Scientific Computing

Jonathan Goodman, Fall, 2025

Syllabus (tentative)

Sept 2, Introduction

- floating point
- relative error
- conditioning, condition number
- recurrence relations

Sept 9, Local Analysis, I (upload Assignment 1 by: **4:50 pm**)

- Big Oh
- asymptotic expansion/approximation
- Taylor series as asymptotic expansions
- an asymptotic expansion that does not converge
- finite difference approximations of derivatives
- order of accuracy

Sept 16, Local Analysis II (upload Assignment 2 by: **4:50 pm**)

- Integration, integration rules
- second order via centering
- Uses of asymptotic error expansions
- interpolation

Sept 23, Linear Algebra I (upload Assignment 3 by: **4:50 pm**)

- review: matrices and linear transformations, image, kernel, basis
- inner product, symmetry, positive definiteness
- data fitting, least squares, over and underdetermined problems
- symmetric and non-symmetric eigenvalue problems
- variational principles

Sept 30, Linear Algebra II (upload Assignment 4 by: **4:50 pm**)

- Factorizations: LU, Cholesky, QR, symmetric and non-symmetric eigenvalue/eigenvector
- applications to linear systems
- SVD
- low rank approximation

Oct 7, Linear Algebra III (upload Assignment 5 by: **4:50 pm**)

- Matrix and eigenvalue perturbation theory

- Conditioning of linear algebra problems
- Elimination and factorization algorithms (overview)
- Block matrices and applications.

Oct 14, No class: classes this Tuesday run on a Monday schedule

Oct 22, Linear Iterative Methods (upload Assignment 6 by: **4:50 pm**)

- What is a sparse matrix?
- Convergence (symmetric, positive definite), role of condition number
- Relation to gradient descent
- Least squares
- Looking for "good" subspaces and low rank approximations
- Halting criteria, good/bad/ugly

Oct 28, Optimization I (upload Assignment 7 by: **4:50 pm**)

- Local and global minimizers, convexity and the Hessian
- Gradient descent, learning rate, line search, conditioning and local linear convergence
- Newton's method, local quadratic convergence, affine invariance
- Safeguards and convergence guarantees

Nov 14, Monte Carlo I (upload Assignment 8 by: **4:50 pm**)

- "Review" of probability, PDF, conditional and marginal, Bayes' rule, central limit theorem
- Random number generators
- Direct sampling via mappings and Cholesky
- Rejection sampling, principles and efficiency
- Histograms, scatterplots, corner plots
- Simulating a random process, event driven simulation

Nov 11, Monte Carlo II (upload Assignment 9 by: **4:50 pm**)

- Error bars, central limit theorem
- Variance reduction via stratified sampling
- Variance reduction via control variates
- Density estimation using histogram and kernel methods
- **The Curse of Dimensionality**

Nov 18, Representing functions (upload Assignment 10 by: **4:50 pm**)

- One variable polynomials, polynomial bases
- One variable splines
- Low dimensional extensions of polynomials and splines
- **The Curse of Dimensionality**.
- Neural nets (overview)

Nov 25, Dynamics (upload Assignment 11 by: **4:50 pm**)

- The ODE initial value problem
- Time stepping methods
- Euler and Runge Kutta methods
- Adaptive methods (overview)

Dec 2, Optimization II (upload Assignment 12 by: **4:50 pm**)

- Autograd in JAX
- Constraints and Lagrange multipliers
- Stochastic approximation and gradient descent
- Improvements: ADAM, minibatch, etc.
- Randomized linear algebra algorithms, "good" subspaces again

Dec 9, Fourier methods (upload Assignment 13 by: **4:50 pm**)

- Fourier series representation of a continuous function
- Discrete Fourier Transform, DFT
- DFT properties: isometry, aliasing,
- Applications: convolution, filtering, etc.
- The Fast Fourier Transform (FFT) algorithm

Dec 16, Final exam, in class, pending final scheduling. Final project upload by **4:50 pm**