MA 511, Session 41

Approximation of Eigenvalues

Let A be a $n \times n$ matrix.

(I) Power Method

Choose an initial vector $u_0 \in \mathbb{R}^n$, and define the sequence

$$u_1 = Au_0, \quad u_2 = Au_1, \quad \ldots, u_k = Au_{k-1}.$$

Then,

$$u_2 = A^2u_0, \quad u_3 = A^3u_0, \quad \ldots, u_k = A^ku_0.$$

This provides an efficient method when A is sparse, i.e. most of its coefficients are zero.

Suppose that A is non-defective, with eigenvectors $x_1, \ldots, x_n$ corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_n$, where $|\lambda_1| \leq |\lambda_2| \leq \cdots \leq |\lambda_{n-1}| < |\lambda_n|$. Let $u_0 = c_1x_1 + \cdots + c_nx_n$ with $c_n \neq 0$. Then,

$$u_k = c_1\lambda_1^kx_1 + \cdots + c_n\lambda_n^kx_n,$$

and

$$\begin{aligned}
\frac{u_k}{\|u_k\|} &= \frac{c_1\lambda_1^k x_1 + \cdots + c_n\lambda_n^k x_n}{\|c_1\lambda_1^k x_1 + \cdots + c_n\lambda_n^k x_n\|} \\
&= \frac{\lambda_n^k \left(c_1\left(\frac{\lambda_1}{\lambda_n}\right)^k x_1 + \cdots + c_{n-1}\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^k x_{n-1} + c_n x_n\right)}{|\lambda_n|^k \left\|c_1\left(\frac{\lambda_1}{\lambda_n}\right)^k x_1 + \cdots + c_{n-1}\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^k x_{n-1} + c_n x_n\right\|} \\
&= d_n^k x_n + \varepsilon_k,
\end{aligned}$$

where

$$\begin{aligned}
|d_n^k| &= \left|\frac{\lambda_n}{|\lambda_n|}\right|^k \frac{|c_n|}{\sqrt{c_1^2\left(\frac{\lambda_1}{\lambda_n}\right)^{2k} + \cdots + c_{n-1}^2\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^{2k} + c_n^2}} \\
&= \frac{1}{\sqrt{\left(\frac{c_1}{c_n}\right)^2\left(\frac{\lambda_1}{\lambda_n}\right)^{2k} + \cdots + \left(\frac{c_{n-1}}{c_n}\right)^2\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^{2k} + 1}} \\
&\longrightarrow 1
\end{aligned}$$

and

$$\varepsilon_k = \frac{\lambda_n^k \left(c_1\left(\frac{\lambda_1}{\lambda_n}\right)^k x_1 + \cdots + c_{n-1}\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^k x_{n-1}\right)}{|\lambda_n|^k \left\|c_1\left(\frac{\lambda_1}{\lambda_n}\right)^k x_1 + \cdots + c_{n-1}\left(\frac{\lambda_{n-1}}{\lambda_n}\right)^k x_{n-1} + c_n x_n\right\|} \longrightarrow 0$$

as $k \to \infty$. Thus, in the limit we obtain an eigenvector corresponding to the largest eigenvalue (in the direction of x_n).

(II) Inverse Power Method

Suppose that A is non-defective, with eigenvectors $x_1, \ldots, x_n$ corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_n$, where $|\lambda_1| < |\lambda_2| \leq \cdots \leq |\lambda_n|$. This method is the same as the previous one but applying iteratively to A^{-1} rather than A. It leads in the limit to an eigenvector corresponding to the smallest eigenvalue (in the direction of x_1).

(III) Hessenberg Form

The Hessenberg form of a matrix A is a matrix B similar to A but with many more vanishing coefficients (i.e. equal to zero) than A has. B will be produced through repeated applications of Householder transformations to A.

Let $u \in \mathbb{C}^n$ be a unit vector (i.e. $\|u\| = 1$). Define the Householder transformation $L : \mathbb{C}^n \longrightarrow \mathbb{C}^n$ as $L(v) = Uv$, where $U = \mathbb{I} - 2uu^H$.

Theorem: U is Hermitian and unitary.

Proof: $U^H = (\mathbb{I} - 2uu^H)^H = \mathbb{I} - 2(u^H)^H u^H = U$, and U is Hermitian. Also,

$$\begin{aligned} U^H U = U^2 &= (\mathbb{I} - 2uu^H)(\mathbb{I} - 2uu^H) \\ &= \mathbb{I} - 4uu^H + 4(uu^H)(uu^H) = \mathbb{I} \end{aligned}$$

since $u^H u = 1$, and thus U is unitary.

Lemma: Let $v = x + \|x\| \, e_1$, where e_1 is the first vector in the standard basis of $\mathbb{R}^n$ (or $\mathbb{C}^n$), $(e_1)_j = \delta_{1j}$, $1 \leq j \leq n$. Let $u = \frac{v}{\|v\|}$ and U be the corresponding Householder matrix. Then, $Hx = -\|x\| e_1$.

<u>Proof</u>: Since $U = \mathbb{I} - 2 \, \dfrac{(x + \|x\| \, e_1)(x + \|x\| \, e_1)^H}{(x + \|x\| \, e_1)^H (x + \|x\| \, e_1)}$, then

$$\begin{aligned} Ux &= x - 2 \, \frac{(x + \|x\| \, e_1)(x + \|x\| \, e_1)^H}{(x + \|x\| \, e_1)^H (x + \|x\| \, e_1)} \, x \\ &= x - (x + \|x\| e_1) \, \frac{2\big(\|x\|^2 + \|x\| x_1\big)}{2\|x\|^2 + 2\|x\| x_1} \end{aligned}$$

where x_1 is the first component of x. As the last factor equals 1, it follows that $Ux = -\|x\| e_1$, as claimed.

Let now A be a $n \times n$ matrix, and take $x_1 = (a_{21}, a_{31}, \ldots, a_{n1})^T \in \mathbb{C}^{n-1}$. Let $e_1^{(k)}$ denote the first vector in the standard basis of $\mathbb{C}^k$. Define the Householder transformation of $\mathbb{C}^{n-1}$ as in the lemma with $x = x_1$, and denote $\tilde{U}_1$ its matrix. Then, from the lemma, $\tilde{U}_1 x_1 = -\|x_1\| e_1^{(n-1)}$. Define now a unitary and symmetric $n \times n$ matrix U_1 by putting $e_1^{(n)}$ as first row and column of U_1 and $\tilde{U}_1$ for the rest of the rows and columns. We have $U_1^{-1} = U_1$ and $U_1^{-1} A U_1$ has its first column equal to $(a_{11}, -\|x_1\|, 0, \ldots, 0)^T$.

In the next step one takes $x_2 \in \mathbb{C}^{n-2}$ to be the last $n-2$ coefficients of the second column of $U_1^{-1} A U_1$, and use the $(n-2) \times (n-2)$ Householder matrix $\tilde{U}_2$ that transforms x_2 into $-\|x_2\|\, e_1^{(n-2)}$. Then we define a unitary and symmetric $n \times n$ matrix U_2 by putting $e_1^{(n)}, e_2^{(n)}$ as the first two rows and columns of U_2 and $\tilde{U}_2$ for the rest of the rows and columns. We have $U_2^{-1} = U_2$ and $U_2^{-1} U_1^{-1} A U_1 U_2$ has its first column equal to $(a_{11}, -\|x_1\|, 0, \ldots, 0)^T$, and its second column to $(*, *, -\|x_2\|, 0, \ldots, 0)^T$, where $*$ stands for some unspecified number.

Repeating this process $n-2$ times, we find a unitary and symmetric $n \times n$ matrix $U = U_1 U_2 \ldots U_{n-2}$ such that $U^{-1}AU$ has zeros below the the first lower diagonal, i.e. $(U^{-1}AU)_{ij} = 0$ for $2 \leq j+1 < i \leq n$. This matrix is the <u>Hessenberg matrix</u> for A.

If A had been Hermitian, since $U_1, \ldots, U_{n-2}$ are all Hermitian, then so would be the Hessenberg matrix $U^{-1}AU$, and therefore, it must be <u>tridiagonal</u>, i.e. $(U^{-1}AU)_{ij} = 0$ for $|i-j| > 1$, $1 \leq i, j \leq n$.

Remark: We should stress the fact that the matrices produced by this method are sparse and have the same eigenvalues than the original one.

(IV) <u>QR Method</u>

Begin with the $n \times n$ matrix A_0. Then use Gram-Schmidt to factor it as $A_0 = Q_0 R_0$, where the columns of Q_0 are linear combinations of the corresponding columns of A_0 and, if A_0 is nonsingular, they are orthonormal. R_0 is upper triangular. Let now $A_1 = R_0 Q_0$. Then,

$$Q_0^{-1} A_0 Q_0 = Q_0^{-1}(Q_0 R_0) q_0 = A_1,$$

so that A_1 is similar to A_0.

Let now $A_1 = Q_1R_1$ and define $A_2 = R_1Q_1$, and so on. This process that defines the similar matrices $A_1, A_2, \ldots$, all similar to the original one A_0 is called the unshifted QR method.

If A_0 were a Hessenberg form of A, then the QR method would converge rapidly to an upper triangular matrix —which would then have the eigenvalues of A on its diagonal.