

# Eigenvalues and eigenvectors

- Eigenvalues and eigenvectors
- Important matrix properties
  - Hermitian, orthogonality,...
- Eigenvalue algorithm
  - Power iteration, a simple numerical algorithm producing a number  $\lambda$ , 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
  - <http://numerical.recipes/>
  - [http://www2.units.it/ipl/students\\_area/imm2/files/Numerical\\_Recipes.pdf](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>

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