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THEORY
4.3 DISTRIBUTIONS OF SUMS OF RANDOM VARIABLES4.4 MULTIRESPONSE NORMAL ERROR DISTRIBUTIONS; 4.5 STATISTICAL INFERENCE AND CRITICISM; PROBLEMS; REFERENCES and FURTHER READING; Chapter 5. Introduction to Bayesian Estimation; 5.1 THE THEOREM; 5.2 BAYESIAN ESTIMATION WITH INFORMATIVE PRIORS; 5.3 INTRODUCTION TO NONINFORMATIVE PRIORS; 5.4 JEFFREYS PRIOR FOR ONE-PARAMETER MODELS; 5.5 JEFFREYS PRIOR FOR MULTIPARAMETER MODELS; 5.6 SUMMARY; PROBLEMS; REFERENCES and FURTHER READING; Chapter 6. Process Modeling with Single-Response Data; 6.1 THE OBJECTIVE FUNCTION S()
6.2 WEIGHTING AND OBSERVATION FORMS6.3 PARAMETRIC SENSITIVITIES; NORMAL EQUATIONS; 6.4 CONSTRAINED MINIMIZATION OF S(); 6.4.1 The Quadratic Programming Algorithm GRQP; 6.4.2 The Line Search Algorithm GRSl; 6.4.3 Final Expansions Around ; 6.5 TESTING THE RESIDUALS; 6.6 INFERENCES FROM THE POSTERIOR DENSITY; 6.6.1 Inferences for the Parameters; 6.6.2 Inferences for Predicted Functions; 6.6.3 Discrimination of Rival Models by Posterior Probability; 6.7 SEQUENTIAL PLANNING OF EXPERIMENTS; 6.7.1 Planning for Parameter Estimation; 6.7.2 Planning for Auxiliary Function Estimation
6.7.3 Planning for Model Discrimination6.7.4 Combined Discrimination and Estimation; 6.7.5 Planning for Model Building; 6.8 EXAMPLES; 6.9 SUMMARY; 6.10 NOTATION; PROBLEMS; REFERENCES and FURTHER READING; Chapter 7. Process Modeling with Multiresponse Data; 7.1 PROBLEM TYPES; 7.2 OBJECTIVE FUNCTION; 7.2.1 Selection of Working Responses; 7.2.2 Derivatives of Eqs. (7.2-1) and (7.2-3); 7.2.3 Quadratic Expansions; Normal Equations; 7.3 CONSTRAINED MINIMIZATION OF s(); 7.3.1 Final Expansions Around ; 7.4 TESTING THE RESIDUALS; 7.5 POSTERIOR PROBABILITIES AND REGIONS 7.5.1 Inferences Regarding Parameters

Sommario/riassunto

Learn to apply modeling and parameter estimation tools and strategies to chemicalprocesses using your personal computer This book introduces readers to powerful parameter estimation and computational methods for modeling complex chemical reactions and reaction processes. It presents useful mathematical models, numerical methods for solving them, and statistical methods for testing and discriminating candidate models with experimental data. Topics covered include: Chemical reaction models Chemical reactor models Probability and statistics Bayesian estimation Process modeling with si