

General Index to Volumes 1 and 2

In this index, page numbers 1 through 934 refer to Volume 1, *Numerical Recipes in Fortran 77*, while page numbers 935 through 1446 refer to Volume 2, *Numerical Recipes in Fortran 90*. Front matter in Volume 1 is indicated by page numbers in the range 1/i through 1/xxxii, while front matter in Volume 2 is indicated 2/i through 2/xx.

- A**bstract data types 2/xiii, 1030
Accelerated convergence of series 160ff.,
 1070
Accuracy 19f.
 achievable in minimization 392, 397, 404
 achievable in root finding 346f.
 contrasted with fidelity 832, 840
 CPU different from memory 181
 vs. stability 704, 729, 830, 844
Accuracy parameters 1362f.
Acknowledgments 1/xvi, 2/ix
Ada 2/x
Adams-Basford-Moulton method 741
Adams' stopping criterion 366
Adaptive integration 123, 135, 703, 708ff.,
 720, 726, 731f., 737, 742ff., 788, 1298ff.,
 1303, 1308f.
 Monte Carlo 306ff., 1161ff.
Addition, multiple precision 907, 1353
Addition theorem, elliptic integrals 255
ADI (alternating direction implicit) method
 847, 861f., 906
Adjoint operator 867
Adobe Illustrator 1/xvi, 2/xx
Advective equation 826
AGM (arithmetic geometric mean) 906
Airy function 204, 234, 243f.
 routine for 244f., 1121
Aitken's delta squared process 160
Aitken's interpolation algorithm 102
Algol 2/x, 2/xiv
Algorithms, non-numerical 881ff., 1343ff.
Aliasing 495, 569
 see also Fourier transform
all() intrinsic function 945, 948
All-poles model 566
 see also Maximum entropy method (MEM)
All-zeros model 566
 see also Periodogram
Allocatable array 938, 941, 952ff., 1197,
 1212, 1266, 1293, 1306, 1336
allocate statement 938f., 941, 953f., 1197,
 1266, 1293, 1306, 1336
allocated() intrinsic function 938, 952ff.,
 1197, 1266, 1293
Allocation status 938, 952ff., 961, 1197,
 1266, 1293
Alpha AXP 2/xix
Alternating-direction implicit method (ADI)
 847, 861f., 906
Alternating series 160f., 1070
Alternative extended Simpson's rule 128
American National Standards Institute (ANSI)
 2/x, 2/xiii
Amoeba 403
 see also Simplex, method of Nelder and
 Mead
Amplification factor 828, 830, 832, 840, 845f.
Amplitude error 831
Analog-to-digital converter 812, 886
Analyticity 195
Analyze/factorize/operate package 64, 824
Anderson-Darling statistic 621
Andrew's sine 697
Annealing, method of simulated 387f., 436ff.,
 1219ff.
 assessment 447
 for continuous variables 437, 443ff., 1222
 schedule 438
 thermodynamic analogy 437
 traveling salesman problem 438ff., 1219ff.
ANSI (American National Standards Institute)
 2/x, 2/xiii
Antonov-Saleev variant of Sobol' sequence
 300, 1160
any() intrinsic function 945, 948
APL (computer language) 2/xi
Apple 1/xxiii
 Macintosh 2/xix, 4, 886
Approximate inverse of matrix 49
Approximation of functions 99, 1043
 by Chebyshev polynomials 185f., 513,
 1076ff.
 Padé approximant 194ff., 1080f.
 by rational functions 197ff., 1081f.
 by wavelets 594f., 782
 see also Fitting
Argument
 keyword 2/xiv, 947f., 1341
 optional 2/xiv, 947f., 1092, 1228, 1230,
 1256, 1272, 1275, 1340
Argument checking 994f., 1086, 1090, 1092,
 1370f.

- Arithmetic
 arbitrary precision 881, 906ff., 1352ff.
 floating point 881, 1343
 IEEE standard 276, 882, 1343
 rounding 882, 1343
- Arithmetic coding 881, 902ff., 1349ff.
- Arithmetic-geometric mean (AGM) method 906
- Arithmetic-if statement 2/xi
- Arithmetic progression 971f., 996, 1072, 1127, 1365, 1371f.
- Array 953ff.
 allocatable 938, 941, 952ff., 1197, 1212, 1266, 1293, 1306, 1336
 allocated with pointer 941
 allocation 953
 array manipulation functions 950
 array sections 939, 941, 943ff.
 of arrays 2/xii, 956, 1336
 associated pointer 953f.
 assumed-shape 942
 automatic 938, 954, 1197, 1212, 1336
 centered subarray of 113
 conformable to a scalar 942f., 965, 1094
 constructor 2/xii, 968, 971, 1022, 1052, 1055, 1127
 copying 991, 1034, 1327f., 1365f.
 cumulative product 997f., 1072, 1086, 1375
 cumulative sum 997, 1280f., 1365, 1375
 deallocation 938, 953f., 1197, 1266, 1293
 disassociated pointer 953
 extents 938, 949
 in Fortran 90 941
 increasing storage for 955, 1070, 1302
 index loss 967f.
 index table 1173ff.
 indices 942
 inquiry functions 948ff.
 intrinsic procedures 2/xiii, 948ff.
 of length 0 944
 of length 1 949
 location of first “true” 993, 1041, 1369
 location of maximum value 993, 1015, 1017, 1365, 1369
 location of minimum value 993, 1369f.
 manipulation functions 950, 1247
 masked swapping of elements in two arrays 1368
 operations on 942, 949, 964ff., 969, 1026, 1040, 1050, 1200, 1326
 outer product 949, 1076
 parallel features 941ff., 964ff., 985
 passing variable number of arguments to function 1022
 of pointers forbidden 956, 1337
 rank 938, 949
 reallocation 955, 992, 1070f., 1365, 1368f.
 reduction functions 948ff.
 shape 938, 944, 949
 size 938
 skew sections 945, 985
 stride 944
 subscript bounds 942
 subscript triplet 944
- swapping elements of two arrays 991, 1015, 1365ff.
- target 938
- three-dimensional, in Fortran 90 1248
- transformational functions 948ff.
- unary and binary functions 949
- undefined status 952ff., 961, 1266, 1293
- zero-length 944
- Array section 2/xiii, 943ff., 960
 matches by shape 944
 pointer alias 939, 944f., 1286, 1333
 skew 2/xii, 945, 960, 985, 1284
 vs. eoshift 1078
- array_copy() utility function 988, 991, 1034, 1153, 1278, 1328
- arth() utility function 972, 974, 988, 996, 1072, 1086, 1127
- replaces do-list 968
- Artificial viscosity 831, 837
- Ascending transformation, elliptic integrals 256
- ASCII character set 6, 888, 896, 902
- Assembly language 269
- assert() utility function 988, 994, 1086, 1090, 1249
- assert_eq() utility function 988, 995, 1022
- associated() intrinsic function 952f.
- Associated Legendre polynomials 246ff., 764, 1122f., 1319
- recurrence relation for 247
 relation to Legendre polynomials 246
- Association, measures of 604, 622ff., 1275
- Assumed-shape array 942
- Asymptotic series 161
 exponential integral 218
- Attenuation factors 583, 1261
- Autocorrelation 492
 in linear prediction 558
 use of FFT 538f., 1254
 Wiener-Khinchin theorem 492, 566f.
- AUTODIN-II polynomial 890
- Automatic array 938, 954, 1197, 1212, 1336
 specifying size of 938, 954
- Automatic deallocation 2/xv, 961
- Autonomous differential equations 729f.
- Autoregressive model (AR) *see* Maximum entropy method (MEM)
- Average deviation of distribution 605, 1269
- Averaging kernel, in Backus-Gilbert method 807
- B**acksubstitution 33ff., 39, 42, 92, 1017
 in band diagonal matrix 46, 1021
 in Cholesky decomposition 90, 1039
 complex equations 41
 direct for computing $A^{-1} \cdot \mathbf{B}$ 40
 with QR decomposition 93, 1040
 relaxation solution of boundary value problems 755, 1316
 in singular value decomposition 56, 1022f.
- Backtracking 419
- in quasi-Newton methods 376f., 1195
- Backus-Gilbert method 806ff.
- Backus, John 2/x
- Backward deflation 363

- Bader-Deuflhard method 730, 735, 1310f.
 Bairstow's method 364, 370, 1193
 Balancing 476f., 1230f.
 Band diagonal matrix 42ff., 1019
 backsubstitution 46, 1021
 LU decomposition 45, 1020
 multiply by vector 44, 1019
 storage 44, 1019
 Band-pass filter 551, 554f.
 wavelets 584, 592f.
 Bandwidth limited function 495
 Bank accounts, checksum for 894
 Bar codes, checksum for 894
 Bartlett window 547, 1254ff.
 Base case, of recursive procedure 958
 Base of representation 19, 882, 1343
 BASIC, Numerical Recipes in 1, 2/x, 2/xviii
 Basis functions in general linear least squares 665
 Bayes' Theorem 810
 Bayesian
 approach to inverse problems 799, 810f., 816f.
 contrasted with frequentist 810
 vs. historic maximum entropy method 816f.
 views on straight line fitting 664
 Bays' shuffle 270
 Bernoulli number 132
 Bessel functions 223ff., 234ff., 936, 1101ff.
 asymptotic form 223f., 229f.
 complex 204
 continued fraction 234, 239
 double precision 223
 fractional order 223, 234ff., 1115ff.
 Miller's algorithm 175, 228, 1106
 modified 229ff.
 modified, fractional order 239ff.
 modified, normalization formula 232, 240
 modified, routines for 230ff., 1109ff.
 normalization formula 175
 parallel computation of 1107ff.
 recurrence relation 172, 224, 232, 234
 reflection formulas 236
 reflection formulas, modified functions 241
 routines for 225ff., 236ff., 1101ff.
 routines for modified functions 241ff., 1118
 series for 160, 223
 series for K_ν 241
 series for Y_ν 235
 spherical 234, 245, 1121f.
 turning point 234
 Wronskian 234, 239
 Best-fit parameters 650, 656, 660, 698, 1285ff.
 see also Fitting
 Beta function 206ff., 1089
 incomplete *see* Incomplete beta function
 BFGS algorithm *see* Broyden-Fletcher-Goldfarb-Shanno algorithm
 Bias, of exponent 19
 Bias, removal in linear prediction 563
 Biconjugacy 77
 Biconjugate gradient method
 elliptic partial differential equations 824
 preconditioning 78f., 824, 1037
 for sparse system 77, 599, 1034ff.
 Bicubic interpolation 118f., 1049f.
 Bicubic spline 120f., 1050f.
 Big-endian 293
 Bilinear interpolation 117
 Binary constant, initialization 959
 Binomial coefficients 206ff., 1087f.
 recurrences for 209
 Binomial probability function 208
 cumulative 222f.
 deviates from 281, 285f., 1155
 Binormal distribution 631, 690
 Biorthogonality 77
 Bisection 111, 359, 1045f.
 compared to minimum bracketing 390ff.
 minimum finding with derivatives 399
 root finding 343, 346f., 352f., 390, 469, 1184f.
 BISYNCH 890
 Bit 18
 manipulation functions *see* Bitwise logical functions
 reversal in fast Fourier transform (FFT) 499f., 525
 bit_size() intrinsic function 951
 Bitwise logical functions 2/xiii, 17, 287, 890f., 951
 Block-by-block method 788
 Block of statements 7
 Bode's rule 126
 Boltzmann probability distribution 437
 Boltzmann's constant 437
 Bootstrap method 686f.
 Bordering method for Toeplitz matrix 85f.
 Borwein and Borwein method for π 906, 1357
 Boundary 155f., 425f., 745
 Boundary conditions
 for differential equations 701f.
 initial value problems 702
 in multigrid method 868f.
 partial differential equations 508, 819ff., 848ff.
 for spheroidal harmonics 764
 two-point boundary value problems 702, 745ff., 1314ff.
 Boundary value problems *see* Differential equations; Elliptic partial differential equations; Two-point boundary value problems
 Box-Muller algorithm for normal deviate 279f., 1152
 Bracketing
 of function minimum 343, 390ff., 402, 1201f.
 of roots 341, 343ff., 353f., 362, 364, 369, 390, 1183f.
 Branch cut, for hypergeometric function 203
 Branching 9
 Break iteration 14
 Brenner, N.M. 500, 517

- Brent's method
 minimization 389, 395ff., 660f., 1204ff.,
 1286
 minimization, using derivative 389, 399,
 1205
 root finding 341, 349, 660f., 1188f., 1286
- Broadcast (parallel capability) 965ff.
- Broyden-Fletcher-Goldfarb-Shanno algorithm
 390, 418ff., 1215
- Broyden's method 373, 382f., 386, 1199f.
 singular Jacobian 386
- btest() intrinsic function 951
- Bubble sort 321, 1168
- Bugs 4
 in compilers 1/xvii
 how to report 1/iv, 2/iv
- Bulirsch-Stoer
 algorithm for rational function interpolation
 105f., 1043
 method (differential equations) 202, 263,
 702f., 706, 716, 718ff., 726, 740, 1138,
 1303ff.
 method (differential equations), stepsize
 control 719, 726
 for second order equations 726, 1307
- Burg's LP algorithm 561, 1256
- Byte 18
- C** (programming language) 13, 2/viii
 and case construct 1010
 Numerical Recipes in 1, 2/x, 2/xvii
- C++ 1/xiv, 2/viii, 2/xvi, 7f.
 class templates 1083, 1106
- Calendar algorithms 1f., 13ff., 1010ff.
- Calibration 653
- Capital letters in programs 3, 937
- Cards, sorting a hand of 321
- Carlson's elliptic integrals 255f., 1128ff.
- case construct 2/xiv, 1010
 trapping errors 1036
- Cash-Karp parameters 710, 1299f.
- Cauchy probability distribution *see* Lorentzian
 probability distribution
- Cauchy problem for partial differential equa-
 tions 818f.
- Cayley's representation of $\exp(-iHt)$ 844
- CCITT (Comité Consultatif International Télé-
 graphique et Téléphonique) 889f., 901
- CCITT polynomial 889f.
- ceiling() intrinsic function 947
- Center of mass 295ff.
- Central limit theorem 652f.
- Central tendency, measures of 604ff., 1269
- Change of variable
 in integration 137ff., 788, 1056ff.
 in Monte Carlo integration 298
 in probability distribution 279
- Character functions 952
- Character variables, in Fortran 90 1183
- Characteristic polynomial
 digital filter 554
 eigensystems 449, 469
 linear prediction 559
 matrix with a specified 368, 1193
 of recurrence relation 175
- Characteristics of partial differential equations
 818
- Chebyshev acceleration in successive over-
 relaxation (SOR) 859f., 1332
- Chebyshev approximation 84, 124, 183, 184ff.,
 1076ff.
- Clenshaw-Curtis quadrature 190
- Clenshaw's recurrence formula 187, 1076
 coefficients for 185f., 1076
 contrasted with Padé approximation 195
 derivative of approximated function 183,
 189, 1077f.
- economization of series 192f., 195, 1080
 for error function 214, 1095
- even function 188
- and fast cosine transform 513
- gamma functions 236, 1118
- integral of approximated function 189,
 1078
- odd function 188
- polynomial fits derived from 191, 1078
- rational function 197ff., 1081f.
- Remes exchange algorithm for filter 553
- Chebyshev polynomials 184ff., 1076ff.
 continuous orthonormality 184
 discrete orthonormality 185
 explicit formulas for 184
 formula for x^k in terms of 193, 1080
- Check digit 894, 1345f.
- Checksum 881, 888
 cyclic redundancy (CRC) 888ff., 1344f.
- Cherry, sundae without a 809
- Chi-by-eye 651
- Chi-square fitting *see* Fitting; Least squares
 fitting
- Chi-square probability function 209ff., 215,
 615, 654, 798, 1272
 as boundary of confidence region 688f.
 related to incomplete gamma function 215
- Chi-square test 614f.
 for binned data 614f., 1272
 chi-by-eye 651
 and confidence limit estimation 688f.
 for contingency table 623ff., 1275
 degrees of freedom 615f.
 for inverse problems 797
 least squares fitting 653ff., 1285
 nonlinear models 675ff., 1292
 rule of thumb 655
 for straight line fitting 655ff., 1285
 for straight line fitting, errors in both coor-
 dinates 660, 1286ff.
 for two binned data sets 616, 1272
 unequal size samples 617
- Chip rate 290
- Chirp signal 556
- Cholesky decomposition 89f., 423, 455, 1038
 backsubstitution 90, 1039
 operation count 90
 pivoting 90
 solution of normal equations 668
- Circulant 585
- Class, data type 7
- Clenshaw-Curtis quadrature 124, 190, 512f.

- Clenshaw's recurrence formula 176f., 191, 1078
 for Chebyshev polynomials 187, 1076
 stability 176f.
- Clocking errors 891
- CM computers (Thinking Machines Inc.) 964
- CM Fortran 2/xv
 cn function 261, 1137f.
- Coarse-grid correction 864f.
- Coarse-to-fine operator 864, 1337
- Coding
 arithmetic 902ff., 1349ff.
 checksums 888, 1344
 decoding a Huffman-encoded message 900, 1349
 Huffman 896f., 1346ff.
 run-length 901
 variable length code 896, 1346ff.
- Ziv-Lempel 896
see also Arithmetic coding; Huffman coding
- Coefficients
 binomial 208, 1087f.
 for Gaussian quadrature 140ff., 1059ff.
 for Gaussian quadrature, nonclassical weight function 151ff., 788f., 1064
 for quadrature formulas 125ff., 789, 1328
- Cohen, Malcolm 2/xiv
- Column degeneracy 22
- Column operations on matrix 29, 31f.
- Column totals 624
- Combinatorial minimization *see* Annealing
- Comité Consultatif International Télégraphique et Téléphonique (CCITT) 889f., 901
- Common block
 obsolescent 2/xif.
 superseded by internal subprogram 957, 1067
 superseded by module 940, 953, 1298, 1320, 1322, 1324, 1330
- Communication costs, in parallel processing 969, 981, 1250
- Communication theory, use in adaptive integration 721
- Communications protocol 888
- Comparison function for rejection method 281
- Compilers 964, 1364
 CM Fortran 968
 DEC (Digital Equipment Corp.) 2/viii
 IBM (International Business Machines) 2/viii
 Microsoft Fortran PowerStation 2/viii
 NAG (Numerical Algorithms Group) 2/viii, 2/xiv
 for parallel supercomputers 2/viii
- Complementary error function 1094f.
see Error function
- Complete elliptic integral *see* Elliptic integrals
- Complex arithmetic 171f.
 avoidance of in path integration 203
 cubic equations 179f.
 for linear equations 41
 quadratic equations 178
- Complex error function 252
- Complex plane
 fractal structure for Newton's rule 360f.
 path integration for function evaluation 201ff., 263, 1138
 poles in 105, 160, 202f., 206, 554, 566, 718f.
- Complex systems of linear equations 41f.
- Compression of data 596f.
- Concordant pair for Kendall's tau 637, 1281
- Condition number 53, 78
- Confidence level 687, 691ff.
- Confidence limits
 bootstrap method 687f.
 and chi-square 688f.
 confidence region, confidence interval 687
 on estimated model parameters 684ff.
 by Monte Carlo simulation 684ff.
 from singular value decomposition (SVD) 693f.
- Confluent hypergeometric function 204, 239
- Conformal arrays 942f., 1094
- Conjugate directions 408f., 414ff., 1210
- Conjugate gradient method
 biconjugate 77, 1034
 compared to variable metric method 418
 elliptic partial differential equations 824
 for minimization 390, 413ff., 804, 815, 1210, 1214
 minimum residual method 78
 preconditioner 78f., 1037
 for sparse system 77ff., 599, 1034
 and wavelets 599
- Conservative differential equations 726, 1307
- Constrained linear inversion method 799ff.
- Constrained linear optimization *see* Linear programming
 Constrained optimization 387
 Constraints, deterministic 804ff.
 Constraints, linear 423
 CONTAINS statement 954, 957, 1067, 1134, 1202
- Contingency coefficient C 625, 1275
- Contingency table 622ff., 638, 1275f.
 statistics based on chi-square 623ff., 1275
 statistics based on entropy 626ff., 1275f.
- Continued fraction 163ff.
 Bessel functions 234
 convergence criterion 165
 equivalence transformation 166
 evaluation 163ff.
 evaluation along with normalization condition 240
 even and odd parts 166, 211, 216
 even part 249, 251
 exponential integral 216
 Fresnel integral 248f.
 incomplete beta function 219f., 1099f.
 incomplete gamma function 211, 1092f.
 Lentz's method 165, 212
 modified Lentz's method 165
 Pincherle's theorem 175
 ratio of Bessel functions 239
 rational function approximation 164, 211, 219f.
 recurrence for evaluating 164f.

- and recurrence relation 175
 sine and cosine integrals 250f.
 Steed's method 164f.
 tangent function 164
 typography for 163
 Continuous variable (statistics) 623
 Control structures 7ff., 2/xiv
 bad 15
 named 959, 1219, 1305
 Convergence
 accelerated, for series 160ff., 1070
 of algorithm for pi 906
 criteria for 347, 392, 404, 483, 488, 679, 759
 eigenvalues accelerated by shifting 470f.
 golden ratio 349, 399
 of golden section search 392f.
 of Levenberg-Marquardt method 679
 linear 346, 393
 of QL method 470f.
 quadratic 49, 351, 356, 409f., 419, 906
 rate 346f., 353, 356
 recurrence relation 175
 of Ridders' method 351
 series vs. continued fraction 163f.
 and spectral radius 856ff., 862
 Conversion intrinsic functions 946f.
 Convex sets, use in inverse problems 804
 Convolution
 denoted by asterisk 492
 finite impulse response (FIR) 531
 of functions 492, 503f.
 of large data sets 536f.
 for multiple precision arithmetic 909, 1354
 multiplication as 909, 1354
 necessity for optimal filtering 535
 overlap-add method 537
 overlap-save method 536f.
 and polynomial interpolation 113
 relation to wavelet transform 585
 theorem 492, 531ff., 546
 theorem, discrete 531ff.
 treatment of end effects 533
 use of FFT 523, 531ff., 1253
 wrapharound problem 533
 Cooley-Tukey FFT algorithm 503, 1250
 parallel version 1239f.
 Co-processor, floating point 886
 Copyright rules 1/xx, 2/xix
 Cornwell-Evans algorithm 816
 Corporate promotion ladder 328
 Corrected two-pass algorithm 607, 1269
 Correction, in multigrid method 863
 Correlation coefficient (linear) 630ff., 1276
 Correlation function 492
 autocorrelation 492, 539, 558
 and Fourier transforms 492
 theorem 492, 538
 treatment of end effects 538f.
 using FFT 538f., 1254
 Wiener-Khinchin theorem 492, 566f.
 Correlation, statistical 603f., 622
 Kendall's tau 634, 637ff., 1279
 linear correlation coefficient 630ff., 658, 1276
 linear related to least square fitting 630, 658
 nonparametric or rank statistical 633ff., 1277
 among parameters in a fit 657, 667, 670
 in random number generators 268
 Spearman rank-order coefficient 634f., 1277
 sum squared difference of ranks 634, 1277
 Cosine function, recurrence 172
 Cosine integral 248, 250ff., 1125f.
 continued fraction 250
 routine for 251f., 1125
 series 250
 Cosine transform *see* Fast Fourier transform (FFT); Fourier transform
 Coulomb wave function 204, 234
 count() intrinsic function 948
 Courant condition 829, 832ff., 836
 multidimensional 846
 Courant-Friedrichs-Lowy stability criterion *see* Courant condition
 Covariance
 a priori 700
 in general linear least squares 667, 671, 1288ff.
 matrix, by Cholesky decomposition 91, 667
 matrix, of errors 796, 808
 matrix, is inverse of Hessian matrix 679
 matrix, when it is meaningful 690ff.
 in nonlinear models 679, 681, 1292
 relation to chi-square 690ff.
 from singular value decomposition (SVD) 693f.
 in straight line fitting 657
 cpu_time() intrinsic function (Fortran 95) 961
 CR method *see* Cyclic reduction (CR)
 Cramer's V 625, 1275
 Crank-Nicholson method 840, 844, 846
 Cray computers 964
 CRC (cyclic redundancy check) 888ff., 1344f.
 CRC-12 890
 CRC-16 polynomial 890
 CRC-CCITT 890
 Creativity, essay on 9
 Critical (Nyquist) sampling 494, 543
 Cross (denotes matrix outer product) 66
 Crosstabulation analysis 623
see also Contingency table
 Crout's algorithm 36ff., 45, 1017
 cshift() intrinsic function 950
 communication bottleneck 969
 Cubic equations 178ff., 360
 Cubic spline interpolation 107ff., 1044f.
see also Spline
 cumprod() utility function 974, 988, 997, 1072, 1086
 cumsum() utility function 974, 989, 997, 1280, 1305
 Cumulant, of a polynomial 977, 999, 1071f., 1192

- Cumulative binomial distribution 222f.
 Cumulative Poisson function 214
 related to incomplete gamma function 214
 Curvature matrix *see* Hessian matrix
 cycle statement 959, 1219
 Cycle, in multigrid method 865
 Cyclic Jacobi method 459, 1225
 Cyclic reduction (CR) 848f., 852ff.
 linear recurrences 974
 tridiagonal systems 976, 1018
 Cyclic redundancy check (CRC) 888ff., 1344f.
 Cyclic tridiagonal systems 67, 1030
- D.C.** (direct current) 492
 Danielson-Lanczos lemma 498f., 525, 1235ff.
 DAP Fortran 2/xi
 Data
 assigning keys to 889
 continuous vs. binned 614
 entropy 626ff., 896, 1275
 essay on 603
 fitting 650ff., 1285ff.
 fraudulent 655
 glitches in 653
 iid (independent and identically distributed) 686
 modeling 650ff., 1285ff.
 serial port 892
 smoothing 604, 644ff., 1283f.
 statistical tests 603ff., 1269ff.
 unevenly or irregularly sampled 569, 574, 648f., 1258ff.
 use of CRCs in manipulating 889
 windowing 545ff., 1254
 see also Statistical tests
 Data compression 596f., 881
 arithmetic coding 902ff., 1349ff.
 cosine transform 513
 Huffman coding 896f., 902, 1346ff.
 linear predictive coding (LPC) 563ff.
 lossless 896
 Data Encryption Standard (DES) 290ff., 1144, 1147f., 1156ff.
 Data hiding 956ff., 1209, 1293, 1296
 Data parallelism 941, 964ff., 985
 DATA statement 959
 for binary, octal, hexadecimal constants 959
 repeat count feature 959
 superseded by initialization expression 943, 959, 1127
 Data type 18, 936
 accuracy parameters 1362f.
 character 1183
 derived 2/xiii, 937, 1030, 1336, 1346
 derived, for array of arrays 956, 1336
 derived, initialization 2/xv
 derived, for Numerical Recipes 1361
 derived, storage allocation 955
 DP (double precision) 1361f.
 DPC (double precision complex) 1361
 I1B (1 byte integer) 1361
 I2B (2 byte integer) 1361
 I4B (4 byte integer) 1361
- intrinsic 937
 LGT (default logical type) 1361
 nrtype.f90 1361f.
 passing complex as real 1140
 SP (single precision) 1361f.
 SPC (single precision complex) 1361
 user-defined 1346
- DAUB4 584ff., 588, 590f., 594, 1264f.
 DAUB6 586
 DAUB12 598
 DAUB20 590f., 1265
 Daubechies wavelet coefficients 584ff., 588, 590f., 594, 1264ff.
 Davidon-Fletcher-Powell algorithm 390, 418ff., 1215
 Dawson's integral 252ff., 600, 1127f.
 approximation for 252f.
 routine for 253f., 1127
 dble() intrinsic function (deprecated) 947
 deallocate statement 938f., 953f., 1197, 1266, 1293
 Deallocation, of allocatable array 938, 953f., 1197, 1266, 1293
 Debugging 8
 DEC (Digital Equipment Corp.) 1/xxiii, 2/xix, 886
 Alpha AXP 2/viii
 Fortran 90 compiler 2/viii
 quadruple precision option 1362
 VAX 4
 Decomposition *see* Cholesky decomposition;
 LU decomposition; QR decomposition;
 Singular value decomposition (SVD)
 Deconvolution 535, 540, 1253
 see also Convolution; Fast Fourier transform (FFT); Fourier transform
 Defect, in multigrid method 863
 Deferred approach to the limit *see* Richardson's deferred approach to the limit
 Deflation
 of matrix 471
 of polynomials 362ff., 370f., 977
 Degeneracy of linear algebraic equations 22, 53, 57, 670
 Degenerate kernel 785
 Degenerate minimization principle 795
 Degrees of freedom 615f., 654, 691
 Dekker, T.J. 353
 Demonstration programs 3, 936
 Deprecated features
 common block 2/xif., 940, 953, 957, 1067, 1298, 1320, 1322, 1324, 1330
 dble() intrinsic function 947
 EQUIVALENCE statement 2/xif., 1161, 1286
 statement function 1057, 1256
 Derivatives
 computation via Chebyshev approximation 183, 189, 1077f.
 computation via Savitzky-Golay filters 183, 645
 matrix of first partial *see* Jacobian determinant
 matrix of second partial *see* Hessian matrix

- numerical computation 180ff., 379, 645, 732, 750, 771, 1075, 1197, 1309
of polynomial 167, 978, 1071f.
use in optimization 388f., 399, 1205ff.
- Derived data type *see* Data type, derived
- DES *see* Data Encryption Standard
- Descending transformation, elliptic integrals 256
- Descent direction 376, 382, 419
- Descriptive statistics 603ff., 1269ff.
see also Statistical tests
- Design matrix 645, 665, 795, 801, 1082
- Determinant 25, 41
- Deviates, random *see* Random deviates
- DFP algorithm *see* Davidon-Fletcher-Powell algorithm
- diagadd() utility function 985, 989, 1004
- diagmult() utility function 985, 989, 1004, 1294
- Diagonal dominance 43, 679, 780, 856
- Difference equations, finite *see* Finite difference equations (FDEs)
- Difference operator 161
- Differential equations 701ff., 1297ff.
accuracy vs. stability 704, 729
Adams-Basforth-Moulton schemes 741
adaptive stepsize control 703, 708ff., 719, 726, 731, 737, 742f., 1298ff., 1303ff., 1308f., 1311ff.
algebraically difficult sets 763
backward Euler's method 729
Bader-Deuflhard method for stiff 730, 735, 1310f.
boundary conditions 701f., 745ff., 749, 751f., 771, 1314ff.
- Bulirsch-Stoer method 202, 263, 702, 706, 716, 718ff., 740, 1138, 1303
- Bulirsch-Stoer method for conservative equations 726, 1307
comparison of methods 702f., 739f., 743
conservative 726, 1307
danger of too small stepsize 714
eigenvalue problem 748, 764ff., 770ff., 1319ff.
embedded Runge-Kutta method 709f., 731, 1298, 1308
equivalence of multistep and multivalue methods 743
Euler's method 702, 704, 728f.
forward Euler's method 728
free boundary problem 748, 776
high-order implicit methods 730ff., 1308ff.
implicit differencing 729, 740, 1308
initial value problems 702
internal boundary conditions 775ff.
internal singular points 775ff.
interpolation on right-hand sides 111
Kaps-Rentrop method for stiff 730, 1308
local extrapolation 709
modified midpoint method 716f., 719, 1302f.
multistep methods 740ff.
multivalue methods 740
order of method 704f., 719
- path integration for function evaluation 201ff., 263, 1138
- predictor-corrector methods 702, 730, 740ff.
reduction to first-order sets 701, 745
relaxation method 746f., 753ff., 1316ff.
relaxation method, example of 764ff., 1319ff.
r.h.s. independent of x 729f.
- Rosenbrock methods for stiff 730, 1308f.
- Runge-Kutta method 702, 704ff., 708ff., 731, 740, 1297f., 1308
- Runge-Kutta method, high-order 705, 1297
- Runge-Kutta-Fehlberg method 709ff., 1298
- scaling stepsize to required accuracy 709
- second order 726, 1307
- semi-implicit differencing 730
- semi-implicit Euler method 730, 735f.
- semi-implicit extrapolation method 730, 735f., 1311ff.
- semi-implicit midpoint rule 735f., 1310f.
- shooting method 746, 749ff., 1314ff.
shooting method, example 770ff., 1321ff.
- similarity to Volterra integral equations 786
- singular points 718f., 751, 775ff., 1315f., 1323ff.
- step doubling 708f.
- stepsize control 703, 708ff., 719, 726, 731, 737, 742f., 1298, 1303ff., 1308f.
stiff 703, 727ff., 1308ff.
- stiff methods compared 739
Stoermer's rule 726, 1307
see also Partial differential equations; Two-point boundary value problems
- Diffusion equation 818, 838ff., 855
- Crank-Nicholson method 840, 844, 846
- Forward Time Centered Space (FTCS) 839ff., 855
- implicit differencing 840
multidimensional 846
- Digamma function 216
- Digital filtering *see* Filter
- Dihedral group D_5 894
- dim optional argument 948
- Dimensional expansion 965ff.
- Dimensions (units) 678
- Diminishing increment sort 322, 1168
- Dirac delta function 284, 780
- Direct method *see* Periodogram
- Direct methods for linear algebraic equations 26, 1014
- Direct product *see* Outer product of matrices
- Direction of largest decrease 410f.
- Direction numbers, Sobol's sequence 300
- Direction-set methods for minimization 389, 406f., 1210ff.
- Dirichlet boundary conditions 820, 840, 850, 856, 858
- Disclaimer of warranty 1/xx, 2/xvii
- Discordant pair for Kendall's tau 637, 1281
- Discrete convolution theorem 531ff.

- Discrete Fourier transform (DFT) 495ff., 1235ff.
 as approximate continuous transform 497
 see also Fast Fourier transform (FFT)
- Discrete optimization 436ff., 1219ff.
- Discriminant 178, 457
- Diskettes
 are ANSI standard 3
 how to order 1/xxi, 2/xvii
- Dispersion 831
- DISPO *see* Savitzky-Golay filters
- Dissipation, numerical 830
- Divergent series 161
- Divide and conquer algorithm 1226, 1229
- Division
 complex 171
 multiple precision 910f., 1356
 of polynomials 169, 362, 370, 1072
- dn function 261, 1137f.
- Do-list, implied 968, 971, 1127
- Do-loop 2/xiv
- Do-until iteration 14
- Do-while iteration 13
- Dogleg step methods 386
- Domain of integration 155f.
- Dominant solution of recurrence relation 174
- Dot (denotes matrix multiplication) 23
- dot_product() intrinsic function 945, 949, 969, 1216
- Double exponential error distribution 696
- Double precision
 converting to 1362
 as refuge of scoundrels 882
 use in iterative improvement 47, 1022
- Double root 341
- Downhill simplex method *see* Simplex, method of Nelder and Mead
- DP, defined 937
- Driver programs 3
- Dual viewpoint, in multigrid method 875
- Duplication theorem, elliptic integrals 256
- DWT (discrete wavelet transform) *see* Wavelet transform
- Dynamical allocation of storage 2/xiii, 869, 938, 941f., 953ff., 1327, 1336
 garbage collection 956
 increasing 955, 1070, 1302
- E**ardley, D.M. 338
- EBCDIC 890
- Economization of power series 192f., 195, 1080
- Eigensystems 449ff., 1225ff.
 balancing matrix 476f., 1230f.
 bounds on eigenvalues 50
 calculation of few eigenvalues 454, 488
 canned routines 454f.
 characteristic polynomial 449, 469
 completeness 450
 defective 450, 476, 489
 deflation 471
 degenerate eigenvalues 449ff.
 elimination method 453, 478, 1231
 factorization method 453
 fast Givens reduction 463
 generalized eigenproblem 455
 Givens reduction 462f.
 Hermitian matrix 475
 Hessenberg matrix 453, 470, 476ff., 488, 1232
 Householder transformation 453, 462ff., 469, 473, 475, 478, 1227f., 1231
 ill-conditioned eigenvalues 477
 implicit shifts 472ff., 1228f.
 and integral equations 779, 785
 invariance under similarity transform 452
 inverse iteration 455, 469, 476, 487ff., 1230
 Jacobi transformation 453, 456ff., 462, 475, 489, 1225f.
 left eigenvalues 451
 list of tasks 454f.
 multiple eigenvalues 489
 nonlinear 455
 nonsymmetric matrix 476ff., 1230ff.
 operation count of balancing 476
 operation count of Givens reduction 463
 operation count of Householder reduction 467
 operation count of inverse iteration 488
 operation count of Jacobi method 460
 operation count of QL method 470, 473
 operation count of QR method for Hessenberg matrices 484
 operation count of reduction to Hessenberg form 479
 orthogonality 450
 parallel algorithms 1226, 1229
 polynomial roots and 368, 1193
 QL method 469ff., 475, 488f.
 QL method with implicit shifts 472ff., 1228f.
 QR method 52, 453, 456, 469ff., 1228
 QR method for Hessenberg matrices 480ff., 1232ff.
 real, symmetric matrix 150, 467, 785, 1225, 1228
 reduction to Hessenberg form 478f., 1231
 right eigenvalues 451
 shifting eigenvalues 449, 470f., 480
 special matrices 454
 termination criterion 484, 488
 tridiagonal matrix 453, 469ff., 488, 1228
- Eigenvalue and eigenvector, defined 449
- Eigenvalue problem for differential equations 748, 764ff., 770ff., 1319ff.
- Eigenvalues and polynomial root finding 368, 1193
- EISPACK 454, 475
- Electromagnetic potential 519
- ELEMENTAL attribute (Fortran 95) 961, 1084
- Elemental functions 2/xiii, 2/xv, 940, 942, 946f., 961, 986, 1015, 1083, 1097f.
- Elimination *see* Gaussian elimination
- Ellipse in confidence limit estimation 688
- Elliptic integrals 254ff., 906
 addition theorem 255

- Carlson's forms and algorithms 255f., 1128ff.
 Cauchy principal value 256f.
 duplication theorem 256
 Legendre 254ff., 260f., 1135ff.
 routines for 257ff., 1128ff.
 symmetric form 255
 Weierstrass 255
- Elliptic partial differential equations 818, 1332ff.
 alternating-direction implicit method (ADI) 861f., 906
 analyze/factorize/operate package 824
 biconjugate gradient method 824
 boundary conditions 820
 comparison of rapid methods 854
 conjugate gradient method 824
 cyclic reduction 848f., 852ff.
 Fourier analysis and cyclic reduction (FACR) 848ff., 854
 Gauss-Seidel method 855, 864ff., 876, 1338, 1341
 incomplete Cholesky conjugate gradient method (ICCG) 824
 Jacobi's method 855f., 864
 matrix methods 824
 multigrid method 824, 862ff., 1009, 1334ff.
 rapid (Fourier) method 824, 848ff.
 relaxation method 823, 854ff., 1332
 strongly implicit procedure 824
 successive over-relaxation (SOR) 857ff., 862, 866, 1332
 elsewhere construct 943
 Emacs, GNU 1/xvi
 Embedded Runge-Kutta method 709f., 731, 1298, 1308
 Encapsulation, in programs 7
 Encryption 290, 1156
 endo statement 12, 17
 Entropy 896
 of data 626ff., 811, 1275
 EOM (end of message) 902
 eoshift() intrinsic function 950
 communication bottleneck 969
 vector shift argument 1019f.
 vs. array section 1078
 epsilon() intrinsic function 951, 1189
 Equality constraints 423
 Equations
 cubic 178ff., 360
 normal (fitting) 645, 666ff., 800, 1288
 quadratic 20, 178
see also Differential equations; Partial differential equations; Root finding
 Equivalence classes 337f., 1180
 EQUIVALENCE statement 2/xif., 1161, 1286
 Equivalence transformation 166
 Error
 checksums for preventing 891
 clocking 891
 double exponential distribution 696
 local truncation 875
 Lorentzian distribution 696f.
 in multigrid method 863
 nonnormal 653, 690, 694ff.
 relative truncation 875
 roundoff 180f., 881, 1362
 series, advantage of an even 132f., 717, 1362
 systematic vs. statistical 653, 1362
 truncation 20f., 180, 399, 709, 881, 1362
 varieties found by check digits 895
 varieties of, in PDEs 831ff.
see also Roundoff error
 Error function 213f., 601, 1094f.
 approximation via sampling theorem 601
 Chebyshev approximation 214, 1095
 complex 252
 for Fisher's z-transformation 632, 1276
 relation to Dawson's integral 252, 1127
 relation to Fresnel integrals 248
 relation to incomplete gamma function 213
 routine for 214, 1094
 for significance of correlation 631, 1276
 for sum squared difference of ranks 635, 1277
 Error handling in programs 2/xii, 2/xvi, 3, 994f., 1036, 1370f.
 Estimation of parameters *see* Fitting; Maximum likelihood estimate
 Estimation of power spectrum 542ff., 565ff., 1254ff., 1258
 Euler equation (fluid flow) 831
 Euler-Maclaurin summation formula 132, 135
 Euler's constant 216ff., 250
 Euler's method for differential equations 702, 704, 728f.
 Euler's transformation 160f., 1070
 generalized form 162f.
 Evaluation of functions *see* Function
 Even and odd parts, of continued fraction 166, 211, 216
 Even parity 888
 Exception handling in programs *see* Error handling in programs
 exit statement 959, 1219
 Explicit differencing 827
 Exponent in floating point format 19, 882, 1343
 exponent intrinsic function 1107
 Exponential deviate 278, 1151f.
 Exponential integral 215ff., 1096f.
 asymptotic expansion 218
 continued fraction 216
 recurrence relation 172
 related to incomplete gamma function 215
 relation to cosine integral 250
 routine for $Ei(x)$ 218, 1097
 routine for $E_n(x)$ 217, 1096
 series 216
 Exponential probability distribution 570
 Extended midpoint rule 124f., 129f., 135, 1054f.
 Extended Simpson's rule 128, 788, 790
 Extended Simpson's three-eighths rule 789
 Extended trapezoidal rule 125, 127, 130ff., 135, 786, 1052ff., 1326
 roundoff error 132
 Extrapolation (so-called) 574, 1261

- Extrapolation 99ff.
 in Bulirsch-Stoer method 718ff., 726, 1305ff.
 differential equations 702
 by linear prediction 557ff., 1256f.
 local 709
 maximum entropy method as type of 567
 polynomial 724, 726, 740, 1305f.
 rational function 718ff., 726, 1306f.
 relation to interpolation 101
 for Romberg integration 134
see also Interpolation
 Extremization *see* Minimization
- F**-distribution probability function 222
 F-test for differences of variances 611, 613, 1271
 FACR *see* Fourier analysis and cyclic reduction (FACR)
 Facsimile standard 901
 Factorial
 double (denoted “!!”) 247
 evaluation of 159, 1072, 1086
 relation to gamma function 206
 routine for 207ff., 1086ff.
 False position 347ff., 1185f.
 Family tree 338
 FAS (full approximation storage algorithm) 874, 1339ff.
 Fast Fourier transform (FFT) 498ff., 881, 981, 1235f.
 alternative algorithms 503f.
 as approximation to continuous transform 497
 Bartlett window 547, 1254
 bit reversal 499f., 525
 and Clenshaw-Curtis quadrature 190
 column-parallel algorithm 981, 1237ff.
 communication bottleneck 969, 981, 1250
 convolution 503f., 523, 531ff., 909, 1253, 1354
 convolution of large data sets 536f.
 Cooley-Tukey algorithm 503, 1250
 Cooley-Tukey algorithm, parallel 1239f.
 correlation 538f., 1254
 cosine transform 190, 511ff., 851, 1245f.
 cosine transform, second form 513, 852, 1246
 Danielson-Lanczos lemma 498f., 525
 data sets not a power of 2 503
 data smoothing 645
 data windowing 545ff., 1254
 decimation-in-frequency algorithm 503
 decimation-in-time algorithm 503
 discrete autocorrelation 539, 1254
 discrete convolution theorem 531ff.
 discrete correlation theorem 538
 at double frequency 575
 effect of caching 982
 endpoint corrections 578f., 1261ff.
 external storage 525
 figures of merit for data windows 548
 filtering 551ff.
 FIR filter 553
 four-step framework 983, 1239
- Fourier integrals 577ff., 1261
 Fourier integrals, infinite range 583
 Hamming window 547
 Hann window 547
 history 498
 IIR filter 553ff.
 image processing 803, 805
 integrals using 124
 inverse of cosine transform 512ff.
 inverse of sine transform 511
 large data sets 525
 leakage 544
 memory-local algorithm 528
 multidimensional 515ff., 1236f., 1241, 1246, 1251
 for multiple precision arithmetic 906
 for multiple precision multiplication 909, 1354
 number-theoretic transforms 503f.
 operation count 498
 optimal (Wiener) filtering 539ff., 558
 order of storage in 501
 parallel algorithms 981ff., 1235ff.
 partial differential equations 824, 848ff.
 Parzen window 547
 periodicity of 497
 periodogram 543ff., 566
 power spectrum estimation 542ff., 1254ff.
 for quadrature 124
 of real data in 2D and 3D 519ff., 1248f.
 of real functions 504ff., 519ff., 1242f., 1248f.
 related algorithms 503f.
 row-parallel algorithm 981, 1235f.
 Sande-Tukey algorithm 503
 sine transform 508ff., 850, 1245
 Singleton's algorithm 525
 six-step framework 983, 1240
 square window 546, 1254
 timing 982
 treatment of end effects in convolution 533
 treatment of end effects in correlation 538f.
 Tukey's trick for frequency doubling 575
 use in smoothing data 645
 used for Lomb periodogram 574, 1259
 variance of power spectrum estimate 544f., 549
 virtual memory machine 528
 Welch window 547, 1254
 Winograd algorithms 503
see also Discrete Fourier transform (DFT);
 Fourier transform; Spectral density
 Faure sequence 300
 Fax (facsimile) Group 3 standard 901
 Feasible vector 424
 FFT *see* Fast Fourier transform (FFT)
 Field, in data record 329
 Figure-of-merit function 650
 Filon's method 583
 Filter 551ff.
 acausal 552
 bilinear transformation method 554
 causal 552, 644

- characteristic polynomial 554
 data smoothing 644f., 1283f.
 digital 551ff.
 DISPO 644
 by fast Fourier transform (FFT) 523,
 551ff.
 finite impulse response (FIR) 531, 552
 homogeneous modes of 554
 infinite impulse response (IIR) 552ff., 566
 Kalman 700
 linear 552ff.
 low-pass for smoothing 644ff., 1283f.
 nonrecursive 552
 optimal (Wiener) 535, 539ff., 558, 644
 quadrature mirror 585, 593
 realizable 552, 554f.
 recursive 552ff., 566
 Remes exchange algorithm 553
 Savitzky-Golay 183, 644ff., 1283f.
 stability of 554f.
 in the time domain 551ff.
 Fine-to-coarse operator 864, 1337
 Finite difference equations (FDEs) 753, 763,
 774
 alternating-direction implicit method (ADI)
 847, 861f.
 art not science 829
 Cayley's form for unitary operator 844
 Courant condition 829, 832ff., 836
 Courant condition (multidimensional) 846
 Crank-Nicholson method 840, 844, 846
 eigenmodes of 827f.
 explicit vs. implicit schemes 827
 forward Euler 826f.
 Forward Time Centered Space (FTCS)
 827ff., 839ff., 843, 855
 implicit scheme 840
 Lax method 828ff., 836
 Lax method (multidimensional) 845f.
 mesh drifting instability 834f.
 numerical derivatives 181
 partial differential equations 821ff.
 in relaxation methods 753ff.
 staggered leapfrog method 833f.
 two-step Lax-Wendroff method 835ff.
 upwind differencing 832f., 837
 see also Partial differential equations
 Finite element methods, partial differential
 equations 824
 Finite impulse response (FIR) 531
 Finkelstein, S. 1/xvi, 2/ix
 FIR (finite impulse response) filter 552
 Fisher's z-transformation 631f., 1276
 Fitting 650ff., 1285ff.
 basis functions 665
 by Chebyshev approximation 185f., 1076
 chi-square 653ff., 1285ff.
 confidence levels related to chi-square val-
 ues 691ff.
 confidence levels from singular value de-
 composition (SVD) 693f.
 confidence limits on fitted parameters 684ff.
 covariance matrix not always meaningful
 651, 690
 degeneracy of parameters 674
 an exponential 674
 freezing parameters in 668, 700
 Gaussians, a sum of 682, 1294
 general linear least squares 665ff., 1288,
 1290f.
 Kalman filter 700
 K-S test, caution regarding 621f.
 least squares 651ff., 1285
 Legendre polynomials 674, 1291f.
 Levenberg-Marquardt method 678ff., 816,
 1292f.
 linear regression 655ff., 1285ff.
 maximum likelihood estimation 652f.,
 694ff.
 Monte Carlo simulation 622, 654, 684ff.
 multidimensional 675
 nonlinear models 675ff., 1292f.
 nonlinear models, advanced methods 683
 nonlinear problems that are linear 674
 nonnormal errors 656, 690, 694ff.
 polynomial 83, 114, 191, 645, 665, 674,
 1078, 1291
 by rational Chebyshev approximation 197ff.,
 1081f.
 robust methods 694ff., 1294
 of sharp spectral features 566
 standard (probable) errors on fitted pa-
 rameters 657f., 661, 667, 671, 684ff.,
 1285f., 1288, 1290
 straight line 655ff., 667f., 698, 1285ff.,
 1294ff.
 straight line, errors in both coordinates
 660ff., 1286ff.
 see also Error; Least squares fitting; Max-
 imum likelihood estimate; Robust esti-
 mation
 Five-point difference star 867
 Fixed point format 18
 Fletcher-Powell algorithm *see* Davidon-Fletcher-
 Powell algorithm
 Fletcher-Reeves algorithm 390, 414ff., 1214
 Floating point co-processor 886
 Floating point format 18ff., 882, 1343
 care in numerical derivatives 181
 IEEE 276, 882, 1343
 floor() intrinsic function 948
 Flux-conservative initial value problems 825ff.
 FMG (full multigrid method) 863, 868, 1334ff.
 FOR iteration 9f., 12
 forall statement 2/xii, 2/xv, 960, 964, 986
 access to associated index 968
 skew array sections 985, 1007
 Formats of numbers 18ff., 882, 1343
 Fortran 9
 arithmetic-if statement 2/xi
 COMMON block 2/xif., 953, 957
 deprecated features 2/xif., 947, 1057,
 1161, 1256, 1286
 dynamical allocation of storage 869, 1336
 EQUIVALENCE statement 2/xif., 1161,
 1286
 evolution of 2/xivff.
 exception handling 2/xii, 2/xvi
 filenames 935
 Fortran 2000 (planned) 2/xvi

- Fortran 95 2/xv, 945, 947, 1084, 1100, 1364
 HPF (High-Performance Fortran) 2/xvf.
 Numerical Recipes in 2/x, 2/xvii,
 obsolescent features 2/xif.
 side effects 960
see also Fortran 90
 Fortran D 2/xv
 Fortran 77 1/xix
 bit manipulation functions 17
 hexadecimal constants 17
 Fortran 8x 2/xi, 2/xiii
 Fortran 90 3
 abstract data types 2/xiii, 1030
 all() intrinsic function 945, 948
 allocatable array 938, 941, 953ff., 1197, 1212, 1266, 1293, 1306, 1336
 allocate statement 938f., 941, 953f., 1197, 1266, 1293, 1306, 1336
 allocated() intrinsic function 938, 952ff., 1197, 1266, 1293
 any() intrinsic function 945, 948
 array allocation and deallocation 953
 array of arrays 2/xii, 956, 1336
 array constructor 2/xii, 968, 971, 1022, 1052, 1055, 1127
 array constructor with implied do-list 968, 971
 array extents 938, 949
 array features 941ff., 953ff.
 array intrinsic procedures 2/xiii, 948ff.
 array of length 0 944
 array of length 1 949
 array manipulation functions 950
 array parallel operations 964f.
 array rank 938, 949
 array reallocation 955
 array section 2/xiif., 2/xiii, 939, 941ff., 960, 1078, 1284, 1286, 1333
 array shape 938, 949
 array size 938, 942
 array transpose 981f.
 array unary and binary functions 949
 associated() intrinsic function 952f.
 associated pointer 953f.
 assumed-shape array 942
 automatic array 938, 954, 1197, 1212, 1336
 backwards-compatibility 935, 946
 bit manipulation functions 2/xiii, 951
 bit_size() intrinsic function 951
 broadcasts 965f.
 btest() intrinsic function 951
 case construct 1010, 1036
 case insensitive 937
 ceiling() intrinsic function 947
 character functions 952
 character variables 1183
 cmplx function 1125
 communication bottlenecks 969, 981, 1250
 compatibility with Fortran 77 935, 946
 compilers 2/viii, 2/xiv, 1364
 compiling 936
 conformable arrays 942f., 1094
 CONTAINS statement 954, 957, 985, 1067, 1134, 1202
 control structure 2/xiv, 959, 1219, 1305
 conversion elemental functions 946
 count() intrinsic function 948
 cshift() intrinsic function 950, 969
 cycle statement 959, 1219
 data hiding 956ff., 1209
 data parallelism 964
 DATA statement 959
 data types 937, 1336, 1346, 1361
 deallocate statement 938f., 953f., 1197, 1266, 1293
 deallocating array 938, 953f., 1197, 1266, 1293
 defined types 956
 deprecated features 947, 1057, 1161, 1256, 1286
 derived types 937, 955
 dimensional expansion 965ff.
 do-loop 2/xiv
 dot_product() intrinsic function 945, 949, 969, 1216
 dynamical allocation of storage 2/xiii, 938, 941f., 953ff., 1327, 1336
 elemental functions 940, 942, 946f., 951, 1015, 1083, 1364
 elsewhere construct 943
 eoshift() intrinsic function 950, 969, 1019f., 1078
 epsilon() intrinsic function 951, 1189
 evolution 2/xivff., 959, 987f.
 example 936
 exit statement 959, 1219
 exponent() intrinsic function 1107
 floor() intrinsic function 948
 Fortran tip icon 1009
 garbage collection 956
 gather-scatter operations 2/xiif., 969, 981, 984, 1002, 1032, 1034, 1250
 generic interface 2/xiii, 1083
 generic procedures 939, 1015, 1083, 1094, 1096, 1364
 global variables 955, 957, 1210
 history 2/xff.
 huge() intrinsic function 951
 iand() intrinsic function 951
 ibclr() intrinsic function 951
 ibits() intrinsic function 951
 ibset() intrinsic function 951
 ieor() intrinsic function 951
 IMPLICIT NONE statement 2/xiv, 936
 implied do-list 968, 971, 1127
 index loss 967f.
 initialization expression 943, 959, 1012, 1127
 inquiry functions 948
 integer model 1144, 1149, 1156
 INTENT attribute 1072, 1092
 interface 939, 942, 1067, 1084, 1384
 internal subprogram 2/xii, 2/xiv, 957, 1057, 1067, 1202f., 1256, 1302
 interprocessor communication 969, 981, 1250
 intrinsic data types 937

- intrinsic procedures 939, 945ff., 987, 1016
 ior() intrinsic function 951
 ishft() intrinsic function 951
 ishftc() intrinsic function 951
 ISO (International Standards Organization)
 2/xf., 2/xiiif.
 keyword argument 2/xiv, 947f., 1341
 kind() intrinsic function 951
 KIND parameter 937, 946, 1125, 1144,
 1192, 1254, 1261, 1284, 1361
 language features 935ff.
 lbound() intrinsic function 949
 lexical comparison 952
 linear algebra 969f., 1000ff., 1018f., 1026,
 1040, 1200, 1326
 linear recurrence 971, 988
 linking 936
 literal constant 937, 1361
 logo for tips 2/viii, 1009
 mask 948, 967f., 1006f., 1038, 1102,
 1200, 1226, 1305, 1333f., 1368, 1378,
 1382
 matmul() intrinsic function 945, 949, 969,
 1026, 1040, 1050, 1076, 1200, 1216,
 1290, 1326
 maxexponent() intrinsic function 1107
 maxloc() intrinsic function 949, 961,
 992f., 1015
 maxval() intrinsic function 945, 948, 961,
 1016, 1273
 memory leaks 953, 956, 1327
 memory management 938, 953ff.
 merge() intrinsic function 945, 950, 1010,
 1094f., 1099f.
 Metcalf and Reid (M&R) 935
 minloc() intrinsic function 949, 961, 992f.
 minval() intrinsic function 948, 961
 missing language features 983ff., 987ff.
 modularization 956f.
 MODULE facility 2/xiii, 936f., 939f.,
 953f., 957, 1067, 1298, 1320, 1322,
 1324, 1330, 1346
 MODULE subprograms 940
 modulo() intrinsic function 946, 1156
 named constant 940, 1012, 1361
 named control structure 959, 1219, 1305
 nearest() intrinsic function 952, 1146
 nested where construct forbidden 943
 not() intrinsic function 951
 nullify statement 953f., 1070, 1302
 numerical representation functions 951
 ONLY option 941, 957, 1067
 operator overloading 2/xiif.
 operator, user-defined 2/xii
 optional argument 2/xiv, 947f., 1092,
 1228, 1230, 1256, 1272, 1275, 1340
 outer product 969f.
 overloading 940, 1083, 1102
 pack() intrinsic function 945, 950, 964,
 969, 991, 1170, 1176, 1178
 pack, for selective evaluation 1087
 parallel extensions 2/xv, 959ff., 964, 981,
 984, 987, 1002, 1032
 parallel programming 963ff.
 PARAMETER attribute 1012
 pointer 2/xiif., 938f., 941, 944f., 952ff.,
 1067, 1070, 1197, 1210, 1212, 1266,
 1302, 1327, 1336
 pointer to function (missing) 1067
 portability 963
 present() intrinsic function 952
 PRIVATE attribute 957, 1067
 product() intrinsic function 948
 programming conventions 937
 PUBLIC attribute 957, 1067
 quick start 936
 radix() intrinsic function 1231
 random_number() intrinsic function 1141,
 1143
 random_seed() intrinsic function 1141
 real() intrinsic function 947, 1125
 RECURSIVE keyword 958, 1065, 1067
 recursive procedure 2/xiv, 958, 1065,
 1067, 1166
 reduction functions 948
 reshape() intrinsic function 950, 969, 1247
 RESULT keyword 958, 1073
 SAVE attribute 953f., 958f., 1052, 1070,
 1266, 1293
 scale() intrinsic function 1107
 scatter-with-combine (missing function)
 984
 scope 956ff.
 scoping units 939
 select case statement 2/xiv, 1010, 1036
 shape() intrinsic function 938, 949
 size() intrinsic function 938, 942, 945,
 948
 skew sections 985
 sparse matrix representation 1030
 specification statement 2/xiv
 spread() intrinsic function 945, 950, 966ff.,
 969, 1000, 1094, 1290f.
 statement functions deprecated 1057
 stride (of an array) 944
 structure constructor 2/xii
 subscript triplet 944
 sum() intrinsic function 945, 948, 966
 tiny() intrinsic function 952
 transformational functions 948
 transpose() intrinsic function 950, 960,
 969, 981, 1247
 tricks 1009, 1072, 1146, 1274, 1278, 1280
 truncation elemental functions 946
 type checking 1140
 ubound() intrinsic function 949
 undefined pointer 953
 unpack() intrinsic function 950, 964, 969
 USE statement 936, 939f., 954, 957, 1067,
 1384
 utility functions 987ff.
 vector subscripts 2/xiif., 969, 981, 984,
 1002, 1032, 1034, 1250
 visibility 956ff., 1209, 1293, 1296
 WG5 technical committee 2/xi, 2/xiii,
 2/xvif.
 where construct 943, 985, 1060, 1291
 X3J3 Committee 2/viii, 2/xff., 2/xv, 947,
 959, 964, 968, 990
 zero-length array 944

- see also* Intrinsic procedures
see also Fortran
 Fortran 95 947, 959ff.
 allocatable variables 961
 blocks 960
 cpu_time() intrinsic function 961
 elemental functions 2/xii, 2/xv, 940, 961,
 986, 1015, 1083f., 1097f.
 forall statement 2/xii, 2/xv, 960, 964, 968,
 986, 1007
 initialization of derived data type 2/xv
 initialization of pointer 2/xv, 961
 minor changes from Fortran 90 961
 modified intrinsic functions 961
 nested where construct 2/xv, 960, 1100
 pointer association status 961
 pointers 961
 PURE attribute 2/xv, 960f., 964, 986
 SAVE attribute 961
 side effects 960
 and skew array section 945, 985
 see also Fortran
 Fortran 2000 2/xvi
 Forward deflation 363
 Forward difference operator 161
 Forward Euler differencing 826f.
 Forward Time Centered Space *see* FTCS
 Four-step framework, for FFT 983, 1239
 Fourier analysis and cyclic reduction (FACR)
 848f., 854
 Fourier integrals
 attenuation factors 583, 1261
 endpoint corrections 578f., 1261
 tail integration by parts 583
 use of fast Fourier transform (FFT) 577ff.,
 1261ff.
 Fourier transform 99, 490ff., 1235ff.
 aliasing 495, 569
 approximation of Dawson's integral 253
 autocorrelation 492
 basis functions compared 508f.
 contrasted with wavelet transform 584,
 594
 convolution 492, 503f., 531ff., 909, 1253,
 1354
 correlation 492, 538f., 1254
 cosine transform 190, 511ff., 851, 1245f.
 cosine transform, second form 513, 852,
 1246
 critical sampling 494, 543, 545
 definition 490
 discrete Fourier transform (DFT) 184,
 495ff.
 Gaussian function 600
 image processing 803, 805
 infinite range 583
 inverse of discrete Fourier transform 497
 method for partial differential equations
 848ff.
 missing data 569
 missing data, fast algorithm 574f., 1259
 Nyquist frequency 494ff., 520, 543, 545,
 569, 571
 optimal (Wiener) filtering 539ff., 558
 Parseval's theorem 492, 498, 544
 power spectral density (PSD) 492f.
 power spectrum estimation by FFT 542ff.,
 1254ff.
 power spectrum estimation by maximum
 entropy method 565ff., 1258
 properties of 491f.
 sampling theorem 495, 543, 545, 600
 scalings of 491
 significance of a peak in 570
 sine transform 508ff., 850, 1245
 symmetries of 491
 uneven sampling, fast algorithm 574f.,
 1259
 unevenly sampled data 569ff., 574, 1258
 and wavelets 592f.
 Wiener-Khinchin theorem 492, 558, 566f.
 see also Fast Fourier transform (FFT);
 Spectral density
 Fractal region 360f.
 Fractional step methods 847f.
 Fredholm alternative 780
 Fredholm equations 779f.
 eigenvalue problems 780, 785
 error estimate in solution 784
 first kind 779
 Fredholm alternative 780
 homogeneous, second kind 785, 1325
 homogeneous vs. inhomogeneous 779f.
 ill-conditioned 780
 infinite range 789
 inverse problems 780, 795ff.
 kernel 779f.
 nonlinear 781
 Nystrom method 782ff., 789, 1325
 product Nystrom method 789, 1328ff.
 second kind 779f., 782ff., 1325, 1331
 with singularities 788, 1328ff.
 with singularities, worked example 792,
 1328ff.
 subtraction of singularity 789
 symmetric kernel 785
 see also Inverse problems
 Frequency domain 490
 Frequency spectrum *see* Fast Fourier transform
 (FFT)
 Frequentist, contrasted with Bayesian 810
 Fresnel integrals 248ff.
 asymptotic form 249
 continued fraction 248f.
 routine for 249f., 1123
 series 248
 Friday the Thirteenth 14f., 1011f.
 FTCS (forward time centered space) 827ff.,
 839ff., 843
 stability of 827ff., 839ff., 855
 Full approximation storage (FAS) algorithm
 874, 1339ff.
 Full moon 14f., 936, 1011f.
 Full multigrid method (FMG) 863, 868, 1334ff.
 Full Newton methods, nonlinear least squares
 683
 Full pivoting 29, 1014
 Full weighting 867
 Function
 Airy 204, 243f., 1121

- approximation 99ff., 184ff., 1043, 1076ff.
 associated Legendre polynomial 246ff.,
 764, 1122f., 1319
 autocorrelation of 492
 bandwidth limited 495
 Bessel 172, 204, 223ff., 234, 1101ff.,
 1115ff.
 beta 209, 1089
 binomial coefficients 208f., 1087f.
 branch cuts of 202f.
 chi-square probability 215, 798
 complex 202
 confluent hypergeometric 204, 239
 convolution of 492
 correlation of 492
 cosine integral 250f., 1123f.
 Coulomb wave 204, 234
 cumulative binomial probability 222f.
 cumulative Poisson 209ff.
 Dawson's integral 252ff., 600, 1127f.
 digamma 216
 elliptic integrals 254ff., 906, 1128ff.
 error 213f., 248, 252, 601, 631, 635,
 1094f., 1127, 1276f.
 evaluation 159ff., 1070ff.
 evaluation by path integration 201ff., 263,
 1138
 exponential integral 172, 215ff., 250,
 1096f.
 F-distribution probability 222
 Fresnel integral 248ff., 1123
 gamma 206, 1085
 hypergeometric 202f., 263ff., 1138ff.
 incomplete beta 219ff., 610, 1098ff., 1269
 incomplete gamma 209ff., 615, 654, 657f.,
 1089ff., 1272, 1285
 inverse hyperbolic 178, 255
 inverse trigonometric 255
 Jacobian elliptic 261, 1137f.
 Kolmogorov-Smirnov probability 618f.,
 640, 1274, 1281
 Legendre polynomial 172, 246, 674, 1122,
 1291
 logarithm 255
 modified Bessel 229ff., 1109ff.
 modified Bessel, fractional order 239ff.,
 1118ff.
 overloading 1083
 parallel evaluation 986, 1009, 1084, 1087,
 1090, 1102, 1128, 1134
 path integration to evaluate 201ff.
 pathological 99f., 343
 Poisson cumulant 214
 representations of 490
 routine for plotting a 342, 1182
 sine and cosine integrals 248, 250ff.,
 1125f.
 sn, dn, cn 261, 1137f.
 spherical harmonics 246ff., 1122
 spheroidal harmonic 764ff., 770ff., 1319ff.,
 1323ff.
 Student's probability 221f.
 variable number of arguments 1022
 Weber 204
- Functional iteration, for implicit equations 740f.
 FWHM (full width at half maximum) 548f.
- G**amma deviate 282f., 1153f.
 Gamma function 206ff., 1085
 incomplete *see* Incomplete gamma function
 Garbage collection 956
 Gather-scatter operations 2/xiif., 984, 1002,
 1032, 1034
 communication bottleneck 969, 981, 1250
 many-to-one 984, 1002, 1032, 1034
 Gauss-Chebyshev integration 141, 144, 512f.
 Gauss-Hermite integration 144, 789
 abscissas and weights 147, 1062
 normalization 147
 Gauss-Jacobi integration 144
 abscissas and weights 148, 1063
 Gauss-Jordan elimination 27ff., 33, 64, 1014f.
 operation count 34, 39
 solution of normal equations 667, 1288
 storage requirements 30
 Gauss-Kronrod quadrature 154
 Gauss-Laguerre integration 144, 789, 1060
 Gauss-Legendre integration 145f., 1059
 see also Gaussian integration
 Gauss-Lobatto quadrature 154, 190, 512
 Gauss-Radau quadrature 154
 Gauss-Seidel method (relaxation) 855, 857,
 864ff., 1338
 nonlinear 876, 1341
 Gauss transformation 256
 Gaussian (normal) distribution 267, 652, 798
 central limit theorem 652f.
 deviates from 279f., 571, 1152
 kurtosis of 606
 multivariate 690
 semi-invariants of 608
 tails compared to Poisson 653
 two-dimensional (binormal) 631
 variance of skewness of 606
 Gaussian elimination 33f., 51, 55, 1014f.
 fill-in 45, 64
 integral equations 786, 1326
 operation count 34
 outer product variant 1017
 in reduction to Hessenberg form 478,
 1231
 relaxation solution of boundary value problems 753ff., 777, 1316
 Gaussian function
 Hardy's theorem on Fourier transforms 600
 see also Gaussian (normal) distribution
 Gaussian integration 127, 140ff., 789, 1059ff.
 calculation of abscissas and weights 142ff.,
 1009, 1059ff.
 error estimate in solution 784
 extensions of 153f.
 Golub-Welsch algorithm for weights and
 abscissas 150, 1064
 for integral equations 781, 783, 1325
 from known recurrence relation 150, 1064

- nonclassical weight function 151ff., 788f., 1064f., 1328f.
 and orthogonal polynomials 142, 1009, 1061
 parallel calculation of formulas 1009, 1061
 preassigned nodes 153f.
 weight function $\log x$ 153
 weight functions 140ff., 788f., 1059ff., 1328f.
- Gear's method (stiff ODEs) 730
- Geiger counter 266
- Generalized eigenvalue problems 455
- Generalized minimum residual method (GMRES) 78
- Generic interface *see* Interface, generic
- Generic procedures 939, 1083, 1094, 1096, 1364
 elemental 940, 942, 946f., 1015, 1083
- Geometric progression 972, 996f., 1365, 1372ff.
- geop() utility function 972, 974, 989, 996, 1127
- Geophysics, use of Backus-Gilbert method 809
- Gershberg-Saxton algorithm 805
- get_diag() utility function 985, 989, 1005, 1226
- Gilbert and Sullivan 714
- Givens reduction 462f., 473
 fast 463
 operation count 463
- Glassman, A.J. 180
- Global optimization 387f., 436ff., 650, 1219ff.
 continuous variables 443f., 1222
- Global variables 940, 953f., 1210
 allocatable array method 954, 1197, 1212, 1266, 1287, 1298
 communicated via internal subprogram 954, 957f., 1067, 1226
 danger of 957, 1209, 1293, 1296
 pointer method 954, 1197, 1212, 1266, 1287, 1302
- Globally convergent
 minimization 418ff., 1215
 root finding 373, 376ff., 382, 749f., 752, 1196, 1314f.
- GMRES (generalized minimum residual method) 78
- GNU Emacs 1/xvi
- Godunov's method 837
- Golden mean (golden ratio) 21, 349, 392f., 399
- Golden section search 341, 389ff., 395, 1202ff.
- Golub-Welsch algorithm, for Gaussian quadrature 150, 1064
- Goodness-of-fit 650, 654, 657f., 662, 690, 1285
- GOTO statements, danger of 9, 959
- Gram-Schmidt
 biorthogonalization 415f.
 orthogonalization 94, 450f., 1039
 SVD as alternative to 58
- Graphics, function plotting 342, 1182f.
- Gravitational potential 519
- Gray code 300, 881, 886ff., 1344
- Greenbaum, A. 79
- Gregorian calendar 13, 16, 1011, 1013
- Grid square 116f.
- Group, dihedral 894, 1345
- Guard digits 882, 1343
- H**alf weighting 867, 1337
- Halton's quasi-random sequence 300
- Hamming window 547
- Hamming's motto 341
- Hann window 547
- Harmonic analysis *see* Fourier transform
- Hashing 293, 1144, 1148, 1156
 for random number seeds 1147f.
- HDLC checksum 890
- Heap (data structure) 327f., 336, 897, 1179
- Heapsort 320, 327f., 336, 1171f., 1179
- Helmholtz equation 852
- Hermite polynomials 144, 147
 approximation of roots 1062
- Hermitian matrix 450ff., 475
- Hertz (unit of frequency) 490
- Hessenberg matrix 94, 453, 470, 476ff., 488, 1231
see also Matrix
- Hessian matrix 382, 408, 415f., 419f., 676ff., 803, 815
 is inverse of covariance matrix 667, 679
 second derivatives in 676
- Hexadecimal constants 17f., 276, 293
 initialization 959
- Hierarchically band diagonal matrix 598
- Hierarchy of program structure 6ff.
- High-order not same as high-accuracy 100f., 124, 389, 399, 705, 709, 741
- High-pass filter 551
- High-Performance Fortran (HPF) 2/xvf., 964, 981, 984
 scatter-with-add 1032
- Hilbert matrix 83
- Home page, Numerical Recipes 1/xx, 2/xvii
- Homogeneous linear equations 53
- Hook step methods 386
- Hotelling's method for matrix inverse 49, 598
- Householder transformation 52, 453, 462ff., 469, 473, 475, 478, 481ff., 1227f.
 operation count 467
 in QR decomposition 92, 1039
- HPF *see* High-Performance Fortran
- Huffman coding 564, 881, 896f., 902, 1346ff.
- huge() intrinsic function 951
- Hyperbolic functions, explicit formulas for
 inverse 178
- Hyperbolic partial differential equations 818
 advective equation 826
 flux-conservative initial value problems 825ff.
- Hypergeometric function 202f., 263ff.
 routine for 264f., 1138
- Hypothesis, null 603
- I**2B, defined 937

- I4B, defined 937
 iand() intrinsic function 951
 ibclr() intrinsic function 951
 ibits() intrinsic function 951
 IBM 1/xxiii, 2/xix
 bad random number generator 268
 Fortran 90 compiler 2/viii
 PC 4, 276, 293, 886
 PC-RT 4
 radix base for floating point arithmetic 476
 RS6000 2/viii, 4
 IBM checksum 894
 ibset() intrinsic function 951
 ICCG (incomplete Cholesky conjugate gradient method) 824
 ICF (intrinsic correlation function) model 817
 Identity (unit) matrix 25
 IEEE floating point format 276, 882f., 1343
 ieor() intrinsic function 951
 if statement, arithmetic 2/xi
 if structure 12f.
 ifirstloc() utility function 989, 993, 1041, 1346
 IIR (infinite impulse response) filter 552ff., 566
 Ill-conditioned integral equations 780
 Image processing 519, 803
 cosine transform 513
 fast Fourier transform (FFT) 519, 523, 803
 as an inverse problem 803
 maximum entropy method (MEM) 809ff.
 from modulus of Fourier transform 805
 wavelet transform 596f., 1267f.
 imaxloc() utility function 989, 993, 1017
 iminloc() utility function 989, 993, 1046, 1076
 Implicit
 function theorem 340
 pivoting 30, 1014
 shifts in QL method 472ff.
 Implicit differencing 827
 for diffusion equation 840
 for stiff equations 729, 740, 1308
 IMPLICIT NONE statement 2/xiv, 936
 Implied do-list 968, 971, 1127
 Importance sampling, in Monte Carlo 306f.
 Improper integrals 135ff., 1055
 Impulse response function 531, 540, 552
 IMSL 1/xxiii, 2/xx, 26, 64, 205, 364, 369, 454
 In-place selection 335, 1178f.
 Included file, superseded by module 940
 Incomplete beta function 219ff., 1098ff.
 for F-test 613, 1271
 routine for 220f., 1097
 for Student's t 610, 613, 1269
 Incomplete Cholesky conjugate gradient method (ICCG) 824
 Incomplete gamma function 209ff., 1089ff.
 for chi-square 615, 654, 657f., 1272, 1285
 deviates from 282f., 1153
 in mode estimation 610
 routine for 211f., 1089
 Increment of linear congruential generator 268
 Indentation of blocks 9
 Index 934ff., 1446ff.
 this entry 1464
 Index loss 967f., 1038
 Index table 320, 329f., 1173ff., 1176
 Inequality constraints 423
 Inheritance 8
 Initial value problems 702, 818f.
 see also Differential equations;
 Partial differential equations
 Initialization of derived data type 2/xv
 Initialization expression 943, 959, 1012, 1127
 Injection operator 864, 1337
 Instability *see* Stability
 Integer model, in Fortran 90 1144, 1149, 1156
 Integer programming 436
 Integral equations 779ff.
 adaptive stepsize control 788
 block-by-block method 788
 correspondence with linear algebraic equations 779ff.
 degenerate kernel 785
 eigenvalue problems 780, 785
 error estimate in solution 784
 Fredholm 779f., 782ff., 1325, 1331
 Fredholm alternative 780
 homogeneous, second kind 785, 1325
 ill-conditioned 780
 infinite range 789
 inverse problems 780, 795ff.
 kernel 779
 nonlinear 781, 787
 Nystrom method 782ff., 789, 1325
 product Nystrom method 789, 1328ff.
 with singularities 788ff., 1328ff.
 with singularities, worked example 792, 1328ff.
 subtraction of singularity 789
 symmetric kernel 785
 unstable quadrature 787f.
 Volterra 780f., 786ff., 1326f.
 wavelets 782
 see also Inverse problems
 Integral operator, wavelet approximation of 597, 782
 Integration of functions 123ff., 1052ff.
 cosine integrals 250, 1125
 Fourier integrals 577ff., 1261
 Fourier integrals, infinite range 583
 Fresnel integrals 248, 1123
 Gauss-Hermite 147f., 1062
 Gauss-Jacobi 148, 1063
 Gauss-Laguerre 146, 1060
 Gauss-Legendre 145, 1059
 integrals that are elliptic integrals 254
 path integration 201ff.
 sine integrals 250, 1125
 see also Quadrature
 Integro-differential equations 782
 INTENT attribute 1072, 1092
 Interface (Fortran 90) 939, 942, 1067

- for communication between program parts 957, 1209, 1293, 1296
 explicit 939, 942, 1067, 1384
 generic 2/xiii, 940, 1015, 1083, 1094, 1096
 implicit 939
 for Numerical Recipes 1384ff.
- Interface block 939, 1084, 1384
- Interface, in programs 2, 8
- Intermediate value theorem 343
- Internal subprogram (Fortran 90) 2/xiv, 954, 957, 1067, 1202f., 1226
 nesting of 2/xii
 resembles C macro 1302
 supersedes statement function 1057, 1256
- International Standards Organization (ISO) 2/xf., 2/xiii
- Internet, availability of code over 1/xx, 2/xvii
- Interpolation 99ff.
 Aitken's algorithm 102
 avoid 2-stage method 100
 avoid in Fourier analysis 569
 bicubic 118f., 1049f.
 bilinear 117
 caution on high-order 100
 coefficients of polynomial 100, 113ff., 191, 575, 1047f., 1078
 for computing Fourier integrals 578
 error estimates for 100
 of functions with poles 104ff., 1043f.
 inverse quadratic 353, 395ff., 1204
 multidimensional 101f., 116ff., 1049ff.
 in multigrid method 866, 1337
 Neville's algorithm 102f., 182, 1043
 Nystrom 783, 1326
 offset arrays 104, 113
 operation count for 100
 operator 864, 1337
 order of 100
 and ordinary differential equations 101
 oscillations of polynomial 100, 116, 389, 399
 parabolic, for minimum finding 395, 1204
 polynomial 99, 102ff., 182, 1043
 rational Chebyshev approximation 197ff., 1081
 rational function 99, 104ff., 194ff., 225, 718ff., 726, 1043f., 1080, 1306
 reverse (extrapolation) 574, 1261
 spline 100, 107ff., 120f., 1044f., 1050f.
 trigonometric 99
see also Fitting
- Interprocessor communication 969, 981
- Interval variable (statistics) 623
- Intrinsic correlation function (ICF) model 817
- Intrinsic data types 937
- Intrinsic procedures
 array inquiry 938, 942, 948ff.
 array manipulation 950
 array reduction 948
 array unary and binary functions 949
 backwards-compatibility 946
 bit manipulation 2/xiii, 951
 character 952
 cmplx 1254
- conversion elemental 946
 elemental 940, 942, 946f., 951, 1083, 1364
 generic 939, 1083f., 1364
 lexical comparison 952
 numeric inquiry 2/xiv, 1107, 1231, 1343
 numerical 946, 951f.
 numerical representation 951
 pack used for sorting 1171
 random_number 1143
 real 1254
 top 10 945
 truncation 946f.
see also Fortran 90
- Inverse hyperbolic function 178, 255
- Inverse iteration *see* Eigensystems
- Inverse problems 779, 795ff.
 Backus-Gilbert method 806ff.
 Bayesian approach 799, 810f., 816f.
 central idea 799
 constrained linear inversion method 799ff.
 data inversion 807
 deterministic constraints 804ff.
 in geophysics 809
 Gerchberg-Saxton algorithm 805
 incomplete Fourier coefficients 813
 and integral equations 780
 linear regularization 799ff.
 maximum entropy method (MEM) 810, 815f.
 MEM demystified 814
 Phillips-Twomey method 799ff.
 principal solution 797
 regularization 796ff.
 regularizing operator 798
 stabilizing functional 798
 Tikhonov-Miller regularization 799ff.
 trade-off curve 795
 trade-off curve, Backus-Gilbert method 809
 two-dimensional regularization 803
 use of conjugate gradient minimization 804, 815
 use of convex sets 804
 use of Fourier transform 803, 805
 Van Cittert's method 804
- Inverse quadratic interpolation 353, 395ff., 1204
- Inverse response kernel, in Backus-Gilbert method 807
- Inverse trigonometric function 255
- ior() intrinsic function 951
- ISBN (International Standard Book Number)
 checksum 894
- ishft() intrinsic function 951
- ishftc() intrinsic function 951
- ISO (International Standards Organization) 2/xf., 2/xiii
- Iterated integrals 155
- Iteration 9f.
 functional 740f.
 to improve solution of linear algebraic equations 47ff., 195, 1022
 for linear algebraic equations 26

- required for two-point boundary value problems 745
in root finding 340f.
- Iteration matrix 856
- ITPACK 71
- Iverson, John 2/xi
- J**acobi matrix, for Gaussian quadrature 150, 1064
- Jacobi polynomials, approximation of roots 1064
- Jacobi transformation (or rotation) 94, 453, 456ff., 462, 475, 489, 1041, 1225
- Jacobian determinant 279, 774
- Jacobian elliptic functions 261, 1137f.
- Jacobian matrix 374, 376, 379, 382, 731, 1197f., 1309
singular in Newton's rule 386
- Jacobi's method (relaxation) 855ff., 864
- Jenkins-Traub method 369
- Julian Day 1, 13, 16, 936, 1010ff.
- Jump transposition errors 895
- K**-S test *see* Kolmogorov-Smirnov test
- Kalman filter 700
- Kanji 2/xii
- Kaps-Rentrop method 730, 1308
- Kendall's tau 634, 637ff., 1279
- Kennedy, Ken 2/xv
- Kepler's equation 1061
- Kermit checksum 889
- Kernel 779
averaging, in Backus-Gilbert method 807
degenerate 785
finite rank 785
inverse response 807
separable 785
singular 788f., 1328
symmetric 785
- Keys used in sorting 329, 889
- Keyword argument 2/xiv, 947f., 1341
- kind() intrinsic function 951
- KIND parameter 946, 1261, 1284
and cmplx() intrinsic function 1125, 1192, 1254
- default 937
- for Numerical Recipes 1361
- for random numbers 1144
- and real() intrinsic function 1125
- Kolmogorov-Smirnov test 614, 617ff., 694, 1273f.
two-dimensional 640, 1281ff.
variants 620ff., 640, 1281
- Kuiper's statistic 621
- Kurtosis 606, 608, 1269
- L**-estimate 694
- Labels, statement 9
- Lag 492, 538, 553
- Lagged Fibonacci generator 1142, 1148ff.
- Lagrange multiplier 795
- Lagrange's formula for polynomial interpolation 84, 102f., 575, 578
- Laguerre polynomials, approximation of roots 1061
- Laguerre's method 341, 365f., 1191f.
- Lanczos lemma 498f.
- Lanczos method for gamma function 206, 1085
- Landen transformation 256
- LAPACK 26, 1230
- Laplace's equation 246, 818
see also Poisson equation
- Las Vegas 625
- Latin square or hypercube 305f.
- Laurent series 566
- Lax method 828ff., 836, 845f.
multidimensional 845f.
- Lax-Wendroff method 835ff.
- lbound() intrinsic function 949
- Leakage in power spectrum estimation 544, 548
- Leakage width 548f.
- Leapfrog method 833f.
- Least squares filters *see* Savitzky-Golay filters
- Least squares fitting 645, 651ff., 655ff., 660ff., 665ff., 1285f., 1288f.
contrasted to general minimization problems 684ff.
- degeneracies in 671f., 674
- Fourier components 570
as M-estimate for normal errors 696
as maximum likelihood estimator 652
as method for smoothing data 645, 1283
- Fourier components 1258
- freezing parameters in 668, 700
- general linear case 665ff., 1288, 1290f.
- Levenberg-Marquardt method 678ff., 816, 1292f.
- Lomb periodogram 570, 1258
- multidimensional 675
- nonlinear 386, 675ff., 816, 1292
- nonlinear, advanced methods 683
- normal equations 645, 666f., 800, 1288
- normal equations often singular 670, 674
- optimal (Wiener) filtering 540f.
- QR method in 94, 668
- for rational Chebyshev approximation 199f., 1081f.
- relation to linear correlation 630, 658
- Savitzky-Golay filter as 645, 1283
- singular value decomposition (SVD) 25f., 51ff., 199f., 670ff., 1081, 1290
- skewed by outliers 653
- for spectral analysis 570, 1258
- standard (probable) errors on fitted parameters 667, 671
- weighted 652
- see also* Fitting
- L'Ecuyer's long period random generator 271, 273
- Least squares fitting
standard (probable) errors on fitted parameters 1288, 1290
weighted 1285
- Left eigenvalues or eigenvectors 451
- Legal matters 1/xx, 2/xvii
- Legendre elliptic integral *see* Elliptic integrals

- Legendre polynomials 246, 1122
 fitting data to 674, 1291f.
 recurrence relation 172
 shifted monic 151
 see also Associated Legendre polynomials;
 Spherical harmonics
- Lehmer-Schur algorithm 369
- Lemarie's wavelet 593
- Lentz's method for continued fraction 165,
 212
- Lepage, P. 309
- Leptokurtic distribution 606
- Levenberg-Marquardt algorithm 386, 678ff.,
 816, 1292
 advanced implementation 683
- Levinson's method 86, 1038
- Lewis, H.W. 275
- Lexical comparison functions 952
- LGT, defined 937
- License information 1/xx, 2/xviif.
- Limbo 356
- Limit cycle, in Laguerre's method 365
- Line minimization *see* Minimization, along a ray
- Line search *see* Minimization, along a ray
- Linear algebra, intrinsic functions for parallelization 969f., 1026, 1040, 1200,
 1326
- Linear algebraic equations 22ff., 1014
 band diagonal 43ff., 1019
 biconjugate gradient method 77, 1034ff.
 Cholesky decomposition 89f., 423, 455,
 668, 1038f.
 complex 41
 computing $\mathbf{A}^{-1} \cdot \mathbf{B}$ 40
 conjugate gradient method 77ff., 599,
 1034
 cyclic tridiagonal 67, 1030
 direct methods 26, 64, 1014, 1030
 Fortran 90 vs. library routines 1016
 Gauss-Jordan elimination 27ff., 1014
 Gaussian elimination 33f., 1014f.
 Hilbert matrix 83
 Hotelling's method 49, 598
 and integral equations 779ff., 783, 1325
 iterative improvement 47ff., 195, 1022
 iterative methods 26, 77ff., 1034
 large sets of 23
 least squares solution 53ff., 57f., 199f.,
 671, 1081, 1290
 LU decomposition 34ff., 195, 386, 732,
 783, 786, 801, 1016, 1022, 1325f.
 nonsingular 23
 overdetermined 25f., 199, 670, 797
 partitioned 70
 QR decomposition 91f., 382, 386, 668,
 1039f., 1199
 row vs. column elimination 31f.
 Schultz's method 49, 598
 Sherman-Morrison formula 65ff., 83
 singular 22, 53, 58, 199, 670
 singular value decomposition (SVD) 51ff.,
 199f., 670ff., 797, 1022, 1081, 1290
 sparse 23, 43, 63ff., 732, 804, 1020f.,
 1030
- summary of tasks 25f.
 Toeplitz 82, 85ff., 195, 1038
 tridiagonal 26, 42f., 64, 109, 150, 453f.,
 462ff., 469ff., 488, 839f., 853, 861f.,
 1018f., 1227ff.
 Vandermonde 82ff., 114, 1037, 1047
 wavelet solution 597ff., 782
 Woodbury formula 68ff., 83
 see also Eigensystems
- Linear congruential random number generator
 267ff., 1142
 choice of constants for 274ff.
- Linear constraints 423
- Linear convergence 346, 393
- Linear correlation (statistics) 630ff., 1276
- Linear dependency
 constructing orthonormal basis 58, 94
 of directions in N -dimensional space 409
 in linear algebraic equations 22f.
- Linear equations *see* Differential equations;
 Integral equations; Linear algebraic equations
- Linear inversion method, constrained 799ff.
- Linear prediction 557ff.
 characteristic polynomial 559
 coefficients 557ff., 1256
 compared to maximum entropy method
 558
 compared with regularization 801
 contrasted to polynomial extrapolation
 560
 related to optimal filtering 558
 removal of bias in 563
 stability 559f., 1257
- Linear predictive coding (LPC) 563ff.
- Linear programming 387, 423ff., 1216ff.
 artificial variables 429
 auxiliary objective function 430
 basic variables 426
 composite simplex algorithm 435
 constraints 423
 convergence criteria 432
 degenerate feasible vector 429
 dual problem 435
 equality constraints 423
 feasible basis vector 426
 feasible vector 424
 fundamental theorem 426
 inequality constraints 423
 left-hand variables 426
 nonbasic variables 426
 normal form 426
 objective function 424
 optimal feasible vector 424
 pivot element 428f.
 primal-dual algorithm 435
 primal problem 435
 reduction to normal form 429ff.
 restricted normal form 426ff.
 revised simplex method 435
 right-hand variables 426
 simplex method 402, 423ff., 431ff., 1216ff.
 slack variables 429
 tableau 427
 vertex of simplex 426

- Linear recurrence *see* Recurrence relation
 Linear regression 655ff., 660ff., 1285ff.
see also Fitting
 Linear regularization 799ff.
 LINPACK 26
 Literal constant 937, 1361
 Little-endian 293
 Local extrapolation 709
 Local extremum 387f., 437
 Localization of roots *see* Bracketing
 Logarithmic function 255
 Lomb periodogram method of spectral analysis 569f., 1258f.
 fast algorithm 574f., 1259
 Loops 9f.
 Lorentzian probability distribution 282, 696f.
 Low-pass filter 551, 644f., 1283f.
 Lower subscript 944
 lower_triangle() utility function 989, 1007,
 1200
 LP coefficients *see* Linear prediction
 LPC (linear predictive coding) 563ff.
 LU decomposition 34ff., 47f., 51, 55, 64, 97,
 374, 667, 732, 1016, 1022
 for $\mathbf{A}^{-1} \cdot \mathbf{B}$ 40
 backsubstitution 39, 1017
 band diagonal matrix 43ff., 1020
 complex equations 41f.
 Crout's algorithm 36ff., 45, 1017
 for integral equations 783, 786, 1325f.
 for inverse iteration of eigenvectors 488
 for inverse problems 801
 for matrix determinant 41
 for matrix inverse 40, 1016
 for nonlinear sets of equations 374, 386,
 1196
 operation count 36, 39
 outer product Gaussian elimination 1017
 for Padé approximant 195, 1080
 pivoting 37f., 1017
 repeated backsubstitution 40, 46
 solution of linear algebraic equations 40,
 1017
 solution of normal equations 667
 for Toeplitz matrix 87
 Lucifer 290
- M&R** (Metcalf and Reid) 935
 M-estimates 694ff.
 how to compute 697f.
 local 695ff.
see also Maximum likelihood estimate
 Machine accuracy 19f., 881f., 1189, 1343
 Macintosh, *see* Apple Macintosh
 Machly's procedure 364, 371
 Magic
 in MEM image restoration 814
 in Padé approximation 195
 Mantissa in floating point format 19, 882,
 909, 1343
 Marginals 624
 Marquardt method (least squares fitting) 678ff.,
 816, 1292f.
 Marsaglia shift register 1142, 1148ff.
 Marsaglia, G. 1142, 1149
- mask 1006f., 1102, 1200, 1226, 1305, 1333f.,
 1368, 1378, 1382
 optional argument 948
 optional argument, facilitates parallelism 967f., 1038
 Mass, center of 295ff.
 MasterCard checksum 894
 Mathematical Center (Amsterdam) 353
 Mathematical intrinsic functions 946, 951f.
 matmul() intrinsic function 945, 949, 969,
 1026, 1040, 1050, 1076, 1200, 1216,
 1290, 1326
 Matrix 23ff.
 add vector to diagonal 1004, 1234, 1366,
 1381
 approximation of 58f., 598f.
 band diagonal 42ff., 64, 1019
 band triangular 64
 banded 26, 454
 bidiagonal 52
 block diagonal 64, 754
 block triangular 64
 block tridiagonal 64
 bordered 64
 characteristic polynomial 449, 469
 Cholesky decomposition 89f., 423, 455,
 668, 1038f.
 column augmented 28, 1014
 complex 41
 condition number 53, 78
 create unit matrix 1006, 1382
 curvature 677
 cyclic banded 64
 cyclic tridiagonal 67, 1030
 defective 450, 476, 489
 of derivatives *see* Hessian matrix; Jacobian
 determinant
 design (fitting) 645, 665, 801, 1082
 determinant of 25, 41
 diagonal of sparse matrix 1033ff.
 diagonalization 452ff., 1225ff.
 elementary row and column operations 28f.
 finite differencing of partial differential
 equations 821ff.
 get diagonal 985, 1005, 1226f., 1366,
 1381f.
 Hermitian 450, 454, 475
 Hermitian conjugate 450
 Hessenberg 94, 453, 470, 476ff., 488,
 1231ff.
 Hessian *see* Hessian matrix
 hierarchically band diagonal 598
 Hilbert 83
 identity 25
 ill-conditioned 53, 56, 114
 indexed storage of 71f., 1030
 and integral equations 779, 783, 1325
 inverse 25, 27, 34, 40, 65ff., 70, 95ff.,
 1014, 1016f.
 inverse, approximate 49
 inverse by Hotelling's method 49, 598
 inverse by Schultz's method 49, 598
 inverse multiplied by a matrix 40
 iteration for inverse 49, 598

- Jacobi transformation 453, 456ff., 462, 1225f.
 Jacobian 731, 1309
 logical dimension 24
 lower triangular 34f., 89, 781, 1016
 lower triangular mask 1007, 1200, 1382
 multiplication denoted by dot 23
 multiplication, intrinsic function 949, 969, 1026, 1040, 1050, 1200, 1326
 norm 50
 normal 450ff.
 nullity 53
 nullspace 25, 53f., 449, 795
 orthogonal 91, 450, 463ff., 587
 orthogonal transformation 452, 463ff., 469, 1227
 orthonormal basis 58, 94
 outer product denoted by cross 66, 420
 partitioning for determinant 70
 partitioning for inverse 70
 pattern multiply of sparse 74
 physical dimension 24
 positive definite 26, 89f., 668, 1038
 QR decomposition 91f., 382, 386, 668, 1039, 1199
 range 53
 rank 53
 residual 49
 row and column indices 23
 row vs. column operations 31f.
 self-adjoint 450
 set diagonal elements 1005, 1200, 1366, 1382
 similarity transform 452ff., 456, 476, 478, 482
 singular 53f., 58, 449
 singular value decomposition 26, 51ff., 797
 sparse 23, 63ff., 71, 598, 732, 754, 804, 1030ff.
 special forms 26
 splitting in relaxation method 856f.
 spread 808
 square root of 423, 455
 symmetric 26, 89, 450, 454, 462ff., 668, 785, 1038, 1225, 1227
 threshold multiply of sparse 74, 1031
 Toeplitz 82, 85ff., 195, 1038
 transpose() intrinsic function 950
 transpose of sparse 73f., 1033
 triangular 453
 tridiagonal 26, 42f., 64, 109, 150, 453f., 462ff., 469ff., 488, 839f., 853, 861f., 1018f., 1227ff.
 tridiagonal with fringes 822
 unitary 450
 updating 94, 382, 386, 1041, 1199
 upper triangular 34f., 91, 1016
 upper triangular mask 1006, 1226, 1305, 1382
 Vandermonde 82ff., 114, 1037, 1047
see also Eigensystems
 Matrix equations *see* Linear algebraic equations
 Matterhorn 606
 maxexponent() intrinsic function 1107
 Maximization *see* Minimization
 Maximum entropy method (MEM) 565ff., 1258
 algorithms for image restoration 815f.
 Bayesian 816f.
 Cornwell-Evans algorithm 816
 demystified 814
 historic vs. Bayesian 816f.
 image restoration 809ff.
 intrinsic correlation function (ICF) model 817
 for inverse problems 809ff.
 operation count 567
see also Linear prediction
 Maximum likelihood estimate (M-estimates) 690, 694ff.
 and Bayes' Theorem 811
 chi-square test 690
 defined 652
 how to compute 697f.
 mean absolute deviation 696, 698, 1294
 relation to least squares 652
 maxloc() intrinsic function 949, 992f., 1015
 modified in Fortran 95 961
 maxval() intrinsic function 945, 948, 961, 1016, 1273
 Maxwell's equations 825f.
 Mean(s)
 of distribution 604f., 608f., 1269
 statistical differences between two 609ff., 1269f.
 Mean absolute deviation of distribution 605, 696, 1294
 related to median 698
 Measurement errors 650
 Median 320
 calculating 333
 of distribution 605, 608f.
 as L-estimate 694
 role in robust straight line fitting 698
 by selection 698, 1294
 Median-of-three, in Quicksort 324
 MEM *see* Maximum entropy method (MEM)
 Memory leak 953, 956, 1071, 1327
 Memory management 938, 941f., 953ff., 1327, 1336
 merge construct 945, 950, 1099f.
 for conditional scalar expression 1010, 1094f.
 contrasted with where 1023
 parallelization 1011
 Merge-with-dummy-values idiom 1090
 Merit function 650
 in general linear least squares 665
 for inverse problems 797
 nonlinear models 675
 for straight line fitting 656, 698
 for straight line fitting, errors in both coordinates 660, 1286
 Mesh-drift instability 834f.
 Mesokurtic distribution 606
 Metcalf, Michael 2/viii
see also M&R
 Method of regularization 799ff.

- Metropolis algorithm 437f., 1219
 Microsoft 1/xxii, 2/xix
 Microsoft Fortran PowerStation 2/viii
 Midpoint method *see* Modified midpoint method;
 Semi-implicit midpoint rule
 Mikado, or Town of Titipu 714
 Miller's algorithm 175, 228, 1106
 MIMD machines (Multiple Instruction Multiple
 Data) 964, 985, 1071, 1084
 Minimal solution of recurrence relation 174
 Minimax polynomial 186, 198, 1076
 Minimax rational function 198
 Minimization 387ff.
 along a ray 77, 376f., 389, 406ff., 412f.,
 415f., 418, 1195f., 1211, 1213
 annealing, method of simulated 387f.,
 436ff., 1219ff.
 bracketing of minimum 390ff., 402, 1201f.
 Brent's method 389, 395ff., 399, 660f.,
 1204ff., 1286
 Broyden-Fletcher-Goldfarb-Shanno algo-
 rithm 390, 418ff., 1215
 chi-square 653ff., 675ff., 1285, 1292
 choice of methods 388f.
 combinatorial 436f., 1219
 conjugate gradient method 390, 413ff.,
 804, 815, 1210, 1214
 convergence rate 393, 409
 Davidon-Fletcher-Powell algorithm 390,
 418ff., 1215
 degenerate 795
 direction-set methods 389, 406ff., 1210ff.
 downhill simplex method 389, 402ff.,
 444, 697f., 1208, 1222ff.
 finding best-fit parameters 650
 Fletcher-Reeves algorithm 390, 414ff.,
 1214
 functional 795
 global 387f., 443f., 650, 1219, 1222
 globally convergent multidimensional 418,
 1215
 golden section search 390ff., 395, 1202ff.
 multidimensional 388f., 402ff., 1208ff.,
 1214
 in nonlinear model fitting 675f., 1292
 Polak-Ribiere algorithm 389, 414ff., 1214
 Powell's method 389, 402, 406ff., 1210ff.
 quasi-Newton methods 376, 390, 418ff.,
 1215
 and root finding 375
 scaling of variables 420
 by searching smaller subspaces 815
 steepest descent method 414, 804
 termination criterion 392, 404
 use in finding double roots 341
 use for sparse linear systems 77ff.
 using derivatives 389f., 399ff., 1205ff.
 variable metric methods 390, 418ff., 1215
see also Linear programming
 Minimum residual method, for sparse system
 78
 minloc() intrinsic function 949, 992f.
 modified in Fortran 95 961
 MINPACK 683
 minval() intrinsic function 948, 961
 MIPS 886
 Missing data problem 569
 Mississippi River 438f., 447
 MMP (massively multiprocessor) machines
 965ff., 974, 981, 984, 1016ff., 1021,
 1045, 1226ff., 1250
 Mode of distribution 605, 609
 Modeling of data *see* Fitting
 Model-trust region 386, 683
 Modes, homogeneous, of recursive filters 554
 Modified Bessel functions *see* Bessel func-
 tions
 Modified Lentz's method, for continued frac-
 tions 165
 Modified midpoint method 716ff., 720, 1302f.
 Modified moments 152
 Modula-2 7
 Modular arithmetic, without overflow 269,
 271, 275
 Modular programming 2/xiii, 7f., 956ff.,
 1209, 1293, 1296, 1346
 MODULE facility 2/xiii, 936f., 939f., 957,
 1067, 1298, 1320, 1322, 1324, 1330,
 1346
 initializing random number generator 1144ff.
 in nr.f90 936, 941f., 1362, 1384ff.
 in nrtype.f90 936f., 1361f.
 in nrutil.f90 936, 1070, 1362, 1364ff.
 sparse matrix 1031
 undefined variables on exit 953, 1266
 Module subprogram 940
 modulo() intrinsic function 946, 1156
 Modulus of linear congruential generator 268
 Moments
 of distribution 604ff., 1269
 filter that preserves 645
 modified problem of 151f.
 problem of 83
 and quadrature formulas 791, 1328
 semi-invariants 608
 Monic polynomial 142f.
 Monotonicity constraint, in upwind differenc-
 ing 837
 Monte Carlo 155ff., 267
 adaptive 306ff., 1161ff.
 bootstrap method 686f.
 comparison of sampling methods 309
 exploration of binary tree 290
 importance sampling 306f.
 integration 124, 155ff., 295ff., 306ff.,
 1161
 integration, recursive 314ff., 1164ff.
 integration, using Sobol' sequence 304
 integration, VEGAS algorithm 309ff.,
 1161
 and Kolmogorov-Smirnov statistic 622,
 640
 partial differential equations 824
 quasi-random sequences in 299ff.
 quick and dirty 686f.
 recursive 306ff., 314ff., 1161, 1164ff.
 significance of Lomb periodogram 570
 simulation of data 654, 684ff., 690
 stratified sampling 308f., 314, 1164

- Moon, calculate phases of 1f., 14f., 936, 1010f.
- Mother functions 584
- Mother Nature 684, 686
- Moving average (MA) model 566
- Moving window averaging 644
- Mozart 9
- MS 1/xxii, 2/xix
- Muller's method 364, 372
- Multidimensional
- confidence levels of fitting 688f.
 - data, use of binning 623
 - Fourier transform 515ff., 1241, 1246, 1251
 - Fourier transform, real data 519ff., 1248f.
 - initial value problems 844ff.
 - integrals 124, 155ff., 295ff., 306ff., 1065ff., 1161ff.
 - interpolation 116ff., 1049ff.
 - Kolmogorov-Smirnov test 640, 1281
 - least squares fitting 675
 - minimization 402ff., 406ff., 413ff., 1208ff., 1214f., 1222ff.
 - Monte Carlo integration 295ff., 306ff., 1161ff.
 - normal (Gaussian) distribution 690
 - optimization 388f.
 - partial differential equations 844ff.
 - root finding 340ff., 358, 370, 372ff., 746, 749f., 752, 754, 1194ff., 1314ff.
 - search using quasi-random sequence 300
 - secant method 373, 382f., 1199f.
 - wavelet transform 595, 1267f.
- Multigrid method 824, 862ff., 1334ff.
- avoid SOR 866
 - boundary conditions 868f.
 - choice of operators 868
 - coarse-to-fine operator 864, 1337
 - coarse-grid correction 864f.
 - cycle 865
 - dual viewpoint 875
 - fine-to-coarse operator 864, 1337
 - full approximation storage (FAS) algorithm 874, 1339ff.
 - full multigrid method (FMG) 863, 868, 1334ff.
 - full weighting 867
 - Gauss-Seidel relaxation 865f., 1338
 - half weighting 867, 1337
 - importance of adjoint operator 867
 - injection operator 864, 1337
 - interpolation operator 864, 1337
 - line relaxation 866
 - local truncation error 875
 - Newton's rule 874, 876, 1339, 1341
 - nonlinear equations 874ff., 1339ff.
 - nonlinear Gauss-Seidel relaxation 876, 1341
 - odd-even ordering 866, 869, 1338
 - operation count 862
 - prolongation operator 864, 1337
 - recursive nature 865, 1009, 1336
 - relative truncation error 875
 - relaxation as smoothing operator 865
 - restriction operator 864, 1337
 - speeding up FMG algorithm 873
 - stopping criterion 875f.
 - straight injection 867
 - symbol of operator 866f.
 - use of Richardson extrapolation 869
 - V-cycle 865, 1336
 - W-cycle 865, 1336
 - zebra relaxation 866
- Multiple precision arithmetic 906ff., 1352ff.
- Multiple roots 341, 362
- Multiplication, complex 171
- Multiplication, multiple precision 907, 909, 1353f.
- Multiplier of linear congruential generator 268
- Multistep and multivalue methods (ODEs) 740ff.
- see also* Differential Equations; Predictor-corrector methods
- Multivariate normal distribution 690
- Murphy's Law 407
- Musical scores 5f.
- N**AG 1/xxiii, 2/xx, 26, 64, 205, 454
- Fortran 90 compiler 2/viii, 2/xiv
 - Named constant 940
 - initialization 1012
 - for Numerical Recipes 1361
 - Named control structure 959, 1219, 1305
 - National Science Foundation (U.S.) 1/xvii, 1/xix, 2/ix
 - Natural cubic spline 109, 1044f.
 - Navier-Stokes equation 830f.
 - nearest() intrinsic function 952, 1146
 - Needle, eye of (minimization) 403
 - Negation, multiple precision 907, 1353f.
 - Negentropy 811, 896
 - Nelder-Mead minimization method 389, 402, 1208
 - Nested iteration 868
 - Neumann boundary conditions 820, 840, 851, 858
 - Neutrino 640
 - Neville's algorithm 102f., 105, 134, 182, 1043
 - Newton-Cotes formulas 125ff., 140
 - Newton-Raphson method *see* Newton's rule
 - Newton's rule 143f., 180, 341, 355ff., 362, 364, 469, 1059, 1189
 - with backtracking 376, 1196
 - caution on use of numerical derivatives 356ff.
 - fractal domain of convergence 360f.
 - globally convergent multidimensional 373, 376ff., 382, 749f., 752, 1196, 1199, 1314f.
 - for matrix inverse 49, 598
 - in multidimensions 370, 372ff., 749f., 752, 754, 1194ff., 1314ff.
 - in nonlinear multigrid 874, 876, 1339, 1341
 - nonlinear Volterra equations 787
 - for reciprocal of number 911, 1355
 - safe 359, 1190
 - scaling of variables 381

singular Jacobian 386
 solving stiff ODEs 740
 for square root of number 912, 1356
 Niederreiter sequence 300
 NL2SOL 683
 Noise
 bursty 889
 effect on maximum entropy method 567
 equivalent bandwidth 548
 fitting data which contains 647f., 650
 model, for optimal filtering 541
 Nominal variable (statistics) 623
 Nonexpansive projection operator 805
 Non-interfering directions *see* Conjugate directions
 Nonlinear eigenvalue problems 455
 Nonlinear elliptic equations, multigrid method 874ff., 1339ff.
 Nonlinear equations, in MEM inverse problems 813
 Nonlinear equations, roots of 340ff.
 Nonlinear instability 831
 Nonlinear integral equations 781, 787
 Nonlinear programming 436
 Nonnegativity constraints 423
 Nonparametric statistics 633ff., 1277ff.
 Nonpolynomial complete (NP-complete) 438
 Norm, of matrix 50
 Normal (Gaussian) distribution 267, 652, 682, 798, 1294
 central limit theorem 652f.
 deviates from 279f., 571, 1152
 kurtosis of 607
 multivariate 690
 semi-invariants of 608
 tails compared to Poisson 653
 two-dimensional (binormal) 631
 variance of skewness of 606
 Normal equations (fitting) 26, 645, 666ff., 795, 800, 1288
 often are singular 670
 Normalization
 of Bessel functions 175
 of floating-point representation 19, 882, 1343
 of functions 142, 765
 of modified Bessel functions 232
 not() intrinsic function 951
 Notch filter 551, 555f.
 NP-complete problem 438
 nr.f90 (module file) 936, 1362, 1384ff.
 nrerror() utility function 989, 995
 nrtype.f90 (module file) 936f.
 named constants 1361
 nrutil.f90 (module file) 936, 1070, 1362, 1364ff.
 table of contents 1364
 Null hypothesis 603
 nullify statement 953f., 1070, 1302
 Nullity 53
 Nullspace 25, 53f., 449, 795
 Number-theoretic transforms 503f.
 Numeric inquiry functions 2/xiv, 1107, 1231, 1343
 Numerical derivatives 180ff., 645, 1075

Numerical integration *see* Quadrature
 Numerical intrinsic functions 946, 951f.
 Numerical Recipes
 compatibility with First Edition 4
 Example Book 3
 Fortran 90 types 936f., 1361
 how to get programs 1/xx, 2/xvii
 how to report bugs 1/iv, 2/iv
 interface blocks (Fortran 90) 937, 941f., 1084, 1384ff.
 no warranty on 1/xx, 2/xvii
 plan of two-volume edition 1/xiii
 table of dependencies 921ff., 1434ff.
 as trademark 1/xiii, 2/xx
 utility functions (Fortran 90) 936f., 945, 968, 970, 972ff., 977, 984, 987ff., 1015, 1071f., 1361ff.
 Numerical Recipes Software 1/xv, 1/xxiiff., 2/xviiff.
 address and fax number 1/iv, 1/xxii, 2/iv, 2/xix
 Web home page 1/xx, 2/xvii
 Nyquist frequency 494ff., 520, 543, 545, 569ff.
 Nystrom method 782f., 789, 1325
 product version 789, 1331

Object extensibility 8
 Objective function 424
 Object-oriented programming 2/xvi, 2, 8
 Oblateness parameter 764
 Obsolete features *see* Fortran, Obsolescent features
 Octal constant, initialization 959
 Odd-even ordering
 allows parallelization 1333
 in Gauss-Seidel relaxation 866, 869, 1338
 in successive over-relaxation (SOR) 859, 1332
 Odd parity 888
 OEM information 1/xxii
 One-sided power spectral density 492
 ONLY option, for USE statement 941, 957, 1067
 Operation count
 balancing 476
 Bessel function evaluation 228
 bisection method 346
 Cholesky decomposition 90
 coefficients of interpolating polynomial 114f.
 complex multiplication 97
 cubic spline interpolation 109
 evaluating polynomial 168
 fast Fourier transform (FFT) 498
 Gauss-Jordan elimination 34, 39
 Gaussian elimination 34
 Givens reduction 463
 Householder reduction 467
 interpolation 100
 inverse iteration 488
 iterative improvement 48
 Jacobi transformation 460
 Kendall's tau 637

- linear congruential generator 268
 LU decomposition 36, 39
 matrix inversion 97
 matrix multiplication 96
 maximum entropy method 567
 multidimensional minimization 413f.
 multigrid method 862
 multiplication 909
 polynomial evaluation 97f., 168
 QL method 470, 473
 QR decomposition 92
 QR method for Hessenberg matrices 484
 reduction to Hessenberg form 479
 selection by partitioning 333
 sorting 320ff.
 Spearman rank-order coefficient 638
 Toeplitz matrix 83
 Vandermonde matrix 83
 Operator overloading 2/xiif., 7
 Operator splitting 823, 847f., 861
 Operator, user-defined 2/xii
 Optimal feasible vector 424
 Optimal (Wiener) filtering 535, 539ff., 558, 644
 compared with regularization 801
 Optimization *see* Minimization
 Optimization of code 2/xiii
 Optional argument 2/xiv, 947f., 1092, 1228, 1230, 1256, 1272, 1275, 1340
 dim 948
 mask 948, 968, 1038
 testing for 952
 Ordering Numerical Recipes 1/xxf., 2/xvif.
 Ordinal variable (statistics) 623
 Ordinary differential equations *see* Differential equations
 Orthogonal *see* Orthonormal functions; Orthonormal polynomials
 Orthogonal transformation 452, 463ff., 469, 584, 1227
 Orthonormal basis, constructing 58, 94, 1039
 Orthonormal functions 142, 246
 Orthonormal polynomials
 Chebyshev 144, 184ff., 1076ff.
 construct for arbitrary weight 151ff., 1064
 in Gauss-Hermite integration 147, 1062
 and Gaussian quadrature 142, 1009, 1061
 Gaussian weights from recurrence 150, 1064
 Hermite 144, 1062
 Jacobi 144, 1063
 Laguerre 144, 1060
 Legendre 144, 1059
 weight function $\log x$ 153
 Orthonormality 51, 142, 463
 Outer product Gaussian elimination 1017
 Outer product of matrices (denoted by cross) 66, 420, 949, 969f., 989, 1000ff., 1017, 1026, 1040, 1076, 1200, 1216, 1275
 outerand() utility function 989, 1002, 1015
 outerdiff() utility function 989, 1001
 outerdiv() utility function 989, 1001
 outerprod() utility function 970, 989, 1000, 1017, 1026, 1040, 1076, 1200, 1216, 1275
 outersum() utility function 989, 1001
 Outgoing wave boundary conditions 820
 Outlier 605, 653, 656, 694, 697
 see also Robust estimation
 Overcorrection 857
 Overflow 882, 1343
 how to avoid in modulo multiplication 269
 in complex arithmetic 171
 Overlap-add and overlap-save methods 536f.
 Overloading
 operator 2/xiif.
 procedures 940, 1015, 1083, 1094, 1096
 Overrelaxation parameter 857, 1332
 choice of 858
- P**ack() intrinsic function 945, 950, 964, 991, 1031
 communication bottleneck 969
 for index table 1176
 for partition-exchange 1170
 for selection 1178
 for selective evaluation 1087
 Pack-unpack idiom 1087, 1134, 1153
 Padé approximant 194ff., 1080f.
 Padé approximation 105
 Parabolic interpolation 395, 1204
 Parabolic partial differential equations 818, 838ff.
 Parallel axis theorem 308
 Parallel programming 2/xv, 941, 958ff., 962ff., 965f., 968f., 987
 array operations 964f.
 array ranking 1278f.
 band diagonal linear equations 1021
 Bessel functions 1107ff.
 broadcasts 965ff.
 C and C++ 2/viii
 communication costs 969, 981, 1250
 counting do-loops 1015
 cyclic reduction 974
 deflation 977ff.
 design matrix 1082
 dimensional expansion 965ff.
 eigenvalues 1226, 1229f.
 fast Fourier transform (FFT) 981, 1235ff., 1250
 in Fortran 90 963ff.
 Fortran 90 tricks 1009, 1274, 1278, 1280
 function evaluation 986, 1009, 1084f., 1087, 1090, 1102, 1128, 1134
 Gaussian quadrature 1009, 1061
 geometric progressions 972
 index loss 967f., 1038
 index table 1176f.
 interprocessor communication 981
 Kendall's tau 1280
 linear algebra 969f., 1000ff., 1018f., 1026, 1040, 1200, 1326
 linear recurrence 973f., 1073ff.
 logo 2/viii, 1009
 masks 967f., 1006f., 1038, 1102, 1200, 1226, 1305, 1333f., 1368, 1378, 1382
 merge statement 1010

- MIMD (multiple instruction, multiple data) 964, 985f., 1084
 MMP (massively multiprocessor) machines 965ff., 974, 984, 1016ff., 1226ff., 1250
 nrutil.f90 (module file) 1364ff.
 odd-even ordering 1333
 one-dimensional FFT 982f.
 parallel note icon 1009
 partial differential equations 1333
 in-place selection 1178f.
 polynomial coefficients from roots 980
 polynomial evaluation 972f., 977, 998
 random numbers 1009, 1141ff.
 recursive doubling 973f., 976f., 979, 988, 999, 1071ff.
 scatter-with-combine 984, 1002f., 1032f.
 second order recurrence 974f., 1074
 SIMD (Single Instruction Multiple Data) 964, 985f., 1009, 1084f.
 singular value decomposition (SVD) 1026
 sorting 1167ff., 1171, 1176f.
 special functions 1009
 SSP (small-scale parallel) machines 965ff., 984, 1010ff., 1016ff., 1059f., 1226ff., 1250
 subvector scaling 972, 974, 996, 1000
 successive over-relaxation (SOR) 1333
 supercomputers 2/viii, 962
 SVD algorithm 1026
 synthetic division 977ff., 999, 1048, 1071f., 1079, 1192
 tridiagonal systems 975f., 1018, 1229f.
 utilities 1364ff.
 vector reduction 972f., 977, 998
 vs. serial programming 965, 987
 PARAMETER attribute 1012
 Parameters in fitting function 651, 684ff.
 Parity bit 888
 Park and Miller minimal standard random generator 269, 1142
 Parkinson's Law 328
 Parseval's Theorem 492, 544
 discrete form 498
 Partial differential equations 818ff., 1332ff.
 advective equation 826
 alternating-direction implicit method (ADI) 847, 861f.
 amplification factor 828, 834
 analyze/factorize/operate package 824
 artificial viscosity 831, 837
 biconjugate gradient method 824
 boundary conditions 819ff.
 boundary value problems 819, 848
 Cauchy problem 818f.
 caution on high-order methods 844f.
 Cayley's form 844
 characteristics 818
 Chebyshev acceleration 859f., 1332
 classification of 818f.
 comparison of rapid methods 854
 conjugate gradient method 824
 Courant condition 829, 832ff., 836
 Courant condition (multidimensional) 846
 Crank-Nicholson method 840, 842, 844, 846
 cyclic reduction (CR) method 848f., 852ff.
 diffusion equation 818, 838ff., 846, 855
 Dirichlet boundary conditions 508, 820, 840, 850, 856, 858
 elliptic, defined 818
 error, varieties of 831ff.
 explicit vs. implicit differencing 827
 FACR method 854
 finite difference method 821ff.
 finite element methods 824
 flux-conservative initial value problems 825ff.
 forward Euler differencing 826f.
 Forward Time Centered Space (FTCS) 827ff., 839ff., 843, 855
 Fourier analysis and cyclic reduction (FACR) 848ff., 854
 Gauss-Seidel method (relaxation) 855, 864ff., 876, 1338, 1341
 Godunov's method 837
 Helmholtz equation 852
 hyperbolic 818, 825f.
 implicit differencing 840
 incomplete Cholesky conjugate gradient method (ICCG) 824
 inhomogeneous boundary conditions 850f.
 initial value problems 818f.
 initial value problems, recommendations on 838ff.
 Jacobi's method (relaxation) 855ff., 864
 Laplace's equation 818
 Lax method 828ff., 836, 845f.
 Lax method (multidimensional) 845f.
 matrix methods 824
 mesh-drift instability 834f.
 Monte Carlo methods 824
 multidimensional initial value problems 844ff.
 multigrid method 824, 862ff., 1009, 1334ff.
 Neumann boundary conditions 508, 820, 840, 851, 858
 nonlinear diffusion equation 842
 nonlinear instability 831
 numerical dissipation or viscosity 830
 operator splitting 823, 847f., 861
 outgoing wave boundary conditions 820
 parabolic 818, 838ff.
 parallel computing 1333
 periodic boundary conditions 850, 858
 piecewise parabolic method (PPM) 837
 Poisson equation 818, 852
 rapid (Fourier) methods 508ff., 824, 848ff.
 relaxation methods 823, 854ff., 1332f.
 Schrödinger equation 842ff.
 second-order accuracy 833ff., 840
 shock 831, 837
 sparse matrices from 64
 spectral methods 825
 spectral radius 856ff., 862
 stability vs. accuracy 830
 stability vs. efficiency 821
 staggered grids 513, 852
 staggered leapfrog method 833f.
 strongly implicit procedure 824

- successive over-relaxation (SOR) 857ff.,
 862, 866, 1332f.
 time splitting 847f., 861
 two-step Lax-Wendroff method 835ff.
 upwind differencing 832f., 837
 variational methods 824
 varieties of error 831ff.
 von Neumann stability analysis 827f.,
 830, 833f., 840
 wave equation 818, 825f.
see also Elliptic partial differential equations; Finite difference equations (FDEs)
- Partial pivoting 29
 Partition-exchange 323, 333
 and pack() intrinsic function 1170
 Partitioned matrix, inverse of 70
 Party tricks 95ff., 168
 Parzen window 547
 Pascal, Numerical Recipes in 2/x, 2/xvii, 1
 Pass-the-buck idiom 1102, 1128
 Path integration, for function evaluation 201ff.,
 263, 1138
 Pattern multiply of sparse matrices 74
 PBCG (preconditioned biconjugate gradient method) 78f., 824
 PC methods *see* Predictor-corrector methods
 PCGPACK 71
 PDEs *see* Partial differential equations
 Pearson's r 630ff., 1276
 PECE method 741
 Pentagon, symmetries of 895
 Percentile 320
 Period of linear congruential generator 268
 Periodic boundary conditions 850, 858
 Periodogram 543ff., 566, 1258ff.
 Lomb's normalized 569f., 574f., 1258ff.
 variance of 544f.
- Perl (programming language) 1/xvi
 Perron's theorems, for convergence of recurrence relations 174f.
- Perturbation methods for matrix inversion 65ff.
- Phase error 831
 Phase-locked loop 700
 Phi statistic 625
 Phillips-Twomey method 799ff.
 Pi, computation of 906ff., 1352ff., 1357f.
- Piecewise parabolic method (PPM) 837
 Pincherle's theorem 175
 Pivot element 29, 33, 757
 in linear programming 428f.
 Pivoting 27, 29ff., 46, 66, 90, 1014
 full 29, 1014
 implicit 30, 38, 1014, 1017
 in LU decomposition 37f., 1017
 partial 29, 33, 37f., 1017
 and QR decomposition 92
 in reduction to Hessenberg form 478
 in relaxation method 757
 as row and column operations 32
 for tridiagonal systems 43
- Pixel 519, 596, 803, 811
 PL/I 2/x
- Planck's constant 842
- Plane rotation *see* Givens reduction; Jacobi transformation (or rotation)
 Platykurtic distribution 606
 Plotting of functions 342, 1182f.
 POCS (projection onto convex sets) 805
 Poetry 5f.
 Pointer (Fortran 90) 2/xiii, 938f., 944f.,
 953ff., 1197, 1212, 1266
 as alias 939, 944f., 1286, 1333
 allocating an array 941
 allocating storage for derived type 955
 for array of arrays 956, 1336
 array of, forbidden 956, 1337
 associated with target 938f., 944f., 952f.,
 1197
 in Fortran 95 961
 to function, forbidden 1067, 1210
 initialization to null 2/xv, 961
 returning array of unknown size 955f.,
 1184, 1259, 1261, 1327
 undefined status 952f., 961, 1070, 1266,
 1302
- Poisson equation 519, 818, 852
 Poisson probability function
 cumulative 214
 deviates from 281, 283ff., 571, 1154
 semi-invariants of 608
 tails compared to Gaussian 653
- Poisson process 278, 282ff., 1153
 Polak-Ribiere algorithm 390, 414ff., 1214
 Poles *see* Complex plane, poles in
 Polishing of roots 356, 363ff., 370f., 1193
 poly() utility function 973, 977, 989, 998,
 1072, 1096, 1192, 1258, 1284
 Polymorphism 8
 Polynomial interpolation 99, 102ff., 1043
 Aitken's algorithm 102
 in Bulirsch-Stoer method 724, 726, 1305
 coefficients for 113ff., 1047f.
 Lagrange's formula 84, 102f.
 multidimensional 116ff., 1049ff.
 Neville's algorithm 102f., 105, 134, 182,
 1043
 pathology in determining coefficients for
 116
 in predictor-corrector method 740
 smoothing filters 645
 see also Interpolation
- Polynomials 167ff.
 algebraic manipulations 169, 1072
 approximate roots of Hermite polynomials
 1062
 approximate roots of Jacobi polynomials
 1064
 approximate roots of Laguerre polynomials
 1061
 approximating modified Bessel functions
 230
 approximation from Chebyshev coefficients
 191, 1078f.
 AUTODIN-II 890
 CCITT 889f.
 characteristic 368, 1193
 characteristic, for digital filters 554, 559,
 1257

- characteristic, for eigenvalues of matrix 449, 469
 Chebyshev 184ff., 1076ff.
 coefficients from roots 980
 CRC-16 890
 cumulants of 977, 999, 1071f., 1192, 1365, 1378f.
 deflation 362ff., 370f., 977
 derivatives of 167, 978, 1071
 division 84, 169, 362, 370, 977, 1072
 evaluation of 167, 972, 977, 998f., 1071, 1258, 1365, 1376ff.
 evaluation of derivatives 167, 978, 1071
 extrapolation in Bulirsch-Stoer method 724, 726, 1305f.
 extrapolation in Romberg integration 134
 fitting 83, 114, 191, 645, 665, 674, 1078f., 1291
 generator for CRC 889
 ill-conditioned 362
 masked evaluation of 1378
 matrix method for roots 368, 1193
 minimax 186, 198, 1076
 monic 142f.
 multiplication 169
 operation count for 168
 orthonormal 142, 184, 1009, 1061
 parallel operations on 977ff., 998f., 1071f., 1192
 primitive modulo 2 287ff., 301f., 889
 roots of 178ff., 362ff., 368, 1191ff.
 shifting of 192f., 978, 1079
 stopping criterion in root finding 366
poly_term() utility function 974, 977, 989, 999, 1071f., 1192
 Port, serial data 892
 Portability 3, 963
 Portable random number generator *see* Random number generator
 Positive definite matrix, testing for 90
 Positivity constraints 423
 Postal Service (U.S.), barcode 894
 PostScript 1/xvi, 1/xxiii, 2/xx
 Powell's method 389, 402, 406ff., 1210ff.
 Power (in a signal) 492f.
 Power series 159ff., 167, 195
 economization of 192f., 1061, 1080
 Padé approximant of 194ff., 1080f.
 Power spectral density *see* Fourier transform; Spectral density
 Power spectrum estimation *see* Fourier transform; Spectral density
 PowerStation, Microsoft Fortran 2/xix
 PPM (piecewise parabolic method) 837
 Precision
 converting to double 1362
 floating point 882, 937, 1343, 1361ff.
 multiple 906ff., 1352ff., 1362
 Preconditioned biconjugate gradient method (PBCG) 78f.
 Preconditioning, in conjugate gradient methods 824
 Predictor-corrector methods 702, 730, 740ff.
 Adams-Basforth-Moulton schemes 741
 adaptive order methods 744
 compared to other methods 740
 fallacy of multiple correction 741
 with fixed number of iterations 741
 functional iteration vs. Newton's rule 742
 multivalue compared with multistep 742ff.
 starting and stopping 742, 744
 stepsize control 742f.
present() intrinsic function 952
 Prime numbers 915
 Primitive polynomials modulo 2 287ff., 301f., 889
 Principal directions 408f., 1210
 Principal solution, of inverse problem 797
 PRIVATE attribute 957, 1067
 Prize, \$1000 offered 272, 1141, 1150f.
 Probability *see* Random number generator; Statistical tests
 Probability density, change of variables in 278f.
 Procedure *see* Program(s); Subprogram
 Process loss 548
product() intrinsic function 948
 Product Nystrom method 789, 1331
 Program(s)
 as black boxes 1/xviii, 6, 26, 52, 205, 341, 406
 dependencies 921ff., 1434ff.
 encapsulation 7
 interfaces 2, 8
 modularization 7f.
 organization 5ff.
 type declarations 2
 typography of 2f., 12, 937
 validation 3f.
 Programming, serial vs. parallel 965, 987
 Projection onto convex sets (POCS) 805
 Projection operator, nonexpansive 805
 Prolongation operator 864, 1337
 Protocol, for communications 888
 PSD (power spectral density) *see* Fourier transform; Spectral density
 Pseudo-random numbers 266ff., 1141ff.
 PUBLIC attribute 957, 1067
 Puns, particularly bad 167, 744, 747
 PURE attribute 2/xx, 960f., 964, 986
put_diag() utility function 985, 990, 1005, 1200
 Pyramidal algorithm 586, 1264
 Pythagoreans 392
- Q_L** *see* Eigensystems
QR *see* Eigensystems
 QR decomposition 91f., 382, 386, 1039f., 1199
 backsubstitution 92, 1040
 and least squares 668
 operation count 92
 pivoting 92
 updating 94, 382, 386, 1041, 1199
 use for orthonormal basis 58, 94
 Quadratic
 convergence 49, 256, 351, 356, 409f., 419, 906
 equations 20, 178, 391, 457

- interpolation 353, 364
 programming 436
 Quadrature 123ff., 1052ff.
 adaptive 123, 190, 788
 alternative extended Simpson's rule 128
 arbitrary weight function 151ff., 789,
 1064, 1328
 automatic 154
 Bode's rule 126
 change of variable in 137ff., 788, 1056ff.
 by Chebyshev fitting 124, 189, 1078
 classical formulas for 124ff.
 Clenshaw-Curtis 124, 190, 512f.
 closed formulas 125, 127f.
 and computer science 881
 by cubic splines 124
 error estimate in solution 784
 extended midpoint rule 129f., 135, 1054f.
 extended rules 127ff., 134f., 786, 788ff.,
 1326, 1328
 extended Simpson's rule 128
 Fourier integrals 577ff., 1261ff.
 Fourier integrals, infinite range 583
 Gauss-Chebyshev 144, 512f.
 Gauss-Hermite 144, 789, 1062
 Gauss-Jacobi 144, 1063
 Gauss-Kronrod 154
 Gauss-Laguerre 144, 789, 1060
 Gauss-Legendre 144, 783, 789, 1059,
 1325
 Gauss-Lobatto 154, 190, 512
 Gauss-Radau 154
 Gaussian integration 127, 140ff., 781,
 783, 788f., 1009, 1059ff., 1325, 1328f.
 Gaussian integration, nonclassical weight
 function 151ff., 788f., 1064f., 1328f.
 for improper integrals 135ff., 789, 1055,
 1328
 for integral equations 781f., 786, 1325ff.
 Monte Carlo 124, 155ff., 295ff., 306ff.,
 1161ff.
 multidimensional 124, 155ff., 1052, 1065ff.
 multidimensional, by recursion 1052,
 1065
 Newton-Cotes formulas 125ff., 140
 open formulas 125ff., 129f., 135
 related to differential equations 123
 related to predictor-corrector methods 740
 Romberg integration 124, 134f., 137, 182,
 717, 788, 1054f., 1065, 1067
 semi-open formulas 130
 Simpson's rule 126, 133, 136f., 583, 782,
 788ff., 1053
 Simpson's three-eighths rule 126, 789f.
 singularity removal 137ff., 788, 1057ff.,
 1328ff.
 singularity removal, worked example 792,
 1328ff.
 trapezoidal rule 125, 127, 130ff., 134f.,
 579, 583, 782, 786, 1052ff., 1326f.
 using FFTs 124
 weight function $\log x$ 153
 see also Integration of functions
 Quadrature mirror filter 585, 593
 Quantum mechanics, Uncertainty Principle
 600
 Quartile value 320
 Quasi-Newton methods for minimization 390,
 418ff., 1215
 Quasi-random sequence 299ff., 318, 881, 888
 Halton's 300
 for Monte Carlo integration 304, 309, 318
 Sobol's 300ff., 1160
 see also Random number generator
 Quicksort 320, 323ff., 330, 333, 1169f.
 Quotient-difference algorithm 164
- R**-estimates 694
 Radioactive decay 278
 Radix base for floating point arithmetic 476,
 882, 907, 913, 1231, 1343, 1357
 Radix conversion 902, 906, 913, 1357
 radix() intrinsic function 1231
 Radix sort 1172
 Ramanujan's identity for π 915
 Random bits, generation of 287ff., 1159f.
 Random deviates 266ff., 1141ff.
 binomial 285f., 1155
 exponential 278, 1151f.
 gamma distribution 282f., 1153
 Gaussian 267, 279f., 571, 798, 1152f.
 normal 267, 279f., 571, 1152f.
 Poisson 283ff., 571, 1154f.
 quasi-random sequences 299ff., 881, 888,
 1160f.
 uniform 267ff., 1158f., 1166
 uniform integer 270, 274ff.
 Random number generator 266ff., 1141ff.
 bitwise operations 287
 Box-Muller algorithm 279, 1152
 Data Encryption Standard 290ff., 1144,
 1156ff.
 good choices for modulus, multiplier and
 increment 274ff.
 initializing 1144ff.
 for integer-valued probability distribution
 283f., 1154
 integer vs. real implementation 273
 L'Ecuyer's long period 271f.
 lagged Fibonacci generator 1142, 1148ff.
 linear congruential generator 267ff., 1142
 machine language 269
 Marsaglia shift register 1142, 1148ff.
 Minimal Standard, Park and Miller's 269,
 1142
 nonrandomness of low-order bits 268f.
 parallel 1009
 perfect 272, 1141, 1150f.
 planes, numbers lie on 268
 portable 269ff., 1142
 primitive polynomials modulo 2 287ff.
 pseudo-DES 291, 1144, 1156ff.
 quasi-random sequences 299ff., 881, 888,
 1160f.
 quick and dirty 274
 quicker and dirtier 275
 in Quicksort 324
 random access to n th number 293

- random bits 287ff., 1159f.
 recommendations 276f.
 rejection method 281ff.
 serial 1141f.
 shuffling procedure 270, 272
 in simulated annealing method 438
 spectral test 274
 state space 1143f.
 state space exhaustion 1141
 subtractive method 273, 1143
 system-supplied 267f.
 timings 276f., 1151
 transformation method 277ff.
 trick for trigonometric functions 280
- Random numbers *see* Monte Carlo; Random deviates
- Random walk 20
- random_number() intrinsic function 1141, 1143
- random_seed() intrinsic function 1141
- RANDU, infamous routine 268
- Range 53f.
- Rank (matrix) 53
 kernel of finite 785
- Rank (sorting) 320, 332, 1176
- Rank (statistics) 633ff., 694f., 1277
 Kendall's tau 637ff., 1279
 Spearman correlation coefficient 634f., 1277ff.
 sum squared differences of 634, 1277
- Ratio variable (statistics) 623
- Rational Chebyshev approximation 197ff., 1081f.
- Rational function 99, 167ff., 194ff., 1080f.
 approximation for Bessel functions 225
 approximation for continued fraction 164, 211, 219f.
 Chebyshev approximation 197ff., 1081f.
 evaluation of 170, 1072f.
 extrapolation in Bulirsch-Stoer method 718ff., 726, 1306f.
 interpolation and extrapolation using 99, 104ff., 194ff., 718ff., 726
 as power spectrum estimate 566
 interpolation and extrapolation using 1043f., 1080ff., 1306
 minimax 198
- Re-entrant procedure 1052
- real() intrinsic function, ambiguity of 947
- Realizable (causal) 552, 554f.
- realloc() utility function 955, 990, 992, 1070, 1302
- Rearranging *see* Sorting
- Reciprocal, multiple precision 910f., 1355f.
- Record, in data file 329
- Recurrence relation 172ff., 971ff.
 arithmetic progression 971f., 996
 associated Legendre polynomials 247
 Bessel function 172, 224, 227f., 234
 binomial coefficients 209
 Bulirsch-Stoer 105f.
 characteristic polynomial of tridiagonal matrix 469
 Clenshaw's recurrence formula 176f.
 and continued fraction 175
- continued fraction evaluation 164f.
 convergence 175
 cosine function 172, 500
 cyclic reduction 974
 dominant solution 174
 exponential integrals 172
 gamma function 206
 generation of random bits 287f.
 geometric progression 972, 996
 Golden Mean 21
 Legendre polynomials 172
 minimal vs. dominant solution 174
 modified Bessel function 232
 Neville's 103, 182
 orthonormal polynomials 142
 Perron's theorems 174f.
 Pincherle's theorem 175
 for polynomial cumulants 977, 999, 1071f.
 polynomial interpolation 103, 183
 primitive polynomials modulo 2 287f.
 random number generator 268
 rational function interpolation 105f., 1043
 recursive doubling 973, 977, 988, 999, 1071f., 1073
 second order 974f., 1074
 sequence of trig functions 173
 sine function 172, 500
 spherical harmonics 247
 stability of 21, 173ff., 177, 224f., 227f., 232, 247, 975
 trig functions 572
 weight of Gaussian quadrature 144f.
- Recursion
 in Fortran 90 958
 in multigrid method 865, 1009, 1336
- Recursive doubling 973f., 979
 cumulants of polynomial 977, 999, 1071f.
 linear recurrences 973, 988, 1073
 tridiagonal systems 976
- RECURSIVE keyword 958, 1065, 1067
- Recursive Monte Carlo integration 306ff., 1161
- Recursive procedure 2/xiv, 958, 1065, 1067, 1166
 as parallelization tool 958
 base case 958
 for multigrid method 1009, 1336
 re-entrant 1052
- Recursive stratified sampling 314ff., 1164ff.
- Red-black *see* Odd-even ordering
- Reduction functions 948ff.
- Reduction of variance in Monte Carlo integration 299, 306ff.
- References (explanation) 4f.
- References (general bibliography) 916ff., 1359f.
- Reflection formula for gamma function 206
- Regula falsi (false position) 347ff., 1185f.
- Regularity condition 775
- Regularization
 compared with optimal filtering 801
 constrained linear inversion method 799ff.
 of inverse problems 796ff.
 linear 799ff.
 nonlinear 813

- objective criterion 802
 Phillips-Twomey method 799ff.
 Tikhonov-Miller 799ff.
 trade-off curve 799
 two-dimensional 803
 zeroth order 797
see also Inverse problems
- Regularizing operator 798
 Reid, John 2/xiv, 2/xvi
 Rejection method for random number generator 281ff.
- Relaxation method
 for algebraically difficult sets 763
 automated allocation of mesh points 774f., 777
 computation of spheroidal harmonics 764ff., 1319ff.
 for differential equations 746f., 753ff., 1316ff.
 elliptic partial differential equations 823, 854ff., 1332f.
 example 764ff., 1319ff.
 Gauss-Seidel method 855, 864ff., 876, 1338, 1341
 internal boundary conditions 775ff.
 internal singular points 775ff.
 Jacobi's method 855f., 864
 successive over-relaxation (SOR) 857ff., 862, 866, 1332f.
see also Multigrid method
- Remes algorithms
 exchange algorithm 553
 for minimax rational function 199
- reshape() intrinsic function 950
 communication bottleneck 969
 order keyword 1050, 1246
- Residual 49, 54, 78
 in multigrid method 863, 1338
- Resolution function, in Backus-Gilbert method 807
- Response function 531
- Restriction operator 864, 1337
- RESULT keyword 958, 1073
- Reward, \$1000 offered 272, 1141, 1150f.
- Richardson's deferred approach to the limit 134, 137, 182, 702, 718ff., 726, 788, 869
see also Bulirsch-Stoer method
- Richtmyer artificial viscosity 837
- Ridders' method, for numerical derivatives 182, 1075
- Ridders' method, root finding 341, 349, 351, 1187
- Riemann shock problem 837
- Right eigenvalues and eigenvectors 451
- Rise/fall time 548f.
- Robust estimation 653, 694ff., 700, 1294
 Andrew's sine 697
 average deviation 605
 double exponential errors 696
 Kalman filtering 700
 Lorentzian errors 696f.
 mean absolute deviation 605
 nonparametric correlation 633ff., 1277
 Tukey's biweight 697
- use of a priori covariances 700
see also Statistical tests
- Romberg integration 124, 134f., 137, 182, 717, 788, 1054f., 1065
- Root finding 143, 340ff., 1009, 1059
 advanced implementations of Newton's rule 386
 Bairstow's method 364, 370, 1193
 bisection 343, 346f., 352f., 359, 390, 469, 698, 1184f.
 bracketing of roots 341, 343ff., 353f., 362, 364, 369, 1183f.
 Brent's method 341, 349, 660f., 1188f., 1286
 Broyden's method 373, 382f., 386, 1199
 compared with multidimensional minimization 375
 complex analytic functions 364
 in complex plane 204
 convergence criteria 347, 374
 deflation of polynomials 362ff., 370f., 1192
 without derivatives 354
 double root 341
 eigenvalue methods 368, 1193
 false position 347ff., 1185f.
 Jenkins-Traub method 369
 Laguerre's method 341, 366f., 1191f.
 Lehmer-Schur algorithm 369
 Maehly's procedure 364, 371
 matrix method 368, 1193
 Muller's method 364, 372
 multiple roots 341
 Newton's rule 143f., 180, 341, 355ff., 362, 364, 370, 372f., 376, 469, 740, 749f., 754, 787, 874, 876, 911f., 1059, 1189, 1194, 1196, 1314ff., 1339, 1341, 1355f.
 pathological cases 343, 356, 362, 372
 polynomials 341, 362ff., 449, 1191f.
 in relaxation method 754, 1316
 Ridders' method 341, 349, 351, 1187
 root-polishing 356, 363ff., 369ff., 1193
 safe Newton's rule 359, 1190
 secant method 347ff., 358, 364, 399, 1186f.
 in shooting method 746, 749f., 1314f.
 singular Jacobian in Newton's rule 386
 stopping criterion for polynomials 366
 use of minimum finding 341
 using derivatives 355ff., 1189
 zero suppression 372
see also Roots
- Root polishing 356, 363ff., 369ff., 1193
- Roots
 Chebyshev polynomials 184
 complex *n*th root of unity 999f., 1379
 cubic equations 179f.
 Hermite polynomials, approximate 1062
 Jacobi polynomials, approximate 1064
 Laguerre polynomials, approximate 1061
 multiple 341, 364ff., 1192
 nonlinear equations 340ff.
 polynomials 341, 362ff., 449, 1191f.
 quadratic equations 178

- reflection in unit circle 560, 1257
 square, multiple precision 912, 1356
see also Root finding
- Rosenbrock method 730, 1308
 compared with semi-implicit extrapolation 739
 stepsize control 731, 1308f.
- Roundoff error 20, 881, 1362
 bracketing a minimum 399
 compile time vs. run time 1012
 conjugate gradient method 824
 eigensystems 458, 467, 470, 473, 476, 479, 483
 extended trapezoidal rule 132
 general linear least squares 668, 672
 graceful 883, 1343
 hardware aspects 882, 1343
 Householder reduction 466
 IEEE standard 882f., 1343
 interpolation 100
 least squares fitting 658, 668
 Levenberg-Marquardt method 679
 linear algebraic equations 23, 27, 29, 47, 56, 84, 1022
 linear predictive coding (LPC) 564
 magnification of 20, 47, 1022
 maximum entropy method (MEM) 567
 measuring 881f., 1343
 multidimensional minimization 418, 422
 multiple roots 362
 numerical derivatives 180f.
 recurrence relations 173
 reduction to Hessenberg form 479
 series 164f.
 straight line fitting 658
 variance 607
- Row degeneracy 22
 Row-indexed sparse storage 71f., 1030
 transpose 73f.
- Row operations on matrix 28, 31f.
- Row totals 624
 RSS algorithm 314ff., 1164
 RST properties (reflexive, symmetric, transitive) 338
- Runge-Kutta method 702, 704ff., 731, 740, 1297ff., 1308
 Cash-Karp parameters 710, 1299f.
 embedded 709f., 731, 1298, 1308
 high-order 705
 quality control 722
 stepsize control 708ff.
- Run-length encoding 901
- Runge-Kutta method
 high-order 1297
 stepsize control 1298f.
- Rybicki, G.B. 84ff., 114, 145, 252, 522, 574, 600
- S**-box for Data Encryption Standard 1148
- Sampling
 importance 306f.
 Latin square or hypercube 305f.
 recursive stratified 314ff., 1164
 stratified 308f.
 uneven or irregular 569, 648f., 1258
- Sampling theorem 495, 543
 for numerical approximation 600ff.
- Sande-Tukey FFT algorithm 503
- SAVE attribute 953f., 958f., 961, 1052, 1070, 1266, 1293
 redundant use of 958f.
- SAVE statements 3
- Savitzky-Golay filters
 for data smoothing 644ff., 1283f.
 for numerical derivatives 183, 645
- scale() intrinsic function 1107
- Scallop loss 548
- Scatter-with-combine functions 984, 1002f., 1032, 1366, 1380f.
- scatter_add() utility function 984, 990, 1002, 1032
- scatter_max() utility function 984, 990, 1003
- Schonfelder, Lawrie 2/xi
- Schrage's algorithm 269
- Schrödinger equation 842ff.
- Schultz's method for matrix inverse 49, 598
- Scope 956ff., 1209, 1293, 1296
- Scoping unit 939
- SDLC checksum 890
- Searching
 with correlated values 111, 1046f.
 an ordered table 110f., 1045f.
 selection 333, 1177f.
- Secant method 341, 347ff., 358, 364, 399, 1186f.
- Broyden's method 382f., 1199f.
 multidimensional (Broyden's) 373, 382f., 1199
- Second Euler-Maclaurin summation formula 135f.
- Second order differential equations 726, 1307
- Seed of random number generator 267, 1146f.
- select case statement 2/xiv, 1010, 1036
- Selection 320, 333, 1177f.
 find m largest elements 336, 1179f.
 heap algorithm 336, 1179
 for median 698, 1294
 operation count 333
 by packing 1178
 parallel algorithms 1178
 by partition-exchange 333, 1177f.
 without rearrangement 335, 1178f.
 timings 336
 use to find median 609
- Semi-implicit Euler method 730, 735f.
- Semi-implicit extrapolation method 730, 735f., 1310f.
 compared with Rosenbrock method 739
 stepsize control 737, 1311f.
- Semi-implicit midpoint rule 735f., 1310f.
- Semi-invariants of a distribution 608
- Sentinel, in Quicksort 324, 333
- Separable kernel 785
- Separation of variables 246
- Serial computing
 convergence of quadrature 1060
 random numbers 1141
 sorting 1167
- Serial data port 892

- Series 159ff.
 accelerating convergence of 159ff.
 alternating 160f., 1070
 asymptotic 161
 Bessel function K_ν 241
 Bessel function Y_ν 235
 Bessel functions 160, 223
 cosine integral 250
 divergent 161
 economization 192f., 195, 1080
 Euler's transformation 160f., 1070
 exponential integral 216, 218
 Fresnel integral 248
 hypergeometric 202, 263, 1138
 incomplete beta function 219
 incomplete gamma function 210, 1090f.
 Laurent 566
 relation to continued fractions 163f.
 roundoff error in 164f.
 sine and cosine integrals 250
 sine function 160
 Taylor 355f., 408, 702, 709, 754, 759
 transformation of 160ff., 1070
 van Wijngaarden's algorithm 161, 1070
- Shaft encoder 886
- Shakespeare 9
- Shampine's Rosenbrock parameters 732, 1308
- shape() intrinsic function 938, 949
- Shell algorithm (Shell's sort) 321ff., 1168
- Sherman-Morrison formula 65ff., 83, 382
- Shifting of eigenvalues 449, 470f., 480
- Shock wave 831, 837
- Shooting method
 computation of spheroidal harmonics 772, 1321ff.
 for differential equations 746, 749ff., 770ff., 1314ff., 1321ff.
 for difficult cases 753, 1315f.
 example 770ff., 1321ff.
 interior fitting point 752, 1315f., 1323ff.
- Shuffling to improve random number generator 270, 272
- Side effects
 prevented by data hiding 957, 1209, 1293, 1296
 and PURE subprograms 960
- Sidelobe fall-off 548
- Sidelobe level 548
- sign() intrinsic function, modified in Fortran 95 961
- Signal, bandwidth limited 495
- Significance (numerical) 19
- Significance (statistical) 609f.
 one- vs. two-sided 632
 peak in Lomb periodogram 570
 of 2-d K-S test 640, 1281
 two-tailed 613
- SIMD machines (Single Instruction Multiple Data) 964, 985f., 1009, 1084f.
- Similarity transform 452ff., 456, 476, 478, 482
- Simplex
 defined 402
 method in linear programming 389, 402, 423ff., 431ff., 1216ff.
- method of Nelder and Mead 389, 402ff., 444, 697f., 1208f., 1222ff.
 use in simulated annealing 444, 1222ff.
- Simpson's rule 124ff., 128, 133, 136f., 583, 782, 788f., 1053f.
- Simpson's three-eighths rule 126, 789f.
- Simulated annealing *see* Annealing, method of simulated
- Simulation *see* Monte Carlo
- Sine function
 evaluated from $\tan(\theta/2)$ 173
 recurrence 172
 series 160
- Sine integral 248, 250ff., 1123, 1125f.
 continued fraction 250
 series 250
see also Cosine integral
- Sine transform *see* Fast Fourier transform (FFT); Fourier transform
- Singleton's algorithm for FFT 525
- Singular value decomposition (SVD) 23, 25, 51ff., 1022
 approximation of matrices 58f.
 backsubstitution 56, 1022f.
 and bases for nullspace and range 53
 confidence levels from 693f.
 covariance matrix 693f.
 fewer equations than unknowns 57
 for inverse problems 797
 and least squares 54ff., 199f., 668, 670ff., 1081, 1290f.
 in minimization 410
 more equations than unknowns 57f.
 parallel algorithms 1026
 and rational Chebyshev approximation 199f., 1081f.
 of square matrix 53ff., 1023
 use for ill-conditioned matrices 56, 58, 449
- use for orthonormal basis 58, 94
- Singularities
 of hypergeometric function 203, 263
 in integral equations 788ff., 1328
 in integral equations, worked example 792, 1328ff.
 in integrands 135ff., 788, 1055, 1328ff.
 removal in numerical integration 137ff., 788, 1057ff., 1328ff.
- Singularity, subtraction of the 789
- SIPSOL 824
- Six-step framework, for FFT 983, 1240
- size() intrinsic function 938, 942, 945, 948
- Skew array section 2/xii, 945, 960, 985, 1284
- Skewness of distribution 606, 608, 1269
- Smoothing
 of data 114, 644ff., 1283f.
 of data in integral equations 781
 importance in multigrid method 865
- sn function 261, 1137f.
- Snyder, N.L. 1/xvi
- Sobol's quasi-random sequence 300ff., 1160f.
- Sonata 9
- Sonnet 9
- Sorting 320ff., 1167ff.
 bubble sort 1168

- bubble sort cautioned against 321
 compared to selection 333
 covariance matrix 669, 681, 1289
 eigenvectors 461f., 1227
 Heapsort 320, 327f., 336, 1171f., 1179
 index table 320, 329f., 1170, 1173ff.,
 1176
 operation count 320ff.
 by packing 1171
 parallel algorithms 1168, 1171f., 1176
 Quicksort 320, 323ff., 330, 333, 1169f.
 radix sort 1172
 rank table 320, 332, 1176
 ranking 329, 1176
 by reshaping array slices 1168
 Shell's method 321ff., 1168
 straight insertion 321f., 461f., 1167, 1227
 SP, defined 937
 SPARC or SPARCstation 1/xxii, 2/xix, 4
 Sparse linear equations 23, 63ff., 732, 1030
 band diagonal 43, 1019ff.
 biconjugate gradient method 77, 599,
 1034
 data type for 1030
 indexed storage 71f., 1030
 in inverse problems 804
 minimum residual method 78
 named patterns 64, 822
 partial differential equations 822ff.
 relaxation method for boundary value prob-
 lems 754, 1316
 row-indexed storage 71f., 1030
 wavelet transform 584, 598
 see also Matrix
 Spearman rank-order coefficient 634f., 694f.,
 1277
 Special functions *see Function*
 Spectral analysis *see Fourier transform; Peri-*
odogram
 Spectral density 541
 and data windowing 545ff.
 figures of merit for data windows 548f.
 normalization conventions 542f.
 one-sided PSD 492
 periodogram 543ff., 566, 1258ff.
 power spectral density (PSD) 492f.
 power spectral density per unit time 493
 power spectrum estimation by FFT 542ff.,
 1254ff.
 power spectrum estimation by MEM 565ff.,
 1258
 two-sided PSD 493
 variance reduction in spectral estimation
 545
 Spectral lines, how to smooth 644
 Spectral methods for partial differential equa-
 tions 825
 Spectral radius 856ff., 862
 Spectral test for random number generator
 274
 Spectrum *see Fourier transform*
 Spherical Bessel functions 234
 routine for 245, 1121
 Spherical harmonics 246ff.
 orthogonality 246
 routine for 247f., 1122
 stable recurrence for 247
 table of 246
 see also Associated Legendre polynomials
 Spheroidal harmonics 764ff., 770ff., 1319ff.
 boundary conditions 765
 normalization 765
 routine for 768ff., 1319ff., 1323ff.
 Spline 100
 cubic 107ff., 1044f.
 gives tridiagonal system 109
 natural 109, 1044f.
 operation count 109
 two-dimensional (bicubic) 120f., 1050f.
 spread() intrinsic function 945, 950, 969,
 1000, 1094, 1290f.
 and dimensional expansion 966ff.
 Spread matrix 808
 Spread spectrum 290
 Square root, complex 172
 Square root, multiple precision 912, 1356f.
 Square window 546, 1254ff.
 SSP (small-scale parallel) machines 965ff.,
 972, 974, 984, 1011, 1016ff., 1021,
 1059f., 1226ff., 1250
 Stability 20f.
 of Clenshaw's recurrence 177
 Courant condition 829, 832ff., 836, 846
 diffusion equation 840
 of Gauss-Jordan elimination 27, 29
 of implicit differencing 729, 840
 mesh-drift in PDEs 834f.
 nonlinear 831, 837
 partial differential equations 820, 827f.
 of polynomial deflation 363
 in quadrature solution of Volterra equation
 787f.
 of recurrence relations 173ff., 177, 224f.,
 227f., 232, 247
 and stiff differential equations 728f.
 von Neumann analysis for PDEs 827f.,
 830, 833f., 840
 see also Accuracy
 Stabilized Kolmogorov-Smirnov test 621
 Stabilizing functional 798
 Staggered leapfrog method 833f.
 Standard (probable) errors 1288, 1290
 Standard deviation
 of a distribution 605, 1269
 of Fisher's z 632
 of linear correlation coefficient 630
 of sum squared difference of ranks 635,
 1277
 Standard (probable) errors 610, 656, 661,
 667, 671, 684
 Stars, as text separator 1009
 Statement function, superseded by internal sub-
 program 1057, 1256
 Statement labels 9
 Statistical error 653
 Statistical tests 603ff., 1269ff.
 Anderson-Darling 621
 average deviation 605, 1269
 bootstrap method 686f.
 chi-square 614f., 623ff., 1272, 1275f.

- contingency coefficient C 625, 1275
 contingency tables 622ff., 638, 1275f.
 correlation 603f.
 Cramer's V 625, 1275
 difference of distributions 614ff., 1272
 difference of means 609ff., 1269f.
 difference of variances 611, 613, 1271
 entropy measures of association 626ff.,
 1275f.
 F-test 611, 613, 1271
 Fisher's z-transformation 631f., 1276
 general paradigm 603
 Kendall's tau 634, 637ff., 1279
 Kolmogorov-Smirnov 614, 617ff., 640,
 694, 1273f., 1281
 Kuiper's statistic 621
 kurtosis 606, 608, 1269
 L-estimates 694
 linear correlation coefficient 630ff., 1276
 M-estimates 694ff.
 mean 603ff., 608ff., 1269f.
 measures of association 604, 622ff., 1275
 measures of central tendency 604ff., 1269
 median 605, 694
 mode 605
 moments 604ff., 608, 1269
 nonparametric correlation 633ff., 1277
 Pearson's r 630ff., 1276
 for periodic signal 570
 phi statistic 625
 R-estimates 694
 rank correlation 633ff., 1277
 robust 605, 634, 694ff.
 semi-invariants 608
 for shift vs. for spread 620f.
 significance 609f., 1269ff.
 significance, one- vs. two-sided 613, 632
 skewness 606, 608, 1269
 Spearman rank-order coefficient 634f.,
 694f., 1277
 standard deviation 605, 1269
 strength vs. significance 609f., 622
 Student's t 610, 631, 1269
 Student's t, for correlation 631
 Student's t, paired samples 612, 1271
 Student's t, Spearman rank-order coeffi-
 cient 634, 1277
 Student's t, unequal variances 611, 1270
 sum squared difference of ranks 635,
 1277
 Tukey's trimean 694
 two-dimensional 640, 1281ff.
 variance 603ff., 607f., 612f., 1269ff.
 Wilcoxon 694
see also Error; Robust estimation
 Steak, without sizzle 809
 Steed's method
 Bessel functions 234, 239
 continued fractions 164f.
 Steepest descent method 414
 in inverse problems 804
 Step
 doubling 130, 708f., 1052
 tripling 136, 1055
 Stieltjes, procedure of 151
 Stiff equations 703, 727ff., 1308ff.
 Kaps-Rentrop method 730, 1308
 methods compared 739
 predictor-corrector method 730
 r.h.s. independent of x 729f.
 Rosenbrock method 730, 1308
 scaling of variables 730
 semi-implicit extrapolation method 730,
 1310f.
 semi-implicit midpoint rule 735f., 1310f.
 Stiff functions 100, 399
 Stirling's approximation 206, 812
 Stoermer's rule 726, 1307
 Stopping criterion, in multigrid method 875f.
 Stopping criterion, in polynomial root finding
 366
 Storage
 band diagonal matrix 44, 1019
 sparse matrices 71f., 1030
 Storage association 2/xiv
 Straight injection 867
 Straight insertion 321f., 461f., 1167, 1227
 Straight line fitting 655ff., 667f., 1285ff.
 errors in both coordinates 660ff., 1286ff.
 robust estimation 698, 1294ff.
 Strassen's fast matrix algorithms 96f.
 Stratified sampling, Monte Carlo 308f., 314
 Stride (of an array) 944
 communication bottleneck 969
 Strongly implicit procedure (SIPSOL) 824
 Structure constructor 2/xii
 Structured programming 5ff.
 Student's probability distribution 221f.
 Student's t-test
 for correlation 631
 for difference of means 610, 1269
 for difference of means (paired samples)
 612, 1271
 for difference of means (unequal variances)
 611, 1270
 for difference of ranks 635, 1277
 Spearman rank-order coefficient 634,
 1277
 Sturmian sequence 469
 Sub-random sequences *see* Quasi-random se-
 quence
 Subprogram 938
 for data hiding 957, 1209, 1293, 1296
 internal 954, 957, 1057, 1067, 1226, 1256
 in module 940
 undefined variables on exit 952f., 961,
 1070, 1266, 1293, 1302
 Subscript triplet (for array) 944
 Subtraction, multiple precision 907, 1353
 Subtractive method for random number genera-
 tor 273, 1143
 Subvector scaling 972, 974, 996, 1000
 Successive over-relaxation (SOR) 857ff., 862,
 1332f.
 bad in multigrid method 866
 Chebyshev acceleration 859f., 1332f.
 choice of overrelaxation parameter 858
 with logical mask 1333f.
 parallelization 1333
 sum() intrinsic function 945, 948, 966

Sum squared difference of ranks 634, 1277
Sums *see* Series
 Sun 1/xxii, 2/xix, 886
 SPARCstation 1/xxii, 2/xix, 4
 Supernova 1987A 640
 SVD *see* Singular value decomposition (SVD)
 swap() utility function 987, 990f., 1015, 1210
 Symbol, of operator 866f.
 Synthetic division 84, 167, 362, 370
 parallel algorithms 977ff., 999, 1048,
 1071f., 1079, 1192
 repeated 978f.
 Systematic errors 653

Tableau (interpolation) 103, 183
 Tangent function, continued fraction 163
 Target, for pointer 938f., 945, 952f.
 Taylor series 180, 355f., 408, 702, 709, 742,
 754, 759
 Test programs 3
 Thermodynamics, analogy for simulated annealing 437
 Thinking Machines, Inc. 964
 Threshold multiply of sparse matrices 74,
 1031
 Tides 560f.
 Tikhonov-Miller regularization 799ff.
 Time domain 490
 Time splitting 847f., 861
 tiny() intrinsic function 952
 Toeplitz matrix 82, 85ff., 195, 1038
 LU decomposition 87
 new, fast algorithms 88f.
 nonsymmetric 86ff., 1038
 Tongue twisters 333
 Torus 297f., 304
 Trade-off curve 795, 809
 Trademarks 1/xxii, 2/xixf.
 Transformation
 Gauss 256
 Landen 256
 method for random number generator 277ff.
 Transformational functions 948ff.
 Transforms, number theoretic 503f.
 Transport error 831ff.
 transpose() intrinsic function 950, 960, 969,
 981, 1050, 1246
 Transpose of sparse matrix 73f.
 Trapezoidal rule 125, 127, 130ff., 134f., 579,
 583, 782, 786, 1052, 1326f.
 Traveling salesman problem 438ff., 1219ff.
 Tridiagonal matrix 42, 63, 150, 453f., 488,
 839f., 1018f.
 in alternating-direction implicit method
 (ADI) 861f.
 from cubic spline 109
 cyclic 67, 1030
 in cyclic reduction 853
 eigenvalues 469ff., 1228
 with fringes 822
 from operator splitting 861f.
 parallel algorithm 975, 1018, 1229f.
 recursive splitting 1229f.
 reduction of symmetric matrix to 462ff.,
 470, 1227f.

serial algorithm 1018f.
see also Matrix
 Trigonometric
 functions, linear sequences 173
 functions, recurrence relation 172, 572
 functions, $\tan(\theta/2)$ as minimal 173
 interpolation 99
 solution of cubic equation 179f.
 Truncation error 20f., 399, 709, 881, 1362
 in multigrid method 875
 in numerical derivatives 180
 Tukey's biweight 697
 Tukey's trimean 694
 Turbo Pascal (Borland) 8
 Twin errors 895
 Two-dimensional *see* Multidimensional
 Two-dimensional K-S test 640, 1281ff.
 Two-pass algorithm for variance 607, 1269
 Two-point boundary value problems 702,
 745ff., 1314ff.
 automated allocation of mesh points 774f.,
 777
 boundary conditions 745ff., 749, 751f.,
 771, 1314ff.
 difficult cases 753, 1315f.
 eigenvalue problem for differential equa-
 tions 748, 764ff., 770ff., 1319ff.
 free boundary problem 748, 776
 grid (mesh) points 746f., 754, 774f., 777
 internal boundary conditions 775ff.
 internal singular points 775ff.
 linear requires no iteration 751
 multiple shooting 753
 problems reducible to standard form 748
 regularity condition 775
 relaxation method 746f., 753ff., 1316ff.
 relaxation method, example of 764ff.,
 1319
 shooting to a fitting point 751ff., 1315f.,
 1323ff.
 shooting method 746, 749ff., 770ff., 1314ff.,
 1321ff.
 shooting method, example of 770ff., 1321ff.
 singular endpoints 751, 764, 771, 1315f.,
 1319ff.
see also Elliptic partial differential equa-
 tions
 Two-sided exponential error distribution 696
 Two-sided power spectral density 493
 Two-step Lax-Wendroff method 835ff.
 Two-volume edition, plan of 1/xiii
 Two's complement arithmetic 1144
 Type declarations, explicit vs. implicit 2

Ubound() intrinsic function 949
 ULTRIX 1/xxiii, 2/xix
 Uncertainty coefficient 628
 Uncertainty principle 600
 Undefined status, of arrays and pointers 952f.,
 961, 1070, 1266, 1293, 1302
 Underflow, in IEEE arithmetic 883, 1343
 Underrelaxation 857
 Uniform deviates *see* Random deviates, uni-
 form

- Unitary (function) 843f.
 Unitary (matrix) *see* Matrix
`unit_matrix()` utility function 985, 990, 1006, 1216, 1226, 1325
 UNIX 1/xxiii, 2/viii, 2/xix, 4, 17, 276, 293, 886
 Upper Hessenberg matrix *see* Hessenberg matrix
 U.S. Postal Service barcode 894
`unpack()` intrinsic function 950, 964
 communication bottleneck 969
 upper subscript 944
`upper_triangle()` utility function 990, 1006, 1226, 1305
 Upwind differencing 832f., 837
 USE statement 936, 939f., 954, 957, 1067, 1384
 USES keyword in program listings 2
 Utility functions 987ff., 1364ff.
 add vector to matrix diagonal 1004, 1234, 1366, 1381
 alphabetical listing 988ff.
 argument checking 994f., 1370f.
 arithmetic progression 996, 1072, 1127, 1365, 1371f.
 array reallocation 992, 1070f., 1365, 1368f.
 assertion of numerical equality 995, 1022, 1365, 1370f.
 compared to intrinsics 990ff.
 complex *n*th root of unity 999f., 1379
 copying arrays 991, 1034, 1327f., 1365f.
 create unit matrix 1006, 1382
 cumulative product of an array 997f., 1072, 1086, 1375
 cumulative sum of an array 997, 1280f., 1365, 1375
 data types 1361
 elemental functions 1364
 error handling 994f., 1036, 1370f.
 generic functions 1364
 geometric progression 996f., 1365, 1372ff.
 get diagonal of matrix 1005, 1226f., 1366, 1381f.
 length of a vector 1008, 1383
 linear recurrence 996
 location in an array 992ff., 1015, 1017ff.
 location of first logical “true” 993, 1041, 1369
 location of maximum array value 993, 1015, 1017, 1365, 1369
 location of minimum array value 993, 1369f.
 logical assertion 994, 1086, 1090, 1092, 1365, 1370
 lower triangular mask 1007, 1200, 1382
 masked polynomial evaluation 1378
 masked swap of elements in two arrays 1368
 moving data 990ff., 1015
 multiply vector into matrix diagonal 1004f., 1366, 1381
 nrutil.f90 (module file) 1364ff.
 outer difference of vectors 1001, 1366, 1380
 outer logical and of vectors 1002
 outer operations on vectors 1000ff., 1379f.
 outer product of vectors 1000f., 1076, 1365f., 1379
 outer quotient of vectors 1001, 1379
 outer sum of vectors 1001, 1379f.
 overloading 1364
 partial cumulants of a polynomial 999, 1071, 1192f., 1365, 1378f.
 polynomial evaluation 996, 998f., 1258, 1365, 1376ff.
 scatter-with-add 1002f., 1032f., 1366, 1380f.
 scatter-with-combine 1002f., 1032f., 1380f.
 scatter-with-max 1003f., 1366, 1381
 set diagonal elements of matrix 1005, 1200, 1366, 1382
 skew operation on matrices 1004ff., 1381ff.
 swap elements of two arrays 991, 1015, 1365ff.
 upper triangular mask 1006, 1226, 1305, 1382
- V**-cycle 865, 1336
`vabs()` utility function 990, 1008, 1290
 Validation of Numerical Recipes procedures 3f.
 Valley, long or narrow 403, 407, 410
 Van Cittert’s method 804
 Van Wijngaarden-Dekker-Brent method *see* Brent’s method
 Vandermonde matrix 82ff., 114, 1037, 1047
 Variable length code 896, 1346ff.
 Variable metric method 390, 418ff., 1215
 compared to conjugate gradient method 418
 Variable step-size integration 123, 135, 703, 707ff., 720, 726, 731, 737, 742ff., 1298ff., 1303, 1308f., 1311ff.
 Variance(s)
 correlation 605
 of distribution 603ff., 608, 611, 613, 1269
 pooled 610
 reduction of (in Monte Carlo) 299, 306ff.
 statistical differences between two 609, 1271
 two-pass algorithm for computing 607, 1269
see also Covariance
 Variational methods, partial differential equations 824
 VAX 275, 293
 Vector(s)
 length 1008, 1383
 norms 1036
 outer difference 1001, 1366, 1380
 outer operations 1000ff., 1379f.
 outer product 1000f., 1076, 1365f., 1379
 Vector reduction 972, 977, 998
 Vector subscripts 2/xiif., 984, 1002, 1032, 1034
 communication bottleneck 969, 981, 1250
 VEGAS algorithm for Monte Carlo 309ff., 1161
 Verhoeff’s algorithm for checksums 894f., 1345

- Viète's formulas for cubic roots 179
 Vienna Fortran 2/xv
 Virus, computer 889
 Viscosity
 artificial 831, 837
 numerical 830f., 837
 Visibility 956ff., 1209, 1293, 1296
 VMS 1/xxii, 2/xix
 Volterra equations 780f., 1326
 adaptive stepsize control 788
 analogy with ODEs 786
 block-by-block method 788
 first kind 781, 786
 nonlinear 781, 787
 second kind 781, 786ff., 1326f.
 unstable quadrature 787f.
 von Neuman, John 963, 965
 von Neumann-Richtmyer artificial viscosity 837
 von Neumann stability analysis for PDEs 827f., 830, 833f., 840
 Vowellish (coding example) 896f., 902
- W**-cycle 865, 1336
 Warranty, disclaimer of 1/xx, 2/xvii
 Wave equation 246, 818, 825f.
 Wavelet transform 584ff., 1264ff.
 appearance of wavelets 590ff.
 approximation condition of order p 585
 coefficient values 586, 589, 1265
 contrasted with Fourier transform 584, 594
 Daubechies wavelet filter coefficients 584ff., 588, 590f., 594, 598, 1264ff.
 detail information 585
 discrete wavelet transform (DWT) 586f., 1264
 DWT (discrete wavelet transform) 586f., 1264ff.
 eliminating wrap-around 587
 fast solution of linear equations 597ff.
 filters 592f.
 and Fourier domain 592f.
 image processing 596f.
 for integral equations 782
 inverse 587
 Lemarie's wavelet 593
 of linear operator 597ff.
 mother-function coefficient 587
 mother functions 584
 multidimensional 595, 1267f.
 nonsmoothness of wavelets 591
 pyramidal algorithm 586, 1264
 quadrature mirror filter 585
 smooth information 585
 truncation 594f.
 wavelet filter coefficient 584, 587
 wavelets 584, 590ff.
 Wavelets *see* Wavelet transform
 Weber function 204
 Weighted Kolmogorov-Smirnov test 621
 Weighted least-squares fitting *see* Least squares fitting
 Weighting, full vs. half in multigrid 867
 Weights for Gaussian quadrature 140ff., 788f., 1059ff., 1328f.
 nonclassical weight function 151ff., 788f., 1064f., 1328f.
 Welch window 547, 1254ff.
 WG5 (ISO/IEC JTC1/SC22/WG5 Committee) 2/xiff.
 where construct 943, 1291
 contrasted with merge 1023
 for iteration of a vector 1060
 nested 2/xv, 943, 960, 1100
 not SIMD 985
 While iteration 13
 Wiener filtering 535, 539ff., 558, 644
 compared to regularization 801
 Wiener-Khinchin theorem 492, 558, 566f.
 Wilcoxon test 694
 Window function
 Bartlett 547, 1254ff.
 flat-topped 549
 Hamming 547
 Hann 547
 Parzen 547
 square 544, 546, 1254ff.
 Welch 547, 1254ff.
 Windowing for spectral estimation 1255f.
 Windows 95 2/xix
 Windows NT 2/xix
 Winograd Fourier transform algorithms 503
 Woodbury formula 68ff., 83
 Wordlength 18
 Workspace, reallocation in Fortran 90 1070f.
 World Wide Web, Numerical Recipes site 1/xx, 2/xvii
 Wraparound
 in integer arithmetic 1146, 1148
 order for storing spectrum 501
 problem in convolution 533
 Wronskian, of Bessel functions 234, 239
- X**.25 protocol 890
 X3J3 Committee 2/viii, 2/xff., 2/xv, 947, 959, 964, 968, 990
 XMODEM checksum 889
 X-ray diffraction pattern, processing of 805
- Y**ale Sparse Matrix Package 64, 71
- Z**-transform 554, 559, 565
 Z-transformation, Fisher's 631f., 1276
 Zaman, A. 1149
 Zealots 814
 Zebra relaxation 866
 Zero contours 372
 Zero-length array 944
 Zeroth-order regularization 796ff.
 Zip code, barcode for 894
 Ziv-Lempel compression 896
 zroots_unity() utility function 974, 990, 999