data sample (by error minimization). The underlying data set is divided into training data (to establish the model) and test data (to validate the model). One distinguishes between batch and incremental learning of ANNs. In batch learning, all runs of the training data are used to update the connection weights simultaneously (by taking the average), while in incremental learning the connection weights are updated step by step according to each single run.

Process Optimization

We define process optimization as the task to determine optimal process parameters (control variables or constant operating conditions as input) with respect to a desired process result (output). We distinguish between offline and online optimization. In the first case, the parameters to be optimized are constant over time, while in the second case, the parameters are time-dependent and have to be optimized for each single time step (also taking into account uncertainties in the result). Examples for process optimization are given as follows. The local blank holder forces of a deep drawing process are optimized over segments and time from simulations in [10]. A (bio)chemical process with time-dependent behavior is optimized considering uncertainties in [11].

Draw Bending Simulation

The two-dimensional draw bending example process is visualized in Figure 2. A metal sheet is clamped between a blank holder and a die. A punch presses the sheet into the die opening such that it is subject to bending. When the bent sheet is unloaded, it undergoes an elastic spring-back that results from the residual stresses in the sheet. We simulate the process with SIMULIA Abaqus according to [12]. The process parameters with their lower and upper limits and the process result are summarized in Table I. The parameters that influence the draw bending process comprise: Young's modulus, Poisson's ratio, blank geometry (width and length), coefficient of friction, blank holder

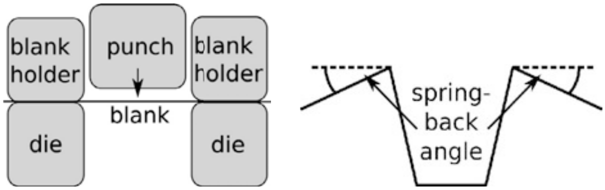

Figure 2: Two-dimensional draw bending process (left) with resulting spring-back (right)

Table I: Process parameters and result

Parameter (input)	Result (output)	Name	ID	Lower limit	Upper limit	Unit
x		Young's modulus	x_1	165	247	GPa
x		Poisson's ratio	x_2	0.24	0.36	-
x		blank width	x_3	4	6	mm
x		blank length	x_4	140	210	mm
x		coefficient of friction	x_5	0.115	0.173	-
x		blank holder force	x_6	-210	-140	N
x		punch velocity	x_7	-18	-12	m/s
	x	spring-back angle	y			°

force and punch velocity. The spring-back angle is the result.

Results

We have implemented the proposed concept in Mathworks MATLAB (with toolboxes: optimization, global optimization, neural network, statistics) and SIMULIA Abaqus (Finite Element Analysis software) with Python scripting. We use deterministic simulations without taking into account uncertainty. We optimize seven time-independent parameters to minimize spring-back in the draw bending process.

Design of Experiments

We create a screening design for all seven process parameters at two levels that correspond to the lower and upper parameter limits (see Table I): a full factorial of all possible parameter combinations with $128 = 2^7$ samples. The screening corresponds to a sensitivity analysis of the process parameters on the result and reveals the relevant parameters. The box plots in Figure 3 indicate a high influence for the Young's modulus (x_1) and the punch velocity (x_7), and a low influence for the coefficient of friction (x_5) and the blank holder force (x_6). The parameters x_5 and x_6 are neglected in the following.

For the ensuing process modeling, we create three advanced designs for the five selected parameters (with fix values for $x_5 = 0.173$ and $x_6 = -210$ N) at three levels (for nonlinearities): full factorial with $243 = 3^5$ samples, d-optimal with 81 samples and central composite with 43 samples. The two latter are (extended) subsets of the former.

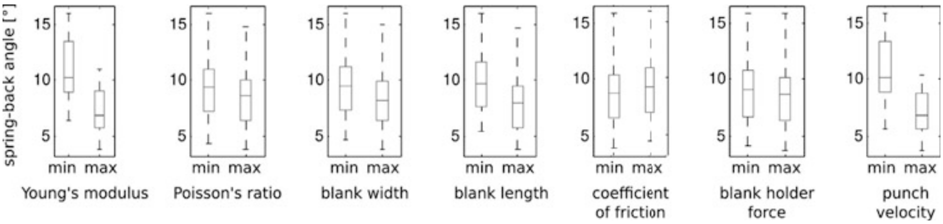

Figure 3: Influence of process parameters on result (full factorial screening design)

Table II: Goodness of fit for approximation models R^2

	PLS	ANN batch		ANN incremental	
Design	linear	nonlinear	linear	nonlinear	linear
full factorial (243 samples)	0.9739	0.9946	0.9739	0.9811	0.9703
d-optimal (81 samples)	0.9747	0.9954	0.9747	0.9874	0.9744
central composite (43 samples)	0.9738	0.9599	0.9735	0.9502	0.9739

Process Modeling

For the three advanced modeling designs, we compare linear PLS (five components) with linear and nonlinear ANNs (five nodes in the hidden layer) with batch and incremental learning in Table II. The goodness of fit for the surrogate process model is quantified by the coefficient of determination:

$$R^2 = 1 - \frac{SSE}{SST}. \tag{1}$$

The sum of squared errors (SSE) is the sum of the squared deviations between the test data set y and the associated predicted results $\hat{y}$ calculated over all N samples:

$$SSE = \sum_{n=1}^{N} (y - \hat{y})_n{}^2. \tag{2}$$

The SST is the total variation in the test data set calculated by the summed squared deviations of the test data from their means. The R^2 (typically between 0.0 and 1.0) has a high value for a good model fit and a low value for a poor fit. For our results, it is averaged over five independent modeling runs with varying random initial conditions.

Table II shows the highest R^2 for nonlinear ANNs in combination with the full factorial design and the d-optimal design, whereas batch learning outperforms incremental learning. The models built on the central composite design are characterized by the lowest R^2, especially in the nonlinear cases. The sample size of the central composite might be too small to describe the nonlinearities of the considered process relation appropriately. PLS yields moderate, but robust results for all designs. We obtain comparable model prediction accuracy for the different designs that vary in sample size considerably.

Process Optimization

We implement the process optimization with the presented batch learning ANN surrogate model to determine the optimal values for the five selected parameters x_1, x_2, x_3, x_4, x_7

Table III: Optimal process parameters x_1, x_2, x_3, x_4, x_7 for minimum spring-back y

Design	x_1	x_2	x_3	x_4	x_7	y
full factorial (243 samples)	247	0.36	6	210	-12	4.9726
d-optimal (81 samples)	247	0.36	6	210	-12	4.8585

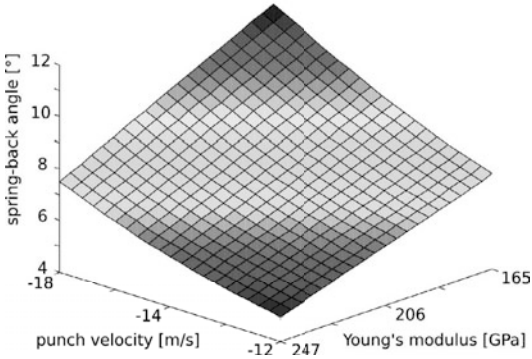

Figure 4: Optimal Young's modulus (x_1) and punch velocity (x_7) for minimum spring-back y (d-optimal design)

for minimum spring-back. We combine a Genetic Algorithm [13] with lower and upper parameter limits for global optimization with a gradient-based Newton algorithm [8] for local optimization (fine-tuning around the global solution).

Table III presents the optimal parameter values for the full factorial and the d-optimal design that match exactly for the investigated case. The spring-back predicted by the batch learning ANNs differs slightly due to the different designs and the resulting varied initial conditions. Figure 4 depicts the Young's modulus x_1 and punch velocity x_7 that lead to minimum spring-back for the d-optimal design. The spring-back is visualized as a surface function over the two-dimensional parameter space with its minimum at $x_1 = 247$ GPa, $x_7 = -12$ m/s.

Extension of the Integrated Approach

We are currently working on extending the proposed integrated approach in view of Sequential DoE. This removes the limitation of initially fixed sample size by adapting the design during the execution of process runs (experiments or simulations) taking into account already existing information. Both extensions (see Figure 5 and Figure 6) contain an initial DoE component to create an initial space filling design (e.g. Latin hypercube or grid sampling [4]). In a next step, Sequential DoE enables the extension of the initial design by taking into account new samples with respect to 1) the design (parameter) space or 2) the response (result) space.

1) Sequential DoE with sample selection with respect to design space

In the extension with sample selection with respect to the design space (Figure 5),

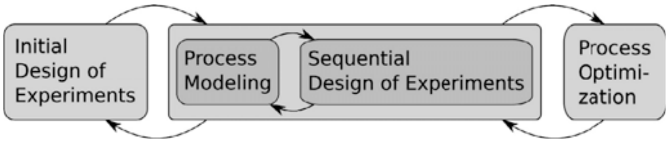

Figure 5: Extension of integrated approach with respect to design space

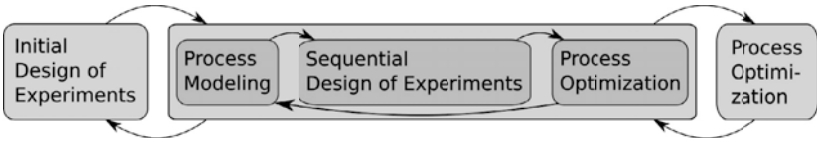

Figure 6: Extension of integrated approach with respect to response space

an initial process model is implemented from the initial design and then incrementally adjusted by each new sample (inner loop). If the model accuracy is satisfactory, it is finally used for process optimization. New samples with respect to the design space can either be selected randomly or with a distance-based criterion. A random selection covers the entire design space for many runs, but does not create a sparse and adaptive data sample. However, this can be achieved by a distance-based sample selection with respect to the design space which is the common procedure in comparison to sample selection with respect to the response space. Nevertheless, the design space is typically multi-dimensional compared to the scalar response, which leads to a high complexity.

2) Sequential DoE with sample selection with respect to response space
The distance-based sample selection with respect to the response space (Figure 6) enables the generation of a sparse and adaptive data sample regarding the actual quantity of interest which is typically only one-dimensional. An initial process model is built from the initial design and then incrementally adjusted by each new sample that is selected with respect to the response space. A process optimization step is required to determine the optimal process parameters (in the design space) from the distance-based selected response. This (inner loop) is repeated until the model is exact enough and it can be applied for the final process optimization to determine the optimal parameters with respect to a desired result. The most crucial point in this case is to use the process model for optimization at an early stage (after initial modeling). This can be addressed by selecting an adequate initial design.

Conclusion

We have introduced an integrated approach for rapid prototyping in process and materials design by combining DoE, surrogate process modeling and process optimization. We have compared different designs and regression models. Our results show that we obtain the same optimal process parameter values for minimum spring-back from a detailed full factorial design (243 samples) as from a reduced d-optimal design (81 samples). We have proposed extensions with Sequential DoE to efficiently create and handle sparse and adaptive data samples for process or material optimization. Future work involves the refinement and evaluation of the extensions and the transfer to more complex tasks.

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