8. Linear algebra

Motivation: transistion from classical (already done a lot) to quantum dynamics

$\rightsquigarrow$ Schrödinger equation $\quad i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$

state $\qquad$ Hamilton operator

Ansatz: $|\Psi(t)\rangle = e^{-iEt/\hbar} |\Psi_E\rangle$

$\hookrightarrow \quad \boxed{E|\Psi_E\rangle = \hat{H}|\Psi_E\rangle}$ Eigenvalue equation

$\hat{=}$ for finite dim. Hilbert space diagonalize the matrix

$H_{ij} = \langle \Psi_i | \hat{H} | \Psi_j \rangle \rightsquigarrow \boxed{E \vec{\Psi}_E = H \vec{\Psi}_E}$

eigenvalue $\qquad$ eigenvector

8.1. Matrix diagonalization

Task: for $N \times N$ matrix A we look for vectors $\vec{x}$ which satisfy $A\vec{x} = \lambda \vec{x}$

$(\vec{A} - \lambda \cdot \mathbb{1})\vec{x} = 0$ for $\vec{x} \neq 0 \rightsquigarrow \det(\lambda \cdot \mathbb{1} - A) = P(\lambda) = 0$

characteristic Polynomial

Naive approach: 1. find roots for $P(\lambda) = 0$ ✓

2. for each root λ_i solve linear sys.

$$A \cdot \vec{x}_i = \lambda_i \vec{x}_i$$

↯ too complicated, rather consider

$A' = Z^{-1} A Z$ (similarity transformation)

$\det(\lambda \mathbb{1} - A') = \cancel{\det} Z^{-1} \det(\lambda \mathbb{1} - A) \cancel{\det} Z = P(z)$

$\rightsquigarrow$ A' has same eigenvalues as A

$$\lambda \vec{X}' = A' \vec{X}' = \lambda \vec{x}' = Z^{-1} A Z \vec{x}'$$

$$\boxed{\vec{X}_i' := Z^{-1} \vec{X}_i}$$

$$\Rightarrow \lambda Z \vec{x}' = A \underbrace{Z \vec{x}'}_{\vec{X}}$$

but different eigenvectors!

Ideally: $\boxed{Z^{-1} A Z = D}$ diagonal matrix

not always possible but guaranteed for

1. real symmetric matrices, with real λ_i & $Z^{-1} = Z^T$
2. hermitian $(A^+ = (A^*)^T = A)$ — " — & $Z^{-1} = Z^+$

important for QM

If possible $A \cdot Z = Z \cdot D$ $\quad \sum A_{ij} Z_{jk} = \lambda_k Z_{ik}$

$\rightsquigarrow$ k'th column of Z is eigenvector $(\vec{X}_k)_i = Z_{ik}$

numeric methods apply sucessive transformations

$A \to \ldots P_2^{-1} P_1^{-1} A \underbrace{P_1 \; P_2 \ldots}_{Z}$ to make A diagonal

8.2. Householder-Algorithm

Find orthogonal P_1 $(P_1^T = P_1^{-1})$ such that

$$P_1^T A P_1 = \left(\begin{array}{c|ccc} a_{11} & k_1 & & 0 \\ \hline k_1 & a'_{22} & \cdots & a'_{2N} \\ \vdots & \vdots & & \vdots \\ 0 & a'_{N2} & \cdots & a'_{NN} \\ \vdots & & & \end{array}\right)$$

and continue with

$$P_2^T P_1^T A P_1 P_2 = \left(\begin{array}{cc|cc} a_{11} & \kappa_1 & & 0 \\ \kappa_1 & a'_{22} & \kappa_2 & \\ \hline & \kappa_2 & a''_{33} & \cdots \\ 0 & & \vdots & \end{array}\right) \quad \text{and so on.}$$

$\leadsto$ After N-2 steps we have a tridiagonal matrix.

Question: How to find P_n?

Ansatz $\underbrace{P_n}_{\text{Householder matrices}} = \left(\begin{array}{c|c} \mathbb{1}_{n\times n} & 0 \\ \hline 0 & S_n \end{array}\right)$ with $S_n^T = S_n$ and $S_n^2 = 1$

$\leadsto$ $S_n = 1 - 2\vec{u}_n \otimes \vec{u}_n$ with $\vec{u}_n^{\,2} = 1$

$\hat{=}$ reflection in $\mathbb{R}^{N-n}$ on an $N-n-1$ dim. hyperplane with normal vector $\vec{u}_n$

How to choose them?

for $n=1$, $P_1^T A P_1 = \left(\begin{array}{c|c} a_{11} & (S_1 \cdot \vec{v})^T \\ \hline S_1 \cdot \vec{v} & A' \end{array}\right)$ with $\vec{v} = \begin{pmatrix} a_{21} \\ \vdots \\ a_{N1} \end{pmatrix}$

$S_1 \cdot \vec{v} = \vec{v} - 2\vec{u}_1(\vec{u}_1 \cdot \vec{v}) = \kappa_1 \cdot \vec{e}_1$ ~ (N-1) dim!

solved by
$$\boxed{\begin{aligned} \kappa_1 &= \pm|\vec{v}| \quad \text{and} \\ \vec{u}_1 &= \frac{\vec{v} - \kappa_1\vec{e}_1}{|\vec{v} - \kappa_1\vec{e}_1|} \end{aligned}}$$

choose $\text{sign}(\kappa_1) = -\text{sign}(a_{21})$

to minimize numerical errors in (no cancellation)

8.3. QR-decomposition (and tridiagonal matrices)

every real matrix can be decomposed into

$A = Q \cdot R$ ~ upper triangular ($\triangledown$)

orthogonal

$\rightsquigarrow \quad Q^T \cdot A = R$

$$Q^T = P_{N-1} \cdot \ldots \cdot P_1 \cdot P_0$$

This time we start with P_0

$$P_0 \cdot A = \left(\begin{array}{c|c} k_0 & * \\ \hline 0 & A' \end{array}\right) \quad \text{with} \quad k_0 = \pm |\vec{v}|, \quad u_0 = \frac{\vec{v} - k_0 \vec{e}_1}{|\vec{v} - k_0 \vec{e}_1|}$$

and so on.

For tridiagonal matrix
$$A = \begin{pmatrix} a_{11} & k_1 & & 0 \\ k_1 & a_{22} & k_2 & \\ 0 & k_2 & a_{33} & \ddots \\ & & \ddots & \end{pmatrix}$$

$Q^T = P_{N-1\,N} \ldots P_{23}\, P_{12}$ with Jacobi-rotation

$$\begin{array}{cc} & \begin{array}{ccccc} & & p & q & \end{array} \\ P_{pq} = \begin{array}{c} \\ p \rightarrow \\ q \rightarrow \\ \end{array} & \begin{pmatrix} 0 & \ldots & & & 0 \\ & & c & \ldots\, s & \\ & & -s & \ldots\, c & \\ 0 & & & & 0 \end{pmatrix} \end{array} \quad \text{with} \quad c = \cos\phi, \quad s = \sin\phi$$

$$\boxed{t = \frac{s}{c} = \frac{k_n}{a_{nn}}, \qquad c = \frac{1}{\sqrt{1+t^2}}, \quad s = tc}$$

QR-iteration

$T_0 = A$

$T_{k-1} = Q_k \cdot R_k$ split and

$T_k = R_k \cdot Q_k$ swap

Theorem: QR-iteration converges nearly always to diagonal matrix.

Summary:
1. Householder to get tridiagonal matrix with very simple QR factorization.
2. QR-iteration (tri-diag $\Rightarrow$ tri-diag) to make A diagonal.