

The eigenvalues and eigenvectors of a tridiagonal Toeplitz matrix

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Introduction

An $N \times N$ matrix A_N is **tridiagonal** when only the main diagonal and the two diagonals immediately surrounding it have non-zero elements, that is, a matrix for which

$$(A_N)_{ij} = 0 \quad \text{if} \quad |i - j| > 1 \quad \text{for} \quad 1 \leq i \leq N \quad \text{and} \quad 1 \leq j \leq N.$$

An $N \times N$ tridiagonal matrix has at most $(3N - 2)$ non-zero elements. For example, the 4×4 matrix below is tridiagonal:

$$\begin{pmatrix} a & b & 0 & 0 \\ c & d & e & 0 \\ 0 & f & g & h \\ 0 & 0 & i & j \end{pmatrix}.$$

An $N \times N$ matrix A_N is **Toeplitz** when elements in each diagonal are all the same, although possibly different between diagonals, that is, a matrix for which

$$(A_N)_{j+k,j} = c_k \quad \text{for} \quad |k| < N \quad \text{and} \quad 1 \leq j + k \leq N, \quad 1 \leq j \leq N,$$

where the c_k values are arbitrary. It has at most $(2N - 1)$ non-zero elements. For example, the 4×4 matrix below is Toeplitz:

$$\begin{pmatrix} a & b & c & d \\ e & a & b & c \\ f & e & a & b \\ g & f & e & a \end{pmatrix}.$$

An $N \times N$ matrix A_N that is both tridiagonal **and** Toeplitz is then fully characterized by at most 3 non-zero values so it stands to reason that its eigenvalues and eigenvectors

should be relatively easy to find. The 4×4 matrix below is an example of a matrix that is both tridiagonal and Toeplitz:

$$\begin{pmatrix} a & b & 0 & 0 \\ c & a & b & 0 \\ 0 & c & a & b \\ 0 & 0 & c & a \end{pmatrix}.$$

The eigenvalues of A_N

We want to solve the eigenvalue problem for a matrix A_N that is both tridiagonal and Toeplitz, that is, we want to find the set of constants $\lambda_{N,n}$ and column vectors $u_{N,n}$ such that

$$A_N u_{N,n} = \lambda_{N,n} u_{N,n},$$

for $1 \leq n \leq N$. The eigenvalues are the N roots of A_N 's *characteristic polynomial*, a polynomial of order N obtained by setting the determinant of $(A_N - \lambda I_N)$ to zero, where I_N is the $N \times N$ identity matrix. Now,

$$\Delta_N(\lambda) \equiv \det(A_N - \lambda I_N) = \begin{vmatrix} (a-\lambda) & b & 0 & 0 & \cdots & 0 \\ c & (a-\lambda) & b & 0 & \cdots & 0 \\ 0 & c & (a-\lambda) & b & \cdots & 0 \\ 0 & 0 & c & (a-\lambda) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & c & (a-\lambda) \end{vmatrix}$$

is an $N \times N$ determinant. We can compute it by using Laplace's method of expansion in cofactors. Defining

$$\alpha \equiv (a - \lambda)$$

and using the last column as our base column, we have:

$$\Delta_N = \boxed{\alpha} (-1)^{N+N} \begin{vmatrix} \alpha & b & 0 & \cdots & 0 & \mathbf{0} \\ c & \alpha & b & \cdots & 0 & \mathbf{0} \\ 0 & c & \alpha & \cdots & 0 & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha & \mathbf{b} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{c} & \boxed{\alpha} \end{vmatrix} + \boxed{b} (-1)^{(N-1)+N} \begin{vmatrix} \alpha & b & 0 & \cdots & 0 & \mathbf{0} \\ c & \alpha & b & \cdots & 0 & \mathbf{0} \\ 0 & c & \alpha & \cdots & 0 & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \alpha & \boxed{b} \\ 0 & 0 & 0 & \cdots & c & \alpha \end{vmatrix},$$

where bold rows and columns are to be removed from the matrix whose determinant is being computed. The first determinant above is clearly just Δ_{N-1} . Thus,

$$\Delta_N = \alpha \Delta_{N-1} - \boxed{b} \begin{vmatrix} \alpha & b & 0 & \cdots & 0 & \mathbf{0} \\ c & \alpha & b & \cdots & 0 & \mathbf{0} \\ 0 & c & \alpha & \cdots & 0 & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \alpha & \boxed{b} \\ 0 & 0 & 0 & \cdots & c & \alpha \end{vmatrix} = \alpha \Delta_{N-1} - b \begin{vmatrix} \alpha & b & 0 & \cdots & 0 & 0 \\ c & \alpha & b & \cdots & 0 & 0 \\ 0 & c & \alpha & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha & b \\ 0 & 0 & 0 & \cdots & 0 & c \end{vmatrix},$$

The remaining $(N-1) \times (N-1)$ determinant can be computed by another pass of Laplace's method, so:

$$\begin{aligned} \Delta_N &= \alpha \Delta_{N-1} - b \boxed{c} (-1)^{(N-1)+(N-1)} \begin{vmatrix} \alpha & b & 0 & \cdots & 0 & \mathbf{0} \\ c & \alpha & b & \cdots & 0 & \mathbf{0} \\ 0 & c & \alpha & \cdots & 0 & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha & \mathbf{b} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \boxed{c} \end{vmatrix} \\ &\quad - b \boxed{b} (-1)^{(N-2)+(N-1)} \begin{vmatrix} \alpha & b & 0 & \cdots & 0 & \mathbf{0} \\ c & \alpha & b & \cdots & 0 & \mathbf{0} \\ 0 & c & \alpha & \cdots & 0 & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \alpha & \boxed{b} \\ 0 & 0 & 0 & \cdots & 0 & c \end{vmatrix}. \end{aligned}$$

The first determinant shown explicitly is clearly Δ_{N-2} and the second is clearly zero, since its last row contains only zeros. Therefore,

$$\Delta_N = \alpha \Delta_{N-1} - bc \Delta_{N-2}.$$

This recurrence relation lets us find Δ_N given its previous values but we need two consecutive starting values. Clearly,

$$\Delta_1 = \alpha \quad \text{and} \quad \Delta_2 = \alpha^2 - bc.$$

In fact, the recurrence is also valid for $N = 0$ if we set $\Delta_0 = 1$. Thus,

$$\Delta_N = \begin{cases} 1 & \text{if } N = 0 \\ \alpha & \text{if } N = 1 \\ \alpha \Delta_{N-1} - bc \Delta_{N-2} & \text{if } N > 1 \end{cases}.$$

Generating functions

Suppose we define a function $f(\xi)$ by a formal power series with coefficients equal to the Δ_N values:

$$f(\xi) \equiv \sum_{n=0}^{\infty} \Delta_n \xi^n.$$

If we can somehow find a closed form for this function, then we can recover the Δ_n values by expanding $f(\xi)$ in a Taylor series around $\xi = 0$:

$$f(\xi) = f(0) + f'(0)\xi + \frac{f''(0)}{2}\xi^2 + \dots = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \xi^n$$

which shows that $\Delta_n = f^{(n)}(0)/n!$. Such a function $f(\xi)$ is called a *generating function* for the recurrence relation in question. In order to find a closed form for it, we start with its definition and make use of the recurrence relation for Δ_n :

$$\begin{aligned} f(\xi) &= \sum_{n=0}^{\infty} \Delta_n \xi^n = \Delta_0 + \Delta_1 \xi + \sum_{n=2}^{\infty} \Delta_n \xi^n \\ &= 1 + \alpha \xi + \sum_{n=0}^{\infty} \Delta_{n+2} \xi^{n+2} \\ &= 1 + \alpha \xi + \sum_{n=0}^{\infty} \left[\alpha \Delta_{n+1} - bc \Delta_n \right] \xi^{n+2} \\ &= 1 + \alpha \xi + \alpha \xi \sum_{n=0}^{\infty} \Delta_{n+1} \xi^{n+1} - bc \xi^2 \sum_{n=0}^{\infty} \Delta_n \xi^n \\ &= 1 + \alpha \xi + \alpha \xi \left[f(\xi) - \Delta_0 \right] - bc \xi^2 f(\xi). \end{aligned}$$

Thus, $f(\xi) = 1 + \alpha \xi f(\xi) - bc \xi^2 f(\xi)$ or, more simply,

$$f(\xi) = \frac{1}{bc \xi^2 - \alpha \xi + 1}.$$

Therefore,

$$\Delta_n = \frac{1}{n!} \frac{d^n}{d\xi^n} \left[\frac{1}{bc \xi^2 - \alpha \xi + 1} \right] \Bigg|_{\xi=0}.$$

Expanding this n -th derivative is far too complicated as it stands but we can use yet another trick. Suppose we can write $f(\xi)$ as follows:

$$f(\xi) = \frac{1}{bc \xi^2 - \alpha \xi + 1} = \frac{(bc)^{-1}}{\xi^2 - \alpha (bc)^{-1} \xi + (bc)^{-1}} = \frac{R}{\xi - r} + \frac{S}{\xi - s}$$

for some as-yet-undetermined constants R , r , S , and s . The n -th derivative then becomes trivial. Finding the constants is very simple:

$$\frac{(bc)^{-1}}{\xi^2 - \alpha(bc)^{-1}\xi + (bc)^{-1}} = \frac{R}{\xi - r} + \frac{S}{\xi - s} = \frac{R(\xi - s) + S(\xi - r)}{(\xi - r)(\xi - s)} = \frac{(R + S)\xi - (Rs + Sr)}{(\xi - r)(\xi - s)},$$

which imply $R + S = 0$ and $Rs + Sr = -(bc)^{-1}$. Thus, $R = -S = (bc)^{-1}(r - s)^{-1}$ and

$$f(\xi) = \frac{1}{bc\xi^2 - \alpha\xi + 1} = \frac{1}{bc(r - s)} \left[\frac{1}{\xi - r} - \frac{1}{\xi - s} \right],$$

provided that r and s are the roots of $\xi^2 - \alpha(bc)^{-1}\xi + (bc)^{-1} = 0$, that is,

$$r = \frac{1}{2bc}(\alpha + \sqrt{\alpha^2 - 4bc}) \quad \text{and} \quad s = \frac{1}{2bc}(\alpha - \sqrt{\alpha^2 - 4bc}).$$

Note that $rs = (bc)^{-1}$ and $(r - s) = (bc)^{-1}\sqrt{\alpha^2 - 4bc}$. Now that we have $f(\xi)$ written in terms of something easier to find multiple derivatives for, we find:

$$\begin{aligned} \Delta_n &= \frac{(bc)^{-1}(r - s)^{-1}}{n!} \frac{d^n}{d\xi^n} \left[(\xi - r)^{-1} - (\xi - s)^{-1} \right] \Big|_{\xi=0} \\ &= \frac{(bc)^{-1}(r - s)^{-1}}{n!} \left[(-1)^n n! (\xi - r)^{-(n+1)} - (-1)^n n! (\xi - s)^{-(n+1)} \right] \Big|_{\xi=0} \\ &= \frac{1}{bc(r - s)} \left[\frac{1}{s^{(n+1)}} - \frac{1}{r^{(n+1)}} \right] = \frac{r^{(n+1)} - s^{(n+1)}}{bc(r - s)(rs)^{(n+1)}} = (bc)^n \left[\frac{r^{(n+1)} - s^{(n+1)}}{(r - s)} \right]. \end{aligned}$$

We've implicitly assumed that $bc \neq 0$, so the eigenvalues of A_N are then given by the roots of $\delta_N(\lambda) = 0$ where

$$\delta_N(\lambda) = \frac{\Delta_N}{(bc)^N} = \frac{r^{(N+1)} - s^{(N+1)}}{(r - s)}.$$

Note that neither r nor s is ever equal to zero. Also, $(r - s) = 0$ only if $\alpha = \pm 2\sqrt{bc}$, that is, only when $\lambda = a \pm 2\sqrt{bc}$. Thus, since

$$\lim_{s \rightarrow r} \delta_N(\lambda) = (N + 1) \lim_{\alpha \rightarrow \pm 2\sqrt{bc}} r^N = (\pm\sqrt{bc})^{-N}(N + 1) \neq 0,$$

we conclude that $\lambda = a \pm 2\sqrt{bc}$ is not a root of $\Delta_N(\lambda) = 0$, for any value of N , so we may assume $r \neq s$. The roots of $\delta_N(\lambda) = 0$ then require that

$$r^{(N+1)} - s^{(N+1)} = 0 \quad \text{or, more simply,} \quad \left(\frac{r}{s} \right)^{N+1} = 1.$$

The only way for this equation to be satisfied with $r \neq s$ is for r and s to be complex numbers. Then, using the fact that $rs = (bc)^{-1}$, we have

$$r^{(N+1)} - s^{(N+1)} = 0 \quad \Rightarrow \quad \left(\frac{r}{s}\right)^{N+1} = (bcr^2)^{N+1} = e^{2\pi n i} \quad \text{where} \quad n \in \mathcal{Z},$$

which has the solution $r^2 = (bc)^{-1} e^{2\pi n i/(N+1)}$, with $1 \leq n \leq N$. This, in turn, can be solved for λ , resulting in the N values:

$$\boxed{\lambda_n = a + 2\sqrt{bc} \cos\left(\frac{n\pi}{N+1}\right), \quad 1 \leq n \leq N.}$$

The eigenvectors of A_N

We now want to find the set of eigenvectors associated with A_N 's eigenvalues, that is, we want to find the set of (column) vectors $\{u_n \mid 1 \leq n \leq N\}$ such that

$$A_N u_n = \lambda_n u_n,$$

for each n . Since multiples of eigenvectors are also eigenvectors, we can arbitrarily choose one component of each vector, so let's define $u_n \equiv (1, u_{n,2}, u_{n,3}, \dots, u_{n,N})^t$. Thus,

$$\begin{aligned} A_N u_n = \lambda_n u_n \quad \Rightarrow \quad \begin{aligned} u_{n,1} &= 1 \\ b u_{n,2} &= (\lambda_n - a) \\ b u_{n,3} &= (\lambda_n - a) u_{n,2} - c \\ b u_{n,4} &= (\lambda_n - a) u_{n,3} - c u_{n,2} \\ &\vdots \\ b u_{n,N} &= (\lambda_n - a) u_{n,N-1} - c u_{n,N-2} \\ (\lambda_n - a) u_{n,N} &= c u_{n,N-1}. \end{aligned} \end{aligned}$$

Excluding the last equation, which can be ignored because the procedure to obtain the eigenvalues has already accounted for it, these are identical in form to the recurrence relation obtained earlier, that is,

$$u_{n,k} = \begin{cases} 1 & \text{if } k = 1 \\ \alpha_n/b & \text{if } k = 2 \\ (\alpha_n/b) u_{n,k-1} - (c/b) u_{n,k-2} & \text{if } k > 2 \end{cases} \quad \text{where} \quad \alpha_n = (\lambda_n - a) \quad \text{and} \quad 1 < k \leq N.$$

We, therefore, proceed just as before, defining a generating function for each eigenvector,

$$f_n(\xi) \equiv \sum_{k=1}^{\infty} u_{n,k} \xi^k = f'_n(0) \xi + \frac{f''_n(0)}{2} \xi^2 + \dots = \sum_{k=1}^{\infty} \frac{f_n^{(k)}(0)}{k!} \xi^k$$

so that $u_{n,k} = f_n^{(k)}(0)/k!$. Then,

$$f_n(\xi) = \frac{(b/c)\xi}{\xi^2 - (\alpha_n/c)\xi + (b/c)} = \frac{(b/c)}{(r-s)} \left[\frac{r}{\xi-r} - \frac{s}{\xi-s} \right],$$

provided that r and s are now the roots of $\xi^2 - (\alpha_n/c)\xi + (b/c) = 0$, that is,

$$r = \frac{1}{2c}(\alpha_n + \sqrt{\alpha_n^2 - 4bc}) \quad \text{and} \quad s = \frac{1}{2c}(\alpha_n - \sqrt{\alpha_n^2 - 4bc}).$$

Note that

$$\alpha_n = \lambda_n - a = 2\sqrt{bc} \cos\left(\frac{n\pi}{N+1}\right)$$

so

$$\alpha_n^2 - 4bc = -4bc \sin^2\left(\frac{n\pi}{N+1}\right)$$

and

$$r = \sqrt{\frac{b}{c}} \exp\left(+i\frac{n\pi}{N+1}\right) \quad \text{and} \quad s = \sqrt{\frac{b}{c}} \exp\left(-i\frac{n\pi}{N+1}\right).$$

Then,

$$u_{n,k} = \frac{f_n^{(k)}(0)}{k!} = \frac{(b/c)}{(rs)^k} \left(\frac{r^k - s^k}{r - s} \right) = \left(\frac{c}{b} \right)^{(k-1)/2} \frac{\sin\left(\frac{kn\pi}{N+1}\right)}{\sin\left(\frac{n\pi}{N+1}\right)}.$$

We may now normalize these eigenvectors, resulting in

$$u_{n,k} = \frac{\left(\frac{c}{b}\right)^{(k-1)/2} \sin\left(\frac{kn\pi}{N+1}\right)}{\sqrt{\sum_{r=1}^N \left(\frac{c}{b}\right)^{(r-1)} \sin^2\left(\frac{rn\pi}{N+1}\right)}} \quad \text{where} \quad 1 \leq n \leq N \quad \text{and} \quad 1 \leq k \leq N.$$

Note, however, that

$$\begin{aligned} \sum_{r=1}^N \left(\frac{c}{b}\right)^{(r-1)} \sin^2\left(\frac{rn\pi}{N+1}\right) &= \sum_{r=1}^N \beta^{r-1} \sin^2(\gamma r) \quad \left(\beta \equiv \frac{c}{b}, \quad \gamma \equiv \frac{n\pi}{N+1}\right) \\ &= \sum_{r=1}^N \beta^{r-1} \left(\frac{e^{i\gamma r} - e^{-i\gamma r}}{2i} \right)^2 = \sum_{r=1}^N \beta^{r-1} \left(\frac{2 - e^{2i\gamma r} - e^{-2i\gamma r}}{4} \right) \\ &= \frac{1}{2\beta} \sum_{r=1}^N \beta^r - \frac{1}{4\beta} \sum_{r=1}^N \beta^r (e^{2i\gamma r} + e^{-2i\gamma r}) \\ &= \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) - \frac{1}{4\beta} \sum_{r=1}^N \left(\beta e^{+2i\gamma} \right)^r - \frac{1}{4\beta} \sum_{r=1}^N \left(\beta e^{-2i\gamma} \right)^r \end{aligned}$$

Now,

$$\sum_{r=1}^N \left(\beta e^{2i\gamma} \right)^r = \left(\beta e^{2i\gamma} \right) \left[\frac{\beta^N e^{2iN\gamma} - 1}{\beta e^{2i\gamma} - 1} \right]$$

so

$$\begin{aligned} & \sum_{r=1}^N \left(\frac{c}{b} \right)^{(r-1)} \sin^2 \left(\frac{rn\pi}{N+1} \right) = \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) - \frac{1}{4\beta} \sum_{r=1}^N \left(\beta e^{+2i\gamma} \right)^r - \frac{1}{4\beta} \sum_{r=1}^N \left(\beta e^{-2i\gamma} \right)^r \\ &= \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) - \frac{1}{4} \left\{ \frac{e^{+2i\gamma} (\beta^N e^{+2iN\gamma} - 1)}{(\beta e^{+2i\gamma} - 1)} + \frac{e^{-2i\gamma} (\beta^N e^{-2iN\gamma} - 1)}{(\beta e^{-2i\gamma} - 1)} \right\} \\ &= \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) - \frac{1}{4} \left\{ \frac{e^{+2i\gamma} (\beta^N e^{+2iN\gamma} - 1) (\beta e^{-2i\gamma} - 1) + e^{-2i\gamma} (\beta^N e^{-2iN\gamma} - 1) (\beta e^{+2i\gamma} - 1)}{(\beta e^{+2i\gamma} - 1) (\beta e^{-2i\gamma} - 1)} \right\} \\ &= \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) - \frac{1}{2} \left\{ \frac{\beta^{N+1} \cos(2N\gamma) - \beta^N \cos[2(N+1)\gamma] - \beta + \cos(2\gamma)}{\beta^2 - 2\beta \cos(2\gamma) + 1} \right\} \\ &= \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) - \frac{1}{2} \left\{ \frac{\beta^{N+1} \cos[2(N+1)\gamma - 2\gamma] - \beta^N \cos[2(N+1)\gamma] - \beta + \cos(2\gamma)}{\beta^2 - 2\beta \cos(2\gamma) + 1} \right\} \\ &= \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) + \frac{1}{2} \left\{ \frac{\beta(\beta^{N-1} + 1) - (\beta^{N+1} + 1) \cos(2\gamma)}{\beta^2 - 2\beta \cos(2\gamma) + 1} \right\} \end{aligned}$$

The **normalized eigenvectors** are, then, given by

$$\begin{aligned} u_{n,k} &= \frac{1}{\sqrt{\Phi_n}} \beta^{(k-1)/2} \sin(k\gamma_n) \\ \Phi_n &\equiv \frac{1}{2} \left(\frac{\beta^N - 1}{\beta - 1} \right) + \frac{1}{2} \left\{ \frac{\beta(\beta^{N-1} + 1) - (\beta^{N+1} + 1) \cos(2\gamma_n)}{\beta^2 - 2\beta \cos(2\gamma_n) + 1} \right\} \quad \text{where} \\ \beta &\equiv \frac{c}{b}, \quad \gamma_n \equiv \frac{n\pi}{N+1}, \quad 1 \leq n \leq N, \quad \text{and} \quad 1 \leq k \leq N. \end{aligned}$$

Note that $\Phi_n = (N+1)/2$ when $\beta = c/b = 1$, that is, when the matrix is symmetric. ■