

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/220693008>

# Numerical Methods for Special Functions

Book · January 2007

DOI: 10.1137/1.9780898717822 · Source: DBLP

---

CITATIONS

148

READS

2,843

3 authors:



Amparo Gil

Universidad de Cantabria

107 PUBLICATIONS 1,148 CITATIONS

[SEE PROFILE](#)



Javier Segura

Universidad de Cantabria

123 PUBLICATIONS 1,202 CITATIONS

[SEE PROFILE](#)



Nico Temme

Centrum Wiskunde & Informatica

268 PUBLICATIONS 2,885 CITATIONS

[SEE PROFILE](#)

Some of the authors of this publication are also working on these related projects:



Computation of Special Functions [View project](#)



Chromaffin cells [View project](#)

# **Numerical Methods for Special Functions**

**Amparo Gil**

Universidad de Cantabria  
Santander, Cantabria, Spain

**Javier Segura**

Universidad de Cantabria  
Santander, Cantabria, Spain

**Nico M. Temme**

Centrum voor Wiskunde en Informatica  
Amsterdam, The Netherlands

# Contents

Preface	xiii
<b>1 Introduction</b>	<b>1</b>
<b>I Basic Methods</b>	<b>13</b>
<b>2 Convergent and Divergent Series</b>	<b>15</b>
2.1 Introduction . . . . .	15
2.1.1 Power series: First steps . . . . .	15
2.1.2 Further practical aspects . . . . .	17
2.2 Differential equations and Frobenius series solutions . . . . .	18
2.2.1 Singular points . . . . .	19
2.2.2 The solution near a regular point . . . . .	20
2.2.3 Power series expansions around a regular singular point .	22
2.2.4 The Liouville transformation . . . . .	25
2.3 Hypergeometric series . . . . .	26
2.3.1 The Gauss hypergeometric function . . . . .	28
2.3.2 Other power series for the Gauss hypergeometric function	30
2.3.3 Removable singularities . . . . .	33
2.4 Asymptotic expansions . . . . .	34
2.4.1 Watson's lemma . . . . .	36
2.4.2 Estimating the remainders of asymptotic expansions . . .	38
2.4.3 Exponentially improved asymptotic expansions . . . . .	39
2.4.4 Alternatives of asymptotic expansions . . . . .	40
<b>3 Chebyshev Expansions</b>	<b>51</b>
3.1 Introduction . . . . .	51
3.2 Basic results on interpolation . . . . .	52
3.2.1 The Runge phenomenon and the Chebyshev nodes . . . .	54
3.3 Chebyshev polynomials: Basic properties . . . . .	56
3.3.1 Properties of the Chebyshev polynomials $T_n(x)$ . . . . .	56
3.3.2 Chebyshev polynomials of the second, third, and fourth kinds . . . . .	60

---

3.4	Chebyshev interpolation . . . . .	62
3.4.1	Computing the Chebyshev interpolation polynomial . . . . .	64
3.5	Expansions in terms of Chebyshev polynomials . . . . .	66
3.5.1	Convergence properties of Chebyshev expansions . . . . .	68
3.6	Computing the coefficients of a Chebyshev expansion . . . . .	69
3.6.1	Clebschaw's method for solutions of linear differential equations with polynomial coefficients . . . . .	70
3.7	Evaluation of a Chebyshev sum . . . . .	75
3.7.1	Clebschaw's method for the evaluation of a Chebyshev sum	75
3.8	Economization of power series . . . . .	80
3.9	Example: Computation of Airy functions of real variable . . . . .	80
3.10	Chebyshev expansions with coefficients in terms of special functions .	83
<b>4</b>	<b>Linear Recurrence Relations and Associated Continued Fractions</b>	<b>87</b>
4.1	Introduction . . . . .	87
4.2	Condition of three-term recurrence relations . . . . .	88
4.2.1	Minimal solutions . . . . .	89
4.3	Perron's theorem . . . . .	92
4.3.1	Scaled recurrence relations . . . . .	94
4.4	Minimal solutions of TTRRs and continued fractions . . . . .	95
4.5	Some notable recurrence relations . . . . .	96
4.5.1	The confluent hypergeometric family . . . . .	96
4.5.2	The Gauss hypergeometric family . . . . .	102
4.6	Computing the minimal solution of a TTRR . . . . .	105
4.6.1	Miller's algorithm when a function value is known . . . . .	105
4.6.2	Miller's algorithm with a normalizing sum . . . . .	107
4.6.3	"Anti-Miller" algorithm . . . . .	110
4.7	Inhomogeneous linear difference equations . . . . .	112
4.7.1	Inhomogeneous first order difference equations. Examples . . . . .	112
4.7.2	Inhomogeneous second order difference equations . . . . .	115
4.7.3	Olver's method . . . . .	116
4.8	Anomalous behavior of some second order homogeneous and first order inhomogeneous recurrences . . . . .	118
4.8.1	A canonical example: Modified Bessel function . . . . .	118
4.8.2	Other examples: Hypergeometric recursions . . . . .	120
4.8.3	A first order inhomogeneous equation . . . . .	121
4.8.4	A warning . . . . .	122
<b>5</b>	<b>Quadrature Methods</b>	<b>123</b>
5.1	Introduction . . . . .	123
5.2	Newton–Cotes quadrature: The trapezoidal and Simpson's rule . . . . .	124
5.2.1	The compound trapezoidal rule . . . . .	126
5.2.2	The recurrent trapezoidal rule . . . . .	129
5.2.3	Euler's summation formula and the trapezoidal rule . . . . .	130
5.3	Gauss quadrature . . . . .	132

---

5.3.1	Basics of the theory of orthogonal polynomials and Gauss quadrature . . . . .	133
5.3.2	The Golub–Welsch algorithm . . . . .	141
5.3.3	Example: The Airy function in the complex plane . . . . .	145
5.3.4	Further practical aspects of Gauss quadrature . . . . .	146
5.4	The trapezoidal rule on $\mathbb{R}$ . . . . .	147
5.4.1	Contour integral formulas for the truncation errors . . . . .	148
5.4.2	Transforming the variable of integration . . . . .	153
5.5	Contour integrals and the saddle point method . . . . .	157
5.5.1	The saddle point method . . . . .	158
5.5.2	Other integration contours . . . . .	163
5.5.3	Integrating along the saddle point contours and examples . . . . .	165
<b>II</b>	<b>Further Tools and Methods</b>	<b>171</b>
<b>6</b>	<b>Numerical Aspects of Continued Fractions</b>	<b>173</b>
6.1	Introduction . . . . .	173
6.2	Definitions and notation . . . . .	173
6.3	Equivalence transformations and contractions . . . . .	175
6.4	Special forms of continued fractions . . . . .	178
6.4.1	Stieltjes fractions . . . . .	178
6.4.2	Jacobi fractions . . . . .	179
6.4.3	Relation with Padé approximants . . . . .	179
6.5	Convergence of continued fractions . . . . .	179
6.6	Numerical evaluation of continued fractions . . . . .	181
6.6.1	Steed's algorithm . . . . .	181
6.6.2	The modified Lentz algorithm . . . . .	183
6.7	Special functions and continued fractions . . . . .	185
6.7.1	Incomplete gamma function . . . . .	186
6.7.2	Gauss hypergeometric functions . . . . .	187
<b>7</b>	<b>Computation of the Zeros of Special Functions</b>	<b>191</b>
7.1	Introduction . . . . .	191
7.2	Some classical methods . . . . .	193
7.2.1	The bisection method . . . . .	193
7.2.2	The fixed point method and the Newton–Raphson method . . . . .	193
7.2.3	Complex zeros . . . . .	197
7.3	Local strategies: Asymptotic and other approximations . . . . .	197
7.3.1	Asymptotic approximations for large zeros . . . . .	199
7.3.2	Other approximations . . . . .	202
7.4	Global strategies I: Matrix methods . . . . .	205
7.4.1	The eigenvalue problem for orthogonal polynomials . . . . .	206
7.4.2	The eigenvalue problem for minimal solutions of TTRRs . . . . .	207
7.5	Global strategies II: Global fixed point methods . . . . .	213
7.5.1	Zeros of Bessel functions . . . . .	213

---

7.5.2	The general case . . . . .	219
7.6	Asymptotic methods: Further examples . . . . .	224
7.6.1	Airy functions . . . . .	224
7.6.2	Scorer functions . . . . .	227
7.6.3	The error functions . . . . .	229
7.6.4	The parabolic cylinder function . . . . .	233
7.6.5	Bessel functions . . . . .	233
7.6.6	Orthogonal polynomials . . . . .	234
<b>8</b>	<b>Uniform Asymptotic Expansions</b>	<b>237</b>
8.1	Asymptotic expansions for the incomplete gamma functions . . . . .	237
8.2	Uniform asymptotic expansions . . . . .	239
8.3	Uniform asymptotic expansions for the incomplete gamma functions .	240
8.3.1	The uniform expansion . . . . .	242
8.3.2	Expansions for the coefficients . . . . .	244
8.3.3	Numerical algorithm for small values of $\eta$ . . . . .	245
8.3.4	A simpler uniform expansion . . . . .	247
8.4	Airy-type expansions for Bessel functions . . . . .	249
8.4.1	The Airy-type asymptotic expansions . . . . .	250
8.4.2	Representations of $a_s(\zeta), b_s(\zeta), c_s(\zeta), d_s(\zeta)$ . . . . .	253
8.4.3	Properties of the functions $A_\nu, B_\nu, C_\nu, D_\nu$ . . . . .	254
8.4.4	Expansions for $a_s(\zeta), b_s(\zeta), c_s(\zeta), d_s(\zeta)$ . . . . .	256
8.4.5	Evaluation of the functions $A_\nu(\zeta), B_\nu(\zeta)$ by iteration .	258
8.5	Airy-type asymptotic expansions obtained from integrals . . . . .	263
8.5.1	Airy-type asymptotic expansions . . . . .	264
8.5.2	How to compute the coefficients $\alpha_n, \beta_n$ . . . . .	267
8.5.3	Application to parabolic cylinder functions . . . . .	270
<b>9</b>	<b>Other Methods</b>	<b>275</b>
9.1	Introduction . . . . .	275
9.2	Padé approximations . . . . .	276
9.2.1	Padé approximants and continued fractions . . . . .	278
9.2.2	How to compute the Padé approximants . . . . .	278
9.2.3	Padé approximants to the exponential function . . . . .	280
9.2.4	Analytic forms of Padé approximations . . . . .	283
9.3	Sequence transformations . . . . .	286
9.3.1	The principles of sequence transformations . . . . .	286
9.3.2	Examples of sequence transformations . . . . .	287
9.3.3	The transformation of power series . . . . .	288
9.3.4	Numerical examples . . . . .	288
9.4	Best rational approximations . . . . .	290
9.5	Numerical solution of ordinary differential equations: Taylor expansion method . . . . .	291
9.5.1	Taylor-series method: Initial value problems . . . . .	292
9.5.2	Taylor-series method: Boundary value problem . . . . .	293
9.6	Other quadrature methods . . . . .	294

---

9.6.1	Romberg quadrature . . . . .	294
9.6.2	Fejér and Clenshaw–Curtis quadratures . . . . .	296
9.6.3	Other Gaussian quadratures . . . . .	298
9.6.4	Oscillatory integrals . . . . .	301
<b>III</b>	<b>Related Topics and Examples</b>	<b>307</b>
<b>10</b>	<b>Inversion of Cumulative Distribution Functions</b>	<b>309</b>
10.1	Introduction . . . . .	309
10.2	Asymptotic inversion of the complementary error function . . . . .	309
10.3	Asymptotic inversion of incomplete gamma functions . . . . .	312
10.3.1	The asymptotic inversion method . . . . .	312
10.3.2	Determination of the coefficients $\varepsilon_i$ . . . . .	314
10.3.3	Expansions of the coefficients $\varepsilon_i$ . . . . .	316
10.3.4	Numerical examples . . . . .	316
10.4	Generalizations . . . . .	317
10.5	Asymptotic inversion of the incomplete beta function . . . . .	318
10.5.1	The nearly symmetric case . . . . .	319
10.5.2	The general error function case . . . . .	322
10.5.3	The incomplete gamma function case . . . . .	324
10.5.4	Numerical aspects . . . . .	326
10.6	High order Newton-like methods . . . . .	327
<b>11</b>	<b>Further Examples</b>	<b>331</b>
11.1	Introduction . . . . .	331
11.2	The Euler summation formula . . . . .	331
11.3	Approximations of Stirling numbers . . . . .	336
11.3.1	Definitions . . . . .	337
11.3.2	Asymptotics for Stirling numbers of the second kind . . . . .	338
11.3.3	Stirling numbers of the first kind . . . . .	343
11.4	Symmetric elliptic integrals . . . . .	344
11.4.1	The standard forms in terms of symmetric integrals . . . . .	345
11.4.2	An algorithm . . . . .	346
11.4.3	Other elliptic integrals . . . . .	347
11.5	Numerical inversion of Laplace transforms . . . . .	347
11.5.1	Complex Gauss quadrature . . . . .	348
11.5.2	Deforming the contour . . . . .	349
11.5.3	Using Padé approximations . . . . .	352
<b>IV</b>	<b>Software</b>	<b>353</b>
<b>12</b>	<b>Associated Algorithms</b>	<b>355</b>
12.1	Introduction . . . . .	355
12.1.1	Errors and stability: Basic terminology . . . . .	356

12.1.2	Design and testing of software for computing functions: General philosophy . . . . .	357
12.1.3	Scaling the functions . . . . .	358
12.2	Airy and Scorer functions of complex arguments . . . . .	359
12.2.1	Purpose . . . . .	359
12.2.2	Algorithms . . . . .	359
12.3	Associated Legendre functions of integer and half-integer degrees . . . . .	363
12.3.1	Purpose . . . . .	363
12.3.2	Algorithms . . . . .	364
12.4	Bessel functions . . . . .	369
12.4.1	Modified Bessel functions of integer and half-integer orders . . . . .	370
12.4.2	Modified Bessel functions of purely imaginary orders . . . . .	372
12.5	Parabolic cylinder functions . . . . .	377
12.5.1	Purpose . . . . .	377
12.5.2	Algorithm . . . . .	378
12.6	Zeros of Bessel functions . . . . .	385
12.6.1	Purpose . . . . .	385
12.6.2	Algorithm . . . . .	385
<b>List of Algorithms</b>		<b>387</b>
<b>Bibliography</b>		<b>389</b>
<b>Index</b>		<b>405</b>