

Index

- absorbance, 26, 45, 48, 160
 accuracy, 17–21, 25, 63, 96, 131, 181
 action lines, in control charts, 92–95
 additive factors, in experimental design, 175, 176, 181
 adjusted coefficient of determination, 134–136
 albumin, serum, determination, 15, 27, 38
 alternating variable search, 185–187
 alternative hypothesis, 75, 76
 American Society for Testing and Materials (ASTM), 21, 22, 32, 98
 analysis of variance (ANOVA), 65–71, 81–84, 89, 90, 98, 157, 169–181
 arithmetic of calculations, 69, 70
 between-block variation in, 171
 between-column variation, 179
 between-row variation in, 179
 between-sample variation in, 68–69, 83, 90, 92
 between-treatment variation in, 171
 correction term, 178
 for comparison of several means, 66–69
 in curve-fitting, 133–137
 least significant difference in, 69
 mean-squares in, 67, 171–174, 179, 184
 one-way, 66–69, 175
 residual mean square in, 173–174, 179
 significant differences in, 69
 sums of squares in, 172, 173, 179, 180
 total variation in, 69, 70
 two-way, 90, 171–181
 within-sample variation in, 66–70, 83, 84, 90, 94
 antibody concentrations in serum, 38, 40, 142
 arithmetic mean, *see* mean
 ARTHUR, pattern recognition method, 201
 artificial intelligence, 30
 assumptions used in linear calibration calculations, 104, 124, 125
 astigmatism, 25
 atomic-absorption spectrometry, 25, 27, 101, 117, 118, 129, 193
 atomic-emission spectrometry, 137
 automatic analysis, 102, 104, 119, 192, 193
 average run length, 94, 96
 background signal, *see* blank
 between-run precision, 19, 20
 bias, *see* systematic error
 binary classification, 197
 binomial distribution, 143, 146
 binomial theorem, 146, 150
 blank, 24, 103, 104, 115–117, 122
 block procedure, for multiple outliers, 64
 blocking, 170–174
 box-and-whisker plot, 145
 breakdown point, 164
 British Standards Institution (BSI), 21, 32
 bulk sampling, 82
 buoyancy effects in weighing, 22, 23
 burette, 21–23
 calculators, 29, 34, 106, 110, 113, 159
 calibration methods, 17, 26, 30, 102–139, 146, 160, 161
 censoring of values in collaborative trials, 90
 central limit theorem, 41, 142
 centrifugal analysers, 193
 centroid, of points in calibration plots, 104, 109, 114, 126–128

- chemometrics, 29, 193
- chi-squared test, 71, 72, 156, 157, 165, 220, 221, 224
- chromium, serum, determination, 25–27
- classifier, 197
- clinical analysis, 102
- clustering, 194, 197–199
- coding values before calculation, 34
- coefficient of determination, 134–136
adjusted, 134–136
- coefficient of non-determination, 134
- coefficient of variation (CV), 35, 49, 124 (*see also* relative standard deviation)
- collaborative trials, 27, 85–92
- colorimetry, 193
- colour blindness, 25
- comparison of experimental result with standard value, 16, 17, 53, 54, 220
of means of several sets of data, 65–69
of means of two sets of data, 17, 31, 55–58, 220
of paired data, 58, 59, 220
of standard deviations of two sets of data, 60–62, 220
- complete factorial design, 181
- complexometric analysis, 101
- concentration determination by calibration methods, 110, 112–115, 119, 126–128
- confidence interval of the mean, 41, 42, 45, 46
- confidence limits of the mean, 30, 41–45, 82
in linear calibration plots, 103, 111–114, 119, 120, 122–124, 127, 128, 139
- consecutive procedure, for multiple outliers, 65
- contour diagrams, 185–193
- control charts, 92–98
- controlled factor, 65, 83, 169, 172, 180
- Cook's distance, 139
- correlation, 29, 101
- correlation coefficient, 73, 104–109, 121, 123, 130, 131, 134
- critical values in statistical tests, 54, 55, 57, 58–64, 68, 72, 84, 90, 91, 157, 166, 173, 174, 179, 222–227
- cubic splines, 137
- cumulative frequency, 72–74
curve, 72–74, 166–167
- curve-fitting, 130, 133–137, 148, 156, 161
- curvilinear regression, *see* regression, non-linear
- cusum (cumulative sum) chart, 94–97
- decision plane, 197–199
- degrees of freedom, 43, 54, 57, 59, 61, 67–70, 72, 84, 89, 108, 110, 111, 113, 115, 122, 124, 134, 135, 156, 172, 173, 178–180, 184, 222–227
- dendrogram, 200
- derivative spectroscopy, 102
- determinate errors, 18
- distance function, 163
- distribution-free methods, *see* non-parametric methods
- distribution of errors, 35–38
- Dixon's Q , 63, 64, 92, 224
- dot plot, 20, 64, 224
- drainage errors, 23
- electrochemical analysis methods, 101, 118
- electronic balance, 50
- emission spectrometry, 101, 118
- enzymatic analysis, 29, 182
- error bars, 125
- errors, *see* gross, random and systematic errors
- errors in significance tests, 75–77
- Euclidian distance, 197
- expected frequency, in chi-squared test, 71, 72
- experimental design, 24, 26, 28, 29, 59, 65, 169–181
- expert systems, 30
- exploratory data analysis (EDA), *see* initial data analysis (IDA)
- F -test, 60–62, 77, 84, 90–92, 154, 173, 174, 185, 223
- factorial designs, 181–185, 188–190
- factors affecting experimental results, 169, 171, 175–177, 181–185, 190–192
- fences, 145
- Fisher, R. A., 170
- five-number summary, 145
- fixed-effect factors, 65, 83, 166, 169
- fluorescence spectrometry, 47, 65–69, 129, 133, 169, 194
- Fourier transform methods, 102
- fractional factorial designs, 88, 185, 201
- frequency, in chi-squared test, 71
- frequency table, 35
- Friedman, M., 156–157
- Friedman's test, 156–157, 220
- gas-liquid chromatography, 101, 137, 156, 193, 194, 200

- Gaussian distribution, *see* normal distribution
 general functions in error propagation, 48
 goodness-of-fit, 165–167, 221, 227
 gravimetric analysis, 25, 101
 gross errors, 17, 23, 91
- heavy-tailed distributions, 142, 143, 161
 hierarchical designs, 175
 high-performance liquid chromatography, 102, 156, 182
 histogram, 36
 hollow-cathode lamp, 129
- immunoassay, 27, 129, 137, 156
 incomplete factorial design, 88, 185, 201
 indeterminate errors, 18
 indicator errors, 23, 24
 influence function, 139
 initial data analysis (IDA), 137, 144, 145, 146
 iner-filter effects, in fluorimetry, 129, 133
 intelligent instruments, 25, 102
 interactions between factors, 29, 157, 175–181, 189, 190
 intercept, of linear calibration graph, 103, 110, 112, 113, 117, 121–124, 126, 127, 159–161
 interlaboratory variation, 85, 86, 90, 91
 International Union of Pure and Applied Chemistry (IUPAC), 38
 interpolation methods in non-linear regression, 137
 interquartile range, 143–145, 162–163
 International Organisation for Standardisation (ISO), 32
 iterative univariate method, 185–187
- Kendall, 159
K-nearest neighbour (KNN) method, 198–199
 knots, in spline functions, 137
 Kolmogorov–Smirnov methods, 74, 165–167, 221, 227
 Kowalski, B. R., 201
 Kruskal–Wallis test, 155–156, 220
 laboratory information management systems (LIMS), 31
 last drop error, 24
 Latin squares, 174–175, 201
 learning machine method, 197–198
 least median of squares (LMS), 164
 least significant difference, in ANOVA, 69
 least-squares method, 31, 109, 133, 160, 161, 164
 levels of experimental factors, 87, 88, 170, 175–177, 181–187, 191, 192
 limit of decision, 116
 limit of detection, 17, 103, 110, 115–117
 limit of determination, 116
 limit of quantitation, 116
 line of regression of x on y , 109
 line of regression of y on x , 109, 124
 linear combinations,
 of random errors, 46
 of systematic errors, 50
 logit transformation, 132
 log-normal distribution, 38, 40, 65, 142
 lower quartile, 144, 145
 luminescence spectrometry, 101
- main-frame computers, 31
 Mann–Whitney *U*-test, 153, 154, 220, 226
 masking, in outlier tests, 64
 mass spectrometry, 101
 matrix effects, 117, 118, 119
 mean, 29, 33–45, 53–59, 63–64, 65–71, 92, 142–143, 165–167
 trimmed, 162, 165
 mean squares, in non-linear regression, 134
 measurement variance, 82–84
 measures of central tendency, 143
 measuring cylinder, tolerance of, 22
 median, 143–147, 149–151, 154, 155, 156, 159, 160, 163, 164, 220
 median absolute deviation (MAD), 163, 164
 Methyl Orange, indicator error due to, 24
 microcomputers, 25, 30–31, 57, 102, 106, 113, 122, 125, 128, 133, 137, 139, 143, 146, 159, 161, 193, 201
 mini-computers, 30
 missing data, in collaborative trials, 91
 modified simplex optimization methods, 191
 monochromators, systematic errors due to, 25–27
 multiple correlation coefficient, *see* coefficient of determination
 multiplicative expressions,
 in random error propagation, 47
 in systematic error propagation, 50
- National Institute for Science and Technology (NIST), 27
 National Physical Laboratory (NPL), 27

- Nernst equation, 49, 50
 nested and cross-classified designs, 175
 non-linear regression, 30, 31, 128–137
 non-parametric methods, 65, 110, 139, 142–144, 146–161, 164, 167, 199, 220, 221
 normal distribution, 37–39, 42, 65, 71, 72–74, 115, 116, 117, 130, 142–143, 145, 161, 165–167, 181
 tests for, 72–74, 165–167, 221, 227
 normal probability paper, 73–74, 165
 null hypothesis, 53–62, 67–69, 71, 72, 75, 76, 108, 146–147, 148–149, 150–151, 153, 154, 155, 156, 157, 159, 166, 167
 number bias, 25
 observed frequency, 71, 72
 one-at-a-time experimental designs and optimization, 181, 185–187
 one-sided test, *see* one-tailed test
 one-tailed test, 59–62, 68, 77, 153, 154, 220, 222, 223, 225–227
 one-way analysis of variance (ANOVA), 65–69, 89
 optimization, 28, 29, 31, 102, 169, 181–193
 outliers, 16, 17, 62–65, 92, 131, 139, 143, 145, 160, 164
 in regression, 137–139
 paired alternate ranking, 154
 paired data, 150
 paired *t*-test, 58–59, 147, 150, 220
 partial least squares, 195
 particle size analysis, 16
 pattern recognition, 131, 193–200
 pattern space, 194
 pattern vector, 194, 195
 periodicity, effects in sampling, 82
 of + and – signs, 149
 pipette, 21–23
 plasma spectrometry, 27, 101, 117, 193
 polynomial equations in curve fitting, 133, 134
 pooled estimate of standard deviation, 55–56
 population measurements, 36, 82
 potentiometric analysis, 49–50
 power of a statistical test, 76, 77, 148, 167
 precision, 18–20, 40, 44, 63, 96, 181
 prediction set, 197, 198, 199
 presentation of results, 44, 45
 principal components analysis, 195, 196, 201
 principal components regression, 195
 process capability, 93, 94, 98
 process mean, 93, 94, 98
 process mean, 93, 94, 96
 product-moment correlation coefficient, 73, 104–109, 121, 123, 130, 131, 215
 propagation of random errors, 28, 35, 46–50
 propagation of systematic errors, 50–51
 pseudo-values, 163–164
Q-test for outliers, 63, 64, 92, 137, 164, 224
 qualitative analysis, 15
 qualitative factors, 169
 quality control, 81–98
 quantitative analysis, 15–17
 quantitative factors, 169
 quartiles, 144
 radiochemical analysis methods, 101
 random-effect factors, 66, 83, 89, 166
 random errors, 17–24, 25, 27, 28, 46, 53, 65, 92, 98
 in collaborative trials, 86, 87, 90, 91
 in regression calculations, 102, 110–121, 124, 130
 random number table, 82, 88, 170, 224
 random sample, 82
 randomization, 170, 171
 randomized block design, 171, 174
 range, 93, 94, 98
 rank correlation, 158–159, 221, 227
 rank sum test, 152–155, 167, 220
 ranking methods, 149–160
 referee laboratory, 87–89, 92
 regression methods, assumptions used in, 104, 124, 125
 for comparing analytical methods, 120–124
 linear, 29, 59, 101–133, 147, 148
 non-linear, 30, 102, 107, 128–137
 non-parametric, 159–161
 relative errors, 35, 47–50
 relative standard deviation (RSD), 35, 47–49, 124, 127
 repeatability, 18–20
 replicates, in experimental design, 177
 reproducibility, 18–20
 residual diagnostics, 137–138
 residuals, in regression calculations, *see* *y*-residuals,
 residuals,
 response surface in optimization, 185–187
 robust methods, 65, 139, 142, 143, 161–165
 rounding of results, 44, 45, 112, 130
 ruggedness test, 87

- runs of + and - signs, 130, 148-149, 221, 225
- sample, 38
- sample of measurements, 36
- sampling, 66, 81-85, 88
- sampling distribution of the mean, 40-41, 68, 75, 76
- sampling variance, 82-85
- scaling, of data before pattern recognition, 198
- sensitivity, 117
- sequences of + and - signs, *see* runs of + and - signs
- sequential use of significance tests, 77
- Shewhart chart, 92-94
- Siegel-Tukey test, 146, 154-155, 221
- sign test, 146-148, 149, 220, 225
- signed rank test, 149-151, 220
- significance levels, 53, 54
- significance tests, 30, 45, 53-80, 92, 145
 errors in the use of, 75-77
 problems in sequential use, 77
- significant figures, 30, 36, 44, 106, 112
- SIMCA, pattern recognition method, 201
- similarity in pattern recognition, 200
- simplex optimization, 190-193, 198, 201
- slope of linear calibration graph, 103, 110-112, 113, 117, 121, 159-161
- Spearman's rank correlation coefficient, 158-159, 221, 227
- speciation problems, 122
- specimen, 39
- spline functions, 137
- spreadsheets, 30
- standard additions method, 103, 117-120
- standard deviation, 29, 33-51, 54-64, 88, 143, 162, 165
 of slope and intercept of linear calibration plot, 110-112, 117, 119, 122, 125, 127, 128
- standard error of the mean (s.e.m.), 40, 44, 76
- standard flask, 21, 22
- standard form, 165
- standard normal variable, 165-167
- standard reference materials, 26, 101
 for volumetric analysis, 22
- steepest ascent, optimization method, 188-190, 201
- sums of squares, in non-linear regression, 134-136
- supervised learning, pattern recognition methods, 195, 197-199
- systematic errors, 17-28, 36, 41, 45, 46, 50, 51, 53, 54, 59, 60, 86, 87, 90, 91, 102, 120-123, 151, 170, 181
- t*-statistic, 43, 45, 54-59, 108, 109, 111, 113, 115, 119, 122, 131, 220, 222
- t*-test, 45, 54-59, 62, 72, 77, 81, 108, 131, 146, 220, 222
- target value, in control charts, 93-96, 98
- temperature effects in volumetric analysis, 23, 24
- test extract, 39
- test increment, 82
- test solution, 39
- Theil's method for regression lines, 159-161
- thermal analysis methods, 101
- tied ranks, 151, 153, 154, 156, 157, 159
- ties, in pattern recognition, 199
- titrimetric analysis, 16-20, 21-24, 25, 46, 48, 101
- tolerances, of glassware and weights, 21, 22
- training set, 197, 199
- transformations, in regression, 128, 131-133
- transmittance, 48
- treatments, 170, 171, 175
- trend, significance test for, 147
- trimmed mean, 162, 165
- true value, 36, 38, 39, 41, 42, 53, 54
- Tukey's quick test, 153, 154, 220
- two-sample plot, 86, 87
- two-sided test, *see* two-tailed test
- two-tailed test, 59, 60, 62, 77, 108, 147, 148, 150, 151, 154, 155, 220, 222-227
- type 1 errors, in significance tests, 75-77, 93
- type 2 errors, in significance tests, 75-77
- uncertainty, 28
- unsupervised learning, pattern recognition methods, 195, 199-201
- unweighted regression methods, 114, 117, 119, 124, 126-128, 131, 132, 133
- upper quartile, 144, 145
- V-mask, 96-98
- variance, 35, 40, 46, 56, 61-62, 67, 68, 69, 70, 71, 77, 83, 163, 171, 173, 184, 221
- volumetric glassware, 21-26
- voting scheme, in pattern recognition, 198
- Wald-Wolfowitz runs tests, 148-149, 221, 225

- warning lines, in control charts, 92–95
- weighing, 21, 22, 23
 - bottle, 21
 - buoyancy effects in, 22, 23
 - by difference, 21, 23, 26, 50
- weighted centroid, 126–129
- weighted regression methods, 124–129, 132, 133
- weights, of points in weighted regression, 125, 126, 128, 132, 133
- Wilcoxon rank sum test, 152–155, 167, 220, 221, 226
- Wilcoxon signed rank test, 149–151, 155, 220, 226
- Winsorization, 164–165
- within-run precision, 18, 19
- Wold, S., 199
- word-processors, 30
- y -residuals, in calibration plots, 109–111, 130, 131, 133, 135, 136, 148–149, 158, 164
- Yates, 72, 184
- Yates's correction, 72
- Youden plot, 86–87
- Youden, W. J., 86, 87