University of Pannonia  
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Doctoral (Ph.D.) thesis

Computational Intelligence based regression techniques and their applications in process engineering

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Introduction

Majority of problems arose in chemical engineering practice requires data-driven modeling of nonlinear relationships between experimental and technological variables. Complexity of nonlinear regression techniques is gradually expanding with the development of analytical and experimental techniques, hence model structure and parameter identification is a current and important topic in the field of nonlinear regression not just by scientific but also from industrial point of view as well.

Model interpretability is the most important key property besides accuracy in regression modeling of technological processes and this is essential characteristic of these models in their application as process controllers.

As it was mentioned above model structure and parameter identification is an actual topic with increasing importance, since identified model needs to be interpretable as well.

In line with these expectations and taking interpretability of regression models as basic requirement robust nonlinear regression identification algorithms were developed in this thesis. Three algorithms were examined in details namely identification of regression trees based hinging hyperplanes, neural networks and support vector regression. Application of these techniques eventuate black box models at first step.
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It is shown in my thesis how interpretability could be maintained during model identification with utilization of applicable visualization and model structure reduction techniques within the fuzzy modeling framework.

First part of the thesis deals with the identification of hinge hyperplane based regression trees. Results of the developed algorithm prove that the implementation of a priori constraints enables fuzzy c-regression clustering technique to identify hinging hyperplane models. Application of this technique recursively on the partitioned input space ends up in a regression tree capable for modeling and even for implementation of model predictive control of technological data coming from real life applications. The next section deals with the validation, visualization and structural reduction of neural networks. It is described in details that the hidden layer of the neural network can be transform to an additive fuzzy rule base. This section is followed by the description of connections between fuzzy regression and support vector regression, and introduces a three-step reduction algorithm to get interpretable fuzzy regression models on the basis of support vector regression.

New scientific results

Thesis I.
I showed that hinging hyperplane models are excellent tools for the identification of models based on technological data. I tailored a new model structure by the hierarchical representation of hinging hyperplane
models and I delivered a new identification algorithm based on fuzzy clustering.

a.) To overcome the problems of original hinge hyperplane identification algorithm delivered by Breimann [1] I adapted a fuzzy c-regression clustering algorithm for hinge identification with incorporating a priori constraints.

b.) As further enhancement of this algorithm I developed hierarchical hinge hyperplane based on regression tree identification technique. I showed performance of the developed tool on multiple examples from the well-know repositories.

c.) I proved that the identified transparent and interpretable models - with the help of the developed algorithm - are suitable for solving process control duties of technological systems. To illustrate this feature I presented model predictive control of a simulated cartridge water heater.

Connected publications: 1, 7, 8, 9, 10, 12, 13, 17, 19, 20, 21, 24, 25
Thesis II.

To reinforce support vector regression methods I worked out a three step reduction technique in order to reduce and transform the support vector model into an interpretable fuzzy rule base. Further reduction of this rule base implies interpretable and robust regression models.

a.) I examined structural equivalency between support vector and fuzzy regression. I worked out a technique with the help of Gaussian kernels to transform the identified support vector model into a fuzzy rule base.

b.) Based on the identified support vector regression model the transformed fuzzy rule base generates large number of rules making the model interpretation and validation difficult. I tailored a three step reduction algorithm to overcome this problem. I used the reduced set method [2] to select the important set of support vectors and I utilized further, similarity based reduction of the generated rule base. The resulted fuzzy rule base is linear in the consequent part, therefore I applied orthogonal least squares algorithm for further reduction.

Connected publications: 2, 5, 6
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Thesis III.
Interpretability of neural network models can be achieved by transforming hidden layer of the neural network into a fuzzy rule base and with using a special, self developed visualization technique of this rule base. Based on the self developed transformation and visualization technique I reduced the generated model with orthogonal least squares and similarity based reduction techniques in order to support proper model structure design.

a.) I examined that validation and interpretability of black box neural network models can be improved by transforming the hidden layer of the neural network models with a special operator to a fuzzy rule base.

b.) I compared calculated membership functions based on similarity measure enabling the analysis of the neural network model and point out possible further model reductions. This model structure is also linear in parameters from the output layer point, so I used the mentioned orthogonal least squares technique for further model reduction.

c.) Visualization of the neurons taking place on the hidden layer of neural network can be achieved by distance measure and multi-dimensional scaling. This technique is also a new tool to examine and validate structure of the neural network. Performance of these techniques is shown on a technological pH. process.

Connected publications: 3, 4, 11, 14, 15, 16, 18, 22, 23

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Utilization of results

The motivation to write my thesis was to integrate data, prior knowledge and extracted information into a single framework that helps model-building procedures with interpretability, visualization and reduction. Utilization of the developed algorithms was shown by section-wise examples taken from the area of chemical engineering. Benchmarks and experimental data were used to perform a most comprehensive test of novel methods.

Due to computational efficiency and easy interpretation, the hierarchical representation of hinging hyperplane model proved to be a promising tool to develop local linear controllers. Interpretable fuzzy regression models initialized by robust support vector regression could help when besides quantitative relationships, qualitative analysis is needed as well. The interpretable property of fuzzy models is a great vehicle for variable quality characterization. Structural validation and visualization of neural network models can support modellers to solve the challenge in case only black box model identification is possible. My self-developed technique gives excellent feedback to determine model structure and evaluate task complexity. In the chemical industry, these problems occur when trying to find connections between complex reaction kinetic relationships and key technology- and product-quality variables.

Future developments of the thesis at hand can branch in various directions in the field of interactive learning where modeller experience combined with
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learning capability of different identification techniques can lead to further successes.

Publications and presentations related to the subject of the thesis

Articles published in scientific papers:


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Presentations:


[13.] Fuzzy Clustering for the Identification of Hinging Hyperplanes Based Regression Trees WILF 2007 - International Workshop on Fuzzy Logic and
Applications, Lecture Notes in Artificial Intelligence 4578

[14.] Petroleum Supply Chain Optimization with Linear Programming APS Forum Balatonfüred, Hungary, Hotel Flamingo 26-27.05.2010


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[17.] Hinging Hyperplanes based Regression tree identified by Fuzzy Clustering WSC16 – 16th Online World Conference on Soft Computing in Industrial Applications

[18.] Visualization and Complexity Reduction of Neural Networks WSC12 -12th Online World Conference on Soft Computing in Industrial Applications


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[22.] Complexity Reduction of Local Linear Models Extracted from Neural Networks VI. Alkalmazott Informatika Konferencia Kaposvár 2007. május 25.

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[23.] Kenesei Tamás, Neurális hálózatok alkalmazási lehetőségei, Molekulák biológiai aktivitásának adat-alapú becslésére alkalmas algoritmusok áttekintése; 2006
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