Contents

I Introduction 1

1 Applications of Numerical Integration 5
- 1.1 Computational Statistics . . . 6
  - 1.1.1 Fundamentals . . . 6
  - 1.1.2 Computation of Stochastic Quantities . . . 6
  - 1.1.3 Bayesian Statistics . . . 8
- 1.2 Integral Transforms . . . 9
  - 1.2.1 Fundamentals . . . 9
  - 1.2.2 Application to Differential Equations . . . 10
  - 1.2.3 Finite Transforms and Fourier Series . . . 11
  - 1.2.4 Computational Aspects . . . 12
- 1.3 Finite Element Methods . . . 13
  - 1.3.1 Variational Equations . . . 13
  - 1.3.2 Galerkin Method . . . 15
  - 1.3.3 Fundamentals of Finite Element Methods . . . 16
- 1.4 Boundary Integral Methods . . . 19
  - 1.4.1 Boundary Integral Equations . . . 19
  - 1.4.2 Collocation Methods . . . 21

2 Fundamentals of Numerical Integration 25
- 2.1 Integration Problems . . . 25
- 2.2 Integration Methods . . . 26
- 2.3 Conditioning of Integration Problems . . . 30
- 2.4 Inherent Uncertainty of Numerical Integration . . . 33

II Mathematical Aspects 35

3 Integrals 37
- 3.1 Riemann Integrals . . . 37
  - 3.1.1 One Dimension . . . 37
  - 3.1.2 Multiple Dimensions . . . 38
- 3.2 Improper Integrals . . . 39
  - 3.2.1 One-Dimensional Improper Integrals . . . 39

3.2.2 Multi-Dimensional Improper Integrals 41
3.3 Special Types of Integrals 42
3.4 Integration Regions 44
3.5 Weight Functions 45
3.6 The Preprocessing of Integrals 47
3.6.1 Transformation of Integrals 47
3.6.2 Decomposition of Integration Regions 54
3.6.3 Iteration of Integrals 55

4 Univariate Integration Formulas **57**
4.1 Construction of Quadrature Formulas 57
4.1.1 Riemann Sums 57
4.1.2 Formula Construction by Approximation 60
4.1.3 Formula Construction by Acceleration 64
4.1.4 Linear Transformation of Quadrature Formulas 66
4.2 Simple Interpolatory Quadrature Formulas 67
4.2.1 Degree of Accuracy 68
4.2.2 Convergence 70
4.2.3 Closed Newton-Cotes Formulas 70
4.2.4 Open Newton-Cotes Formulas 73
4.2.5 Clenshaw-Curtis Formulas 74
4.2.6 Gauss Formulas 75
4.2.7 Radau und Lobatto Formulas 78
4.2.8 Gauss-Kronrod Formulas 78
4.3 Compound Formulas 79
4.3.1 Compound Trapezoidal Rule 82
4.3.2 IMT Formulas 84
4.4 Romberg Formulas 85
4.5 Nonlinear Extrapolation Methods 87

5 Multivariate Integration Formulas **91**
5.1 Construction Principles 92
5.1.1 Riemann Sums 92
5.1.2 Construction by Approximation 92
5.1.3 Construction by Transformation 93
5.1.4 Construction by Iteration 94
5.1.5 Construction by Decomposition 97
5.2 Polynomial Rules 99
5.2.1 Multivariate Polynomials 99
5.2.2 Construction of Interpolatory Formulas 103
5.2.3 Simple Interpolatory Formulas 113
5.2.4 Compound Formulas 117
5.3 Low-Discrepancy Formulas 118
5.3.1 Formula Construction by Equidistribution 118

5.3.2 One-Dimensional Low-Discrepancy Sequences 124
5.3.3 Multi-Dimensional Low-Discrepancy Sequences 128
5.4 Pseudorandom Methods 134
5.4.1 Basic Monte Carlo Techniques 134
5.4.2 Variance Reduction Schemes 137
5.4.3 Generation of Pseudorandom Numbers 140
5.4.4 Generation of Uniform Random Numbers 141
5.4.5 Generation of Non-Uniform Random Numbers 144
5.5 Lattice Rules 147
5.5.1 Formula Construction by Harmonic Analysis 147
5.5.2 Basic Definitions 149
5.5.3 Practical Representation of Lattice Rules 151
5.5.4 Error Analysis of Lattice Rules 152
5.5.5 Efficiency of Lattice Rules 159
5.6 Various Special Methods 161

III Algorithmic and Computational Aspects **163**

6 Integration Algorithms **165**
6.1 Error Estimation 166
6.1.1 Fundamental Uncertainty 166
6.1.2 Use of Two Integration Formulas with Different Accuracy 167
6.1.3 Use of Null Rules 169
6.1.4 Use of the Same Formula on Different Subdivisions 173
6.1.5 Use of Randomized Formulas 174
6.2 Sampling Strategy 176
6.2.1 Efficiency Assessment 177
6.2.2 Non-Adaptive Algorithms 179
6.2.3 Adaptive Algorithms 179
6.3 Reliability Enhancement 184
6.3.1 Noise Detection 184
6.3.2 Detection of Non-Integrable Functions 185
6.4 Efficiency Enhancement 187
6.4.1 Extrapolation in Non-Adaptive Algorithms 187
6.4.2 Extrapolation in Adaptive Algorithms 187
6.5 Integration of Multiple Integrands 190

7 Load Distribution **193**
7.1 Static Load Distribution 195
7.2 Dynamic Load Distribution 196
7.2.1 Dynamic Load Balancing Algorithms 197
7.2.2 Asynchronous Single Task Pool Methods 198
7.2.3 Synchronous Single Task Pool Methods 200

7.2.4 Multiple Task Pool Methods 201
7.2.5 Synchronous Multiple Task Pool Methods 205
7.2.6 Asynchronous Multiple Task Pool Methods 206
7.2.7 Hierarchical Methods 209

8 Potential Parallelism in Integration Algorithms 211
8.1 Integrand Level 211
8.2 Global Extrapolation Level 214
8.3 Subdivision Level 215
8.4 Subregion Level 218
8.5 Local Extrapolation Level 219
8.6 Integration Formula Level 219
8.7 Integrand Evaluation Level 221

9 Parallelization Schemes for Integration Algorithms 223
9.1 Constituent Parts of Parallel Tasks 226
9.2 Performance Characteristics of Parallel Tasks 227
9.2.1 Algorithmic Efficiency 227
9.2.2 Degree of Parallelism 228
9.2.3 Kind of Parallelism 228
9.2.4 Predictability of Execution Times 229
9.2.5 Locality of Reference 229

10 Practical Parallelization of Integration Algorithms 233
10.1 Computer Systems for Parallel Integration 233
10.1.1 Pipelined Processors 234
10.1.2 SIMD Computers 235
10.1.3 MIMD Systems 235
10.2 Vectorization of Integration Methods 236
10.2.1 Integrand Evaluation Level 236
10.2.2 Integration Formula Level 237
10.2.3 Integrand Level 237
10.2.4 Multiple Level Vectorization 237
10.3 Parallelization of Integration Methods 238
10.3.1 Integration Formula Level 238
10.3.2 Subregion Level 239
10.3.3 Subdivision Level 240
10.3.4 Subdivision and Subregion Level 246
10.3.5 Subdivision, Subregion, and Integration Formula Level 251
10.4 Vectorization and Parallelization of Extrapolation Methods 251
10.5 Vectorization and Parallelization of Abscissa Computations 252
10.6 Vectorization and Parallelization of Reduction Operations 254

11 Parallel Data Management 257
11.1 Data Structures for Global Subdivision Strategies 259
11.1.1 Heaps 259
11.1.2 Other Implementations of Priority Queues 263
11.2 Concurrent Access to Data Structures 269
11.2.1 Concurrent Access to Priority Queues 270
11.2.2 New Types of Data Structures 274

IV Software Aspects 277

12 Assessment of Numerical Integration Software 279
12.1 Assessment Criteria 279
12.1.1 Reliability 280
12.1.2 Performance 282
12.1.3 Portability 283
12.2 Techniques of Assessment 285
12.2.1 Test Batteries and Performance Profiles 286
12.2.2 Fundamental Approaches to Assessing Numerical Integration Software 290

13 Architecture Adaptive Integration Algorithms 293
13.1 Required Information 294
13.2 Practical Experience 300

Glossary of Notation 303

Bibliography 309

Authors 329

Index 334