0.0.1 Jacobi eigenvalue algorithm

A basic problem in numerical Linear Algebra is to find the eigenvalues and eigenvectors of a real-symmetric $N \times N$ matrix. An old but effective algorithm is the Jacobi eigenvalue algorithm. This algorithm uses planar rotations to systematically decrease the size of off-diagonal elements while increasing the size of diagonal elements. A bit of linear algebra is the foundation of the algorithm.

Planar rotations

Recall that a 2×2 rotation matrix has the form

$$R_2 = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}.$$

We can restrict θ in the range $\pi \le \theta \le \pi$. Notice that if we apply this matrix to the standard basis vectors we get

$$R_2 E_1 = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix},$$

$$R_2 E_2 = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin(\theta) \\ \cos(\theta) \end{pmatrix},$$

so as given this matrix multiplication gives a counterclockwise rotation in the plane.

The next step is to extend this rotation to two of N coordinates in $\mathbb{R}^N$. Pick two distinct indices m, n, with $1 \le m < n \le N$. Define the $N \times N$ matrix $R_{m,n}(\theta)$ which is the identity, except for replacement of the m-th row and the n-th row. For notational convenience we will sometimes suppress the argument θ, writing $R_{m,n}$ for $R_{m,n}(\theta)$. The new m, n-th rows have zero entries except for

$$R_{m,n}(m,m) = R_{m,n}(n,n) = \cos(\theta), \quad R_{m,n}(n,m) = \sin(\theta) = -R_{m,n}(m,n).$$

As an example with $N = 4$,

$$R_{2,4}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & 0 & -\sin(\theta) \\ 0 & 0 & 1 & 0 \\ 0 & \sin(\theta) & 0 & \cos(\theta) \end{pmatrix}.$$

Such rotation matrices are orthogonal. That is, the inverse is the transpose, and multiplication by $R = R_{m,n}(\theta)$ does not change vector length,

$$\|X\|^2 = X \bullet X = R^{-1}RX \bullet X = R^TRX \bullet X = RX \bullet RX = \|RX\|^2.$$

Suppose A, with entries $A(i,j)$ is an $N \times N$ real symmetric matrix, that is $A = A^T$. Since in general $(AB)^T = B^TA^T$ we get

$$[R_{m,n}(\theta)^TAR_{m,n}(\theta)]^T = R_{m,n}(\theta)^TAR_{m,n}(\theta).$$

Moreover, since $R_{m,n}^T = R_{m,n}^{-1}$, this conjugation replaces A with a new symmetric matrix, but leaves the eigenvalues fixed. That is

$$AX = \lambda X, \quad AR_{m,n}R_{m,n}^{-1}X = \lambda X, \quad \big(R_{m,n}^{-1}AR_{m,n}\big)R_{m,n}^{-1}X = \lambda R_{m,n}^{-1}X$$

In addition, the mapping from $A \to R_{m,n}(\theta)^TA$ leaves the lengths of the columns unchanged, while the mapping $R_{m,n}(\theta)^TA \to (R_{m,n}(\theta)^TA)R_{m,n}(\theta)$ leaves the lengths of the rows unchanged, so the square of the matrix norm

$$\|A\|^2 = \sum_{i,j=1}^{N} A(i,j)^2$$

is unchanged by the conjugation.

Recall that dot products with the standard basis vectors $E_1, \dots, E_N$ give matrix entries,

$$A(i,j) = E_i \bullet AE_j.$$

This fact helps compute the entries of $R_{m,n}(\theta)^TAR_{m,n}(\theta)$. If $i \ne m,n$ and $j \ne m,n$, then multiplication by $R_{m,n}$ leaves E_i and E_j fixed, so

$$E_i \bullet R_{m,n}^TAR_{m,n}E_j = R_{m,n}E_i \bullet AR_{m,n}E_j = E_i \bullet AE_j = A(i,j).$$

That is, there is no effect on the matrix entries unless the row or column is m or n. It may help to use the 4×4 case as an illustration.

Now consider the new rows m,n and columns m,n. If the row is m and the column is j then the (m,j) entry is

$$R_{m,n}E_m \bullet AR_{m,n}E_j = \big(\cos(\theta)E_m + \sin(\theta)E_n\big) \bullet AR_{m,n}E_j.$$

Now if the row is n and the column is j then the (n,j) entry is

$$R_{m,n}E_n \bullet AR_{m,n}E_j = \big(-\sin(\theta)E_m + \cos(\theta)E_n\big) \bullet AR_{m,n}E_j.$$

If $j \neq m, n$ then $R_{m,n} E_j = E_j$.

Consider the diagonal entries of $R^T_{m,n} A R_{m,n}$. Using $A(m,n) = A(n,m)$, the (m,m) entry $B_1(\theta)$ is

$$R_{m,n} E_m \bullet A R_{m,n} E_m = \big(\cos(\theta) E_m + \sin(\theta) E_n\big) \bullet A\big(\cos(\theta) E_m + \sin(\theta) E_n\big)$$

$$= \cos^2(\theta) A(m,m) + \sin^2(\theta) A(n,n) + 2\sin(\theta)\cos(\theta) A(m,n).$$

$$= A(m,m) + \sin^2(\theta)[A(n,n) - A(m,m)] + 2\sin(\theta)\cos(\theta) A(m,n)$$

$$= A(m,m) + \frac{1-\cos(2\theta)}{2}[A(n,n) - A(m,m)] + \sin(2\theta) A(m,n).$$

Similarly, the (n,n) entry $B_2(\theta)$ is

$$R_{m,n} E_n \bullet A R_{m,n} E_n = \big(-\sin(\theta) E_m + \cos(\theta) E_n\big) \bullet A\big(-\sin(\theta) E_m + \cos(\theta) E_n\big)$$

$$= A(n,n) + \sin^2(\theta)[A(m,m) - A(n,n)] - 2\sin(\theta)\cos(\theta) A(m,n)$$

$$= A(n,n) + \frac{1-\cos(2\theta)}{2}[A(m,m) - A(n,n)] - \sin(2\theta) A(m,n).$$

Write the sum of the squares of the new diagonal entries as $B_1(\theta)^2 + B_2(\theta)^2$. Since this function is continuous and periodic with period π, it must have maxima and minima. $B_1(\theta)^2 + B_2(\theta)^2$ is extremized when

$$2B_1 \frac{dB_1}{d\theta} + 2B_2 \frac{dB_2}{d\theta} = 0.$$

The derivative terms are

$$\frac{dB_1}{d\theta} = \sin(2\theta)[A(n,n) - A(m,m)] + 2\cos(2\theta) A(m,n) = -\frac{dB_2}{d\theta}.$$

We want either $dB_1/d\theta = 0$, or $B_1 = B_2$.

If the derivatives are zero we get

$$\tan(2\theta) = 2\frac{A(m,n)}{A(m,m) - A(n,n)}. \tag{0.0.1}$$

If $B_1 = B_2$ then simplifying leads to

$$\cos(2\theta)[A(n,n) - A(m,m)] = 2\sin(2\theta) A(m,n),$$

and this value of θ then gives

$$B_1 = B_2 = \frac{1}{2}[A(n,n) + A(m,m)],$$

so

$$B_1^2 + B_2^2 = \frac{1}{2}[A(n,n)^2 + 2A(m,m)A(n,n) + A(m,m)^2].$$

From

$$0 \leq (\alpha - \beta)^2 = \alpha^2 - 2\alpha\beta + \beta^2, \quad 2\alpha\beta \leq \alpha^2 + \beta^2,$$

we see that

$$\frac{(A(m,m) + A(n,n)^2}{2} < A(m,m)^2 + A(n,n)^2$$

unless the values are equal. It is (0.0.1) that we want.

Jacobi algorithm

The algorithm is much easier to describe than to justify. Pick an $\epsilon > 0$, for example $\epsilon = 10^{-6}$.

Sweep: First do a *sweep*: for $n = 1, \ldots, N$ and $m = 1, \ldots, n$, determine θ as in (0.0.1). Replace A by $R_{m,n}(\theta)^T A R_{m,n}(\theta)$.

Iterate: At the end of the sweep, check to see if the sum of the squares of the off-diagonal elements is less than ϵ. If so, stop. Otherwise perform another sweep.

The original version of the algorithm was slightly different. You were supposed to find the maximum $|A(m,n)|$ for off-diagonal entries and then replace A by $R_{m,n}(\theta)^T A R_{m,n}(\theta)$. Then repeat until the sum of the squares of the off-diagonal elements (or some other measure of goodness) is less than ϵ. Since the original algorithm was described in the middle of the 1800's, the matrices were probably small and the maximum $|A(m,n)|$ could be seen by eye. With modern computers, large matrices, and small ϵ, the repeated searches for maxima seems inefficient.