

Table of Contents

1	Introduction	1
1.1	Advice for Quick Readers	1
1.2	Structure of the Book	2
1.3	Typography	3
1.4	Algorithmic Notation	3
1.5	Implementation	4
1.6	Computational Environment	6
1.7	Why Numerical Result Verification?	6
1.7.1	A Brief History of Computing	6
1.7.2	Arithmetic on Computers	7
1.7.3	Extensions of Ordinary Floating-Point Arithmetic	9
1.7.4	Scientific Computation with Automatic Result Verification	11
1.7.5	Program Verification versus Numerical Verification	14
I	Preliminaries	15
2	The Features of PASCAL-XSC	17
2.1	Predefined Data Types, Operators, and Functions	18
2.2	The Universal Operator Concept	21
2.3	Overloading of Procedures, Functions, and Operators	22
2.4	Module Concept	23
2.5	Dynamic Arrays and Subarrays	24
2.6	Data Conversion	26
2.7	Accurate Expressions (#-Expressions)	27
2.8	The String Concept	28
2.9	Predefined Arithmetic Modules	28
2.10	Why PASCAL-XSC?	30
3	Mathematical Preliminaries	31
3.1	Real Interval Arithmetic	31
3.2	Complex Interval Arithmetic	38
3.3	Extended Interval Arithmetic	40
3.4	Interval Vectors and Matrices	42
3.5	Floating-Point Arithmetic	43
3.6	Floating-Point Interval Arithmetic	45
3.7	The Problem of Data Conversion	47

3.8 Principles of Numerical Verification	51
II One-Dimensional Problems	55
4 Evaluation of Polynomials	57
4.1 Theoretical Background	57
4.1.1 Description of the Problem	57
4.1.2 Iterative Solution	58
4.2 Algorithmic Description	59
4.3 Implementation and Examples	61
4.3.1 PASCAL-XSC Program Code	61
4.3.1.1 Module rpoly	61
4.3.1.2 Module rpeval	62
4.3.2 Examples	64
4.3.3 Restrictions and Hints	67
4.4 Exercises	67
4.5 References and Further Reading	68
5 Automatic Differentiation	69
5.1 Theoretical Background	69
5.2 Algorithmic Description	71
5.3 Implementation and Examples	73
5.3.1 PASCAL-XSC Program Code	73
5.3.1.1 Module ddf_ari	73
5.3.2 Examples	83
5.3.3 Restrictions and Hints	86
5.4 Exercises	86
5.5 References and Further Reading	86
6 Nonlinear Equations in One Variable	87
6.1 Theoretical Background	87
6.2 Algorithmic Description	89
6.3 Implementation and Examples	92
6.3.1 PASCAL-XSC Program Code	92
6.3.1.1 Module xi_ari	93
6.3.1.2 Module nlfzero	96
6.3.2 Example	101
6.3.3 Restrictions and Hints	103
6.4 Exercises	103
6.5 References and Further Reading	104
7 Global Optimization	105
7.1 Theoretical Background	105
7.1.1 Midpoint Test	106
7.1.2 Monotonicity Test	107
7.1.3 Concavity Test	108

7.1.4	Interval Newton Step	108
7.1.5	Verification	109
7.2	Algorithmic Description	109
7.3	Implementation and Examples	115
7.3.1	PASCAL-XSC Program Code	115
7.3.1.1	Module lst1_ari	115
7.3.1.2	Module gop1	119
7.3.2	Examples	125
7.3.3	Restrictions and Hints	128
7.4	Exercises	128
7.5	References and Further Reading	130
8	Evaluation of Arithmetic Expressions	131
8.1	Theoretical Background	131
8.1.1	A Nonlinear Approach	131
8.2	Algorithmic Description	134
8.3	Implementation and Examples	137
8.3.1	PASCAL-XSC Program Code	137
8.3.1.1	Module expreval	138
8.3.2	Examples	146
8.3.3	Restrictions, Hints, and Improvements	150
8.4	Exercises	150
8.5	References and Further Reading	151
9	Zeros of Complex Polynomials	152
9.1	Theoretical Background	152
9.1.1	Description of the Problem	152
9.1.2	Iterative Approach	153
9.2	Algorithmic Description	156
9.3	Implementation and Examples	161
9.3.1	PASCAL-XSC Program Code	161
9.3.1.1	Module cpoly	161
9.3.1.2	Module cipoly	162
9.3.1.3	Module cpzero	164
9.3.2	Example	169
9.3.3	Restrictions and Hints	170
9.4	Exercises	171
9.5	References and Further Reading	171
III	Multi-Dimensional Problems	173
10	Linear Systems of Equations	175
10.1	Theoretical Background	175
10.1.1	A Newton-like Method	175
10.1.2	The Residual Iteration Scheme	176
10.1.3	How to Compute the Approximate Inverse	176

10.2 Algorithmic Description	177
10.3 Implementation and Examples	181
10.3.1 PASCAL-XSC Program Code	181
10.3.1.1 Module matinv	181
10.3.1.2 Module linsys	185
10.3.2 Example	189
10.3.3 Restrictions and Improvements	191
10.4 Exercises	192
10.5 References and Further Reading	193
11 Linear Optimization	195
11.1 Theoretical Background	195
11.1.1 Description of the Problem	195
11.1.2 Verification	196
11.2 Algorithmic Description	198
11.3 Implementation and Examples	204
11.3.1 PASCAL-XSC Program Code	204
11.3.1.1 Module lop_ari	204
11.3.1.2 Module rev_simp	208
11.3.1.3 Module lop	211
11.3.2 Examples	218
11.3.3 Restrictions and Hints	223
11.4 Exercises	223
11.5 References and Further Reading	224
12 Automatic Differentiation for Gradients, Jacobians, and Hessians	225
12.1 Theoretical Background	225
12.2 Algorithmic Description	228
12.3 Implementation and Examples	230
12.3.1 PASCAL-XSC Program Code	230
12.3.1.1 Module hess_ari	230
12.3.1.2 Module grad_ari	245
12.3.2 Examples	256
12.3.3 Restrictions and Hints	262
12.4 Exercises	263
12.5 References and Further Reading	263
13 Nonlinear Systems of Equations	264
13.1 Theoretical Background	264
13.1.1 Gauss-Seidel Iteration	265
13.2 Algorithmic Description	267
13.3 Implementation and Examples	271
13.3.1 PASCAL-XSC Program Code	271
13.3.1.1 Module nlss	272
13.3.2 Example	278
13.3.3 Restrictions, Hints, and Improvements	280

13.4 Exercises	281
13.5 References and Further Reading	281
14 Global Optimization	282
14.1 Theoretical Background	282
14.1.1 Midpoint Test	283
14.1.2 Monotonicity Test	283
14.1.3 Concavity Test	284
14.1.4 Interval Newton Step	284
14.1.5 Verification	285
14.2 Algorithmic Description	286
14.3 Implementation and Examples	293
14.3.1 PASCAL-XSC Program Code	293
14.3.1.1 Module lst_ari	293
14.3.1.2 Module gop	297
14.3.2 Examples	306
14.3.3 Restrictions and Hints	310
14.4 Exercises	310
14.5 References and Further Reading	311
A Utility Modules	313
A.1 Module b_util	313
A.2 Module r_util	313
A.3 Module i_util	314
A.4 Module mvi_util	318
Bibliography	319
Index of Special Symbols	325
Index	327