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Nota di contenuto	Nonlinear Systems and Optimization for the Chemical Engineer: Solving Numerical Problems; Contents; Preface; 1 Function Root-Finding; 1.1 Introduction; 1.2 Substitution Algorithms; 1.3 Bolzano's Algorithm; 1.4 Function Approximation; 1.4.1 Newton's Method; 1.4.2 The Secant Method; 1.4.3 Regula Falsi Method; 1.4.4 Muller's Method or Parabolic Interpolation; 1.4.5 Hyperbolic Interpolation Method; 1.4.6 Inverse Polynomial Interpolation Method; 1.4.7 Inverse Rational Interpolation Method; 1.5 Use of a Multiprocessor Machine with a Known Interval of Uncertainty 1.6 Search for an Interval of Uncertainty1.7 Stop Criteria; 1.8 Classes for Function Root-Finding; 1.9 Case Studies; 1.9.1 Calculation of the Volume of a Nonideal Gas; 1.9.2 Calculation of the Bubble Point of Vapor-Liquid Equilibrium; 1.9.3 Zero-Crossing Problem; 1.9.4 Stationary Condition in a Gravity-Flow Tank; 1.10 Tests for BzzFunctionRoot and BzzFunctionRootMP Classes; 1.11 Some Caveats; 2 One-Dimensional Optimization; 2.1 Introduction; 2.2 Measuring the Efficiency of the Search for the Minimum; 2.3 Comparison Methods; 2.4 Parabolic Interpolation; 2.5 Cubic Interpolation 2.6 Gradient-Based Methods2.7 Combination of Algorithms in a General Program; 2.8 Parallel Computations; 2.9 Search for the Interval of Uncertainty; 2.10 Stop Criteria; 2.11 Classes for One-Dimensional Minimization; 2.12 Case Studies; 2.12.1 Optimization of Unimodal Functions; 2.12.2 Optimization of a Batch Reactor; 2.12.3 Maximum Level in a Gravity-Flow Tank in Transient Conditions; 2.13 Tests; 3 Unconstrained Optimization; 3.1 Introduction; 3.1.1 Necessary and Sufficient Conditions; 3.1.2 Quadratic Functions; 3.1.3 Directions of Function Decrease 3.1.4 Comparison with the One-Dimensional Case3.1.5 Classification of Methods; 3.2 Heuristic Methods; 3.2.1 Modified Hooke-Jeeves Method; 3.2.2 The Rosenbrock Method; 3.2.3 The Nelder-Mead Simplex Method; 3.2.4 Robust Optnov Method Combined with the Simplex Method; 3.3 Gradient-Based Methods; 3.4 Conjugate Direction Methods; 3.5 Newton's Method; 3.6 Modified Newton Methods; 3.6.1 Singular or Nonpositive Definite Hessian Matrix; 3.6.2 Convergence Problems; 3.6.3 One-Dimensional Search; 3.6.4 Trust Region Methods; 3.6.5 Use of Alternative Methods; 3.7 Quasi-Newton Methods 3.8 Narrow Valley Effect3.9 Stop Criteria; 3.10 BzzMath Classes for Unconstrained Multidimensional Minimization; 3.11 Case Study; 3.11.1 Optimization of a Batch Reactor; 3.11.2 Optimal Adiabatic Bed Reactors for Sulfur Dioxide with Cold Shot Cooling; 3.11.3 Global Optimization; 3.12 Tests; 4 Large-Scale Unconstrained Optimization; 4.1 Introduction; 4.2 Collecting a Sparse Symmetric Matrix; 4.3 Ordering the Hessian Rows and Columns; 4.4 Quadratic Functions; 4.5 Hessian Evaluation; 4.6 Newton's Method; 4.7 Inexact Newton Methods; 4.8 Practical Preconditioners; 4.9 openMP Parallelization 4.10 Class for Large-Scale Unconstrained Minimization
Sommario/riassunto	This third in a suite of four practical guides is an engineer's companion to using numerical methods for the solution of complex mathematical problems. It explains the theory behind current numerical methods and shows in a step-by-step fashion how to use them.The volume focuses on optimization from experimental to large-scale processes, detailing the algorithms needed to solve real-life problems. It describes the methods, innovative techniques and strategies that are all implemented in a well-established, freeware mathematical toolbox called BzzMath, which is developed and maintained by th