Mathematics 307—December 5, 1995

Practical mathods of finding eigenvalues and eigenvectors

Recall that if T is a linear transformation, an eigenvector of T is a non-zero vector v such that T takes v into a multiple of itself. The scalar multiple which occurs here is the associate eigenvalue. The only method for finding eigenvectors and eigenvalues which we know so far is this: if λ is an eigenvalue for the eigenvector v and A is a matrix for T then the system of equations

$$Av = \lambda v, \quad (A - \lambda I)v = 0$$

has a non-trivial solution v, which means that the matrix $A - \lambda I$ must be singular, or equivalently

$$\det(A - \lambda I) = 0$$

Therefore the eigenvalues of T are the roots of the characteristic polynomial, and the eigenvectors are the non-zero solutions of the system above.

This method works fine for 2×2 matrices, but fails to be practical for ones of larger size, in the face of inevitable roundoff errors. There are several reasons for this, but the most obvious one is that it will usually be impossible to find a characteristic root exactly, so that the matrix $A - \lambda I$ will not usually be in fact singular. There is as far as I know no reasonable way to get around this difficulty. There turn out to be other reasons not to use this simple metod to find eigenvalues and eigenvectors: (•) a small amount of roundoff error in the characteristic polynomial can lead to huge errors in finding its roots; (•) this method is completely impractical when the matrix is huge, as it often will be in real applications.

The upshot is that no good computer programs for finding eigenvalues and eigenvectors proceed in this fashion. There are a variety of practical methods implemented in current software. They are as robust and efficient as possible, but not easy to understand. After all, they have been developed over a period of at least 40 years.

In this course I shall only attempt to explain some simple techniques. Better ones have much in common with them, so the ones explained here are more instructive than they might appear. Their limitations, in fact, only arise with matrices of much larger size than the ones we shall look at.

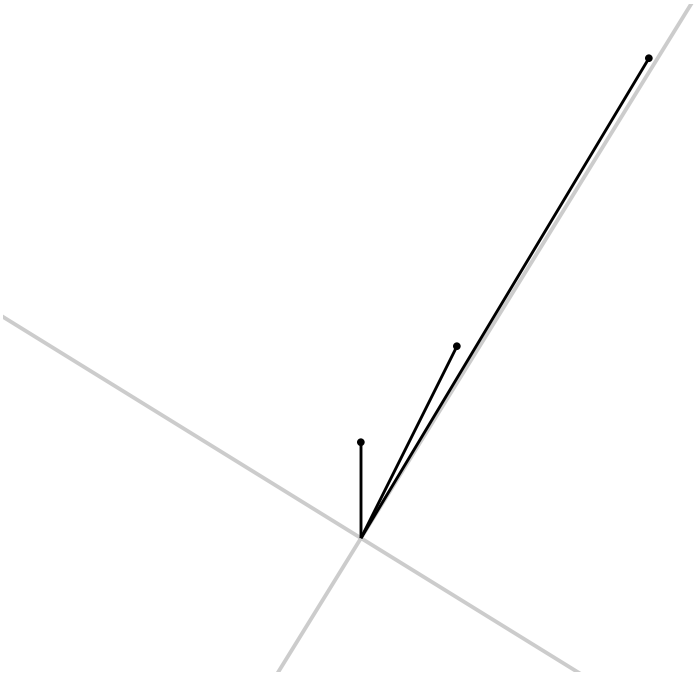
The power method

Let A be the matrix

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

Its eigenvalues are $\lambda = 3/2 \pm \sqrt{5}/2$, approximately $2.618,\ 0.382$. Let $v_1 \sim (0.526, 0.851)$ be its first (normalized) eigenvector, $v_2 \sim (-0.851, 0.526)$ its second. We know that A scales by a factor of $\lambda_1 > 1$ in the direction of $\pm v_1$, by a factor of $\lambda_2 < 1$ in the complementary direction. The point of the power method is that *if one applies A repeatedly to almost any initial vector, then as the number of repetitions goes up the direction of the vector one gets will tend more and more towards the direction of an eigenvector whose eigenvalue is largest in magnitude.*

Here is a picture of what happens when we start with $(0, 1)$.



The picture suggests how to approximate the eigenvector v_1. We start with a vector v_0 chosen randomly, apply A and normalize over and over again until we seem to be getting the same vector again on each iteration — that is to say, until the process has converged to the number of decimal places we are working with.

(1) Set $v_{*,n} = Av_{n-1}$. (2) Set $v_n = v_{*,n}/\|v_{*,n}\|$.

In the example above, for example, we get

v	$v_* = Av$
[0.000000 1.000000]	[1.00000 2.00000]
[0.447214 0.894427]	[1.34164 2.23607]
[0.514496 0.857493]	[1.37199 2.22948]
[0.524097 0.851658]	[1.37576 2.22741]
[0.525493 0.850798]	[1.37629 2.22709]
[0.525696 0.850672]	[1.37637 2.22704]
[0.525726 0.850654]	[1.37638 2.22703]
[0.525730 0.850651]	[1.37638 2.22703]
[0.525731 0.850651]	[1.37638 2.22703]
[0.525731 0.850651]	

The only problem with doing this is that it is conceivable that we shallstart with a vector in the plane perpendicular to v_1. But in practice, because of rounding erriors, even this causes no problems. Besides, no matter what happens we have to get some eigenvector in the end.

This method is something you'd never carry out by hand, but it works very well with even the simplest programmable calculator. Once we have the eigenvector we want, we find its eigenvalue by applying A once more and calculating the ratio of Au to u.

How fast this process converges depends on the ratio between the two largest eigenvalues — the larger this ratio, the more rapid the convergence. In other words, the process has trouble separating eigenvectors for eigenvalues which are very close. This is typical of all such processes, and reflects a real difficulty which

occurs when an eigenvalue has multiplicity greater than one. The convergence is at any rate **linear**: *the amount of work we have to do is roughly proportional to the number of accurate decimal places we want.*

Once we have one eigenvector, how do we find others? In two dimensions the answer is very simple: the other eigenvector is perpendicular to the one we have already. In higher dimensions we perform a more complicated calculation called **deflation**: we look at the linear transformation we get by considering the original one acting on vectors perpendicular to the one we have found. They form a vector space of dimension one less than the original. Then we continue on with decreasing dimensions. This process is conceptually simple, but complicated by technical details. I will probably come back to this point later.

Jacobi's method

In contrast to the power method, Jacobi's method has no (apparent) geometric basis. But it is fairly effective, and has generally faster convergence than the first method. Convergence is in fact **quadratic** which means that we double at each stage the number of accurate decimals.

Given a symmetric matrix A, our ultimate goal is to find an orthogonal matrix X such that $XAX^{-1} = XA\,{}^tX$ is diagonal. It will be convenient if we have a name for the matrix XAX^{-1}: it is called the **conjugation** of A by X. If we have such a matrix, then we know that the eigenvectors of A are the columns of X^{-1}; since X is orthogonal, its inverse is its tarnspose, so the eigenvectors are the *rows* of X. The basic idea of Jacobi's method (which was invented by the German mathematician Jacobi around 1830, in order to find by hand the eigenvalues of a certain 7×7 matrix occurring in the theory of planetary orbits) is to conjugate A successively by very simple orthogonal matrices in order to make it closer and closer to a diagonal matrix.

The procedure depends completely on the simplest case, when A is 2×2. Here we can do everything explicitly, using the quadratic formula for finding eigenvalues, and a single linear equation in two unknowns to find eigenvectors. In order to make it a bit easier to carry out the full Jacobi process, I recall what is involved here, in a form best suited to Jacobi's method.

Suppose we are given a symmetric 2×2 matrix

$$A = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$$

We know that we can find

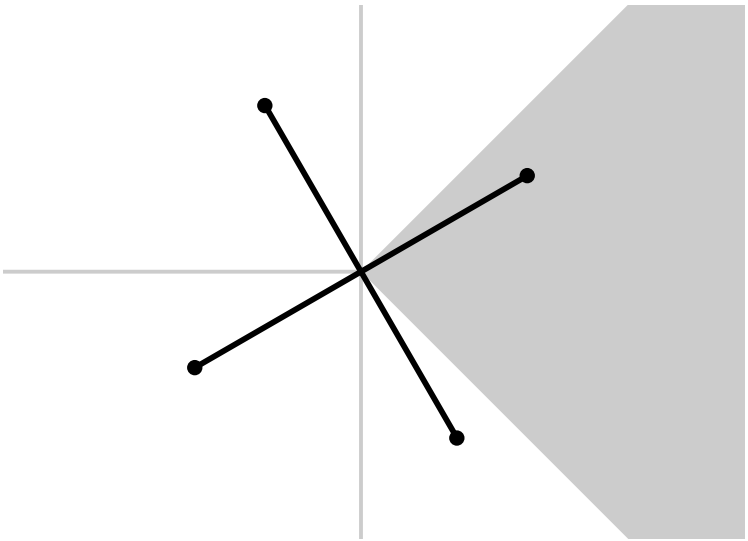
$$X = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

such that

$$X\,A\,X^{-1} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

There are several ways to find the matrix X, or equivalently $c = \cos\theta$ and $s = \sin\theta$, but it pays to do it in a slightly complicated way, in order to minimize roundoff errors, which can build up easily here since so many calculations are carried out.

The rows of X are eigenvectors v of of A with $\|v\| = 1$, and since X is a rotation we know X if we know just one of its rows. But there are still some choices to be made, since there are exactly four eigenvectors v of A with $\|v\| = 1$.



As the diagram illustrates, there will be exactly one eigenvector in the (shaded) region $|y| \leq x$, $x > 0$ unless the eigenvectors lie on the lines $y = \pm x$. In Jacobi's method, it is this eigenvector, generally unique, which we want to pick out. We shall next see some formulas for it.

We know that the λ_i are the roots of the characteristic polynomial

$$\lambda^2 - (a+c)\lambda + (ac - b^2) = 0$$

$$\lambda = \frac{a+c}{2} \pm \frac{\sqrt{(a+c)^2 - 4(ac-b^2)}}{2} = \frac{a+c}{2} \pm \frac{\sqrt{(a-c)^2 + 4b^2}}{2} = \frac{a+c}{2} \pm \sqrt{\left(\frac{a-c}{2}\right)^2 + b^2}$$

The eigenvector equation is

$$(a - \lambda)x + by = 0$$

so that an eigenvector is

$$\begin{aligned} x &= b \\ y &= \lambda - a \\ &= \frac{c-a}{2} \pm \sqrt{\left(\frac{c-a}{2}\right)^2 + b^2} \end{aligned}$$

which we can scale (dividing by b) to

$$\begin{aligned} x &= 1 \\ y &= \lambda - a \\ &= \frac{c-a}{2b} \pm \sqrt{\left(\frac{c-a}{2b}\right)^2 + 1} \\ &= \zeta \pm \sqrt{\zeta^2 + 1}, \quad \zeta = \frac{c-a}{2b} \end{aligned}$$

This makes sense only if $b \neq 0$, but in case $b = 0$ the original matrix is diagonal so there is no work to be done. We have $x > 0$ here, and we have only to choose the sign of the square root to get $|y| \leq 1$. The best formula for this involves a simple algebraic trick. The numbers

$$\zeta \pm \sqrt{\zeta^2 + 1}$$

are the roots of the equation

$$t^2 - 2\zeta t - 1 = 0$$

The two roots t_1 and t_2 of this equation satisfy

$$t_1 t_2 = -1$$

Therefore if t_i is a root, so is $1/t_i$. This means that

$$\zeta \pm \sqrt{\zeta^2 + 1} = \frac{-1}{\zeta \mp \sqrt{\zeta^2 + 1}}$$

But in this form it is easy to see how to choose the sign so as to get a number of magnitude at most 1. It depends on the sign of ζ, since if $\zeta > 0$ then $\zeta + \sqrt{\zeta^2 + 1} \geq 1$, while if $\zeta < 0$ then it is $\zeta - \sqrt{\zeta^2 + 1}$ that we want. This can be summarized in the formula

$$y = \frac{-\text{sign}(\zeta)}{|\zeta| + \sqrt{\zeta^2 + 1}}$$

where

$$\text{sign}(\zeta) = \frac{\zeta}{|\zeta|}$$

if $\zeta \neq 0$, and if $\zeta = 0$ can be taken to be either ± 1. Note that if $\zeta = 0$ then $y = \pm 1$, and this ambiguity matches with the cases where the eigenvectors lie on lines $y = \pm x$. So we know how to get the eigenvectors we want, and we must finally normalize to get eigenvectors of length 1. Recalling that it is the rows of X which are to be the eigenvectors, all in all we perform the sequence of calculations

$$\begin{aligned}
\zeta &= \frac{c - a}{2b} \\
t &= \frac{\text{sign}(\zeta)}{|\zeta| + \sqrt{1 + \zeta^2}} \\
c &= \frac{1}{\sqrt{1 + t^2}} \\
s &= ct \\
X &= \begin{bmatrix} c & -s \\ s & c \end{bmatrix}
\end{aligned}$$

where $t = -y$ in the discussion above. Recall again that if $b = 0$ then there is nothing to do! This recipe will always give us c and s for the smallest possible angle θ, which is a good idea since if we don't have to rotate by a large angle we shouldn't. The variable t represents $\tan\theta$, and these formulas, which are essentially equivalent to the standard ones, work because of various trigonometric identities. The eigenvalues themselves can finally be obtained according to the recipe

$$\begin{aligned}
\lambda &= a - bt \\
\mu &= c + bt
\end{aligned}$$

so the calculations in the 2×2 case are all easily laid out in terms of t.

As for the full Jacobi procedure, I will illustrate how it goes by an example. Let

$$A = \begin{bmatrix} 1 & 1/2 & 1/3 \\ 1/2 & 1/3 & 1/4 \\ 1/3 & 1/4 & 1/5 \end{bmatrix} \sim \begin{bmatrix} 1.000000 & 0.500000 & 0.333333 \\ 0.500000 & 0.333333 & 0.250000 \\ 0.333333 & 0.250000 & 0.200000 \end{bmatrix}$$

In each stage of Jacobi's method we will make two opposite off-diagonal terms of our symmetric equal to zero, affecting the others as little as possible. The entries we choose to make zero will be the largest ones. In our example, those are 0.500. So we focus only on the 2×2 matrix containing those terms. It is

$$\alpha = \begin{bmatrix} 1.000000 & 0.500000 \\ 0.500000 & 0.333333 \end{bmatrix}$$

We find a 2×2 rotation matrix χ such that $\chi A_* \chi^{-1}$ is diagonal, say by applying the above formulas. Here

$$\begin{aligned} \zeta &= \frac{c-a}{2b} \\ &= -0.666667 \\ t &= \frac{\text{sign}(\zeta)}{|\zeta| + \sqrt{1+\zeta^2}} \\ &= -0.535184 \\ c &= \frac{1}{\sqrt{1+t^2}} \\ &= 0.881675 \\ s &= ct \\ &= -0.471858 \\ \chi &= \begin{bmatrix} c & -s \\ s & c \end{bmatrix} \\ &= \begin{bmatrix} 0.881675 & 0.471858 \\ -0.471858 & 0.881675 \end{bmatrix} \\ \chi\alpha\chi^{-1} &= \begin{bmatrix} 1.26759 & \\ & 0.0657414 \end{bmatrix} \end{aligned}$$

How do we use this 2×2 rotation? We embed it into a 3×3 rotation.

$$X = \begin{bmatrix} \chi & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0.881675 & 0.471858 & \\ -0.471858 & 0.881675 & \\ & & 1 \end{bmatrix}$$

and then calculate

$$XAX^{-1} = \begin{bmatrix} 1.26759 & & 0.411856 \\ & 0.065741 & 0.063132 \\ 0.411856 & 0.063132 & 0.200000 \end{bmatrix}$$

Note that this new matrix is symmetric, and that its off-diagonal entries are on the average somewhat smaller than those of A. We shall see in a moment that we can make this assertion more precise.

We do the same thing again to this new symmetric matrix, which I'll call A_1, to distinguish it from A_0. So far, we can write

$$A_1 = X_0 A_0 X_0^{-1}$$

We make the entry 0.411856 equal to 0 now. We do this by looking at the matrix

$$\begin{bmatrix} 1.26759 & 0.411856 \\ 0.411856 & 0.200000 \end{bmatrix}$$

sitting at the corners of A_1. We find

$$\chi_1 = \begin{bmatrix} 0.946502 & 0.322698 \\ -0.322698 & 0.946502 \end{bmatrix}$$

$$X_1 = \begin{bmatrix} 0.946502 & & 0.322698 \\ & 1 & \\ -0.322698 & & 0.946502 \end{bmatrix}$$

$$X_1 A_1 X_1^{-1} = \begin{bmatrix} 1.40801 & 0.0203728 & \\ 0.0203728 & 0.0657414 & 0.0597552 \\ & 0.0597552 & 0.0595827 \end{bmatrix}$$

This is even closer to being diagonal. In the next stage we make the entry 0.0597552 equal to 0. Here

$$\chi_2 = \begin{bmatrix} 0.725074 & 0.688671 \\ -0.688671 & 0.725074 \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & & \\ & 0.725074 & 0.688671 \\ & 0.688671 & 0.725074 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} 1.40801 & 0.0147718 & -0.0140302 \\ 0.0147718 & 0.122497 & \\ -0.0140302 & & 0.0028276 \end{bmatrix}$$

In the next step

$$\chi_3 = \begin{bmatrix} 0.999934 & -0.0114887 \\ 0.0114887 & 0.999934 \end{bmatrix}$$

Note that this is very close to an identity matrix, or a rotation of 0°. Then

$$A_4 = \begin{bmatrix} 1.40818 & & -0.0140292 \\ & 0.122327 & .000161188 \\ -0.0140292 & .000161188 & 0.0028276 \end{bmatrix}$$

etc. In the limit we get

$$A_\infty = \begin{bmatrix} 1.40832 & & \\ & 0.122327 & \\ & & 0.00268735 \end{bmatrix}$$

There are some observations which can make this business a bit faster, but until you have tried a few yourself they won't make much sense.

(•) Suppose at some step we are about to make zero the entries $a_{i,j} = a_{j,i}$ where $i > j$. Then we first make up a 2×2 matrix

$$\begin{bmatrix} a_{j,j} & a_{j,i} \\ a_{i,j} & a_{i,i} \end{bmatrix}$$

and diagonalize it by means of some 2×2 matrix

$$\chi = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$$

which we then make into an $n \times n$ matrix by embedding χ into the four places where rows and columns i, j intersect. We then multiply X on the left of A and X^{-1} on the right. There is no serious objection to just

multiplying these out in the straightforward way, but a great deal of work can be saved through the following observations: (♠) when we multiply on the left by X, only rows j and i are affected. To be precise, the entries $x_{j,\ell}$, $x_{i,\ell}$ are replaced by the coordinates of the two dimensional vector we get by rotating it, which is

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} x_{j,\ell} \\ x_{i,\ell} \end{bmatrix}$$

Furthermore, we don't have to make this calculation for $\ell = i$ or $\ell = j$, since we know how these entries will wind up. For $n = 3$, for example, we have just a single two dimensional rotation to calculate. (♣) When we multiply on the right by X^{-1}, we only affect the columns i and j. But here we know in advance what we are going to get, because we know the final result is going to be symmetric. So instead of actually performing these calculations, we can just copy across the diagonal the entries we have already calculated. For 3×3, for example, suppose $j = 1$, $i = 2$. Then we just set

$$a_{1,1} = \lambda_1, \quad a_{2,2} = \lambda_2, \quad a_{1,2} = a_{2,1} = 0$$

Then we calculate

$$\begin{bmatrix} a_{1,3} \\ a_{2,3} \end{bmatrix} := \begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} a_{1,3} \\ a_{2,3} \end{bmatrix}$$

and finally set

$$a_{3,1} = a_{1,3}, \quad a_{3,2} = a_{2,3}$$

(•) How to get the matrix X? We have

$$X = \ldots X_3 X_2 X_1 X_0$$

Again, keep in mind that the eigenvectors of the original A are the *rows* of X, not its columns.

(•) Why does it work? At each stage consider the sum of the squares of the off-diagonal entries

$$\sigma_n = \sum_{i<j} a_{i,j}^2$$

Then in going from one stage to the next we kill one of the off-daigonal entries a_{i_n,j_n}. Then

$$\sigma_{n+1} = \sigma_n - a_{i_n,j_n}^2$$

Thus σ_n decreases by a known amount in each stage, and it turns out that this does the trick. Why is this identity tue? Precisely because, as I mentioned a moment ago, multiplying by X_i amounts to rotating the rows of A. This concerns only off-diagonal entries, except at one place, where we just mae the off diagonal entry 0. But rotation preserves the sums of squares of these pairs, so the change in the total sum of squares of off-diagonal enttries is just to subtract the entries made 0.