

Contents

I	Framework of Least-Squares Method	1
1	Introduction to Data-Fitting Problems	3
1.1	What is data fitting?	3
1.2	Notation	5
1.3	Linear vs. nonlinear problems	5
1.4	Example applications of linear data fitting	10
1.4.1	Estimation of a constant value	10
1.4.2	Estimation for a straight line (linear regression)	11
1.4.3	Polynomial function	11
1.4.4	Multiple linear regression	12
1.4.5	Wiener filter	19
1.5	Selected nonlinear data-fitting problems	19
1.5.1	Exponential functions	19
1.5.2	Composite Gaussian bell functions	21
1.5.3	Circle function	21
1.5.4	Neural networks	23
1.6	Test questions	25
2	Estimation of Model Parameters by the Method of Least Squares	26
2.1	What are “Least Squares”?	26
2.2	A general algorithm for minimisation problems	28
2.3	Pitfalls	31
2.4	Simplifications for linear model functions	32
2.5	Curve approximation in case of unknown model function	33
2.6	Example computations	36
2.6.1	Constant value	36
2.6.2	Straight line	37
2.6.3	Polynomial approximation	38
2.6.4	Plane approximation	38
2.6.5	Linear prediction	39
2.6.6	Cosine function	39

2.6.7	Rotation and translation of coordinates	40
2.6.8	Exponential model function	41
2.6.9	Composite Gaussian bell functions	42
2.6.10	Circle function	43
2.6.11	Neural networks	44
2.7	Test questions	47
3	Weights and Outliers	48
3.1	What are the weights good for?	48
3.2	Outliers	50
3.3	Estimation of weights	51
3.3.1	Estimation by binning	53
3.3.2	Weights estimation using deviates	54
3.4	Approaches towards outlier detection	56
3.4.1	Standardised residuals	57
3.4.2	Cluster criterion	60
3.4.3	Random sample consensus (RANSAC)	70
3.5	Application of weighted data fitting and outlier detection	76
3.5.1	Constant value	77
3.5.2	Straight line	79
3.5.3	Plane approximation	85
3.5.4	Coordinates transformation	87
3.5.5	Linear prediction	90
3.5.6	Cosine function	91
3.5.7	Exponential model function	98
3.5.8	Composite Gaussian bell functions	100
3.5.9	Circle	104
3.5.10	Comparison of binning and deviate-based weights estimation	106
3.6	Conclusions	108
3.6.1	Evaluation of weighting	109
3.6.2	Comparison of outlier detectors	110
3.6.3	Usefulness of weights	111
3.7	Test questions	112
4	Uncertainty of Results	113
4.1	Goodness-of-fit, precision and accuracy	113

4.1.1	Consistence of statistical model and data	113
4.1.2	Sample variance	114
4.2	Uncertainty of estimated parameters	116
4.3	Uncertainty of data approximation	119
4.4	Inspection of plots	120
4.5	Example computations	121
4.5.1	Constant value	122
4.5.2	Straight line	123
4.5.3	Cosine function	125
4.5.4	Model mismatch	126
4.6	Test questions	133
II	Mathematics, Optimisation Methods, and Add ons	135
5	Matrix Algebra	137
5.1	Basics	137
5.2	Determinants	141
5.3	Numerical solutions for matrix inversion	143
5.3.1	Cofactor-matrix method	143
5.3.2	Inversion via Gauss-Jordan elimination	144
5.3.3	Inversion via LU decomposition	146
5.3.4	Inversion by singular value decomposition (SVD)	153
5.4	Test questions	155
6	The Idea behind Least Squares	156
6.1	Normal distribution	156
6.2	Maximum likelihood principle	157
6.3	Fitting of linear model functions	159
6.3.1	Standard approach	159
6.3.2	Solution using singular value decomposition (SVD)	161
6.3.3	Scaling of conditions	162
6.4	Fitting of nonlinear model functions	163
6.4.1	Error-surface approximation	163
6.4.2	Gauss-Newton method	164
6.4.3	Gradient-descent method	167

6.4.4	Levenberg-Marquardt method	168
6.4.5	Example of finding the minimum	169
6.5	Test questions	179
7	Supplemental Tools and Methods	180
7.1	Alternative parameter estimation	180
7.1.1	Recursive adaptation of parameters	180
7.1.2	Gradient descent by trial and error	182
7.1.3	Evolutionary approach	183
7.1.4	Training of neural networks using backpropagation	183
7.2	Chauvenet's criterion for outlier detection	190
7.3	Propagation of errors	193
7.4	Manual calculation of linear least squares	196
7.4.1	Fitting of a straight line using manual derivation	197
7.4.2	Wiener filter	199
7.5	Combined treatment of different model functions	202
7.5.1	Example 1: Coordinate transformation	205
7.5.2	Example 2: Circular movement	206
7.6	Weighted least squares with correlated data	209
7.7	Total least squares	215
7.7.1	Orthogonal fitting of a circle	216
7.7.2	General approach	218
7.8	Test questions	221
A	Comparison of Approaches to Outlier Detection	223
A.1	Normally distributed data	223
A.1.1	Data sets without outliers	223
A.1.2	Data sets containing outliers	225
A.2	Non-Gaussian distribution	228
A.2.1	Laplace distribution	228
A.2.2	Uniformly distributed data	228
A.3	Discussion	231
B	Implementation	234
B.1	Functionality	234
B.2	Manual	234

B.2.1	Input and output	236
B.2.2	Initialisation of model parameters	241
B.2.3	Processing control	243
B.2.4	Weights and outliers	243
B.3	General organisation of source code	251
B.4	Model functions	253
B.4.1	Numerical differentiation	253
B.4.2	Handling of multi-dimensional conditions	254
B.4.3	Limitation of parameter space	254
B.4.4	Initialisation of parameters	255
B.5	Special algorithms	256
B.5.1	LU decomposition	256
B.5.2	Singular value decomposition	257
B.5.3	Sorting	257
B.6	Possible optimisations	257
B.7	Performance Test	258
B.7.1	Fitting linear systems	259
B.7.2	Fitting nonlinear systems	262
List of symbols		267
Bibliography		271
Index		277
S	The Source Code (accessible via internet)	1
S.1	Licence and Disclaimer	1
S.2	Main functions	2
S.3	Model functions	26
S.4	Initialisation of nonlinear models	34
S.5	Matrix processing	41
S.5.1	Utils	41
S.5.2	Allocation and matrix handling	44
S.6	Command-line parsing	50
S.7	Error Handling	52
S.8	Other	53