Eigensystems

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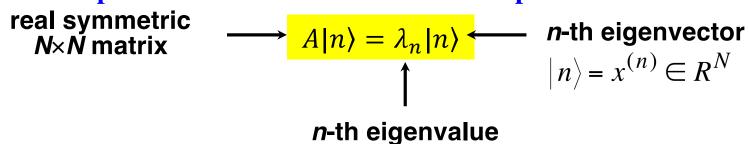
- Matrix diagonalization methods in the context of quantum mechanics
- Matrix decompositions
- Vector space: projection & rotation





Eigenvalue Problem

Eigenvalue problem in N-dimensional vector space



or

$$\sum_{j=1}^{N} A_{ij} x_j^{(n)} = \lambda_n x_i^{(n)}$$

i-th element of the n-th eigenvector

Orthonormal Basis

• The basis set $\{|n\rangle|n=1,...,N\}$ can be made orthonormal, i.e.,

$$\langle m|n\rangle = \sum_{i=1}^{N} x_i^{(m)} x_i^{(n)} = \delta_{mn}$$

• Orthogonal matrix: $U = [x^{(1)} x^{(2)} ... x^{(N)}]$ or $U_{in} = x_i^{(n)}$

$$U^T U = I$$

(Proof: orthogonality)

For Hermitian matrix:

$$\lambda_{m} \neq \lambda_{n} \qquad \langle m|A|n \rangle = \lambda_{n} \langle m|n \rangle \qquad \begin{pmatrix} A^{+} \end{pmatrix}_{ij} = A_{ji}^{*} = A_{ij}$$

$$-) \qquad \langle m|A|n \rangle = \lambda_{m} \langle m|n \rangle \qquad \begin{array}{c} \langle m|A|m \rangle = \lambda_{m} \langle n|m \rangle \\ \hline 0 = (\lambda_{n} - \lambda_{m}) \langle m|n \rangle \qquad \text{(real eigenvalue)} \end{array}$$

- $\lambda_m = \lambda_n$ (degenerate): use Gram-Schmidt orthogonalization procedure
 - 1. Orthogonal projection: $|n'\rangle \leftarrow |n\rangle |m\rangle\langle m|n\rangle = (1 |m\rangle\langle m|)|n\rangle$ $\langle m|n'\rangle = \langle m|n\rangle - \langle m|m\rangle\langle m|n\rangle = \langle m|n\rangle - \langle m|n\rangle = 0$
 - 2. Normalization: $|n'\rangle \leftarrow |n'\rangle/\langle n'|n'\rangle^{1/2}$ $\langle n'|n'\rangle = 1$

Completeness

• Arbitrary N-dimensional vector can be represented as a linear combination of (linearly independent) N vectors

$$|\psi\rangle = \sum_{n=1}^{N} |n\rangle\langle n|\psi\rangle$$

i.e.,
$$\sum_{n=1}^{N} |n\rangle\langle n| = 1$$
 or equivalently $\sum_{n=1}^{N} x_i^{(n)} x_j^{(n)} = \delta_{ij}$

Orthogonal matrix

$$U^T U = U U^T = I$$

$$\therefore U^{-1} = U^T$$

... Column-aligned eigenvectors, $U = [x^{(1)} x^{(2)} ... x^{(N)}]$, can be made an orthogonal matrix

Orthogonal Transformation

$$\sum_{i=1}^{N} \sum_{j=1}^{N} x_i^{(m)} A_{ij} x_j^{(n)} = \lambda_n \sum_{i=1}^{N} x_i^{(m)} x_i^{(n)} = \lambda_n \delta_{mn}$$
 orthogonality

Matrix eigenvalue problem = find an orthogonal transformation matrix

Spectral
decomposition
$$U^TAU = \Lambda$$

 $\Lambda_{mn} = \lambda_m \delta_{mn}$

Grand strategy: Nudge the matrix A towards diagonal form by a sequence of orthogonal transformations (successive elimination of off-diagonal elements)

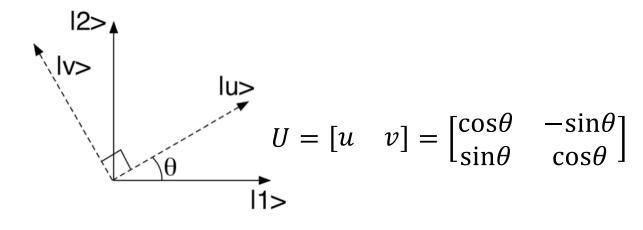
$$A \to P_1^T A P_1 \to P_2^T P_1^T A P_1 P_2 \to \cdots$$

$$U = P_1 P_2 \cdots$$

Rotation

- General real symmetric 2×2 matrix: $H = \begin{bmatrix} \varepsilon_1 & \delta \\ \delta & \varepsilon_2 \end{bmatrix}$
- General orthonormal matrices: $|u\rangle = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} = \cos\theta |1\rangle + \sin\theta |2\rangle; |v\rangle = \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}$

• Eigenvalue solution



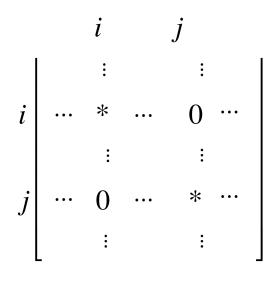
$$\begin{bmatrix} \lambda - \varepsilon_1 & -\delta \\ -\delta & \lambda - \varepsilon_2 \end{bmatrix} \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \det(\lambda I - H) = \begin{vmatrix} \lambda - \varepsilon_1 & -\delta \\ -\delta & \lambda - \varepsilon_2 \end{vmatrix} = (\lambda - \varepsilon_1)(\lambda - \varepsilon_2) - \delta^2 = 0$$

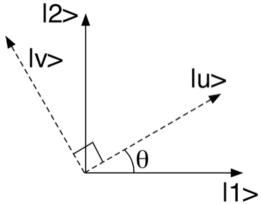
$$\lambda_{\pm} = \frac{\varepsilon_1 + \varepsilon_2 \pm \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\delta^2}}{2}$$

$$\theta = \tan^{-1} \left(\frac{-\varepsilon_1 + \varepsilon_2 + \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\delta^2}}{2\delta} \right) \xrightarrow{\delta \to 0} \frac{\delta}{\varepsilon_1 - \varepsilon_2}$$

Jacobi Transformation

• Successive 2D rotations to eliminate off-diagonal (i,j)–(j,i) pairs



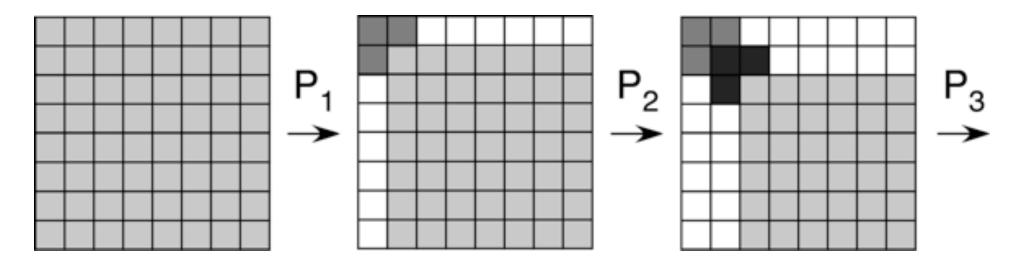




Carl Jacobi (1804-1851)

Householder Transformation

• Eliminate an entire row (but the first 2 elements) at a time



• The outcome is a tridiagonal matrix



Alston Householder (1904-1993)

Projection Matrix

• Let an N-dimensional vector $v \in \mathbb{R}^N$ & the projection matrix

$$P = I - \frac{2vv^{T}}{v^{T}v} = I - \frac{2|v\rangle\langle v|}{\langle v|v\rangle}$$

then P is symmetric & orthonormal, i.e.,

$$P^T P = PP = I$$

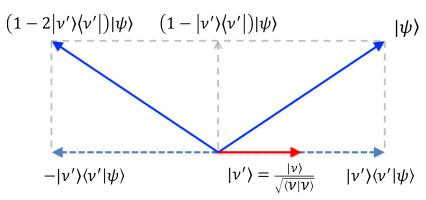
(Proof)

$$P_{ij} = \delta_{ij} - \frac{2v_i v_j}{\sum_{k=1}^{N} v_k^2} \leftarrow \text{symmetric w.r.t. } i \leftrightarrow j$$

$$PP = \left(I - \frac{2vv^T}{v^Tv}\right)\left(I - \frac{2vv^T}{v^Tv}\right) = I - \frac{4vv^T}{v^Tv} + \frac{4vv^Tvv^T}{\left(v^Tv\right)^2}$$

$$= I - \frac{4vv^T}{v^Tv} + \frac{4vv^T}{v^Tv} = I$$

Mirror image: reflect twice = do nothing



Householder Matrix

• For $x \in \mathbb{R}^N$, let $v = x \mp ||x||_2 e_1$ where

$$e_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix}$$
 & the vector 2-norm is $||x||_2 = \sqrt{x^T x} = \sqrt{\sum_{i=1}^N x_i^2}$

then the Householder matrix below, when multiplied, eliminates all the elements of x but one:

$$Px = \left(I - \frac{2vv^T}{v^Tv}\right)x = \mp \|x\|_2 e_1$$

(Proof)

$$v^T v = (x^T \pm ||x||_2 e_1^T) (x \pm ||x||_2 e_1) = ||x||_2^2 \pm 2||x||_2 x_1 + ||x||_2^2 = 2||x||_2 (||x||_2 \pm x_1)$$

$$Px = x - \frac{2vv^{T}}{2\|x\|_{2}(\|x\|_{2} \pm x_{1})}x = x - \frac{(x \pm \|x\|_{2}e_{1})(x^{T} \pm \|x\|_{2}e_{1}^{T})x}{\|x\|_{2}(\|x\|_{2} \pm x_{1})}$$

$$= x - \frac{(x \pm \|x\|_{2}e_{1})\|x\|_{2}(\|x\|_{2} \pm x_{1})}{\|x\|_{2}(\|x\|_{2} \pm x_{1})} = x - x \mp \|x\|_{2}e_{1} = \mp \|x\|_{2}e_{1}$$

Tridiagonalization

Householder matrix can be used for tridiagonalization: Let

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & & & \\ \vdots & & & \\ a_{N1} & & & \end{bmatrix} = \begin{bmatrix} a_{11} & A_{12} = A_{21}^T \\ & & & \\ A_{21} & & & A_{22} \end{bmatrix}$$

$$v \in \mathbb{R}^{N-1} = A_{21} + \operatorname{sign}(a_{21}) ||A_{21}||_2 e_1$$

then

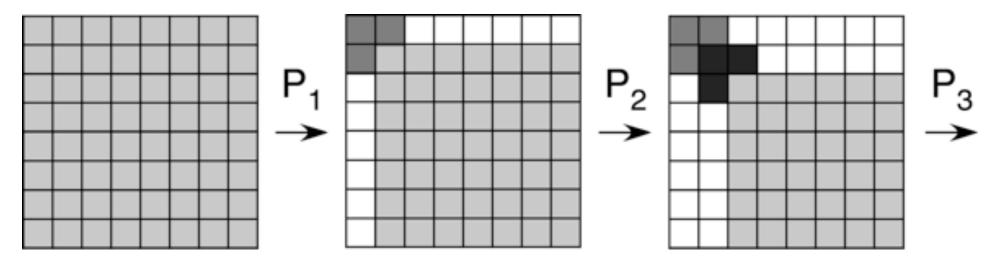
$$\overline{P}A_{21} = \left(I_{N-1} - \frac{2vv^T}{v^Tv}\right)A_{21} = -\operatorname{sign}(a_{21}) ||A_{21}||_2 e_1 = ke_1$$

$$PAP = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & \overline{P} & 0 \end{bmatrix} \begin{bmatrix} a_{11} & A_{21}^T & & \\ A_{21} & & A_{22} & \\ & & & \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & \overline{P} & 0 \end{bmatrix}$$

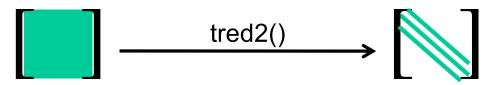
$$= \begin{bmatrix} a_{11} & A_{21}^T \\ k & \\ 0 & \overline{P}A_{22} \\ \vdots & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \\ \vdots & \overline{P} & \\ 0 \end{bmatrix} = \begin{bmatrix} a_{11} & k & 0 & \cdots & 0 \\ k & \\ 0 & & \overline{P}A_{22}\overline{P} \\ \vdots & \\ 0 & & \end{bmatrix}$$

Householder Transformation

• After (N-2) such transformations, all the off-diagonal elements but the diagonal & upper/lower sub-diagonal elements are eliminated



• The outcome is a tridiagonal matrix (done in tred2() in *Numerical Recipes*)



QR Decomposition

- Used for the diagonalization of a tridiagonal matrix
- Let A = QR, where Q is orthogonal & R is upper-triangular, $R_{ij} = 0$ for i > j
- QR decomposition by Householder transformation

$$A = \begin{bmatrix} a_{11} \\ \vdots \\ a_{N1} \end{bmatrix} = \begin{bmatrix} A_1 & A_2 \end{bmatrix} \quad v \quad (\in \mathbb{R}^N) = A_1 + \text{sign}(a_{11}) ||A_1||_2 e_1$$

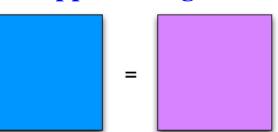
$$PA_1 = \left(I_N - \frac{2vv^T}{v^T v} \right) A_1 = -\text{sign}(a_{11}) ||A_1||_2 e_1 = ke_1$$

$$PA = \begin{bmatrix} PA_1 & PA_2 & \\ PA_1 & PA_2 & \\ 0$$

• After (N-1) transformations, the matrix is upper-triangular

$$P_{N-1} \cdots P_2 P_1 A = R$$

$$A = P_1^{-1} P_2^{-1} \cdots P_{N-1}^{-1} R \equiv QR$$





Orthogonal Transformation by QR

$$A = QR \quad A' = RQ$$

$$R = Q^{-1}A = Q^{T}A$$

$$A \rightarrow A' = Q^{T}AQ$$

(QR algorithm)

$$\begin{cases} 1. Q_s R_s \leftarrow A_s \\ 2. A_{s+1} \leftarrow R_s Q_s \end{cases} \quad s = 1, 2, \dots$$

(Theorem)

- 1. $\lim_{s\to\infty}A_s$ is upper-triangular
- 2. The eigenvalues appear on its diagonal
- tqli() in *Numerical Recipes* uses QL algorithm instead to obtain lowertriangular matrix
- Fast -O(N) operations per iteration for a tridiagonal matrix