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Chemical Process Performance Evaluation

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TO MINE, BEDIRHAN AND TO THE MEMORY OF MY PARENTS
(A. CINAR)

TO MINE, AYCAN, OMER AND MY PARENTS
(A. PALAZOGLU)

TO GULSEVIN, ARKAN, TARHAN AND TO THE MEMORY OF MY PARENTS
(F. KAYIHAN)

FOR THEIR LOVE, SUPPORT AND INSPIRATION.

Preface

As the demand for profitability and competitiveness increases in the global marketplace, industrial manufacturing operations face a growing pressure to maintain safety, flexibility and environmental compliance. This is a result of pushing the operational boundaries to maximize productivity that may sometimes compromise the safe and rational operational practices. To minimize costly plant shut-downs and to diminish the probability of accidents and catastrophic events, an industrial plant is kept under close surveillance by computerized process supervision and control systems that collect data from process units and analyze the data to assess process status. Over the years, analysis and diagnosis methods have evolved from simple control charts to more sophisticated statistical techniques and signal processing capabilities. The goal of this book is to introduce the reader to the fundamentals and applications of a variety of process performance evaluation approaches, including process monitoring, controller performance monitoring and fault diagnosis. The material covered represents a culmination of decades of theoretical and practical research carried out by the authors and is based on the early notes that supported several short courses that the authors gave over the years. It is intended as advanced study material for graduate students and can be used as a textbook for undergraduate or graduate courses on process monitoring. By emphasizing the balance between the practice and the theory of statistical monitoring and fault diagnosis, it would also be an excellent reference for industrial practitioners, as well as a resource for training courses.

The reader is expected to have a rudimentary knowledge of statistics and have an awareness of general monitoring and control concepts such as fault detection, diagnosis and feedback control. The book will be constructed upon these basic building blocks, introducing new concepts and techniques when necessary. The early chapters of the book present the reader with the use of multivariate statistics and various tools that one can use for process monitoring and diagnosis. This includes a chapter on empirical process modeling and another chapter on the modeling of process signals. In later chapters, several fault diagnosis methods and the means to discriminate between sensor faults and process upsets are discussed in detail. Then, the statistical modeling techniques are extended to the assessment of control performance. The book concludes with an extensive discussion on the use of data analysis techniques for the special case of web and sheet processes. Several case studies are included to demonstrate the implementation of the discussed methods and hopefully to motivate the readers to explore these ideas further in solving their own specific problems. The focus of this

book is on continuous processes. However, there are a number of process applications, especially in pharmaceuticals and specialty chemicals, where the batch mode of operation is used. The monitoring of such processes has been discussed in detail in another book by Cinar *et al.* [41].

For further information on the authors, the readers are referred to the individual Web pages: Ali Cinar, www.chee.iit.edu/~cinar/, Ahmet Palazoglu, www.chms.ucdavis.edu/research/web/pse/ahmet/, and Ferhan Kayihan, ietek.net/. Furthermore, for supplementary materials and corrections, the readers can access the publisher's Web site www.crcpress.com¹.

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 Ahmet Palazoglu
 Ferhan Kayihan

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Nomenclature

Symbols

a	Number of principal components retained for a PC model
$a_{i \rightarrow j}$	Transition probability between states i and j
A , B	State and input coefficient matrices in continuous state-space systems
b_i	Inner relation regression coefficient in PLS
b_j	Probability distribution for observation j
$d_i^Q(\mathbf{x})$	Quadratic discrimination score for the i th population
c_A	Concentration of species A
$CONT_{i,j}^{T^2}$	Total contribution of variable x_j to T^2
$cont_{i,j}^{T^2}$	Contribution of variable x_j to the normalized score $t_i \ll S_i^2$
C , D	State and input coefficient matrices in output equation of state-space systems
$d(\mathbf{x}, \mathbf{y})$	Distance between \mathbf{x} and \mathbf{y}
$d_i(\mathbf{x})$	Linear discriminant score for the i th population
E	Residuals matrix ($n \times m$)
$e(k)$	Prediction error (residual) at time k
$E_{[a \rightarrow b]}$	Episode of a signal between points a and b
F	Residuals matrix of quality variables in PLS
F	Feature space

$F_L(d), F_H(d)$	Soft-thresholding and hard-thresholding wavelet filters
$F_W(d)$	Wiener wavelet filter
F, G	State and input coefficient matrices in discrete-time state-space systems
J	Cost function, CPM performance measure
$K(\mathbf{u}, \mathbf{v})$	Kernel function
M	Sphering matrix in ICA
M	Control horizon in MPC
m	Number of process variables in a data set
n	Number of samples in a data set
O	An observable output sequence in a HMM
P	Loadings matrix ($m \times a$)
p	Loadings vector ($m \times 1$)
p_i	PC loading i , ordered eigenvector i of $\mathbf{X}^T \mathbf{X}$
P	Prediction horizon in MPC
Q	Weight matrix of quality variables in PLS
q	Flow rate
q	Number of quality variables in a data set
q	Shift operator in time series models
q^{-1}	Backward shift operator in time series models
Q, R	Positive definite weight matrices in MPC
R	Residuals block matrix in multipass sensor FDD
R_i	Range of variable i
r_i	Residual based on the PC model for fault i
r_l	Autocorrelation at lag l
r_{sindex}	Sensor index of residuals

$r_{x,y}$	Crosscorrelation between x and y
$RCI_{j,\alpha}$	Residual contribution index for j th variable with confidence level α
S	Covariance matrix
S	A Markov state
s_i	Score distance based on the PC model for fault i
s_i^2	Variance of variable i
$SCI_{j,\alpha}$	Scores contribution index for j th variable with confidence level α
S_B	Between-class scatter matrix
S_W	Within-class scatter matrix
S_Y	Total scatter matrix
T	Scores matrix ($n \times a$)
\mathbf{t}	Scores vector ($n \times 1$)
T	Length of observation sequence in a HMM
T	Temperature
T^2	Hotelling's T^2 statistic
$TRAN$	Matrix defined in Eq. 7.2
U	Scores matrix of quality variables in PLS
v	An observation symbol in a HMM
\mathbf{v}_P	Plant noise
\mathbf{v}_y	Output sensor noise
\mathbf{w}	FDA vectors to maximize scatter between classes
$w(t - \tau)$	A STFT window function centered at τ
$\mathbf{W}_1, \mathbf{W}_2$	Disturbance coefficients matrix to state variables and outputs, respectively
W	Weight matrix of process variables in PLS

W	Projection matrix
\bar{x}	Sample mean of variable x
X	Process variables data matrix ($x \times m$)
Y	Quality variables data matrix ($x \times q$)
$z(k)$	A discrete signal evaluated at time instant k
$z(t)$	A continuous signal evaluated at time t

Greek Characters

β	Low-pass filter constant
β	Vector of regression coefficients
Δ	Magnitude of step change
ϵ	Random variation (uncorrelated zero-mean Gaussian), measurement error
$\gamma\#$	CPM performance measures ($\#$: <i>hist, des</i>)
κ	Ridge parameter
λ	A HMM
λ	Forgetting factor
λ_i	i th eigenvalue
ω	Frequency
π	Initial HMM state distribution
π_i	Classes of events such as distinct operation modes $i = 1 \dots g$
Σ	Covariance matrix
σ	Standard deviation
θ	Model parameters vector
θ_E	Euclidian angle between points a and b with vertex at the origin

θ_M	Mahalanobis angle between a and b with vertex at origin
τ	Target for the mean, first-order system time constant
Φ	MPC cost function
ϕ	Autoregressive parameter, residual Mahalanobis angle
$\phi(k)$	MPC cost function at time k
$\phi : X \rightarrow F$	Nonlinear map from input space X to feature space F
$\psi(t)$	A wavelet function
$\psi_{s \cdot u}$	A wavelet function with dilation parameter s and translation parameter u

Subscripts

$0 \cdot 0$	Initial conditions
c	Coolant
f	Feed
min	Minimum value of a variable
m, max	Maximum values of a variable
r	Reference state/value
s	Steady-state

Superscripts

T	Transpose of a matrix
-----	-----------------------

Abbreviations

AIC	Akaike information criteria
ANN	Artificial neural network
AR	Autoregressive

ARIMA	Autoregressive integrated moving average
ARL	Average run length
ARMA	Autoregressive moving average
ARMAX	Autoregressive moving average with exogenous inputs
ARX	Autoregressive model with exogenous inputs
ASM	Abnormal situation management
ASR	Automatic speech recognition
BESI	Backward elimination sensor identification
BJ	Box-Jenkins
BSSIR	Backward substitution for sensor identification and reconstruction
<i>CC</i>	Correlation coefficient
<i>CWT</i>	Continuous wavelet transform
CLP	Closed-loop potential
CPCA	Consensus principal components analysis
CPM	Controller performance monitoring
CQI	Continuous quality improvement
CSTR	Continuous stirred tank reactor
CUMPRESS	Cumulative prediction sum of squares
CUSUM	Cumulative sum
CV	Canonical variate
CVA	Canonical variates analysis
CVSS	Canonical variate state space (models)
<i>CL</i>	Centerline of SPM chart
<i>DWT</i>	Discrete wavelet transform
DCS	Distributed control system
DMC	Dynamic matrix control

<i>ECM</i>	Expected cost of misclassification
EM	Expectation maximization
EWMA	Exponentially weighted moving average
FDA	Fisher's discriminant analysis
FDD	Fault detection and diagnosis
FFT	Fast Fourier transform
FPE	Final prediction error
FT	Fourier transform
GUI	Graphical user interface
HMM	Hidden Markov model
HMT	Hidden Markov tree
HPCA	Hierarchical principal components analysis
HPLS	Hierarchical partial least squares
HTST	High-temperature short-time pasteurization
ICA	Independent component analysis
KBS	Knowledge-based system
KDE	Kernel density estimation
<i>LCL</i>	Lower control limit
<i>LWL</i>	Lower warning limit
LFCM	Liquid-fed ceramic melter
LQG	Linear quadratic Gaussian (control problem)
LV	Latent variable
<i>MSE</i>	Mean square error
MA	Moving average
MBPCA	Multiblock principal components analysis
MBPLS	Multiblock partial least squares