Neurocomputing 149 (2015) 1216–1224

Contents lists available at ScienceDirect

Neurocomputing

journal homepage: www.elsevier.com/locate/neucom

Optimal online soft sensor for product quality monitoring in propylene polymerization process

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ARTICLE INFO

Article history:
Received 15 May 2014
Received in revised form
28 August 2014
Accepted 1 September 2014
Communicated by J. Zhang
Available online 16 September 2014

Keywords:
Polypropylene
Melt index prediction
Soft-sensor
Least squares support vector machine
Particle swarm optimization
Online correction

ABSTRACT

In the real-time propylene polymerization manufacturing process, melt index (MI), as the key product quality variable, is hard to be measured on-line, which brings difficulties to the control and optimization of this process. However, a large amount of data of other relative process variables in this process can be routinely recorded online by the distributed control system (DCS). An optimal soft-sensor of least squares support vector machine (LS-SVM) is therefore proposed to implement the on-line estimation of MI with the above real-time DCS records, where LS-SVM is employed for developing a data-driven model of the above industry process. In view of that the input variable selection and parameter setting are crucial for the learning results and generalization ability of LS-SVM, the nonlinear isometric feature mapping technique and particle swarm optimization algorithm are then structurally integrated into the model to search the optimal values of those parameters. Considering the process time-varying nature, an online correction strategy is further switched on to update the modeling data and revise the model configuration parameters via adaptive behavior. Finally, the explored soft sensor model is illustrated with a real plant of propylene polymerization, and the results show the predictive accuracy and validity of the proposed systematic approach.

1. Introduction

As an important material, polypropylene has been widely used in many different fields including chemical, optical and medical sectors. The quality of polypropylene is conventionally assessed by the melt index (MI) in practical manufacturing processes [1]. However, due to the challenging engineering activity and the complexity of the process, MI is usually evaluated offline with an analytical procedure that takes almost two hours to complete in the laboratory [2]. Therefore, this will cause a time delay to the quality control system, since the process is without any quality indicator during this period of time. An alternative way is to install an online analyzer, such as those based on near infrared spectroscopy or ultrasound for measuring the melt index [3], but the very high price and the following considerable maintenance efforts result in a limited adoption of the online analyzers in real plants.

Since the propylene polymerization process is quite complex, the rigorous theoretical modeling approaches are often impractical or even impossible. Recently, with the wide utilization of the distributed control system (DCS) in industrial processes, a large amount of process data can be routinely recorded. In such case, obtaining the process model based on the measured data using data-driven techniques is a feasible option [4]. These recorded data, also referred to as historical data, serve as the input signals of the soft sensor. To date, different soft sensors have been developed for the prediction of the MI. Lou et al. [5] proposed a novel multiple-priori-knowledge based neural network inferential model for melt index prediction. By embedding priori knowledge, the model ensured the safety in controlling the quality of melt index. Jiang et al. [6] devised an optimal soft sensor, named the least squares support vector machines with ant colony-immune clone particle swarm optimization (AC-ICPSO-LSSVM), to predict the MI successfully. Ge et al. [7] developed a so-called combined local Gaussian process regression and it gained the best MI prediction results in contrast with several other methods, such as the Gaussian mixture model, the fuzzy-learning based model, multiple local partial least squares, artificial neural network and the support vector regression model. Park et al. [8] employed partial least squares (PLS) and support vector regression to predict the MI in the high-density polyethylene process. The simulation results showed that PLS and support vector regression both exhibited excellent predicting performances even for operating situations accompanying severely frequent grade changes. Han et al. [9] introduced three different approaches, including supported vector machine, PLS and back propagation neural network, to estimate the MI and concluded that the standard support vector

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http://dx.doi.org/10.1016/j.neucom.2014.09.006
0925-2312/

Nomenclature

MI	melt index
DCS	distributed control system
SVM	support vector machine
LS-SVM	least squares support vector machine
PLS	partial least squares
ISOMAP	isometric feature mapping
PSO	particle swarm optimization
OCS	online correction strategy
PCA	principal component analysis
GA	genetic algorithms
Iso-LS-SVM	least squares support vector machine with isometric feature mapping
Pso-LS-SVM	least squares support vector machine with isometric feature mapping and particle swarm optimization
Sys-LS-SVM	systematic LS-SVM approach, i.e., least squares support vector machine with isometric feature mapping, particle swarm optimization and online correction strategy
RMSE	root mean square error
MAXE	maximum absolute error
MAE	mean absolute error
MRE	mean relative error
STD	standard deviation
TIC	Theil's inequality coefficient
T	temperature
P	pressure
H	level of liquid
a	percentage of hydrogen in vapor phase
$f1, f2, f3$	flow rates of three streams of propylene
$f4$	flow rate of catalyst
$f5$	flow rate of aid catalyst

machine yielded the best prediction. Nowadays, neural networks have been widely applied to model and control dynamic processes because of their extremely powerful adaptive capabilities in response to the nonlinear behaviors [10,11]. Zhang et al. [12] set up a novel RBF prediction model under chaotic theory (RBF-chaos) for MI prediction. Zhang et al. [13] proposed a sequential training method of neural networks to infer the polymer MI for an industrial plant and obtained quite good performances. Rallo et al. [14] provided a fuzzy ARTMAP neural system and two hybrid networks to infer the MI of six different low density polyethylene grades produced in a tubular reactor. Although these methods have achieved better and better MI prediction accuracy, they may be only locally valid or deteriorate as time elapses due to high level noises and disturbances in the samples or the time-variant characteristics of industrial processes caused by the catalyst deactivation, equipment aging, sensor and process drifting. For example in the AC-ICPSO-LSSVM modeling, the integrated ant colony-immune clone particle swarm optimization (AC-ICPSO) has the only one purpose to find the global optimal values of the LS-SVM model parameters. These optimal values are also only matched with the current modeling samples. Since the collected new samples are not homogeneous duo to the process changes, a newer model must be built from scratch.

As is well known, the polymerization of propylene is a highly nonlinear process evidenced by mechanistic analysis of the reactions and plants. So, nonlinear soft sensors should be considered. Now, the least squares support vector machines (LS-SVM) method is widely used in the areas of nonlinear system identification, optimal control and pattern recognition [15–17]. As a soft sensing method, its learning and generalization abilities are greatly affected by the parameter setting. If you take a step forward, you will find that the appropriate parameters of the LS-SVM model vary with the selection of input variables and vice verse, so the input variables selection and parameter setting must be operated simultaneously. Accordingly, the aim of this paper is to present a systematic data-driven soft sensor based on the feature selection and parameter optimization technique. As a result, an optimal LS-SVM model is proposed, in which the nonlinear isometric feature mapping (ISOMAP) technique [18] is in charge of selecting the model input variables and the particle swarm optimization (PSO) algorithm [19] is responsible for optimizing the model parameters. In this devised procedure, the input variables selection and parameter setting of LS-SVM can be regarded as a combination optimal problem, and the optimal objective function based on the root mean square error is constructed. Moreover, when addressing the process time-varying nature, online correction strategy (OCS) is explored to self-adaptively update the modeling data and adjust the values of model configuration parameters. This scheme in a fashion to minimize the prediction error is only activated on whenever the model mismatch happens by adding the new data and removing the older ones recursively.

The remaining part of this paper will be organized as follows. In Section 2, theoretical aspects of the ISOMAP, PSO and OCS are introduced, which is followed by the detailed description of the proposed systematic LS-SVM soft sensor. In Section 4, to verify the effectiveness of this proposed method, it is then applied to the polypropylene manufacturing process data and compared with several other soft sensors in terms of performances. Finally, a short discussion and some conclusions are provided.

2. Methodology

2.1. Isometric feature mapping

ISOMAP, as a very general-purpose projection technique, holds the capability of learning the structure of certain curved manifolds. Here, it is used to extract relevant nonlinear features and concurrently obtain fewer ISOMAP variates that are maximally independent from each other. In a comparative study, Ivakhno et al. [20] investigated three feature extraction approaches, i.e., principal component analysis (PCA), PLS and ISOMAP. The results showed that ISOMAP can generally perform better than PCA and PLS for multi-variable nonlinear systems.

Given a set of data points $\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n$ in the p-dimensional space, the ISOMAP algorithm takes as input the Euclidean distances $h(\boldsymbol{x}_i, \boldsymbol{x}_j)$ between all pairs $\boldsymbol{x}_i$, $\boldsymbol{x}_j$ from all these data points. After choosing its free parameter (the number of nearest neighbors k or the fixed radius δ), the ISOMAP algorithm outputs coordinate vectors (underlying variables or secondary variables) $\boldsymbol{s}_i \in \Re^d$ $(i = 1, 2, \cdots, n)$ in the d-dimensional space. These underlying variables have a compact $(d < p)$ and optimal description of the data set and best preserve the intrinsic structure in the data. The complete ISOMAP procedure for solving the underlying variables can be referred to its original paper [18].

2.2. PSO algorithm

In the last two decades, genetic algorithms (GA) [21] and PSO, the population-based optimization algorithms have been proven