Feb 21, 2006

< Eigenvalue problems >

$$\left[-\frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i<j} V(r_{ij})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

$$\vec{r} = (r_1, r_2, \ldots, r_N)$$

$N \times N$ matrix A has an eigenvector x and corresponding eigenvalue λ if $Ax = \lambda x$.

Only if $\det|A - \lambda I| = 0$, there exist non-trivial solutions x.

Numerically solving eigenvalue problems (Jacobi, Householder, QL algorithm) use similarity transform.

- <u>Similarity transformation</u> :

$$D = R^T A R$$

A: real $\quad R$: orthogonal matrix $\quad R^T = R^{-1}$

$\quad$ complex $\quad$ unitary matrix $\quad R^\dagger = R^{-1}$

D: diagonal matrix

$$\det|\overbrace{R^T A R}^{D} - \lambda I| = \det|R^T(A - \lambda I)R|$$

$$= \cancel{\det|R| \cdot \det|A - \lambda I| \det|R^T|}$$

$$= \det|A - \lambda I|$$

Eigenvalues of D = Eigenvalues of A

- Strategy of all modern eigensystem routines :

(i) Diagonalize the matrix A by applying a sequence of similarity transformations

$$A \to P_1^{-1} A P_1 \to P_2^{-1}(P_1^{-1} A P_1) P_2$$

$$\to P_3^{-1}(P_2^{-1} P_1^{-1} A P_1 P_2) P_3 \to \cdots$$

(ii) If we obtain the diagonal matrix, then the eigenvectors are columns of the accumulated transformation

$$X_R = P_1 \cdot P_2 \cdot P_3 \cdots$$

- If we are interested only in $\boxed{\text{eigenvalue}}$ not eigenvectors, it is enough to transform the matrix A to be triangular (upper or lower triangular). → Gaussian elimination
  Eigenvalue : diagonal elements of upper or lower triangular matrix

- How to implement the strategy :

  (i) Construct individual P_i's to perform specific tasks such as zeroing a particular off-diagonal element (Jacobi transformation) or zeroing a whole particular row or column (Householder transformation).
  Then iterate the finite sequence of the transformations until the deviation of the matrix from diagonal is negligibly small.

  (ii) Use the finite sequence of transformations to go most of the way and follow up with factorization method. (QR or QL method)

  factorization method :

  $$\text{matrix } A = F_L \cdot F_R \quad \text{or} \quad F_L^{-1} \cdot A = F_R \quad \cdots \text{①}$$

  Similarity tr. if F_L orthogo

  Multiply by F_L from the right $F_L^{-1} \cdot A \cdot F_L = F_R \cdot F_L$

$$\begin{pmatrix} a_{11} & a_{12} & & & 0 \\ a_{12} & a_{22} & a_{23} & & \\ & a_{32} & a_{33} & \ddots & \\ 0 & & & \ddots & a_{nn} \end{pmatrix}$$

- Eigenpackages of Canned Eigenroutines

http://www.netlib.org/

Always a good idea to think first ① what kind of matrices you want to diagonalize

(e.g. - real, symmetric, tridiagonal
- real, symmetric, banded (only a small # of sub- or superdiagonals are nonzero)
- real, symmetric
- real, nonsymmetric
- complex, Hermitian
- Complex, non Hermitian)

& ② what you want to calculate

(e.g. - some eigenvalues, and no eigenvectors
- all eigenvalues and no eigenvectors
- all eigenvalues and some corresponding eigenvectors
- all eigenvalues and all corresponding eigenvectors)

⇒ This will save compute time and storage.

Often many eigenpackages deal with generalized eigenvalue problem

$$A \cdot x = \lambda B \cdot x$$

A, B : matrices

<Motivation of dealing with diagonalization of real symmetric matrices>

- Many physics problems deal with eigenproblems of Hermitian matrices

- A : Hermitian matrix

  $A = B + iC$ $\quad$ B, C : real matrices

  $n\times n$ complex eigenvalue problem:

  $$Ax = \lambda x \qquad x = y + iz$$

  $$\Rightarrow (B+iC)(y+iz) = \lambda(y+iz) \quad \cdots\cdots ①$$

  $\Rightarrow$ $2n\times 2n$ real eigenvalue problem:

  $$\underbrace{\begin{bmatrix} B & -C \\ C & B \end{bmatrix}}_{\text{this is a } 2n\times 2n \text{ real, symmetric matrix}} \begin{bmatrix} y \\ z \end{bmatrix} = \lambda \begin{bmatrix} y \\ z \end{bmatrix} \quad \cdots\cdots ②$$

for a given λ, $\begin{bmatrix} -z \\ y \end{bmatrix}$ is also an eigenvector because $i(y+iz)$ can also satisfy the equation ①

So if $\lambda_1, \lambda_2, \cdots, \lambda_n$ are eigenvalues of A,
$2n$ eigenvalues of Eq. ② are $\lambda_1, \lambda_1, \lambda_2, \lambda_2, \cdots, \lambda_n, \lambda_n$.

$\Rightarrow$ Solving eigenvalue problem of $n\times n$ complex Hermitian matrix
= Eigenvalue problem of $2n\times 2n$ real, symmetric matrix

$A^T = A$: Hermitian

$$A = \begin{pmatrix} b_{11} + i c_{11} & b_{12} + i c_{12} \\ b_{21} + i c_{21} & b_{22} + i c_{22} \end{pmatrix}$$

$$A^T = \begin{pmatrix} b_{11} - i c_{11} & b_{21} - i c_{21} \\ b_{12} - i c_{12} & b_{22} - i c_{22} \end{pmatrix}$$

$$A^T = A \Rightarrow c_{11} = 0, \quad c_{22} = 0$$
$$b_{21} = b_{12}, \quad c_{21} = -c_{12}$$

$$A = \begin{pmatrix} b_{11} & b_{12} + i c_{12} \\ b_{12} - i c_{12} & b_{22} \end{pmatrix}$$

$$Ax = \lambda x$$

$$\begin{pmatrix} b_{11} & b_{12} + i c_{12} \\ b_{12} - i c_{12} & b_{22} \end{pmatrix} \begin{pmatrix} y_1 + i z_1 \\ y_2 + i z_2 \end{pmatrix} = \lambda \begin{pmatrix} y_1 + i z_1 \\ y_2 + i z_2 \end{pmatrix}$$

$$b_{11}(y_1 + i z_1) + (b_{12} + i c_{12})(y_2 + i z_2) = \lambda(y_1 + i z_1)$$
$$(b_{12} - i c_{12})(y_1 + i z_1) + b_{22}(y_2 + i z_2) = \lambda(y_2 + i z_2)$$

$\lambda(y_1 + i z_1)$
$\lambda(y_2 + i z_2)$

$\begin{pmatrix} -z_1 \\ -z_2 \\ y_1 \\ y_2 \end{pmatrix}$ is also eigenvector

$$b_{11} y_1 + b_{12} y_2 - c_{12} z_2 = \lambda y_1$$
$$b_{11} z_1 + b_{12} z_2 + c_{12} y_2 = \lambda z_1$$
$$b_{12} y_1 + c_{12} z_1 + b_{22} y_2 = \lambda y_2$$
$$b_{12} z_1 - c_{12} y_1 + b_{22} z_2 = \lambda z_2$$

$$-b_{11} z_1 - b_{12} z_2 - c_{12} y_2 = -\lambda z_1$$
$$-b_{12} z_1 - b_{22} z_2 + c_{12} y_1 = -\lambda z_2$$
$$-c_{12} z_2 + b_{11} y_1 + b_{12} y_2 = \lambda y_1$$
$$+c_{12} z_1 + b_{12} y_1 + b_{22} y_2 = \lambda y_2$$

$$\left(\begin{array}{cc|cc} b_{11} & b_{12} & 0 & -c_{12} \\ b_{12} & b_{22} & c_{12} & 0 \\ \hline 0 & c_{12} & b_{11} & b_{12} \\ -c_{12} & 0 & b_{12} & b_{22} \end{array}\right) \begin{pmatrix} y_1 \\ y_2 \\ z_1 \\ z_2 \end{pmatrix} = \lambda \begin{pmatrix} y_1 \\ y_2 \\ z_1 \\ z_2 \end{pmatrix}$$

$(\lambda_1, \lambda_2, \cdots, \lambda_n)$

$\Rightarrow$ Eigenvalue problem of $n \times n$ complex Hermitian matrix

$=$ Eigenvalue problem of $2n \times 2n$ real symmetric matrix

$(\lambda_1, \lambda_1, \lambda_2, \lambda_2, \cdots, \lambda_n, \lambda_n)$ Solve Eq. (2) and choose one eigenvalue and eigenvector from each pair

Hermitian Eigenvalue problem :

- Eigenvalues of a Hermitian matrix are all real.

$$\underset{\uparrow}{\mathcal{H}} \Psi = \underset{\uparrow}{E} \Psi$$

Schrödinger eq. energy

- Eigenvectors of a Hermitian matrix can be made orthonormal
- Similarity transformation : Hermitian $\rightarrow$ diagonalized

Discuss algorithms to calculate all eigenvalues and eigenvectors of a complex, Hermitian matrix and a real, symmetric, tridiagonal matrix

< Jacobi Transformations of a Symmetric Matrix >

Essense : Applying a sequence of orthogonal similarity transformations (each transformation consisting of a plane rotation designed to <u>annihilate one of the off-diagonal elements</u>) until the matrix becomes diagonal to machine precision.

Eigenvectors : columns of the matrix consisting of the product of the transformations

Eigenvalues : diagonal elements of the final diagonal matrix

For matrices of order > 10, use the QR or QL method.

- Transform the matrix A to A'

$$A' = P_{pq}^{T} \cdot A \cdot P_{pq} \quad \cdots ③$$

φ: rotation angle

$c \equiv \cos\phi$

$s \equiv \sin\phi$

where P_{pq} = (Jacobi rotation)

$$\begin{array}{c} \text{q th column} \\ \begin{bmatrix} 1 & & & & 0 & \\ & \ddots & & & & \\ & & c & \cdots & s & \\ & & \vdots & 1 & \vdots & \\ 0 & & -s & \cdots & c & \\ & & & & & \ddots \;\; 1 \end{bmatrix} \end{array} \leftarrow \text{p th row}$$

$P_{pq}^T \cdot A$ = changes only rows p and q of A

$A \cdot P_{pq}$ = " " columns p and q.

$$A' = \begin{bmatrix} & \cdots & a'_{1p} & \cdots & a'_{1q} & \cdots & \\ \vdots & & \vdots & & \vdots & & \vdots \\ a'_{p1} & \cdots & a'_{pp} & \cdots & a'_{pq} & \cdots & a'_{pn} \\ \vdots & & \vdots & & \vdots & & \vdots \\ a'_{q1} & \cdots & a'_{qp} & \cdots & a'_{qq} & \cdots & a'_{qn} \\ \vdots & & \vdots & & \vdots & & \\ & \cdots & a'_{np} & & a'_{nq} & \cdots & \end{bmatrix}$$

Eq.③ + $(A^T = A)$

$\Rightarrow$ changed elements

$$\left.\begin{aligned} a'_{rp} &= c\,a_{rp} - s\,a_{rq} \\ a'_{rq} &= c\,a_{rq} + s\,a_{rp} \end{aligned}\right\} \quad r \neq p,\ r \neq q \quad \cdots ④$$

$$a'_{pp} = c^2 a_{pp} + s^2 a_{qq} - 2sc\,a_{pq} \quad \cdots ⑤$$

$$a'_{qq} = s^2 a_{pp} + c^2 a_{qq} + 2sc\,a_{pq} \quad \cdots ⑥$$

$$a'_{pq} = (c^2 - s^2)\,a_{pq} + sc\,(a_{pp} - a_{qq}) \quad \cdots ⑦$$

$a'_{pq} = 0$ (a'_{qp}) $\Rightarrow$ $\theta \equiv \cot 2\phi = \dfrac{c^2 - s^2}{2sc} = \dfrac{a_{pp} - a_{qq}}{2a_{pq}}$ $\cdots$ ⑧

θ is determined by a_{pp}, a_{pq}, a_{qq}.

Let $t \equiv \frac{s}{c}$. $\quad t^2 + 2t\theta - 1 = 0$

If $0 < \theta \leq \frac{\pi}{4}$ choose smaller root of the eq. such as

$$t = \frac{\mathrm{sgn}(\theta)}{|\theta| + \sqrt{\theta^2 + 1}} \quad \cdots ⑨$$

If $\theta \gg 1$, $t \approx \frac{1}{2\theta}$ ... (10)

From $c^2+s^2=1 \Rightarrow c = \frac{1}{\sqrt{1+t^2}}$

$$s = tc.$$

- To reduce round off error, replace Eq. (7) by $a'_{pq}=0$.

Replace Eqs. (4), (5), (6) by (old value + a small correction).

$$a'_{pp} = (1-s^2)a_{pp} + s^2 a_{qq} - 2sc\, a_{pq}$$

$$= a_{pp} - s^2(a_{pp}-a_{qq}) - 2sc\, a_{pq}$$

using eq. (8)

$$= a_{pp} + s^2 \frac{c^2-s^2}{sc} a_{pq} - 2sc\, a_{pq}$$

$$= a_{pp} - \frac{s\,\overbrace{(s^2+c^2)}^{1}}{c} a_{pq}$$

$$= a_{pp} - t\, a_{pq}$$

$$a'_{qq} = a_{qq} + t\, a_{pq}$$

$$a'_{rp} = a_{rp} - s(a_{rq} + \tau a_{rp})$$

$$a'_{rq} = a_{rq} + s(a_{rp} - \tau a_{rq})$$

where $\tau = \tan\frac{\phi}{2} = \frac{s}{1+c}$

- Convergence of Jacobi method:

Successive transformations undo previously set zeros but the off-diagonal elements get smaller at each rotation.

Use $S = \sum_{r \neq s} |a_{rs}|^2$

$$a_{rp}'^2 + a_{rq}'^2 = (c\,a_{rp} - s\,a_{rq})^2 + (c\,a_{rq} + s\,a_{rp})^2$$

$$= c^2 a_{rp}^2 + s^2 a_{rq}^2 + c^2 a_{rq}^2 + s^2 a_{rp}^2 - \cancel{2sc\,a_{rp}a_{rq}}$$

$$\cancel{+ 2a_{rp}a_{rq}cs}$$

$$= a_{rp}^2 + a_{rq}^2$$

So $S' = S - 2|a_{pq}|^2$

$S'' = S' - 2|a_{p'q'}|^2 - 2|a_{pq}|^2$

$\vdots$

If diagonal elements are larger compared to off-diagonal elements, you may diagonalize

$(A - kI)$ where k is the maximum value among the diagonal elements

Then the eigenvalues are $\lambda_i - k$

$$S' = \sum_{r \neq s} |a'_{rs}|^2 = S - 2|a_{pq}|^2 \geq 0$$

$\Rightarrow$ S value is bounded below by zero.

S value converges monotonically.

- Eigenvalues and eigenvectors :

$$D = V^T \cdot A \cdot V$$

diagonal matrix

where $V = P_1 \cdot P_2 \cdot P_3 \cdots$

Jacobi rotation matrix

diagonal elements of D : eigenvalues

columns of V : eigenvectors

At each stage of calculation, columns of V can be obtained by

$$V' = V \cdot P_i$$

Initially, $V = I$

$$v'_{rs} = v_{rs} \quad (s \neq p,\ s \neq q)$$

$$v'_{rp} = c\, v_{rp} - s\, v_{rq}$$

$$v'_{rq} = s\, v_{rp} + c\, v_{rq}$$

- Order in which the elements are annihilated :

$P_{12}, P_{13}, \cdots P_{1n} \; ; \; P_{23}, P_{24}, \cdots P_{2n} ; \cdots ; P_{n\,n-1}$

$a_{12}, a_{13}, \cdots, a_{1n} \; ; \; a_{23}, a_{24}, \cdots$ are killed

- One sweep : $\frac{n(n-1)}{2}$ rotations

Fortran

```
DO ISweep=1, 50      <- 50 iterations or sweeps
  DO IP=1, N-1
    DO IQ=IP+1, N
      { Jacobi transformation : Jacobi matrix P_IP,IQ }
    END DO
  END DO
END DO
```

one sweep

C

```
for (i=0; i<=49; i++){      <- 50 iterations or sweeps
  for (ip=0; ip<=n-2; ip++){
    for (iq=ip+1; iq<=n-1; iq++){
      { Jacobi transformation : P_ip,iq }
    }
  }
}
```

- Two refinements :

(i) During the first three sweeps, carry out the Jacobi transformation or rotation for (p,q) element only if $|a_{pq}| > \frac{1}{5}\frac{S_0}{n^2}$ where $S_0 = \sum_{r<s} |a_{rs}|$

(ii) After four sweeps, if $|a_{pq}| \ll |a_{pp}|$ and $|a_{pq}| \ll |a_{qq}|$, set $|a_{pq}| = 0$ and skip the rotation.

< Reduction of a symmetric matrix to Tridiagonal form : Givens and Householder reduction >

- Reduce a real, symmetric matrix to a tridiagonal form using Givens or Householder method
- Find eigenvalue and eigenvectors of the tridiagonal matrix using QR or QL algorithm

① Givens method :

Similar to the Jacobi transformation.

Using the sequence

$$P_{23}, P_{24}, \cdots, P_{2n} ; P_{34}, \cdots, P_{3n} ; \cdots ; P_{n-1\,n},$$

annihilate $a_{31}, a_{41}, \cdots, a_{n,1} ; a_{42}, a_{52}, \cdots ; a_{n\,n-2}$

(Here P_{pq} is used to make $a_{q,p-1}$ zero)

From Eq. ④ (EVP-8), $a'_{q\,p-1} = a'_{p-1\,q} = 0$

$$\Rightarrow c\,a_{p-1\,q} + s\,a_{p-1\,p} = 0 \Rightarrow \frac{s}{c} = \tan\phi = -\frac{a_{p-1\,q}}{a_{p-1\,p}}$$

$$\phi = \tan^{-1}\left[-\frac{a_{p-1\,q}}{a_{p-1\,p}}\right] \quad \text{if } r = p-1$$

We can find out a'_{rp}, a''_{rq}, a'_{pp}, a'_{qq}, a'_{pq} using the calculated ϕ.

$c \equiv \cos\phi$, $s \equiv \sin\phi$

② Householder method:

Reduce an $n \times n$ symmetric matrix A to a tridiagonal form by $n-2$ orthogonal transformations. Each transformation annihilates the required part of a whole column and whole corresponding row.

- Householder matrix $P = 1 - 2\vec{w}\cdot\vec{w}^T$ $\quad w^T w = 1$

  where w = a real vector with $|\vec{w}|^2 = 1$

P is orthogonal because

$$P^2 = (1 - 2w\cdot w^T)(1 - 2w\cdot w^T)$$

$$= 1 - 4w\cdot w^T + 4w\underbrace{(w^T\cdot w)}_{1 \text{ because } |w|^2=1} w^T$$

$$= 1$$

$$P = P^{-1}$$

$$P^T = (1 - 2ww^T)^T$$

$$= 1 - 2ww^T = P$$

$$\boxed{P^T = P^{-1}}$$

$n\times n$ matrix

Rewrite $P = 1 - \frac{\vec{u}\cdot\vec{u}^T}{H}$ where $H \equiv \frac{1}{2}|\vec{u}|^2$

Suppose that $\vec{x}$: first column vector of A

Choose $\vec{u} = \vec{x} \mp |\vec{x}|\hat{e}_1$ $\hat{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$

What does P do to $\vec{x}$?

$$P\cdot x = \left[1 - \frac{\vec{u}\cdot\vec{u}^T}{H}\right]\cdot\vec{x}$$

$$= \vec{x} - \frac{\vec{u}\cdot(\vec{x}\mp|\vec{x}|\hat{e}_1)^T\cdot\vec{x}}{H}$$

$$= \vec{x} - \frac{2\vec{u}\,(|\vec{x}|^2 \mp |\vec{x}|\,x_1)}{2|\vec{x}|^2 \mp 2|\vec{x}|\,x_1}$$

$$= \vec{x} - \vec{u} = \pm|\vec{x}|\hat{e}_1$$

Applying P to $\vec{x}$ $\Rightarrow$ make all the elements in the vector $\vec{x}$ zero but the first one.

- $A \to$ tridiagonal form :

(1) Choose $\vec{x}$ for the first Householder matrix P_1 as lower $n-1$ elements of the first column of A

$(n-1)\times(n-1)$ matrix

$$^{(n-1)}P_1 = I - \frac{\vec{u}\cdot\vec{u}^T}{H}$$

$\vec{u} = \vec{x} \mp |\vec{x}|\hat{e}_1$ $\vec{x} = \begin{pmatrix} a_{21} \\ a_{31} \\ \vdots \\ a_{n1} \end{pmatrix}$ $\hat{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$

$$A'' = P_2 \cdot A' \cdot P_2$$

$$= P_2 P_1 A P_1 P_2$$

$$= \left[\begin{array}{cc|ccc} a_{11} & k & 0 & \cdots & 0 \\ k & a'_{22} & k' & 0 \cdots & 0 \\ \hline 0 & k' & & & \\ 0 & 0 & & & \\ \vdots & \vdots & & & \\ 0 & 0 & & & \end{array}\right]$$

$\Rightarrow$ $n-2$ transformations $\rightarrow$ A : tridiagonal

- In real implementation of this algorithm:

Instead of carrying out $P \cdot A \cdot P$ compute a vector

$$\vec{p} \equiv \frac{A \cdot \vec{u}}{H}$$

$$A \cdot P = A \cdot \left(1 - \frac{\vec{u} \cdot \vec{u}^T}{H}\right) = A - \vec{p} \cdot \vec{u}^T$$

$$A' = P \cdot A \cdot P = \left(1 - \frac{\vec{u} \cdot \vec{u}^T}{H}\right)\left(A - \vec{p} \cdot \vec{u}^T\right)$$

$$= A - \vec{p} \cdot \vec{u}^T - \vec{u} \cdot \vec{p}^T + 2K\, \vec{u} \cdot \vec{u}^T$$

$$K \equiv \frac{\vec{u}^T \cdot \vec{p}}{2H} \qquad H \equiv \frac{1}{2}|\vec{u}|^2$$

$$\vec{q} \equiv \vec{p} - K\vec{u}$$

$$\boxed{A' = A - \vec{q} \cdot \vec{u}^T - \vec{u} \cdot \vec{q}^T}$$

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- In the original algorithm,
  zeroing the elements starts from n^{th} column of A
  not the first column.

- Variables are calculated in the following order:
  $\vec{u}$, H, $\vec{p}$, $\vec{K}$, $\vec{q}$, A'

- At any stage m, A is tridiagonal in its last
  m-1 rows and columns.

• Eigenvectors of matrix A
  : If the eigenvectors $\vec{v}_K$ of the final tridiagonal
  matrix are found (using the QR or QL algorithm),
  the eigenvectors of A =

$$Q\vec{v}_K = (P_1 \cdot P_2 \cdot \cdots P_{n-2})\vec{v}_K$$

algorithm real implementation

- Determine Q from recursion after all the P's are
  obtained.
  Since we start with n^{th} column,

$$Q_{n-2} = P_{n-2}$$

$$Q_j = P_j \cdot Q_{j+1} \quad (j = n-3, \cdots, 1)$$

$$Q = Q_1$$

$\vec{u} = \vec{x} \mp |\vec{x}| \hat{e}_1$

- Refinement :
  - At the stage m $(=1, 2, \cdots, n-2)$,

    the vector $\vec{u}^T = [a_{i1}, a_{i2}, \cdots, a_{i,i-2}, a_{i,i-1} \pm k, 0, \cdots 0]$

    where $i \equiv n-m+1 = n, n-1, \cdots, 3$

    $$k \equiv \sqrt{a_{i1}^2 + \cdots + a_{i\,i-1}^2}$$

    Define $\epsilon = \sum_{k=1}^{i-1} |a_{ik}|$

    If ϵ is very small, skip the transformation

    Otherwise rescale a_{ik} by ϵ.

    $$a_{ik} \rightarrow a_{ik}/\epsilon$$

    use the scaled variables for the transformation

  - When you have a matrix whose elements vary over many orders of magnitude,

    <u>permute the matrix elements such that</u>

    <u>the smaller elements go to the top left-hand</u>

    <u>corner.</u> This is because we start our reduction from the bottom right-hand corner, and that mixing small and large elements can cause significant roundoff errors.

With tridiagonal matrix, QL, QR $\Rightarrow O(N)$ calculation per iteration EVP-19

⟨Eigenvalues and eigenvectors of Tridiagonal Matrix⟩ – QR and QL algorithms.

Essence: Perform a sequence of the following orthogonal transformations until off-diagonal elements become zero.

$\boxed{QL}$

$$A_s = Q_s \cdot L_s$$

tridiagonal, orthogonal matrix, lower triangular

$$\tilde{A}_s = L_s \cdot Q_s = Q_s^T \cdot A_s \cdot Q_s$$

diagonal matrix

When A_s is a real, symmetric, tridiagonal matrix, if we use QL algorithm,

off-diagonal elements converge zero like

$$a_{ij}^{(s)} \sim \left(\frac{\lambda_i}{\lambda_j}\right)^s \quad , \lambda_i < \lambda_j$$

eigenvalues of A.

The convergence can be slow if λ_i is close to λ_j.

In this case, do <u>shifting</u> of the eigenvalues such as

$$A_s - k_s I = Q_s \cdot L_s \qquad k_s : \text{constant.}$$

$$\tilde{A}_s = L_s \cdot Q_s + k_s I$$

$$= Q_s^T \cdot A_s \cdot Q_s$$

$\Rightarrow$ convergence depends on $\frac{\lambda_i - k_s}{\lambda_j - k_s}$ not $\frac{\lambda_i}{\lambda_j}$

if $\lambda_i \sim k_s$, convergence can be very fast.

- Rule of thumb: Take a submatrix $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ of A

and find eigenvalues of the submatrix.

k_s = eigenvalue closer to a_{11}

- To annihilate the off-diagonal elements in the tridiagonal matrix, use Jacobi rotation matrices. P_{pq}.

$P_{12}, P_{23}, P_{34}, \cdots, P_{n-1n}$ will annihilate

$a_{12}, a_{23}, a_{34}, \cdots, a_{n-1n}$

(by symmetry, $a_{21}, a_{32}, a_{43}, \cdots, a_{nn-1}$ as well)

$$\boxed{Q_s^T = P_{12}^{(s)} P_{23}^{(s)} \cdots P_{n-1n}^{(s)}}$$

$$(L = Q^T A)$$

QL algorithm w/ implicit shifts.