Eigenvalues and eigenvectors

- Eigenvalues and eigenvectors
- Important matrix properties
  - Hermitian, orthogonality,...
- Eigenvalue algorithm
  - Power iteration, a simple numerical algorithm producing a number λ, the greatest (in absolute value) eigenvalue of a matrix A, and the corresponding eigenvector v, such that $Av=\lambda v$.
  - LR algorithm, developed by Heinz Rutishauser (1958 ?)
  - QR algorithm

Applications

- collisional relaxation
- population dynamics, evolution (stationary population pyramid)
- normal modes analysis (molecular vibrations)
- PCA (principal component analysis)
- Schrödinger equation in quantum mechanics, molecular orbitals (Hartree–Fock theory)

Python libraries

- NumPy (more portability)
  - numpy.linalg
    - linalg.eig(a) Compute the eigenvalues and right eigenvectors of a square array
- SciPy (more complete wrapper on LAPACK fortran package)
  - scipy.linalg
    - scipy.linalg.eig Solve an ordinary or generalized eigenvalue problem of a square matrix
    - Decompositions (LU, QR,...)

References

- Numerical recipes, The Art of Scientific Computing 3rd Edition, William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, 2007, isbn: 9780521880688
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  - http://www2.units.it/ipl/students_area/imm2/files/Numerical_Recipes.pdf, chapter 11 Eigensystems p 456...
  - http://apps.nrbook.com/empanel/index.html#
- Python NumPy vs SciPy : *cf.* https://stackoverflow.com/questions/6684238/whats-the-fastest-way-to-find-eigenvalues-vectors-in-python