Jacobi's rotation method

- We want ~~to~~ diagonalize A using similarity transf., or in other words, find S such that $S^T A S = D$

- Will do it by a series of sim. transf $S_1, S_2, \dots, S_M$

$$\begin{aligned}
A &\equiv A^{(1)} \\
S_1^T A S_1 &\equiv A^{(2)} \\
S_2^T S_1^T A S_1 S_2 &\equiv A^{(3)} \\
&\vdots
\end{aligned}$$

until we get an $A^{(i)}$ that is <u>close enough</u> to diagonal:

$$S_{M-1}^T \cdots S_2^T S_1^T A S_1 S_2 \dots S_{M-1} \equiv A^{(M)} \approx D$$

- Then we have $S \approx S_1 S_2 \dots S_M$
    - S contains eigen<u>vectors</u> of A
    - D contains eigen<u>values</u> of A

- Notation in our algorithm: $\boxed{A^{(m+1)} = S_m^T A^{(m)} S_m}$

For bookkeeping

- Start from $A^{(1)} = A$

$$A^{(2)} = S_1^T A^{(1)} S_1$$

$$A^{(3)} = S_2^T A^{(2)} S_2$$

$$\vdots$$

until $A^{(M)} \approx D$

eigen<u>values</u>

$$A^{(m)} = \begin{bmatrix} a_{11}^{(m)} & a_{12}^{(m)} & \dots \\ a_{21}^{(m)} & a_{22}^{(m)} & \dots \\ \vdots & & \\ & & \end{bmatrix}$$

For bookkeeping!

- $\boxed{R^{(m+1)} = R^{(m)} S_m}$

- Start from $R^{(1)} = I$

$$R^{(2)} = R^{(1)} S_1 = S_1$$

$$R^{(3)} = R^{(2)} S_2 = R^{(1)} S_1 S_2 = S_1 S_2$$

$$\vdots$$

until $R^{(M)} = R^{(M-1)} S_{M-1} = S_1 S_2 \dots S_{M-1}$

- S_m matrices are rotation matrices

$$S_m = \begin{array}{c c} & \begin{array}{c c} \quad k & \quad l \\ \quad\downarrow & \quad\downarrow \end{array} \\ \begin{array}{c} \\ k \rightarrow \\ \\ l \rightarrow \\ \\ \end{array} & \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & \cos\theta & \cdots & \sin\theta & & \\ & & \vdots & \ddots & \vdots & & \\ & & -\sin\theta & \cdots & \cos\theta & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{bmatrix} \end{array}$$

4x4 examples

$$S_m = \begin{bmatrix} \cos\theta & \sin\theta & 0 & 0 \\ -\sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$ Rotation in (x_1, x_2) plane

$$S_m = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & 0 & \sin\theta \\ 0 & 0 & 1 & 0 \\ 0 & -\sin\theta & 0 & \cos\theta \end{bmatrix}$$ Rotation in (x_2, x_4) plane

- Here S_m is defined as clockwise rotation to match Morten's lecture notes.
  Then S_m^T is a counterclockwise rotation

- Note : S_m is fully specified by (k, l, θ)
  (Never need to construct the full S_m)

- Look at 2×2 case to see where the algorithm will come from.

  - Symmetric A $(a_{21} = a_{12})$

$$A^{(1)} = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} \end{bmatrix}$$

  - We want $A^{(2)} = \begin{bmatrix} a_{11}^{(2)} & a_{12}^{(2)} \\ a_{21}^{(2)} & a_{22}^{(2)} \end{bmatrix} = \begin{bmatrix} a_{11}^{(2)} & 0 \\ 0 & a_{22}^{(2)} \end{bmatrix}$

  - So need transf. S_1 that gives $a_{12}^{(2)} = 0$ $(k=1, l=2)$

  - Let $S_1 = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \equiv \begin{bmatrix} c & s \\ -s & c \end{bmatrix}$

  - Write out $A^{(2)} = S^T A^{(1)} S$

$$\begin{bmatrix} a_{11}^{(2)} & a_{12}^{(2)} \\ a_{12}^{(2)} & a_{22}^{(2)} \end{bmatrix} = \begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} \\ a_{12}^{(1)} & a_{22}^{(1)} \end{bmatrix} \begin{bmatrix} c & s \\ -s & c \end{bmatrix}$$

  - We get:
    - $a_{11}^{(2)} = a_{11}^{(1)} c^2 - 2a_{12}^{(1)} cs + a_{22}^{(1)} s^2$
    - $a_{22}^{(2)} = a_{22}^{(1)} c^2 + 2a_{12}^{(1)} cs + a_{11}^{(1)} s^2$
    - $a_{12}^{(2)} = (a_{11}^{(1)} - a_{22}^{(1)}) cs + a_{12}^{(1)} (c^2 - s^2)$

  - Require $a_{12}^{(2)} = 0$

$$\Rightarrow \left(\frac{a_{11}^{(1)} - a_{22}^{(1)}}{a_{12}^{(1)}}\right) cs + c^2 - s^2 = 0 \qquad (*)$$

- Notation: $\tan\theta \equiv t = \frac{s}{c}$

$$\tau \equiv \frac{a_{22} - a_{11}}{2 a_{12}}$$

- Then (*) $\Rightarrow$ $s^2 + 2\tau cs - c^2 = 0$

- Divide by c^2: $\boxed{t^2 + 2\tau t - 1 = 0}$ 2nd ord. eq. for t

- Solutions: $t = -\tau \pm \sqrt{1 + \tau^2}$ [These choices of $\tan\theta$ (so angle θ) ensures that $a_{12}^{(2)} = 0$]

- Compute: $c = \frac{1}{\sqrt{1+t^2}}$

$$s = ct$$

- Can now compute $a_{11}^{(2)}$ and $a_{22}^{(2)}$

[No need to compute $a_{12}^{(2)}$ or $a_{21}^{(2)}$ — they are 0 by our choice of θ]

$\Rightarrow$ Have the new $A^{(2)} = \begin{bmatrix} a_{11}^{(2)} & 0 \\ 0 & a_{22}^{(2)} \end{bmatrix}$ Eigenvalues of A

- Eigenvectors: $R^{(2)} = R^{(1)} S_1 = I S_1 = \left[\begin{pmatrix} c \\ -s \end{pmatrix} \begin{pmatrix} s \\ c \end{pmatrix} \right]$ Eigenvectors of A

Problems

- For $N \times N$ matrix we need <u>many</u> iterations, because S_m also affect other elements along rows/colums k and l

- Can end in situation where element a_{ij} that have prev. been set to $a_{ij} = 0$ is transformed back to $a_{ij} \neq 0$ at later iteration.

Algorithm

1) • Choose tolerance ε, e.g. $\varepsilon = 10^{-8}$

• Let $A^{(1)} = A$

• Let $R^{(1)} = I$

2) Find indices (k,l) of max off-diagonal element in A

3) While $|a_{kl}^{(m)}| > \varepsilon$

3.1) Compute $\tau = \dfrac{a_{ll}^{(m)} - a_{kk}^{(m)}}{2a_{kl}^{(m)}}$

Notation:
$\sin\theta \equiv s$
$\cos\theta \equiv c$
$\tan\theta \equiv t$

3.2) Compute $\tan\theta, \cos\theta, \sin\theta$ (t, c, s):

• $t = -\tau \pm \sqrt{1+\tau^2}$

[Choose solution that gives smallest t,
i.e. smallest angle θ
So: if $\tau > 0$, use $t = -\tau + \sqrt{1+\tau^2} = \dfrac{1}{\tau + \sqrt{1+\tau^2}}$
if $\tau < 0$, use $t = -\tau - \sqrt{1+\tau^2} = \dfrac{-1}{-\tau + \sqrt{1+\tau^2}}$

• $c = \dfrac{1}{\sqrt{1+t^2}}$

If $a_{kl}^{(m)} = 0$:
$c = 1$
$s = 0$
$t = 0$

• $s = ct$

[Now we know S_m, since we have $k, l, \cos\theta, \sin\theta$]

3.3) Transform current A matrix,

$$A^{(m)} \to A^{(m+1)} = S_m^T A^{(m)} S_m$$

by updating elements:

- $a_{kk}^{(m+1)} = a_{kk}^{(m)} c^2 - 2 a_{kl}^{(m)} c s + a_{ll}^{(m)} s^2$
- $a_{ll}^{(m+1)} = a_{ll}^{(m)} c^2 + 2 a_{kl}^{(m)} c s + a_{kk}^{(m)} s^2$
- $a_{kl}^{(m+1)} = 0$
- $a_{lk}^{(m+1)} = 0$

This was the requirement we used to determine $\tan\theta$, i.e. that these elements should be transf. to 0.

- For all $i \neq k, l$:
  - $a_{ik}^{(m+1)} = a_{ik}^{(m)} c - a_{il}^{(m)} s$
  - $a_{ki}^{(m+1)} = a_{ik}^{(m+1)}$
  - $a_{il}^{(m+1)} = a_{il}^{(m)} c + a_{ik}^{(m)} s$
  - $a_{li}^{(m+1)} = a_{il}^{(m+1)}$

Must keep separate copies of some elements, i.e. don't use the new $a_{ik}^{(m+1)}$ here

3.4) Update the overall rotation matrix,

$$R^{(m)} \to R^{(m+1)} = R^{(m)} S_m$$

by updating elements:

- For all i:
  - $r_{ik}^{(m+1)} = r_{ik}^{(m)} c - r_{il}^{(m)} s$
  - $r_{il}^{(m+1)} = r_{il}^{(m)} c + r_{ik}^{(m)} s$

Again, make sure to use the correct value here!

3.5) Find the (k,l) indices of the new max off-diag. element

[While loop returns to 3)]