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Mathematical Tripos Part II: Michaelmas Term 2021

Numerical Analysis – Lecture 21

5 Eigenvalues and eigenvectors

We consider in this chapter the problem of computing eigenvalues and eigenvectors of matrices. 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 in general, and $\boldsymbol{w}$ is a nonzero vector. If A is diagonalizable, then the eigenvectors form a basis of $\mathbb{R}^n$. If A is symmetric, we know that the eigenvalues are all real, and that the eigenvectors form an orthonormal basis of $\mathbb{R}^n$.

We start by describing algorithms to compute a single eigenvalue/eigenvector pair for A.

5.1 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 $A\boldsymbol{x}^{(k)}$, so that $\|\boldsymbol{x}^{(k+1)}\| = 1$.

POWER ITERATION: for $k = 0, 1, 2, \ldots$

- Set $\boldsymbol{y} = A\boldsymbol{x}^{(k)}$
- $\boldsymbol{x}^{(k+1)} = \boldsymbol{y}/\|\boldsymbol{y}\|$

The next theorem shows that the sequence $\boldsymbol{x}^{(k)}$ converges to an eigenvector of A associated with the largest eigenvalue in modulus.

Theorem 5.1 *Let $A\boldsymbol{w}_i = \lambda_i \boldsymbol{w}_i$, where the eigenvalues of A satisfy $|\lambda_1| \le \cdots \le |\lambda_{n-1}| < |\lambda_n|$ and the eigenvectors are of unit length $\|\boldsymbol{w}_i\| = 1$. Assume $\boldsymbol{x}^{(0)} = \sum_{i=1}^n c_i \boldsymbol{w}_i$ with $c_n \neq 0$. Then $\|\boldsymbol{x}^{(k)} - \pm \boldsymbol{w}_n\| = \mathcal{O}(\rho^k)$ as $k \to \infty$, where $\rho = |\lambda_{n-1}/\lambda_n| < 1$.*

Proof. Given $x^{(0)}$ as in the assumption, $\boldsymbol{x}^{(k)}$ is a multiple of

$$A^k \boldsymbol{x}^{(0)} = \sum_{i=1}^n c_i \lambda_i^k \boldsymbol{w}_i = c_n \lambda_n^k \Big(\boldsymbol{w}_n + \sum_{i=1}^{n-1} \tfrac{c_i}{c_n} \big(\tfrac{\lambda_i}{\lambda_n}\big)^k \boldsymbol{w}_i \Big).$$

Since $\|\boldsymbol{x}^{(k)}\| = \|\boldsymbol{w}_n\| = 1$, we conclude that $\boldsymbol{x}^{(k)} = \pm \boldsymbol{w}_n + \mathcal{O}(\rho^k)$, where the sign is that of $c_n \lambda_n^k$ and the ratio $\rho = \frac{|\lambda_{n-1}|}{|\lambda_n|} < 1$ characterizes the rate of convergence.[1] □

The *Rayleigh quotient* at a nonzero vector $\boldsymbol{x}$ is defined by

$$r(\boldsymbol{x}) = \frac{\boldsymbol{x}^T A \boldsymbol{x}}{\boldsymbol{x}^T \boldsymbol{x}}.$$

If $A\boldsymbol{x} = \lambda \boldsymbol{x}$ then clearly $r(\boldsymbol{x}) = \lambda$. In general, $r(\boldsymbol{x}) = \arg\min_\mu \|A\boldsymbol{x} - \mu \boldsymbol{x}\|_2^2$, since $\|A\boldsymbol{x} - \mu\boldsymbol{x}\|_2^2 = \mu^2 \boldsymbol{x}^T\boldsymbol{x} - 2\mu \boldsymbol{x}^T A \boldsymbol{x} + \|A\boldsymbol{x}\|^2$, which is minimized precisely at $\mu = r(\boldsymbol{x})$. One can show, using the same proof as the theorem above, that the sequence of Rayleigh quotients $r(\boldsymbol{x}^{(k)})$ converges to λ_n at the rate $\mathcal{O}(\rho^k)$.

Discussion 5.2 (Deficiencies of the power method) The power method may perform adequately if $c_n \neq 0$ and $|\lambda_{n-1}| < |\lambda_n|$, where we are using the notation of Theorem 5.1, but often it is unacceptably slow. The difficulty of $c_n = 0$ is that, theoretically, in this case the method should find

[1] The assumption that $|\lambda_{n-1}| < |\lambda_n|$ implies that λ_n is real: indeed since our matrix A has real entries, all eigenvalues come in complex conjugate pairs, so if $\rho(A)$ was attained with a complex eigenvalue λ_n then $\overline{\lambda_n} \neq \lambda_n$ would also be an eigenvalue and has the same modulus.

an eigenvector $\boldsymbol{w}_m$ with the largest m such that $c_m \neq 0$, but practically computer rounding errors can introduce a small nonzero component of $\boldsymbol{w}_n$ into the sequence $\boldsymbol{x}^{(k)}$, 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. Next, we will study the inverse iterations (with *shifts*), because they can be highly useful, particularly in the more efficient methods for eigenvalue calculations that will be considered later.

5.2 Inverse iteration

Inverse iteration is the power method applied to the matrix $(A - sI)^{-1}$, for some *shift* $s \in \mathbb{R}$. The eigenvalues of $(A-sI)^{-1}$ are equal to $\frac{1}{\lambda_i - s}$ where λ_i are the eigenvalues of A, and the eigenvectors are the same. Let λ be the eigenvalue of A closest to s, and let λ' be the eigenvalue second-closest to s, so that $|\lambda - s| < |\lambda' - s|$. Then, from the analysis of the power method, we know that inverse iteration will converge to an eigenvector of λ with rate ρ^k, where $\rho = \frac{|\lambda - s|}{|\lambda' - s|} < 1$.

INVERSE ITERATION: for $k = 0, 1, 2, \ldots$

- $\lambda = r(\boldsymbol{x}^{(k)})$
- Solve $(A - sI)\boldsymbol{y} = \boldsymbol{x}^{(k)}$ (in $\boldsymbol{y}$, using e.g., LU decomposition)
- $\boldsymbol{x}^{(k+1)} = \boldsymbol{y}/\|\boldsymbol{y}\|$

The advantage of inverse iteration is the choice of the parameter s: if we have a good estimate of the eigenvalue λ, then the iterations converge very fast.

Rayleigh quotient iteration In the algorithm above, the Rayleigh quotient $r(\boldsymbol{x}^{(k)})$ gives us an estimate of the eigenvalue closest to s. In turn, we know that the convergence of inverse iteration depends on how well the shift s approximates the eigenvalue. In Rayleigh quotient iteration, we update the shift at each iteration by the Rayleigh quotient, namely:

RAYLEIGH QUOTIENT ITERATION: for $k = 0, 1, 2, \ldots$

- $s_k = r(\boldsymbol{x}^{(k)})$
- Solve $(A - s_k I)\boldsymbol{y} = \boldsymbol{x}^{(k)}$
- $\boldsymbol{x}^{(k+1)} = \boldsymbol{y}/\|\boldsymbol{y}\|$

In practice, the convergence of Rayleigh quotient iteration is *extremely fast*.

Example: consider the matrix

$$A = \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}$$

with $n = 5$, and the initial vector $\boldsymbol{x}^{(0)} = (1, \ldots, 1)/\sqrt{5}$. We know that the eigenvalues of A are equal to $4\sin^2(\ell\pi/(2(n+1)))$, $\ell = 1, \ldots, n$, and that the eigenvectors correspond to sinusoidal vectors with frequencies $\ell = 1, \ldots, n$. The initial vector $\boldsymbol{x}^{(0)}$ here is constant, so it makes sense to think that the Rayley quotient iteration will converge to the eigenvalue corresponding to the smallest frequency, i.e., $\ell = 1$, which in this case is $4\sin^2(\pi/12) \approx 0.267949192431$. After 3 iterations of Rayleigh quotient iteration we obtain the approximation 0.267949192649 which is correct up to 9 digits!