Numerical Analysis – Lecture 5[1]

2 Eigenvalues and eigenvectors

Remarks 2.1 (Introduction to matrix eigenvalue calculations). Let A be a real $n \times n$ matrix. The eigenvalue equation is $A\boldsymbol{w} = \lambda \boldsymbol{w}$, where λ is a scalar, which may be complex if A is not symmetric. There exists a nonzero vector $\boldsymbol{w} \in \mathbb{R}^n$ satisfying this equation if and only if $\det(A - \lambda I) = 0$. The function $p(\lambda) = \det(A - \lambda I)$, $\lambda \in \mathbb{C}$, is a polynomial of degree n, but calculating the eigenvalues by finding the roots of p is a disaster area because of loss of accuracy due to rounding errors.
If the polynomial has some multiple roots and if A is not symmetric, then the number of linearly independent eigenvectors may be fewer than n, but there are always n mutually orthogonal real eigenvectors in the symmetric case. We assume in all cases, however, that the eigenvalue equations $A\boldsymbol{w}_j = \lambda_j \boldsymbol{w}_j$, $j = 1, 2, \ldots, n$, are satisfied by eigenvectors $\boldsymbol{w}_j$, $j = 1, 2, \ldots, n$, that are linearly independent, which can be achieved by making an arbitrarily small change to A if necessary.

Method 2.2 (The power method). The iterative algorithms that will be studied for the calculation of eigenvalues and eigenvectors are all closely related to the power method, which has the following basic form for generating a single eigenvalue and eigenvector of A.

We pick a nonzero vector $\boldsymbol{x}^{(0)}$ in $\mathbb{R}^n$. Then, for $k = 0, 1, 2, \ldots$, we let $\boldsymbol{x}^{(k+1)}$ be a nonzero multiple of $A\boldsymbol{x}^{(k)}$, typically

$$\boldsymbol{x}^{(k+1)} = A\boldsymbol{x}^{(k)}/\|A\boldsymbol{x}^{(k)}\|, \qquad k = 0, 1, 2, \ldots.$$

Note that $\boldsymbol{x}^{(k)} \in \mathcal{K}_{k+1}(A, \boldsymbol{x}^{(0)})$.
If $\boldsymbol{x}^{(k)}$ were an eigenvector of A, then $\boldsymbol{x}^{(k+1)}$ would be a multiple of $\boldsymbol{x}^{(k)}$. Therefore the calculation is terminated if this condition is achieved up to sufficient accuracy. Herewith the details of an implementation of the procedure.

0. Pick $\boldsymbol{x}^{(0)} \in \mathbb{R}^n$ satisfying $\|\boldsymbol{x}^{(0)}\| = 1$. Let ε be a small positive tolerance. Set $k = 0$.

1. Calculate $\tilde{\boldsymbol{x}}^{(k+1)} = A\boldsymbol{x}^{(k)}$ and find the real number λ that minimizes $f(\lambda) = \|\tilde{\boldsymbol{x}}^{(k+1)} - \lambda \boldsymbol{x}^{(k)}\|$.

2. Accept λ as an eigenvalue and $\tilde{\boldsymbol{x}}^{(k+1)}$ as the corresponding eigenvector if $f(\lambda) \leq \varepsilon$.

3. Otherwise, let $\boldsymbol{x}^{(k+1)} = \tilde{\boldsymbol{x}}^{(k+1)}/\|\tilde{\boldsymbol{x}}^{(k+1)}\|$, increase k by one and go back to **1.**

A useful starting point in the analysis of this algorithm is to express $\boldsymbol{x}^{(0)}$ as a linear combination of the eigenvectors of A.

Theorem 2.3 *(Termination of the power method). If A has n eigenvalues of different magnitude then the implementation in the previous paragraph terminates.*

Proof Let the eigenvalue equations be $A\boldsymbol{w}_j = \lambda_j \boldsymbol{w}_j$, $j = 1, 2, \ldots, n$, where $|\lambda_1| < |\lambda_2| < \cdots < |\lambda_n|$. We express $\boldsymbol{x}^{(0)}$ in the form $\boldsymbol{x}^{(0)} = \sum_{j=1}^n \theta_j \boldsymbol{w}_j$, and let m be the largest integer in $\{1, \ldots, n\}$ such that $\theta_m \neq 0$. Then $\boldsymbol{x}^{(k)}$ is a multiple of $A^k\boldsymbol{x}^{(0)} = \sum_{j=1}^m \theta_j \lambda_j^k \boldsymbol{w}_j$. Hence, after **1** of the implementation, the formula $\boldsymbol{x}^{(k)} = A^k\boldsymbol{x}^{(0)}/\|A^k\boldsymbol{x}^{(0)}\|$ provides

$$\|\tilde{\boldsymbol{x}}^{(k+1)} - \lambda \boldsymbol{x}^{(k)}\| = \min_\eta \|\tilde{\boldsymbol{x}}^{(k+1)} - \eta \boldsymbol{x}^{(k)}\| \leq \|\tilde{\boldsymbol{x}}^{(k+1)} - \lambda_m \boldsymbol{x}^{(k)}\| = \|A\boldsymbol{x}^{(k)} - \lambda_m \boldsymbol{x}^{(k)}\|$$

$$= \frac{\|\sum_{j=1}^m \theta_j \lambda_j^{k+1} \boldsymbol{w}_j - \lambda_m \sum_{j=1}^m \theta_j \lambda_j^k \boldsymbol{w}_j\|}{\|\sum_{j=1}^m \theta_j \lambda_j^k \boldsymbol{w}_j\|} = \frac{\|\sum_{j=1}^{m-1} \theta_j (\lambda_j - \lambda_m)(\lambda_j/\lambda_m)^k \boldsymbol{w}_j\|}{\|\sum_{j=1}^m \theta_j (\lambda_j/\lambda_m)^k \boldsymbol{w}_j\|}.$$

[1] Please email all corrections and suggestions to these notes to `A.Iserles@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartII/Handouts.html`.

We see that, as $k \to \infty$, the numerator and denominator of the right hand side tend to 0 and $\|\theta_m \boldsymbol{w}_m\|$, respectively, which implies $\|\tilde{\boldsymbol{x}}^{(k+1)} - \lambda \boldsymbol{x}^{(k)}\| \to 0$. Therefore termination occurs. □

Discussion 2.4 (Deficiencies of the power method). The power method may perform adequately if $\theta_n \neq 0$ and $|\lambda_{n-1}| < |\lambda_n|$, where we are using the notation of Theorem 2.3, but often it is unacceptably slow. The difficulty of $\theta_n = 0$ is that computer rounding errors can introduce a small nonzero component of $\boldsymbol{w}_n$ into the sequence $\boldsymbol{x}^{(k)}$, $k = 0, 1, 2, \ldots$, and then $\boldsymbol{w}_n$ may be found eventually, but one has to wait for the small component to grow. Moreover, $|\lambda_{n-1}| = |\lambda_n|$ is not uncommon when A is real and nonsymmetric, because the spectral radius of A may be due to a complex conjugate pair of eigenvalues. The technique of the next paragraph is designed for that case. Then the use of *shifts* will be studied, because they can be highly useful, particularly in the more efficient methods for eigenvalue calculations that will be considered later.

Algorithm 2.5 (Pairs of eigenvalues). Let Method 2.2 be applied when the eigenvalues of A are in increasing order of magnitude and satisfy $|\lambda_{n-2}| < |\lambda_{n-1}| = |\lambda_n|$ and $\lambda_{n-1} \neq \lambda_n$. We assume $\boldsymbol{x}^{(0)} = \sum_{j=1}^{n} \theta_j \boldsymbol{w}_j$, where both θ_{n-1} and θ_n are nonzero. Then, as $k \to \infty$, the vectors $\boldsymbol{x}^{(k)}$, $\boldsymbol{x}^{(k+1)}$ and $\boldsymbol{x}^{(k+2)}$ tend to be linearly dependent, because they tend to lie in the two-dimensional space spanned by $\boldsymbol{w}_{n-1}$ and $\boldsymbol{w}_n$. This is true even if λ_{n-1} and λ_n have nonzero imaginary parts but $\boldsymbol{x}^{(0)} \in \mathbb{R}^n$ (and hence the entire calculation can be carried out in real atithmetic, an important advantage).

The *two-stage power method* is a development of Method 2.2 for this situation, typical details being given in the following implementation.

0. Pick $\boldsymbol{x}^{(0)} \in \mathbb{R}^n$ satisfying $\|\boldsymbol{x}^{(0)}\| = 1$. Let $0 < \varepsilon \ll 1$. Set $k = 0$ and $\tilde{\boldsymbol{x}}^{(1)} = A\boldsymbol{x}^{(0)}$.

1. Calculate $\tilde{\boldsymbol{x}}^{(k+2)} = A\tilde{\boldsymbol{x}}^{(k+1)}$ and α, β that minimize $f(\alpha, \beta) = \|\tilde{\boldsymbol{x}}^{(k+2)} + \alpha\tilde{\boldsymbol{x}}^{(k+1)} + \beta\boldsymbol{x}^{(k)}\|$.

2. If $f(\alpha, \beta) \leq \varepsilon$, solve $\lambda^2 + \alpha\lambda + \beta = 0$ and let its roots be λ_+ and λ_-. They are accepted as eigenvalues of A, estimating their eigenvectors as $\tilde{\boldsymbol{x}}^{(k+1)} - \lambda_- \boldsymbol{x}^{(k)}$ and $\tilde{\boldsymbol{x}}^{(k+1)} - \lambda_+ \boldsymbol{x}^{(k)}$, respectively.

3. Otherwise, scale $\boldsymbol{x}^{(i)} = \tilde{\boldsymbol{x}}^{(i)}/\|\tilde{\boldsymbol{x}}^{(i)}\|$, $i = k+1, k+2$, increase k by one and return to **1.**

Step **2** is justified by the eigenvalue equation

$$\boldsymbol{0} = \tilde{\boldsymbol{x}}^{(k+2)} + \alpha\tilde{\boldsymbol{x}}^{(k+1)} + \beta\boldsymbol{x}^{(k)} = \tilde{\boldsymbol{x}}^{(k+2)} - (\lambda_+ + \lambda_-)\tilde{\boldsymbol{x}}^{(k+1)} + \lambda_+\lambda_-\boldsymbol{x}^{(k)}.$$

Hence, for example, $A(\tilde{\boldsymbol{x}}^{(k+1)} - \lambda_+\boldsymbol{x}^{(k)}) = \tilde{\boldsymbol{x}}^{(k+2)} - \lambda_+\tilde{\boldsymbol{x}}^{(k+1)} = \lambda_-(\tilde{\boldsymbol{x}}^{(k+1)} - \lambda_+\boldsymbol{x}^{(k)})$ and $\tilde{\boldsymbol{x}}^{(k+1)} - \lambda_+\boldsymbol{x}^{(k)}$ is an eigenvector corresponding to λ_-.

Technique 2.6 (The power method with shifts). This technique is based on the elementary remark that the eigenvectors of $A - sI$, $s \in \mathbb{R}$, are also eigenvectors of A. Specifically, the *power method with shifts* is Method 2.2, except that **1** and **2** of the implementation are replaced by

1. Choose $s^{(k)} \in \mathbb{R}$ and let $\tilde{\boldsymbol{x}}^{(k+1)} = (A - s^{(k)}I)\boldsymbol{x}^{(k)}$. Find λ minimizing $f(\lambda) = \|\tilde{\boldsymbol{x}}^{(k+1)} - \lambda\boldsymbol{x}^{(k)}\|$.

2. Accept $\lambda + s^{(k)}$ as an eigenvalue and $\tilde{\boldsymbol{x}}^{(k)}$ as an eigenvector if $f(\lambda) \leq \varepsilon$.

The reason for the new step **2** is that $f(\lambda) = 0$ implies that $\boldsymbol{x}^{(k)}$ satisfies $A\boldsymbol{x}^{(k)} = (\lambda + s^{(k)})\boldsymbol{x}^{(k)}$.

It follows from the expansion $\boldsymbol{x}^{(0)} = \sum_{j=1}^{n} \theta_j \boldsymbol{w}_j$, introduced already, that $\boldsymbol{x}^{(k+1)}$ is a multiple of

$$\prod_{l=0}^{k}(A - s^{(l)}I)\boldsymbol{x}^{(0)} = \sum_{j=1}^{n} \theta_j \left[\prod_{l=0}^{k}(\lambda_j - s^{(l)})\right] \boldsymbol{w}_j.$$

Therefore, if we are seeking the eigenvector $\boldsymbol{w}_n$ and $\theta_n \neq 0$, then it is suitable to employ shifts that render $\left|\prod_{l=0}^{k}(\lambda_j - s^{(l)})/(\lambda_n - s^{(l)})\right|$, $j = 1, 2, \ldots, n-1$, very small. Occasionally some good choices are clear. For example, if it is known that A has $n-1$ real eigenvalues in the interval $[100, 101]$ and that λ_n exceeds 101, then a shift of $s^{(k)} = 100.5$ for every k would be very useful. Another possibility is that the difference between $\tilde{\boldsymbol{x}}^{(k+1)}$ and the required eigenvector may be dominated by just one other eigenvector, and then the shift should be an estimate of the eigenvalue of this other eigenvector.