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Finites Element Procedure, Klaus-Jürgen Bathe

Chapter 11:

Solution of Eigenproblems

$$\mathbf{K}\boldsymbol{\phi} = \lambda \mathbf{M}\boldsymbol{\phi}$$

Chapter 11: Solution of Eigenproblems

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Example 11.4

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Difference between Iterations

Inverse Iteration:	In general we can calculate all Eigen values, but with very small convergence. Only the first Eigen value has a good convergence
Forward Iteration:	Gives the last Eigen value
Shifting in Vector Iteration:	Gives the last Eigen value using the inverse iteration
Gram-Schmidt Orthogonalization:	Gives the starting vector to calculate all Eigen values using the inverse iteration

Forward Iteration

EXAMPLE 11.4: Use forward iteration as given in (11.36) to (11.41) with $tol = 10^{-6}$ in (11.20) to evaluate λ_4 and $\boldsymbol{\phi}_4$ of the eigenproblem $\mathbf{K}\boldsymbol{\phi} = \lambda\mathbf{M}\boldsymbol{\phi}$, where

$$\mathbf{K} = \begin{bmatrix} 5 & -4 & 1 & 0 \\ -4 & 6 & -4 & 1 \\ 1 & -4 & 6 & -4 \\ 0 & 1 & -4 & 5 \end{bmatrix}; \qquad \mathbf{M} = \begin{bmatrix} 2 & & & \\ & 2 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

Start vector: $$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Iteration Scheme

Procedure:

$$\mathbf{y}_1 = \mathbf{K}\mathbf{x}_1$$

$$\mathbf{M}\overline{\mathbf{x}}_{k+1} = \mathbf{y}_k$$

$$\overline{\mathbf{y}}_{k+1} = \mathbf{K}\overline{\mathbf{x}}_{k+1}$$

$$\rho(\overline{\mathbf{x}}_{k+1}) = \frac{\overline{\mathbf{x}}_{k+1}^T \overline{\mathbf{y}}_{k+1}}{\overline{\mathbf{x}}_{k+1}^T \mathbf{y}_k}$$

$$\mathbf{y}_{k+1} = \frac{\overline{\mathbf{y}}_{k+1}}{(\overline{\mathbf{x}}_{k+1}^T \mathbf{y}_k)^{1/2}}$$

Eigen Values:

$$\lambda_n \doteq \rho(\overline{\mathbf{x}}_{l+1})$$

$$\boldsymbol{\phi}_n \doteq \frac{\overline{\mathbf{x}}_{l+1}}{(\overline{\mathbf{x}}_{l+1}^T \mathbf{y}_l)^{1/2}}$$

Tolerance:

$$\frac{|\lambda_1^{(k+1)} - \lambda_1^{(k)}|}{\lambda_1^{(k+1)}} \leq tol$$

Results

TABLE E11.4

k	$\overline{\mathbf{x}}_{k+1}$	$\overline{\mathbf{y}}_{k+1}$	$\rho(\overline{\mathbf{x}}_{k+1})$	$\mathbf{y}_{k+1}$	$\dfrac{\lvert\lambda_4^{(k+1)} - \lambda_4^{(k)}\rvert}{\lambda_4^{(k+1)}}$
1	1	6	5.93333	2.1909	—
	−0.5	−1		−0.3651	
	−1	−11		−4.0166	
	2	13.5		4.9295	
2	1.0954	2.1909	8.57887	0.3345	0.3084
	−0.1826	15.5188		2.3694	
	−4.0166	−41.9921		−6.4112	
	4.9295	40.5315		6.1882	
3	0.1672	−10.3137	10.15966	−1.1372	0.1556
	1.1847	38.2720		4.2198	
	−6.4112	−67.7914		−7.4745	
	6.1882	57.7704		6.3696	
8	−1.1285	−24.2083	10.63838	−2.2756	0.00003304
	2.7044	57.7298		5.4267	
	−7.7481	−82.4222		−7.7478	
	5.9969	63.6811		5.9861	
9	−1.1378	−24.2902	10.63844	−2.2833	0.000005584
	2.7133	57.8086		5.4340	
	−7.7478	−82.4224		−7.7476	
	5.9861	63.6351		5.9816	
10	−1.1416	−24.3237	10.63845	−2.2864	0.0000009437
	2.7170	57.8405		5.4369	
	−7.7476	−82.4219		−7.7476	
	5.9816	63.6157		5.9798	

Example 11.5

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Shifting in Vector Iteration

EXAMPLE 11.5: Use inverse iteration as given in (11.16) to (11.22) in order to calculate $(\lambda_1, \boldsymbol{\phi}_1)$ of the problem $\mathbf{K}\boldsymbol{\phi} = \lambda\mathbf{M}\boldsymbol{\phi}$, where $\mathbf{K}$ and $\mathbf{M}$ are given in Example 11.4. Then impose the shift $\mu = 10$ and show that in the inverse iteration convergence occurs toward λ_4 and $\boldsymbol{\phi}_4$.

$$\mathbf{K} = \begin{bmatrix} 5 & -4 & 1 & 0 \\ -4 & 6 & -4 & 1 \\ 1 & -4 & 6 & -4 \\ 0 & 1 & -4 & 5 \end{bmatrix}; \qquad \mathbf{M} = \begin{bmatrix} 2 & & & \\ & 2 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

Start vector:

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Iteration Scheme

Procedure:

$$(\mathbf{K} - \mu\mathbf{M})\boldsymbol{\phi} = \eta\mathbf{M}\boldsymbol{\phi}$$

Same Iteration as in inverse iteration
(But: K = K-μM, M = ηM)

$$\mathbf{K}\overline{\mathbf{x}}_{k+1} = \mathbf{y}_k$$

$$\overline{\mathbf{y}}_{k+1} = \mathbf{M}\overline{\mathbf{x}}_{k+1}$$

$$\rho(\overline{\mathbf{x}}_{k+1}) = \frac{\overline{\mathbf{x}}_{k+1}^T \mathbf{y}_k}{\overline{\mathbf{x}}_{k+1}^T \overline{\mathbf{y}}_{k+1}}$$

$$\mathbf{y}_{k+1} = \frac{\overline{\mathbf{y}}_{k+1}}{(\overline{\mathbf{x}}_{k+1}^T \overline{\mathbf{y}}_{k+1})^{1/2}}$$

Eigen Values:

$$\lambda_1 \doteq \mu + \rho(\overline{\mathbf{x}}_l)$$

$$\boldsymbol{\phi}_1 \doteq \frac{\overline{\mathbf{x}}_{l+1}}{(\overline{\mathbf{x}}_{l+1}^T \overline{\mathbf{y}}_{l+1})^{1/2}}$$

Mathematica-Code

Comparing

Forward Iteration (4 Iterations)	$\lambda 4 = 10.6264$	$\Phi 4 = \begin{pmatrix} 0.10358 \\ 0.251875 \\ 0.728457 \\ 0.566578 \end{pmatrix}$
Shifting in Vector Iteration (4 Iterations)	$\lambda 4 = 10.63844$	$\Phi 4 = \begin{pmatrix} 0.107154 \\ 0.255504 \\ 0.728127 \\ 0.562409 \end{pmatrix}$
Convergence Result	$\lambda 4 = 10.63845$	$\Phi 4 = \begin{pmatrix} \mathbf{0.1076} \\ \mathbf{0.2556} \\ \mathbf{0.7283} \\ \mathbf{0.5620} \end{pmatrix}$

Example 11.8

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Gram-Schmidt Orthogonalization

EXAMPLE 11.8: Calculate, using Gram-Schmidt orthogonalization, an appropriate starting iteration vector for the solution of the problem $\mathbf{K}\boldsymbol{\phi} = \lambda\mathbf{M}\boldsymbol{\phi}$, where $\mathbf{K}$ and $\mathbf{M}$ are given in Example 11.4. Assume that the eigenpairs $(\lambda_1, \boldsymbol{\phi}_1)$ and $(\lambda_4, \boldsymbol{\phi}_4)$ are known as obtained in Example 11.5 and that convergence to another eigenpair is sought.

$$\mathbf{K} = \begin{bmatrix} 5 & -4 & 1 & 0 \\ -4 & 6 & -4 & 1 \\ 1 & -4 & 6 & -4 \\ 0 & 1 & -4 & 5 \end{bmatrix}; \qquad \mathbf{M} = \begin{bmatrix} 2 & & & \\ & 2 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

From inverse iteration:

$$\lambda_1 \doteq 0.09654; \qquad \boldsymbol{\phi}_1 \doteq \begin{bmatrix} 0.3126 \\ 0.4955 \\ 0.4791 \\ 0.2898 \end{bmatrix}$$

From forward or shifting in vector iteration:

$$\lambda_4 \doteq 10.63845; \qquad \boldsymbol{\phi}_4 \doteq \begin{bmatrix} -0.10731 \\ 0.25539 \\ -0.72827 \\ 0.56227 \end{bmatrix}$$

Procedure

$$\tilde{\mathbf{x}}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \alpha_1 \boldsymbol{\phi}_1 - \alpha_4 \boldsymbol{\phi}_4$$

$$\alpha_1 = \boldsymbol{\phi}_1^T \mathbf{M} \mathbf{x}_1; \qquad \alpha_4 = \boldsymbol{\phi}_4^T \mathbf{M} \mathbf{x}_1$$

$$\alpha_1 = 2.385; \qquad \alpha_4 = 0.1299$$

$$\tilde{\mathbf{x}}_1 = \begin{bmatrix} 0.2683 \\ -0.2149 \\ -0.04812 \\ 0.2358 \end{bmatrix}$$

With we can now get λ2 and Φ2 using inverse iteration: Mathematica-Code

11.3 Transformation Methods

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The Aim of Transformation Methods

$$\mathbf{K}_2 = \mathbf{P}_1^T \mathbf{K}_1 \mathbf{P}_1$$

$$\mathbf{K}_3 = \mathbf{P}_2^T \mathbf{K}_2 \mathbf{P}_2$$

$$\vdots$$

$$\mathbf{K}_{k+1} = \mathbf{P}_k^T \mathbf{K}_k \mathbf{P}_k$$

$$\vdots$$

$$\mathbf{M}_2 = \mathbf{P}_1^T \mathbf{M}_1 \mathbf{P}_1$$

$$\mathbf{M}_3 = \mathbf{P}_2^T \mathbf{M}_2 \mathbf{P}_2$$

$$\vdots$$

$$\mathbf{M}_{k+1} = \mathbf{P}_k^T \mathbf{M}_k \mathbf{P}_k$$

$$\vdots$$

Find P_k Matrices to bring M and K into a diagonal form

$$\mathbf{K}_{k+1} \longrightarrow \operatorname{diag}(K_r)$$

$$\text{as } k \longrightarrow \infty$$

$$\mathbf{M}_{k+1} \longrightarrow \operatorname{diag}(M_r)$$

11.3.1 The Jacobi Method

$$
\begin{array}{cc}
 & \begin{array}{ccccccccccc} & & & i\text{th} & & & & j\text{th column} & & & \end{array} \\
\mathbf{P}_k = & \left[\begin{array}{ccccccccccc}
1 & & & & & & & & & & \\
 & \ddots & & & & & & & & & \\
 & & 1 & & & & & & & & \\
 & & & \cos\theta & & & & -\sin\theta & & & \\
 & & & & 1 & & & & & & \\
 & & & & & \ddots & & & & & \\
 & & & & & & 1 & & & & \\
 & & & \sin\theta & & & & \cos\theta & & & \\
 & & & & & & & & 1 & & \\
 & & & & & & & & & \ddots & \\
 & & & & & & & & & & 1
\end{array}\right]
\begin{array}{l} \\ \\ \\ i\text{th} \\ \\ \\ \\ j\text{th row} \\ \\ \\ \\ \end{array}
\end{array}
$$

$$\tan 2\theta = \frac{2k_{ij}^{(k)}}{k_{ii}^{(k)} - k_{jj}^{(k)}} \qquad \theta = \frac{\pi}{4} \quad \text{for } k_{ii}^{(k)} = k_{jj}^{(k)}$$

Example 11.9

$$\mathbf{K} = \begin{bmatrix} 5 & -4 & 1 & 0 \\ -4 & 6 & -4 & 1 \\ 1 & -4 & 6 & -4 \\ 0 & 1 & -4 & 5 \end{bmatrix}$$

$i = 1, j = 2$: $\quad \cos\theta = 0.7497; \quad \sin\theta = 0.6618$

$$\mathbf{P}_1 = \begin{bmatrix} 0.7497 & -0.6618 & 0 & 0 \\ 0.6618 & 0.7497 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{P}_1^T\mathbf{K}\mathbf{P}_1 = \begin{bmatrix} 1.469 & 0 & -1.898 & 0.6618 \\ 0 & 9.531 & -3.661 & 0.7497 \\ -1.898 & -3.661 & 6 & -4 \\ 0.6618 & 0.7497 & -4 & 5 \end{bmatrix}$$

For $i = 1, j = 3$:

$$\cos\theta = 0.9398; \qquad \sin\theta = 0.3416$$

$$\mathbf{P}_2 = \begin{bmatrix} 0.9398 & 0 & -0.3416 & 0 \\ 0 & 1 & 0 & 0 \\ 0.3416 & 0 & 0.9398 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{P}_2^T\mathbf{P}_1^T\mathbf{K}\mathbf{P}_1\mathbf{P}_2 = \begin{bmatrix} 0.7792 & -1.250 & 0 & -0.7444 \\ -1.250 & 9.531 & -3.440 & 0.7497 \\ 0 & -3.440 & 6.690 & -3.986 \\ -0.7444 & 0.7497 & -3.986 & 5 \end{bmatrix}$$

For $i = 1, j = 4$:

$$\cos\theta = 0.9857; \qquad \sin\theta = 0.1687$$

$$\mathbf{P}_3 = \begin{bmatrix} 0.9857 & 0 & 0 & -0.1687 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0.1687 & 0 & 0 & 0.9857 \end{bmatrix}$$

$$\mathbf{P}_3^T\mathbf{P}_2^T\mathbf{P}_1^T\mathbf{K}\mathbf{P}_1\mathbf{P}_2\mathbf{P}_3 = \begin{bmatrix} 0.6518 & -1.106 & -0.6725 & 0 \\ -1.106 & 9.531 & -3.440 & 0.9499 \\ -0.6725 & -3.440 & 6.690 & -3.928 \\ 0 & 0.9499 & -3.928 & 5.127 \end{bmatrix}$$

For $i = 2, j = 3$:

$$\cos\theta = 0.8312; \qquad \sin\theta = -0.5560$$

$$\mathbf{P}_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.8312 & 0.5560 & 0 \\ 0 & -0.5560 & 0.8312 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{P}_4^T\mathbf{P}_3^T\mathbf{P}_2^T\mathbf{P}_1^T\mathbf{K}\mathbf{P}_1\mathbf{P}_2\mathbf{P}_3\mathbf{P}_4 = \begin{bmatrix} 0.6518 & 0.5453 & -1.174 & 0 \\ -0.5453 & 11.83 & 0 & 2.974 \\ -1.174 & 0 & 4.388 & -2.737 \\ 0 & 2.974 & -2.737 & 5.127 \end{bmatrix}$$

For $i = 2, j = 4$:

$$\cos\theta = 0.9349; \qquad \sin\theta = 0.3549$$

$$\mathbf{P}_5 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.9349 & 0 & -0.3549 \\ 0 & 0 & 1 & 0 \\ 0 & 0.3549 & 0 & 0.9349 \end{bmatrix}$$

$$\mathbf{P}_5^T\mathbf{P}_4^T\mathbf{P}_3^T\mathbf{P}_2^T\mathbf{P}_1^T\mathbf{K}\mathbf{P}_1\mathbf{P}_2\mathbf{P}_3\mathbf{P}_4\mathbf{P}_5 = \begin{bmatrix} 0.6518 & 0.5098 & -1.174 & 0.1935 \\ -0.5098 & 12.96 & 0.9713 & 0 \\ -1.174 & -0.9713 & 4.388 & -2.559 \\ 0.1935 & 0 & -2.559 & 3.999 \end{bmatrix}$$

To complete the sweep, we zero element (3, 4), using

$$\cos\theta = 0.7335; \qquad \sin\theta = -0.6797$$

$$\mathbf{P}_6 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0.7335 & 0.6797 \\ 0 & 0 & -0.6797 & 0.7335 \end{bmatrix}$$

$$\mathbf{\Lambda} \doteq \mathbf{P}_6^T \ldots \mathbf{P}_1^T \mathbf{K} \mathbf{P}_1 \ldots \mathbf{P}_6$$

$$\mathbf{\Lambda} \doteq \begin{bmatrix} 0.6518 & -0.5098 & -0.9926 & -0.6560 \\ -0.5098 & 12.96 & -0.7124 & -0.6602 \\ -0.9926 & -0.7124 & 6.7596 & 0 \\ -0.6560 & -0.6602 & 0 & 1.6272 \end{bmatrix}$$

Λ is not very diagonal yet, so the procedure has to be repeated until the error can be tolerated

$$\frac{|k_{ii}^{(l+1)} - k_{ii}^{(l)}|}{k_{ii}^{(l+1)}} \leq 10^{-s}; \qquad i = 1, \ldots, n$$

$$\left[\frac{(k_{ij}^{(l+1)})^2}{k_{ii}^{(l+1)} k_{jj}^{(l+1)}}\right]^{1/2} \leq 10^{-s}; \qquad \text{all } i, j;\ i < j$$

$$\mathbf{\Phi} \doteq \mathbf{P}_1 \ldots \mathbf{P}_6$$

$$\mathbf{\Phi} \doteq \begin{bmatrix} 0.6945 & -0.4233 & -0.4488 & -0.3702 \\ 0.6131 & 0.6628 & 0.4152 & -0.1113 \\ 0.3367 & -0.5090 & 0.4835 & 0.6275 \\ 0.1687 & 0.3498 & -0.6264 & 0.6759 \end{bmatrix}$$

After the second sweep we obtain

$$\mathbf{\Lambda} \doteq \begin{bmatrix} 0.1563 & -0.3635 & 0.0063 & -0.0176 \\ -0.3635 & 13.08 & -0.0020 & 0 \\ 0.0063 & -0.0020 & 6.845 & 0 \\ -0.0176 & 0 & 0 & 1.910 \end{bmatrix}$$

$$\mathbf{\Phi} \doteq \begin{bmatrix} 0.3875 & -0.3612 & -0.6017 & -0.5978 \\ 0.5884 & 0.6184 & 0.3710 & -0.3657 \\ 0.6148 & -0.5843 & 0.3714 & 0.3777 \\ 0.3546 & 0.3816 & -0.6020 & 0.6052 \end{bmatrix}$$

And after the third sweep we have

$$\mathbf{\Lambda} \doteq \begin{bmatrix} 0.1459 & & & \\ & 13.09 & & \\ & & 6.854 & \\ & & & 1.910 \end{bmatrix}$$

$$\mathbf{\Phi} \doteq \begin{bmatrix} 0.3717 & -0.3717 & -0.6015 & -0.6015 \\ 0.6015 & 0.6015 & 0.3717 & -0.3717 \\ 0.6015 & -0.6015 & 0.3717 & 0.3717 \\ 0.3717 & 0.3717 & -0.6015 & 0.6015 \end{bmatrix}$$

11.3.2 The Generalized Jacobi Method

$$
\mathbf{P}_k = \begin{array}{c}
\begin{array}{ccccccc} & & i\text{th} & & j\text{th column} & & \end{array} \\
\left[\begin{array}{ccccccc}
1 & & & & & & \\
 & \ddots & & & & & \\
 & & 1 & & \alpha & & \\
 & & & \ddots & & & \\
 & & \gamma & & 1 & & \\
 & & & & & \ddots & \\
 & & & & & & 1
\end{array}\right]
\end{array}
\begin{array}{l}
\\ \\ \\ i\text{th} \\ \\ j\text{th row} \\ \\ \\
\end{array}
$$

$$\alpha k_{ii}^{(k)} + (1 + \alpha\gamma) k_{ij}^{(k)} + \gamma k_{jj}^{(k)} = 0$$

$$\alpha m_{ii}^{(k)} + (1 + \alpha\gamma) m_{ij}^{(k)} + \gamma m_{jj}^{(k)} = 0$$

α and γ

$$\gamma = -\frac{\bar{k}_{ii}^{(k)}}{x}; \qquad \alpha = \frac{\bar{k}_{jj}^{(k)}}{x}$$

$$\bar{k}_{ii}^{(k)} = k_{ii}^{(k)} m_{ij}^{(k)} - m_{ii}^{(k)} k_{ij}^{(k)}$$

$$\bar{k}_{jj}^{(k)} = k_{jj}^{(k)} m_{ij}^{(k)} - m_{jj}^{(k)} k_{ij}^{(k)}$$

$$\bar{k}^{(k)} = k_{ii}^{(k)} m_{jj}^{(k)} - k_{jj}^{(k)} m_{ii}^{(k)}$$

$$x = \frac{\bar{k}^{(k)}}{2} + \operatorname{sign}(\bar{k}^{(k)}) \sqrt{\left(\frac{\bar{k}^{(k)}}{2}\right)^2 + \bar{k}_{ii}^{(k)} \bar{k}_{jj}^{(k)}}$$

The Householder-QR-Inverse Iteration Solution

1. Householder transformations are employed to reduce the matrix $\mathbf{K}$ to tridiagonal form.
2. QR iteration yields all eigenvalues.
3. Using inverse iteration the required eigenvectors of the tridiagonal matrix are calculated. These vectors are transformed to obtain the eigenvectors of $\mathbf{K}$.

(1) Householder Reduction

Aim: get K into a tridiagonal form:

$$\begin{pmatrix} a_{1,1} & a_{1,2} & 0 & \dots & 0 \\ a_{2,1} & a_{2,2} & a_{2,3} & \ddots & \vdots \\ 0 & a_{3,2} & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & a_{n-1,n} \\ 0 & \dots & 0 & a_{n,n-1} & a_{n,n} \end{pmatrix}$$

(1) $\overline{\mathbf{w}}_1 = \mathbf{k}_1 + \operatorname{sign}(k_{21}) \| \mathbf{k}_1 \|_2 \mathbf{e}_1$

(2) $\mathbf{w}_1 = \begin{bmatrix} 0 \\ \hline \overline{\mathbf{w}}_1 \end{bmatrix}$

(3) $\theta = \dfrac{2}{\mathbf{w}_k^T \mathbf{w}_k}$

(4) $\mathbf{P}_k = \mathbf{I} - \theta \mathbf{w}_k \mathbf{w}_k^T$

(5) $\mathbf{K}_2 = \mathbf{P}_1^T \mathbf{K}_{11} \mathbf{P}_1$

(6) Repeat for $\overline{\mathbf{K}}_2$

$$\mathbf{K}_2 = \left[\begin{array}{c|cccc} k_{11} & \times & 0 & \dots & 0 \\ \hline \times & & & & \\ 0 & & & & \\ \vdots & & & \overline{\mathbf{K}}_2 & \\ 0 & & & & \end{array}\right]$$

(2) The QR Iteration

$$\mathbf{P}_{n,n-1}^T \ldots \mathbf{P}_{3,1}^T \mathbf{P}_{2,1}^T \mathbf{K} = \mathbf{R} \qquad \mathbf{Q} = \mathbf{P}_{2,1} \mathbf{P}_{3,1} \ldots \mathbf{P}_{n,n-1}$$

Jacobi rotation matrix $\mathbf{P}_{j,i}^T$

$$\mathbf{P}_{j,i}^T = \begin{array}{c} \left[\begin{array}{ccccccccc} 1 & & & & & & & & \\ & \ddots & & & & & & & \\ & & 1 & & & & & & \\ & & & \cos\theta & & \sin\theta & & & \\ & & & & 1 & & & & \\ & & & & & \ddots & & & \\ & & & & & & 1 & & \\ & & & -\sin\theta & & \cos\theta & & & \\ & & & & & & 1 & & \\ & & & & & & & \ddots & \\ & & & & & & & & 1 \end{array}\right] \begin{array}{l} \\ \\ \\ i\text{th row} \\ \\ \\ \\ j\text{th row} \\ \\ \\ \\ \end{array} \end{array}$$

$$\sin\theta = \frac{\bar{k}_{ji}}{(\bar{k}_{ii}^2 + \bar{k}_{ji}^2)^{1/2}}; \qquad \cos\theta = \frac{\bar{k}_{ii}}{(\bar{k}_{ii}^2 + \bar{k}_{ji}^2)^{1/2}}$$

$$\mathbf{K}_{k+1} = \mathbf{R}_k \mathbf{Q}_k$$

$$\mathbf{K}_{k+1} \rightarrow \mathbf{\Lambda} \quad \text{and} \quad \mathbf{Q}_1 \cdots \mathbf{Q}_{k-1} \mathbf{Q}_k \rightarrow \mathbf{\Phi} \qquad \text{as } k \rightarrow \infty$$

(3) Calculation of Eigen Vectors

The QR iteration gives us only the Eigen vectors of the tridiagonalized K-matrix. So we have to transform them back.

Original Eigen vector

Eigen vector of the tridiagonalized matrix

$$\boldsymbol{\phi}_i = \mathbf{P}_1\mathbf{P}_2 \; . \; . \; . \; \mathbf{P}_{n-2}\boldsymbol{\psi}_i$$

Same P-matrices as in Householder Reduction

Compare of Householder-QR-Inverse Iteration Solution and the generalized Jacobi Solution

TABLE 11.2 *Summary of Householder-QR-inverse iteration solution*

Operation	Calculation	Number of operations	Required storage
Householder transformation	$\mathbf{K}_{k+1} = \mathbf{P}_k^T \mathbf{K}_k \mathbf{P}_k$; $k = 1, 2, \ldots, n-2$; $\mathbf{K}_1 = \mathbf{K}$	$\frac{2}{3}n^3 + \frac{3}{2}n^2$	
QR iterations	$\mathbf{T}_{k+1} = \mathbf{Q}_k^T \mathbf{T}_k \mathbf{Q}_k$; $k = 1, 2, \ldots$ $\mathbf{T}_1 = \mathbf{K}_{n-1}$	$9n^2$	Using symmetry of matrix
Calculation of p eigenvectors	$(\mathbf{K}_{n-1} - \lambda_i \mathbf{I})\mathbf{x}_i^{(k+1)} = \mathbf{x}_i^{(k)}$; $k = 1, 2$; $i = 1, 2, \ldots, p$	$10pn$	$\frac{n}{2}(n+1) + 6n$
Transformation of eigenvectors	$\boldsymbol{\phi}_i = \mathbf{P}_1 \ldots \mathbf{P}_{n-2}\mathbf{x}_i^{(3)}$; $i = 1, 2, \ldots, p$	$pn(n-1)$	
Total for all eigenvalues and p eigenvectors		$\frac{2}{3}n^3 + \frac{21}{2}n^2 + pn^2 + 9pn$	

TABLE 11.1 *Summary of generalized Jacobi solution*

Operation	Calculation	Number of operations	Required storage
Calculation of coupling factors	$\dfrac{(k_{ij}^{(k)})^2}{k_{ii}^{(k)}k_{jj}^{(k)}}; \quad \dfrac{(m_{ij}^{(k)})^2}{m_{ii}^{(k)}m_{jj}^{(k)}}$	6	
Transformation to zero elements (i, j)	$\bar{k}_{ii}^{(k)} = k_{ii}^{(k)}m_{ij}^{(k)} - m_{ii}^{(k)}k_{ij}^{(k)}$ $\bar{k}_{jj}^{(k)} = k_{jj}^{(k)}m_{ij}^{(k)} - m_{jj}^{(k)}k_{ij}^{(k)}$ $\bar{k}^{(k)} = k_{ii}^{(k)}m_{jj}^{(k)} - k_{jj}^{(k)}m_{ii}^{(k)}$ $x = \dfrac{\bar{k}^{(k)}}{2} + (\text{sign } \bar{k}^{(k)})\sqrt{\left(\dfrac{\bar{k}^{(k)}}{2}\right)^2 + \bar{k}_{ii}^{(k)}\bar{k}_{jj}^{(k)}}$ $\gamma = -\dfrac{\bar{k}_{ii}^{(k)}}{x}, \; \alpha = \dfrac{\bar{k}_{jj}^{(k)}}{x}$ $\mathbf{K}_{k+1} = \mathbf{P}_k^T\mathbf{K}_k\mathbf{P}_k, \quad \mathbf{M}_{k+1} = \mathbf{P}_k^T\mathbf{M}_k\mathbf{P}_k$	$4n + 12$	Using symmetry of matrices $n(n + 2)$
Calculation of eigenvectors	$(\mathbf{P}_1 \ldots \mathbf{P}_{k-1})\mathbf{P}_k$	$2n$	n^2
Total for one sweep		$3n^3 + 6n^2$	$2n^2 + 2n$