

# Index

- $\chi^2$ , *see* chi squared
- $\zeta$  function, *see* Riemann zeta function
- 0-indexing, 5, 11, 19, 86, 98, 275, 300, 320, 343, 567
- $\pm 0$ , 563
- $\pm\infty$ , 562
- absolute error, 30–34, 36, 37, 42, 43, 45, 54, 57, 58,  
76, 89–95, 104, 118, 173, 399–401, 405, 406,  
410–416, 418, 420, 427, 436, 465, 501, 519
- acceleration, 177, 495
- acceptance probability, 470–473, 482, 493
- acceptance rate, 473, 485
- action functional, 297
- action-angle coordinates, 490
- Acton, Forman Sinnickson, xiv, xvi, 441
- Adams–Bashforth method, 553
- adaptive integration, 396, 414, 415, 419, 421, 487,  
518, 522
- adaptive stepping, 518, 553
- addition rule, 455, 571, 572
- air resistance, 495, 555
- Aitken acceleration, 177
- algebraic multiplicity, 125
- algorithmic differentiation, *see* automatic  
differentiation
- aliasing, 351
- Anaconda distribution, 559
- analytical differentiation, 86
- analytical manipulation, 49, 55, 78, 125, 268, 391, 441
- angular momentum, 207, 211, 221, 223, 226, 242
- Ansatz, 331, 475, 506, 511
- approximating function, 314, 316, 317, 361–363
- approximation error, 30, 52, 89–93, 95, 101, 104,  
397–399, 401, 405, 410, 414
- arbitrary precision, 560
- argument, *see* keyword argument, positional argument
- Aristotle, xvi, 28, 439
- arithmetic, 5, 40, 105, 106, 108, 227, 312, 400, 405,  
410, 454, 455, 457, 466, 492, 561
- array, *see* NumPy array
- assignment, *see* augmented assignment, multiple  
assignment, pass-by-assignment
- associative, 8, 47, 224
- astrophysics, xvi, 60, 494, 546
- asymptotic error constant, 249
- asymptotic notation, *see* big-O notation
- atom, xvi, 394, 475
- attribute, 16, 18, 20
- augmented assignment, 5
- augmented matrix, 153–156, 166
- autocorrelation, 492
- autocovariance, 492
- automatic differentiation, xiv, 86, 105, 108, 119
- autonomous ODE, 497, 512, 553
- average, 111, 313, 331, 454, 455, 457, 466, 471, 492,  
510
- azimuthal quantum number, *see* quantum number
- back substitution, 148, 152, 154, 156, 162–164, 167,  
172, 186, 391
- backtracking, 265, 310
- backward difference, 89, 91, 92
- backward Euler, 504, 505, 510, 516, 517, 524, 533,  
553, 555
- backward recursion, 57, 81, 82
- banded, 157, 171, 335, 568
- Barker’s algorithm, 493
- barrier, 120
- barycentric formula, 324, 326, 328, 329, 341, 387
- Basel problem, 81
- basis, *see* momentum basis, monomial basis, position  
basis, [product basis](#)
- basis functions, 313–315, 317, 319–323, 362, 368,  
374
- Bernoulli number, 83, 84, 406, 441
- Bernoulli polynomial, 83, 406
- Bessel function, 81, 555
- bias, 561, 562, 564
- biased estimator, *see* unbiased estimator
- big-O notation, 88, 151
- bikeshedding, 3
- binning, 471
- binomial theorem, 66, 67
- bisection method, 256–258, 264, 269, 271, 272, 279,  
305
- bit, *see* byte (one eighth of it)
- black body, 377, 378
- Boltzmann, Ludwig Eduard, *see* Stefan–Boltzmann  
law
- boltzmannons, *see* Maxwell–Boltzmann statistics
- Bolzano’s theorem, 257
- Bonnet’s formula, *see* recurrence relation
- Boole’s rule, 411, 487
- Born rule, 111

- Bose–Einstein statistics, 475
- bound state, 112
- boundary condition, *see* Dirichlet boundary condition, Neumann boundary condition, periodic boundary
- boundary-value problem, 496, 497, 529–532, 536, 546, 552
- Box–Muller method, 491
- bra, *see* state vector
- bracketing method, 246, 247, 264, 269, 271–273, 306
- broadcasting, 17, 19, 20, 478, 479
- Broyden’s method, 287, 296
- burn-in, 472
- byte, 560
- C++, 2, 8
- cache misses, 2
- cardinal number, 120, 242, 275, 557
- cardinal polynomials, 322–324, 332, 387, 402, 403, 407, 430, 431, 433
- Cartesian, 22, 24, 119, 121, 122, 229, 297, 474, 476, 478, 486, 491
- catastrophic cancellation, 34, 35, 41, 42, 58, 67, 78, 398
- Cauchy distribution, 377
- Cauchy product, 83
- Cauchy–Schwarz inequality, 139
- central difference, 89, 91–93, 95–97, 99, 100, 102, 103, 117, 118, 303, 310, 311
- central limit theorem, 457, 491
- change of variables, 437, 442–445, 459, 461, 462, 467, 471, 489
- characteristic equation, 124, 277
- characteristic function, 491
- characteristic polynomial, 125, 136, 278
- Chebyshev inequality, 490
- Chebyshev point, xiv, 84, 318, 319, 323, 326, 329, 331, 341, 387, 553
- Chebyshev polynomial, 84, 318, 439, 440
- chi squared, 362, 364
- Christoffel–Darboux identity, 434, 440, 488
- clamped spline, 388
- classes, *see* object orientation
- classical mechanics, xv, 85, 111, 115, 297, 298, 311
- classical statistics, *see* Maxwell–Boltzmann statistics
- Clebsch–Gordan coefficient, 214, 223
- Clenshaw–Curtis quadrature, 439, 448
- closed methods, 395, 442
- closures, 9, 539
- coefficient matrix, 123, 124, 127, 128, 137, 153, 154, 171, 235, 247, 321, 335, 338, 368, 370, 535, 536, 543
- colleague matrix, 278
- column major, *see* row major
- column vector, 20, 124, 125, 130, 138, 149, 164, 188, 189, 203, 208–210, 214, 215, 221, 222, 224, 225, 239, 278, 279, 287, 293, 295, 314, 316, 370, 374, 567, 568
- commutative, 224, 228, 232
- companion matrix, 278, 279, 307
- comparing floats, 44
- compensated summation, xiv, 47–49, 74, 81
- compilation, 12
- complete pivoting, 171
- complex plane, 274, 354
- composite rule, 404, 412, 428
- computing the exponential, 50
- comrade matrix, 278
- condition number, 131–143, 145, 164, 233, 234, 247, 248, 372, 387, 390
- conditional expression, 5, 13
- conditioning, *see* condition number, ill-conditioned, well-conditioned
- constant vector, 124, 127, 128, 132, 136, 147, 149, 153, 161, 162, 164, 536
- continued fraction, 80
- continuity, *see* Lipschitz continuity
- contour line, 291, 292, 295
- control flow, 5, 8
- convergence criterion, *see* termination criterion
- convergent method, 248, 309
- convolution, 22
- coroutines, 3
- correlation length, 492
- correlations, 449, 451, 452, 483
- correspondence principle, 111
- cosmology, *see* Hubble’s law
- Coulomb potential, 60, 61, 66
- coupled differential equations, *see* simultaneous differential equations
- coupled representation, 214, 222, 223, 226, 230
- covariance, 366, 373, 390, 391, 492, 571
- critical point, 287, 288, 290, 291, 295, 296, 370, 372
- cubic spline, 336, 348, 388
- cumulative distribution function, 459, 491
- curse of dimensionality, 448
- Danielson–Lanczos lemma, 356
- data structures, 6
- data types, 16
- DC component, 353, 550
- de Moivre’s formula, 343, 349, 388
- decorators, 3
- deflation, 177, 306
- degrees of freedom, 206, 211, 382, 394, 473, 490
- dependent variable, 106, 496, 498, 507, 510, 512, 515, 522, 523, 546
- derivative, *see* analytical differentiation, automatic differentiation, backward difference, central difference, forward difference, *second derivative*
- design matrix, 370
- detailed balance, 468–471, 491, 493
- determinant, 124, 125, 127–132, 134, 139, 165, 182, 193, 194, 233–235, 240, 278, 279, 321, 387, 467, 493, 569

- deviates, 452, 453, 491
- DFT, *see* discrete Fourier transform
- diagonalize, 176, 193, 209, 223, 226, 230, 527
- diagonally dominant, 171, 173, 175, 176, 237, 338, 568, 569
- dictionary, 8, 10, 11, 23, 26, 63, 69, 71, 112–116, 120, 417
- differential equations, *see* autonomous ODE,
  - boundary-value problem, [eigenvalue problem](#),
  - initial-value problem, Legendre differential equation, matrix approach, ordinary differential equation, partial differential equation, RK4, shooting method, [simultaneous differential equations](#)
- Diogenes Laërtius, xvi, 558
- Diogenes the Cynic, 558
- dipole, 72, 73, 82
- Dirac, Paul Adrian Maurice, 206, 241, 493, 579
- direct method, 81, 147, 171
- Dirichlet boundary condition, 529
- discontinuous derivative, 442
- discrete Fourier transform, 351, 389, 494
- discretization, 242, 299, 304, 310, 351, 499, 501, 524, 528, 530, 532, 538, 542, 546–548, 557, 558
- dispersive, 545
- divide-and-conquer, 26, 357, 360
- dominant eigenvalue, 178, 179, 528
- dominant eigenvector, 178, 179
- Doolittle, 160, 161, 165, 234
- dot product, 20, 66, 149, 220, 221, 226, 229, 290, 361
- double precision, 39, 42, 45, 52, 54, 57, 166, 564
- doubling the number of panels, *see* adaptive integration, adaptive stepping
- drag coefficient, 495
- Dryden, John, 311
- dual numbers, 105, 106
- efficiency, 2, 26, 157, 303, 329, 412, 536, 544
- eigenenergy, 115, 242, 498
- eigenfunction, 109, 110, 112, 115, 119, 541, 543, 545, 557
- eigenstate, 120, 206–208, 241, 480, 481
- eigenvalue problem, 109, 122, 124, 135, 140–142, 172, 175, 176, 193, 206, 222, 247, 277, 278, 308, 473, 496, 498, 529, 536, 537, 539, 541, 543, 556–558
- eigenvalue shifting, 183, 184, 201
- eigenvector, *see* left eigenvectors, right eigenvectors
- Einstein, Albert, 28, 29, 475, 494, 578
- electric charge, 121, 211, 393, 546
- electric field, 21–25, 27, 28, 60–62, 85, 552
- electromagnetism, xiii, xv, 60, 72, 85, 393, 546, 558
- electron, 28, 207, 211, 242, 561
- electrostatic potential, 60–63, 65, 121, 393, 412, 437, 461
- elementary interval, 401–404, 407–409, 411, 412, 428, 433, 486
- elementary row operations, 123
- elementwise product, *see* Hadamard product
- elimination, *see* Gaussian elimination
- elliptic, 490, 545, 546
- emacs, *see* vim
- Emerson, Ralph Waldo, 10
- encapsulation, *see* separation of concerns
- entropy, 379
- equally spaced grid, 98, 340, 341, 345, 396, 402, 411, 428, 499
- equation of state, 243, 494
- equidistribution test, 452, 490
- equilibrium, 391, 468, 470, 471, 485, 494, 533
- equilibrium method (BVPs), *see* matrix approach
- ergodic, 468
- error, *see* absolute error, approximation error, error bound, [error creep](#), error formula, error function, error propagation, error scaling, [global error](#), local error, [maximal error](#), rounding error, standard error, truncation error
- error bound, 31–36, 38, 42, 43, 45, 125, 133, 138, 139, 233, 249
- error creep, 98, 283, 412
- error formula, 329, 331, 333, 341, 387, 404, 409, 430, 435, 436, 486
- error function, 394
- error propagation, 32, 33, 36, 37, 45, 76, 247
- error scaling, xiv, 430, 435, 436, 441
- estimator, *see* unbiased estimator
- Euclidean norm, 129–131, 133, 233, 286, 316, 371
- Euler's method, 499, 508, 509
- Euler–Lagrange equation, 304
- Euler–Maclaurin summation formula, 83, 406, 441
- everything slice, 17
- exceptions, 3
- expectation value, 114, 480, 481
- experimental measurement, 28, 29, 33, 316, 381
- explicit trapezoid method, 509, 552
- extrapolation, *see* Richardson extrapolation
- extremization, *see* minimization
- extremum test, 288
- factorial, 25, 26, 51, 55, 113, 436, 441, 489
- false-position method, *see* regula falsi
- fast Fourier transform, xv, 315, 348, 354, 357, 358, 360, 548
- Fermi–Dirac statistics, 493
- Feynman, Richard Phillips, 207
- FFT, *see* fast Fourier transform
- field equations, 494
- field lines, 21, 22, 24, 27
- field theory, 85, 468
- finite difference, *see* backward difference, central difference, forward difference
- finite-difference method, *see* matrix approach
- fitting, *see* least-squares fitting

- fixed-point iteration, 247, 249–252, 254–256, 259, 263, 268, 279, 304, 305, 308
- fixed-point representation, 561
- floating-point number, 30, 39, 40, 42, 44, 47, 52, 54, 57, 60, 77, 166, 449, 560–565
- floor division, 5
- for-else, 3, 12, 13, 175, 184, 252, 253, 417
- format string, 13–15, 93
- Fortran, 2, 4, 21
- forward difference, 87–90, 92, 95, 96, 100, 102, 103, 117, 119, 282, 283, 299, 300, 312
- forward Euler, 499–505, 510, 511, 515, 516, 524, 528, 529, 531, 553
- forward recursion, 81
- forward substitution, 147–149, 152, 162, 164, 186
- Fourier coefficients, 342, 351, 359
- Fourier differentiation, *see* spectral differentiation
- Fourier series, 82, 342, 343, 348, 351, 358, 388
- Fourier transform, *see* discrete Fourier transform, fast Fourier transform
- frequency, 28, 109, 342, 352, 353, 359
- Frobenius norm, 129
- Fubini's theorem, 446
- function, *see* user-defined function
- functional, *see* action functional
- fundamental theorem of algebra, 272
- g-factor, 211, 221
- Gauss–Chebyshev, 440, 444
- Gauss–Hermite, 440, 446, 489
- Gauss–Kronrod, 439
- Gauss–Laguerre, 440, 446, 492
- Gauss–Legendre, 69, 324, 428–430, 433, 435–440, 442, 446, 448, 465, 466, 488–491, 493, 512, 558
- Gauss–Newton, 377
- Gauss–Seidel method, 172, 175, 236, 237, 536
- Gaussian elimination, 125, 152–167, 170, 171, 173, 235, 240, 282, 285, 297, 314, 319, 338, 340, 366, 368, 370, 382, 535
- Gaussian quadrature, *see* Gauss–Chebyshev, Gauss–Hermite, Gauss–Kronrod, Gauss–Laguerre, Gauss–Legendre
- general relativity, 494
- generating function, 67, 83, 118
- Gibbs phenomenon, 82, 342
- global error, 500–503, 513, 517, 518, 521
- global minimum, 288, 291, 294–296
- global variables, 301, 382
- Go, 1
- Goethe, Johann Wolfgang von, xvi, 1
- golden ratio, 267
- Golub–Welsch algorithm, 307, 430, 488
- gradient descent, 292, 294–296, 304
- gradient vector, 290, 291, 300, 303, 312, 567
- Gram–Schmidt, 188, 190–193, 196, 237, 238, 275, 431, 432
- Grassmann variable, 105
- gravitation, 60, 244, 494, 546
- Green's function, 558
- grid points, *see* points on a grid
- Hadamard product, 20
- Hamilton's principle, 298, 299, 304
- Hamiltonian, 109, 206, 210, 211, 221, 222, 225, 226, 228–230, 232, 242, 474–476, 478–481, 557
- harmonic oscillator, 109–112, 115, 119, 241, 474, 475, 557
- heat equation, 545
- heat-bath update, 485
- Heraclitus of Ephesus, xiv, xvi, 243
- Hermite interpolation, 331, 333, 387, 388, 430, 432, 433, 440
- Hermite polynomial, 110, 113, 307, 440, 489
- Hermitian conjugate, 138, 569
- Hermitian matrices, 171, 568
- Hero of Alexandria, 245
- Hesiod, xvi, 121
- Hessenberg form, 203
- Hessian matrix, 290, 291, 296, 301, 372, 567
- Heun's method, 509
- hexadecapole, 72
- hidden bit, 561
- Higham, Nicholas John, 46
- Hilbert space, 190, 206, 212, 213, 223
- Horner's rule, 46, 79, 80, 274
- Householder transformation, 177, 193, 203, 239
- Hubble's law, 312, 313
- hyperbolic, 393, 545
- ideal gas, 243, 394
- identity matrix, 18, 124, 162, 164, 195, 216, 218, 225, 229, 282, 286, 308, 324, 568, 569
- IEEE 754, 561
- if, *see* conditional expression
- ill-conditioned, 133–137, 140, 142, 145, 146, 176, 234, 248, 249, 264, 273, 274, 319, 321, 322, 324, 368, 372, 391, 516
- imaginary unit, 105, 273, 343, 352, 547
- immutable object, 7, 9
- implicit midpoint method, 510
- implicit trapezoid method, 511, 553
- importance sampling, 461–465
- improper integral, 444, 454
- indentation, 5, 8, 12
- independent variable, *see* dependent variable
- induction, 197, 198, 201, 387
- inequality, *see* Cauchy–Schwarz inequality, Chebyshev inequality, triangle inequality
- infinite interval, 444, 446, 448
- infinite-dimensional, 190, 241
- infinity norm, 129, 131, 233, 237, 341
- infix, 20, 559
- inflection point, 288
- information hiding, *see* separation of concerns

- initial-value problem, 48, 495–498, 515–517, 522, 529–531, 539, 546
- instability, *see* unstable
- integer division, *see* floor division
- integral equation, 558
- integration, *see* Gaussian quadrature, Monte Carlo integration, Newton–Cotes methods
- integration by substitution, 459
- interacting spins, 219, 221, 222, 226, 473, 496
- intermediate-value theorem, 257
- interpolating polynomial, 312, 320, 321, 323, 324, 326, 328, 329, 331, 332, 334, 340, 344–346, 349–351, 358, 359, 361, 388, 401, 430, 435
- interpolation, *see* barycentric formula, cubic spline, Hermite interpolation, Lagrange interpolation, Newton interpolation, polynomial interpolation, trigonometric interpolation
- interpreter, 2, 4, 18, 43, 559
- inverse, *see* inverse DFT, inverse-power method, inverse transform sampling, matrix inverse
- inverse DFT, 350, 351, 353, 358, 390, 549, 550
- inverse transform sampling, 459, 467
- inverse-power method, 176, 181–184, 186, 187, 202, 204, 205, 242
- iterative method, 171–173, 176, 181, 192, 235, 236, 248, 250, 251, 256, 280, 282, 536
- Jacobi matrix, 307, 488
- Jacobi method, 172, 173, 176, 177, 236, 250
- Jacobian matrix, 281–283, 285, 286, 296, 307, 382
- joint probabilities, 571
- Julia, 1
- Jupyter Notebook, 559
- Kahan, William Morton, xvi, 48, 49, 81, 126
- Kant, Immanuel, xvi, 560
- Kernighan, Brian Wilson, 3
- ket, *see* state vector
- keys, 8, 10, 11, 26, 27, 63, 417
- keyword argument, 9, 14, 15, 21
- kinetic energy, 28, 97, 109, 111, 114, 115, 120, 206, 297, 474–476, 478, 479
- kinetic theory, 391
- Klein–Gordon equation, 496
- knot, 333
- Kronecker delta, 122, 300, 323
- Kronecker product, 216–220, 224–229, 232, 242
- L'Hôpital's rule, 58, 78, 442, 555
- Lagrange interpolation, 322, 329, 331, 333, 336, 340, 341, 348, 368, 387, 388, 401, 430, 486, 553
- Lagrange polynomial, *see* cardinal polynomials
- Lagrange remainder, 90, 566
- Lagrangian, xiii, 85, 297, 298, 468
- Laguerre polynomial, 440
- Laguerre's method, 277
- LAPACK, 169, 180
- Laplacian, 474, 478, 479, 548
- lattice Monte Carlo, 85, 485
- Laurent polynomial, 349
- law of large numbers, 490
- leading error, 101–103, 400, 405, 410, 419–423, 442, 447, 486
- leakage, 351
- leapfrog method, 554
- least-squares fitting, 315–317, 361, 362, 364, 366, 368, 374, 376, 377, 380
- left eigenvectors, 138, 140
- Legendre differential equation, 526, 531, 539
- Legendre polynomial, 60, 65–69, 71, 82, 83, 110, 118, 190, 239, 275–277, 307, 319, 331, 387, 432–437, 440, 488, 526, 531
- lemma, *see* Danielson–Lanczos lemma
- Levenberg–Marquardt, 377
- line style, 14
- line-search, 295, 309
- linear algebra, *see* eigenvalue problem, ill-conditioned, linear system
- linear congruential generator, 449
- linear fitting, *see* least-squares fitting
- linear system, 122, 125–127, 131–135, 137, 138, 141, 164, 182, 183, 186, 194, 233–236, 238, 241, 248, 280, 282, 283, 285, 287, 292, 296, 314, 319, 321, 322, 324, 336, 338, 339, 344, 365, 368, 370, 374, 377, 382, 533, 548, 549
- linearly independent, 123, 144, 175, 188, 190, 195, 198, 314, 321, 371
- Lipschitz continuity, 501
- list, *see* Python list
- list comprehension, 3, 10, 13, 15, 24, 49, 65, 76, 93, 229, 231
- literal, 5, 12, 45, 58
- local energy, 476, 478, 479, 481–483, 485
- local error, 501, 508, 510–513, 520–522, 553, 554
- local kinetic energy, 109, 114, 115, 476, 478, 479
- local minimum, 287, 288, 290–292, 372
- local update, 485
- logarithm, 16, 25, 27, 31, 36, 254, 377, 380, 381, 392, 412
- logistic map, 305
- loop, *see* Python keywords
- Lotka–Volterra equations, 555
- LU decomposition, 159–164, 169, 183, 186, 187, 194, 203, 234, 235
- Lummer and Pringsheim, 380, 381, 392
- machine number, 38, 42, 44, 45, 561
- machine precision, 40–42, 105, 108, 166, 192, 341, 393
- Maclaurin series, 51, 58, 502, 566
- magnetic field, 210, 211, 221–223, 225, 226, 230, 232, 391
- mantissa, 38, 40, 561–565
- many-particle, 473, 474, 476, 478, 480, 493
- marginal probabilities, *see* joint probabilities
- marker, 14, 70, 71

- Markov chain, 468–473, 483
- Mathieu equation, 537, 539, 541–543, 545, 557
- matrix approach, 532–537, 541, 543, 556, 558
- matrix inverse, 135, 164
- matrix multiplication, 20, 26, 151, 189, 192, 201, 203, 209, 218, 219, 229, 241, 242, 279, 357, 370, 373, 568
- matrix norm, 129, 130
- matrix representation, 208, 209, 211, 214, 218, 219, 224
- matrix-vector multiplication, 151, 179, 181, 183, 209, 354, 355, 370, 374, 568
- Matthew effect, 322
- maximal error, 31, 33, 46, 365
- maximization, *see* minimization
- maximum likelihood, 363
- Maxwell, James Clerk, 379, 391, 394, 475
- Maxwell–Boltzmann statistics, 394, 475
- mean-value theorem, 255, 256, 330, 405, 436, 487
- mechanics, *see* classical mechanics, quantum mechanics, statistical mechanics
- Mersenne prime, 453
- mesh points, *see* points on a grid
- Metropolis ratio, 485
- Metropolis–Hastings algorithm, 458, 465, 470, 471, 493
- midpoint rule, 398, 400, 401, 405, 411, 428, 486, 488, 510
- Millikan, Robert Andrews, 28, 29, 313
- minimax approximation, 316
- minimization, 287, 289, 292, 296, 297, 299–302, 304, 309, 317, 363, 370, 377, 378, 382, 384, 482, 486
- model selection, 382
- modified Gram–Schmidt, 193, 237, 238
- modules
  - cmath, 112
  - copy, 7
  - functools, 384
  - jax, 105, 119, 559
  - math, 5
  - matplotlib, 13, 559
  - numpy.linalg, 125, 150, 179, 234
  - numpy.random, 453
  - numpy, 2, 16, 559
  - random, 453
  - scipy, 2, 555, 559
  - sympy, 87, 117, 559
  - timeit, 26, 389
- molecular dynamics, xiii, 554
- moment of inertia, 122
- momentum basis, 558
- monic polynomial, 278, 279, 330, 431, 432, 440, 488
- monomial basis, 319–322, 324, 326, 329, 334
- Monte Carlo integration, 46, 396, 454, 457, 458, 464, 466, 467, 481, 491
- multidimensional integral, 394, 446, 448, 474, 481
- multidimensional minimization, 289, 292, 297, 299, 301, 304, 309, 370, 377, 378
- multiple assignment, 5, 168
- multiple roots, 263, 264, 273, 305
- multiplication, *see* matrix multiplication, matrix-vector multiplication
- multipole expansion, 60, 65, 71–76, 84, 275, 546
- multistep method, *see* Adams–Bashforth method
- $n$ -th roots of unity, 354
- NaN, *see* not a number
- natural spline, 334, 336, 388
- near-singular, 130–132
- nested functions, 9
- nesting, 319, 439
- Neumann boundary condition, 529, 556
- neutron, 207, 475
- Newton interpolation, 322
- Newton potential, 60, 66
- Newton’s method, 249, 256, 260–265, 267, 269, 272, 274, 275, 279, 281, 282, 287, 295, 296, 299, 300, 305–309, 382, 384–386, 531, 532, 555, 556
- Newton–Cotes methods, 395, 396, 402, 411, 427, 435, 436, 512
- Newton–Raphson method, *see* Newton’s method
- Nietzsche, Friedrich Wilhelm, xvi, 566
- nodal abscissas, 395, 427, 432, 488
- node polynomial, 324–326, 330, 331, 387, 431, 433, 436
- noisy data, 86, 312
- non-bracketing method, *see* bracketing method
- noncentral difference, *see* backward difference, forward difference
- nonlinear equation, 243–247, 251, 254, 272, 274, 279, 280, 296, 297, 308, 321, 378, 382, 386, 429
- nonlinear fitting, 382
- nonsymmetric matrices, 121, 122, 171, 176, 321, 335, 527
- norm, *see* Euclidean norm, Frobenius norm, infinity norm, matrix norm
- normal distribution, 374, 491
- normal equations, 317, 368–370, 377, 384, 391
- normal number, 38, 42, 81, 563
- normalization, 190, 197, 238, 239, 436, 440, 458–461, 464, 472, 492, 538, 539, 550
- not a number, 166, 442, 562
- nuclear physics, *see* neutron, proton
- numerical analysis, xiv, 494
- numerology, 449
- Numerov’s method, 554, 555
- NumPy array, xiv, 15–17, 19, 21, 23–27, 149, 205, 226, 227, 229, 235
- NumPy functions
  - arange(), 16
  - argmax(), 17, 27, 168, 340
  - argsort(), 489
  - array(), 16

- concatenate(), 17, 361
- conjugate(), 550
- copy(), 17
- dot(), 20
- empty(), 149
- fill\_diagonal(), 21, 27, 303, 338, 536, 543
- kron(), 227
- linalg.det(), 234
- linalg.eig(), 179
- linalg.inv(), 234
- linalg.solve(), 150
- linspace(), 16
- logspace(), 16
- meshgrid(), 21, 550
- nonzero(), 27
- ones(), 16
- outer(), 20, 287
- polynomial.hermite.hermgauss(), 307
- polynomial.legendre.leggauss(), 277
- random.randn(), 374
- random.seed(), 374, 453
- random.uniform(), 453, 483
- sort(), 489, 543
- sqrt(), 17
- sum(), 17
- transpose(), 20
- where(), 17, 27, 328
- zeros(), 16
- object orientation, 3, 119, 301, 382
- octupole, 72
- one-dimensional quantum mechanics, *see* barrier, harmonic oscillator, particle in a box, quantum pendulum, square well
- one-pass, 79
- open methods, 395, 411
- operation count, xiv, 151, 152, 158, 163, 181, 186, 203, 241, 282, 354, 357
- operator, 6, 20, 109, 206–216, 218–221, 223–225, 227, 241, 242, 548, 559
- order of convergence, 248, 249, 267, 305, 306
- ordinary differential equation, 48, 495, 496, 498, 502, 515, 522
- orthogonal iteration, *see* simultaneous iteration
- orthogonal matrix, 187–190, 194, 200, 233, 240, 569
- orthogonal polynomial, 430, 432, 488
- orthogonalization, 188, 190, 193, 196, 275, 372, 431, 432, 436
- orthonormal, 188–190, 196–198, 207, 208, 215, 238, 239, 432, 480
- oscillator, *see* harmonic oscillator, quartic oscillator
- outer product, 20, 287
- overdetermined, 316, 362
- overfitting, 363, 368, 376, 390
- overflow, 38, 39, 51, 77, 253, 560, 561, 564, 565
- page faults, 2
- panel, *see* subinterval
- parabolic, 545
- parameter estimation, 363, 382
- partial differential equation, 496, 498, 545, 554
- partial pivoting, *see* pivoting
- partial sum, 48
- particle in a box, 111, 120, 557
- partition function, 394
- pass-by-assignment, 9
- pass-by-reference, 9
- pass-by-value, 9
- pathological, 126, 272, 319, 421, 424, 441, 502
- Pauli spin matrices, 208, 219, 220, 226
- pendulum, *see* quantum pendulum, simple pendulum
- PEP 8, 3
- periodic boundary, 236, 552
- periodic function, 346, 351, 441, 442, 541
- perturbation theory, xiv, 125, 475, 557
- photoelectric effect, 28, 29, 313
- photon, 28, 391
- piecewise interpolation, *see* cubic spline
- Pindar, xv
- pivot element, 156, 166–168, 170
- pivot row, 153–160, 165–168, 170, 171
- pivoting, 124, 159, 165, 167–171, 173, 235, 283, 319, 338, 340, 374, 536
- Planck, Max Karl Ernst Ludwig, 28, 109, 298, 379, 392
- Plato, xvi, 317, 559
- points on a grid, 97, 99, 100, 119, 298, 314, 353, 395, 396, 533, 547
- Poisson's equation, 498, 545, 546, 548, 549
- polynomial interpolation, 315, 317, 319, 320, 322, 329, 331, 333, 341, 346, 349, 402, 404, 428, 437
- polynomials, *see* Bernoulli polynomial, Chebyshev polynomial, Hermite polynomial, Laguerre polynomial, Laurent polynomial, Legendre polynomial, orthogonal polynomial
- population mean, 454, 455, 457, 458, 466, 490, 491
- population variance, 454, 456, 458, 466, 490, 491
- posit, *see* unum
- position basis, 109, 241, 496, 558
- positional argument, 13, 15
- positive definite, 171, 290, 291, 296, 371, 372
- positive semidefinite, 370
- potential energy, 28, 109, 115, 301, 474, 475, 478, 479
- potential well, *see* square well
- power method, 176, 177, 181–184, 186, 187, 194–196, 198, 202, 204, 205, 237, 242, 528
- precision, *see* arbitrary precision, double precision, machine precision, single precision
- predator-prey, *see* Lotka–Volterra equations
- pressure, 243, 379, 391, 494, 495
- principal axes, 122
- principle of superposition, 21, 61, 122
- probability, *see* acceptance probability, joint



- probabilities, probability density, proposal probability
- probability density, 110, 111, 454, 458, 459, 467–469, 572
- Proclus Lycaeus, 402
- product basis, 212
- projectile, 495, 555
- proof by contradiction, 488
- proof by induction, *see* induction
- proof by intimidation, xiv
- proof by omission, xiv
- propagation of error, *see* error propagation
- proposal probability, 470
- proton, 207, 211, 475
- pseudorandom, 449, 451
- Python built-ins and library functions
  - `abs()`, 44
  - `deepcopy()`, 7, 23
  - `default_timer()`, 26, 389
  - `enumerate()`, 11
  - `exp()` from `cmath`, 113
  - `exp()` from `math`, 8
  - `format()`, 8
  - `partial()`, 384
  - `random()`, 453
  - `range()`, 5
  - `reversed()`, 11
  - `seed()`, 453
  - `sqrt()`, 5
  - `zip()`, 11
- Python keywords
  - `break`, 5, 12, 13, 175
  - `continue`, 5, 328
  - `def`, 8
  - `else`, 5, 12
  - `for`, 5
  - `global`, 9
  - `if`, 5
  - `import`, 5
  - `lambda`, 9
  - `None`, 9
  - `nonlocal`, 9
  - `return`, 9
  - `True`, 5
  - `while`, 5
- Python list, 2, 15, 16, 18, 24, 98, 149, 226, 478
- Python modules, *see* modules
- Python versions
  - Python 2, 559
  - Python 3, xiv, 2, 20, 559
- QR decomposition, 187, 190–193, 196, 197, 200, 202, 203, 238, 240, 241, 368, 391
- QR method, 176, 187, 192, 193, 199–203, 205, 241, 543, 544
- quadratic convergence, 249, 264, 272, 287, 307
- quadratic equation, 35, 77, 269, 306, 553
- quadrature, *see* Gaussian quadrature, Monte Carlo integration, Newton–Cotes methods
- quadrupole, 72, 82
- quantization, 28, 110
- quantum mechanics, xv, 109, 111, 190, 206–208, 214, 241, 243, 244, 312, 473, 480, 481, 538, 545, 557
- quantum Monte Carlo, 115
- quantum number, 111, 112, 114, 207, 208, 214, 476
- quantum pendulum, 545
- quantum statistics, *see* Bose–Einstein statistics, Fermi–Dirac statistics
- quartic oscillator, 301, 310
- Racah W-coefficients, 223
- random number, 374, 396, 448–453, 458–461, 466, 467, 472, 479, 483, 484, 570
- random variable, 46, 454–456, 458, 459, 466, 469, 490, 491, 570–572
- random walk, 468, 469, 471, 482, 492
- rational function, 46, 47, 80, 326
- Rayleigh quotient, 178, 179, 181, 182, 184, 186, 196, 198, 202, 240
- Rayleigh–Ritz principle, 480, 481
- real numbers, 30, 33, 35, 38, 42–44, 47, 52, 60, 105, 106, 108, 112, 343, 451, 527, 561
- recoupling, 223, 242
- rectangle rule, 299, 395, 397–401, 404, 407, 409, 412, 416–418, 501, 510
- rectangular matrix, 369, 374, 391
- recurrence relation, 60, 67–69, 82–84, 110, 118, 307, 308, 441, 488
- recursion, *see* backward recursion, forward recursion, recurrence relation
- reduced QR decomposition, 391
- regula falsi, 306
- reinventing the wheel, 4
- relative error, 30, 32, 34–38, 41–43, 46, 49, 54, 76, 84, 90, 173, 417, 519
- relativity, *see* general relativity, special relativity
- relaxation method, *see* iterative method
- remainder, *see* Lagrange remainder
- residual vector, 126, 173, 191, 316, 362
- residuals, 382, 384, 390
- resolution of the identity, 210, 219, 221, 480, 481, 558
- reversibility condition, 468
- Riccati equation, 515, 521, 525, 553, 554
- Richardson extrapolation, 101–104, 119, 315, 396, 419–424, 441, 518, 557
- Ridders’ method, 257, 269, 271, 272
- Riemann integral, 398
- Riemann zeta function, 81
- right eigenvectors, 138, 140, 144, 145, 176
- RK4, 511–513, 516–519, 521, 522, 527, 529, 531–533, 539, 542, 553–555
- rocket surgery, 415
- Rodrigues’ formula, 118, 432
- Rolle’s theorem, 330



- Romberg integration, 396, 407, 419, 421, 424, 425, 427, 448, 488
- root suppression, *see* suppress an already-found root
- root-finding, 172, 246, 256, 264, 273–275, 277, 287, 288, 295, 304, 309, 317, 378, 384, 494, 505, 516, 526, 531–533, 537, 539, 555
- roots of unity, *see*  $n$ -th roots of unity
- rotation, 121, 122
- rounding error, 30, 45, 46, 48, 58, 77, 78, 80, 125, 128, 283
- row major, 21
- row vector, 20, 138, 568
- rule of thumb, 10, 134, 145, 363
- Runge function, 322, 341
- Runge–Kutta method, 506, 511, 512, 515–517, 553
- Runge–Kutta–Fehlberg method, 554
- RuntimeWarning, 442, 550
- saddle point, 288, 289, 292, 296
- safety factor, 521
- sample mean, 454–458, 464–467, 473, 482, 483, 486, 490, 491
- sample variance, 456
- sampling, *see* importance sampling, inverse transform sampling, uniform sampling, weighted sampling
- scalar function, 60, 287, 289, 291, 293, 295, 296, 299, 466, 566
- Schrödinger equation, 109, 111, 115, 206, 210, 211, 221, 225, 241, 243, 473, 475, 496, 498, 545, 558
- scientific notation, 38, 561
- secant method, 247, 249, 265–268, 272, 285, 288, 306, 308, 532, 539
- second derivative, 86, 91, 96, 97, 100, 109, 114–120, 261, 262, 288, 296, 300, 301, 333, 334, 336–338, 371, 388, 389, 405, 409, 474, 478, 493, 496, 501, 533, 542, 557
- seed, 374, 375, 450, 452, 453, 463, 464, 483–485, 583, 584
- self-correcting, 172, 256
- seminormal equations, 391
- separation of concerns, 13, 69, 149, 275, 464
- serial test, 452
- series, *see* Basel problem, Fourier series, Maclaurin series, Taylor series, telescoping series
- Shakespeare, William, xvi, 85
- shifted DFT, 352
- shifting, *see* eigenvalue shifting
- shooting method, 530–533, 536–539, 541–543, 556, 557
- sign bit, 561, 563
- signed zero, *see*  $\pm 0$
- significant figure, 561
- significand, 561
- significant figure, 39, 42, 43, 58, 78, 126, 417, 561, 564, 565
- similarity transformation, 187, 193, 194, 198
- simple eigenvalue, 135, 137, 139, 145
- simple pendulum, 490
- Simpson’s rule, 403, 407–412, 414–419, 425, 427, 429, 436, 441, 447, 448, 487–489, 512, 518
- simultaneous differential equations, 495, 522, 531
- simultaneous iteration, 187, 194–196, 199–201, 240
- single precision, 562, 563, 565
- singularity, 321, 341, 395, 442–446, 448, 489
- Slater determinant, 493
- slicing, 3, 6, 7, 16, 19, 149, 168, 169, 175, 303, 338, 346, 361, 479, 489, 536
- Sophocles, xvi, 393, 494
- sorting, 2, 48, 489, 544
- sparse, 147, 157, 171, 176, 235, 282, 354, 391, 568
- special relativity, 496
- spectral differentiation, 312, 389
- spin matrices, *see* Pauli spin matrices
- spinor, 208, 209
- spline, *see* clamped spline, cubic spline, natural spline
- Spyder, 559
- square matrix, 187, 567, 568
- square well, 243, 557
- stability, 57, 165, 171, 319, 372, 502, 503, 505, 516, 518, 527–529, 534, 552, 555
- standard deviation, 34, 46, 366, 390, 454, 455, 457, 465, 466, 482, 483, 485, 570
- standard error, 31, 46, 365
- standard form, 124, 444
- standard order of DFT, *see* shifted DFT
- state vector, 206, 208–216, 218, 220, 223, 224, 480, 496, 557
- stationary, 287, 298, 304, 468–472, 491, 492, 585
- stationary distribution, 468, 469, 471, 472
- statistical inference, 363
- statistical mechanics, xv, 243, 394, 468
- statistics, *see* autocovariance, average, covariance, population mean, population variance, sample mean, sample variance, standard error, [variance](#)
- steepest descent, *see* gradient descent
- Stefan–Boltzmann law, 377, 379–381, 385
- Steffensen’s method, 307
- stellar structure, 494
- stencil, *see* discretization
- step size, 92–94, 99–102, 115, 117, 419, 472, 478, 479, 493, 499, 503, 515–522, 528, 529, 557
- stiffness, 516, 527
- Stirling’s formula, 436
- stochastic, 46, 374, 396, 449, 479, 480
- stress-energy tensor, 391
- Sturm–Liouville form, 537
- subinterval, 98, 315, 333, 334, 336, 338, 396, 399, 400, 405
- subnormal, 38, 81, 563
- subtract off the singularity, 443, 489
- subtractive cancellation, *see* catastrophic cancellation
- summation, *see* Basel problem, compensated summation, Euler–Maclaurin summation formula, partial sum

- superlinear convergence, 267, 272
- superposition, *see* principle of superposition
- suppress an already-found root, 274, 306
- Swift, Jonathan, 131
- symbolic differentiation, *see* analytical differentiation
- symmetric matrices, 121, 140, 171, 176, 198, 335, 568
- synthetic division, 306
- Taylor series, 30, 54, 81, 83, 86–89, 97, 102, 103, 118, 119, 399, 409, 410, 436, 441, 487, 566
- telescoping series, 234, 406, 488
- temperature, 32, 243, 378, 379, 381, 385, 391, 394
- tensor product, 212, 213, 216, 218, 220, 223, 224
- termination criterion, 173, 174, 198, 202, 241, 250, 256, 258, 259, 276, 281, 283, 304, 305, 386
- test equation, 502–505, 513, 517, 527, 528, 552, 553
- test function, 115, 116, 205
- theorem, *see* binomial theorem, Bolzano's theorem, central limit theorem, Fubini's theorem, fundamental theorem of algebra, intermediate-value theorem, mean-value theorem, Rolle's theorem, Weierstrass approximation theorem
- thermodynamic, 379, 391
- thin QR decomposition, *see* reduced QR decomposition
- timing, 26, 389, 552
- Tolman–Oppenheimer–Volkoff, 494
- trace, 21, 242, 391, 568
- trajectory, 295, 297, 298, 303, 304, 555
- transcendental equation, 243, 244
- transpose, 20, 126, 138, 179, 187, 191, 192, 200, 205, 370, 568, 569, 583
- trapeziform, *see* trapezoid rule
- trapezoid rule, 402–409, 411, 412, 414–416, 418, 420, 421, 423, 424, 427, 435, 441–443, 448, 487, 489, 490, 511, 512
- Trefethen, Lloyd Nicholas, xvi, 317
- triangle inequality, 33, 35, 130, 501
- triangular matrix, 134, 136, 147, 151, 152, 157–160, 162, 165, 170, 187, 188, 190, 198, 233, 236, 238, 240, 424, 569
- tridiagonal, 235, 236, 241, 301, 308, 335, 338, 488, 535, 536, 543, 568
- trigonometric interpolation, 315, 341, 343, 344, 346, 348, 351, 358, 389
- truncation error, 500, 501, 504, 506, 508, 533, 542
- tuple, 7–9, 11, 17, 18, 69, 71, 76, 212, 226, 227, 229, 276, 328, 452
- two-dimensional FFT, 549, 550
- two-pass, 79
- type hints, 3
- unbiased estimator, 456
- unconditionally stable, 505
- uncoupled representation, *see* coupled representation
- underdetermined, 285
- underflow, 38–40, 51, 77, 561, 564, 565
- unequally spaced abscissas, 396, 428
- uniform distribution, 458
- uniform sampling, 463–465, 467
- uniqueness, 325, 432
- unit circle, 318, 349, 354
- unit roundoff, 41
- unitary, 194, 569
- unshifted DFT, 351
- unsigned integer, 560, 561
- unstable, 54, 170, 319, 322, 429, 503, 516, 517, 528, 529
- unum, 561
- upper bound, 473, 474, 480, 481, 486
- user-defined function, 8, 20
- van der Waals, 243
- Vandermonde matrix, 321, 322, 324, 368, 387, 429
- variance, 79, 364, 366, 372–374, 382, 390–392, 454–458, 461, 462, 464, 466, 473, 483, 490–492, 570–572
- variational method, 479
- variational Monte Carlo, 481
- variational principle, *see* Rayleigh–Ritz principle
- vector field, 21, 22
- vectorization, 17
- velocity, 85, 311, 313, 391, 394, 495, 554
- Vergil (Publius Vergilius Maro), xvi, 311
- Verlet algorithm, 300, 554
- vibrations, 85, 537
- vim, 559
- virial expansion, 243
- visualization, xiii, 1, 60, 62, 546
- w-orthogonal, 440
- walker, 468, 472, 478, 479, 482, 483, 485, 492
- Waring, Edward, 322
- wave equation, 545
- wave function, 97, 109–117, 120, 244, 312, 473–476, 478–483, 485, 492, 493, 496, 545
- wave number, 112, 342, 352, 356, 359, 548
- wave vector, 120
- Weierstrass approximation theorem, 317
- weight function, 439, 440, 458, 460–462, 464, 467, 482, 485
- weighted sampling, 465, 467, 468
- well-conditioned, 125, 133, 134, 136, 140–142, 145, 165, 166, 170, 176, 248, 319, 516
- Wigner 6j-symbols, 223
- Wilkinson, James Hardy, xvi, 125, 135, 241, 273, 274
- windowing, 351
- Wordsworth, William, xiii, xv
- Yang–Mills Lagrangian, xiii
- Zeeman effect, 230
- zero-point motion, 110
- ZeroDivisionError, 50, 442
- zeros of polynomials, 272, 274, 297
- zeta function, *see* Riemann zeta function