Some analytic expressions for symmetric tridiagonal and pentadiagonal matrices

In the course of learning a bit about compact finite differences, I discovered a couple of papers that provide analytic expressions for the determinants and inverses of a few specialized tridiagonal matrices. I wanted to understand this and see if I could reproduce it for symmetric, pentadiagonal matrices as well as generalized versions.

Consider the following $k \times k$, symmetric, tridiagonal matrix

$$M = \begin{pmatrix} D & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 1 & D & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & D & 1 & \cdots & 0 & 0 & 0 & 0 \\ & \vdots & & & \vdots & & & \vdots & \\ 0 & 0 & 0 & 0 & \cdots & 1 & D & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & D & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & D \end{pmatrix}$$

where D is a constant and sits only on the diagonal. We will refer to the determinant of this matrix as M_k. It can be shown that M_k satisfies the three term recursion relation

$$M_k = D\, M_{k-1} - M_{k-2}$$

with "initial conditions" $M_0 = 1$ and $M_1 = D$. This recursion relation can be solved by setting $M_k = r^k$ and finding the roots of

$$0 = r^k - D\, r^{k-1} + r^{k-2}$$

or

$$0 = r^2 - Dr + 1$$

which has solutions

$$r_\pm = \frac{1}{2}\, D \pm \frac{1}{2}\sqrt{D^2 - 4}$$

Thus, we can write for M_k

$$M_k = A\, r_+^k + B\, r_-^k$$

where, from the initial conditions,

$$A = \frac{D + \sqrt{D^2 - 4}}{2\sqrt{D^2 - 4}}$$

$$B = \frac{-D + \sqrt{D^2 - 4}}{2\sqrt{D^2 - 4}}$$

so

$$M_k = \frac{1}{2^{k+1}}\, \frac{1}{\sqrt{D^2 - 4}} \left[\left(D + \sqrt{D^2 - 4}\right)^{k+1} - \left(D - \sqrt{D^2 - 4}\right)^{k+1} \right]$$

Reparameterizing D, we set

$$D = \begin{cases} -2\cosh\lambda & D \leq -2 \\ 2\,\cos\lambda & |D| < 2 \\ 2\cosh\lambda & D \geq 2 \end{cases}$$

It can then be shown that

$$M_k = \begin{cases} \dfrac{(-1)^k \sinh\big((k+1)\lambda\big)}{\sinh\lambda} & D \leq -2 \\ \dfrac{\sin\big((k+1)\lambda\big)}{\sin\lambda} & |D| < 2 \\ \dfrac{\sinh\big((k+1)\lambda\big)}{\sinh\lambda} & D \geq 2 \end{cases}$$

With the determinant in hand, we can now try to find the exact form of the inverse of this matrix as well. Recall that the inverse can be given in terms of the cofactor expansion. More particularly, if we have a (nonsingular) $k \times k$ matrix, A, the inverse, A^{-1}, is given by $\mathrm{adj(A)}/\det(\mathrm{A})$ where adj(A) is the adjoint or adjugate matrix. The adjoint matrix, in turn, is the transpose of the cofactor matrix, C:

$$\mathrm{adj}(A) = C^T$$

and the cofactor matrix, C, is made from the cofactors of A. If the elements of A are given by a_{ij}, the elements, c_{ij}, of C are found by calculating the determinant of the $(k-1) \times (k-1)$ matrix formed by taking A and striking out the i^{th} row and j^{th} column (and multiplying by $(-1)^{i+j}$).

In our current case, one can show that the cofactor matrix is symmetric and that its elements can be written as

$$c_{ij} = (-1)^{i+j} M_{i-1} M_{k-j} \quad i \leq j$$

Using the above relation for M_k, we have for the inverse of M

$$\begin{aligned}
(M^{-1})_{ij}\Big|_{i \leq j} &= \frac{c_{ij}}{M_k} \\
&= (-1)^{i+j} \frac{M_{i-1} M_{k-j}}{M_k} \\
&= \begin{cases} -\dfrac{\sinh(i\lambda)\, \sinh[(k+1-j)\lambda]}{\sinh\lambda\, \sinh[(k+1)\lambda]} & D \leq -2 \\ (-1)^{i+j} \dfrac{\sin(i\lambda)\, \sin[(k+1-j)\lambda]}{\sin\lambda\, \sin[(k+1)\lambda]} & |D| < 2 \\ (-1)^{i+j} \dfrac{\sinh(i\lambda)\, \sinh[(k+1-j)\lambda]}{\sinh\lambda\, \sinh[(k+1)\lambda]} & D \geq 2 \end{cases} \\
&= \begin{cases} -\dfrac{\cosh[(k+1-j+i)\lambda] - \cosh[(k+1-j-i)\lambda]}{2\sinh\lambda\, \sinh[(k+1)\lambda]} & D \leq -2 \\ (-1)^{i+j+1} \dfrac{\cos[(k+1-j+i)\lambda] - \cos[(k+1-j-i)\lambda]}{2\sin\lambda\, \sin[(k+1)\lambda]} & |D| < 2 \\ (-1)^{i+j} \dfrac{\cosh[(k+1-j+i)\lambda] - \cosh[(k+1-j-i)\lambda]}{2\sinh\lambda\, \sinh[(k+1)\lambda]} & D \geq 2 \end{cases}
\end{aligned}$$

If we want the case that $i > j$, then we can simply swap i and j in the above expressions. However, to write a general expression, we have to recognize a subtlety associated with using finite ranges in i and j by invoking an absolute value, namely

$$(M^{-1})_{ij} = \begin{cases} -\dfrac{\cosh[(k+1-|j-i|)\lambda] - \cosh[(k+1-j-i)\lambda]}{2\sinh\lambda\, \sinh[(k+1)\lambda]} & D \leq -2 \\ (-1)^{i+j+1} \dfrac{\cos[(k+1-|j-i|)\lambda] - \cos[(k+1-j-i)\lambda]}{2\sin\lambda\, \sin[(k+1)\lambda]} & |D| < 2 \\ (-1)^{i+j} \dfrac{\cosh[(k+1-|j-i|)\lambda] - \cosh[(k+1-j-i)\lambda]}{2\sinh\lambda\, \sinh[(k+1)\lambda]} & D \geq 2 \end{cases}$$

This, then, is the exact inverse of our tridiagonal matrix for any real value of D.

"Periodic" boundaries

Of course, the last matrix can be understood as the difference approximation of a derivative of a function. But the first and last rows will not be the same (or even correct) difference approximations. However, if we were to assume a function with periodic boundary conditions, our matrix would become

$$\tilde{M} = \begin{pmatrix} D & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 \\ 1 & D & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & D & 1 & \cdots & 0 & 0 & 0 & 0 \\ & \vdots & & & \vdots & & & \vdots & \\ 0 & 0 & 0 & 0 & \cdots & 1 & D & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & D & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & D \end{pmatrix}$$

This becomes a new matrix whose determinant is clearly related to M_k. Indeed, one can show that $\tilde{M}_k \equiv \det(\tilde{M})$ can be written as

$$\tilde{M}_k = DM_{k-1} - 2M_{k-2} + 2(-1)^{k+1}$$

Using our previous results, it can then be shown that

$$\tilde{M}_k = \begin{cases} 2(-1)^k\big[1-\cosh(k\lambda)\big] & D \le -2 \\ 2\big[(-1)^{k+1}+\cos(k\lambda)\big] & |D| < 2 \\ 2\big[(-1)^{k+1}+\cosh(k\lambda)\big] & D \ge 2 \end{cases}$$

The cofactors needed for the inverse take the form

$$c_{ij}\Big|_{i\le j} = (-1)^{i+j}\Big[M_{i-1}M_{k-j} - M_{i-2}M_{k-1-j} + (-1)^k M_{j-i-1}\Big]$$

The corresponding inverse takes the form

$$(\tilde{M}^{-1})_{ij} = \begin{cases} \dfrac{(-1)^{k+1}}{2\sinh\lambda}\,\dfrac{\sinh[(k-|j-i|)\lambda]+\sinh[|j-i|\lambda]}{1-\cosh(k\lambda)} & D \le -2 \\ \dfrac{(-1)^{i+j}}{2\sin\lambda}\,\dfrac{\sin[(k-|j-i|)\lambda]+(-1)^k\sin[|j-i|\lambda]}{(-1)^{k+1}+\cos(k\lambda)} & |D| < 2 \\ \dfrac{(-1)^{i+j}}{2\sinh\lambda}\,\dfrac{\sinh[(k-|j-i|)\lambda]+(-1)^k\sinh[|j-i|\lambda]}{(-1)^{k+1}+\cosh(k\lambda)} & D \ge 2 \end{cases}$$

A pentadiagonal system

We want to extend the previous analysis to systems more complicated than a tridiagonal system. To begin, let us try with a $k \times k$, symmetric, pentadiagonal matrix of the form

$$N = \begin{pmatrix} D & a & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ a & D & a & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & a & D & a & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & a & D & a & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ & \vdots & & & \vdots & & & \vdots & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & a & D & a & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & a & D & a & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & a & D & a \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & a & D \end{pmatrix}$$

where a and D are real numbers. Unsurprisingly, the determinant, $\det N \equiv N_k$, is more complicated. Doing the straightforward evaluation requires evaluating a new determinant, S_k, of a (secondary?) matrix given by

$$S = \begin{pmatrix} a & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ a & D & a & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & a & D & a & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & a & D & a & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 \\ & \vdots & & & \vdots & & & \vdots & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & a & D & a & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & a & D & a & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & a & D & a \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & a & D \end{pmatrix}$$

where, clearly, the first row and first column are different from the matrix N. The remainder of S, of course, is otherwise identical and the corresponding determinant, S_k, will be related to N_k. Indeed, with a little work, one can show that the recursion relation now takes the form of a coupled system

$$\begin{aligned} N_k &= D(N_{k-1} - N_{k-3}) - a(S_{k-1} - S_{k-2}) + N_{k-4} \\ S_k &= aN_{k-1} - S_{k-1} \end{aligned}$$

These can be uncoupled to yield

$$0 = N_k - (D-1)N_{k-1} - (D-a^2)N_{k-2} + (D-a^2)N_{k-3} + (D-1)N_{k-4} - N_{k-5}$$

and, surprisingly (at least to me), S_k satisfies exactly the same equation. We can solve this by substituting $N_k = r^k$ and rewriting the resulting fifth order polynomial in r:

$$0 = r^5 - (D-1)r^4 - (D-a^2)r^3 + (D-a^2)r^2 + (D-1)r - 1$$

There is, of course, no "quintic" formula, but we nonetheless would like to solve this. To that end, we first note that $r = 1$ is a solution of the equation. Dividing out this solution, we reduce the polynomial by one degree and get

$$0 = r^4 + (2-D)r^3 + (2-2D+a^2)r^2 + (2-D)r + 1$$

This looks daunting, but Mathematica is able to find solutions, namely four simple roots given by

$$\begin{aligned} r_1 &= \frac{1}{4}\left[\alpha - \beta - \sqrt{\gamma - \delta}\right] \\ r_2 &= \frac{1}{4}\left[\alpha - \beta + \sqrt{\gamma - \delta}\right] \\ r_3 &= \frac{1}{4}\left[\alpha + \beta - \sqrt{\gamma + \delta}\right] \\ r_4 &= \frac{1}{4}\left[\alpha + \beta + \sqrt{\gamma + \delta}\right] \end{aligned}$$

where

$$\begin{aligned} \alpha &= D - 2 \\ \beta &= \sqrt{(D+2)^2 - 4a^2} \\ \gamma &= 2(D^2-4) - 4a^2 = \alpha^2 + \beta^2 - 16 \\ \delta &= 2(D-2)\sqrt{(D+2)^2 - 4a^2} = 2\alpha\beta \end{aligned}$$

Curiously, one can show that $r_1 r_2 = 1$ and $r_3 r_4 = 1$, so (in an abuse of notation) we will set $r_1 = r$ and $r_3 = s$. In addition, we have the following observation. We have

$$\sqrt{\gamma \pm \delta} = \sqrt{(\alpha \pm \beta)^2 - 16}$$

which leads to an idea for a reparameterization of the constants as

$$\begin{aligned} \alpha - \beta &= 4\cosh\sigma \\ \alpha + \beta &= 4\cosh\mu \end{aligned}$$

which leads to

$$\begin{aligned} \alpha &= 2(\cosh\sigma + \cosh\mu) \\ \beta &= 2(\cosh\mu - \cosh\sigma) \end{aligned}$$

and

$$\begin{aligned} r &= \cosh\sigma - \sinh\sigma = e^{-\sigma} \\ s &= \cosh\mu - \sinh\mu = e^{-\mu} \end{aligned}$$

With this form, we can write the general solution for the determinant as

$$N_k = A + Br^k + Cr^{-k} + D's^k + Es^{-k}$$

where A, B, C, D' and E are constants that will depend on D and a and can be found from our "initial conditions" as a 5 dimensional system of equations:

$$\begin{aligned}
A + B + C + D' + E &= N_0 = 1 \\
A + Br + Cr^{-1} + D's + Es^{-1} &= N_1 = D \\
A + Br^2 + Cr^{-2} + D's^2 + Es^{-2} &= N_2 = \begin{vmatrix} D & a \\ a & D \end{vmatrix} \\
A + Br^3 + Cr^{-3} + D's^3 + Es^{-3} &= N_3 = \begin{vmatrix} D & a & 1 \\ a & D & a \\ 1 & a & D \end{vmatrix} \\
A + Br^4 + Cr^{-4} + D's^4 + Es^{-4} &= N_4 = \begin{vmatrix} D & a & 1 & 0 \\ a & D & a & 1 \\ 1 & a & D & a \\ 0 & 1 & a & D \end{vmatrix}
\end{aligned}$$

On inverting this for the coefficients, we can find lengthier expressions for them which, on simplification, leads to

$$\begin{aligned}
N_k = &\frac{2rs}{(r-1)^2(s-1)^2} \\
&+ \frac{1}{(r-1)^2(r+1)(r-s)(rs-1)} \Big\{ sr^2(1+r)\big(r^{k+2} + r^{-k-2}\big) - (1+s+s^2)r\big(r^{k-2} + r^{-k+2}\big) \cdot \\
&\qquad \big[r^4 + 1 + \frac{r}{s}(1+s)^2(1+r^2) + \frac{r^2}{s^2}\big(1 + 2s + 4s^2 + 2s^3 + s^4\big)\big] \Big\} \\
&- \frac{1}{(s-1)^2(s+1)(r-s)(rs-1)} \Big\{ rs^2(1+s)\big(s^{k+2} + s^{-k-2}\big) - (1+r+r^2)s\big(s^{k-2} + s^{-k+2}\big) \cdot \\
&\qquad \big[s^4 + 1 + \frac{s}{r}(1+r)^2(1+s^2) + \frac{s^2}{r^2}\big(1 + 2r + 4r^2 + 2r^3 + r^4\big)\big] \Big\}
\end{aligned}$$

An important question surrounding any finite difference scheme is whether or not it is stable. The same holds for these compact finite difference schemes. We will attempt to sketch a possible proof of the stability of a CFD scheme though I suspect it will be highly dependent on the choice of boundary conditions.

To review a simple stability argument, consider the advection equation

$$u_{,t} = v u_{,x}$$

where v is the velocity of the wave. We will (semi-)discretize in space leaving the problem continuous in t: $u(t,x) \to u(t,x_i) \equiv u_i(t)$. A simple FD approximation becomes

$$u_{i,t} = \frac{v}{h}\big(u_i - u_{i-1}\big)$$

which, on Fourier transforming with $\tilde{u}(t,k) = \frac{1}{\sqrt{2\pi}} \int e^{-ikx} u(t,x) dx$ becomes

$$\tilde{u}_{,t}(t,k) = \frac{v}{h}(1 - e^{-ikh})\, \tilde{u}(t,k)$$

which can be integrated in t to give

$$\tilde{u}(t,k) = \tilde{u}(0,k)\, e^{ikvt\sin(kh)/kh}\, e^{vt(1-\cos(kh))/h}$$

for which all $k > 0$ modes grows exponentially in time. Hence the scheme is unstable. To note a stable alternative, consider the centered FDA given by

$$u_{i,t} = \frac{v}{2h}\big(u_{i+1} - u_{i-1}\big)$$

which, on Fourier transforming yields

$$\tilde{u}(t,k) = \tilde{u}(0,k)\, e^{ikvt\sin(kh)/kh}$$

so that for a mode with k, the velocity becomes $v' = v\sin(kh)/kh$, and we have dispersion, but not unbounded growth. Hence this scheme is stable.

If we apply this to a compact finite difference scheme for the above advection equation with periodic boundary conditions, we can write the semi-discrete equation as

$$u_{i,t} = v\, C_{ij} u_j(t)$$

where the matrix $C = A^{-1}B$ comes from our CFD scheme which approximates the derivative via

$$A_{ij} {u_j}' = B_{ij} u_j$$

and where the prime denotes the derivative with respect to x. If we take a three point stencil for both u and its derivative, in the interior of the grid, we would have something like

$$\alpha u'_{i-1} + u'_i + \alpha u'_{i+1} = \frac{a}{2h}(u_{i+1} - u_{i-1})$$

where α and a are chosen for to get as high an order of accuracy for the smallest stencil. In this case, if we would like an a $\mathcal{O}(h^4)$ accurate scheme, we would set $\alpha = 1/4$ and $a = 3/2$. As a result, the matrix A will look like our earlier matrix M ($\tilde{M}$, really as we have periodic boundary conditions), i.e. $A = \alpha\tilde{M}$ where $D = 1/\alpha$. The (rescaled) matrix B_{ij} will then best be represented by ones and negative ones as

$$B_{ij} = \delta_{i,j-1} - \delta_{i,j+1} + \delta_{i,N-1}\delta_{j,0} - \delta_{i,0}\delta_{j,N-1}$$

where the indices i and j here take values from 0 to $N-1$ (we assume that we have a total of N points), the first term is for the first superdiagonal of B, the second term gives the first subdiagonal of B, the third term gives the upper rightmost element of B and the final terms is the lower leftmost element of B.

So, our full CFD scheme would look like

$$\alpha \tilde{M}_{ij} u'_j = \frac{a}{2h} B_{ij} u_j$$

On taking the inverse, we have

$$u'_i = \frac{a}{2h\alpha} (\tilde{M}^{-1})_{ij} B_{jk} u_k$$

such that our earlier matrix, C, becomes $C_{ik} = a/(2h\alpha)(\tilde{M}^{-1})_{ij} B_{jk}$. Using previous expressions, we can now write this as

$$C_{ij} u_j = \frac{a(4h\alpha \sinh\lambda)^{-1}}{(-1)^{N+1} + \cosh(N\lambda)} \sum_{j=0}^{N-1} (-1)^{i+j} \Big\{ \sinh\big[(N - |j-i|)\lambda\big] + (-1)^N \sinh\big[|j-i|\lambda\big] \Big\} \big(u_{j+1} - u_{j-1}\big)$$

where $\lambda = \cosh^{-1}(1/2\alpha)$ and recall $\alpha = 1/4$ for the CFD scheme we are considering.

At this point, we can Fourier transform our semi-discrete differential equation and we see that we again get a $2i\sin(kh)\,\tilde{u}_j$. So, provided The stuff under the summation is real and positive definite, the integration of our ODE in time should now yield modes that propagate in the same direction, possibly with dispersion, but without exponential growth; hence the CFD scheme should be stable. To show this, note that the quantity under the sum can be written as

$$2\tilde{u}_j\,(-1)^{|j-i|} \begin{cases} \sinh\big(\frac{N\lambda}{2}\big) \cosh\Big[\big(\frac{N}{2} - |j-i|\big)\lambda\Big] & N \text{ even} \\ \cosh\big(\frac{N\lambda}{2}\big) \sinh\Big[\big(\frac{N}{2} - |j-i|\big)\lambda\Big] & N \text{ odd} \end{cases}$$