Advanced Process Monitoring using Wavelets and Non-linear Principal Component Analysis

by

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ADVANCED PROCESS MONITORING USING WAVELETS AND NON-LINEAR PRINCIPAL COMPONENT ANALYSIS

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SYNOPSIS

The aim of this study was to propose a nonlinear multiscale principal component analysis (NLMSPCA) methodology for process monitoring and fault detection based upon multilevel wavelet decomposition and nonlinear principal component analysis via an input-training neural network.

Prior to assessing the capabilities of the monitoring scheme on a nonlinear industrial process, the data is first pre-processed to remove heavy noise and significant spikes through wavelet thresholding. The thresholded wavelet coefficients are used to reconstruct the thresholded details and approximations. The significant details and approximations are used as the inputs for the linear and nonlinear PCA algorithms in order to construct detail and approximation conformance models. At the same time non-thresholded details and approximations are reconstructed and combined which are used in a similar way as that of the thresholded details and approximations to construct a combined conformance model to take account of noise and outliers. Performance monitoring charts with non-parametric control limits are then applied to identify the occurrence of non-conforming operation prior to interrogating differential contribution plots to help identify the potential source of the fault.

A novel summary display is used to present the information contained in bivariate graphs in order to facilitate global visualization. Positive results were achieved.

Keywords: Process monitoring; Fault detection; Non-linear Principal Component Analysis

SINOPSIS

Die hoofdoel van hierdie ondersoek was om 'n nuwe metode voor te stel vir nie-lineêre multivlak hoofkomponent-analise vir prosesmonitering en foutopsporing. Die beginsel is gebaseer op multivlak "wavelet"-ontbinding en nie-lineêre hoofkomponent-analise deur middel van 'n inset-verandering neurale netwerk.

Normale bedryfsdata vanaf 'n nie-lineêre industriële proses word eers vooraf verwerk om hewige geraas en beduidende uitskietpieke in die data te verwyder. Dit word gedoen deur eers die data deur middel van "wavelet"-analise te ontbind in detail- en benaderings- "wavelet"-koëffisiënte en dan die "wavelet"-koëffisiënte groter as 'n sekere limiet uit te filter. Die gefilterde "wavelet"-koëffisiënte word dan gebruik vir die hersamestelling van gefilterde details en benaderings. Die beduidende details en benaderings word gebruik as insette vir die lineêre en nie-lineêre hoofkomponent-analise-algoritmes sodat detail- en benadering-konformasiemodelle saamgestel kan word. Terselfdertyd word ongefilterde details en benaderings herkonstrueer vanaf ongefilterde detail- en benaderingskoëffisiënte wat dan gekombineer word om 'n gekombineerde konformasiemodel saam te stel met die hoofdoel om geraas en uitlopers in nuwe data in ag te neem.

Werkverrigtingsmoniteringsgrafieke met nie-parametriese beheerlimiete word dan gebruik om die voorkoms van nie-konformerende of abnormale bedryf op te spoor. Nadere ondersoek mbv differensiële bydrae grafieke word gebruik om te help met die opsporing van die moontlike oorsaak van die fout.

'n Nuwe metode om die inligting in bivariate grafieke in 'n kompakte en eenvoudiger wyse voor te stel is gebruik en gee 'n beter geheelbeeld van die prosesverloop. Die geskiktheid van die moniteringstelsel is getoets op nuwe data en positiewe resultate is verkry.

Sleutelwoorde: Prosesmonitering; Foutopsporing, Nie-lineêre Hoofkomponent-Analise

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Steven Fourie

Pretoria

If a tool could do its job
after obeying a command or its own feeling
. . .
neither the architects (experts) would require assistants
nor the masters slaves.

Aristotle, Politics A4, 1253b34 - 1254a1

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LIST OF SYMBOLS

A	approximation in wavelet multiresolution analysis
a	wavelet dilation parameter
a_0, b_0	discrete wavelet transform parameters
b	Bias / wavelet translation parameter
D	detail in wavelet multiresolution analysis
$DWTf$	discrete wavelet coefficient
$\mathbf{e}$	Vector of network errors
E	Sum of squares function
$f(t)$	a function in the time domain
g	Current gradient (propagated error) at current node
$g(k)$	the *k*th wavelet synthesis filter
H	wavelet analysis filter
$h(k)$	the *k*th wavelet analysis filter
$\mathbf{I}$	identity matrix
J	Jacobian
k	Number of principal components retained
l	Characteristic roots
$\mathbf{L}$	Diagonal Matrix
m, n	discrete wavelet transform parameters
n	Number of samples per variable
p	Number of correlated variables
r	Correlation coefficient
$\mathbf{S}$	Covariance Matrix

t	Original network output / time
$\mathbf{u}$	Characteristic vectors / Eigenvectors
V	Input weights
w	Network weights
W	Network weights
$\mathbf{W}$	weight matrix
x	Input data point to Neural Network
$\mathbf{x}$	Input vector to Neural Network / Original variable
$\bar{\mathbf{x}}$	Mean of $\mathbf{x}$
z	Output data (IT-net approximation) / Uncorrelated variables

Greek and other symbols

δ	Propagated error at hidden layer
α	Learning rate
ϕ	Nonlinear mapping function relating NN outputs to inputs / wavelet scale function or orthogonal function
σ	Sigmoidal transfer function
σ	standard deviation
ψ	wavelet function
$\lVert \cdot \rVert$	Euclidean norm

Subscripts

p	pth training sample
n	Number of observed variables
k	Observed variable number
j	jth hidden node
T	Transpose
^	estimation

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LIST OF DEFINITIONS

Cross-validation – Cross-validation is widely used as an automatic procedure to choose a smoothing parameter in many statistical settings. The classical cross-validation method is performed by systematically expelling a data point from the construction of an estimate, predicting what the removed value would have been and comparing the prediction with the value of the expelled point.

Covariance matrix – For a given data matrix **X** with *m* rows and *n* columns the covariance matrix of **X** is defined as

$$\mathrm{cov}(\mathbf{X}) = \frac{\mathbf{X}^T\mathbf{X}}{m-1}$$

This assumes that the columns of **X** have been 'mean centered', i.e. adjusted to have a zero mean by subtracting of the original mean of each column.

Correlation matrix – Referring to the definition of covariance matrix, if the columns of **X** have been 'autoscaled', i.e. adjusted to zero mean and unit variance by dividing each column by its standard deviation, the equation for calculating the covariance gives the correlation matrix of **X**.

Details – Details, generally known as the wavelet coefficients, are coefficients that capture the details of the signal lost when moving from an approximation at one scale to the next coarser scale.

Epochs – One training cycle after which the neural network parameters (weights and biases) are updated.

Floor(x) – Rounds the elements of *x* to the nearest integers towards minus infinity.

FMH – Finite impulse response median hybrid filter (Heinonen and Neuvo, 1987). A FMH is a median filter which has a pre-processed input from M linear FIR filters. Thus, the FMH filter output is the median of only M values, which are the outputs of M FIR filters. FMH filters are nonlinear filters, are most effective when applied to piecewise constant signals contaminated with white noise, require careful selection of the filter length, and are limited to off-line use.

Hessian Matrix – For a given data matrix **X**, the hessian matrix is given by Equation 8.25 (see Chapter 8).

Jacobian Matrix – The jacobian matrix is a matrix that contains the first derivatives of the network errors with respect to the weights and biases of a neural network and is given by Equation 8.26 (see Chapter 8).

Loadings – The loadings of a data matrix **X** containing *n* variables (columns) with *m* samples (rows) each are transformed variable vectors containing information on how the *variables* in **X** relate to each other and are the eigenvectors of the covariance matrix of **X**.

MSE – Mean Squared Error

Orthonormal – An orthonormal matrix A is a square matrix with the following properties:

1. $|\mathbf{A}| = \pm 1$, where $|\mathbf{A}|$ is the determinant of $\mathbf{A}$.
2. $\sum_{i=1}^{p} a_{ij}^2 = \sum_{j=1}^{p} a_{ij}^2 = 1$ for al $i = j$. The sum of squares of any row or column is equal to unity.
3. $\sum_{i=1}^{p} a_{ij} a_{ik} = 0$ for all $j \neq k$. The sum of crossproducts of any two columns is equal to zero and implies that the coordinate axes, which these two columns represent, intersect at an angle of 90°.

This implies that $\mathbf{AA}' = \mathbf{I}$. If $\mathbf{A}$ is orthonormal, $\mathbf{A}^{-1} = \mathbf{A}'$ where $\mathbf{A}^{-1}$ is the inverse of $\mathbf{A}$.

Orthogonal – Referring to the definition of a orthonormal matrix, a matrix is orthogonal if it satisfies Condition 3 of orthonormality but not Conditions 1 and 2.

PCA – Principal Component Analysis finds combinations of variables that describe major trends in a data set. It also summarises the data in terms of a smaller number of latent variables which are linear combinations of the original variables.

Rotation – Rotation is a method by which a set of data vectors is converted to what is called simple structure. The object of simple structure is to produce a new set of vectors, each one involving primarily a subset of the original variables with as little overlap as possible so that the original variables are divided into groups somewhat independent of each other. This is, in essence, a method of clustering variables that might aid in the examination of the structure of a multivariate data set.

Scales – The scales or extend of the time-frequency localisation corresponds to the wavelet decomposition level and is the contribution in different regions of the time-frequency space into which a signal is decomposed by varying the scaling parameter of the scaling function. The scaling functions are smoother versions of the original signal and the degree of smoothness increases as the scale increases. As the scaling parameter changes, the wavelet covers different frequency ranges (large values of the scaling parameter correspond to small frequencies, or large scale; small values of the scaling parameter correspond to high frequencies, or very fine scale).

Scores – The scores of a data matrix **X** with *n* variables (columns) with *m* samples (rows) each are vectors containing information on how the *samples* in **X** relate to each other. They are thus individual transformed observations of **X** and weighted sums of the original variables.

SPE – Squared prediction error

Threshold – A threshold is certain chosen or calculated limit that has the effect of zeroing a value, variable or coefficient if it is larger than the specified threshold and leaving it unchanged if it smaller or equal to the threshold.

Wavelet – The wavelet transform is a tool that cuts up data, functions or operators into different frequency components, and then studies each component with a resolution matched to its scale. It is an extension of the Fourier transform that projects the original signal down onto wavelet basis functions, providing a mapping from the time domain to the time-scale plane. In general wavelets have the following three properties:

1. Wavelets are building blocks for general functions
2. Wavelets have space-frequency localisation
3. Wavelets have fast transform algorithms