Scientific Computing

Jonathan Goodman, Fall, 2022

Syllabus

Section 1, Introduction. floating point arithmetic, conditioning, recurrence relations

Section 2, Linear algebra 1. review and notation of basics, matrix functions (inverse, exponential), factorizations, conditioning, variational principles.

Section 3, Linear algebra 2. solving problems using factorizations: linear systems (LU, Cholesky, LDL^t), least squares (QR, SVD), low rank approximation (SVD)

Section 4, Linear algebra 3. perturbation theory and conditioning, elimination/factorization algorithms, performance (as time permits: cache, data locality, data re-use, coding for performance)

Section 5, Iterative methods. linear iterations (including role and pitfalls of eigenvalue analysis), gradient descent and variational principles, role of condition number, non-linear iterations (linearization, local and global convergence), convergence/halting criteria.

Section 6, Optimization. gradient descent, local and global minimizers, step size and line search, Newton's method with local quadratic convergence, safeguards (modified factorization, sufficient decrease criteria).

Section 7, Monte Carlo 1. random number generators, sampling methods (inverse CDF, rejection, Cholesky for multi-variate normal), simulating random processes, error bars (uncertainty quantification).

Section 8, Monte Carlo 2. random number generators, sampling methods (inverse CDF, rejection, Cholesky for multi-variate normal), simulating random processes, error bars (uncertainty quantification), Robbins Monro and stochastic gradient descent (time permitting).

Section 9, Local approximations. Taylor series as asymptotic approximations, low order finite difference approximations, panel method integrations, order of accuracy.

Section 10, asymptotic error approximations. basic definitions, convergence analysis and acceleration, adaptive methods.

Section 11, function representation. polynomial interpolation, splines.

Section 12, Fourier methods. Fourier series, discrete Fourier transform, isometry (Bessel, Plancharel), differentiation and convolution, FFT algorithm (sketch) and software.

Section 13, Dynamics. ordinary differential equation initial value problem, time stepping methods, Euler and Runge Kutta, adaptive methods.