SCIENTIFIC COMPUTING – Part I
Extended Syllabus
Prof. Giulio Giunta

PART I - Data Science and Simulation (first semester)

Review of basic Numerical Linear Algebra: dot product and orthogonal projection – norms – linear combination of vectors - matrix-vector and matrix-matrix product – bases of linear space and projectors - Eigenvalues and eigenvectors - spectral decomposition - Power method. Review of basic MATLAB. Class hours: 4. Lab hours: 4.

Matrix factorizations: orthogonal matrices - QR factorization - Singular value decomposition (SVD) - Applications to Data Science: the idea of data dimensionality reduction, data analysis in bioinformatics, image analysis and compression, semantic indexing of texts, Principal component analysis: Lab applications in MATLAB. Class hours: 8. Lab hours: 4.

Solving systems of nonlinear equations: Newton's methods - fixed point method - application to computer graphics. Lab applications in MATLAB. Class hours: 2. Lab hours: 2.

Constrained and unconstrained minimization: gradient, Hessian, Jacobian, Lagrange multipliers - gradient descent and SGD methods - Newton methods - Levenberg-Marquardt method - nonlinear least squares - applications to data analysis, image processing, maximization of likelihood: Lab applications in MATLAB. Class hours: 6. Lab hours: 4.

Google Pagerank algorithm: graphs and matrices - computing the score vector of web pages as a (dominant) eigenvector problem - interpretation of Pagerank as a random process - Markov chains - application of Markov chains to data analysis: Lab applications in MATLAB. Class hours: 4. Lab hours: 4.

Computing derivatives: Finite differences, derivation of FD formulas, the choice of the stepsize, differentiation matrices - Symbolic differentiation - Automatic differentiation, computational graph, Forward mode, Reverse mode, backpropagation in trainig a neural network: Lab applications in MATLAB. Class hours: 4. Lab hours: 2