

Eigensystems

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations

Department of Computer Science

Department of Physics & Astronomy

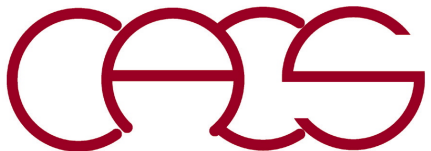
Department of Chemical Engineering & Materials Science

Department of Quantitative & Computational Biology

University of Southern California

Email: anakano@usc.edu

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



Eigenvalue Problem

- Eigenvalue problem in N -dimensional vector space

real symmetric
 $N \times N$ matrix

$$A|n\rangle = \lambda_n |n\rangle$$

n -th eigenvector
 $|n\rangle = x^{(n)} \in R^N$

n -th eigenvalue

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 $\{|n\rangle | n = 1, \dots, N\}$ can be made orthonormal, i.e.,

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

- Orthogonal matrix: $U = [\mathbf{x}^{(1)} \mathbf{x}^{(2)} \dots \mathbf{x}^{(N)}]$ or $U_{in} \equiv x_i^{(n)}$

$$U^T U = I \quad \because \sum_{i=1}^N x_i^{(m)} x_i^{(n)} = \sum_{i=1}^N \overbrace{U_{im}^T}^{U_{mi}^T} U_{in} = (U^T U)_{mn} = \delta_{mn}$$

(Proof: orthogonality)

For Hermitian matrix:

- $\lambda_m \neq \lambda_n$ $\langle m | A | n \rangle = \lambda_n \langle m | n \rangle$ $(A^+)_{ij} = A_{ji}^* = A_{ij}$
 $\quad \quad \quad -) \quad \langle m | A | n \rangle = \lambda_m \langle m | n \rangle$ $\xleftarrow{\text{complex conjugate (real eigenvalue)}} \langle n | A | m \rangle = \lambda_m \langle n | m \rangle$
 $\quad \quad \quad \hline 0 = (\lambda_n - \lambda_m) \langle m | n \rangle$

$$\lambda_n \langle n | n \rangle = \langle n | A | n \rangle = \langle n | A^+ | n \rangle = \lambda_n^* \langle n | n \rangle$$

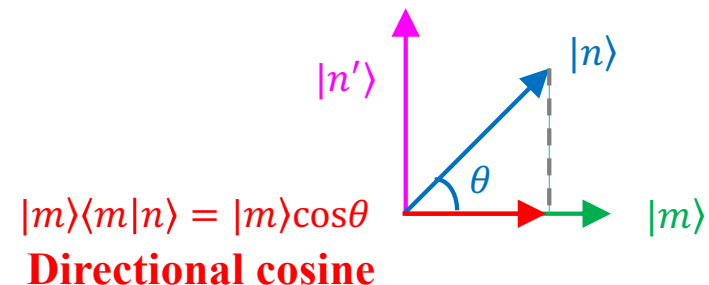
$$0 = (\lambda_n - \lambda_n^*) \langle n | n \rangle \Leftrightarrow \lambda_n = \lambda_n^*$$

- $\lambda_m = \lambda_n$ (degenerate): use **Gram-Schmidt orthogonalization procedure**

- Orthogonal projection: $|n'\rangle \leftarrow |n\rangle - \overbrace{|m\rangle \langle m | n \rangle}^1 = (1 - |m\rangle \langle m|) |n\rangle$

$$\langle m | n' \rangle = \langle m | n \rangle - \overbrace{\langle m | m \rangle}^1 \langle m | n \rangle = 0$$

- Normalization: $|n'\rangle \leftarrow |n'\rangle / \langle n' | n' \rangle^{1/2}$
 $\langle n' | n' \rangle = 1$



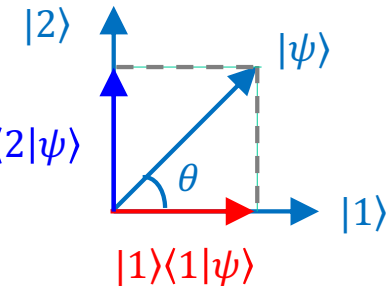
Completeness

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

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

2D example

(just Cartesian coordinates)



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

$$\psi_i = \sum_{n=1}^N x_i^{(n)} \sum_{j=1}^N x_j^{(n)} \psi_j = \sum_{j=1}^N \overbrace{\sum_{n=1}^N x_i^{(n)} x_j^{(n)}}^{\delta_{ij}} \psi_j$$

- Orthogonal matrix

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

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

$$\delta_{ij} = \sum_{n=1}^N x_i^{(n)} x_j^{(n)} = \sum_{n=1}^N U_{in} \overbrace{U_{jn}^T}^{\widetilde{U}_{jn}} = (U U^T)_{ij}$$

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

Orthogonal Transformation

$$\sum_{i=1}^N x_i^{(m)} \times \left(\sum_{j=1}^N A_{ij} x_j^{(n)} = \lambda_n x_i^{(n)} \right)$$

$$\sum_{i=1}^N \sum_{j=1}^N \overbrace{x_i^{(m)}}^{U_{mi}^T} A_{ij} \overbrace{x_j^{(n)}}^{U_{jn}} = \lambda_n \sum_{i=1}^N x_i^{(m)} x_i^{(n)} \stackrel{\text{orthogonality}}{=} \overbrace{\lambda_n \delta_{mn}}^{\equiv \Lambda_{mn}}$$

- Matrix eigenvalue problem = find an orthogonal transformation matrix

Spectral
decomposition

$$U^T A U = \Lambda$$

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

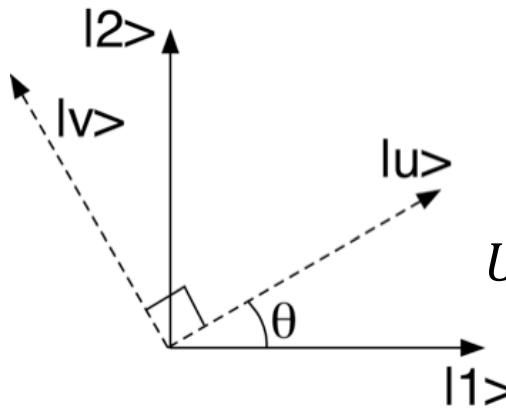
- Grand strategy:** Nudge the matrix A towards diagonal form by a sequence of orthogonal transformations (successive elimination of off-diagonal elements)

$$A \rightarrow P_1^T A P_1 \rightarrow P_2^T P_1^T A P_1 P_2 \rightarrow \dots$$

$$\begin{bmatrix} \text{matrix} \end{bmatrix} \xrightarrow{U = P_1 P_2 \dots} \begin{bmatrix} \text{diagonal} \end{bmatrix}$$

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**

$$U = [u \quad v] = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

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

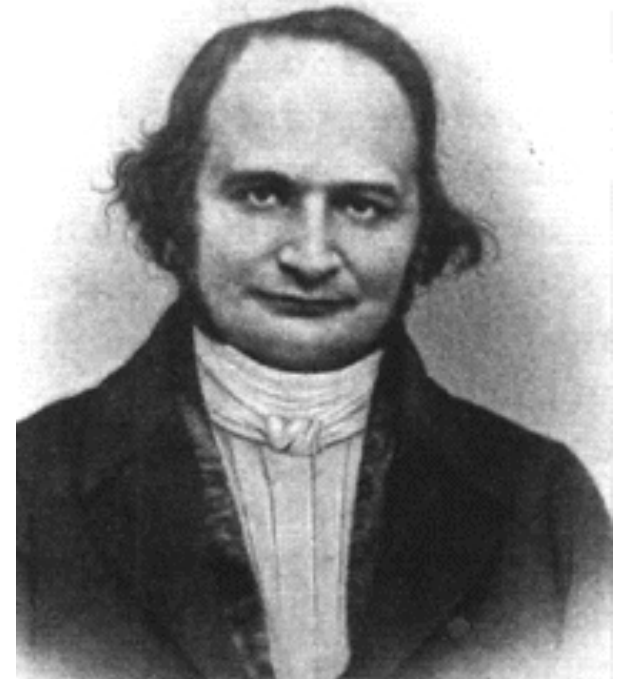
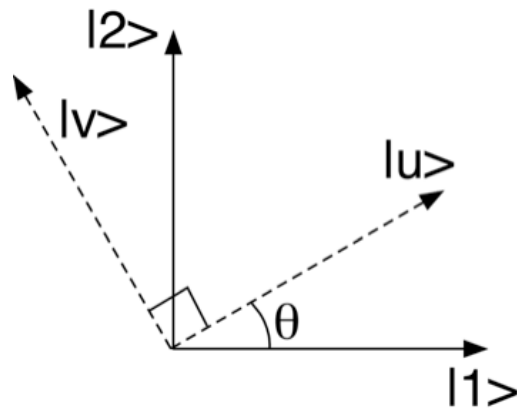
$$\lambda_{\pm} = \frac{\varepsilon_1 + \varepsilon_2 \pm \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\delta^2}}{2}$$

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

Jacobi Transformation

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

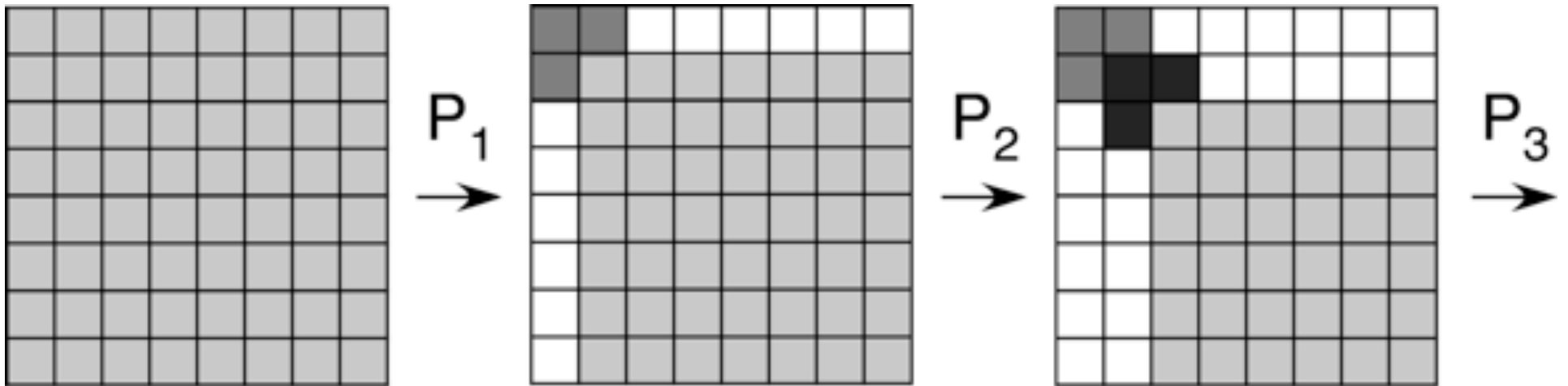
$$\begin{array}{c} i \quad j \\ \vdots \quad \vdots \\ i \quad \dots \quad * \quad \dots \quad 0 \quad \dots \\ \vdots \quad \vdots \\ j \quad \dots \quad 0 \quad \dots \quad * \quad \dots \\ \vdots \quad \vdots \end{array} \left[\begin{array}{cc} i & j \\ \vdots & \vdots \\ \vdots & \vdots \\ \vdots & \vdots \end{array} \right]$$



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.,

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

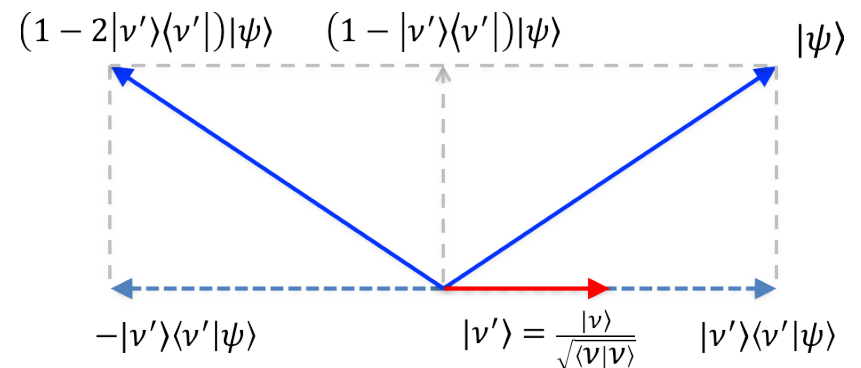
(Proof)

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

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

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

Mirror image: reflect twice = do nothing



Householder Matrix

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

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

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

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

(Proof)

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

$$\begin{aligned} Px &= x - \frac{2vv^T}{2\|x\|_2(\|x\|_2 \pm x_1)} x = x - \frac{(x \pm \|x\|_2 e_1)(x^T \pm \|x\|_2 e_1^T)x}{\|x\|_2(\|x\|_2 \pm x_1)} \\ &= x - \frac{(x \pm \|x\|_2 e_1)\|x\|_2(\|x\|_2 \pm x_1)}{\|x\|_2(\|x\|_2 \pm x_1)} = x - x \mp \|x\|_2 e_1 = \mp \|x\|_2 e_1 \end{aligned}$$

Tridiagonalization

- Householder matrix can be used for tridiagonalization: Let

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

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

then

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

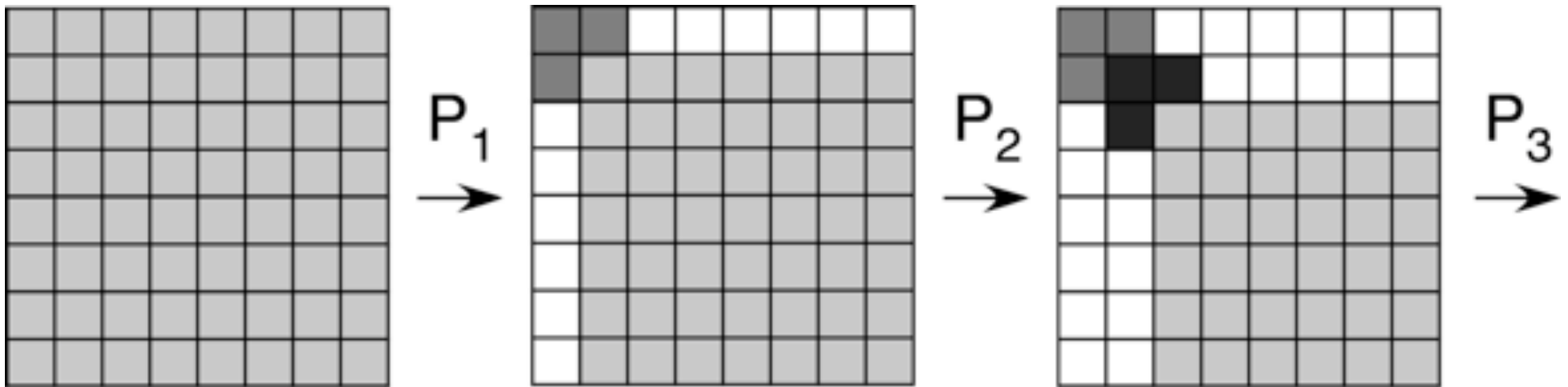
$$PAP \equiv \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & \bar{P} & & \\ 0 & & & \end{bmatrix} \begin{bmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & \bar{P} & & \\ 0 & & & \end{bmatrix} \quad \begin{matrix} N-1 \times N-1 & N-1 \times 1 \\ \bar{\bar{P}} & \widehat{A_{21}} \end{matrix} = \begin{bmatrix} k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

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

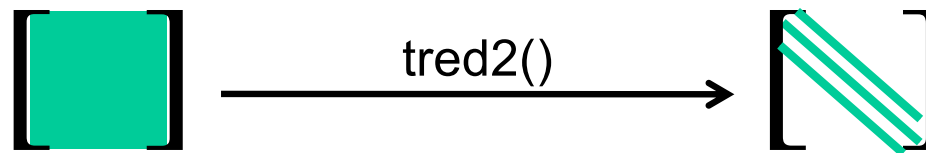
Householder Transformation

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

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



- 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

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

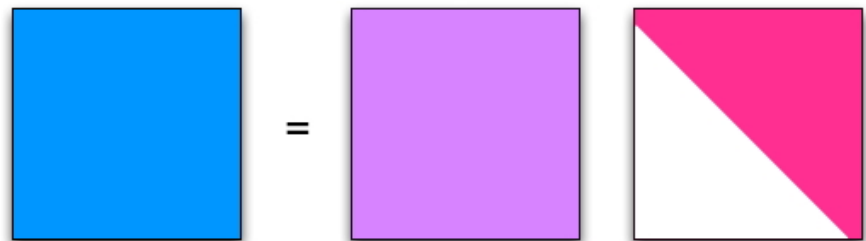
$$PA_1 \equiv \left(I_N - \frac{2vv^T}{v^T v} \right) A_1 = -\text{sign}(a_{11})\|A_1\|_2 e_1 \equiv ke_1$$

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

- 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

$$\begin{aligned} A &= QR & A' &= RQ \\ &\quad \downarrow & R &= Q^{-1}A = Q^T A \\ A &\rightarrow A' = Q^T A Q \end{aligned}$$

(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. $\lim_{s \rightarrow \infty} A_s$ is upper-triangular
2. The eigenvalues appear on its diagonal

- `tqli()` in *Numerical Recipes* uses QL algorithm instead to obtain lower-triangular matrix
- Fast — $O(N)$ operations per iteration — for a tridiagonal matrix
- In `tqli()` in *Numerical Recipes* to diagonalize a tridiagonal matrix, a sequence of rotations are applied to eliminate subdiagonal elements

Top 10 algorithms in history
IEEE CiSE, Jan/Feb ('00)

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method