

Index

- β -carotene, 336, 337
 Abney W, 7
 Accuracy/classification rate, *see* Non-error rate (NER)
 Acousto-optical tunable filter (AOTF), 126, 385
 Agricultural Chamber Lower Saxony, 265
 Ahlemer Institute of the Landwirtschaftskammer Hannover, 265
 Air bearings, 157
 Air-cooled sources, 157
 Albumen quality, 402–5
Alicyclobacillus, 368
 Aliphatic chain, 11–12, 13
 Allium species, 343–5
 American Association of Cereal Chemists (AACC), 121
 Amylose, 287, 332
 Analytical Spectral Devices (ASD), 134, 135
 Anharmonic oscillator, 9
 Apodization, 153–4
 Apple, 322–3
 Artificial neural networks (ANNs), 64, 98–100, 385
 back-propagation learning rule, 68–70
 definition, 65
 neural networks, architecture of, 66–7
 transfer functions, 67
 Asynchronous two-dimensional correlation spectroscopy, 199
 At-line analysis, 245–7
 Atlantic salmon, 217
- Attenuated total reflectance (ATR), 20, 168, 169, 170, 323, 334, 336, 339, 367
 Automated single seed NIR spectroscopy sorters, 295
 Autoscaling, 74
- Back-propagation learning rule, 68–70
 Balmer JJ, 6
 Banana, 327
 Barley analysis, NIR in, 287, 289
 Baseline correction technique, 36–8, 39
 Beckman IR-1, 120, 132
 Beef and beef products:
 adulteration:
 with offal/organ meat, 190
 with other meat, 190
 fresh meat versus frozen-then-thawed meat, 191
 microbial spoilage, 191–3
 proximate composition:
 online NIR spectroscopy, 184
 packaged beef, 183–4
 semi-frozen beef, 184–5
 temperature fluctuation and water phase shifts, compensation for, 185–6
 quality attributes:
 cooking end-point temperature, 187–8
 instrumental beef tenderness determination, 187
 intramuscular fat/marbling, 186
 sensory meat tenderness determination, 186–7
 spinal cord contamination, detection of, 188–9

- Beer, 377
 composition, 387–8
 hops, 386
 malt and wort analysis, 386–7
 process control, 388–9
 yeast analysis and identification, 389–90
- Beer's law, 29–30
- Best-fit model, 228
- Biliverdin, 406
- Binary classification, 92, 93, 94, 97
- Blood and meat spots, in egg, 406–7
- Bohr N, 7
- Bolometers, 129
- Bone adulteration, of meat, 203
- “Boxcar” apodization, 154
- Brackett FS, 7
- Brassica species, 342
- Brix hydrometer, 358
- Brown-shelled eggs, 401, 405
- Butter-making machine, 251, 252, 253
- Calibration:
 calculation of calibration model, 72–8
 calibration method, selection of, 75
 number of factors, selection of, 76–7
 outliers, 78
 spectral range, selection of, 75–6
 spectral scaling and pre-treatments, 73–5
 definition, 51–2
 samples, selection of, 70–2
 transfer methods, 105
 alternative methods for, 114–16
 case study, 109–14
 data set and transfer set selection, 106–9
 transfer issue, 106
 variable reduction process, 59–64
- Canadian Grain Commission, 121, 285
- Canonical variate analysis (CVA), 95, 102
- Capsaicin, 331
- Carbonyl group, 15
- Carrots, 341–2
- Cassava and potato, 332–6
- Centerburst, 150
- Cereals and cereal products, 275
 future development, 311–12
 infrared spectroscopy, unreasonable efficiency of, 306–11
 MIR versus NIR, 276–8
 NIR endosperm model, 304–6
 NIR spectra, reproducibility of, 296–9
- NIR spectroscopy, current practice in:
 instrumentation, 278
 as reproducible physiochemical fingerprint, 279–82
 seed batch analytical applications, 285–94
 single seed quality, exploiting variation in, 294–6
 spectral interval selection, for simple and complex traits, 282–5
 spectral pre-treatment, 279
 variables affecting, 278–9
- NIR spectroscopy data, classification of, 299–303
- Cheddar cheese, 261
- Cheese production, 252–62
- Chemometric techniques, 361
- Chicken and chicken products:
 microbial spoilage, 203, 204
 proximate composition, 197
 quality attributes:
 chilled and frozen storage effects, 197–200
 processing parameters, 200–1
 texture measurement, 201–2
 thermal processing, 200
 unhealthy carcasses, liver analysis of, 202
- Chilli fruits and paprika, 331
- Citrus fruits, 323–7
- City-block, *see* Taxicab norm
- Class-modelling method, 85, 86, 87
- Classes, definition of, 84–5
- Classical calibration, 53
- Classical least squares, 55–7
- Classification methods, 83
 artificial neural networks, 98–100
 classification and regression trees (CART) analysis, 100–2
 discriminant analysis method, 95–6
 evaluation, 88–94
 K-nearest neighbour (KNN) method, 95
 nearest mean classifier (NMC) method, 94–95
 new classifiers, 102
 partial least squares-discriminant analysis (PLS-DA), 97
- principles of classification:
 categories, 85–7
 classes, 84–5
 validation and variable selection procedures, 87–8

- soft independent modeling of class analogy (SIMCA), 97–8
- support vector machines (SVMs), 100
- Classification and influence matrix analysis (CAIMAN), 102
- Classification and regression trees (CART) analysis, 100–2
- Cluster analysis, 86
- Coblenz WW, 7
- Commercial infrared instruments:
- laboratory analyzers, 132–3
 - process analyzers, 133–5
- Confusion matrix, 89, 91, 92, 93
- Continuum sources, 123
- Cooking end-point temperature, 187–8
- Coomans plots, 234
- Counterpropagation ANN, 99
- Covariance matrices, of g-th class, 96
- Crescenza cheese, 262
- Cucumber, 342–3
- Cucumber mosaic virus (CMV), 342, 343
- Curd cheese, 247, 254
- Cuticle, 338, 401
- D-optimal algorithm, 71
- D-Squared Development, Inc., 132, 137, 138
- Data pre-processing, 29
- alternative methods, 39–40
 - baseline correction, 36–8
 - case study, 43
 - data, 43
 - methods, 43–4
 - results and discussion, 44–7
- multiplicative signal correction family, 31–5
- pre-processing techniques, overview of, 31
- reference-dependent techniques, 42–3
- reference-independent methods, example of, 40–2
- Savitzky–Golay (SG) routine, 38–9, 40
- standard normal variate and normalization, 35–6, 37
- Degrees of freedom, 10–11
- DeLight, 132
- Democrite, 6
- Dendrogram, 263, 264
- Descartes, René, 6
- Detectors, in IR instrument, 128–30
- Deuterated triglycine sulfate (DTGS) detector, 129, 130, 158
- Diffraction grating, 126–7, 152
- Diffuse reflectance, 136, 137, 169–70, 228–9
- Diode laser, 106, 124
- Direct standardization (DS), 111, 113, 114
- Discrete Fourier transformation, 155
- Discriminant analysis, 95–6
- Discriminant function analysis (DFA), 338
- Dispersive and multiple beam instruments, 152–3
- Distillation, of wine, 384–5
- Double-beam optics, 120–1, 130–1
- Double transmission, 171
- DPA-20 spectrophotometer, 136
- Dry extract spectroscopy by infrared reflection (DESIR), 232, 380, 388
- Duplex algorithm, 71
- Echelon spectroscope, 152
- Egg and egg products, 399
- composition, 401
 - cuticle, 401
 - eggshell, 400–1
 - shell membranes, 401–2
 - white (albumen), 402
 - yolk, 402
- Vis/NIR application in:
- albumen quality, 402–5
 - blood and meat spots, 406–7
 - compositional analysis, 408–9
 - hatching eggs, 407–8
 - shell pigmentation, 405–6
- Eggshell, 400–1, 405
- Electromagnetic wave, 4
- Electronically tunable filters, 126
- Ellis JW, 7
- Emmental cheeses, 262, 263
- “Environome”, 304
- Error rate (ER), 89
- Erwinia carotovora*, 336
- Euclidean norm, 36, 37, 45
- Evanescence wave, 169
- Extended canonical variate analysis (ECVA), 102
- Extended multiplicative signal correction (EMSC), 32, 279
- Fabry–Pérot etalon interferometer, 152
- False positive rate (FPR), 92, 93
- Far-infrared radiation, 182
- Far-infrared spectroscopy, 215
- Far-ultraviolet region, 4–5
- Federal Food, Drug, and Cosmetic Act, 357

- Fect, 153
 Fellgett advantage, 150–1
 Festing ER, 7
 Filters:
 in near-infrared (NIR) spectroscopy, 125–6
 Fingerprint region, 165, 277
 Finite impulse response (FIR) filter, 115
 Fish and related products, 215
 qualitative analysis:
 fresh and frozen-thawed fish,
 differentiation between, 231–6
 freshness, 228–9
 process verification, 229–31
 quantitative analysis:
 chemical composition, 216–21
 surimi and minced fish, 221–7
 Foucault L, 6
 Fourier analysis, 154
 fast Fourier transforms (FFT), 155–6
 applications of, 156
 Fourier transform infrared (FTIR) spectroscopy,
 16, 146, 122, 191, 192, 216, 242, 322,
 329
 advantages and limitations, 159–60
 commercial FTIR instruments and
 accessories, 173
 comparison of FT-NIR and FT-MIR, 166–7
 factors affecting, 172–3
 Fourier analysis, 154
 fast Fourier transforms (FFT), 155–6
 Fourier transform mid-infrared (FT-MIR)
 spectroscopy:
 applications of, 165–6
 fundamentals of, 164–5
 Fourier transform near-infrared (FT-NIR)
 spectroscopy, 160
 applications of, 162–3
 fundamentals of, 161–2
 hardware, 156
 beam splitters, 158
 detectors, 158–9
 interferometers, 157
 IR source, 157–8
 laser, 159
 history of, 146–8
 interferometer:
 advantages, 150–1
 apodization, 153–4
 construction and working principle, 148–50
 disadvantages, 151–2
 dispersive and multiple beam instruments,
 152–3
 phase correction, 154
 slow and rapid scan interferometers, 153
 of pork water-holding capacities, 196–7
 sampling techniques:
 attenuated total reflectance (ATR), 169
 diffuse reflectance, 169–70
 microspectroscopy, 172
 photoacoustic spectroscopy (PAS),
 171–2
 reflectance, 168–9
 specular reflectance, 170–1
 transmittance, 167–8
 spectra, collection of, 159
 Fourier transformation (FT), 155
 Fresh and frozen-thawed fish:
 differentiation between, 231–6
 Fruit juices, 355
 components of:
 mineral content, 359–60
 organic acids, 358–9
 sugars, 358
 water, 357, 358
 infrared technology, application of, 360
 authentication and classification, 369–71
 composition and quality parameters,
 analyses of, 366–7
 detection and determination, of biological
 contaminants, 367–9
 spectral features, 362–6
 process, 356
 Fruits:
 apple, 322–3
 banana, 327
 citrus fruits, 323–7
 grapes, 330–1
 melon, 331–2
 papaya, 328
 paprika and chilli fruits, 331
 peach, 329
 pear, 328
 strawberries, 329–30
 FTIR-photoacoustic spectroscopy (FTIR-PAS),
 204–5, 323
Gadus morhua, 228
 Garlic oil, 344

- Gas sampling technique, 138–9
 Gelatinization, starch, 333
 Genetic algorithm (GA), 191, 338
 German Accreditation Council (DAP), 265
 Germanium (Ge), 158
 Globar sources, 157
 Golay detectors, 129
 Good laboratory practice (GLP), for IR calibrations, 263
 networking, 265
 service network, 265
 surveillance network, 265–6
 Grapes, 330–1
 of wine, 378–9
 Green banana, 327
- Halogen gas, 123
 Hard-to-cook (HTC) beans, 340
 Harmonic oscillator, 9
 Harmonization network, 266
 Hatching eggs, 407–8
 Haugh unit (HU), 403
 Helium neon (HeNe) lasers, 124, 125
 Herschel W, 7, 120
 High-performance liquid chromatography (HPLC), 366
 Hops, 386
 Huygens C, 6
 Hydroxyl group, 12–14
 Hyper-leverage, 102
- In-line analysis, 247–8
 Incoming product control:
 milk and dairy products, 244–5
 Indirect calibration, 56
 Indium antimonide (InSb), 129
 Indium gallium arsenide (InGaAs), 129, 158
 Infrared (IR) spectroscopy, 3, 181–3, 119, 215, 241–2
 history of, 5, 120–2
 spectroscopic techniques, development of, 7–8
 theoretical bases, of spectroscopy, 6–7
 theories of light, across centuries, 6
 infrared band and spectral interpretation, 139–41
 near- and mid-infrared regions, spectral bands in, 11
 protein, lipid and carbohydrate absorption bands, 16–23, 24
 rules of assignment, 11–16
 optical systems in, 122
 commercial infrared instruments, 132–5
 detectors, 128–30
 double-beam optics, 130
 radiation source, 123–5
 single-beam optics, 130
 software, 131–2
 wavelength selection devices, 125–8
 sampling techniques, 135
 gas sample, 138–9
 liquid sample, 136
 solid sample, 136–8
 vibrational spectroscopy, 8
 polyatomic molecules, 9–11
 vibrational models, development of, 9
 Infrared technology to juice analyses,
 application of, 360
 authentication and classification, of fruit juices, 369
 infrared methods, 370–1
 methods for, 369–70
 composition and quality parameters, analyses of, 366–7
 detection and determination, of biological contaminants, 367–9
 spectral features, of fruit juices, 362
 organic acid, 365–6
 sugar, 364–5
 water, 362–4
 Instrumental beef tenderness determination, 187
 Integrating sphere, 170
 Interference filters, 125–6
 Interferogram, 149–50
 mathematical processing of, 153–4
 Interferometer, 128, 157
 advantages:
 Fellgett advantage, 150–1
 Jacquinot advantage, 151
 apodization, 153–4
 construction and working principle, 148–50
 disadvantages, 151–2
 dispersive and multiple beam instruments, 152–3
 phase correction, 154
 slow and rapid scan interferometers, 153

- Interval extended canonical variate analyses (iECVAs), 285, 286
- Interval partial least squares regression (iPLS), 282, 284
- Inverse calibration, 53
- Inverse least squares (ILS), 57–9
- Inverse linear regression (ILR), 57
- Iterative polynomial baseline fitting (IPBF), 36, 37, 38
- Jack-knife algorithm, 76
- Jacquinot advantage, of interferometry, 151
- Japan Oil Chemists' Society, 220
- Julius WH, 7
- K*-nearest neighbour (KNN) method, 95
- Kamaboko gels, 221, 229, 230
- Kennard–Stone algorithm, 71, 108–9
- KJT-270, 133, 134
- Kohonen maps, 98–9
- Laboratory analyzers, in NIR spectroscopy, 132–3
- Lasers, 124, 159
- Latentix software, 278, 282
- Lead selenide (PbSe), 129, 158
- Lead sulfide (PbS), 120, 158
- Least-squared support vector machine (LS-SVM), 331
- Least squares regression (LSR), 52, 58
- Leave-one-out method, 76
- Legumes, 340–1
- Light, theories of, 6
- Light-emitting diode (LED), 124
- Lignin, 329
- Line sources, 123, 124
- Linear discriminant analysis (LDA), 96, 232
- Linear methods, 53
- Liquid crystal tunable filter (LCTF), 126
- Liquid sampling technique, 136
- Locally weighted regression (LWR), 385
- Loss matrix, 90
- Luminiferous aether, 148
- Lummer–Gehrcke interferometer, 152
- Lycopene, 336, 337
- Lys3*, 303, 304, 306
- Mahalanobis distance, 96
- Maillard reaction, 403
- Maize analysis, NIR in, 288
- Malt and wort analysis, 386–7
- Malting barley production, NIR for, 289–92
- MatLab, 216
- Maxwell JC, 6
- Mean centering, 44, 74
- Mean square error (MSE), 73
- Mean square error of prediction by cross-validation (MSECV), 76, 77
- Meat and meat products, 181
- beef and beef products:
 - adulteration and contamination, detection of, 188–90
 - adulteration with other meat, 190
 - fresh meat versus frozen-then-thawed meat, 191
 - microbial spoilage, 191–3
 - proximate composition, 183–6
 - quality attributes, 186–8
 - chicken and chicken products:
 - microbial spoilage, 203
 - proximate composition, 197
 - quality attributes, 197–202
 - miscellaneous applications:
 - bone adulteration, 203
 - FTIR-photoacoustic spectroscopy, 204–5
 - NIR fiber-optic reflectance probe, dimensions of, 203–4
 - pork and pork products:
 - proximate composition, 193–4
 - quality attributes, 194–7
 - Mechanical bearings, 157
 - Melon, 331–2
 - Mercury cadmium telluride (MCT) detectors, 129, 130, 158
 - Methyl esterification degree (MED), of pectins, 328
 - Michelson, Albert Abraham, 148
 - Microspectroscopy, FTIR, 168, 172
 - Microwave region, 5
 - Mid-infrared (MIR) regions, 5
 - spectral bands in, 11
 - aliphatic chain, 11–12, 13
 - carbonyl group, 15
 - hydroxyl group, 12–14
 - nitrogen group, 15–16
 - protein, lipid and carbohydrate absorption bands, 16–23, 24

- Mid-infrared (MIR) spectroscopy, 119–41, 192–3, 215, 241, 406
 versus near-infrared (NIR) spectroscopy, 276–8
- Milk and dairy products, 241
 cheese production, 252–62
 final product control, 262–3, 264
 future trends, 266–7
- GLP, for IR calibrations, 263
 networking, 265
 service network, 265
 surveillance network, 265–6
- harmonization network, 266
- incoming product control, 244–5
- milk powder production, 248–51
- oil and fat production, 251–2, 253
- process control, 245
 at-line analysis, 245–7
 in-line analysis, 247–8
 off-line analysis, 245
 production, 242–3
- MilkoScan™ FT, 120, 243
- Misclassification risk (MR), 90
- Monochromator, 126, 128
 diffraction grating, 126–7
 prism, 126
- Mozzarella cheese production, 248, 258, 260
- Multilayer feed-forward networks (MLFs), 65
- Multiple linear regression (MLR), 52, 55, 57, 229, 230, 323, 378
- Multiplex advantage, of interferometry, 150–1
- Multiplicative scatter correction (MSC), 30, 31–5, 74–5, 218, 337, 405
- Multivariate calibration, for quantitative analysis, 51
 advantages, 53–4
 artificial neural networks, 64
 back-propagation learning rule, 68–70
 neural networks, architecture of, 66–7
 transfer functions, 67
 construction, 70
 calculation, of calibration model, 72–8
 calibration samples, selection of, 70–2
 reference methods and analytical signal, 72
 routine analyses, 78
 validation, of model, 78
- methods, 52–3, 54, 59
 partial least squares regression, 63–4, 65
- principal component analysis, 60–1
 principal component regression, 61–3
 stepwise multiple linear regression, 55
 classical least squares, 55–7
 inverse least squares, 57–9
- Muskmelon, 331–2
- Myrcene, 324
- Near-infrared (NIR) regions, 5
 spectral bands in, 11
 aliphatic chain, 11–12, 13
 carbonyl group, 15
 hydroxyl group, 12–14
 nitrogen group, 15–16
 protein, lipid and carbohydrate absorption bands, 16–23, 24
- Near-infrared (NIR) spectroscopy, 119–41, 182, 183, 192–3, 197, 215–16, 228–9, 241, 227, 409
 classification by principal component analysis, 299–303
 endosperm model to overview phenome, 304–6
 instrumentation, 278
 reproducibility, 296–9
 as reproducible physiochemical fingerprint, 279–82
- seed batch analytical applications:
 barley, 287
 maize, 288
 rice, 287–8
 wheat, 285, 287
 without commercial calibration models, 288–94
- single seed quality, exploiting variation in, 294–6
- spectral interval selection, for simple and complex traits, 282–5, 286
- spectral pre-treatment, 279
- variables affecting, 278–9
- versus mid-infrared (MIR) spectroscopy, 276–8
- Near-near-infrared spectroscopy (NNIR), 404
- Nearest mean classifier (NMC) method, 94
- Nernst glower source, 125, 158
- Net analyte pre-processing (NAP), 43
- Net analyte signal (NAS), 43
- Neural networks, architecture of, 66–7
- Newton I, 6

- NIR Systems Inc., 183
 NIR/NIT TriQ single seed sorter, 295
 Nitrogen group, 15–16
 No-model error rate (NOMER), 89–90
 Non-error rate (NER), 89, 92
 Non-fat dry milk (NDM), 250
 Non-linear iterative partial least squares (NIPALS) algorithm, 63, 97
 Non-linear methods, 53
 Non-thermal food-processing techniques, 409
 Normal vibration mode, 10
 Normalization, 35, 39
 Norris, Karl, 121, 278
 Norris–Williams (NW) derivation, 30, 39–40
 NSAS (Near-Infrared Spectral Analysis Software), 216
- Off-line analysis, 245
 Oil and fat production, 251–2, 253
Oncorhynchus mykiss, 229
 Onion oil, 343
 Online NIR spectroscopy, for beef analysis, 184
 Optical path difference (OPD), 149
 Optimized scaling, 43
 OptiSim, 72
 Organic acids, 358–9, 365–6
 Orthogonal signal correction (OSC), 42, 115
 Orthogonalization, 42
 Outlier, definition of, 78
- P*-cymene, 326
 Papaya, 328
 Paprika and chilli fruits, 331
 Partial least squares (PLSR) regression, 41, 43, 54, 59, 63–4, 65, 97, 166, 186, 201, 217, 229, 242, 361, 378, 404
 Partial least squares-discriminant analysis (PLS-DA), 97
 Peach, 329
 Pear, 328
 Pectin, 326
 Pelagic fish, 217
 Perkin-Elmer Inc., 120, 122
 Phase correction, 154
Phaseolus vulgaris, 340
 Phi correlation coefficient, 92
 Photoacoustic spectroscopy (PAS), 171–2
 Photon-sensitive detectors, 129
- Photonic spectroscopy, 3
 Piecewise direct standardization (PDS), 113, 114
 Pittsburgh Conference (Pittcon), 132
 Planck's constant, 6
 Polar qualification system (PQS), 332
 Polyatomic molecules, 9–11
 Pooled covariance matrix, 96
 Pork and pork products:
 proximate composition, 193–4
 quality attributes:
 fatty acid composition, 194–5
 pH, 195–6
 Rendement Napole gene, 197
 water-holding capacity, 196–7
 Positive predictive value (PPV), 92
 Potassium bromide (KBr), 126, 158
 Potato and cassava, 332–6
 Pre-processing techniques, *see* Data pre-processing
 Precision, 91
 see also Positive predictive value (PPV)
 Predicted residual error sum of squares (PRESS), 73
 Pressure-assisted thermal processing (PATP), 165–6
 Principal component analysis (PCA), 60–1, 86, 99, 109, 299, 300–3
 Principal component regression (PCR), 54, 59, 60, 61–3, 184
 Prior class probability, 90
 Prism, 126
 Process analytical technology (PAT), 292–4
 Process analyzers, 133–5
 Protein, lipid and carbohydrate absorption bands, 16–23, 24
 Protoporphyrin, 401, 406
 Pure classification method, 85, 86, 87
 Pyroelectric detectors, 129
- Quadratic discriminant analysis (QDA), 96
 Quality index method (QIM), 228
 QualitySpec® BT system, 135
 Quartz tungsten halogen (QTH) lamps, 124
- Radiation source, 123–5
 Radiofrequency region, 5
 Raman spectroscopy, 266, 267
 Random ER, 90

- Rapid scan interferometers, 153
 Red sea bream, 232, 233, 235
 Reference beam, 131
 Reference-dependent techniques, 31, 42–3
 Reference-independent technique, 30
 - derivation methods, 30
 - example of, 40–2
 - scatter correction methods, 30
 Reference methods, and analytical signal, 72
 Reflectance sampling techniques, 168–9
 - attenuated total reflectance (ATR), 169
 - diffuse reflectance, 169–70
 - specular reflectance, 170–1
 Refractometer, *see* Brix hydrometer
 Registration advantage, of interferometry, 151
 Relative standard error (RSE), 73
 Rendement Napole (RN) gene, 197
 Rice analysis, NIR in, 287–8
 Rigid methods, 53
 ROC curves, 93, 94
 Root mean square error (RMSE), 73
 Root mean squared error of prediction (RMSEP), 41, 44
 Rotation movement, 10
 Routine analyses, 78, 366
 Rowland, Henry A, 127
 RPD value, 226

Salmo salar, *see* Atlantic salmon
 Sample beam, 131
 Sardine, 217
Sardinops melanostictus, 217
 Savitzky–Golay (SG) routine, 30, 38–9, 40, 74, 111, 218
 Scatter correction methods, 30
 Scattering, 137, 218, 236
 Schrödinger E, 7
 Seed-sorting system, 295, 296
 Semiconductor detectors, 129
 Sensitivity, 90
 - see also* True positive rate (TPR)
 Sensory meat tenderness determination, 186–7
 Service network, 265
 Shell:
 - membranes, 401–2
 - pigmentation, 405–6
 Short-wavelength near-infrared (SW-NIR) spectra, 108, 120, 137, 138, 139, 140
 Side lobes, 153
 Signal-to-noise ratio (SNR), 150, 151, 159, 173
 Silicon photodiode array detector, 129
 SIMPLS, 63
 Single-beam optics, 130–1, 159
 Slow scan interferometers, 153
 Soft cheese production, 258, 259
 Soft independent modeling by class analogy (SIMCA), 97–8, 163, 232, 233, 380
 Solid sampling technique, 136–8, 167
 Soluble solid content (SSC), 322–3, 369
 Specificity, 90–1
 Spectra, derivation of, 74
 Spectral interference subtraction (SIS), 32
 Spectral range, selection of, 75–6
 Spectral regions of interest, for analytical purposes, 4, 5
 Spectral scaling and pre-treatments, 73–5
 - autoscaling, 74
 - derivation, of spectra, 74
 - mean centering, 74
 - multiplicative scattering correction, 74–5
 - standard normal variate, 75
 Spectroscopes instruments, 152
 Spectroscopy:
 - definition, 6–7
 - techniques, development of, 7–8
 Specular reflectance, 137, 170–1
 Standard error of calibration (SEC) value, 226
 Standard error of cross-validation (SECV), 325–6
 Standard normal variate (SNV), 35–6, 37, 75
 Stepwise ascending method, 59
 Stepwise discriminant analysis (SWDA), 96
 Stepwise multiple linear regression, 55
 - classical least squares, 55–7
 - inverse least squares, 57–9
 Strawberries, 329–30
 Sugar beet, 339–40
 Sugars, 358, 364–5
 Support vector machines (SVMs), 100
 Surimi and minced fish, 221–7
 Surveillance network, 265–6
 Synchronous two-dimensional correlation spectroscopy, 199

 Taxicab norm, 36
 Ternary mixtures, design of, 107
 Terpene, 325

- Theragra chalcogramma*, 221
- Thermal detectors, 129
- Thermal processing (TP), 165–6, 200
- Thermistors, 129
- Thermo Fisher Scientific Inc., 132, 134
- Thermo Nicolet Antaris Near-infrared analyzer, 134, 135
- Thermocouples, 129, 229
- Thin layer chromatography (TLC), 331
- Throughput advantage, of interferometry, 151
- Tomato, 336–9
- Total absolute sum, *see* Taxicab norm
- Total internal reflection, 169
- Transfer functions, in ANNs, 67
- Transfer matrix, 113
- Translation movement, 10
- Transmission mode, 136
- Transmittance sampling techniques, 167–8
- True positive rate (TPR), 92, 93
- Tunable carbon dioxide laser, 124
- Tungsten halogen lamps, 123, 124
- Two dimensional correlation spectroscopy, 199–200
- UNEQ (unequal class modeling), 96
- Unhealthy chicken carcasses, liver analysis of, 202
- “Unreasonable efficiency”, of IR spectroscopy, 306–11
- Unscrambler, 216, 278
- US Department of Agriculture, 8, 121
- Variable-compression methods, 53
- Vegetables:
- allium species, 343–5
 - brassica species, 342
 - carrots, 341–2
 - cucumber, 342–3
 - legumes, 340–1
 - potato and cassava, 332–6
 - sugar beet, 339–40
 - tomato, 336–9
- Vibrational spectroscopy, 8
- polyatomic molecules, 9–11
 - vibrational models, development of, 9
- Visible region, 5
- Visible/near-infrared (Vis/NIR) spectroscopy:
- application, in egg and egg products:
 - albumen quality, 402–5
 - blood and meat spots, 406–7
 - compositional analysis, of egg products, 408–9
 - hatching eggs, 407–8
 - shell pigmentation, 405–6
 - measurement system, 137, 138
- “Vision”, 216, 222
- Water:
- fruit juices component, 357, 358, 362–4
- Water-cooled sources, 157
- Water-holding capacity (WHC), 196
- Water-soluble nitrogen (WSN), 261
- Watermelon, 331–2
- Wavelength, 4
- selection devices, in near-infrared (NIR)
 - instruments:
 - filters, 125–6
 - interferometer, 128
 - monochromator, 126–8
- Wavenumber, 4
- Wheat analysis, near-infrared (NIR)
- spectroscopy in, 285, 287
- White (albumen), 402
- White-shelled eggs, 401
- Wilks’ lambda, 88
- Wine, 377
- composition, 379–82
 - distillation, 384–5
 - online analysis and process control, 382
 - quality grading, 382–4
 - wine grapes, 378–9
 - yeast identification, 385–6
- X-ray region, 4
- Yeast identification:
- in beer, 389–90
 - in wine, 385–6
- Yolk, 402
- Young T, 6
- Zero path difference (ZPD), 149