Linear Eigenvalue Equations

PHYSICS 598 CPA : Problem Set 8

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1 Eigenvalues of a tridiagonal matrix

The `tred2` and `tqli` routines in the Numerical Recipes are used for calculating the eigenvalues of the matrix. The `tred2` routine returns the transformation matrix **Q** which is orthogonal, and it is used in the QL algorithm in the `tqli` routine. After that, the eigenvalues of the matrix computed by numerical method are resulted. The numerical and analytic results are compared (see the table at the back), the relative errors between the two results are also listed. As the `double` precision is used in the calculation, and the language `C` is used, the relative error is controlled at $\sim 10^{-14}$.

2 Coupled harmonic oscillator

2.1 Equation of motion

Since the two ends of the spring are attached to a wall, the displacement of those two ends must be 0. (i.e. $x_0 = x_{n+1} = 0$)

For the points $1 \leq j \leq n$, take the direction towards the $(n+1)$-th particle be positive. The resultant force acting on the j-th particle is:

$$\begin{aligned} F_j = m\ddot{x}_j &= K\left(x_j - x_{j+1}\right) + K\left(-x_j + x_{j-1}\right) \\ \Rightarrow m\ddot{x}_j &= K\left(x_{j-1} - 2x_j + x_{j+1}\right) \end{aligned} \tag{1}$$

2.2 Eigenvalue equation for the normal modes of oscillation

Let $x_j = X_j e^{i\omega t}$, where X_j is the amplitude of the displacement. Then $\ddot{x}_j = -\omega^2 X_j e^{i\omega t}$. Plug into Eqn. (1):

$$\begin{aligned} m\left(-\omega^2 X_j e^{i\omega t}\right) &= K\left(X_{j-1} - 2X_j + X_{j+1}\right)e^{i\omega t} \\ \Rightarrow -\frac{K}{m}X_{j-1} + \left(\frac{2K}{m} - \omega^2\right)X_j - \frac{K}{m}X_{j+1} &= 0 \end{aligned} \tag{2}$$

2.3 Numerical routine

For $n = 2$, then $x_0 = x_3 = 0$. Also, set $K = m = 1$, then ω^2 possesses the unit of K/m. The equations of motion become:

$$\begin{aligned} 2X_1 - X_2 &= \omega^2 X_1 \\ -X_1 + 2X_2 &= \omega^2 X_2 \end{aligned}$$

In matrix representation:

$$\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \omega^2 \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$$

This is equivalent to finding the eigenvalues and eigenvectors of the matrix equations. Solving analytically:

$$\begin{vmatrix} 2-\omega^2 & -1 \\ -1 & 2-\omega^2 \end{vmatrix} = 0$$

$$\begin{aligned} \left(2-\omega^2\right)^2 - 1 &= 0 \\ \left(3-\omega^2\right)\left(1-\omega^2\right) &= 0 \\ \omega^2 &= 3 \text{ or } 1 \end{aligned}$$

Since $\omega \geq 0$, so $\omega = \sqrt{3}$ or 1. For $\omega^2 = 3$ (or $3K/m$) , the equations become:

$$\begin{cases} X_1 + X_2 = 0 \\ X_1 + X_2 = 0 \end{cases}$$

So, a normalized eigenvector would be:

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

For $\omega^2 = 1$ (or K/m), the equations become:

$$\begin{cases} X_1 - X_2 = 0 \\ -X_1 + X_2 = 0 \end{cases}$$

So, a normalized eigenvector would be:

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Using the same routines `tred2` and `tqli` as Q.1., the eigenvalues ω^2 can be found. In fact, the `tqli` routine can also compute the corresponding eigenvectors of those eigenvalues. To check with the analytic solution for the above case, set $N = 2$. From the code, we get two eigenstates.

$$
\begin{aligned}
\omega^2 &= 3, (X_1, X_2) = (-0.707106781186548, 0.707106781186547) \\
\omega^2 &= 1, (X_1, X_2) = (-0.707106781186548, -0.707106781186547)
\end{aligned}
$$

which agree with the analytical result with relative error lower than 10^{-14}, with the sign difference due to the different definition of the normalization factor.

For $N = 32$, the equations of motion of the particles can be written as:

$$
\begin{cases}
2X_1 - X_2 = \omega^2 X_1 \\
-X_1 + 2X_2 - X_3 = \omega^2 X_2 \\
-X_2 + 2X_3 - X_4 = \omega^2 X_3 \\
\qquad\qquad \vdots \\
-X_30 + 2X_31 - X_32 = \omega^2 X_31 \\
-X_31 + 2X_32 = \omega^2 X_32
\end{cases}
$$

In matrix form, it can be written as:

$$
\begin{pmatrix}
2 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
-1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\
0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\
0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\
0 & 0 & 0 & 0 & \cdots & 0 & -1 & 2
\end{pmatrix}
\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ \vdots \\ X_{30} \\ X_{31} \\ X_{32} \end{pmatrix}
= \omega^2
\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ \vdots \\ X_{30} \\ X_{31} \\ X_{32} \end{pmatrix}
$$

It is exactly the same matrix equation as Q.1., with $N = 32$, and $\omega^2 = \lambda_n$. The normalization factor A is calculated by:

$$
A^2 = \left[\sum_{j=1}^{N} \sin^2 \left(j \frac{r\pi}{n+1} \right) \right]^{-1} \tag{3}
$$

Again, the numerical and analytical eigenvalues agree with each other with error lower than 10^{-14}. For the eigenvectors, they generally agree with that accuracy as well, except for the extremely small value of X_{jr}'s, with values $\leq 10^{-16}$, do they not agree quite well. It is due to the round up error resulted from two large numbers subtracting each other, yielding an inaccurate estimate of a small number.