

## Index

### **a**

abduction 326  
 accreditation 384–385  
 accuracy 105, 106, 284, 380, 382  
     of analysis 106  
 adaptive neuro-fuzzy inference system  
     (ANFIS) 361–362  
 adaptive splines 85  
 adjacency matrix 304, 352  
 aggregation, performance characteristics  
     108–110  
 alignment methods  
     DTW 91  
     left panel, simulated chromatogram 91  
 allele 366  
 alternating conditional expectations (ACE)  
     281, 286–290  
 alternating least squares (ALS) 182, 184  
 alternative, compound propositions 325  
 alternative hypothesis. *See* hypothesis  
 American Food and Drug Administration  
     (FDA) 385  
 analog-to-digital converter (ADC) 4, 5, 8  
 analysis of variance (ANOVA)  
     ASCA 52–56  
     definition 45  
     MANOVA. *See* multidimensional analysis  
         of variance (MANOVA)  
     multi dimensional 51  
     multi-way 48, 51. *See also* multi-way  
         analysis of variance  
     one-way 45. *See also* one-way analysis of  
         variance

regression analysis 236  
 sums of squares (SS) 235  
 two-way 48. *See also* two-way analysis of  
     variance  
 analytical databases  
     coding of chemical structures. *See* chemical  
         structures coding  
     coding of spectra 298–301  
     examples 295, 296  
     exchange files 297–298  
     information types 296  
     laboratory information and management  
         systems (LIMS) 308–309  
     source and library files 297  
     structure 296, 297  
     working and index file 308  
 analytical range 105  
 analyzers 10, 323  
 Anthranilic acid 289–290  
 apodization function 82  
 area determination 61, 74, 75  
 artificial intelligence (AI) 2, 11–13, 316, 321  
     definition 321  
     knowledge acquisition and processing  
         329, 330  
     methods 323  
     modules 321, 322  
 artificial neural networks 321, 330–332, 343,  
     345. *See also* neural networks  
 artificial neuron 331  
 assembler language 8  
 associative learning law 337  
 atomic absorption spectrometry 37, 104

atomic emission spectroscopy 91, 323  
 inductively coupled plasma (ICP-AES) 91  
 autocorrelation 61, 92, 93, 95, 99  
 correlated data 97  
 correlogram 95  
 drift and periodicities 97  
 empirical 96  
 function 96, 98  
 measure 93  
 point-wise 94  
 stationary process 94  
 time lag 93, 95  
 uncorrelated data 96  
 autocovariance 93–95  
 automation 1, 3, 9  
 autoregression 99  
 autoscaling 148, 149  
 axiom 325  
 axon 331

**b**

background correction 61, 76, 82, 84  
 backpropagation 337, 343, 344, 370  
 networks 341  
 backtracking 326  
 bagging 218–220  
 BASIC 8, 326  
 Bayes' theorem 205  
 Bayesian classification 205  
 Bayesian regulation backpropagation  
 algorithm 344  
 Beer's law 259, 260, 263, 264, 281  
 best linear unbiased estimator (BLUE) 250  
 bias 16, 45, 106, 112, 274, 294, 337, 343.  
*See also* error; systematic  
 bidirectional associative memory (BAM)  
 333, 337, 377  
 binary number system 4  
 biological fluids 91  
 biplot 159, 160  
 bit 1, 4, 6–8, 309, 312–313, 366–367, 369,  
 370, 372  
 blank 104, 105, 361, 380–382  
 samples 381  
 blind source separation problem 178  
 blocking 113, 118, 119, 134  
 blood 10, 16, 91, 188, 189, 198, 217, 384

bond electron (BE) matrix 304  
 boosting 219  
 bootstrapping 219, 285, 347  
 box-and-whisker plots 25  
 Box–Behnken design 125  
 bulk storage devices 7  
 bus 7  
 byte 6

**c**

C 8, 326  
 calcium 188  
 calibration 231  
 curved 104, 105  
 direct 261, 263  
 function 232, 380  
 indirect 263, 264  
 inverse 265–268, 272  
 K-matrix approach 264  
 P-matrix approach 265  
 calibration function 104, 105  
 canonization 307  
 cardinality 359, 360, 377  
 centering 147, 149, 227, 255  
 central composite design 125–127  
 central limit theorem 21  
 central processing unit (CPU) 7  
 certified reference materials 384  
 ceteris paribus principle 111  
 change and hope optimization procedure  
 135  
 chaos 13  
 chemical databases 295. *See also* analytical  
 databases  
 chemical structure 12, 295–298, 300–311,  
 314–316  
 matrix representation 161, 303–306  
 chemical structures coding  
 canonization 307  
 connection table 306–307  
 fragmentation codes 301–303  
 Markush structures 307  
 matrix representation 303–306  
 chemometrics  
 in Analytical Chemistry 1  
*computer-based methods. See*  
*computer-based laboratory*

- data evaluation and interpretation methods
  - 11
  - definition 1
- Chernoff faces 196, 197
- chromatographic response function (CRF) 109
- chromatography 10, 108, 109, 128, 145, 173, 177, 179, 279, 300, 323, 364
- chromosome 366, 367, 370, 378
- city-block distance 186, 187
- class 12, 17, 23, 39, 145–147, 198, 200, 203, 205–208, 211–215, 217, 219, 226, 307, 312, 336, 338, 339, 347, 363
- classification
  - by *k*-nearest neighbors (*k*NN) 192
  - by discriminant analysis 201, 213, 215, 290
  - by *k*-nearest neighbors (*k*NN) 207
  - by soft independent modeling of class analogies (SIMCA) 198, 210, 211
- classification and regression trees (CART) 216–221, 225, 226, 229, 291
- class width 16, 17
- cluster analysis 12, 145, 185, 216, 311, 312, 336, 364
  - distance measures 186
  - hierarchical 188–193
  - nonhierarchical 194–196
  - similarity measures 187
- clustering 146
  - crisp 194, 313, 353, 354
  - fuzzy 194, 364, 365
  - hierarchical 188
  - nonhierarchical 194, 195
- c-means algorithm 194, 195
- c-means clustering 196
- coding
  - chemical structures 301–319
  - spectra 295
- coefficient
  - of determination 239, 272
  - of variation 23
- Coiflet 86
- collinearity 264
- common factors 153, 161–164, 171, 172, 174
- communalities 163
- competitive learning law(s) 346
  - steps 337
- supervised 338
- unsupervised 338
- compiler 8
- complement 358
- compositional rule of inference 360
- computer application in analytics (COMPANA) 1
- computer-based analytical chemistry (COBAC) 1
- computer-based information systems 12
- computer-based laboratory 3
  - analog and digital data 3
  - analog-to-digital converters (ADCs) 5
  - binary vs. decimal number system 4
  - central processing units and buses 7
  - computer terminology 6
  - digital-to-analog converters (DACs) 6
  - input/output-systems 8
  - memory 7
  - networking 8
  - programming 8
  - robotics and automation 9
- computer program 3, 6, 8, 328
- conditioning 10, 250
- condition number 227, 250, 251
- confidence
  - band 243, 244, 285
  - interval 24, 241, 252, 294, 347
- confidence interval 24, 381
- confounding 114, 125
  - parameter estimations 125
- confusion matrix 202, 352
- conjunction 325
- connection table 306–307, 314, 315, 318
  - bond atoms and bonds 306
  - connection matrix of atoms 306
  - nonredundant 307
- continuous/discrete continuous quantities 104
- control
  - chart 382–383
  - sample 382
- convolution 61, 76, 80
- Cook's distance 273, 275
- correlation
  - coefficient 91, 93, 94, 150, 164, 239, 311

- correlation (*contd.*)
  - matrix 150, 151, 156, 158, 160, 162–166, 168, 169, 171, 189, 333, 335
  - reduced 163, 164
  - measure 16, 159
- corticoids 311
- cortisone 311
- counting rates 20
- covariance matrix 69, 92, 150, 163, 202, 206, 207, 210, 241, 243, 285, 290
- cross-correlation 61, 92, 98
- crossover 367, 368
- cross-validation 86, 156, 179, 208, 218–220, 225, 255, 257, 268, 273, 274, 276, 291
- cross-validation principal components 211
  
- d**
- data
  - analog 3
  - correlated 16, 61, 97, 99
  - digital 3, 5
  - interpretation 11
  - missing 147
  - preprocessing 145, 147, 149
  - random 11, 16, 61, 208
  - set characterization 21, 148, 151, 156, 157, 179, 185, 188, 203, 219, 225, 229, 270, 287–289, 300, 309, 313, 343, 362, 364
  - three-way 179, 183, 185, 279, 280
  - transfer
    - parallel 7
    - serial 7
  - two-way 48, 179, 278
- database
  - analytical 295–320
  - model 308
  - structure 296
- data preprocessing
  - correlation matrix 150, 151
  - mean centering 148
  - missing data 147
  - scaling 148
  - variance-covariance matrix 150
- data reduction 79, 82, 84, 300, 308
- Daubechies 86
- decimal number system 4
- decision boundary 199, 201, 214, 345
- deconvolution 61, 76, 81, 82
- deduction 325
- degrees of freedom 24, 31, 32, 36, 38, 47, 51, 116, 235, 239, 270, 273, 383
- delta rule 337, 342
- dendrite 331
- dendrogram 191, 193
- density function. *See* frequency function
- derivation algorithm 11
- descriptive statistics
  - box-and-whisker plots 25
  - confidence interval 24
  - dispersion measure 23
  - error propagation 25, 27
  - geometric mean 22
  - harmonic mean 22
  - median 23
  - quartiles 23
  - random numbers. *See* random number distribution
  - uncertainty and error 28
- detection limit 105, 361, 380
- diagnostic statistics
  - hat matrix 268
  - influential observations 270, 271, 275
  - inverse calibration model 268
  - outliers 269, 270
  - residuals and prediction error 269
  - SEC 268
- digit
  - least significant 4
  - most significant 4, 83
- digital smoothing and filtering
  - advantages 62
  - filter selection process 64, 67
  - Kalman filter 68, 69
  - moving average filter 62
  - Savitzky–Golay filter. *See* Savitzky–Golay filter
  - Simpson rules 75
  - trapezoidal rules 74
- digital-to-analog converter (DAC) 6, 8
- discrete analyzers 10
- discrete membership functions 357
- discrete quantities 104
- discriminant analysis

- linear (LDA) 201, 225, 226
- quadratic (QDA) 207, 225, 226
- regularized (RDA) 207
- dispersion 15, 18, 23, 106, 152, 162, 166, 381, 382
  - matrix 152, 162, 166. *See also* variance
  - measure 23
- dissimilarity measures 312
- distance
  - matrix 188–190, 192
  - measure 186, 189, 191, 311, 312, 337, 346
- distribution
  - binomial 21
  - F* 36, 37
  - function 19, 29, 40, 354
  - Gaussian. *See* normal distribution
  - kurtosis 20, 21, 24, 172
  - moment 19
  - Poisson 20
  - skewness 19
  - Student's 24, 31, 32, 381
- Dixon's Q-test 43
- drift 61, 69, 80, 86, 93, 97, 112
- dynamical system model 68
- dynamic range 105
- dynamic time warping (DTW) 91
  
- e**
- eigenvalue 52, 156, 157, 251, 265, 268
  - one criterion 156
- eigenvector
  - analysis 152, 165
  - projection 151
- elemental composition 51, 146, 147, 158, 173, 177, 204
- ensemble methods 218, 219
- enzyme 114, 120, 123, 131, 133, 140
  - ceruloplasmin (CP) 130, 131
- equivalence 146, 325
- error
  - first and second kind 41
  - integral. *See* distribution function
  - propagation 15, 25, 27, 72, 74, 108
  - random 16, 37, 45, 48, 99, 106, 245, 248
  - real 171
  - round-off 3, 26, 62, 251
- of second kind 41
- systematic 16, 105, 112, 379
- $\alpha$  error 41
- $\beta$  error 41–42
- ESPRIT 330
- Euclidean distance 186–188, 193, 337
- European Union regulation 33
- evolutional component 365
- evolutionary strategies 12, 13
- evolving factor analysis (EVA) 177
- exchange file 297–298
- exclusive OR 312, 313, 339, 340
- experimental design
  - balanced 114
  - blocking factors 113
  - Box–Behnken 125, 126, 128, 130
  - central composite 125–127
  - ceteris paribus principle 111
  - confounding 114
  - factorial experiments 113
  - fractional factorial 115, 118
  - full factorial 114, 115, 121, 124–126, 135
  - Latin square 118, 119
  - lattice 129
  - mixture 128, 129
  - Plackett and Burman 118
  - randomization 112
  - replication 111
  - response surface. *See* three-level
  - saturated 118
  - screening. *See* two-level
  - star 125, 126
  - supersaturated 119
  - symmetry 114
  - three-level 124, 126
  - three-level designs. *See* response surface designs
  - two-level 114, 115, 117
  - two-level designs. *See* screening designs
- expert systems 5, 8, 12, 323, 364
  - aims 328
  - analytical chemistry 330
  - definition 328
  - development tools 329
  - structure 329, 330
- explained variance principal components 156

- extended *t*-test and *F*-test 37  
externally studentized residual 270
- f**
- factor
- coding 132, 133
  - experimental 15, 143
  - loadings 164, 165
  - rotation methods 161
  - score determination 169
  - score matrix 169
  - significance 102
- factor analysis (FA)
- evolving 177
  - factorial methods 177
  - parallel 179, 279
  - vs. singular value decomposition 170
- factor effects 52, 101, 114, 116, 120–122, 129, 130, 133, 135
- estimation 120–122, 124
- vs. regression parameters 133
- relation with regression parameters 252, 268
- factorial
- experiments 113, 116
  - methods 151, 155, 182, 336
    - factor analysis 161, 177
    - principal component analysis 152
    - singular value decomposition 161
- factorial methods 86
- fast Hadamard transformation (FHT) 79
- feature 33, 90, 146, 148, 152, 159, 163, 164, 168, 171, 172, 186–189, 194, 196, 198, 199, 203, 213, 215, 217, 218, 274, 298, 310, 312, 319, 345, 366, 378, 379
- figure-of-merit. *See* objective function
- filter
- high-pass 80
  - Kalman 61, 68, 69
  - low-pass 80
  - moving average 62, 63
  - polynomial 61, 68, 71, 72, 86
  - recursive 68
  - Savitzky–Golay 64, 67, 71, 72
  - width 62–64, 67, 100
- filtering algorithm 69
- fixed-size simplex optimization method 137, 138
- flowing system 10
- forecasting. *See* prediction
- FORTRAN 8
- forward directed learning algorithm 342
- Fourier transformation (FT)
- conventional spectroscopy 77
  - convolution and deconvolution 80–82
  - data reduction and background correction 82
  - discrete 77
  - integration 82
  - inverse 77
  - Nyquist frequency 76
  - signal filtering 80
  - time domain 76
- fractal structures 13
- fractional factorial designs 115, 118
- fragmentation codes 301–303, 314
- HORD code 302
  - HOSE code 301, 302
  - structure generator 303
- frame 324, 379
- frequency
- aliased 77
  - function 18
- F*-tests 36
- full factorial design 114, 115
- fuzzy arithmetic 364
- fuzzy clustering 194
- fuzzy inferences 364
- fuzzy inference systems 360
- fuzzy logic 360, 364
- fuzzy set 194, 314, 321, 352–354, 358, 360, 364
- operation 358
- fuzzy theory 12, 352
- applications 364, 365
  - cardinality 359
  - complement 358, 359
  - intersection 358
  - relative cardinality 359, 360
  - set theory 353
  - union 358, 359
- F* value 36, 37, 47, 46, 50, 240, 241, 244

***g***

gas chromatography 145, 279, 300, 364  
 GC/MS 8  
 Gaussian distribution 17, 18. *See also*  
     normal distribution  
 Gaussian elimination 251  
 Gauss–Jordan elimination 251  
 general least squares (GLM) 53  
 generic structure. *See* Markush structure  
 genetic algorithms 13, 321, 365  
     applications 369, 370  
     computer heredity 366  
     crossover 367  
     initial population 366  
     mutations 367  
     selection/reproduction 366  
     simulated annealing (SA) 370–372  
     tabu search (TS) 372, 373, 375  
 geometric mean 22  
 global search strategies. *See* genetic  
     algorithms  
 glucose 16, 91, 97  
 good laboratory practice (GLP) 385  
 goodness-of-fit test 39, 239, 240, 272  
 $\chi^2$  goodness-of-fit test 38, 39  
 graph theory 303  
 Grubbs's test 44

***h***

Haar 86, 87  
 Hadamard transformation (HT)  
     data reduction and background correction  
         83  
     FHT 79  
     Walsh function 78  
     wavelet transformations 77  
 hair 146, 147, 156–159, 172, 193, 197, 199,  
     203, 204  
 Hamming distance 312  
 hard disk 8  
 hardware 6, 62  
 harmonic mean 22  
 hat matrix 268  
 Hebb learning. *See* learning, associative  
 Hebb's law 337

heredity 366  
 Hessian matrix 284  
 heteroscedasticity 245, 246  
 hexadecimal number 5  
 hidden layer 216, 331, 338, 340–343  
 hierarchical cluster analysis  
     centroid linkage 192  
     complete linkage 192  
     first reduced matrix 189  
     fourth reduced matrix 190  
     median linkage 193  
     second reduced matrix 190  
     single linkage 192  
     third reduced matrix 190  
     unweighted average linkage 192  
 Ward's method 193  
     weighted average linkage 192  
 hierarchically ordered ring description  
     (HORD) code 302. *See also* HORD  
     code  
 hierarchically ordered spherical description of  
     environment (HOSE) code 301, 302.  
     *See also* HOSE code  
 hierarchical search trees 311  
 histogram 17, 18, 245  
 hit list 311  
 homoscedasticity 246  
 horn clause 328  
 householder reduction 251  
 human being 9, 322  
 3-hydroxypropanal 305  
 hypotheses testing 20  
     comparison of mean with true value 31  
     comparison of two means 35, 36  
     comparison of variances 36  
         error of first and second kind 41  
     distribution. *See* hypotheses distribution  
     mean vs. true value 35  
     steps 30  
 hypothesis  
     alternative 30–32, 34, 40  
     null 40, 41, 43, 44, 46, 52, 251, 252, 270  
     testing 28, 30, 34, 35, 41  
 hypothetical distribution  
      $\chi^2$  goodness-of-fit test 39  
     Kolmogorov–Smirnov's test 39

***i***

ICA. *See* Independent Component Analysis (ICA)  
 identification 308, 343, 365  
 identity matrix 69, 165, 207  
 image processing 11  
 implication 325, 330  
 in-breadth searching 326  
 Independent Component Analysis (ICA) 177, 178  
 in-depth search 330  
 indicator function 171  
 induction 326  
 inferences 11, 15, 16, 325, 360, 364  
   abduction 325, 326  
   deduction 325  
   engine 330  
   induction 326  
   logical connectives 325  
   rule 325  
 influential observation 246, 270, 271, 275  
 information and system theory 11  
 infra red spectroscopy 231, 259  
   NIR 231, 257, 259, 272, 273, 343  
 initial population 366, 368  
 integration algorithm 82  
 interface  
   IEEE-488 7  
 interference noise 80  
 interlaboratory comparison 36, 47, 49  
 interpolating splines 84, 85  
 interpretable factors 161  
 interquartile range 22, 23, 25  
 intersection 309, 314, 358, 377, 359  
 inverse sensitivity 104  
 inverted lists 309–310  
   library search 309, 311  
 I/O system 8

***j***

jackknifed residual 270, 274, 275. *See also*  
   studentized residual  
 Jacobian matrix 284  
 JCAMP/DX exchange file 297–298  
 joint committee on atomic and molecular data  
   (JCAMP/DX) 297

***k***

Kalman filter 68, 69  
 Karhunen–Loéve expansion 159  
 kernel functions 215  
 kinetic–enzymatic oxidation 120, 123  
 K-matrix approach 264–266  
 k-nearest neighbor (*k*-NN) method 192  
   classification 208, 210  
 knowledge  
   processing 12  
   acquisition 12, 329  
   base 326, 329  
   processing 321  
   representation 323, 324  
 knowledge processing and soft computing. *See*  
   artificial intelligence (AI); expert  
   systems; fuzzy theory; genetic  
   algorithms; neural networks  
 known factors 113  
 Kohonen networks 336, 345  
 Kolmogoroff–Smirnov's test 39  
 kurtosis. *See* distribution

***l***

laboratory-information-and-management  
 system (LIMS) 8, 308–309  
 lack-of-fit test 240  
 Lagrangian theory 214  
 lasso regression 276  
 latent variable 153, 227, 254, 288  
 Latin square. *See* experimental design  
 Latin square factorial design 118, 119  
 learning  
   algorithm 332, 338, 341, 342, 346, 370  
   associative 337, 339, 347  
   competitive 337, 338, 346  
   law 337, 338, 377  
   paradigm 336  
   supervised 336, 339, 343, 364  
   unsupervised 145, 151, 185, 186, 336, 345,  
    364  
 Leary criterion 108  
 legal inference 325, 326  
 level attained. *See* *p*-level  
 library file 297  
 library search 207, 295, 309–316, 365

- hierarchical search trees 311  
 inverted lists 309–310  
 sequential search 309  
 similarity measures for chemical structures 314–316. *See also* similarity measures for spectra  
 library spectrum 311–313  
 limit of determination 105, 380, 386  
 limited selective method 107  
 linear discriminant analysis (LDA) 201, 225, 226  
 linearization method 282–285  
 linear learning machine (LLM) 198, 200  
 linear model 232, 240, 283  
 linguistic modifiers 356, 357  
 linguistic variables 356, 357, 361  
 linkage  
     centroid 192  
     complete 192  
     median 193  
     single 192  
     unweighted average 192  
     weighted average 192  
 liquid chromatography 128, 173  
     HPLC 111, 129, 139, 173, 281, 289, 290, 299, 312, 330, 343, 370  
 liquid handling 10  
 list processing language (LISP) 8, 322, 326–327, 330  
 local area networks (LANs) 8  
 location parameter 21  
 logical connective 5, 312, 325
- m**
- Machine code 8  
 machine learning 12, 322, 323, 330, 347  
 Mahalanobis distance 186, 207, 269  
 Manhattan distance 186, 312  
 manipulation 9, 12, 61, 309  
     software 308  
 MANOVA. *See* analysis of variance, multidimensional  
 Markush chemical structures 307  
 Markush structure 307  
 Marquardt algorithm 285  
 mass spectrometry 88, 89, 145, 182, 279, 300, 312, 313, 323  
 electrospray-ionization (ESI-MS) 182, 184, 185  
 matrix inversion 266  
 mean  
     arithmetic 18, 21, 24  
     centering 148  
     geometric 22, 24  
     harmonic 22  
 c-means algorithm 364  
 measurement 2, 4, 8, 10, 11, 15, 23–25, 27, 28, 30, 31, 40, 48, 49, 51, 103–106, 109, 111, 120, 130, 232–236, 240, 247, 253, 279, 295, 300, 379, 382  
     model 68, 77, 83, 84, 91, 93, 95, 98, 99  
     uncertainty 16  
 median 23, 24, 193, 382  
 membership functions 194, 353–356, 358, 360, 362  
     characteristic function 353  
     discrete 357, 358  
     fuzzy observations 354  
     linguistic variables 356  
     truth values 357  
 memory  
     random access (RAM) 7, 310  
     read-only (ROM) 7  
 method of steepest descent 282, 285  
 Mexican hat 86, 87, 346, 347  
 Minkowski distance 187  
 missing data 147  
 mixture design 128  
 mode 3, 23, 163, 183, 279  
 model adequacy test 116, 233, 234, 236, 239, 240  
 model(ing)  
     empirical 124, 130, 131, 231, 281, 284, 290  
     linear 116, 130, 232, 240, 283, 336  
     mechanistic 130, 284, 290  
     power 211, 212  
 moments of distribution 19  
 Monte Carlo method 285  
 Moore–Penrose-matrix. *See* pseudo inverse matrix  
 Morgan’s algorithm 307  
 Morlet 86, 87  
 multicomponent analysis 69, 107, 108, 249, 259, 267, 366, 370, 372

multicriteria optimization 364, 366  
 multidimensional analysis of variance (MANOVA) 51  
 multilayer perceptrons 341, 342  
 multiple linear regression  
   diagnostic statistics. *See* diagnostic statistics  
   direct calibration method 261, 263  
   indirect calibration method 263, 264  
   OLS. *See* ordinary least squares (OLS)  
   regression  
   PCR 249, 251, 253, 266, 274  
   PLS 249, 251, 253, 255, 257, 266, 267, 274, 276  
   *P*-matrix approach 265  
   soft modeling 265, 266, 268  
   spectrometric multicomponent analysis 249  
 multivariate adaptive regression splines (MARS) 281, 288, 289  
 multivariate curve resolution 155  
 multivariate regression spline model 288  
 multi-way analysis of variance 51  
 multiway decompositions 179  
 mutation 366, 367

***n***

negation 309, 325  
 Nelder and Mead method 101, 136  
 network 3, 8, 13, 215, 281, 295, 300, 308, 312, 333, 334, 336–339  
   worldwide 8  
 Network Common Data Format (Netcdf) 300  
 neural networks 13, 312, 330, 370  
   aggregation 332  
   applications 343  
   architecture 338, 339  
   artificial neuron 331  
   associative learning law 337  
   backpropagation algorithm 341  
   bidirectional associative memory (BAM) 333  
   competitive learning law 337, 338  
   convolutional 349  
   deep learning 348  
   hidden layer 331  
   Kohonen network 345

learning paradigm 336, 337  
 long short-term memory (LSTM) 349  
 models 336  
 perceptron models 339  
 recurrent 348  
 transfer functions 332, 333  
 weights of synapses 332  
 neuron 331, 336, 341–343, 345–347  
 nitrate 33–35  
 noise  
   interference 80  
   signal derivatives 71, 72, 74  
 non-hierarchical cluster analysis  
   c-means clustering 194–196  
   fuzzy clustering 194  
 nonlinear iterative partial least squares (NIPALS) algorithm 153, 154, 160, 210, 211, 255  
 nonlinear partial least squares (NPLS) 281, 287–290  
 nonlinear regression (NLR)  
   chemical equilibria 281  
   grid search method 285  
   Hessian matrix 284  
   Jacobian matrix 284  
   Marquardt algorithm 285  
   Monte Carlo method 285  
   parameters 281  
   regression diagnostics 285  
   simplex method 285  
   steepest descent 282, 283  
 nonparametric test 231, 281, 289, 290  
 normal distribution 18, 20, 21, 24, 28, 39, 40, 43, 205, 206, 210, 245  
 normalization 27, 64, 149, 227, 283  
 nuclear magnetic resonance (NMR) 77, 297, 299, 316, 317, 323  
 null hypothesis 31–36. *See also* hypothesis  
 N-way PLS (N-PLS) 280  
 Nyquist frequency 76

***o***

object 22, 147, 152, 157, 160, 186, 188–191, 194, 195, 203, 205, 207, 208, 210–213, 384  
 objective criterion 11, 109, 140, 382, 383  
   aggregation of 189

objective function 103, 282, 285, 337, 364, 366, 367, 369, 372  
accuracy of analysis 106  
aggregation, performance characteristics 109, 110  
calibration function 104, 105  
detection limit and limit of determination 105  
polyoptimization 110, 111  
specificity and selectivity 106–108  
time, cost and risk 108  
oblimax criterion 172  
one-variable *t*-test  
calculated value vs. tabulated value 32, 33  
nonparametric tests 33  
null hypothesis 31  
one-sided *t*-test 33  
*p*-level 35  
significance level 31  
standard deviation 31  
two-sided *t*-test 33  
one-way analysis of variance 45  
OPLS. *See* orthogonal PLS (OPLS)  
optimization  
poly 110  
sequential 103, 135  
simultaneous 109  
systematic 101, 102  
ordinal scaled values 104  
ordinary least squares (OLS) regression  
definition 250  
matrix notation 250  
parameter estimation 250  
parameter significance 251, 252  
prediction 252, 253  
singular value decomposition (SVD) 251  
Organization for Economic Cooperation and Development (OECD) 385  
orthogonal PLS (OPLS) 257  
outlier 15, 23, 25, 43, 44, 192, 200, 205, 211, 212, 246, 249, 267, 269–271, 275  
Dixon's Q-test 43  
Grubb's test 44  
out-of-bag classification error 224  
overfitting 179, 218, 251

**p**  
parallel factor analysis 179, 182  
parameter estimation 125, 130, 131, 133, 146, 233, 241, 249, 250, 252, 284, 285, 337, 343, 366  
Pareto optimality 110  
Pareto scaling 148  
partial least squares (PLS) 153, 198, 249, 251, 257, 267, 276  
regression 253–256  
partition 17, 45, 114, 194–196, 216, 217, 291  
pattern 194–196, 216, 217  
pattern recognition 11, 12, 43, 145  
pattern recognition and classification. *See* cluster analysis; supervised learning methods; unsupervised learning methods  
PCR. *See* regression, principal component peak separation after Kaiser 109, 110  
peak shape  
Gaussian 67  
Lorentz 67, 72  
peak list 299  
Pearson distance 186  
percentile 23  
perceptron 216, 339, 343, 377  
performance characteristic 104, 109, 110, 308, 380, *See also* objective function  
periodicity 93, 95  
pH monitoring 91  
pharmaceutical industry 128, 259  
phenol 30  
phosgene 303, 304, 306  
phosphate 188  
photomultiplier 3, 20, 80  
*p*-level 35, 50, 52, 272  
Poisson distribution 20  
polycyclic aromatic hydrocarbons (PAHs) 43, 173  
polyoptimization 110, 111  
potassium 46, 47, 51  
Powell's method 139  
p-phenylenediamine (PPD) 120, 123, 130–133, 140, 142  
precision 10, 16, 101, 102, 106, 114, 251, 255, 256, 263, 380, 381  
predicate logic 323

- prediction 2, 69, 93, 99, 176, 218, 219, 233, 243, 244, 247, 252, 253, 255, 257, 267, 268, 272, 274, 287, 291, 345, 347, 370  
 error 269, 274, 291  
 principal component 157, 210, 211, 228, 249, 255, 257, 263, 267–269, 276, 287, 312  
 principal component analysis (PCA) 150–154, 157, 158, 160, 162, 164, 165, 168, 169, 171, 177–179  
 principal component regression (PCR) 253, 266, 274  
 principal factor analysis 164, 168  
 probability 16, 18–20, 24, 27, 28, 30, 37, 206, 207, 240, 252, 353, 354, 367–370, 372  
 probability density function. *See* frequency function  
 probability function of Poisson distribution 20, 370  
 productivity 10  
 programming 3, 8, 10, 322, 326, 328  
 programming in logic (PROLOG) 322, 327–330, 377  
 language 8, 322, 328–330, 377  
 protein 88, 90, 182, 185, 231, 257, 259, 271–274, 300  
     apomyoglobin 183  
 proximity matrix 224  
 pruning 217  
 pseudo-inverse matrix 253
- q**
- Q analysis 162, 163, 170  
 quadratic discriminant analysis (QDA) 207  
 quality assurance  
     external 384  
     internal 381–382  
 quality control 11, 365, 379–383  
 quality, definition 380  
 quantile 21, 23, 31, 32, 381  
 quartimax criterion 172
- r**
- R analysis 162, 163, 166, 170  
 radial basis function 215  
 random access memory (RAM) 7. *See also* memory, random access
- random errors 16, 106  
 randomization 112, 113, 143  
 random forest 222  
 random number distribution  
     analytical 380, 381  
     central limit theorem 21  
     classes 16  
     dynamic 380, 381  
     frequency distribution 17  
     Gaussian distribution 17, 18  
     moments of distribution 19  
     Poisson distribution 20  
     scaling 148  
     spectrophotometric measurements 17  
 random process 97  
 range  
     analytical 80, 104  
     dynamic 105  
 rank 21, 104, 165, 171, 269, 274  
 rank annihilation 151  
 read-only memory (ROM). *See* memory; read-only (ROM)  
 recovery function 273, 285, 292, 380  
 recursive filter 68, 69  
 reduced correlation matrix 163, 164, 168  
 regression  
     linear 86, 97, 99, 173, 176, 202, 231, 232, 234, 235, 238, 245, 246, 284, 285, 316, 372, 380  
     multiple linear 173, 176, 231, 249, 316  
     multiway 278–280  
     nonlinear 231, 281–283, 287, 289, 290  
     nonparametric 290  
     ordinary least squares 249–251, 253, 263, 266, 272–274  
     partial least squares 253–255, 257  
     principal component 249, 253, 266, 274  
     robust 248, 249  
     tree-based regression 291  
     univariate linear 232  
     weighted 245–248  
 regression diagnostic 231, 246, 249, 267, 273, 285  
 regression spline. *See* spline  
 regression trees 290, 291  
 relative cardinality 360  
 replication 111, 114, 125, 126, 128, 236

- residual
  - analysis 245, 246
  - studentized 270, 271
- resolution
  - analytical 107
  - chromatographic 109
  - visual 62, 71, 72
- response 51, 52, 101, 102, 109, 111, 116, 124, 126, 128–130, 132, 135, 137, 139, 141, 142, 200, 216–218, 231, 252, 280, 281, 291, 367, 368
- response surface designs
  - factor effects vs. regression parameters 133, 134
  - blocking of experiments 134
  - Box–Behnken design 126–128
  - central composite design 125, 126
  - mixture design 128, 129
  - response surface methods 129–132
- response surface methods (RSM) 101, 103, 129, 130, 132, 231
- ridge regression 276
- risk 24, 29–31, 36, 41, 44, 52, 109, 205, 232, 240, 252, 270
- robot
  - geometry 9
  - robotics and automation 9
- robustness 101, 249, 270, 380, 381, 386
- robust regression 248
- round-robin test 381, 384
- rotation
  - oblique 171
  - orthogonal 172
  - target 172
- rotation of factors 171, 172
- round-robin test 49
- rule 2, 3, 10, 15, 30, 64, 74, 75, 78, 123, 153, 183, 205, 213, 299, 306, 324, 325, 328, 330, 337, 360
- rule-based fuzzy systems 360–362
  
- S**
- sample 6, 15, 91, 107, 108, 145, 233, 296–298, 357, 366, 380
- Savitzky–Golay filter
  - filter coefficients 64
- signal derivatives 71, 73, 74
- scaling 86, 88, 104, 114, 148, 154, 172, 186, 249, 270, 379
- auto 148, 149, 227
- methods 148
- range 148, 227
- score 152, 154, 157, 158, 160–162, 168, 169, 174, 203, 211, 227, 254–257, 268, 269, 287
- Scree plot 157
- scree test 156, 157, 171
- scree test principal components 157
- screening designs
  - factor effects estimation 114, 120
  - fractional factorial designs 115, 120
  - full factorial design 114
- search methods 103, 282, 285, 295
- search problems. *See* genetic algorithms
- search strategies 295, 309, 326
- seed 186
- selection 64, 67, 102, 113, 246, 309, 312, 323, 330, 339, 343, 366, 368, 374, 378
- selective analytical method 106
- selectivity 102, 106–110, 139, 259, 384
- self-organizing feature maps 345. *See also* Kohonen networks
- self-organizing nets. *See* Kohonen networks
- semantic nets 324
- sensitivity 101, 102, 104, 113
- separation 2, 10, 109, 110, 139, 178, 201, 203, 207, 208, 213, 215, 281, 282, 300, 330, 339, 340
- sequential optimization 103, 136
- sequential search strategy 309
- sequential strategies 103
- shell 8, 329, 330, 377
- shot noise. *See* noise, white
- signals 74
  - derivative 71, 73, 74
  - Gaussian 178
  - integration 74, 75
  - Lorentz 84
  - processing 11, 61, 99
- signal smoothing 84
- signal-to-background ratio 108, 109
- signal-to-noise ratio 80, 101, 108

- significance  
 level 30, 33, 35, 36, 39, 40, 43, 45, 50,  
 240–242, 244, 252, 272, 381, 382  
 of parameters 251, 252
- significant factors 171
- similarity measure 186, 187, 311
- similarity measures for spectra  
 correlation measures 311  
 dissimilarity measure 312  
 grouping and feature selection 312  
 logical operations 312
- simplex method 11, 101, 136, 137, 139, 285,  
 371, 377  
 fixed-size 137–138  
 optimization method 138  
 variable-size 135–141
- Simpson rules 74, 75
- simulated annealing (SA) 370
- simultaneous strategies 102
- singular value decomposition (SVD)  
 151–153, 160, 170, 251, 253, 265, 266,  
 280
- skewness 19, 21, 24
- smoothing algorithm 287
- smoothing splines 86
- soft computing 12, 321
- soft independent modeling of class analogies  
 (SIMCA) 198
- soft modeling 265–267
- software 2, 6, 10, 35, 40, 51, 52, 62, 118, 142,  
 157, 168, 267, 308
- soil 43, 91, 228
- source file 297
- specific analytical method 107
- specificity 107
- spectra interpretation 12, 330
- spectra simulation 316–318
- spectrometric multicomponent analysis  
 259
- spline  
 adaptive 85  
 function 288  
 interpolating 84  
 regression 281, 288–290  
 smoothing 61
- spline functions 84  
 defined 85
- interpolating splines 85  
 smoothing 86
- standard deviation  
 of the procedure 380  
 relative 21, 23, 24
- standard error of calibration (SEC) 268, 272
- standard error of prediction (SEP) 256, 269,  
 273
- standard normal distribution 28, 31. *See also*  
 normal distribution
- standard normal variate (SNV) 259
- standard operating procedure (SOP) 381
- standard solution 294, 380, 381
- Staphylococcus nuclease (SNase) 89
- star and sun-ray plots 196, 197
- star design. *See* experimental design
- star plot 197
- stationary process 94, 97
- statistical testing  
*hypotheses. See* hypotheses testing  
 normal distribution 31  
 outlier. *See* outlier testing
- statistical tests 28, 33, 35, 43, 101, 102, 113,  
 234
- statistics  
 descriptive 16, 96  
 inference 11, 15, 16
- steel 37, 49, 51, 309, 323, 330
- storage  
 bulk 7, 297, 298  
 optical 3, 20, 52, 179, 339
- straight-line model. *See also* regression,  
 univariate linear
- ANOVA 234, 235, 236, 238
- coefficient of determination 239
- confidence bands 243, 244
- confidence intervals 241, 242, 252
- correlation coefficient 239
- lack-of-fit test 240
- parameter estimation 233, 250, 251
- prediction 233, 252
- residual analysis 245
- residual variance 233
- robust regression 248
- standard deviation 233, 247, 283
- standard generalization 233
- weighted regression 246–248

- structure–activity relationships 2, 318, 375  
 structure generator 303  
 Student's *t* value 31, 34, 121, 252, 270  
 studentized residual 270, 271  
 substructure search 307, 314  
 sulfate 93, 217  
 sum of residuals 238  
 sum of squares  
   mean (MSS) 234, 237, 239  
 predictive residual (PRESS) 269, 272, 274,  
   276, 289  
 sun-ray plot 197  
 supervised competitive learning 338  
 supervised learning methods 336, 339, 343,  
   364, 365  
   discriminant analysis 201–207  
   *k*-nearest neighbor method 207, 208  
   linear learning machine 198–200  
   soft independent modeling of class  
     analogies 210, 211  
   support vector machines 215, 216  
   tree-based classification 216  
 supervision 10  
 support vector machines (SVMs) 198, 213,  
   215, 216  
 symbolic knowledge processing 360, 377  
   inferencing 325  
   knowledge representation 323, 324  
 programming 326, 328  
   search strategies 326  
 symbolic programming 322, 323, 326  
 symmetry 125  
 Symmlet 87  
 systematic errors 16, 105  
 systematic optimizations 101, 102
- t***  
 tabu search (TS) 372  
 tail area 28, 30  
 target-transform factor analysis (TTFA)  
   162  
 Taylor expansion 284  
 ternary mixtures 129  
 test  
   chi-square 38  
   distribution 15, 20, 30, 31, 38  
   *F* 33  
   for distributions 38  
 Kolmogorov–Smirnov 38, 40  
 nonparametric 33, 207  
 outlier 43  
*t*-, extended 37  
*t*-, general 30, 36  
*t*-, one-sided 32–35  
*t*-, one-variable 31  
*t*-, two-sided 15, 33, 35, 37  
*t*-, two-variable 35  
 Wilk's 52  
 textile industry 128  
 time-series analysis 16, 61, 99  
   autocorrelation. *See* autocorrelation  
   autocovariance 94  
   autoregression 99  
   cross-correlation 98  
 titanium 36, 37  
 transfer function 332, 333, 377  
 transformation  
   Fourier 11, 76, 227, 297  
     discrete 77  
     inverse 77  
   Hadamard 11, 61, 76–79  
   wavelet discrete (DWT) 88, 89  
 traceability 384  
 trapezoidal rule 74  
 tree-based classification 217  
   CART 216–220, 225, 229  
   classification 216  
   ensemble methods 218, 219  
   recursive binary partitioning 216  
 trueness 10, 16, 101, 106, 380, 381, 384  
 truth value 5, 16, 31, 33, 106, 254, 328, 357,  
   358, 384  
 Tucker models 179, 183, 185, 279  
 two-variable *t*-tests 35  
 two-way analysis of variance 48, 50
- u***  
 uncertainty 15, 16, 25, 27, 28, 69, 354, 355.  
   *See also* measurement uncertainty  
   vs. error 28  
   error propagation 25  
   measurement uncertainty 16  
   random and systematic errors 16  
   sources 26

- uncertainty (*contd.*)  
 vagueness 16  
 variability 15
- uncontrolled factors 113
- undirected graphs 303
- univariate linear regression 232  
 straight-line model 232, 233. *See also*  
 straight-line model
- unknown factors 113
- unselective or partially selective method 107
- unsupervised competitive learning 338
- unsupervised learning methods 336, 365  
 cluster analysis 185  
 factorial methods 151, 152  
 graphical methods 196
- urine 97
- UV spectroscopy 173
- V**
- vagueness 15, 16
- validation 10, 86, 156, 157, 362, 380, 384
- variability 15, 16, 364
- variable-size simplex optimization method 138
- variance  
 explained 156  
 meaningful 212  
 residual 157, 211–213, 233, 241
- variance–covariance matrix 150. *See also*  
 covariance matrix
- variate 20, 28  
 standard normal 28, 31
- varimax criterion 172
- W**
- Walsh function 77, 84
- Walter Shewhart 383
- Ward's method 193
- warping 91
- water 30, 33, 35, 46, 51, 91, 129, 231, 259,  
 311, 356
- wavelet analysis 86, 88, 90
- weighing 10, 279, 280
- weight 43, 74, 109, 128, 199, 200, 214, 219,  
 246, 247, 255, 257, 331–333, 335–338,  
 347, 361, 377
- weighted regression 245–248
- Welch test 36
- Wilcoxon test 33
- Word 3, 6, 32, 152, 240
- working range 104, 105. *See also* range,  
 analytical
- X**
- X-ray analysis 20
- X-ray diffraction spectrometry 297
- X-ray fluorescence analysis (XRF) 109, 323,  
 353, 354, 365, 370
- XOR problem 312, 340