Chapter 7

Simultaneous vector or subspace iterations

7.1 Basic subspace iteration

We have learned in subsection 6.6 how to compute several eigenpairs of a matrix, one after the other. This turns out to be quite inefficient. Some or several of the quotients λ_{i+1}/λ_i may close to one. The following algorithm differs from Algorithm 6.6 in that it does not perform p individual iterations for computing the, say, p smallest eigenvalues, but a single iteration with p vectors simultaneously.

Algorithm 7.1 Basic subspace iteration

1: Let $X \in \mathbb{F}^{n\times p}$ be a matrix with orthnormalized columns, $X^*X = I_p$. This algorithmus computes eigenvectors corresponding to the p smallest eigenvalues $\lambda_1 \le \cdots \le \lambda_p$ of A.
2: Set $X^{(0)} := X, \quad k = 1,$
3: **while** $\|(I - X^{(k)}X^{(k)^*})X^{(k-1)}\| > tol$ **do**
4: $\quad k := k + 1$
5: $\quad Z^{(k)} := AX^{(k-1)}$
6: $\quad X^{(k)}R^{(k)} := Z^{(k)}$/* QR factorization of $Z^{(k)}$ */
7: **end while**

The QR factorization in step 6 of the algorithm prevents the columns of the $X^{(k)}$ from converging all to the eigenvector of largest modulus.

Notice that in the QR factorization of $Z^{(k)}$ the j-th column affects only the columns to its right. If we would apply Algorithm 7.1 to a matrix $\hat{X} \in \mathbb{F}^{n\times q}$, with $X\mathbf{e}_i = \hat{X}\mathbf{e}_i$ for $i = 1, \ldots, q$ then, for all k, we would have $X^{(k)}\mathbf{e}_i = \hat{X}^{(k)}\mathbf{e}_i$ for $i = 1, \ldots, j$. This, in particular, means that the first columns $X^{(k)}\mathbf{e}_1$ perform a simple vector iteration.

Problem 7.1 Show by recursion that the QR factorization of $A^kX = A^kX^{(0)}$ is given by

$$A^kX = X^{(k)}R^{(k)}R^{(k-1)}\cdots R^{(1)}.$$

7.2 Convergence of basic subspace iteration

In analyzing the convergence of the basic subspace iteration we can proceed very similarly as in simple vector iteration. We again assume that A is **diagonal** and that the p largest eigenvalues in modulus are separated from the rest of the spectrum,

$$A = \operatorname{diag}(\alpha_1, \alpha_2, \ldots, \alpha_n), \qquad |\alpha_1| \geq \cdots \geq |\alpha_p| > |\alpha_{p+1}| \geq \cdots \geq |\alpha_n|. \tag{7.1}$$

We are going to show that the angle between $\mathcal{R}(X^{(k)})$ and the subspace $\mathcal{R}(E_p)$, $E_p = [\mathbf{e}_1, \ldots, \mathbf{e}_p]$ spanned by the eigenvectors corresponding to the largest eigenvalues in modules tends to zero as k tends to ∞. From Problem 7.1 we know that

$$\vartheta^{(k)} := \angle(\mathcal{R}(E_p), \mathcal{R}(X^{(k)})) = \angle(\mathcal{R}(E_p), \mathcal{R}(A^k X^{(0)})). \tag{7.2}$$

We partition the matrices A and $X^{(k)}$,

$$A = \operatorname{diag}(A_1, A_2), \quad X^{(k)} = \begin{bmatrix} X_1^{(k)} \\ X_2^{(k)} \end{bmatrix}, \qquad A_1, X_1^{(k)} \in \mathbb{F}^{p\times p}.$$

From (7.1) we know that A_1 is nonsingular. Let us also assume that $X_1^{(k)} = E_p^* X^{(k)}$ is invertible. This simply means, that $X^{(k)}$ has components in the direction of all eigenvectors of interest. Then,

$$A^k X^{(0)} = \begin{bmatrix} A_1^k X_1^{(k)} \\ A_2^k X_2^{(k)} \end{bmatrix} = \begin{bmatrix} I_p \\ S^{(k)} \end{bmatrix} A_1^k X_1^{(k)}, \qquad S^{(k)} := A_2^k X_2^{(k)} {X_1^{(k)}}^{-1} A_1^{-k}. \tag{7.3}$$

(7.2) and (7.3) imply that

$$\begin{aligned} \sin\vartheta^{(k)} &= \|(I - E_p E_p^*) X^{(k)}\| \\ &= \left\| (I - E_p E_p^*) \begin{bmatrix} I_p \\ S^{(k)} \end{bmatrix} \right\| \Big/ \left\| \begin{bmatrix} I_p \\ S^{(k)} \end{bmatrix} \right\| = \frac{\|S^{(k)}\|}{\sqrt{1 + \|S^{(k)}\|^2}}. \end{aligned} \tag{7.4}$$

Likewise, we have

$$\cos\vartheta^{(k)} = \|E_p^* X^{(k)}\| = \frac{1}{\sqrt{1 + \|S^{(k)}\|^2}},$$

such that by (7.2)

$$\tan\vartheta^{(k)} = \|S^{(k)}\| \leq \|A_2^k\| \|S^{(0)}\| \|A_1^{-k}\| \leq \left| \frac{\alpha_{p+1}}{\alpha_p} \right|^k \tan\vartheta^{(0)}. \tag{7.5}$$

In summary we have proved

Theorem 7.2 *Let $U_p := [\mathbf{u}_1, \ldots, \mathbf{u}_p]$ be the matrix formed by the eigenvectors corresponding to the p eigenvalues $\alpha_1, \ldots, \alpha_p$ of A largest in modulus. Let $X \in \mathbb{F}^{n\times p}$ such that $X^* U_p$ is nonsingular. Then, if $|\alpha_p| < |\alpha_{p+1}|$, the iterates $X^{(k)}$ of the basic subspace iteration with initial subpace $X^{(0)} = X$ converges to U_p, and*

$$\tan\vartheta^{(k)} \leq \left| \frac{\alpha_{p+1}}{\alpha_p} \right|^k \tan\vartheta^{(0)}, \qquad \vartheta^{(k)} = \angle(\mathcal{R}(U_p), \mathcal{R}(X^{(k)})). \tag{7.6}$$

Let us elaborate on this result. Let us assume that not only $W_p := X^* U_p$ is nonsingular but that *each* principal submatrix

$$W_j := \begin{pmatrix} w_{11} & \cdots & w_{1j} \\ \vdots & & \vdots \\ w_{j1} & \cdots & w_{jj} \end{pmatrix}, \quad 1 \leq j \leq p,$$

of W_p is nonsingular. Then we can apply Theorem 7.2 to each set of columns $[\mathbf{x}_1^{(k)}, \ldots, \mathbf{x}_j^{(k)}]$, $1 \le j \le p$, provided that $|\alpha_j| < |\alpha_{j+1}|$. If this is the case, then

$$\tan \vartheta_j^{(k)} \le \left| \frac{\alpha_{j+1}}{\alpha_j} \right|^k \tan \vartheta_j^{(0)}, \tag{7.7}$$

where $\vartheta_j^{(k)} = \angle(\mathcal{R}([\mathbf{u}_1, \ldots, \mathbf{u}_j]), \mathcal{R}([\mathbf{x}_1^{(k)}, \ldots, \mathbf{x}_j^{(k)}]))$.

We can even say a little more. We can combine the statements in (7.7) as follows.

Theorem 7.3 *Let $X \in \mathbb{F}^{n\times p}$. Let $|\alpha_{q-1}| > |\alpha_q| \ge \ldots \ge |\alpha_p| > |\alpha_{p+1}|$. Let W_q and W_p be nonsingular. Then*

$$\sin \angle(\mathcal{R}([\mathbf{x}_q^{(k)}, \ldots, \mathbf{x}_p^{(k)}]), \mathcal{R}([\mathbf{u}_q, \ldots, \mathbf{u}_p])) \le c \cdot \max\left\{ \left| \frac{\alpha_q}{\alpha_{q-1}} \right|^k, \left| \frac{\alpha_{p+1}}{\alpha_p} \right|^k \right\}. \tag{7.8}$$

Proof. Recall that the sine of the angle between two subspaces S_1, S_2 of equal dimension is the norm of the projection on $S_2^\perp$ restricted to S_1, see (2.53). Here, $S_1 = \mathcal{R}([\mathbf{x}_q^{(k)}, \ldots, \mathbf{x}_p^{(k)}])$ and $S_2 = \mathcal{R}([\mathbf{u}_q, \ldots, \mathbf{u}_p])$.

Let $\mathbf{x} \in S_1$ with $\|\mathbf{x}\| = 1$. The orthogonal projection of $\mathbf{x}$ on S_2 reflects the fact, that $\mathbf{y} \in \mathcal{R}([\mathbf{u}_q, \ldots, \mathbf{u}_p])$ implies that $\mathbf{y} \in \mathcal{R}([\mathbf{u}_1, \ldots, \mathbf{u}_p])$ as well as $\mathbf{y} \in \mathcal{R}([\mathbf{u}_1, \ldots, \mathbf{u}_q])^\perp$,

$$U_{q-1}U_{q-1}^*\mathbf{x} + (I - U_pU_p^*)\mathbf{x}.$$

To estimate the norm of this vector we make use of Lemma 2.39 and (7.4),

$$\begin{aligned}
\|U_{q-1}U_{q-1}^*\mathbf{x} + (I - U_pU_p^*)\mathbf{x}\|^2 &= \left(\|U_{q-1}U_{q-1}^*\mathbf{x}\|^2 + \|(I - U_pU_p^*)\mathbf{x}\|^2\right)^{1/2} \\
&\le \left(\sin^2 \vartheta_{q-1}^{(k)} + \sin^2 \vartheta_p^{(k)}\right)^{1/2} \le \sqrt{2} \cdot \max\left\{\sin \vartheta_{q-1}^{(k)}, \sin \vartheta_p^{(k)}\right\} \\
&\le \sqrt{2} \cdot \max\left\{\tan \vartheta_{q-1}^{(k)}, \tan \vartheta_p^{(k)}\right\}.
\end{aligned}$$

Then, inequality (7.8) is obtained by applying (7.7) that we know to hold true for both $j = q-1$ and $j = p$. ■

Corollary 7.4 *Let $X \in \mathbb{F}^{n\times p}$. Let $|\alpha_{j-1}| > |\alpha_j| > |\alpha_{j+1}|$ and let W_{j-1} and W_j be nonsingular. Then*

$$\sin \angle(\mathbf{x}_j^{(k)}, \mathbf{u}_j) \le c \cdot \max\left\{ \left| \frac{\alpha_j}{\alpha_{j-1}} \right|^k, \left| \frac{\alpha_{j+1}}{\alpha_j} \right|^k \right\}. \tag{7.9}$$

Example 7.5 Let us see how subspace iteration performs with the matrix

$$A = \mathrm{diag}(1, 3, 4, 6, 10, 15, 20, \ldots, 185)^{-1} \in \mathbb{R}^{40\times 40}$$

if we iterate with 5 vectors. The critical quotients appearing in Theorem 7.3 are

j	1	2	3	4	5
$\lvert\alpha_{j+1}\rvert/\lvert\alpha_j\rvert$	1/3	3/4	2/3	3/5	2/3

So, according to the Theorem, the first column $\mathbf{x}_1^{(k)}$ of $X^{(k)}$ should converge to the first eigenvector at a rate 1/3, $\mathbf{x}_2^{(k)}$ *and* $\mathbf{x}_3^{(k)}$ should converge at a rate 3/4 and the last two columns should converge at the rate 2/3. The graphs in Figure 7.1 show that convergence takes place in exactly this manner.

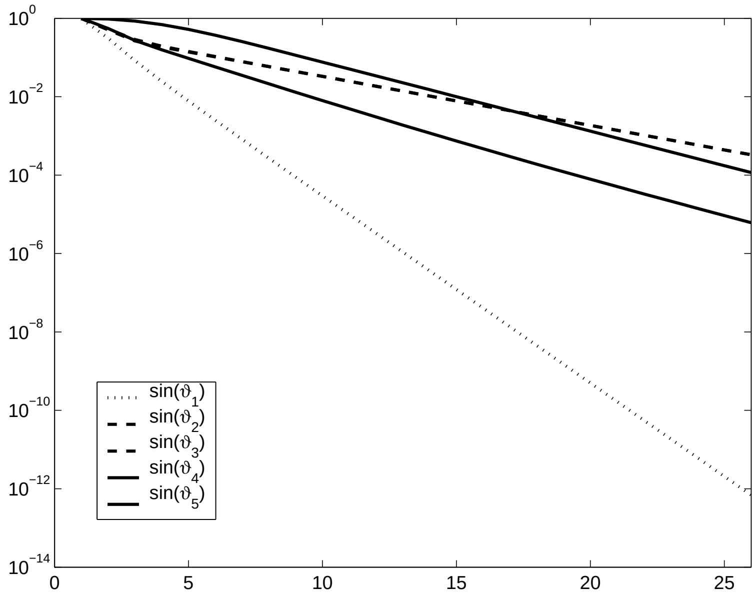

Figure 7.1: Basic subspace iteration with $\tau I_{40} - T_{40}$

Similarly as earlier the eigenvalue approximations $\lambda_j^{(k)}$ approach the desired eigenvalues more rapidly than the eigenvectors. In fact we have

$$\lambda_j^{(k+1)^2} = \|\mathbf{z}_j^{(k+1)}\|^2 = \frac{\mathbf{x}_j^{(k)^*} A^2 \mathbf{x}_j^{(k)}}{\mathbf{x}_j^{(k)^*} \mathbf{x}_j^{(k)}} = \mathbf{x}_j^{(k)^*} A^2 \mathbf{x}_j^{(k)},$$

since $\|\mathbf{x}_j^{(k)}\| = 1$. Let $\mathbf{x}_j^{(k)} = \mathbf{u} + \mathbf{u}^\perp$, where $\mathbf{u}$ is the eigenvalue corresponding to λ_j. Then, since $\mathbf{u} = \mathbf{x}_j^{(k)} \cos\phi$ and $\mathbf{u}^\perp = \mathbf{x}_j^{(k)} \sin\phi$ for a $\phi \le \vartheta^{(k)}$, we have

$$\begin{aligned}
\lambda_j^{(k+1)^2} &= \mathbf{x}_j^{(k)^*} A^2 \mathbf{x}_j^{(k)} = \mathbf{u}^* A \mathbf{u} + \mathbf{u}^{\perp^*} A \mathbf{u}^\perp = \lambda_j^2 \mathbf{u}^* \mathbf{u} + \mathbf{u}^{\perp^*} A \mathbf{u}^\perp \\
&\le \lambda_j^2 \|\mathbf{u}\|^2 + \lambda_1^2 \|\mathbf{u}^\perp\|^2 \\
&\le \lambda_j^2 \cos^2\vartheta^{(k)} + \lambda_1^2 \sin^2\vartheta^{(k)} \\
&= \lambda_j^2 (1 - \sin^2\vartheta^{(k)}) + \lambda_1^2 \sin^2\vartheta^{(k)} = \lambda_j^2 + (\lambda_1^2 - \lambda_j^2) \sin^2\vartheta^{(k)}.
\end{aligned}$$

Thus,

$$|\lambda_j^{(k+1)} - \lambda_j| \le \frac{\lambda_1^2 - \lambda_j^{(k+1)^2}}{\lambda_j^{(k+1)} + \lambda_j} \sin^2\vartheta^{(k)} = O\left(\max\left\{\left(\frac{\lambda_j}{\lambda_{j-1}}\right)^k, \left(\frac{\lambda_{j+1}}{\lambda_j}\right)^k\right\}\right).$$

A numerical example

Let us again consider the test example introduced in subsection 1.6.3 that deals with the accustic vibration in the interior of a car. The eigenvalue problem for the Laplacian is solved by the finite element method as introduced in subsection 1.6.2. We use the finest grid in Fig. 1.9. The matrix eigenvalue problem

$$A\mathbf{x} = \lambda B\mathbf{x}, \qquad A, B \in \mathbb{F}^{n\times n}, \tag{7.10}$$

k	$\frac{\lambda_1^{(k-1)}-\lambda_1}{\lambda_1^{(k)}-\lambda_1}$	$\frac{\lambda_2^{(k-1)}-\lambda_2}{\lambda_2^{(k)}-\lambda_2}$	$\frac{\lambda_3^{(k-1)}-\lambda_3}{\lambda_3^{(k)}-\lambda_3}$	$\frac{\lambda_4^{(k-1)}-\lambda_4}{\lambda_4^{(k)}-\lambda_4}$	$\frac{\lambda_5^{(k-1)}-\lambda_5}{\lambda_5^{(k)}-\lambda_5}$
1	0.0002	0.1378	-0.0266	0.0656	0.0315
2	0.1253	0.0806	-0.2545	0.4017	-1.0332
3	0.1921	0.1221	1.5310	0.0455	0.0404
4	0.1940	0.1336	0.7649	-3.0245	-10.4226
5	0.1942	0.1403	0.7161	0.9386	1.1257
6	0.1942	0.1464	0.7002	0.7502	0.9327
7	0.1942	0.1522	0.6897	0.7084	0.8918
8	0.1942	0.1574	0.6823	0.6918	0.8680
9	0.1942	0.1618	0.6770	0.6828	0.8467
10	0.1942	0.1652	0.6735	0.6772	0.8266
11	0.1943	0.1679	0.6711	0.6735	0.8082
12	0.1942	0.1698	0.6694	0.6711	0.7921
13	0.1933	0.1711	0.6683	0.6694	0.7786
14	0.2030	0.1720	0.6676	0.6683	0.7676
15	0.1765	0.1727	0.6671	0.6676	0.7589
16		0.1733	0.6668	0.6671	0.7522
17		0.1744	0.6665	0.6668	0.7471
18		0.2154	0.6664	0.6665	0.7433
19		0.0299	0.6663	0.6664	0.7405
20			0.6662	0.6663	0.7384
21			0.6662	0.6662	0.7370
22			0.6662	0.6662	0.7359
23			0.6661	0.6662	0.7352
24			0.6661	0.6661	0.7347
25			0.6661	0.6661	0.7344
26			0.6661	0.6661	0.7343
27			0.6661	0.6661	0.7342
28			0.6661	0.6661	0.7341
29			0.6661	0.6661	0.7342
30			0.6661	0.6661	0.7342
31			0.6661	0.6661	0.7343
32			0.6661	0.6661	0.7343
33			0.6661	0.6661	0.7344
34			0.6661	0.6661	0.7345
35			0.6661	0.6661	0.7346
36			0.6661	0.6661	0.7347
37			0.6661	0.6661	0.7348
38			0.6661	0.6661	0.7348
39			0.6661	0.6661	0.7349
40			0.6661	0.6661	0.7350

Table 7.1: Example of basic subspace iteration.
The convergence criterion $\|(I - X^{(k-1)}X^{(k-1)^*})X^{(k)}\| < 10^{-6}$ was satisfied after 87 iteration steps

has the order $n = 1095$. Subspace iteration is applied with five vectors as an *inverse iteration* to

$$L^{-1}AL^{-T}(L\mathbf{x}) = \lambda(L\mathbf{x}), \qquad B = LL^T. \quad \text{(Cholesky factorization)}$$

$X^{(0)}$ is chosen to be a random matrix. Here, we number the eigenvalues from small to big. The smallest six eigenvalues of (7.10) shifted by 0.01 to the right are

$$\begin{aligned} \hat\lambda_1 &= 0.01, & \hat\lambda_4 &= 0.066635, \\ \hat\lambda_2 &= 0.022690, & \hat\lambda_5 &= 0.126631, \\ \hat\lambda_3 &= 0.054385, & \hat\lambda_6 &= 0.147592. \end{aligned}$$

and thus the ratios of the eigenvalues that determine the rate of convergence are

$$\begin{aligned} (\hat\lambda_1/\hat\lambda_2)^2 &= 0.194, & (\hat\lambda_4/\hat\lambda_5)^2 &= 0.277, \\ (\hat\lambda_2/\hat\lambda_3)^2 &= 0.174, & (\hat\lambda_5/\hat\lambda_6)^2 &= 0.736, \\ (\hat\lambda_3/\hat\lambda_4)^2 &= 0.666. \end{aligned}$$

So, the numbers presented in Table 7.1 reflect quite accurately the predicted rates. The numbers in column 6 are a little too small, though.

The convergence criterion

$$\max_{1\le i\le p} \|(I - X^{(k)}X^{(k)*})\mathbf{x}_i^{(k-1)}\| \le \epsilon = 10^{-5}$$

was not satisfied after 50 iteration step.

7.3 Accelerating subspace iteration

Subspace iteration potentially converges very slowly. It can be slow even it one starts with a subspace that contains all desired solutions! If, e.g., $\mathbf{x}_1^{(0)}$ and $\mathbf{x}_2^{(0)}$ are both elements in $\mathcal{R}([\mathbf{u}_1, \mathbf{u}_2])$, the the vectors $\mathbf{x}_i^{(k)}$, $i = 1, 2, \ldots$, still converge linearly towards $\mathbf{u}_1$ und $\mathbf{u}_2$ although they could be readily obtained from the 2×2 eigenvalue problem,

$$\begin{bmatrix} \mathbf{x}_1^{(0)*} \\ \mathbf{x}_2^{(0)*} \end{bmatrix} A \left[\mathbf{x}_1^{(0)}, \mathbf{x}_2^{(0)}\right] \mathbf{y} = \lambda\mathbf{y}$$

The following theorem gives hope that the convergence rates can be improved if one proceeds in a suitable way.

Theorem 7.6 *Let $X \in \mathbb{F}^{n\times p}$ as in Theorem 7.2. Let $\mathbf{u}_i$, $1 \le i \le p$, be the eigenvectors corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_p$ of A. Then we have*

$$\min_{\mathbf{x}\in\mathcal{R}(X^{(k)})} \sin \angle(\mathbf{u}_i, \mathbf{x}) \le c\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k$$

Proof. In the proof of Theorem 7.2 we have seen that

$$\mathcal{R}(X^{(k)}) = \mathcal{R}\left(U \begin{pmatrix} I_p \\ \mathbf{S}^{(k)} \end{pmatrix}\right), \qquad \mathbf{S}^{(k)} \in \mathbb{F}^{(n-p)\times p},$$

where

$$s_{ij}^{(k)} = s_{ij}\left(\frac{\lambda_j}{\lambda_{p+i}}\right)^k, \qquad 1 \le i \le n-p, \quad 1 \le j \le p.$$

But we have

$$\begin{aligned}
\min_{\mathbf{x}\in\mathcal{R}(X^{(k)})} \sin \angle(\mathbf{u}_i, \mathbf{x}) &\le \sin \angle\left(\mathbf{u}_i, U \begin{pmatrix} I_p \\ \mathbf{S}^{(k)} \end{pmatrix} \mathbf{e}_i\right), \\
&= \left\| (I - \mathbf{u}_i{\mathbf{u}_i}^*) U \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ s_{1i}(\lambda_i/\lambda_{p+1})^k \\ \vdots \\ s_{n-p,i}(\lambda_i/\lambda_n)^k \end{pmatrix} \right\| \Big/ \left\| \begin{pmatrix} I_p \\ \mathbf{S}^{(k)} \end{pmatrix} \mathbf{e}_i \right\| \\
&\le \left\| (I - \mathbf{u}_i{\mathbf{u}_i}^*) \left(\mathbf{u}_i + \sum_{j=p+1}^{n} s_{j-p,i}\left(\frac{\lambda_i}{\lambda_{p+j}}\right)^k \mathbf{u}_j \right) \right\| \\
&= \sqrt{\sum_{j=1}^{n-p} s_{ji}^2 \frac{\lambda_i^{2k}}{\lambda_{p+j}^{2k}}} \le \left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k \sqrt{\sum_{j=1}^{n-p} s_{ji}^2}.
\end{aligned}$$

■

These considerations lead to the idea to complement Algorithm 7.1 by a so-called **Rayleigh-Ritz step**. Here we give an 'inverted algorithm' to compute the smallest eigenvalues and corresponding eigenvectors.

Algorithm 7.2 Subspace or simultaneous inverse iteration combined with Rayleigh-Ritz step

```
Let X ∈ F^{n×p} with X*X = I_p:
Set X^(0) := X.
for k = 1, 2, ... do
   Solve AZ^(k) := X^(k−1)
   Q^(k)R^(k) := Z^(k)        /* QR factorization of Z^(k) (or modified Gram–Schmidt) */
   Ĥ^(k) := Q^(k)* A Q^(k),
   Ĥ^(k) =: F^(k) Θ^(k) F^(k)*      /* Spectral decomposition of Ĥ^(k) ∈ F^{p×p} */
   X^(k) = Q^(k) F^(k).
end for
```

Remark 7.1. The columns $\mathbf{x}_i^{(k)}$ of $X^{(k)}$ are called **Ritz vectors** and the eigenvalues $\vartheta_1^{(k)} \le \cdots \le \vartheta_p^{(k)}$ in the diagonal of Θ are called **Ritz values**. According to the Rayleigh-Ritz principle 2.17 we have

$$\lambda_i \le \vartheta_i^{(k)} \qquad 1 \le i \le p, \quad k > 0.$$

□

The solution of the *full* eigenvalue problems $\hat{H}^{(k)}\mathbf{y} = \vartheta\mathbf{y}$ is solved by the symmetric QR algorithm.

The computation of the matrix $\hat{H}^{(k)}$ is expensive as matrix-vector products have to be executed. The following considerations simplify matters. We write $X^{(k)}$ in the form

$$X^{(k)} = Z^{(k)}G^{(k)}, \qquad G^{(k)} \in \mathbb{F}^{p\times p}\text{nonsingular}$$

Because $X^{(k)}$ must have orthonormal columns we must have

$$G^{(k)^*}Z^{(k)^*}Z^{(k)}G^{(k)} = I_p. \tag{7.11}$$

Furthermore, the columns of $Z^{(k)}G^{(k)}$ are the Ritz vectors in $\mathcal{R}(A^{-k}X)$ of A^2,

$$G^{(k)^*}Z^{(k)^*}A^2Z^{(k)}G^{(k)} = \Delta^{(k)^{-2}},$$

where $\Delta^{(k)}$ is a diagonal matrix. Using the definition of $Z^{(k)}$ in Algorithm 7.2 we see that

$$G^{(k)^*}X^{(k-1)^*}X^{(k-1)}G^{(k)} = G^{(k)^*}G^{(k)} = \Delta^{(k)^{-2}},$$

and that $Y^* := G^{(k)}\Delta^{(k)}$ is orthogonal. Substituting into (7.11) gives

$$Y^{(k)^*}Z^{(k)^*}Z^{(k)}Y^{(k)} = \Delta^{(k)^2}.$$

The columns of $Y^{(k)}$ are the normalized eigenvectors of $H^{(k)} := Z^{(k)^*}Z^{(k)}$, too.

Thus we obtain a second variant of the inverse subspace iteration with Rayleigh-Ritz step.

Algorithm 7.3 Subspace or simultaneous inverse vector iteration combined with Rayleigh-Ritz step, version 2

1: Let $X \in \mathbb{F}^{n\times p}$ with $X^*X = I_p$.
2: Set $X^{(0)} := X$.
3: **for** $k = 1, 2, \ldots$ **do**
4: $\quad AZ^{(k)} := X^{(k-1)}$;
5: $\quad H^{(k)} := Z^{(k)^*}Z^{(k)}$ $\quad$ /* $= X^{(k-1)^*}A^{-2}X^{(k-1)}$ */
6: $\quad H^{(k)} =: Y^{(k)}\Delta^{(k)^2}Y^{(k)^*}$ $\quad$ /* Spectral decomposition of $H^{(k)}$ */
7: $\quad X^{(k)} = Z^{(k)}Y^{(k)}\Delta^{(k)^{-1}}$ $\quad$ /* $= Z^{(k)}G^{(k)}$ */
8: **end for**

Remark 7.2. An alternative to Algorithm 7.3 is the subroutine `ritzit`, that has been programmed by Rutishauser [3] in ALGOL, see also [1, p.293]. □

We are now going to show that the Ritz vectors converge to the eigenvectors, as Theorem 7.6 lets us hope. First we prove

Lemma 7.7 ([1, p.222]) *Let $\mathbf{y}$ be a unit vector and $\vartheta \in \mathbb{F}$. Let λ be the eigenvalue of A closest to ϑ and let $\mathbf{u}$ be the corresponding eigenvector. Let*

$$\gamma := \min_{\lambda_i(A)\neq\lambda} |\lambda_i(A) - \vartheta|$$

and let $\psi = \angle(\mathbf{y}, \mathbf{u})$. Then

$$\sin\psi \le \frac{\|\mathbf{r}(\mathbf{y})\|}{\gamma} := \frac{\|A\mathbf{y} - \vartheta\mathbf{y}\|}{\gamma},$$

where $\mathbf{r}(\mathbf{y}, \vartheta) = A\mathbf{y} - \vartheta\mathbf{y}$ plays the role of a ***residual****.*

Proof. We write $\mathbf{y} = \mathbf{u}\cos\psi + \mathbf{v}\sin\psi$ with $\|\mathbf{v}\| = 1$. Then

$$\begin{aligned}\mathbf{r}(\mathbf{y},\vartheta) = A\mathbf{y} - \vartheta\mathbf{y} &= (A-\vartheta I)\mathbf{u}\cos\psi + (A-\vartheta I)\mathbf{v}\sin\psi,\\ &= (\lambda-\vartheta)\cos\psi + (A-\vartheta I)\mathbf{v}\sin\psi.\end{aligned}$$

Because $\mathbf{u}^*(A-\vartheta I)\mathbf{v} = 0$, Pythagoras' theorem implies

$$\|\mathbf{r}(\mathbf{y},\vartheta)\|^2 = (\lambda-\vartheta)^2\cos^2\psi + \|(A-\vartheta I)\mathbf{v}\|^2\sin^2\psi \ge \gamma^2\|\mathbf{v}\|^2\sin^2\psi. \qquad \blacksquare$$

Theorem 7.8 ([1, p.298]) *Let the assumptions of Theorem 7.2 be satisfied. Let* $\mathbf{x}_j^{(k)} = X^{(k)}\mathbf{e}_j$ *be the* j*-th Ritz vector as computed be Algorithm 7.3, and let* $\mathbf{y}_i^{(k)} = U\begin{pmatrix} I \\ \mathbf{S}^{(k)}\end{pmatrix}\mathbf{e}_i$ *(cf. the proof of Theorem 7.2). Then the following inequality holds*

$$\sin\angle(\mathbf{x}_i^{(k)},\mathbf{y}_i^{(k)}) \le c\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k, \qquad 1 \le\ i \le p.$$

Proof. The columns of $U\begin{pmatrix} I_p \\ \mathbf{S}^{(k)}\end{pmatrix}$ form a basis of $\mathcal{R}(X^{(k)})$. Therefore, we can write

$$\mathbf{x}_i^{(k)} = U\begin{pmatrix} I_p \\ S^{(k)}\end{pmatrix}\mathbf{t}_i, \qquad \mathbf{t}_i \in \mathbb{F}^p.$$

Instead of the special eigenvalue problem

$$X^{(k-1)^*}A^{-2}X^{(k-1)}\mathbf{y} = H^{(k)}\mathbf{y} = \mu^{-2}\mathbf{y}$$

in the orthonormal 'basis' $X^{(k)}$ we consider the equivalent eigenvalue problem

$$\left[I_p, S^{(k)^*}\right]UA^{-2}U\begin{pmatrix} I_p \\ S^{(k)}\end{pmatrix}\mathbf{t} = \mu^{-2}\left[I_p, S^{(k)^*}\right]\begin{pmatrix} I_p \\ S^{(k)}\end{pmatrix}\mathbf{t}. \tag{7.12}$$

Let $(\mu,\mathbf{t})$ be an eigenpair of (7.12). Then we have

$$\begin{aligned}0 &= \left[I_p, S^{(k)^*}\right]UA^{-2}U\begin{pmatrix} I_p \\ S^{(k)}\end{pmatrix}\mathbf{t} - \mu^{-2}\left[I_p, S^{(k)^*}\right]\begin{pmatrix} I_p \\ S^{(k)}\end{pmatrix}\mathbf{t}\\ &= \left(\Lambda_1^{-2} + S^{(k)^*}\mathbf{\Lambda}_2^{-2}S^{(k)}\right)\mathbf{t} - \mu^{-2}\left(I_p + S^{(k)^*}S^{(k)}\right)\mathbf{t},\\ &= \left((\Lambda_1^{-2} - \mu^{-2}I) + S^{(k)^*}(\Lambda_2^{-2} - \mu^{-2}I)S^{(k)}\right)\mathbf{t} \qquad (7.13)\\ &= \left((\Lambda_1^{-2} - \mu^{-2}I) + \Lambda_1^k S^{(0)^*}\Lambda_2^{-k}(\Lambda_2^{-2} - \mu^{-2}I)\Lambda_2^{-k}S^{(0)}\Lambda_1^k\right)\mathbf{t}\\ &= \left((\Lambda_1^{-2} - \mu^{-2}I) + \left(\frac{1}{\lambda_{p+1}}\Lambda_1\right)^k H_k\left(\frac{1}{\lambda_{p+1}}\Lambda_1\right)^k\right)\mathbf{t}\end{aligned}$$

with

$$H_k = \lambda_{p+1}^{2k}S^{(0)^*}\Lambda_2^{-k}(\Lambda_2^{-2} - \mu^{-2}I)\Lambda_2^{-k}S^{(0)}.$$

As the largest eigenvalue of Λ_2^{-1} is $1/\lambda_{p+1}$, H_k is bounded,

$$\|H_k\| \le c_1 \qquad \forall k > 0.$$

Thus,

$$\left(\left(\frac{1}{\lambda_{p+1}}\Lambda_1\right)^k H_k\left(\frac{1}{\lambda_{p+1}}\Lambda_1\right)^k\right)\mathbf{t} \quad \xrightarrow[\lambda\to\infty]{} \quad 0.$$

Therefore, in (7.13) we can interpret this expression as an perturbation of the diagonal matrix $\Lambda_2^{-2} - \mu^{-2}I$. For sufficiently large k (that may depend on i) there is a μ_i that is close to λ_i, and a $\mathbf{t}_i$ that is close to $\mathbf{e}_i$. We now assume that k is so big that

$$|\mu_i^{-2} - \lambda_i^{-1}| \le \rho := \frac{1}{2}\min_{\lambda_j\neq\lambda_i}|\lambda_i^{-2} - \lambda_j^{-2}|$$

such that μ_i^{-2} is closer to λ_i^{-2} than to any other λ_j^{-2}, $j \neq i$.

We now consider the orthonormal 'basis'

$$B = \begin{pmatrix} I_p \\ S^{(k)} \end{pmatrix}\left(I_p + S^{(k)^*}S^{(k)}\right)^{-1/2}.$$

If $(\mu_i, \mathbf{t}_i)$ is an eigenpair of (7.12) or (7.13), respectively, then $\left(\mu_i^{-2}, \left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{t}_i\right)$ is an eigenpair of

$$B^*A^{-2}B\mathbf{t} = \mu^{-2}\mathbf{t}. \tag{7.14}$$

As, for sufficiently large k, $(\lambda_i^{-2}, \mathbf{e}_i)$ is a good approximation of the eigenpair $(\mu_i^{-2}, \mathbf{t}_i)$ of (7.13), then also $\left(\lambda_i^{-2}, \left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{e}_i\right)$ is a good approximation to the eigenpair $\left(\mu_i^{-2}, \left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{t}_i\right)$ of (7.14). We now apply Lemma **??** with

$$\begin{aligned}
\gamma = \rho, \qquad \vartheta &= \lambda_i^{-2}, \\
\mathbf{y} &= \left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{e}_i \Big/ \left\|\left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{e}_i\right\|, \\
\mathbf{u} &= \left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{t}_i \Big/ \left\|\left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{t}_i\right\|.
\end{aligned}$$

Now we have

$$\begin{aligned}
\|\mathbf{r}(\mathbf{y})\| &= \left\|(B^*A^{-2^*}B - \lambda_i^{-2}I)\left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{e}_i\right\| \Big/ \left\|\left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{e}_i\right\| \\
&\le \left\|\left(I_p + S^{(k)^*}S^{(k)}\right)^{-\frac{1}{2}}\left[\left[I_p, \mathbf{S}^{(k)^*}\right]UA^{-2}U\begin{pmatrix} I_p \\ S^{(k)} \end{pmatrix} - \frac{1}{\lambda_i^2}\left(I_p + S^{(k)^*}S^{(k)}\right)\right]\mathbf{e}_i\right\| \\
&\le \left\|\left(I_p + S^{(k)^*}S^{(k)}\right)^{-1/2}\right\| \left\|\left[\Lambda_1^{-2} - \lambda_i^{-2}I + \left(\lambda_{p+1}^{-1}\mathbf{\Lambda}_1\right)^k H_k\left(\lambda_{p+1}^{-1}\mathbf{\Lambda}_1\right)^k\right]\mathbf{e}_i\right\| \\
&\le \left\|\left(\lambda_{p+1}^{-1}\mathbf{\Lambda}_1\right)^k H_k\left(\lambda_{p+1}^{-1}\Lambda_1\right)^k\mathbf{e}_i\right\| \\
&\le \left\|\lambda_{p+1}^{-1}\Lambda_1\right\|^k \|H_k\| \left\|\left(\lambda_{p+1}^{-1}\Lambda_1\right)^k e_i\right\| \le c_1\left(\frac{\lambda_p}{\lambda_{p+1}}\right)^k\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k.
\end{aligned}$$

Then, Lemma **??** implies that

$$\sin\angle(x_i^{(k)}, \mathbf{y}_i^{(k)}) = \sin\angle\left(\left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{t}_i, \left(I_p + S^{(k)^*}S^{(k)}\right)^{1/2}\mathbf{e}_i\right) \le \frac{c_1}{\rho}\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k.$$

■

In the proof of Theorem 7.6 we showed that

$$\angle(\mathbf{u}_i, \mathbf{y}_i^{(k)}) \le c\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k.$$

In the previous theorem we showed that

$$\angle(\mathbf{x}_i^{(k)}, \mathbf{y}_i^{(k)}) \le c_1\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k.$$

By consequence,

$$\angle(\mathbf{x}_i^{(k)}, \mathbf{u}_i) \le c_2\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^k$$

must be true for a constant c_2 independent of k.

As earlier, for the eigenvalues we can show that

$$|\lambda_i - \lambda_i^{(k)}| \le c_3\left(\frac{\lambda_i}{\lambda_{p+1}}\right)^{2k}.$$

A numerical example

For the previous example that is concerned with the accustic vibration in the interior of a car the numbers listed in Table 7.2 are obtained. The quotients $\hat{\lambda}_i^2/\hat{\lambda}_{p+1}^2$, that determine the convergence behavior of the eigenvalues are

$$\begin{aligned}
(\hat{\lambda}_1/\hat{\lambda}_6)^2 &= 0.004513, & (\hat{\lambda}_4/\hat{\lambda}_6)^2 &= 0.2045,\\
(\hat{\lambda}_2/\hat{\lambda}_6)^2 &= 0.02357, & (\hat{\lambda}_5/\hat{\lambda}_6)^2 &= 0.7321.\\
(\hat{\lambda}_3/\hat{\lambda}_6)^2 &= 0.1362, & &
\end{aligned}$$

The numbers in the table confirm the improved convergence rate. The convergence rates of the first four eigenvalues have improved considerably. The predicted rates are not clearly visible, but they are approximated quite well. The convergence rate of the fifth eigenvalue has not improved. The convergence of the 5-dimensional *subspace* $\mathcal{R}([\mathbf{x}_1^{(k)}, \ldots, \mathbf{x}_5^{(k)}])$ to the searched space $\mathcal{R}([\mathbf{u}_1, \ldots, \mathbf{u}_5])$ has not been accelerated. Its convergence rate is still $\approx \lambda_5/\lambda_6$ according to Theorem 7.2

By means of the Rayleigh-Ritz step we have achieved that the columns $\mathbf{x}_i^{(k)} = \mathbf{x}^{(k)}$ converge in an optimal rate to the individual eigenvectors of A.

7.4 Relation of the simultaneous vector iteration with the QR algorithm

The connection between (simultaneous) vector iteration and the QR algorithm has been investigated by Parlett and Poole [2].

Let $X_0 = I_n$, the $n \times n$ identity matrix.

k	$\frac{\lambda_1^{(k-1)}-\lambda_1}{\lambda_1^{(k)}-\lambda_1}$	$\frac{\lambda_2^{(k-1)}-\lambda_2}{\lambda_2^{(k)}-\lambda_2}$	$\frac{\lambda_3^{(k-1)}-\lambda_3}{\lambda_3^{(k)}-\lambda_3}$	$\frac{\lambda_4^{(k-1)}-\lambda_4}{\lambda_4^{(k)}-\lambda_4}$	$\frac{\lambda_5^{(k-1)}-\lambda_5}{\lambda_5^{(k)}-\lambda_5}$
1	0.0001	0.0017	0.0048	0.0130	0.0133
2	0.0047	0.0162	0.2368	0.0515	0.2662
3	0.0058	0.0273	0.1934	0.1841	0.7883
4	0.0057	0.0294	0.1740	0.2458	0.9115
5	0.0061	0.0296	0.1688	0.2563	0.9195
6		0.0293	0.1667	0.2553	0.9066
7		0.0288	0.1646	0.2514	0.8880
8		0.0283	0.1620	0.2464	0.8675
9		0.0275	0.1588	0.2408	0.8466
10			0.1555	0.2351	0.8265
11			0.1521	0.2295	0.8082
12			0.1490	0.2245	0.7921
13			0.1462	0.2200	0.7786
14			0.1439	0.2163	0.7676
15			0.1420	0.2132	0.7589
16			0.1407	0.2108	0.7522
17			0.1461	0.2089	0.7471
18			0.1659	0.2075	0.7433
19			0.1324	0.2064	0.7405
20				0.2054	0.7384
21				0.2102	0.7370
22				0.2109	0.7359
23					0.7352
24					0.7347
25					0.7344
26					0.7343
27					0.7342
28					0.7341
29					0.7342
30					0.7342
31					0.7343
32					0.7343
33					0.7344
34					0.7345
35					0.7346
36					0.7347
37					0.7348
38					0.7348
39					0.7349
40					0.7350

Table 7.2: Example of accelerated basic subspace iteration.

Then we have

$$
\begin{aligned}
AI = A_0 = AX_0 = Y_1 &= X_1 R_1 && (SVI)\\
A_1 = X_1^* A X_1 &= X_1^* X_1 R_1 X_1 = R_1 X_1 && (QR)\\
AX_1 = Y_2 &= X_2 R_2 && (SVI)\\
A_1 &= X_1^* Y_2 X_1^* X_2 R_2 && (QR)\\
A_2 &= R_2 X_1^* X_2 && (QR)\\
&= X_2^* X_1 \underbrace{X_1^* X_2 R_2}_{A_1} X_1^* X_2 = X_2^* A X_2 && (QR)
\end{aligned}
$$

More generaly, by induction, we have

$$
\begin{aligned}
AX_k &= Y_{k+1} = X_{k+1} R_{k+1} && (SVI)\\
A_k &= X_k^* A X_k = X_k^* Y_{k+1} = X_k^* X_{k+1} R_{k+1}\\
A_{k+1} &= R_{k+1} X_k^* X_{k+1} && (QR)\\
&= X_{k+1}^* \underbrace{X_k \underbrace{X_k^* X_{k+1} R_{k+1}}_{A_k} X_k^*}_{A} X_{k+1} = X_{k+1}^* A X_{k+1} && (QR)
\end{aligned}
$$

Relation to QR: $Q_1 = X_1$, $Q_k = X_k^* X_{k+1}$.

$$
\begin{aligned}
A^k &= A^k X_0 = A^{k-1} A X_0 = A^{k-1} X_1 R_1\\
&= A^{k-2} A X_1 R_1 = A^{k-2} X_2 R_2 R_1\\
&\vdots\\
&= X_k \underbrace{R_k R_{k-1} \cdots R_1}_{U_k} = X_k U_k && (QR)
\end{aligned}
$$

Because U_k is *upper triangular* we can write

$$
A^k[\mathbf{e}_1, \ldots, \mathbf{e}_p] = X_k U_k [\mathbf{e}_1, \ldots, \mathbf{e}_p] = X_k U_k(:, 1:p) = X_k(:, 1:p) \begin{bmatrix} u_{11} & \cdots & u_{1p} \\ & \ddots & \vdots \\ & & u_{pp} \end{bmatrix}
$$

This holds for all p. We therefore can interpret the QR algorithm as a nested simultaneous vector iteration.

Relation to simultaneous inverse vector iteration.

Let us assume that A is invertible. Then we have,

$$
\begin{gathered}
AX_{k-1} = X_{k-1} A_{k-1} = X_k R_k\\
X_k R_k^{-*} = A^{-*} X_{k-1}, \qquad R_k^{-*} \text{ is lower triangular}\\
X_k \underbrace{R_k^{-*} R_{k-1}^{-*} \cdots R_1^{-*}}_{U_k^{-*}} = \left(A^{-*}\right)^k X_0
\end{gathered}
$$

Then,

$$X_k[\mathbf{e}_\ell, \ldots, \mathbf{e}_n] \begin{bmatrix} \bar{u}_{\ell,\ell} & & \\ \vdots & \ddots & \\ \bar{u}_{n,\ell} & & \bar{u}_{n,n} \end{bmatrix} = \left(A^{-*}\right)^k X_0[\mathbf{e}_\ell, \ldots, \mathbf{e}_n]$$

By consequence, the last $n-\ell+1$ columns of X_k execute a simultaneous *inverse* vector iteration. Shifts in the QR algorithm correspond to shifts in inverse vector iteration.

7.5 Addendum

Let $A = H$ be an *irreducible* Hessenberg matrix and $W_1 = [\mathbf{w}_1, \ldots, \mathbf{w}_p]$ be a basis of the p-th dominant invariant subspace of H^*,

$$H^* W_1 = W_1 S, \qquad S \text{ invertible.}$$

Notice that the p-th dominant invariant subspace if $|\lambda_p| > |\lambda_{p+1}|$.

Let further $X_0 = [\mathbf{e}_1, \ldots, \mathbf{e}_p]$. Then we have the

Theorem 7.9 *$W_1^* X_0$ is nonsingular.*

Remark 7.3. If $W_1^* X_0$ is nonsingular then $W_k^* X_0$ for all $k > 0$. □

Proof. If $W_1^* X_0$ were singular then there was a vectro $\mathbf{a} \in \mathbb{F}^p$ with $X_0^* W_1 \mathbf{a} = \mathbf{0}$. Thus, $\mathbf{w} = W_1 \mathbf{a}$ is orthogonal to $\mathbf{e}_1, \ldots, \mathbf{e}_p$. Therefore, the first p components of $\mathbf{w}$ are zero.

From, $H^* W_1 = W_1 S$ we have that $(H^*)^k \mathbf{w} \in \mathcal{R}(W_1)$ for all k.

But we have

$$\mathbf{w} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \times \\ \vdots \\ \times \end{bmatrix} \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} p \text{ zeros}$$

These vectors evidently are linearly independent.

Sp, we have constructed $p+1$ linearly independent vectors $\mathbf{w}, \ldots, (H^*)^p \mathbf{w}$ in the p-dimensional subspace $\mathcal{R}(W_1)$. This is a contradiction. ■

Bibliography

[1] B. N. Parlett, *The Symmetric Eigenvalue Problem*, Prentice Hall, Englewood Cliffs, NJ, 1980. (Republished by SIAM, Philadelphia, 1998.).

[2] B. N. Parlett and W. G. Poole, *A geometric theory for the QR, LU, and power iterations*, SIAM J. Numer. Anal., 8 (1973), pp. 389–412.

[3] H. Rutishauser, *Simultaneous iteration method for symmetric matrices*, Numer. Math., 16 (1970), pp. 205–223. Reprinted in: Linear Algebra, J.H. Wilkinson, C. Reinsch (eds.), pp. 284–301, Springer, Berlin, 1971.