

过程系统工程

LSSVM过程建模中超参数选取的梯度优化算法

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摘要

基于结构风险最小的最小二乘支持向量机 (least squares support vector machine, LSSVM) 为标准支持向量机 (SVM) 的约简;训练简易;性能良好。其模型精度受超参数影响;常规的网络搜索法很难搜得最佳超参数。在快速留一法的基础上;以全样本留一预测误差平方和最小化为目标;导出基于梯度的最优化算法;用以优选为LSSVM超参数;进而构建G-LSSVM模型。以柠檬酸发酵过程为算例对G-LSSVM进行检验;结果表明G-LSSVM的超参数选取耗时少;模型稳定性良好;且拟合和预报性能都优于标准SVM和神经网络。有望适用于机理不明、高度非线性、小样本的化工过程建模。

关键词

[最小二乘支持向量机](#) [建模](#) [优选超参数](#) [最速下降法](#) [快速留一法](#) [柠檬酸发酵](#)

分类号

Gradient algorithm for selecting hyper parameters of LSSVM in process modeling

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Abstract

Least squares support vector machine (LSSVM) based on structural risk minimization, which is a simplified version of standard support vector machine (SVM), is easy to be trained and has good modeling performance. The model precision of LSSVM is decided by its hyper parameters, while it is difficult to find the optimal hyper parameters of LSSVM via grid search and cross validation method. Based on the fast leave one out (LOO) method selecting hyper parameters of LSSVM, with the LOO prediction error on the entire training sample being the object of optimization, the gradient-based optimal algorithm was proposed in this paper to find the optimal hyper parameters of LSSVM. The LSSVM model whose hyper parameters found in this way is called G-LSSVM. To validate the performance of G-LSSVM, a citric acid fermentation process was taken as the benchmarking problem. The result showed that the modeling was time-economized and stable; while both the fitting and predicting performance of G-LSSVM were superior to standard SVM and artificial neural network whose hyper parameters and net structure are chosen by trial. G-LSSVM is recommended to model the chemical engineering process with high non-linearity and small size training sample whose mechanism is not clear.

Key words

[least squares support vector machines](#) [modeling](#) [optimal hyper parameters](#) [gradient decent](#) [fast leave one out](#) [citric acid fermentation](#)

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