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Melt index prediction by support vector regression

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***Abstract*—Melt index is considered one of the most important variables in determining chemical product quality and thus reliable prediction of melt index (MI) is essential in practical propylene polymerization processes. In this paper, a fuzzy support vector regression (FSVR) based model for propylene polymerization process is developed to predict the MI of polypropylene from other easily measured process variables. Support vector data description (SVDD) is introduced in this model as a novel fuzzy membership function and to reducing the effect of outliers and noises. A detailed comparison between the standard SVR and SVDD-FSVR models is carried out on a real plant. The research results have confirmed the effectiveness of the presented method.**

Keywords—Support vector regression; support vector data description; melt index; propylene polymerization

I. INTRODUCTION

Production of polypropylene is a multi-billion business which has great influences to the world in aspects of industry, military, economy and so on. Melt index is considered the most important parameter in determining the product grade and quality control of polypropylene produced in practical industrial processes. It is usually evaluated offline with particular procedures in the laboratory, which is costly and time-consuming[1], leaving the process without any real-time quality indicator during this period. Such situations can lead to a significant production of off-grades and result in enormous losses in profit. An alternative is to develop on-line indicator of product quality based on available process information which allows the supervision of the overall process and to avoid mismatch of product quality during product grade transitions.

The mechanistic modeling approaches for the prediction of the melt index are often challenged by the engineering activity and the relatively high complexity of the kinetic behavior and operation of the polymer plants[2], which makes it difficult to obtain detailed predictions in real time. Instead, some production plants use machine learning methods to provide information for product and process design, monitoring, and control on the basis of real-time database systems where a considerable amount of data about the studied process is available[3]. Several works have been carried out to predict melt indices with various types of modeling methods. Liu et al. provided a fuzzy neural networks and PSO algorithm with online correction strategy to infer the melt index[4]. Han et al. compared the performance of support vector machines, partial least squares, and artificial neural networks for MI estimation of San and PP processes, and concluded that the standard SVM yields the best prediction among the three toward the studied problems[5]. Unfortunately, further research on SVM regarding this topic has not been carried out.

In this paper, a fuzzy support vector regression model of propylene polymerization process is first developed to infer the MI of polypropylene from other readily measurable process variables. Considering the Methodological consistency, the support vector data description based membership function is adopted in the modeling process to obtain a robust estimation of melt index of polypropylene. Up to now, litter, however, has appeared in the literature on these matters. The standard SVR model of propylene polymerization process proposed by Han is also developed as a basis of comparison research. The performance of the models have been illustrated and evaluated with an actual propylene polymerization. The results obtained are then discussed and concluding remarks about the methods are finally presented..

II. SUPPORT VECTOR REGRESSION

A. Standard Support Vector Regression

Support vector machine introduced by Vapnik is a valuable tool for solving classification problems. SVMs can be applied to regression problems by the introduction of an alternative loss function. Consider regression in the following set of functions:

$$f(x) = w^T \varphi(x) + b \tag{1}$$

with given training data $\{x_i, y_i\}_{i=1}^{M}$, where M denotes the number of training data, x*i* is the input data, and y*i* is the output data. The nonlinear mapping φ maps the input data into a high dimensional feature space, where a linear regression problem is obtained and solved. In the support vector method one aims at minimizing the regularized risk

$$R(w,b) = \gamma \frac{1}{M} \sum_{i=1}^{M} L_\varepsilon(y_i, f(x_i)) + \frac{1}{2} w^T w \tag{2}$$

where

$$L_\varepsilon(y_i, f(x_i)) = \begin{cases} 0, & |y_i - f(x_i)| \le \varepsilon \\ |y_i - f(x_i)| - \varepsilon & otherwise \end{cases} \tag{3}$$

L_ε is the so-called ε-insensitive loss function, which

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indicates that it does not penalize errors below ε. The second term $w^T w/2$, is used as a flatness measurement of function1 and γ is a regularized constant determining the tradeoff between the training error and the model flatness. The estimation problem is then formulated as the optimization problem:

$$\min_{w,b,\xi^*,\xi} R(w,\xi^*,\xi)=\frac{1}{2}w^T w+\gamma\left\{\sum_{i=1}^{M}\xi_i^*+\sum_{i=1}^{M}\xi_i\right\} \tag{4}$$

subject to the constraints

$$\begin{cases} y_i - w^T\varphi(x_i)-b\le\varepsilon+\xi_i^* \\ -y_i + w^T\varphi(x_i)+b\le\varepsilon+\xi_i \\ \xi_i^*,\xi_i \ge 0 \end{cases} \tag{5}$$

where ξ, ξ * are slack variables.

By introducing Lagrange multipliers α*,α to the constraints and exploiting the resulting quadratic program,

$$w=\sum_{i=1}^{M}(\alpha_i^*-\alpha_i)\varphi(x_i) \tag{6}$$

Then the decision function takes following form:

$$f(x)=\sum_{i=1}^{M}(\alpha_i^*-\alpha_i)K(x,x_i)+b \tag{7}$$

where the kernel function K corresponds to:

$$K(x,x_i)=\varphi(x_i)^T\varphi(x) \tag{8}$$

according to Mercer's condition.

B. Fuzzy Support Vector Regression

In many real-world applications, the effects of the training samples are different. It is noted that some training samples are more important than others in the regression problem. We would require that the meaningful training samples must be correctly estimated and may not care about some training samples like noises whether or not they are rigorously fitted.

Given a training dataset with associated fuzzy membership $\{x_i,y_i,s_i\}_{i=1}^{M}$. Each x_i has a fuzzy membership which satisfies $\sigma\le s_i\le 1$ with a sufficiently small constant $\sigma>0$.

As the fuzzy membership s_i is the attitude of the corresponding sample x_i toward the regression and the parameter ξ_i is a measure of error, the term $s_i\xi_i$ is a measure of error with different weighting. The optimization problems turn to:

$$\min_{w,b,\xi^*,\xi} R(w,\xi^*,\xi)=\frac{1}{2}w^T w+\gamma\left\{\sum_{i=1}^{M}s_i\xi_i^*+\sum_{i=1}^{M}s_i\xi_i\right\} \tag{9}$$

subject to

$$\begin{cases} y_i - w^T\varphi(x_i)-b\le\varepsilon+\xi_i^* \\ -y_i + w^T\varphi(x_i)+b\le\varepsilon+\xi_i \\ \xi_i^*,\xi_i \ge 0 \end{cases} \tag{10}$$

Again, by standard Lagrange multiplier techniques, the dual optimization problem

$$\begin{aligned} \max_{\alpha_i,\alpha_i^*} W=&-\frac{1}{2}\sum_{i=1}^{M}\sum_{j=1}^{M}(\alpha_i-\alpha_i^*)(\alpha_j-\alpha_j^*)K(x_i,x_j) \\ &-\varepsilon\sum_{i=1}^{M}(\alpha_i+\alpha_i^*)+\sum_{i=1}^{M}y_i(\alpha_i-\alpha_i^*) \\ \textit{subject to}\quad &\sum_{i=1}^{M}(\alpha_i-\alpha_i^*)=0 \qquad \alpha_i,\alpha_i^*\in[0,\gamma s_i] \end{aligned} \tag{11}$$

can be solved.

Methodological consistency has been a major design principle and is expected to improve the comprehensibility of the modeling paradigm. Support Vector Data Description (SVDD) is inspired by the support vector machine classifier, which searches for a spherically shaped boundary around a dataset to detect novel data or outliers. A SVDD fuzzy membership function is proposed for FSVR, which is defined in the feature space as well.

Assume a hypersphere with center *a* and radius *R*, the cost function is defined as below:

$$\begin{aligned} &\min\ R^2+C\sum_{i=1}^{l}\xi_i \\ &\textit{subject to} \\ &\quad \|(\varphi(x_i)-a)\|^2\le R^2+\xi_i\ ,\ \xi_i\ge 0\ \ i=1,2,...,l \end{aligned} \tag{12}$$

where ξ_i are slack variables, and the parameter *C* controls the trade-off between the volume and the violation.

The training samples with nonzero α_i are support vectors and are used to describe the hypersphere boundary.

Denote *a* as the centers of the samples in the feature space, according to K-T condition:

$$a=\sum\alpha_i x_i \tag{13}$$

The radius is then defined by

$$r=\max|a-\varphi(x_i)| \tag{14}$$

The square of the distance between any sample x_i and the center *a* in the feature space can be calculated as:

$$d_i^2=K(x_i,x_i)-2\sum_j\alpha_j K(x_j,x_i)+\sum_i\sum_j\alpha_i\alpha_j K(x_i,x_j) \tag{15}$$

By definition , the radius *r* is the distance from the center a of the hypersphere to any of its support vectors on the boundary

$$r=d_{sv} \tag{16}$$

Then the fuzzy membership s_i of each input sample x_i can be defined as follows:

$$s_i=1-\sqrt{d_i^2/(r^2+\delta)} \tag{17}$$

where $\delta>0$ is a small constant used to avoid the case $s_i=0$.

III. RESULTS

The history data used for training and testing the prediction model are retrieved from the historical logs recorded in a real propylene polymerization plant. Data are filtered to discard abnormal situations and to improve the quality of the

prediction system. Totally, nine process variables (t, p, l, a,f_1, f_2, f_3, f_4, f_5) have been chosen to develop the MI prediction model, where t is the process temperature, p is the pressure, l is the level of liquid, a is the percentage of hydrogen in vapor phase, f_1–f_3 are flow rates of three streams of propylene, and f_4 is the flow rate of catalyst as well as f_5 is the flow rate of aid catalyst, respectively. A collection of 170 pairs of input–output data are used in this research. It is noted that the test set is obtained from the same batch as the training set, whereas the generalization set is derived from another batch.

The detailed comparison of test performance between SVDD-FSVR and standard SVR is listed in Table I. The difference between the output of the models and the desired output is referred to as the error and can be measured in different ways. Here, mean absolute error (MAE), mean relative error (MRE), root mean squared error (RMSE), standard deviation of absolute errors (STD), and Theil's Inequality Coefficient (TIC), are adopted as derivation measurements between measured and predicted values. They are defined as the following, respectively:

$$MAE = \frac{1}{N}\sum_{i=1}^{N} | y_i - \hat{y}_i | \tag{18}$$

$$MRE = \frac{1}{N}\sum_{i=1}^{N} \frac{| y_i - \hat{y}_i |}{y_i} \tag{19}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N} (y_i - \hat{y}_i)^2} \tag{20}$$

$$TIC = \frac{\sqrt{\sum_{i=1}^{N} (y_i - \hat{y}_i)^2}}{\sqrt{\sum_{i=1}^{N} y_i^{\,2}} + \sqrt{\sum_{i=1}^{N} \hat{y}_i^{\,2}}} \tag{21}$$

where yi and $\hat{y}_i$ denote the measured value and predicted result, respectively.

TABLE I. PERFORMANCE FOR THE TESTING DATASET

Methods	MAE	MRE (%)	RMSE	TIC
SVDD-FSVR	0.0008	0.03	0.0002	0.0002
SVR	0.0057	0.22	0.0017	0.0018

The data listed in Table I indicates that the SVDD-FSVR model functions better than SVR, with mean absolute error of 0.0008, compared with that of 0.0057 obtained from the corresponding SVR models. The RMSE listed also in Table I have confirmed the prediction accuracy of the proposed methods. TIC of SVDD-FSVR is quite acceptable when compared with that of standard SVR, which indicates a good level of agreement between the proposed model and the studied process. A visual impression of the agreement between the measured MI and the models output can be obtained from Figure 2, where the SVDD-FSVR model yields consistently good predictions.

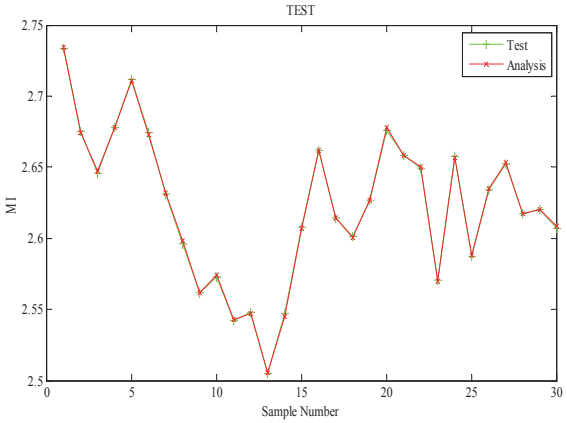

Fig. 1. Estimation via SVDD-FSVR for testing dataset

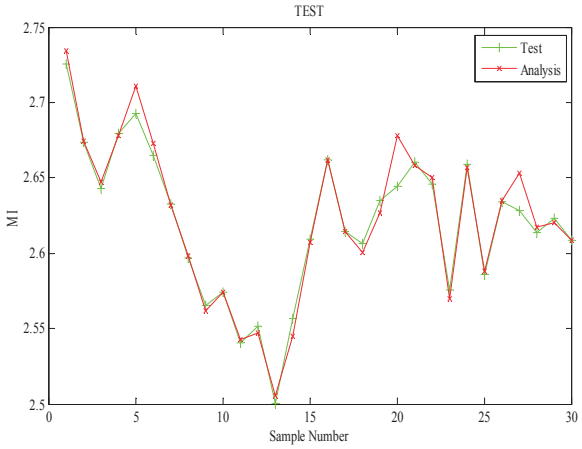

Fig. 2. Estimation via SVR for testing dataset

TABLE II. PERFORMANCE FOR THE GENERALIZATION DATASET

Methods	MAE	MRE (%)	RMSE	TIC
SVDD-FSVR	0.0011	0.04	0.0004	0.0003
SVR	0.0049	0.19	0.0017	0.0014

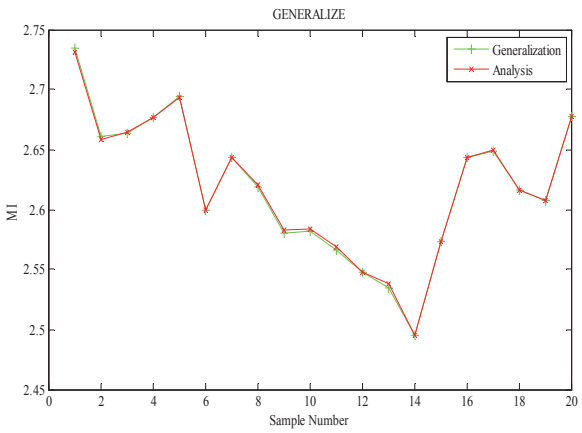

Fig. 3. Estimation via SVDD-FSVR for generalization dataset

To illustrate the universality of the proposed model, a detailed comparison of the generalization data set is presented in Table II. It is noted that the performance is consistent with the above test results. The mean absolute error of SVDD-FSVR

is 0.0011, compared with 0.0049 of SVR, showing an error decrease of approximately 80%. Similar behaviors are observed in terms of MRE, RMSE, and TIC

IV. Conclusions

This paper has presented methods for using SVDD-FSVR to infer MI of polypropylene from other process variables. Comparing with standard SVR, SVDD-FSVR involves support vector data description membership function, which reduced the effect of noise and outliers and greatly improved the prediction accuracy. The SVDD-FSVR model predict MI with mean relative error of approximately 0.03% when appropriately trained, compared with that of 0.22% obtained from the corresponding SVR models. The results indicate that the proposed method provides prediction reliability and accuracy and supposed to have promising potential for practical use.

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