Bibliography

[1] K. Abraham, H. Mielke, W. Huisinga, and U. Gundert-Remy. Elevated internal exposure of children in simulated acute inhalation of volatile organic compounds: Effects of concentration and duration. *Arch Toxicol*, 79:63–73, 2005.

[2] K. Abraham, H. Mielke, W. Huisinga, and U. Gundert-Remy. Elevated internal exposure of children in simulated acute inhalation of volatile organic compounds: Dependency on properties of the chemical. *Basic and Clinical Pharmacology and Toxicology*, pages 242–243, 2005.

[3] F. J. Aherne, N. A. Thacker, and P. I. Rockett. The Bhattacharyya metric as an absolute similarity measure for frequency coded data. *Kybernetika*, 32(4):1–7, 1997.

[4] H. Akaike. Statistical predictor identication. *Ann. Inst. Statist. Math.*, 21:203–217, 1970.

[5] H. Akaike. Information theory as an extension of the maximum likelihood principle. In B. N. Petrov and F. Csaksi, editors, *2nd International Symposium on Information Theory*, pages 267–281, 1973.

[6] H. Akaike. A new look at the statistical identification model. *IEEE Transactions on Automatic Control*, 19:716–723, 1974.

[7] H. Akaike. Factor analysis and aic. *Psychometrika*, 52:317–332, 1987.

[8] J. H. Albert. Criticism of a hierachical model using Bayes factors. Bowling Green State University.

[9] S. M. Ali and S. D. Silvey. A general class of coefficients of divergence of one distribution from another. *Journal of the Royal Statistical Society*, 28:131–142, 1966.

[10] H. Amann. *Gewöhnliche Differentialgleichungen.* Walter de Gruyter and Co., 1983.

[11] S. M. Anderson, J. I. Zink, and D. Neuhaeuser. A simple and accurate approximation for a coupled system-bath: locally propagated Gaussians. Department of Chemistry and Biochemistry University of California, Los Angeles, 1998.

[12] C. Andrieu, A. Doucet, and C. P. Robert. Computational advances for and from Bayesian analysis. *Statistical Science*, 19(1):118–127, 2004.

[13] L. Armijo. Minization of functions having Lipschitz continuous first partial derivatives. *Pacific Journal of Mathematics*, 16(1):1–3, 1966.

[14] S. F. Arnold. *The theory of linear models and multivariante analysis.* Wiley Series in Probability and Mathematical Statistics. John Wiley & Sons, Inc., 1981.

[15] S. F. Arnold. *Mathematical Statistics.* Prentice-Hall, 1990.

[16] W. I. Arnold. *Ordinary Differential Equations.* Springer Verlag Berlin Heidelberg New York, 1992.

[17] A. C. Atkinson. A test for discrimination between models. *Biometrika*, 56:337–347, 1969.

[18] A. C. Atkinson and R. A. Bailey. One hundred years of designed experiments on and off the pages of "biometrika". *Biometrika*, 88, 2001.

[19] A. C. Atkinson, B. Bogacka, and A. Zhigljavsky, editors. *Optimum Design 2000.* Kluwer Scientific Publications, 2001.

[20] A. C. Atkinson and A. N. Donev. *Optimum experimental design.* Oxford: Clarendon Press, 1992.

[21] A. C. Atkinson and V. V. Fedorov. The design of experiments for discriminating between two rival models. *Biometrika*, 62:57–70, 1975.

[22] A. C. Atkinson and V. V. Fedorov. Optimal design: experiments for discriminating between several models. *Biometrika*, 62:289–303, 1975.

[23] A. C. Atkinson and L. M. Haines. Designs for nonlinear and generalized linear models. In S. Ghosh and C.R.Rao, editors, *Design of Experiments*, volume 13 of *Handbook of Statistics*, chapter 28, pages 437–475. Elsevier Science B.V., 1996.

[24] J. E. Bailey and D. F. Ollis. *Biochemical engineering Fundamentals.* McGrawHill, Inc., second edition, 1986.

[25] Y. Bard. *Nonlinear parameter estimation.* Academic Press, Inc., 1974.

[26] W. G. Bardley and P. B. McGinlay. Optimal design for model discrimination using the F-test with nonlinear biochemical models. criteria for choosing the number and spacing for experimental points. *Journal of theoretical biology,* 139:85–102, 1989.

[27] C. Barner-Kowollik, J. F. Quinn, D. R. Morsley, and T. P. Davis. Modeling the reversible addition-fragmentation chain transfer process in cumyl dithiobenzoate-mediated styrene homoppolymerizations: Assessing rate coefficients for addition-fragmentation equilibrium. *Journal of Polymer Science,* 39:1353–1365, 2001.

[28] M. J. Bayarri and J. O. Berger. The interplay of Bayesian and Frequentist analysis. *Statistical Science,* 19(1):58–80, 2004.

[29] H. J. C. Berendsen. Molecular dynamics simulations: The limits and beyond, 2000.

[30] A. Bhattacharyya. On a measure of divergence between two statistical populations defined by their probability distributions. *Bulletin of the Calcutta Mathematical Society,* 35:99–110, 1943.

[31] P. J. Bickel and K. A. Doksum. *Mathematical Statistics.* Holden-Day, Inc. Oakland, California, 1977.

[32] P. J. Bickel, Y. Ritov, and T. M. Stoker. Tailor–made tests for goodness of fit for semiparametric hypotheses. to appear in The Annals of Statistics 2006, 2003.

[33] J. A. Bilmes. A gentle tutorial of the EM-algorithm and its application to parameter estimation for Gaussian mixture and hidden Markov models. Technical Report TR–97–021, International Computer Science Institue, Berkeley, April 1998.

[34] D. R. Bingham and H. A. Chipman. Optimal designs for model selection. Technical Report 388, University of Michigan, Department of Statistics, 2003. tentatively accepted at Technometrics.

[35] A. Biswas and P. Chaudhuri. An efficient design for model discrimination and parameter estimation in linear models. *Biometrika*, 89(3):709–718, 2002.

[36] F. A. Bornemann. An adaptive multilevel approach to parabolic equations: I. General theory and 1D implementation. *Impact of computing in science and engineering*, 2:279–317, 1990.

[37] D. S. Borowiak. *Model discrimination for nonlinear regression models*. Marcel Dekker, INC., 1989.

[38] G. E. P. Box. Science and statistics. *J. Am. Statist. Ass.*, 71:791–799, 1976.

[39] G. E. P. Box and W. J. Hill. Discrimination among mechanistic models. *Technometrics*, 9(1):57–71, February 1967.

[40] G. E. P. Box, W. G. Hunter, and J. S. Hunter. *Statistics for Experimenters: An Introduction to Design, Data Analysis, and Model Building*. Wiley series in Probability and Mathematical Statistics. John Wiley and Sons, Inc., 1978.

[41] G. E. P. Box and H. L. Lucas. Design of experiments in nonlinear situations. *Biometrika*, 46:77–90, 1959.

[42] G. E. P. Box and G. C. Tiao. *Bayesian inference in statistical analysis*. Addison-Wesley, 1973.

[43] L. Breiman. Statistical modeling: The two cultures. *Statistical Science*, 16(3):199–231, 2001.

[44] M. Brettel, S. Hungeling, and D. Meier. Quo Vadis, Kausalanalyse? Preprint, Lehrstuhl für Wirtschaftswissenschaften an der RWTH-Aachen.

[45] S. P. Brooks, N. Friel, and R. King. Classical model selection via simulated annealing. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 65(2):503–520, 2003.

[46] A. L. Burke, T. A. Duever, and A. Penlidis. Discriminating between the terminal and penultimate models using designed experiments: An overview. *Industrial and engineering chemistry research*, 36:1016–1035, 1997.

[47] K. P. Burnham and D. R. Anderson. *Model Selection and Inference – A practical information-theoretic approach*. Springer New York, Inc., 1998.

[48] K. P. Burnham and D. R. Anderson. *Model Selection and Multimodel Inference: A Practical Information-Theoretical Approach.* Springer-Verlag, New York, second edition, 2002.

[49] K. P. Burnham and D. R. Anderson. Multimodel inference – understanding aic and bic in model selection. *Sociological Methods & Research*, 33(2):261–304, 2004. DOI: 10.1177/0049124104268644.

[50] K. Burrage, T. Tian, and P. Burrage. A multi-scale approach for simulating chemical reaction systems. Advanced computational modelling centre, The University of Queensland, Australia, 2003.

[51] M. Busch. Modeling kinetics and structural properties in high-pressure fluid-phase polymerization. *Macromolecular theory simulation*, 10(5):408–429, 2001.

[52] G. Buzzi-Ferraris and P. Forzatti. A new sequential experimental design procedure for discriminating among rival models. *Chemical Engineering Science*, 38(2):225–232, 1983.

[53] K. Chaloner and I. Verdinelli. Bayesian experimental design: A review. *Statistical science*, 23:273–304, 1995.

[54] C. Chatfield. Model uncertainty, data mining and statistical inference. *Journal of the Royal Statistical Society*, 158(3):419–466, 1995.

[55] S. Chatterjee and A. S. Hadi. *Sensitivity Analysis in Linear Regression.* Wiley series in probability and mathematical statistics. John Wiley & Sons, Inc., 1988.

[56] H. Chernoff. A measure of asymptotic efficiency for tests of a hypothesis based on the sum of observations. *Annals of Mathematical Statistics*, pages 493–507, 1952.

[57] H. Chernoff. Locally optimal diesngs for estimating parameters. *Annals of Mathematical Statistics*, 24:586–602, 1953.

[58] S. Chib. Markov Chain Monte Carlo technology. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter II.3, pages 72–102. Springer–Verlag Berlin Heidelberg, 2004.

[59] B. Choi. *ARMA model identification.* Springer New York, 1992.

[60] M. Clyde and E. I. George. Model uncertainty. *Statistical Science*, 19(1):81–94, 2004.

[61] A. Cohen and H. B. Sackrowitz. An approach to inference following model seection with applications to transformation–based and adaptive inference. *Journal of American Statistical Association*, 82:1123–1130, 1987.

[62] A. Cornish-Bowden. *Fundamentals of enzyme kinetcs*. Portland Press, London, 1995.

[63] G. A. Csanady, A. L. Mendrala, R. J. Nolan, and J. G. Filser. A physiologic pharmacokinetic model for styrene and styrene–7,8–oxide in mouse, rat and man. *Arch Toxicol*, 68:143–157, 1994.

[64] T. Dasu, S. Krishnan, S. Venkatasubramanian, and K. Yi. An information-theoretic approach to detecting changes in multi-dimensional data streams. Preprint. AT&T Labs–Research and Duke University., 2005.

[65] B. de Finetti. *Theory of Probability*, volume I. John Wiley & Sons, Inc., 1974.

[66] B. de Finetti. *Theory of Probability*, volume II. John Wiley & Sons, Inc., 1975.

[67] J. G. de Gooijer, B. Abraham, A. Gould, and L. Robinson. Methods for determining the order of an autoregressive-moving average process. *International Statistical Review*, 53:301–329, 1985.

[68] J. de Leeuw. Model selection in multinomial experiments. In T. K. Dijkstra, editor, *On model unvertainty and its statistical implications*, pages 118–138. Springer Berlin, 1988.

[69] M. Dellnitz and O. Junge. On the approximation of complicated dynamical behavior. *SIAM Journal of Numerical Analysis Annals*, 36(2), 1999.

[70] A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the EM-algorithm. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 39:1–38, 1977.

[71] H. Dette and R. Kwiecien. A comparison of sequential and nonsequential designs for discrimination between nested regression models. *Biometrika*, 91(1):165–176, 2004.

[72] H. Dette, V. B. Melas, A. Pepelyshev, and N. Strigul. Efficient design of experiments in Monod model. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 65(3):725–740, 2003.

[73] H. Dette and T. E. O'Brien. Optimality criteria for regression models based on predicted variance. *Biometrika*, 86:93–106, 1999.

[74] P. Deuflhard. *Newton Methods for Nonlinear Problems. Affine Invariance and Adaptive Algorithms*, volume 35 of *Springer Series Computational Mathematics*. Springer, 2004.

[75] P. Deuflhard and F. Bornemann. *Scientific Computing with Ordinary Differential Equiations - Texts in Applied Mathematics*. Springer, 2002.

[76] P. Deuflhard, J. Lang, and U. Nowak. Recent progress in dynamical process simulation. In H. Neunzert, editor, *Progress in Industrial Mathematics*, pages 122–137. 8th Conference of the European Consortium for Mathematics in Industry (ECMI 94), Wiley & Teubner Publishers, 1996.

[77] E. Diederichs. *Dimension Reduction in chemical system*. PhD thesis, Freie Universität Berlin, 2003. in progress.

[78] D. Draper. Assessment and propagation of model uncertainty. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 57:45–97, 1995.

[79] D. Draper, J. S. Hodges, E. E. Morris, C. N. Morris, and D. B. Rubin. A research agenda for assessment and propagation of model uncertainty. Technical Report N-2683-RC, Rand Cooperation, Santa Monica, 1987.

[80] J.-M. Dufour, L. Khalaf, and M.-C. Beaulieu. Exact skewness-kurtosis test for multivariate normality and goodness-of-fit in multivariate regressions with applications to asset pricing models. CIRANO, March 2003.

[81] B. Efron. How biased is the apparent error rate of a prediction rule. *Journal if the American Statistical Association*, 81:461–470, 1986.

[82] S. P. Ellis. Instability of least squares, least absolute deviation and least median of squares linear regression. *Statistical Science*, 13(4):337–350, 1998.

[83] M. Evans, N. Hastings, and J. B. Peacock. *Statistical Distributions*. Wiley series in probability and statistics. John Wiley & Sons, Inc., third edition, 2000.

[84] L. Fahrmeir and G. Tutz. *Multivariate Statistical Modelling Based on Generalized Linear Models.* Springer series in statistics. Springer, 1994.

[85] C. P. Fall, E. S. Marland, J. M. Wagner, and J. J. Tyson. *Computational Cell Biology*, volume 20 of *Interdisciplinary Applied Mathematics.* Springer Verlag New York Inc., 2002.

[86] H. Faure. Discrépance de suites associées à un système de numération. *Bull. Soc. Math. France*, 109(2), 1981.

[87] V. V. Fedorov. *Theory of Optimal Experiments.* Probability and mathematical statistics. Academic Press, New York and London, 1972.

[88] V. V. Fedorov and V. Khabarov. Duality of optimals for model discrimination and parameter estimation. *Biometrika*, 73(1):183–190, 1986.

[89] D. Fell. *Understanding the Control of Metabolism*, volume 2 of *Frintiers in Metabolism.* Portland Press, 1997.

[90] R. Fierro, G. Golub, P. Hansen, and D. O'Leary. Regularization by truncated total least squares. *SIAM Journal on Scientific Computing*, 18(4):1223–1241, July 1997.

[91] R. Fildes and S. Howell. On selecting a forecasting model. *TIMS Stud. Mangmnt Sci.*, 12:297–312, 1979.

[92] D. A. Freedman. A note on screening regression equations. *The American Statistican*, 37:152–155, 1983.

[93] D. A. Freedman. Statistical models and shoe leather with discussion by Richard A. Berk, Hubert M. Blalock, Jr., William M. Mason. In P. Mardsen, editor, *Sociologyical Methodolog*, chapter 10, pages 291–358. American Sociological Association: Washington, D.C., 1991.

[94] D. A. Freedman. From association to causation via regression. *Advances in Applied Mathematics*, 18(1):59–110, 1997.

[95] S. Frühwirth-Schnatter. Bayesian model discrimination and Bayes factor for linear gaussian state space models. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 57:237–246, 1995.

[96] S. Frühwirth-Schnatter. Model likelihood and Bayes factors for switching and mixture models. Technical report, SFB Adaptive Information Systems

and Modelling in Economics and Management Science, http://www.wu-wien.ac.at/am/reports.htm, 2002.

[97] C. W. Gardiner. *Handbook of Stochastic Methods. For Physics, Chemistry and the Natural Sciences*, volume 13 of *Springer Series in Synergetics*. Springer Verlag Berlin Heidelberg, second edition, 2002.

[98] A. Gelfand and D. Dey. Bayesian model choice: Asypmptotic and exact calculations. *1994*, 56:501–514, Journal of the Royal Statistical Society: Series B (Statistical methodology).

[99] A. Gelfand and A. Smith. Sampling-based approaches to calculating marginal densities. *Journal of American Statistical Association*, 85:398–409, 1990.

[100] A. B. Gelman, J. S. Carlin, H. S. Stern, and D. B. Rubin. *Bayesian Data Analysis*. Chapman and Hall/CRC, 2000.

[101] D. T. Gillespie. Exact stochastic simulation of coupled chemical reactions. *Journal of Physical Chemistry*, 81(25):2340–2361, 1977.

[102] L. J. Gleser. Assessing uncertainty in measurement. *Statistical Science*, 13(3):277–290, 1998.

[103] G. E. Golub and C. F. van Loan. *Matrix Computation*. The Johns Hopkins University Press, third edition, 1996.

[104] P. Green. Reversible jump MCMC computation and Bayesian model determination. *Biometrika*, 82:711–732, 1995.

[105] P. J. Green. On the use of the EM–algorithm for penalized likelihood estimation. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 52(4):443–452, 1990.

[106] C. Gu. *Smoothing spline ANOVA models*. Springer Verlag, New York, 2002.

[107] M. H. Hansen and B. Yu. Model selection and the principle of minimum description length. *Journal of the American Statistical Association*, 96:746–774, 2001.

[108] T. Hastie and R. Tibshirani. *Generalized Additive Models*. Chapman and Hall, 1990.

[109] T. Hastie, R. Tibshirani, and J. Friedman. *The Elements of Statistical Learning.* Springer New York Inc., 2002.

[110] W. Hastings. Monte Carlo sampling methods using Markov chains and their applications. *Biometrika*, pages 97–109, 1970.

[111] E. J. Heller. Frozen Gaussians: A very simple semiclassical approximation. *Journal of chemical physics*, 75(6):2923–2931, September 1981.

[112] U. Hjorth. On model selection in computer age. *Journal statistical planning inf.*, 23:101–115, 1989.

[113] U. Hjorth. Model selection needs resampling methods. Technical report, Linköping University, 1990.

[114] U. Hjorth. *Computer intensive statistical methods – validation model selection and bootstrap.* London: Chapman and Hall, 1994.

[115] J. S. Hodges. Uncertainty policy analysis and statistics. *Statistical Science*, 2:259–291, 1987.

[116] J. A. Hoeting, D. Madigan, A. E. Raftery, and C. Volinsky. Bayesian model averaging: A tutorial. *Statistical Science*, 14(4):382–417, 1999.

[117] R. V. Hogg and E. A. Tanis. *Probability and Statistical Inference.* Macmillan Publishing Co., Inc. New York, 2nd edition, 1983.

[118] A. Hohmann. *Inexact Newton Methods for Parameter Dependent Nonlinear Problems.* Reports on Mathematics, Shaker Verlag, Aachen, 1994.

[119] I. Horenko. *Modeling and numerical simulation of quantum effects in molecular dynamics.* PhD thesis, Free University Berlin, Germany, Arnimallee 2-6, 14195 Berlin, Germany, 2004.

[120] I. Horenko, S. Lorenz, C. Schütte, and W. Huisinga. Adaptive approach for nonlinear sensitivity analysis of reaction kinetics. *Journal of Computational Chemistry*, 26(9):941–948, July 2005.

[121] I. Horenko and M. Weiser. Adaptive integration of multidimensional molecular dynamics with quantum initial conditions. ZIB-Report 02-29, July 2002.

[122] I. Horenko and M. Weiser. Adaptive integration of molecular dynamics. *Journal of Computational Chemistry*, 24(15):1921–1929, 2003.

[123] I. Horenko, M. Weiser, B. Schmidt, and C. Schütte. Fully adaptive propagation of the quantum–classical liouville equation. accepted Journal of chemical physics, 2004.

[124] C. M. Hurvich and C. L. Tsai. Regression and time series model selection in small samples. *Biometrika*, 76:297–307, 1989.

[125] R. A. Hutchinson. Modeling of chain length and long–chain branching distributions in free–radical polymerization. *Macromolecular Theory Simulation*, 10(3):144–157, 2001.

[126] P. D. Iedema, C. Willems, G. van Vliet, W. Bunge, S. M. P. Mutsers, and H. C. J. Hoefsloot. Using molecular weight distributions to determine the kinetics of peroxide-induced degradation of polypropylene. *Chemical Engineering Science*, 56:3659–3669, 2001.

[127] A. M. Jacobs and J. Grainiger. Models of visual word recognition – sampling the state of the art. *Journal of Experimental Psychology: Human perception and performance*, 29:1311–1334, 1994.

[128] W. Jeffreys and J. O. Berger. Ockham's razor and Bayesian analysis. *American Scientist*, 80:64–72, 1992.

[129] D. H. Johnson and S. Sinanovi´c. Symmetrizing the kullback–leibler distance. Unpublished.

[130] G. G. Judge and M. E. Bock. *The statistical implications of pre-test and Stein-rule estimators in Econometrics*. Amsterdam: North-Holland, 1978.

[131] R. E. Kaas and A. E. Raftery. Bayes factors. *Journal of the American Statistical Association*, 90(430):773–795, June 1995.

[132] I. Karatzas and S. S. Shreve. *Brownian Motion and Stochastic Calculus*, volume 113 of *Graduate Texts in Mathematics*. Springer Verlag New York Inc., second edition, 1999.

[133] A. Keese. A review of recent developments in the numerical solution of stochastic partial differential equations (stochastic finite elements). Informationbericht 2003-6, Department of Computer Science, Technical University Braunschweig, Brunswick, Germany, Institute of Scientific Computing, Technische Universität Braunschweig, Hans-Sommer-Straße 65, D-38106 Braunschweig, October 2002.

[134] W. J. Kennedy and J. E. Gentle. *Statistical computing*. Marcel Dekker, Inc. New York, USA, 1980.

[135] J. Kiefer. Optimum experimental designs. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 21:272–319, 1959.

[136] J. Kiefer. Optimum designs in regression problems II. *Annals of Mathematical Statistics*, 32:298–325, 1961.

[137] J. Kiefer. General equivalence theory for optimum design (approximate theory). *Annals of Statistics*, 2:849–879, 1974.

[138] J. Kiefer. Optimum design: Variation in structure and performance under change of criterion. *Biometrika*, 62:277–288, 1975.

[139] J. Kiefer and J. Wolfowitz. The equivalence of two extremum problems. *Canadian Journal of Mathematics*, 12:363–366, 1960.

[140] M. Kleiber and T. D. Hien. *The stochastic finite element method, Basic perturbation technique and computer implementation*. John Wiley & Sons, Inc., 1992.

[141] J. P. C. Kleijnen. Design and analysis of Monte Carlo experiments. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter III.3, pages 498–516. Springer–Verlag Berlin Heidelberg, 2004.

[142] D. Krewski, Y. Wang, S. Bartlett, and K. Krishnan. Uncertainty, variability and sensitivity analysis in physiological pharmocokinetic models. *Journal of biopharmaceutical statistics*, 5(3):245–271, 1995.

[143] W. J. Krzanowski. Distance between populations using mixed continuous and categorical variables. *Bioemtrika*, 70:235–243, 1983.

[144] J. Kuha. AIC and BIC – comparisons of asumptions and performance. *Sociological methods and research*, 33(2):188–229, November 2004.

[145] S. Kullback. *Information theory and statistics*. Wiley Inc., New York, 1959.

[146] S. Kullback and R. A. Leibler. On information and sufficiency. *Annals of Mathematical Statistics*, 22:79–86, 1951.

[147] A. J. Lacey, N. A. Thacker, and N. L. Seed. Feature tracking and motion classification using a switchable model kalman filter. In *Proc. BMVC*, 1994.

[148] J. C. Lagarias, J. A. Reeds, M. H. Wright, and P. E. Wright. Convergence properties of the nelder-mead simplex method in low dimensions. *SIAM Journal of Optimization*, 9(1):112–147, 1998.

[149] A. Lasota and M. C. Mackey. *Chaos, Fractals, and Noise – Stochastic Aspects of Dynamics*, volume 97 of *Applied Mathematical Sciences*. Springer Verlag New York, second edition, 1994.

[150] A. Lübbert and S. B. Jørgensen. Bioreactor performance: a more scientific approach for practice. *Journal of Biotechnology*, 85:187–212, 2001.

[151] E. E. Leamer. Testing trade theory. Working Paper 3957. National Bureau of Economic Research.

[152] E. E. Leamer. *Specification searches: Ad hoc inference with experimental data*. Wiley, New York, 1978.

[153] E. E. Leamer. Sensitivity analysis would help. *Am. Econ. Rev.*, 75:308–313, 1985.

[154] E. E. Leamer. Sensitivity analysis would help. In C. W. J. Granger, editor, *Modelling Economic Series*. Claredon Press, 1990.

[155] E. E. Leamer. Testing trade theory. In D. Greenaway and L. A. Winters, editors, *Surveys in International Trade*. Blackwell Publishers, 1994. England, Oxford.

[156] P. L'Ecuyer. Random number generation. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter II.2, pages 36–70. Springer–Verlag Berlin Heidelberg, 2004.

[157] W. Ledermann and E. Lloyd, editors. *Handbook of Applicable Mathematics*, volume VI – part B, chapter Bayesian Statistics. John Wiley & Sons, Inc., 1984.

[158] K. A. Levenberg. A method for the solution of certain problems in least squares. *Quarterly Applied Mathematics*, 2(2):164–168, July 1944.

[159] H. Linhart and W. Zucchini. *Model selection*. Wiley series in probability and mathematical statistics. John Wiley & Sons, Inc., 1986.

[160] S. Lorenz, E. Diederichs, R. Telgmann, and C. Schütte. Discrimination of dynamical system models for biological and chemical processes. submitted to Journal of computational chemistry, reviewing process, December 2003.

[161] E. Läuter. Experimental design in a class of models. *Mathematische Operationsforschung und Statistik*, 5(4/5):379–398, 1974.

[162] E. Läuter. Optimal multipurpose designs for regression models. *Mathematische Operationsforschung und Statistik*, 7(1):51–68, 1976.

[163] D. Madigan and A. E. Raftery. Model selection and accounting for model uncertainty in graphical models using occam's window. *Journal of American Statistical Association*, 89:1535–1546, 1994.

[164] P. Marenbach. *Rechnergestützte Methoden zur interaktiven Modellierung biotechnologischer Prozesse*. PhD thesis, Technische Universität Darmstadt, 1999. D17 Darmstädter Dissertationen 1999.

[165] D. W. Marquardt. An algorithm for least squares estimation of nonlinear parameters. *SIAM Journal Applied Mathematics*, 11:431–441, 1963.

[166] T. J. Martinez, M. Ben-Nun, and G. Ashkenazi. Classical/quantal method for multistate dynamics: A compuational study. *Journal of Chemical Physics*, 104(8):2847–2856, February 1996.

[167] T. J. Martinez, M. Ben-Nun, and R. D. Levine. Multi-electronic-state molecular dynamics: A wave function approach with applications. *Journal of physical chemistry*, 100:7884–7895, 1996.

[168] H. G. Matthies and M. Meyer. Nonlinear galerkin methods for the model reduction of nonlinear dynamical systems. Informationsberich 2002-3, Department of Computer Science, Technical University Braunschweig, Brunswick, Germany, March 2002. submitted to special issue of Computers and Structures, Revised and extended version of a contribution to the EUROMECH Colloquium, 427, ENS Cachan France, September 2001.

[169] K. Matusita. Decision rules based on distance for problems of fit. two samples and estimation. *Annals of Mathematical Statistics*, 26:631–641, 1955.

[170] P. McCullagh and J. Nelder. *Generalized Linear Models*. Chapman and Hall, London, 1989.

[171] G. J. McLachlan. *Discriminant analysis and statistical pattern recognition*. Wiley Inc., New York, 1992.

[172] P. Mendes and D. B. Kell. Non-linear optimization of biochemical pathways: applications to metabolic engineering and parameter estimation. *Bioinformatics*, 14(10):869–883, 1998.

[173] X. Meng and W. Wong. Simulating ratios of normalizing constants via a simple identity. *Statistical Sinica*, 6:831–860, 1996.

[174] T. Miazhynskaia, S. Frühwirth-Schnatter, and G. Dorffner. A comparison of Bayesian model selection based on MCMC with an application to GARCH-type models. report 83, Vienna University of Economics and Business Administration, 2003.

[175] L. Michaelis and M. L. Menten. Die Kinetik der Invertinwirking. *Biochemische Zeitschrift*, 49:333–369, 1913.

[176] P. Müller and F. A. Quintana. Nonparametric Bayesian data analysis. *Statistical Science*, 19(1):95–110, 2004.

[177] A. Monetti, G. Versini, and G. Dalpiaz. Sugar adulterations control in concentrated rectified grape musts by finite mixture distribution analysis of the myo- and scyllo-inositol content and the d/h methyl ratio of fermentative ethanol. *Journal of Agricultural Food Chemistry*, 44:2194–2201, 1996.

[178] D. S. Moore. Tests of the chi-squared type. In R. B. D'Agostino and M. A. Stephens, editors, *Goodness–Of–Fit Techniques*. Marcel Dekker, Inc. New York, 1974.

[179] F. Mosteller and J. Tukey. *Data analysis and regression*. Addison–Wesley, Redding, MA, 1977.

[180] J. Myung and M. A. Pitt. Model comparison methods. In L. Brand and M. L. Johnson, editors, *Numericals computer methods. Part D*, volume 383 of *Methods in Enzymology*, pages 351–366. Elsevier Inc., 2004.

[181] I. Nestorov. Whole body pharmacokinetic models. *Clinial Pharmocokinetic*, 42(10):883–908, 2003.

[182] P. Newbold, C. Agiakloglou, and J. Miller. Long–term inference based on short–term forcasting models. In T. S. Roa, editor, *Developments in time-series analysis*, pages 9–25. Chapman and Hall, London, 1993.

[183] M. Newton and A. Raftery. Approximate bayesian inference by the weighted likelihood bootstrap. *Journal of Royal Statistical Society: Series B (Statistical methodology)*, 56:1–48, 1994.

[184] S. K. Ng, T. Krishnan, and G. J. McLachlan. The EM–algorithm. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter II.5, pages 138–168. Springer–Verlag Berlin Heidelberg, 2004.

[185] H. Niederreiter. Random number generation and quasi-monte carlo methods. *SIAM*, 1992.

[186] J. E. Oakley and A. O'Hagan. Probabilistic sensitivity analysis of complex models: a Bayesian approach. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 66(3):751–769, 2004.

[187] T. E. O'Brien and G. M. Funk. A gentle introduction to optimal design for regression models. *The American Statistician*, 57(4):265–267(3), 2003.

[188] T. E. O'Brien and J. E. Rawling. A nonsequential design procedure for parameter estimation and model discrimination in nonlinear regression models. *Journal of Statistical Planning and Inference*, 55:77–93, 1996.

[189] R. R. Picard and R. D. Cook. Cross-validation of regression model. *Journal of the American Statistical Association*, 79:575–583, 1984.

[190] D. S. Poskitt and A. R. Tremayne. Determining a portfolio of linear time series models. *Biometrika*, 1987.

[191] B. M. Pötscher. Effects of model selection on inference. *Econometric Theory*, 7:163–185, 1991.

[192] F. Pukelsheim. *Optimal Design of experiments*. Wiley series in probability and mathematical statistics. John Wiley & Sons, Inc., 1993.

[193] A. E. Raftery. Choosing models for cross-classification. *American Sociological Review*, 51:145–146, 1986.

[194] A. E. Raftery. Bayesian model selection in social research. In K. Bollen and J. Long, editors, *Testing Structural Equation Models*, pages 163–180. Sage, Newburg Park, CA, 1993.

[195] A. E. Raftery, D. M. Madigan, and Hoeting. Model selection and accounting for model uncertainty in linear regression models. Technical Report 262, University of Washington, Department of Statistics, 1993.

[196] J. C. Ramsey and M. E. Andersen. A physiologically based description of inhalation pharmacokinetics of styrene in rats and humans. *Toxicology and Applied Pharmacology*, 73:159–175, 1984.

[197] C. R. Rao and H. Toutenburg. *Linear Models – Least Squares and Alternatives*. Springer Series in Statistics. Springer, 1995.

[198] R. A. Redner and H. F. Walker. Mixture density, maximum likelihood and the EM algorithm. *SIAM Review*, 26(2):195–239, April 1984.

[199] C. Ren, D. Sun, and D. K. Dey. Comparison of bayesian and frequentist estimation and prediction for a normal population. *The Indian Journal of Statistics*, 66(4):678–706, 2004.

[200] H. Risken. *The Fokker-Planck Equation. Methods of Solution and Applications*, volume 18 of *Springer Series in Synergetics*. Springer Verlag, second edition, 1996.

[201] J. Rissanen. A universal prior for integers and estimation by minimum description length. *Annals of Statistics*, 11:416–431, 1983.

[202] J. Rissanen. Fisher information and stochastic complexity. *IEEE Trans. Infformation Theory*, 42:40–47, 1996.

[203] C. P. Robert. Bayesian computational methods. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter III.11, pages 721–765. Springer–Verlag Berlin Heidelberg, 2004.

[204] E. Rothe. Zweidimensionale parabolische Randwertaufgabe als Grenzfall eindimensionaler Randwertaufgaben. *Mathematische Annalen*, 102:650–670, 1930.

[205] A. Saltelli, K. Chan, and M. Scott, editors. *Special Issue on sensitivity analysis*, volume 117. Computer Physics Communications, 1999.

[206] A. Saltelli, K. Chan, and M. Scott, editors. *Sensitivity analysis*. Probability and Statistics series. John Wiley & Sons, 2000.

[207] A. Saltelli, S. Tarantola, and F. Campolongo. Sensitivity analysis as an ingredient of modeling. *Statistical Science*, 15(4):377–395, 2000.

[208] A. Saltelli, S. Tarantola, and K. Chan. A quantitative, model independent method for global sensitivity analysis of model output. *Technometrics*, 41(1):39–56, 1999.

[209] J. L. Schoendorff, H. J. Korsch, and N. Moiseyev. Semiclassical quantization of a system with mixed regular/chaotic dynamics. *Europhysics Letters*, 44(3):292–297, November 1998.

[210] C. Schütte. Conformational dynamics: Modelling, theory, algorithm, and application to biomolecules. Habilitation thesis in Mathematics, 1999. Free University Berlin.

[211] C. Schütte, E. Diederichs, S. Lorenz, and R. Telgmann. Experimentally controlled discrimination of models, parameter identification and overlap optimization. Postersession BMBF–Statusseminar: Neue mathematische Verfahren in Industrie und Dienstleistungen, 2002.

[212] C. Schütte, W. Huisinga, and P. Deuflhard. Transfer operator approach to conformational dynamics in biomolecular systems. In B. Fiedler, editor, *Ergodic Theory, Analysis, and Efficient Simulation of Dynamical Systems*, pages 191–223. Springer Press, 2001.

[213] C. Schütte, R. Telgmann, E. Diederichs, and S. Lorenz. Internal documentation: Svd-application. Internal Working paper, 2002.

[214] G. Schwarz. Estimation the dimension of a model. *Annals of Statistics*, 6:461–464, 1978.

[215] P. Sebastiani and H. P. Wynn. Maximum entropy sampling and optimal Bayesian experimental design. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 62(1):145–157, 2000.

[216] S. D. Silvey. *Optimal Design*. London: Chapman and Hall, 1980.

[217] K. Smith. On the standard deviation of adjusted and interpolated values of an oberserved polynomial function and its constants and the guidance they give towards a proper choice of the distribution of observations. *Biometrika*, 12:1–85, 1918.

[218] I. M. Sobol. The distribution of points in a cube and the approximate evaluation of integrals. *USSR Comput. Math. Math. Phys.*, 1967.

[219] H.-J. Sommers and K. Zyczkowski. Bures volume of the set of mixed quantum states. arXiv:quant-ph/0304041v3170205, 2005. Preprint.

[220] J. C. Spall. Stochastic optimization. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter II.6, pages 170–197. Springer–Verlag Berlin Heidelberg, 2004.

[221] D. J. Spiegelhalter, N. G. Best, B. P. Carlin, and A. van der Linde. Bayesian measures of model complexity and fit. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 64(4):583–639, 2002.

[222] B. J. Stanley and G. Guiochon. Numerical estimation of adsorption energy distribution from adsorption isotherm data with the expectation-maximization method. *Journal of Physical Chemistry*, 97:8098–8104, 1993.

[223] J. E. Stapleton. *Linear statistical models.* Wiley series in probability and statistics. John Wiley & Sons, Inc., 1995.

[224] M. Stone. Cross-validatory choice and assessment of statistical predictions. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 36:111–147, 1974.

[225] B. Sudret and A. D. Kiuregian. Stochastsic finite element methods and reliablity – a state-of-the-art report. Report UCB/SEMM-2000/08, Department of civil and environmental engineering, University of California, Berkley, November 2000.

[226] R. Takors, W. Wiechert, and D. Weuster-Botz. Experimental design of the identification of macrokinetic models and model discrimination. *Biotechnology and Bioengineering*, 56(5):564–576, 1997.

[227] R. Telgmann. *Numerical aspects of the model–overlap–concept.* PhD thesis, Freie Universität Berlin, 2006. in progress.

[228] N. A. Thacker and J. E. W. Mayhew. Designing a network for context sensitive pattern classification. *Neural Networks*, 3(3):291–299, 1990.

[229] N. A. Thacker, P. A. Riocreux, and R. B. Yates. Assessing the completeness properties of pairwise geometric histograms. *Image and Vision Computing*, 13(5):423–429, 1995.

[230] R. S. Tsay. Comment on a paper by chatfield. *Journal Business Econ. Statistics*, 11:140–142, 1993.

[231] R. S. Tsay and C. G. Tiao. Some advances in non–linear and adaptive modelling in time–series. *J. Forecast.*, 13:109–131, 1994.

[232] J. W. Tukey. More honest foundations for data analysis. *American Statistical Association Meeting, Toronto.*

[233] D. Ucinski and B. Bogacka. T–optimal designs for discrimination between two multiresponse dynamic models. *Journal of the Royal Statistical Society: Series B (Statistical methodology)*, 67(1):3–18, 2005.

[234] P. Čižek. (Non)linear regression modeling. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter III.8, pages 622–654. Springer–Verlag Berlin Heidelberg, 2004.

[235] C. M. Villa, B. L. V. Horn, and W. H. Ray. Dynamics of polymerization reactors with evaporative cooling and wall heat transfer. *Polymer reaction engineering*, 7(2):151–194, 1999.

[236] M. Wagner and J. Timmer. Model selection in nonnested hidden Markov models. *Journal of theoretical biology*, 208, 2001.

[237] G. Wahba. Spline models for observational data. In *CBMS-NSF Regional Conference Series in Applied Mathematics*, volume 59, Philadelphia, 1990. SIAM.

[238] Y. Wang. Model selection. In J. E. Gentle, W. Härdle, and Y. Mori, editors, *Handbook of computational statistics – Concepts and methods*, chapter III.1, pages 438–466. Springer–Verlag Berlin Heidelberg, 2004.

[239] L. Wassermann. Bayesian model selection and model averaging. *Journal of Mathematical Psychology*, 44:92–107, 2000.

[240] S. Weisberg. *Applied linear regression.* Wiley series in probability and mathematical statistics. John Wiley & Sons, Inc., 1980.

[241] H. V. Westerhoff and D. Kell. What biotechnologists knew all along ... ? *Journal of theoretical Biology*, 182:411–420, 1996.

[242] D. Xie, A. Tropsha, and T. Schlick. An efficient projection protocol for chemical databases: Singular value decomposition combined with truncated-newton minimization. *Journal Chemical Inf. Compuational Science*, 40(167–177), 2000.

[243] P. Zhang. Inference after variable selection in linear regression models. *Biometrika*, 79:741–746, 1992.

[244] X. Zhou, L. Joseph, D. B. Wolfson, and P. Belisle. A Bayesian A-optimal and model robust design criterion. *Biometrics*, 59:1082–1088, December 2003.