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Enhanced prediction of misalignment conditions from spectral data using feature selection and filtering

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Abstract

This paper proposes a novel method for the use of genetic algorithm-based feature selection and signal filtering to construct reliable calibration models of shaft misalignment. Determination and selection of the key feature(s) is crucial to the predictive performance of calibration models. Even with proper feature selection, the predictive performance of calibration models can be enhanced by filtering the raw spectral data. This improvement results because a filter removes the unwanted variation of predictor variables that is orthogonal to response variables. This is the first work that attempts to develop a systematic calibration model based on genetic algorithm-based feature selection and orthogonal filtering. A case study shows that the proposed calibration model for shaft misalignment conditions produces better predictive performance than traditional multivariate statistical approaches such as principal component regression and partial least squares.

Keywords: Calibration model; Partial least squares (PLS); Principal component regression (PCR); Genetic algorithm (GA); Feature selection; Orthogonal signal filter; Parallel and angular misalignment

1. Introduction

A shaft transmission system is one of the fundamental and most important parts of rotating machinery. Although the vibration problems associated with out-of-balance shafts are commonly known, misalignment – a condition in which the shafts of coupled machines do not share the same centerline – is just as common and a source of similar vibration problems. Misalignment produces both radial and axial vibrations and usually occurs with loose, bent shafts, inertial imbalance, etc. (Arkan, Calis, & Tağluk, 2005). Perfect alignment of the driving and driven shafts cannot be achieved in practice, and some degree of misalignment almost always exists. However, the closer that alignment can be brought to perfection, the lower the axial and radial forces that will be brought to bear on the most vulnerable parts of a machine system such as its bearings, seals, and couplings (Wowk, 2000). The ability to estimate and predict shaft alignment or misalignment accurately can significantly improve the efficiency and effectiveness of the predictive maintenance tasks of a production system. Thus, monitoring and predicting shaft alignment condition is important to making intelligent decisions on when to perform alignment maintenance (Sinha, Lees, & Friswell, 2004).

Prediction of shaft misalignment conditions can be stated as a multivariate calibration problem. A major objective of this proposed calibration model is to predict misalignment conditions from experimental or historical data. However, the high dimensionality and collinearity of such data makes it difficult to construct a calibration model (Qin, 2003). The need to model such data has led to the adoption of multivariate calibration models using such techniques as partial least squares (PLS). PLS is a dimension reduction technique that seeks to find a set of latent variables by maximizing the covariance of two

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variable blocks (i.e., predictor **X** and response **Y**). It has proven useful in solving various calibration problems (Kourti, 2005; Chiang, Russell, & Braatz, 2000; Rosipal & Trejo, 2001; Omitaomu, Jeong, Badiru, & Hines, 2006). In particular, PLS has been shown to be a powerful technique for multivariate calibration of noisy, collinear, high-dimensional, and ill-conditioned data (Qin, 2003).

The predictor variable **X**, in general, contains unwanted variations that are unrelated (or orthogonal) to response variable **Y**. In such a case, the unwanted variation may degrade the predictive ability of a calibration model. In addition, these calibration models are likely to need a large number of latent components to perform satisfactorily (Wold, Antti, Lindgren, & Öhman, 1998). To overcome this problem, calibration data are often preprocessed or corrected before data analysis. Common approaches for preprocessing include multiplicative signal correction (Geladi, MacDougall, & Martens, 1985), standard normal variate (Barnes, Dhanoa, & Lister, 1989), and principal component analysis (PCA) (Sun, 1997).

Wold et al. (1998) developed the orthogonal signal correction (OSC) method to remove from **X** unwanted variations that are unrelated or orthogonal to **Y**. OSC can selectively remove the largest variation of **X** that has no correlation with **Y**. This is possible because OSC uses the response Y to construct a kind of signal filter for **X** (Eriksson, Trygg, Johansson, Bro, & Wold, 2000). Of course, the other preprocessing methods can be also regarded as different cases of filtering. Compared with the other methods, OSC is a PLS-based solution and is mathematically well-defined. It has been successfully applied to multivariate calibration of near-infrared (NIR) spectroscopy data and to classification of nuclear magnetic resonance (NMR) spectra data (Wold et al., 1998; Eriksson et al., 2000; Westerhuis, de Jong, & Smilde, 2001; Griffin et al., 2002).

Variable or feature selection in multivariate analysis is an essential step because the exclusion of noninformative variables will produce better results even with simple models. When calibration techniques such as PLS and principal component regression (PCR) were introduced, it was thought that feature selection played little role in any of these techniques. However, it has since been widely recognized that feature selection can be useful in producing a calibration model with better predictive ability (Broadhurst, Goodacre, Jones, Rowland, & Kell, 1997; Ding, Small, & Arnold, 1998; Leardi & Gonzalez, 1998). Several approaches to feature selection in calibration have been developed. These include as iterative feature selection (Lindgren, Geladi, Rännar, & Wold, 1994), uninformative variable elimination (Centner et al., 1996), and iterative predictor weighting (Forina, Casolino, & Pizarro, 1999). Recently, it has been shown that genetic algorithms (GA) can be successfully used as a very efficient feature selection technique for PLS (Leardi, 2001; Gourvénec, Capron, & Massart, 2004; Esteban-Díez, González-Sáiz, Gómez-Cámara, & Pizarro Millan, 2006). The selection of variables for calibration can be considered as an optimization problem. In this respect, GA is a very efficient technique for feature selection because the size of the search domain (2^N-1 combinations for N variables) is enormous and many local optima exist.

The first objective of this paper is to present the use of a GA-based variables selection technique for multivariate calibration of shaft misalignment conditions. This illustrates the advantage and the importance of using a feature selection procedure to predict misalignment conditions. The second objective is to investigate in the course of building a calibration model of misalignment conditions the advantage of using an OSC preprocessing technique in order to remove unwanted variation of **X** orthogonal to **Y**. The third objective is to compare the predictive performance of the feature selection-based calibration model with "full" calibration models of PCR and PLS.

The remainder of this paper is organized as follows. First, Section 2 contains a review of PLS, OSC, and GA. Section 3 outlines a prediction problem of some misalignment conditions and the description of the experimental datasets. Prediction results and performance comparisons for misalignment conditions are presented in Section 4. Finally, Section 5 contains the conclusions.

2. Methods

2.1. Principal component regression and partial least squares

PCR and PLS are two multivariate calibration techniques that have been widely used in various calibration problems. PCR first uses standard PCA to construct a linear projection mapping of the data. Principal components (PCs) are usually computed by singular value decomposition on a predictor matrix **X**. Here eigenvectors and scores of PCA, which represent the largest common variations in **X**, are obtained, and then a regression method is used to develop the prediction model for scores against a response matrix **Y**. That is, it finds regression coefficients by minimizing least squares error between the projected data and **Y**.

PLS was developed to model the relation between a predictor matrix **X** and a response matrix **Y**. It seeks to find a set of latent variables that maximizes the covariance between **X** ($n \times N$) and **Y** ($n \times M$). PLS decomposes **X** and **Y** into the form as follows (Kourti, 2005):

$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \tag{1}$$

$$\mathbf{Y} = \mathbf{U}\mathbf{Q}^T + \mathbf{F} \tag{2}$$

where **T** and **U** are ($n \times A$) matrices of the extracted A score vectors, **P** ($N \times A$) and **Q** ($M \times A$) loading matrices, and **E** ($n \times N$) and **F** ($n \times M$) residual matrices.

The PLS method based on nonlinear iterative partial least squares (NIPALS) algorithm (Wold et al., 1998) searches for weight vectors **w** and **c** that maximize the sample covariance between **t** and **u**. The NIPALS algorithm repeats a sequence of the following steps until convergence: