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A Software Framework for Optimization of Process Parameters in Material Production

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Abstract. A framework for optimization of process parameters in material processing and production is described. The framework is designed for effective set up and solution of optimization problems as part of process design, as well as to support development of numerical models by inverse identification of model parameters. The general framework is outlined, which has been supplemented by a neural networks module in order to enable real time decision support. Simulator based on meshless method with radial basis functions (RBF) has been utilized.

Optimization Framework

The optimization part of the framework is designed as a stand-alone optimization system. Its development was centered around a library of optimization techniques for industrial problems where optimization is carried out on basis of computationally expensive numerical simulations whose results contain substantial level of numerical noise [1,2]. This has been predominantly treated by algorithms based on adaptive approximation of the response functions. Successive approximations of sampled response over suitably sized domains enable exploitation of higher order function information. Restricted step approach is used to ensure global convergence, and adaptive sampling strategies play significant role in reducing the necessary number of evaluations of the response functions.

Work was initiated as an attempt to re-implement the C library IOptLib [1-3] in a rigorous object oriented manner in order to more easily master complexity of the developed algorithms and to speed up the development process. The framework is being extended in order to enable straight forward inclusion and seamless use of third party optimizers. This requires careful design of abstraction levels and standardization of input/output and calling conventions, which is achieved by suitable wrappers when third party software is incorporated. Further steps will be made towards more unified treatment of different kinds of problems such as constrained/unconstrained or single objective/multiobjective optimization. Multidisciplinary approach is also considered in a way that different simulators may be used for different problem fields involved in definition of an optimization problem.

Neural Networks Approximation Module. In several practical cases the process design parameters must be adapted quickly in order to produce results that comply with customer requests. With classical approach to optimization of process parameters, long computational times needed for each run of the process simulation at trial design parameters can therefore limit applicability of optimization in industrial environment. Solution has been conceived in the form of approximation of system response, which is calculated on basis of sampled response prepared in advance either by runs of numerical model or by measurements previously performed on the process of interest with varying process parameters. The optimization procedure that produces process design parameters consistent with the current requirements is then performed on the surrogate model based on the approximated response.

In the current work, approximation based on neural networks has been utilized. A convenient characteristic of neural networks is that approximation is calculated in two separate stages (Fig. 1). In the training stage, the network is trained by using the sampled response (either measured or calculated by a numerical model). Training algorithm iterates until sufficient agreement is reached between the data from training set and the corresponding outputs of the network. In the approximation stage, trained network is used for calculation of approximated response at arbitrary values of input parameters.

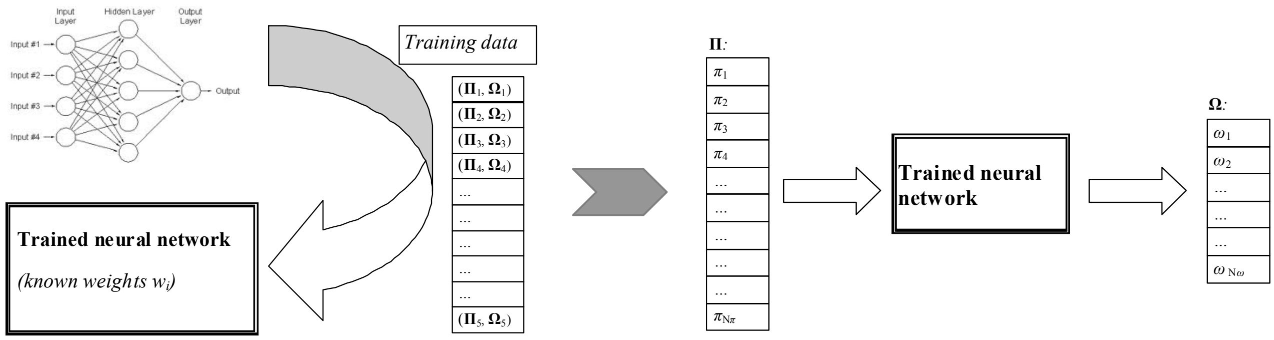

Fig. 1 Approximation with neural networks: traing a network with presented data (left) and calculation of approximated response with trained network (right)

At the beginning, use of various commercial neural network approximation systems was considered. However, such solutions turned inflexible and an in-house software module was built based on general purpose neural network libraries. It features modular design such that new underlying libraries can easily be utilized (open source libraries Aforge.Net [6] and NeuronDotNet [7] are currently used). This also provides good flexibility in integration with other software, enables designing training strategies, filtering training data, verification of results, automatically testing and comparing different network layouts, etc. This flexibility is crucial when approximating behavior of material processing systems with large number of processing parameters. Data obtained from such systems is often inaccurate or even corrupted due to practical limitations in acquisition procedures. Response sampling can not be planned in advance but is accommodated to production schedules in the factory. Information available can be deficient in some regions of parameter space for obtaining satisfactory response approximation. Verification of results plays en especially important role in such scenarios.

Since the final goal is to optimize process parameters according to design goals, we need to approximate the dependence of objective and constraint functions on optimization parameters. The presented software system also supports a different approach where the neural network is trained with data that contains all influential parameters of the process and a number of rough output values sampled in the process. Specific optimization problems can then be defined on such approximated response by defining input mapping between optimization parameters and input parameters of the neural networks, and output mapping between the approximated output values and response functions (constraint and objective functions) of the optimization problem according to their precise definitions. In this way we can solve diverse optimization problems by using the same trained network, without the need to repeat the expensive training procedure when problem definition changes.

Application to Continuous Casting of Steel

The presented optimization system has been applied to optimization of parameters of continuous casting process [8,9] in order to obtain the desired quality of produced steel billets.. Melted steel is poured into tundish, from which it flows to the mold where solidification begins. A partially solidified steel billet is transported from the mold by a series of supporting rolls. During transport the billet is bent into horizontal position and solidifies from the surface towards interior, which is accelerated by spray cooling. At the end of this stage, the billet is cut and prepared for further processing.

Several requirements must be met in order that the process runs smoothly and without defects in output material. At the mold outlet, the solidifying shell must be thick enough that the billet is not torn, which limits the affordable casting speed. In the region when bending occurs, the billet must not solidify too much because bending would cause cracking of the shell. On the other hand, the billet cross section must be fully solidified before the cutoff point.

The described process conditions are predominantly controlled by the temperature of the molten steel, casting speed, cooling in the mold, and spray cooling at different stages. Together with chemical composition, this affects the final mechanical properties of produced material.

A calibrated numerical model has been developed for simulation of the process [8-10], based on meshless spatial discretization method with radial basis functions (RBF). The model was used for generation of test training data set for a neural network. A total of 90 corresponding sets of output values were generated for chosen combinations of 19 influential parameters. These consisted of chemical composition parameters (concentrations of alloying elements Cr, Cu, Mn, Mo, Ni, Si, V, C, P, S), billet dimension, casting temperature, casting superheat, casting speed, temperature difference of cooling water in the mould, cooling flow rate in the mould, cooling water temperature in sprays, cooling flow rate in wreath spray system, and cooling flow rate in first spray system. Metallurgical length, shell thickness at the end of the mould and billet surface temperature at the straightening start position were considered on the output side.

Sampled data has been used to train a two layer artificial neural network with sigmoid activation function. The quality of approximation was verified by leaving different random combinations of training samples out of the learning process, and then checking approximation errors in these points. After training, the network state was saved in order to serve for approximation of the selected process output values dependent on input parameters. An optimization procedure was then performed on the approximate model, with the objective to achieve favorable process behavior with respect to the metallurgical length, shell thickness and billet surface temperature.

A modified Nelder-Mead algorithm [3] has been applied in order to solve the optimization problem. Typically it took between 1000 and 2000 evaluations of the approximated response in order to calculate the solution. Table 1 shows the obtained optimal parameters and Table 2 shows the resulting values of observed output values (for brevity, concentrations of ten alloying elements are not shown in Table 1).

Table 1 Process design parameters

Description & units	Range in the training set	Optimal value
Casting temperature [C]	1515 - 1562	1534
Casting superheat [C]	15 - 59	43
Casting speed [m/min]	1.03 - 1.86	1.74
Temperature difference of cooling water in the mould [C]	5 - 10	8
Cooling flow rate in the mould [l/min]	1050 - 1446	1134
Cooling water temperature in sprays [C]	18 - 33	19
Cooling flow rate in wreath spray system [l/min]	10 - 39	18
Cooling flow rate in 1st spray system [l/min]	28 - 75	48

Table 2 Observed output values of the process

Description & units	Range in the training set	Target value	Optimal value
0: Metallurgical length [m]	8.6399 - 12.54	10.31	10.3137
1: Shell thickness at the end of the mould [m]	0.0058875 - 0.0210225	0.0124	0.01259
2: Billet surface temperature [C]	1064.5 - 1163.5	1121	1120.3296

Conclusion

A procedure of optimization of process parameters based on approximated response obtained by a neural network is described, and a software framework to support the approach has been developed.

The described procedure was carried out as proof of concept, and its application is foreseen in quick adjustment of casting process parameters. The main advantage of the procedure is that neural network is trained with the available data in advance, and can be later used for quick evaluations of the approximate system response. This enables optimization of process parameters in times that are acceptable for industrial purposes.

Although the concept has been tested, some work still needs to be done in assurance and verification of the quality of approximated response obtained from neural networks. Further steps will be directed towards approximation of response for a series of processes (such as casting, heat treatment and rolling). This would have great practical value because final product properties (that are also widely tested in production facilities) are achieved only after the last processing in the chain. Such procedures are challenging due to larger number of influential parameters that need to be considered, difficulties associated with accurate modeling of a chain of processing procedures, and possibility of defects in the data. The next application of the system is foreseen to be the arc-discharge cell for production of fullerenes.

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