Jacobi Methods

Recall that any Hermitian (symmetric) matrix is diagonalizable via a unitary (orthogonal) transformation and that the eigenvectors are the columns of that transformation matrix.

\[
A = A^H \\
Aq = q\lambda \\
\lambda \in \mathbb{R} \\
AQ = Q\Lambda \\
QQ^H = Q^HQ \\
= I \\
\Lambda = \text{diag}(\lambda_1, \cdots, \lambda_n)
\]

Jacobi methods produce \( Q \) as a convergent product of rotations.
Basic Idea for Symmetric Matrices

\[ A_1 \equiv A \]
\[ A_{k+1} = U_k A_k U_k^T \]

- The matrix $U_k$ is orthogonal and represents the action of the $k$-th sweep through the matrix

- $U_k$ is the product of $n(n - 1)/2$ rotations depending on the method.
- Given’s rotations are used to define the basic update

- They are usually called Jacobi rotations in this context.

- The constraints used to determine the angle $\theta$ are more stringent than those we have seen thus far.

- Essentially the Jacobi rotations are the eigenvectors of a $2 \times 2$ symmetric matrix.
Classical Jacobi

In the classical Jacobi method, $U_k$ is defined as a product of rotations each of which is defined by its action on $e_i^T A_k e_j$ and by symmetry $e_j^T A_k e_i$. The elements in rows $i$ and $j$ and columns $i$ and $j$ are also modified.

$i$ and $j$ are chosen by finding the off-diagonal element that has the largest magnitude. (So this is done $n(n - 1)/2$ in a single sweep.)

We have

$$G_{ij} = \begin{pmatrix} I_{i-1} & 0 & 0 \\ 0 & \gamma_{ij} & \cdots & \sigma_{ij} \\ 0 & \vdots & I_{j-i+1} & \vdots & 0 \\ -\sigma_{ij} & \cdots & \gamma_{ij} & I_{n-j} \end{pmatrix}$$

where

$$\gamma_{ij} = \cos \theta_{ij}$$
$$\sigma_{ij} = \sin \theta_{ij}$$
The angle $\theta_{ij}$ is chosen so that

$$e_i^T A_{k+1} e_j = e_j^T A_{k+1} e_i = 0$$

To see how this is done we will consider the $2 \times 2$ problem that determines $\theta_{ij}$

$$R = \begin{pmatrix} \gamma_{ij} & \sigma_{ij} \\ -\sigma_{ij} & \gamma_{ij} \end{pmatrix}$$

$$\tilde{A}_k = \begin{pmatrix} \alpha_{ii}^{(k)} & \alpha_{ji}^{(k)} \\ \alpha_{ij}^{(k)} & \alpha_{jj}^{(k)} \end{pmatrix}$$

$$R\tilde{A}_k R^T = \begin{pmatrix} \alpha_{ii}^{(k+1)} & 0 \\ 0 & \alpha_{jj}^{(k+1)} \end{pmatrix}$$

i.e., $\alpha_{ij}^{(k+1)} = \alpha_{ji}^{(k+1)} = 0$. 
Simplifying the notation we have

\[
\begin{pmatrix}
\gamma & \sigma \\
-\sigma & \gamma
\end{pmatrix}
\begin{pmatrix}
\alpha & \beta \\
\beta & \delta
\end{pmatrix}
\begin{pmatrix}
\gamma & -\sigma \\
\sigma & \gamma
\end{pmatrix}
\]

And letting \( \tau = \tan \theta \) yields

\[
\gamma^2 \begin{pmatrix}
1 & \tau \\
-\tau & 1
\end{pmatrix}
\begin{pmatrix}
\alpha & \beta \\
\beta & \delta
\end{pmatrix}
\begin{pmatrix}
1 & \tau \\
-\tau & 1
\end{pmatrix}
\]

with the updated elements given by

\[
\begin{align*}
\alpha' &= \gamma^2(\alpha + 2\tau\beta + \tau^2\delta) \\
\delta' &= \gamma^2(\delta - 2\tau\beta + \tau^2\alpha) \\
\beta' &= \gamma^2(\beta - \tau\alpha + \tau\delta - \tau^2\beta)
\end{align*}
\]
So we want

\[ 0 = \gamma^2(\beta - \tau\alpha + \tau\delta - \tau^2\beta) \]
\[ 0 = \tau^2 + \frac{\alpha - \delta}{\beta} \tau - 1 \]
\[ = \tau^2 + 2\eta \tau - 1 \]
\[ \eta = \frac{\alpha - \delta}{2\beta} \]

The roots are

\[ \tau_{\pm} = -\eta \pm \sqrt{\eta^2 + 1} \]

which are always real.
Recalling how we stably evaluate the quadratic formula,

\[ \tau_1 = -\text{sign}(\eta)(|\eta| + \sqrt{\eta^2 + 1}) \]
\[ \tau_2 = \frac{-\text{sign}(\eta)}{(|\eta| + \sqrt{\eta^2 + 1})} \]

\( \tau_2 \) is always smaller and we have \( \tau_2 = \tan \theta \) where

\[-1 \leq \tau_2 \leq 1\]
\[-\frac{\pi}{4} \leq \theta \leq \frac{\pi}{4}\]

which is necessary for the proof of convergence.
Given \( \tau = \tau_2 \) we have

\[
\gamma = \frac{1}{\sqrt{1 + \tau^2}} \\
\sigma = \gamma \tau
\]

The updated diagonal elements have a simpler form as well

\[
\alpha' = \gamma^2 (\alpha + 2\tau \beta + \tau^2 \delta) \\
\delta' = \gamma^2 (\delta - 2\tau \beta + \tau^2 \alpha)
\]
To see the $\alpha'$ identity when $\tau \neq 0$ recall the following (when $\tau = 0$ it is trivially true)

\[
\eta = \frac{\alpha - \delta}{2\beta} = \frac{1 - \tau^2}{2\tau} \\
\delta - \alpha = \frac{\beta(\tau^2 - 1)}{\tau} \\
\sigma^2 + \gamma^2 = \frac{1}{\tau} \frac{\sigma}{\gamma}
\]
\[ \begin{align*}
\alpha' &= \gamma^2 \alpha + 2\gamma^2 \tau \beta + \gamma^2 \tau^2 \delta \\
&= \gamma^2 \alpha + \sigma^2 \delta + 2\gamma^2 \tau \beta \\
&= \alpha + \sigma^2 (\delta - \alpha) + 2\gamma^2 \tau \beta \\
&= \alpha + \sigma^2 \left[ \frac{\beta (\tau^2 - 1)}{\tau} \right] + 2\gamma^2 \tau \beta \\
&= \alpha + \sigma^2 \left[ \beta \tau - \frac{\beta^2}{\tau} \right] + 2\gamma^2 \tau \beta \\
&= \alpha + \beta \tau \left[ \sigma^2 - \frac{\sigma^2}{\tau^2} + 2\gamma^2 \right] \\
&= \alpha + \beta \tau \left[ \sigma^2 - \gamma^2 + 2\gamma^2 \right] \\
&= \alpha + \beta \tau 
\end{align*} \]

The \( \delta' \) identity follows similarly.
So we can now characterize what happens to the matrix $A_k$ once the pair $(i,j)$ is chosen and the associated Jacobi rotation is applied.

$$
\begin{align*}
\alpha_{ii}^{(k+1)} &= \alpha_{ii}^{(k)} + \tau_{ij} \alpha_{ij}^{(k)} \\
\alpha_{jj}^{(k+1)} &= \alpha_{jj}^{(k)} - \tau_{ij} \alpha_{ij}^{(k)} \\
\alpha_{ij}^{(k+1)} &= 0 \\
\alpha_{ji}^{(k+1)} &= 0
\end{align*}
$$

We also have for the rest of rows $i$ and $j$

$$
\begin{pmatrix}
\alpha_{ir}^{(k+1)} \\
\alpha_{jr}^{(k+1)}
\end{pmatrix}
= 
\begin{pmatrix}
\gamma_{ij} & \sigma_{ij} \\
-\sigma_{ij} & \gamma_{ij}
\end{pmatrix}
\begin{pmatrix}
\alpha_{ir}^{(k)} \\
\alpha_{jr}^{(k)}
\end{pmatrix}
$$

$$
1 \leq r \leq n \quad \text{and} \quad r \neq i \quad \text{and} \quad r \neq j
$$

The columns $i$ and $j$ are recovered via symmetry.
$$i = 3 \quad j = 2 \quad n = 7$$

Note that, except for the 4 elements that are updated by both rotations, elements are a combination of two off-diagonal elements of $A_k$ via an orthogonal transformation.

So any change in the balance between the norms of the diagonal and off-diagonal elements comes from the 4 doubly updated elements.
This norm argument can be made more formal.

Let $A_k = D_k + L_k + L_k^T$ where $D_k$ is the main diagonal and 0 everywhere else and $L_k$ comprises the elements below the main diagonal and 0 everywhere else.

Since the Frobenius norm is unitarily invariant we have

$$\|A_{k+1}\|_F^2 = \|U_k A_k U_k^T\|_F^2$$
$$= \|D_k\|_F^2 + \|L_k\|_F^2 + \|L_k^T\|_F^2$$

So to make the $A_k$ converge to a diagonal we must increase $\|D_k\|_F^2$ and decrease $\|L_k\|_F^2$. 
The same is true after a single Jacobi transformation is applied, i.e.,

\[ \| \tilde{A}_k \|_F^2 = \| G_{ij} A_k G_{ij}^T \|_F^2 \]
\[ = \| \tilde{D}_k + \tilde{L}_k + \tilde{L}_k^T \|_F^2 \]
\[ \| \tilde{D}_k \|_F^2 = \| D_k \|_F^2 + 2(\alpha_{ij}^{(k)})^2 \]
\[ \| \tilde{L}_k \|_F^2 = \| L_k \|_F^2 - (\alpha_{ij}^{(k)})^2 \]
• Sweeps that visit each \((i, j)\) exactly once before visiting any position again are more efficient than classical Jacobi and can also be shown to converge.

• The choice of sweep is affected by the architecture, e.g., parallel architectures are typically required for Jacobi to be competitive on a general symmetric matrix.

• If \(A\) is almost diagonal then Jacobi can be more efficient than other algorithms for computing all of the eigenvalues and vectors. This can happen, for example, when you have a good estimate of the eigenvectors initially, i.e., \(Q^T AQ \approx \Lambda\).

• If the large elements of \(A\) are few and have a nice pattern Jacobi can be very efficient. Consider the simple case of a diagonal matrix plus a single off-diagonal element in the lower part (and symmetrically in the upper part) plus possibly a matrix of elements below your tolerance for small.
Convergence is quadratic for classical and any useful sweep

\[ \|L_{k+1}\|_F \leq C\|L_k\|_F^2 \]

for \( k > k_0 \).