Flexible Process Modeling Determined by Existing Human Expert Domain Knowledge Bases

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***Abstract*— The evaluation of final workpiece properties at process end can be realized by process modeling instead of destructive testing methods. In this paper, we give an overview about different modeling strategies. They are focused on the amount of available domain knowledge. White box models try to model the reality by physical principles and black box models are mainly data driven. Grey box models are hybrid variants. The different strategies are applied to the domain of resistance spot welding. The proposed approaches are able to improve the quality of resistance spot welding.**

Keywords- Intelligent Systems; Machine Learning Manufacturing.

I. INTRODUCTION

Several methods exist to model the dynamics of nonlinear complex systems [1]. Conceptually, they can be split into two classes. The first class includes prior domain knowledge from human experts. For example, numerical simulations like finite elements or phase field methods describe the behavior of systems with domain knowledge from human experts. The second class is characterized by the use of phenomenological or general basis function models, which try to fit the observed behavior of the systems as good as possible. The latter approach includes many Machine Learning, Data Mining and statistical methods.

The second class can be further refined in modeling via symbolic [2, 3] (e.g., general formula expressions) and subsymbolic (e.g., dedicated base function class, support vector machines or neural networks) representations. Symbolic learning representations can be interpreted by human domain experts and they can help to understand the process in a more formal way. Therefore, this class does not only aim to model the system behavior. Sometimes the human experts are able to identify previously unknown facts of the observed process.

In contrast, subsymbolic representations are black box models. In most cases, it is very difficult or impossible to interpret the behavior of the learnt representation [3].

The proposed methods in this paper can be interpreted as modeling the dynamic of processes. A generic process model is depicted in Fig. 1 with an observer and a controller. This representation enables a universal process description by means of the observable quantities, the characteristic process state and the process parameters that allow manipulating the process purposefully. The observer can predict the characteristic state and the workpiece properties for quality evaluation from static or dynamic observable quantities. The observer model depends on the embedded domain knowledge (white, grey or black box). Independently from this, the observer model that represents the process dynamics might be of static or dynamic model type. The controller can then determine the optimal process parameters from the evolution of the characteristic state by solving a multi-stage optimization problem compensating the process noise.

The purpose of this paper is twofold. It can be used as a guideline and introduction for the creation of a model for system processes with different constraints on the amount of existing prior domain knowledge and/or insufficient experimental data. On the other hand, it attempts to give an overview of our developments concerning intelligent systems. The application domain is resistance spot welding. To this end, we decided to summarize the results of some of our projects, give some background information and refer to some of our already published papers. This article is organized as follows. We start in Section II by giving a brief overview of different modeling strategies, which are predetermined by the amount of existing prior system knowledge and the amount of observed experimental system data. These approaches include in general white box and black box models. Grey box models represent a compromise between both ideas. Section III gives a brief overview on resistance spot welding. Section IV reviews some basic ideas of the used Machine Learning, Data Mining and parameter fitting techniques and section V summarizes how we use them. We conclude with a discussion of open questions and future steps of our project. Most of the results and conducted

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experiments have been published elsewhere, but this paper focuses on an comprehensive overview.

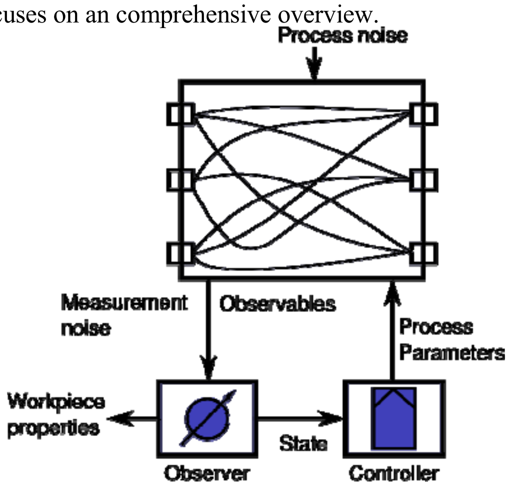

Figure 1. A generic process model.

II. PROCESS MODELING

The basis of system identification is always a model illustrating an idea of the physical reality. In principle, two major modeling approaches can be identified. They are different in terms of the used structure and the free parameters of the model. The structure determines the general behavior and the complexity of the model (qualitative model description) and the parameters determine the specific behavior of a given structure (quantitative model description). Generally, the approaches depend on the existing prior knowledge about the modeled system.

White box models: White box models result from complete understanding of the system behavior and theoretical analysis. This analysis is performed by formulating physical or geometric equations. The predefined model structure and the precise match of the internal model parameters and known physical parameters (e.g., from textbooks) are characteristic for white box models. From this point of view, the parameters are interpretable in a symbolic way which includes a predefined semantic. The model parameters can be compared and fitted to measurements. White box models usually have a high accuracy. However, they assume that the system behavior was analyzed in great detail, which can often be very time-consuming or even impossible. White box models are from this point of view parametric models and the parameters are interpretable by human experts.

Black box models: Sometimes the complicated and time consuming theoretical analysis is not possible. The lack of knowledge of the underlying system principles requires alternative approaches. Most of them make use of the experimental observation data and thus the learning process is mainly data driven. This means that the free parameters of the model are optimized to reproduce the observations of the system as good as possible. The optimized model is a so-called black box model or grey box model. The difference between the two model types is determined by the amount of prior knowledge which is integrated into the model. The characteristic property of black box models is that there is no or very limited prior knowledge about the behavior and structure of the observed system. Typically, the free parameters of the model have no direct link to the physical meaning of the system. In this case, we refer to non-parametric models (aka subsymbolic knowledge representation). It reflects only the input and output of the system and the physical parameters are represented implicitly by the values of the weighting functions (e.g., the basis functions in neural networks). The parameters of a black box model are not interpretable by a human expert.

Grey box models: Grey box models are a mixture of white box and black box models. They generally involve information from physical equations and data as well as qualitative information in form of rules. Grey box models often judge on the basis of assumptions about the structure of the system and the process. In this case, the free parameters of the system have a physical meaning of the system and we refer to parametric models (aka symbolic representation).

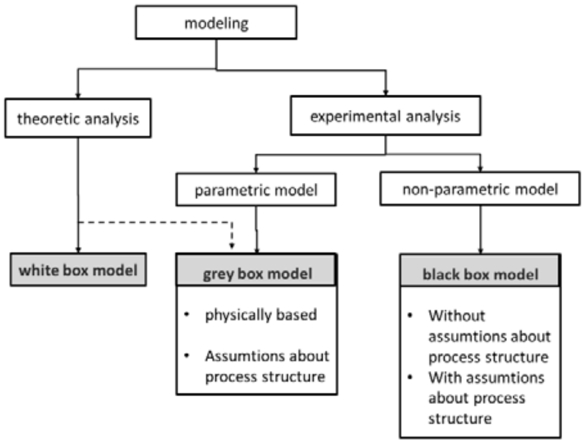

Figure 2. Process modeling.

TABLE I. PROCESS MODEL AND PROPOSED METHODS

	Proposed Methods
white box model	Simulations (e.g., Sorpas)
grey box model	Phenomonologic Model, Symbolic Regression
black box model	SVR

Which type of model is chosen depends on the amount of prior knowledge about the system and the intended use of the extracted model. From a control theory standpoint [4, 5], internal system states are mandatory. This includes white and grey box models. The dynamics of the system (e.g., the behavior of resistance spot welding proposed in this paper) are modeled and the internal states are used to (re-)adjust the parameters in order to optimize the parameters of a goal function. This goal function can be of completely diverse nature, but in most cases it involves reducing costs.

In some use cases, a mapping from the input of a system to its output is sufficient. In these cases, black box models can be applied and experimental data can be used for the learning process. In this case, the dynamics of the system are not modeled. Consequentially, readjusting parameters during operational time is not possible. Even though, the goal function can also be optimized since a mapping from the starting parameters to the final states is constructed and a good starting point from the parameters can be chosen.

Table I summarizes the methods which we elaborated in the course of our projects. Support Vector Regression (see Section IV) is a black box model and is able to map the starting parameters to the final states in an efficient way. Phenomonologic models (which are also expanded by a correction term found by Symbolic Regression) are used to model the system dynamics in a sense of control theory. That means, that the parameters can be readjusted during the service time to further improve the quality of the process.

In the following section, we will introduce the application of resistance spot welding following by a brief introduction to the used methods (Section IV).

III. RESISTANCE SPOT WELDING

In resistance spot welding (RSW, see [8, 9] for more details), two metal sheets are joined together by means of an evolving welding spot that results from local melting of the sheet material. The melting is caused by the electrical current flow and an associated temperature increase through the application of an electrode force and an electrical current. The experimental RSW environment with its tools, namely the electrodes, the two sheets and the individual resistance components that describe the combined dynamic resistance is depicted in Fig. 3. The temporal evolution of the dynamic resistance is shown in Fig. 4. The diameter of the welding spot serves as a visual, nondestructive quality indicator for the processed experiments. During RSW, quantities such as the electrical current, the voltage, the electrode force and the electrode displacement can be measured. The electrical resistance can then be calculated from the current and the voltage.

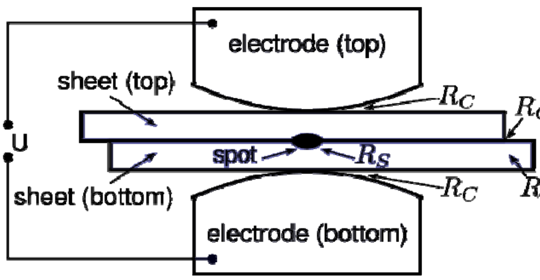

Figure 3. Experimental resistance spot welding environment: tools, sheets and resistance components.

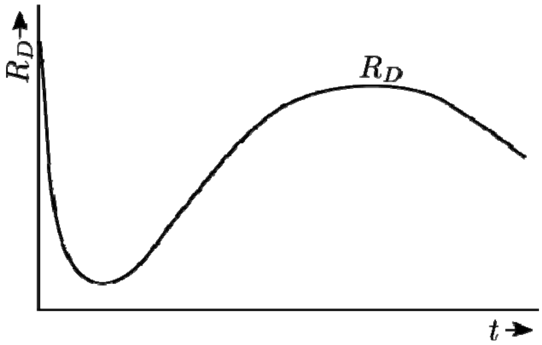

Figure 4. Temporal evolution of the dynamic resistance during resistance spot welding.

Analytical resistance model

In our previous work [6, 7], we have formulated an analytical model of the dynamic resistance that is composed of the individual resistance components as indicated in Fig. 1. The combined dynamic resistance $R_D(t)$ is composed of the bulk resistance $R_B(t)$, the contact resistance $R_C(t)$, the spot resistance $R_S(t)$ and the static resistance $R_0(t)$:

$$R_D(t) = R_0(t) + R_B(t) + R_C(t) + R_S(t)\,. \qquad (1)$$

The bulk resistance

$$R_B(t) = \alpha_{BL} \cdot (1 - \exp(-\alpha_{BC} \cdot t)) \qquad (2)$$

describes the rising resistivity in the bulk material with increasing temperature. The contact resistance

$$R_C(t) = R_{CF}(t) + R_{CC}(t) = \alpha_{CFD} \cdot \exp(-\alpha_{CFC} \cdot t) + \alpha_{CCD} \cdot \exp(-\alpha_{CCC} \cdot t) \qquad (3)$$

consists of the contact film resistance $R_{CF}(t)$ caused by contaminations on the sheet surface and the contact constriction resistance $R_{CC}(t)$. The contact resistance decreases with increasing contact area. The spot resistance

$$R_S(t) = -\alpha_{SH} \cdot \frac{1}{1 + \exp(-\alpha_{SC} \cdot (t - \alpha_{SD}))} \qquad (4)$$

drops with the evolution of the welding spot. The static resistance

$$R_0(t) = \alpha_O = const. \qquad (5)$$

comprises the constant percentages of all previously introduced resistance components. The meaningful features of the dynamic resistance can then be represented by the model parameters

$$[\alpha_O, \alpha_{BL}, \alpha_{BC}, \alpha_{CCD}, \alpha_{CCC}, \alpha_{CFD}, \alpha_{CFC}, \alpha_{SC}, \alpha_{SH}, \alpha_{SD}]$$

which can be determined by fitting the model to experimental data. A fitted model instance from [2, 7] is depicted in Fig. 5.

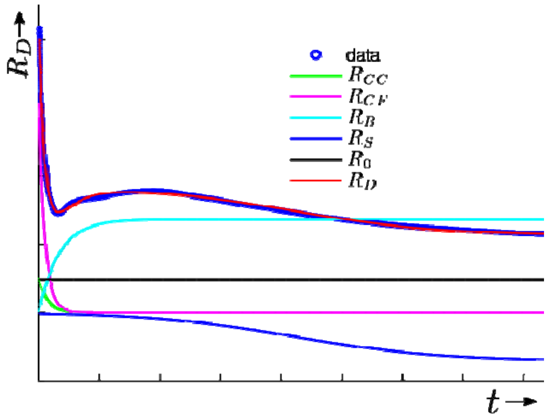

Figure 5. Analytical resistance model fitted to data.

IV. MODELING APPROACHES

This section provides a brief overview of the used methods. Due to a lack of space of this paper, we have to limit the explained methods. For example, the proposed Support Vector Machines should be reread in the literature (see [1] for more details)

A. Nonlinear Curve Fitting + Partial Least Squares

A grey box model for predicting the welding spot diameter as a quality measure from the meaningful features of the dynamic resistance has been introduced in [8, 9]. In a first step, the analytical resistance model described in the previous section is fitted to experimental data for each sample by Nonlinear Curve Fitting (NCF). This results in a low-dimensional feature representation for each individual experiment. In a second step, a Partial Least Squares Regression (PLS) is performed with the features as regression input and the welding spot diameter as regression output.

In NCF, the free model parameters are determined by nonlinear optimization. The objective function is formulated by means of the deviation between the model and the data, e.g., the Sum of Squared Errors (SSE) which is to be minimized. Then, the model represents the real process given by the experimental data in an optimal manner.

PLS combines linear regression with dimension reduction in regression input and output. The dimension reduction is performed similarly as in Principal Component Analysis (PCA) which finds orthogonal directions of largest variance in the data and projects the data to a lower-dimensional space of only the selected components. In PLS, the single steps of dimension reduction in input and output as well as the linear regression are interconnected by an iterative procedure, such that the covariance between the input and the output is maximized. As a result, PLS does not solely provide an efficient regression method to establish a model for the prediction of a target quantity. It additionally reveals the influences of the input on the target quantity.

B. Classical Regression Analysis and Symbolic Regression

Regression analysis [10] is one of the basic tools of scientific investigation. It enables the identification of functional relationships between independent and dependent variables and the general task is defined as the estimation of a functional relationship between the independent variables $\mathbf{x} = [x1, x2, \dots, xn]$ and dependent variables $\mathbf{y} = [y1, y2, \dots, ym]$, where n is the number of independent variables in each observation and m is the number of dependent variables.

The task is often reduced from the identification of an arbitrary functional relationship f to the estimation of the parameter values of a predefined (e.g., linear) function. That means that the structure of the function is predefined by a human expert and only the free parameters are adjusted. From this point of view, Symbolic Regression goes much further.

Like other statistical and machine learning regression techniques, Symbolic Regression also tries to fit experimental data. But unlike the well-known regression techniques in statistics and machine learning, Symbolic Regression is used to identify an analytical mathematical description and it has more degrees of freedom in building it. Therefore, a set of predefined (basic) operators is defined (e.g., add, multiply, sin, cos) and the algorithm is mostly free in concatenating them. In contrast to the classical regression approaches, which optimize only the parameters of a predefined structure, here also the structure of the function is free and the algorithm both optimizes the parameters and the structure of the basis functions.

Since Symbolic Regression operates on discrete representations of mathematical formulas, non-standard optimization methods are needed to fit the data. The main idea of the algorithm is to focus the search on promising areas of the target space while abandoning unpromising solutions (see [11, 12] for more details). In order to achieve this, the Symbolic Regression algorithm uses the main mechanisms of Genetic and Evolutionary Algorithms. In particular, these are mutation, crossover and selection [12] which are applied to an algebraic mathematical representation.

The representation is encoded in a tree [12] (see Fig. 6). Both the parameters and the form of the equation are subject to search in the target space of all possible mathematical expressions of the tree. The operations are nodes in the tree (Fig. 6 represents the formula 6x+2) and can be expressed by mathematical operations such as additions (add), multiplications (mul), abs, exp and others. The terminal values of the tree consist of the function's input variables and real numbers. The input variables are replaced by the values of the training dataset.

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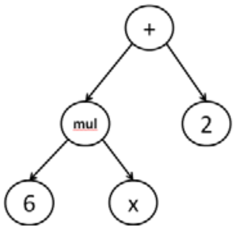

Figure 6. Tree representation of the equation 6x+2.

In Symbolic Regression, many initially random symbolic equations compete to model experimental data in the most promising way. Promising are those solutions, which are a good compromise between correct prediction quality of the predicted data and the length of the computed mathematical formula.

Mutation in a symbolic expression can change the mathematical type of formula in different ways. For example, a div is changed to an add, the arguments of an operation are replaced (e.g., change 2*x to 3*x), an operation is deleted (e.g., change 2*x+1 to 2*x), or an operation is added (e.g., change 2*x to 2*x+1).

The fitness objective in Symbolic Regression, like in other machine learning and data mining mechanisms, is to minimize the regression error on the training set. After an equation reaches a desired level of accuracy, the algorithm returns the best equation or a set of good solutions (the pareto front). In many cases, the solution reflects the underlying principles of the observed system.

V. EXPERIMENTS AND RESULTS

In this section we summarize the basic ideas of the used methods. For more details we refer to the literature.

A. Support Vector Regression

In [13], we describe and evaluate the use of Support Vector Regression to determine a statistical model for a welding spot function associated with a resistance spot welding process (see section III). Based on the training data a Support Vector Regression is used to extract a welding spot diameter function (our goal function) of five variables: current, welding time, force, sheet thickness of material. According to this diameter function, we developed a description of our optimized method needed by an intelligent welding machine.

The SVR represents a black box model (subsymbolic representation), which incorporates no prior domain knowledge. The results were very promising (see [13] for more details). A maximum error value of 0.29mm in the welding spot diameter in a typical range of 2.5 and 6.5mm indicates a good model quality.

B. Nonlinear Curve Fitting + Partial Least Squares

A model for the welding spot diameter based on the meaningful features of the dynamic resistance has been created in [7]. Domain knowledge is embedded through an analytical resistance model, which is fitted to experimental data by NCF. Then, the welding spot diameter is determined from the fitted model parameters as the features of the dynamic resistance by a PLS model. The prediction quality is characterized by a mean relative error value of 8%.

C. Improving a Phenomonological Model by Symbolic Regression

In [6, 7] the process dynamics are modeled by a parameterized phenomenological base model with fixed structure (see Section III). Additionally, Symbolic Regression is used to add a flexible correction term [6], which reflects process effects not considered in the base model. The full model is formed by simultaneous parameter fitting and adding a correction term found by Symbolic Regression. While the phenomenological model covers the major effects that occur in the Resistance Spot Welding process, the correction term can explain further hidden procedures in the residuals of the former. The phenomenological model has been created by use of expert knowledge and the formation of a grey box model. The symbolic correction term found by Symbolic Regression might be interpretable by a human expert again. In the paper, it has been shown that the phenomenological model yields good results, which are further improved by the correction term added by Symbolic Regression.

VI. CONCLUSIONS AND FUTURE WORK

Different approaches have been proposed in this paper that try to improve the quality of resistance spot welding by modeling the process dynamics. Throughout the last years different approaches have been evaluated. In this paper, we propose a scheme to select an adequate model based on the prior domain knowledge.

The different approaches have been successfully applied to the domain of resistance spot welding. Our next step is to demonstrate that this approach is general enough to be applied to other domains.

Future work includes modeling the system dynamics. That means, the described methods will utilize the measured process inputs and outputs to construct static process model components. Therefore we use system information of time step t to predict time step t+1. In the future, we will use time series to model the system information as continuous process dynamics. Instead of using measured output data of the previous time step as input for the current time step, the output is represented as a function of the previous time step. Thus, the process output can be modeled as a function of the previous input and model output: $\hat{y} = f(u(k-1), \dots, u(k-1), \dots, \hat{y}(k-1), \dots, \hat{y}(k-1)$ where $\hat{y}(k-i)$ is the previous model output and $u(k-i)$ the past values of the input. Hence, the output of the dynamic model is connected with the input in terms of recurrent structures. At the current stage of our project, one consideration is to use recurrent neural networks. The connections of a recurrent neural network form a directed circle, allowing the modeling of dynamic behavior. Examples of recurrent networks are the Elman Network [14] or the Hopfield Network [15], these or extended versions of these architectures are often found in publications to identify dynamic systems. Our future research targets the creation of a dynamic model, integrating knowledge of structural features of the desired function (grey box) and minimizing the complexity of the model. Dimension reduction will be applied to realize an efficient process control (based on an observer, see Fig. 1) to improve the quality of the welding process.

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