

## Index

Note: Page numbers in *italics* and **bold** refers to figures and tables respectively.

### **a**

accuracy of sensor 3  
 adaptive hierarchical *K*-models (AHKM)  
     10, 170–173  
 analysis of variance (ANOVA) 111–112, 140  
 asymmetric DTW algorithm 94–95  
 asymmetric synchronization 98  
 asynchronism  
     class I 114  
     class II 114  
     class III 114  
     class IV 114  
     detection 115–117  
 at-line sensors 4  
 autocorrelation 170  
 auto-covariances 153–154  
 auto-scaling 146

### **b**

Bartlett’s test 26  
 batch data analysis 183  
     historical batch data analysis 183–188  
     practical issues 192–198  
 batch dynamic (BD) 152, 162–164, 173,  
     179–180  
 batch multivariate statistical process  
     control (BMSPC) 9, 144, 162, 188, 189,  
     193–198  
 batch process modeling 5  
     data-driven models 6  
     hybrid models 7  
     knowledge-based models 5–6  
 batch process monitoring  
     bilinear modeling cycle for 7–11  
     post-batch process monitoring 189–190

real-time process monitoring 190–192  
 batch-wise (BW) 10  
     phases in batch-wise data 174–177  
     unfolding 152–158  
 bilinear modeling 165  
     cycle for batch process monitoring 7–11  
 biplot 43

### **c**

calibration batches 196  
 compression 13–18  
 conditional mean replacement (CMR) 47  
 consensus matrix 170  
 contribution plots 187  
 control charts 186  
 correlation matrix distance (CMD) 132  
 covariance matrix 151  
 criterion of goodness of fit (CGF) 26  
 cross-validation 26, 30  
 cumulative distance matrix 95, 97  
 cumulative weighted local distance 91  
 curve registration 82  
 cyclostationary 144

### **d**

data array 13  
 data-driven models 6, 13  
 data preprocessing 21, 38, 147–149  
 degrees of freedoms (DOFs) 28  
 Digital Signal Processing 56  
 direct estimation 47  
 dissimilarity index 132, 140  
 dynamic locus analysis 82  
 dynamic partial maps 132  
 dynamic programming 95

dynamic time warping (DTW) 82, 90, 94–95  
 algorithm 94–95  
 end-of-batch synchronization 97–100  
 optimization problem 95–97  
 parametric mapping of trajectories 91  
 warping function constraints 92–94  
 warping information 100–105

**e**

eigenvalue 18, 20  
 eigenvectors 18, 20  
 elution time variation 98  
 endpoint constraints 92  
 equalization 10, 55, 60  
 equalized variables 59, 60  
 evolving modeling 165  
 expectation-maximization (EM)  
 algorithm 52  
 exponential function 167  
 exponentially weighted evolving window  
 (EWEW) model 10, 165, 167  
 exponentially weighted moving average  
 (EWMA) model 170

**f**

false alarm rate 191  
 Fisher Z-transformed correlation  
 coefficients 111  
 forgetting factor 166  
 fuzzy logic for multiphase modeling 174  
 fuzzy theory 174

**g**

geometric average 100  
 global constraints 93–94  
 grey component analysis (GCA) 7

**h**

hierarchical-model approach 10, 151,  
 170–173  
 historical batch data analysis 183–188  
 Hotelling's  $T^2$  185, 187  
 hybrid models 7

**i**

industrial batch processes 1–3  
 inline sensors 4  
 instantaneous-dynamic partial maps 132  
 instantaneous relationships of process  
 variables 153  
 interpolation 64–66, 83, 87  
 Itakura parallelogram 93, 94  
 iterative batch synchronization 121–130  
 iterative imputation 47, 49–51

**k**

Kalman filters 7  
 K-models approach 10, 151, 164, 165  
 knowledge-based models 5–6

**l**

lagged cross-correlation 170  
 lagged cross-covariances 153–154  
 lagged measurement vectors (LMVs) 68  
 lags 163, 168  
 Landmark Feature 184  
 latent variable models (LVMs) 13, 16, 37–38,  
 55, 79, 144, 151, 185  
 latent variables 29  
 least significant difference (LSD)  
 intervals 112, 113  
 limit of detection of sensor 3  
 linearity, sensor 3  
 linear regression problem for two-way  
 matrices 33  
 loading plots 43  
 loading vector 154  
 local continuity constraints 93  
 local models 167, 173

**m**

Mann–Kendall test 82  
 mathematical filter 82  
 matrix factorization 45  
 matrix of regressors 34  
 mean centering 145–146, 147  
 missing data (MD) 29, 46  
 imputation and MSPC 52–53  
 by model building 52–53  
 by model exploitation 47–52  
 recovery using multiphase  
 model 69–70  
 missing-data method for exploratory data  
 analysis (MEDA) 29  
 Mixtures of Probabilistic PCA 174  
 monotonicity conditions 92  
 Moving Window models 166  
 multiblock approach 176  
 multinormal distribution 185  
 multiphase approach, 173. *see also*  
 single-model approach  
 batch dynamic data, phases in 179–180  
 batch-wise data, phases in 174–177  
 missing data recovery using 69–70  
 variable-wise data, phases in 177–179  
 multirate system 57, 74  
 multisynchro approach 114, 115, 124, 129  
 asynchronism detection 115–117  
 batch synchronization with 124–130  
 case-based reasoning 118–119

- iterative batch synchronization and anomaly detection procedure 121–130
  - specific batch synchronization 117–121
  - trajectories of acetate concentration 125
  - warping information 126, 127
  - multivariate curve resolution (MCR) model 7
  - multivariate exploratory data analysis (MEDA) 43–45
  - multivariate statistical process control (MSPC) 29, 81
  - multi-way analysis 16
- n**
- noisy data 83
  - “non-equalized” data 79
  - nonequalized variables 59, 60
  - noninvasive sensors 4
  - nonlinear dynamics 175
  - nonlinear iterative partial least squares (NIPALS) algorithm 18
  - normalized squared difference (NSD) 154
  - normal operating conditions (NOC) 2, 56, 81, 183
  - Nyquist–Shannon sampling theorem 56, 62, 85
- o**
- observation wise unfolding (OWU) 89–90, 152
  - observation-wise unfolding-T scores
    - batch-wise unfolding (OWU-TBWU) 87
  - offline DTW algorithm 104
  - offline post-batch monitoring 123
  - offline sensors 4
  - online sensors 4
  - online synchronization 105
  - ordinary least squares (OLS) 33
  - out-of-control signals 197
- p**
- parallel factor analysis (PARAFAC) 7, 16
  - parameters stability 30–33, 154
  - parametric uncertainty 157
  - partial least squares (PLS) 6, 35–38, 79, 81, 151, 185
    - regression models vs. 42–43
  - partial linear regression problem 36
  - Pearson’s correlation coefficient 110
  - pipe network example 17–18
  - precision, sensor 3
  - prediction error sum of squares (PRESS) 27–28, 30, 42
  - preprocessing 21–26, 38, 143, 147–149
    - mean centering 145–146, 147
    - scaling 97, 146–149
  - principal component analysis (PCA) 6, 18, 79, 151, 185
    - data preprocessing 21–26
    - distribution of observations in space 20
    - effect of measurement noise
      - measurement in 31
    - geometrical illustration 19
    - model exploitation, missing values at 49–52
  - principal component regression (PCR) 35–36, 42–43
  - principal components (PCs) 18–19
  - pseudo-batches 81
  - pseudo-covariance matrix 162
  - pseudo-online process monitoring 190
  - pseudo-online version of DTW 82
- q**
- Q statistic values 197
- r**
- range, sensor 3
  - real-time DTW synchronization for batch monitoring 104–105
  - real-time process monitoring 190–192
  - reference batch selection 97
  - regression 33–35
    - models based on latent variables 35–43
  - relaxed greedy time warping (RGTW) 83, 105, 147, 155
    - algorithm 106
    - batch synchronization with 111–114
    - cross-validation for estimation of parameters 110–114
    - distortion of batch time 113
    - global constraints 107–110
    - iterative procedure 110
    - online synchronization 108
    - optimal paths 109
  - reliability of sensor 3
  - residual error 27
  - residual vector 185, 189
  - response time of sensor 3
  - robust derivative dynamic time warping (RDDTW) 83
  - row-wise leave-one-out cross-validation 27
  - Runge’s phenomenon 65
- S**
- Saccharomyces cerevisiae* cultivation
    - process
      - biomass concentration 85, 87
      - offline synchronization of variable trajectories 86, 88
      - simulation time of 84
  - Sakoe–Chiba band 93, 94
  - Savitzky–Golay filter 83

- scaling 97, 146–149
  - score plots 190
  - score vector 185, 189
  - SCREE plot 26
  - selectivity of sensor 4
  - sensitivity of sensor 4
  - sensors
    - at-line 4
    - biosensor 3
    - inline 4
    - noninvasive 4
    - online 4
    - performance of 3–4
    - soft-sensors 33
    - types of 3–4
  - Shewhart SPE control chart 186–187
  - single-model approach 10, 151–152, 153
    - batch dynamic unfolding 162–164
    - batch-wise unfolding 152–158
    - variable-wise unfolding 158–162
  - single-phase dynamic model 67–69
  - single-phase non-dynamic model 66–67
  - singular points 82
  - singular value decomposition (SVD) 20
  - slope constraint 93
  - soft independent modelling of class analogy (SIMCA) 81
  - soft-sensors 33
  - squared prediction error (SPE) 123, 185
  - statistical process control (SPC) 8, 9, 183
  - stretching, compressing, and translating (SCT)-based methods 131
  - sum of squared residuals (SSR) 65
  - sum of squares (SS) 154, 157, 160, 161, 164
  - symmetric DTW algorithm 94–95, 96
    - with warping function constraints 98
  - synchronization 79
    - dynamic time warping (DTW) 90–105
      - effects on correlation structure 130–141
      - indicator variable (IV) 83–87
      - multisynchro 114–130
      - relaxed greedy time warping (RGTW) 105–114
      - time linear expanding/compressing 87–90
      - total variance-covariance matrices 133, 136, 138, 140
    - synchronization based on DTW 100–104, 103
- t**
- three-way to two-way transformation
    - K-models approach 164–173
    - multiphase approach 173–180
    - single-model approach 152–164
  - time linear expanding/compressing (TLEC)
    - observation level and 89–90
    - synchronization method 81, 87–90
    - TLEC-DTW 130–131, 138–141
    - TLEC-events 130–131, 138–141
  - time-varying static relationships 163
  - time-varying trajectories 183
  - total partial maps 132
  - trajectory centering 145
  - trajectory-wise centering and scaling (trajectory C&S) 10, 143–144, 146–148, 155, 156–159, 164
  - trimmed score imputation (TRI) 47–52
  - trimmed score regression (TSR) 47, 64
  - trimmed score regression model building (TSR-MB) 64, 78
  - truncated-Q statistic 186
  - Tucker-3 16
  - two-way LVM 37–38
- u**
- unconditional mean replacement (UMR) 46
  - unfolding method 15–16, 190
  - uniformly weighted moving window (UWMW) 10, 165, 167
  - univariate interpolation 64
- v**
- variable centering and scaling (variable C&S) 10, 143–144, 146–148, 159
  - variable trajectories 80
  - variable-wise (VW) unfolding 10, 152, 158–162, 161, 177–179
  - variable-wise unfolding after trajectory centering and scaling (VW-TCS) 161
  - variable-wise unfolding after variable centering and scaling (VW-VCS) 161
- w**
- warping function constraints 92–94
  - warping information 114
  - warping profiles 125
  - weighting factor 170
  - weight matrix 98–99, 102