

论文

烟草组分的近红外光谱和支持向量机分析

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摘要:

测定了120个产自福建、安徽和云南烟草样品的近红外光谱。在利用支持向量机(SVM)技术建立其定量、定性分析模型之前,用小波变换技术对光谱变量进行了有效的压缩,然后采用径向基核函数建立了75个烟草样品的分类模型,同时建立了总糖、还原糖、烟碱和总氮4个组分的定量分析模型,并利用45个烟草样品对模型进行了检验。仿真实验表明,建立的SVM分类模型分类准确率达到100%,而4个组分的定量分析模型的预测决定系数(R^2)、预测均方差(RMSEP)和平均相对误差(RME)3个指标值显示其模型泛化能力非常强,预测效果良好,可见这是一种有效的近红外光谱的建模分析方法。

关键词: 近红外光谱 支持向量机 小波变换 烟草

Analysis of Tobacco by Near-infrared Spectroscopy and Support Vector Machine

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Abstract:

In this study, in order to establish analysis models of near-infrared spectroscopy(NIR) of tobacco, 120 samples of tobacco from different cultivation area were surveyed by near-infrared(NIR) spectroscopy. As the new pattern recognition, support vector machine(SVM) can avoid over-fitting problem and owns the superior generalization ability and prediction accuracy, were applied in this study. The quantitative and qualitative analysis models of tobacco samples were studied separately in this experiment using radial basis function(RBF) SVM. For reducing dimension and moving noise, the spectrum variables were highly effectively compressed using the wavelet transformation(WT) technology and the haar wavelet was selected to decompose the spectroscopy signals. Simultaneously, the parameters of the models were also discussed in detail. The best experimental results were obtained using the RBF SVM regression with kernel parameter $\sigma=1.0, 1.2, 1.4, 0\wedge6$, separately corresponds to total-sugar, reducing sugar, nicotine, total-nitrogen, and RBF SVM classifier with kernel parameter $\sigma=1.6$. Meanwhile, the values of appraisal index, namely coefficient of determination(R^2), root mean squared error of prediction(RMSEP) and mean relative error(RME), indicate its excellent generalization for quantitative and qualitative analysis results and high prediction accuracy. The overall results show that NIR spectroscopy combined with SVM can be efficiently utilized for rapid and accurate analysis of chemical compositions in tobacco and discrimination of tobacco of different origins. On the other hand, the research can show that SVM is effective modeling tools to NIR spectroscopy and can provide technical support for quantitative and quantitative analysis of other NIR applications.

Keywords: Near-infrared spectroscopy Support vector machine Wavelet transformation Tobacco

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