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**

real symmetric
$N \times N$ matrix

$$\boxed{A|n\rangle = \lambda_n |n\rangle}$$

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

n-th eigenvalue

or more explicitly

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

i-th element of the n-th eigenvector

Orthonormal Basis

- **The basis set** $\{|n\rangle | n = 1, \ldots, N\}$ **can be made orthonormal, *i.e.*,**
  $\langle m|n\rangle = \sum_{i=1}^{N} x_i^{(m)} x_i^{(n)} = \delta_{mn}$

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

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

(Proof: orthogonality)

For Hermitian matrix:

$$\left(A^\dagger\right)_{ij} = A_{ji}^* = A_{ij}$$

- $\lambda_m \neq \lambda_n$

$$\begin{array}{rl} & \langle m|A|n\rangle = \lambda_n \langle m|n\rangle \\ -) & \langle m|A|n\rangle = \lambda_m \langle m|n\rangle \\ \hline & 0 = (\lambda_n - \lambda_m)\,\langle m|n\rangle \end{array}$$

$$\xleftarrow[\text{(real eigenvalue)}]{\text{complex conjugate}} \langle n|A|m\rangle = \lambda_m \langle n|m\rangle$$

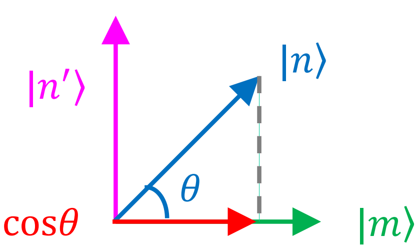
$$\lambda_n \langle n|n\rangle = \langle n|A|n\rangle = \left\langle n\middle|A^\dagger\middle|n\right\rangle = \lambda_n^* \langle n|n\rangle$$
$$0 = (\lambda_n - \lambda_n^*)\langle n|n\rangle \Leftrightarrow \lambda_n = \lambda_n^*$$

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

1. **Orthogonal projection:** $|n'\rangle \leftarrow |n\rangle - |m\rangle\langle m|n\rangle = (1 - |m\rangle\langle m|)|n\rangle$

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

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



$|m\rangle\langle m|n\rangle = |m\rangle\cos\theta$

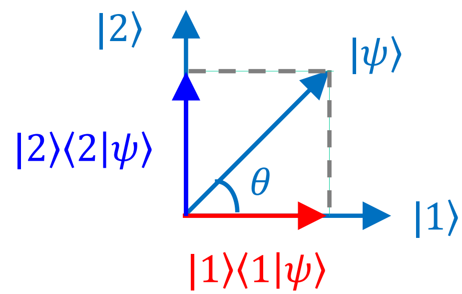
Directional cosine

Completeness

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

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

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**

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

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

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

Orthogonal Transformation

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

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

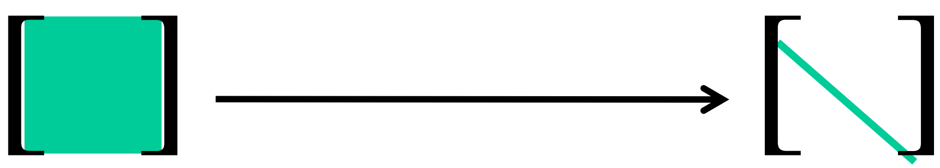
- **Matrix eigenvalue problem = find an orthogonal transformation matrix**

Spectral decomposition

$$\boxed{\begin{gathered} U^T A U = \Lambda \\ \Lambda_{mn} = \lambda_m \delta_{mn} \end{gathered}}$$

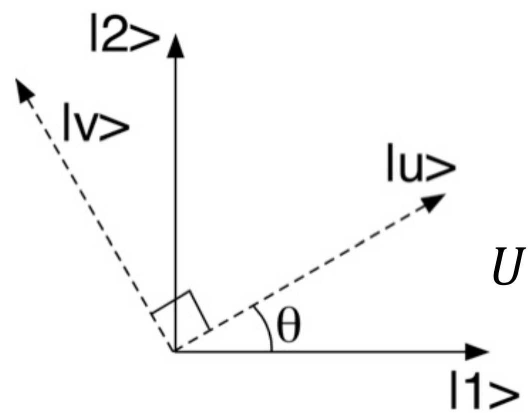
- **Grand strategy: Nudge the matrix *A* towards diagonal form by a sequence of orthogonal transformations (successive elimination of off-diagonal elements)**

$$A \to P_1^T A P_1 \to \overbrace{P_2^T P_1^T}^{U^T} A \overbrace{P_1 P_2}^{U} \to \cdots$$
$$U = P_1 P_2 \cdots$$



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**



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

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

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

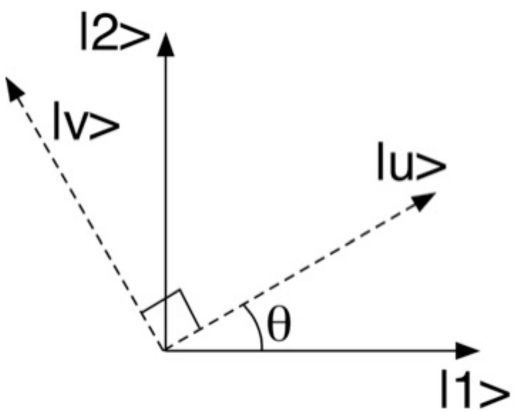
$$\theta = \tan^{-1}\left(\frac{-\varepsilon_1 + \varepsilon_2 + \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\delta^2}}{2\delta}\right) \xrightarrow{\delta \to 0} \frac{\delta}{\varepsilon_1 - \varepsilon_2}$$

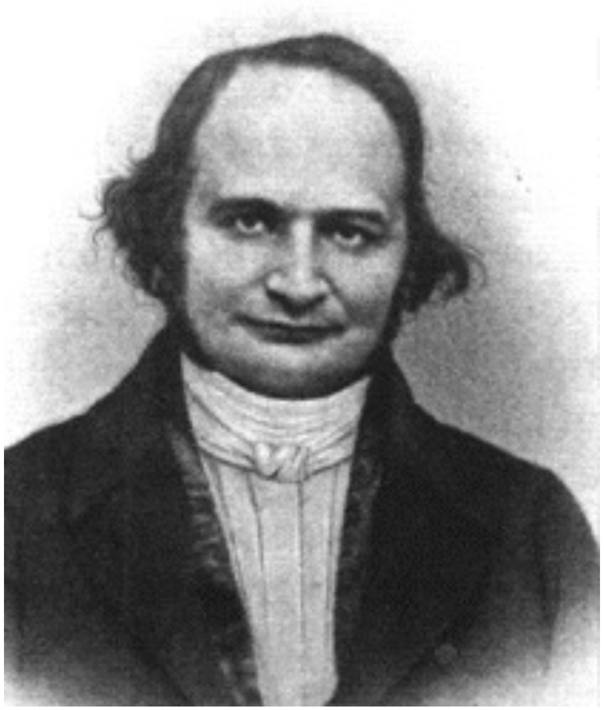
for λ_+ and $\varepsilon_1 > \varepsilon_2$

Jacobi Transformation

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

$$\begin{array}{cc} & \begin{array}{ccccc} & i & & j & \end{array} \\ \begin{array}{c} \\ i \\ \\ j \\ \\ \end{array} & \begin{bmatrix} & \vdots & & \vdots & \\ \cdots & * & \cdots & 0 & \cdots \\ & \vdots & & \vdots & \\ \cdots & 0 & \cdots & * & \cdots \\ & \vdots & & \vdots & \end{bmatrix} \end{array}$$

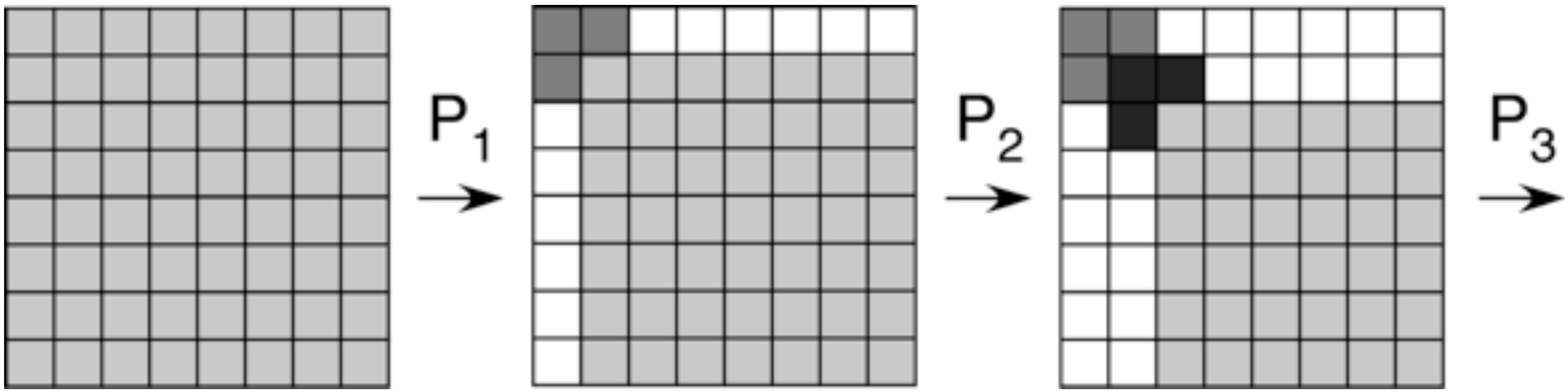




Carl Jacobi
(1804-1851)

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** $v\ (\in \Re^N)$ **& the projection matrix**

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

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

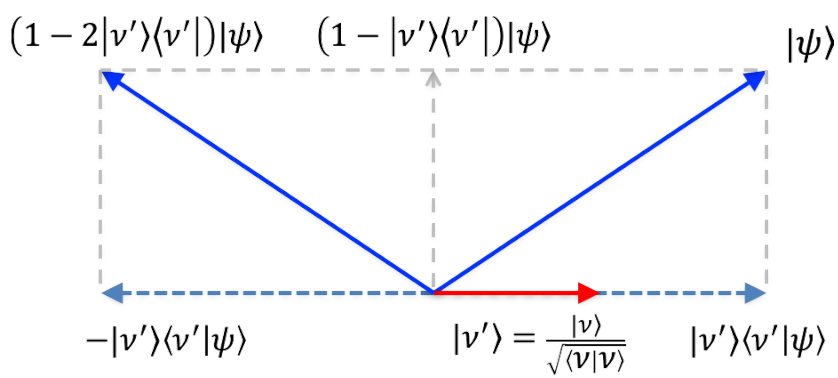
$$P^TP = PP^T = I$$

(Proof)

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

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

Mirror image: reflect twice = do nothing



Householder Matrix

- **For x ($\in$ 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:

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

(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**

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

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

then

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

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

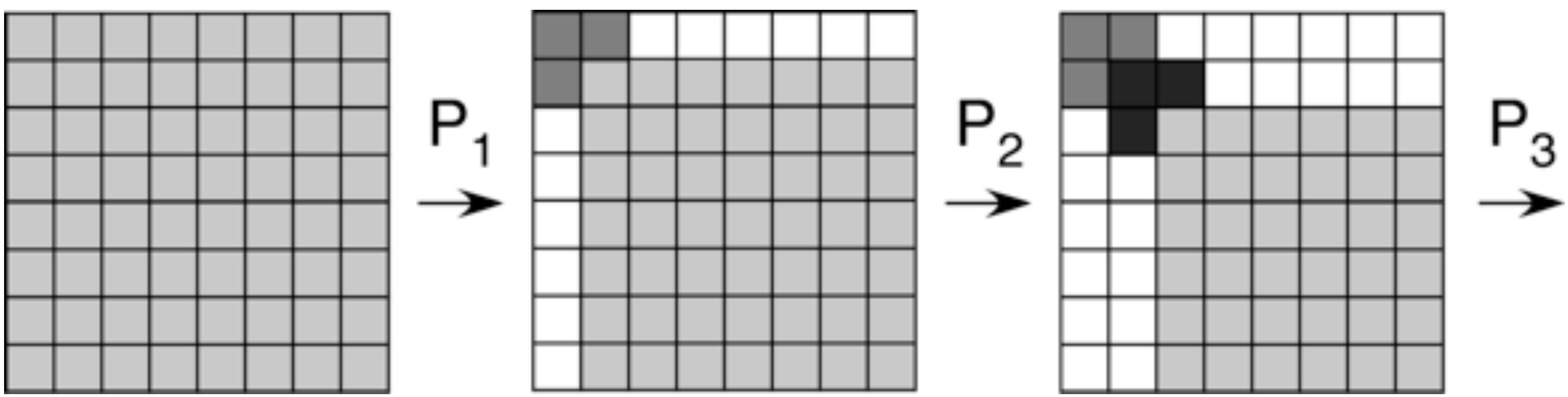
$$\overbrace{\bar{P}}^{N-1 \times N-1} \; \overbrace{A_{21}}^{N-1 \times 1} = \begin{bmatrix} k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

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

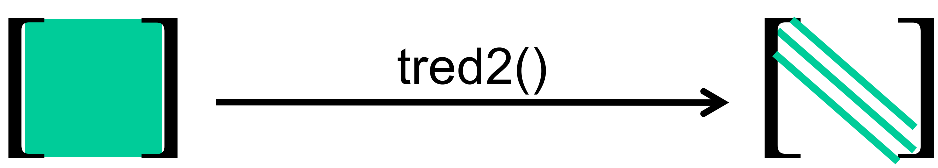
Householder Transformation

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

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



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



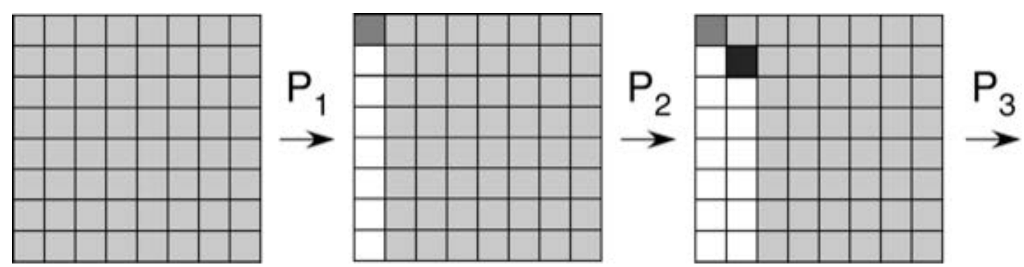
QR Decomposition

- **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**

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

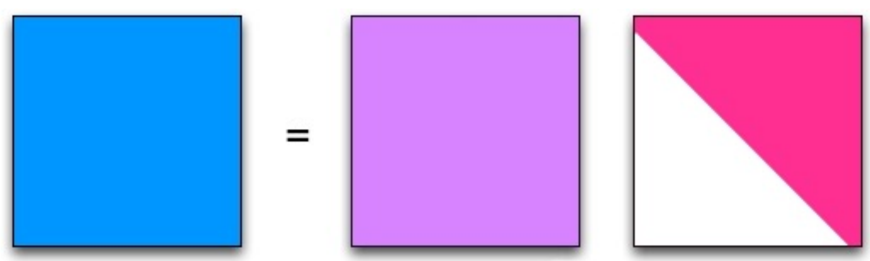
$$PA_1 \equiv \left(I_N - \frac{2vv^T}{v^T v}\right) A_1 = \text{-}\mathrm{sign}(a_{11}) \|A_1\|_2 e_1 \equiv k e_1$$

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



- **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

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

$$\Downarrow \; R = Q^{-1}A = Q^T A$$

$$A \rightarrow A' = Q^T A Q$$

(QR algorithm)

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

(Theorem)

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

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

- **tqli() in *Numerical Recipes* uses QL algorithm instead to obtain lower-triangular matrix**
- **Fast — *O*(*N*) operations per iteration — for a tridiagonal matrix**
- **tqli() diagonalizes a tridiagonal matrix by a sequence of rotations to eliminate subdiagonal elements, in addition to eigenvalue-shift to accelerate the convergence**