

List of Algorithms

1	Kahan's Summation Formula	17
2	Recursive Calculation of Variance and Mean	19
3	Mean, Variance, Minimum and Maximum of a Sample	21
4	Calculation of the Covariance	22
5	Levenberg-Marquardt Method	45
6	Truncated SVD Method	46
7	Evaluation According to GUM	84
8	Construction of a Unit-Triplet	100
9	Multiplication of Two Unit-Triplets	101
10	Addition of Two Unit-Triplets	101
11	Greedy Decomposition of an SI-Vector	103
12	Finding the Range for Optimal λ	105
13	Decomposing an SI-vector with "Best Next" Strategy	106
14	Niceness of a Partial Reduction	108
15	Distributing Prefixes	109
16	Pretty Printing a Unit Vector	110

List of Figures

1	Different random variable samples	14
2	Process of a Calibration Measurement	32
3	Fitting a linear function	50
4	Fitting an Exponential Function	51
5	Fitting a Power Function	53
6	Fitting a Sigmoid Function	54
7	Syntax Tree	58
8	Graphical Representation of an EBNF Production Rule	60
9	Graphical Representation for a Unit in M	64
10	Schematic Architecture of MUSAC	94
11	Elementwise Contributions to 1-norm	105
12	Syntax Tree Transformed to a DAG	118
13	CED in <i>Uncertainty Manager</i>	123
14	Screen Shot of <i>Uncertainty Manager</i>	124
15	Schematic Illustration of ICP-OES Torch	128
16	NIST Report 839.01-00-518	137
17	NIST Report 839.01-00-518 cont.	138
18	NIST Report 839.01-00-518 cont.	139
19	Calibration Type Selection	141
20	Dilution of One Calibration Point	141
21	CED for ICP-OES	142
22	Visualization of Uncertainty Budget	166

List of Tables

1	Algorithms for computing a large sum	20
2	Comparison of TSVD and Levenberg-Marquardt	48
3	Subset of EBNF Reproduction Rules	61
4	Tokens in M	62
5	Distribution Mnemonics	71
6	List of Known and Accepted Units and Engineering Prefixes .	73
7	Regression Functions in MUSAC	82

Bibliography

- [1] *ISO 5725:1994 Accuracy (trueness and precision) of measurement methods and results*, volume 1–6. International Organization for Standardization (ISO), Central Secretariat, 1994. See ISO 5725-5:1998 for alternative methods of estimating precision.
- [2] *Guide to the Expression of Uncertainty in Measurement*. International Organization for Standardization (ISO), Central Secretariat, Geneva, 1 edition, 1995.
- [3] *ISO/IEC 14977*. International Organization for Standardization (ISO), Central Secretariat, Geneva, 1996.
- [4] *ISO/IEC 17025:1999 General Requirement for the Competence of Calibration and Testing Laboratories*. ISO, Geneva, 1999.
- [5] *ISO 6143*, chapter B.2, pages 18–31. International Organization for Standardization (ISO), Central Secretariat, 2000.
- [6] Erwin Achermann and Oscar Chinellato. Estimating measurement uncertainty. Technical Report 346, Department of Computer Science, ETH Zürich, 2000. available at <http://www.inf.ethz.ch/publications/>.
- [7] Jesse Barlow. Error analysis of a pairwise summation algorithm to compute the sample variance. *Numer. Math.*, 58(6):583–590, 1991.
- [8] Kent Beck. *Extreme Programming Explained: Embrace Change*. Addison-Wesley Publishing Company, 2000.

- [9] Joseph Berkson. Are there two regressions? *Journal of the American Statistical Association*, 45(250):164–180, June 1950.
- [10] Åke Björck. *Numerical Methods for Least Squares Problems*. SIAM, Philadelphia, 1996.
- [11] Paul T. Boggs, Richard H. Byrd, and Robert B. Schnabel. A stable and efficient algorithm for nonlinear orthogonal distance regression. *SIAM Journal Sci. and Stat. Computing*, 8(6):1052–1078, November 1987.
- [12] Wolfram Bremser and Werner Hässelbarth. Controlling uncertainty in calibration. *Analytica Chimica Acta*, 348:61–69, 1997.
- [13] Raymond J. Carroll, David Ruppert, and Len A. Stefanski. *Measurement Error in Nonlinear Models*. Number 63 in Monographs on Statistics and Applied Probability. Chapman and Hall, London, 1995.
- [14] Tony Chan, Gene H. Golub, and Randall LeVeque. Algorithms for computing the sample variance: analysis and recommendations. *American Statistician*, 37(3):242–247, August 1983.
- [15] Maurice Cox. Gum — the next generation. Private Communications, November 2001.
- [16] Bureau International des Poids et Mesures. *Comptes rendus des séances de la onzième conférence général des poids et mesures*, 11-20 Octobre 1960.
- [17] Cornelius F. Dietrich. *Uncertainty, calibration and probability*. Adam-Hilger (Bristol), 2 edition, 1991.
- [18] Steve L. R. Ellison, Matthias Rösslein, and Alex Williams, editors. *Quantifying Uncertainty in Analytical Measurement*. EURACHEM / CITAC, 2 edition, 2000. available at <http://www.eurachem.bam.de/guides/quam2.pdf>.
- [19] Trevor Farrant. *Practical Statistics for the Analytical Scientist*. Royal Society of Chemistry, 1997.
- [20] Ulrich Feller. Über Grössen, Einheiten und Einheitensysteme. *OFMET-Info*, 5(1), 1998.

-
- [21] Richard Feynman. *The Feynman Lectures on Physics*, volume 1. Addison-Wesley Publishing Company, London, 1963.
- [22] Wayne A. Fuller. *Measurement Error Models*. Wiley Series in Probability and Mathematical Statistics. John Wiley & Sons, Inc., 1987.
- [23] Erich Gamma, Richard Helm, Ralph Johnson, and John Vlissides. *Entwurfsmuster*. Addison-Wesley Publishing Company, 1996.
- [24] Philip E. Gill, Walter Murray, and Margaret H. Wright. *Practical Optimization*. Academic Press Inc., London, 1981.
- [25] Philip E. Gill, Walter Murray, and Margaret H. Wright. *Numerical Linear Algebra and Optimization*, volume 1. Addison-Wesley Publishing Company, 1991.
- [26] David Goldberg. What every computer scientist should know about floating-point arithmetic. *ACM Computing Surveys*, 23(1), March 1991.
- [27] Gene H. Golub and Charles F. van Loan. *Matrix Computation*. The Johns Hopkins University Press and North Oxford Academic, 3 edition, 1996.
- [28] Jim G. Kalbfleisch. *Probability and Statistical Inference*, volume 1: Probability. Springer-Verlag, 2 edition, 1985.
- [29] Jim G. Kalbfleisch. *Probability and Statistical Inference*, volume 2: Statistical Inference. Springer-Verlag, 2 edition, 1985.
- [30] Donald E. Knuth. *Seminumerical Algorithms*, volume 2 of *The Art of Computer Programming*. Addison-Wesley Publishing Company, 2 edition, 1981.
- [31] Douglas L. MacTaggart and Sherry O. Farwell. Analytical use of linear regression. *Journal of AOAC International*, 75(4):594–608, July 1992. ISSN 1060-3271.
- [32] Scott Meyers. *Effektiv C++ programmieren*. Addison-Wesley Publishing Company, 2 edition, 1995.
- [33] Zbigniew Michalewicz and David B. Fogel. *How to Solve It: Modern Heuristics*. Springer-Verlag, 2 edition, 2000.

- [34] Martin Müller. Entwicklung eines Algorithmus zur automatische Anordnung eines Ursachen-Wirkungs-Diagramms. Semester Projekt, Technische Universität München, Lehrstuhl für effiziente Algorithmen, 2001.
- [35] Arnold Neumaier. Solving ill-conditioned and singular linear systems: a tutorial on regularization. *SIAM Review*, 40(3):636–666, September 1998.
- [36] William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. *Numerical Recipes in C*. Cambridge University Press, 2 edition, 1996.
- [37] Axel Reichert. *units.sty, A Package For Setting Units Typographically Correct*. CTAN, 8 1998. available at CTAN.
- [38] John A. Rice. *Mathematical Statistics and Data Analysis*. Duxbury Press, 2 edition, 1995.
- [39] Jordi Riu and F. Xavier Rius. Univariate regression models with errors in both axes. *Journal of Chemometrics*, 9:343–362, 1995.
- [40] Alan Rüegg. *Wahrscheinlichkeitsrechnung und Statistik*. Oldenburg, München, 1986.
- [41] Marc L. Salit and Greory C. Turk. A drift correction procedure. *Anal. Chem.*, 70(15):3184–3190, August 1998.
- [42] Hans R. Schwarz. *Numerische Mathematik*. B.G. Teubner, Stuttgart, 4 edition, 1997.
- [43] Sabine Van Huffel, editor. *Recent Advances in Total Least Squares Techniques and Errors-In-Variables Modelling*, Proceedings of the 2nd International Workshop. Society for Industrial and Applied Mathematics, SIAM, 1997.
- [44] Edward A. Youngs and Elliot M. Cramer. Some results relevant to choice of sum and sum-of-product algorithms. *Technometrics*, 13:657–665, 1971.