

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
 - e.g. [Collisional relaxation via eigenfunction-eigenvalue expansion: Analysis of a simple case](#) Wendell Forst, J. Chem. Educ., 1989, 66 (2), p 142 DOI: 10.1021/ed066p142
- population dynamics, evolution (stationary [✖ population pyramid](#))
 - [✖ Leslie matrix](#)
 - [Leslie Matrix Model in Population Dynamics - CiteSeerX](#)
 - <http://personal.denison.edu/~ludwig/2011populationdynamicsandma.pdf>,...
- 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, 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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