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Physics 39907 Computational Physics
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Problem Set 4

Question 1. *Special Matrices:* Create a MATLAB function to calculate the four special matrices that we discussed in class: K, T, B, and C for any size N.

$$K = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

$$T = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

$$B = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

$$C = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \dots & -1 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & -1 & 2 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 2 & -1 \\ -1 & \dots & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

As a start:

```matlab
function [K,T,B,C]=ktbc(N)
% ktbc <Special 2nd diff matrices.>
% Usage:: [K,T,B,C]=ktbc(N[5])
%

% revision history:
% 09/17/2023 Mark D. Shattuck <mds> ktbc.m

%% Parse Input
if(~exist('N','var') || isempty(N))
    N=5;
end

%% Main
K=toeplitz([2 -1 zeros(1,N-2)]);
```

Question 2. *Second-order Differences:* Consider the effect of one row far from the boundaries of the second-order difference operator:

$$\frac{\mathbf{\Delta}^2}{h^2} = -\frac{K}{h^2} = \frac{1}{h^2}\begin{bmatrix} \ddots & & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & & \ddots \end{bmatrix},$$

which operates on a the points of a discrete function $f_n = f(nh)$. The result gives

$$\frac{1}{h^2}\mathbf{\Delta}^2 f = g,$$

and as a sum gives,

$$g_n = \frac{1}{h^2}\sum_k \mathbf{\Delta}^2_{nk} f_k.$$

We can use this simple calculation

$$g_n = g(nh) = \frac{1}{h^2}\begin{bmatrix}1 & -2 & 1\end{bmatrix}\begin{bmatrix}f(nh-h)\\ f(nh)\\ f(nh+h)\end{bmatrix} = \frac{1}{h^2}\begin{bmatrix}1 & -2 & 1\end{bmatrix}\begin{bmatrix}f((n-1)h)\\ f(nh)\\ f((n+1)h)\end{bmatrix}$$

to evaluate g_n. For example if $f_n = C$, where C is a constant then,

$$g_n = g(nh) = \frac{1}{h^2}\begin{bmatrix}1 & -2 & 1\end{bmatrix}\begin{bmatrix}C\\ C\\ C\end{bmatrix} = \frac{C}{h^2}(1-2+1) = 0.$$

(1) Use the Taylor expansion around nh show that

$$g_n = g(nh) = \frac{1}{h^2}\begin{bmatrix}1 & -2 & 1\end{bmatrix}\begin{bmatrix}f(nh-h)\\ f(nh)\\ f(nh+h)\end{bmatrix} \simeq f''(nh) + \frac{1}{12}f^{(4)}(nh)h^2 + \mathcal{O}(h^4)$$

(2) Find g_n for:
  (a) $f(x) = Cx$, $f_n = Cnh$, where C is a constant.
  (b) $f(x) = Cx^2$, $f_n = C(nh)^2$, where C is a constant.
  (c) $f(x) = Cx^3$, $f_n = C(nh)^3$, where C is a constant.
  (d) $f(x) = Cx^4$, $f_n = C(nh)^4$, where C is a constant.
  (e) $f(x) = Ce^{ikx}$, $f_n = Ce^{iknh}$, where C and k are a constants, and i is the imaginary number.
  (f) $f(x) = C\sin kx$, $f_n = C\sin(knh)$, where C and k are a constants.
  (g) $f(x) = C\cos kx$, $f_n = C\cos(knh)$, where C and k are a constants.

(3) For which of the previous, is g_n *equal* to the exact second derivative of $f(x)$ and why?

Question 3. *Fixed-Fixed:* Solve the following problem:

$$-\frac{d^2u(x)}{dx^2} = f(x), \quad u(0) = 0, u(1) = 0.$$

Solve analytically and using finite differences with $h = 1/6$, $1/11$, and $1/50$ for

(1) $f(x) = 1$
(2) $f(x) = \delta(x - \frac{2}{3})$
(3) $f(x) = \sin \pi x$

For each forcing function make a plot with the analytic and 3 finite difference solutions. Hint: It would probably be useful to make a function or script which depends on `x` and `f`. For example, here is a start:

```
function u=solveFixFix(f,x)
% solveFixFix <Solve -u'(x)=f(x) with u(a)=0, u(b)=0 on the interval x=[a:h:b]>
% Usage:: u=solveFixFix(f,x[0:1/6:1])
%

% revision history:
% 10/05/2023 Mark D. Shattuck <mds> solveFixFix.m

%% Parse Input
% x is optional
if(~exist('x','var') || isempty(x))
    x=0:1/6:1;
end

%% Main

N=length(x);    % size of x
h=x(2)-x(1);    % size of h nb: should check N>=2

if length(f)~=N-2
  disp('length(f) must be length(x)-2');
  u=-1;
  return
end

K=ktbc(N-2);
u=% add code to solve problem here %
```

This can be used in conjunction with a plotting script like the following:

```
%% Plot multiple
clf; % clear figure

xx=0:.01:1;  % x-values for exact solution

hlist=[1/6 1/11 1/50];  % list of h values
mk={'square','+','o'};  % list of markers

plot(xx,(1-xx).*xx/2,'k--','linewidth',3);  % plot exact
hold all;                                   % turn on over plot
for nh=1:length(hlist)
  h=hlist(nh);                    % set h
  x=0:h:1;                        % make new x
  N=length(x);                    % length of x
  u=solveFixFix(ones(N-2,1),x);   % solution
  % plot
  plot(x,u,mk{nh},'markersize',10,'linewidth',2);
end;
hold off;   % turn off over plot

set(gca,'fontsize',15)
xlabel('Position');
ylabel('Displacement')
```

Question 4. *Free-Fixed:* Solve the following problem:

$$-\frac{d^2u(x)}{dx^2} = f(x), \quad u'(0) = 0, u(1) = 0.$$

Solve analytically and using finite differences to second-order accuracy with $h = 1/6$, $1/11$, and $1/50$ for

(1) $f(x) = 1$
(2) $f(x) = 1 - x$
(3) $f(x) = \delta(x - \frac{1}{3})$

For each forcing function make a plot with the analytic and 3 finite difference solutions.

Question 5. *Free-Free:* Consider the following problem:

$$-\frac{d^2u(x)}{dx^2} = f(x), \quad u'(0) = 0, u'(1) = 0.$$

(1) What is the discrete and analytic condition(s) on $f(x)$ for a solution to exist?
(2) What happens if those conditions are not met?
(3) If a solution exist, solve analytically and using finite differences to second-order accuracy with $h = 1/6$, $1/11$, and $1/50$ for
   (a) $f(x) = 1$
   (b) $f(x) = \delta(x - \frac{1}{3}) - \delta(x - \frac{2}{3})$
   (c) $f(x) = \sin 2\pi x$

   Make a plot with the analytic and 3 finite difference solutions. Describe the solution in words or using a picture.

Question 6. *Delta functions:* Consider the following piece-wise linear functions:

$$R(x-a) = \begin{cases} 0 & x \le a \\ x-a & x > a \end{cases} \quad R_{n-k} = \begin{cases} 0 & n \le k \\ n-k & n > k \end{cases} = \begin{bmatrix} \vdots & \\ 0 & \\ \vdots & \\ 0 & (k^{\text{th}}\text{row}) \\ 1 & \\ \vdots & \\ n-k & (n^{\text{th}}\text{row}) \\ \vdots & \end{bmatrix}$$

$$v(x) = 3R(x-4) \qquad V_n = 3R_{n-4} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 3 \\ 6 \\ \vdots \end{bmatrix}$$

$$u(x) = \begin{cases} Cx & x \le 0 \\ Dx & x > 0 \end{cases} \qquad U_n = \begin{cases} Cn & n \le 0 \\ Dn & n > 0 \end{cases} = \begin{bmatrix} \vdots \\ -2C \\ -C \\ 0 \\ D \\ 2D \\ \vdots \end{bmatrix}$$

(1) Write $u(x)$ in terms of $R(x)$ and write U_n in terms of R_n

(2) Find the second derivatives $R''(x)$, $v''(x)$, and $u''(x)$ and second difference $\mathbf{\Delta}^2 R_{n-k}$, $\mathbf{\Delta}^2 V_n$, and $\mathbf{\Delta}^2 U_n$. The following definitions may be useful:

$$S(x-a) = \begin{cases} 0 & x \le a \\ 1 & x > a \end{cases} \quad S_{n-k} = \begin{cases} 0 & n \le k \\ 1 & n > k \end{cases} = \begin{bmatrix} \vdots & \\ 0 & (k^{\text{th}}\text{row}) \\ 1 & \\ \vdots & \end{bmatrix}$$

$$\delta(x-a) = \begin{cases} \infty & x = a \\ 0 & else \end{cases} \quad \delta_{n-k} = \begin{cases} 1 & n = k \\ 0 & else \end{cases} = \begin{bmatrix} \vdots & \\ 0 & \\ 1 & (k^{\text{th}}\text{row}) \\ 0 & \\ \vdots & \end{bmatrix}$$

where

$$\int_{-\infty}^{\infty} \delta(x-a)\, dx = 1$$

and

$$\int_{-\infty}^{\infty} \delta(x-a) f(x)\, dx = f(a)$$

.

Question 7. *First Differences:* Consider the following definition of the forward difference operator:

$$du_n = \sum_k D_{nk} u_k = u_{n+1} - u_n,$$

where

$$D_{nk} = \mathbf{D} = \begin{bmatrix} -1 & 1 & 0 & & \\ 0 & -1 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & -1 & 1 \end{bmatrix}$$

$$= \texttt{toeplitz([-1 zeros(1,N-2)],[-1 1 zeros(1,N-2)])}.$$

For example,

$$\mathbf{D}_4 u = \begin{bmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} u_2 - u_1 \\ u_3 - u_2 \\ u_4 - u_3 \end{bmatrix}.$$

(1) If $\mathbf{D}_N$ operates on an $N \times 1$ vector u how big is $\mathbf{D}$?
(2) Why is $\mathbf{D}$ not square?
(3) Is $\mathbf{D}$ invertible?
(4) The inverse of differentiation is integration. The discrete version of integration is summation. The summation matrix $\mathbf{S}$ is a lower-triangular matrix of all ones. For example,

$$\mathbf{S}_4 u = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} u_1 \\ u_1 + u_2 \\ u_1 + u_2 + u_3 \\ u_1 + u_2 + u_3 + u_4 \end{bmatrix}.$$

Therefore another candidate for the difference operator would be the inverse of $\mathbf{S}$, $\mathcal{D} = \mathbf{S}^{-1}$. How does $\mathcal{D}$ differ from $\mathbf{D}$?
(5) Show that:

$$\mathbf{S} \begin{bmatrix} \mathbf{0} \\ \mathbf{D} \end{bmatrix} u = u - u_1,$$

and that it is the discrete version of the fundamental theorem of calculus:

$$\int_0^x f'(x)\, dx = f(x) - f(0).$$

(6) Show that:
  (a) $K = \mathbf{D}\mathbf{D}^T$,
  (b) $B = \mathbf{D}^T\mathbf{D}$,
  (c) $T = \mathcal{D}^T\mathcal{D}$,
  What would $\mathcal{D}\mathcal{D}^T$ represent?

Question 8. *Summation by parts:* Find and verify the discrete equivalent for integration by parts:

$$\int_{-\infty}^{\infty} u(x)v'(x)dx = -\int_{-\infty}^{\infty} u'(x)v(x)dx$$

using first-order finite differences.

Question 9. *LDL^T:* K_4 is a symmetric matrix so it has an `ldl` decomposition given by:

$$K_4 = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 & 0 \\ 0 & -\frac{2}{3} & 1 & 0 \\ 0 & 0 & -\frac{3}{4} & 1 \end{bmatrix} \begin{bmatrix} \frac{2}{1} & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 \\ 0 & 0 & \frac{4}{3} & 0 \\ 0 & 0 & 0 & \frac{5}{4} \end{bmatrix} \begin{bmatrix} 1 & -\frac{1}{2} & 0 & 0 \\ 0 & 1 & -\frac{2}{3} & 0 \\ 0 & 0 & 1 & -\frac{3}{4} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The sequence $d = \left[\frac{2}{1}, \frac{3}{2}, \frac{4}{3}, \frac{5}{4}\right]$ can be realized concisely in MATLAB using `d=(2:5)./(1:4)`. Complete the following MATLAB function to calculate the `L` and `d` and optionally `D=diag(d)` for any value of `N` by extending the pattern in `d` and `L`.

```
function [L,d,D]=ldlK(N)
% ldlK <Calculate the LDL' decomposition of K.>
% Usage:: [L,d,[D]]=ldlK(N[4])
% then L*diag(d)*L'=L*D*L'=K
%

% revision history:
% 10/05/2023 Mark D. Shattuck <mds> ldlK.m

%% Parse Input
if(~exist('N','var') || isempty(N))
    N=4;
end

%% Main

d=(2:5)./(1:4);          % correct for N=4 fix for N
L=eye(N)-diag(???,-1);   % fill in to get correct L

% optional full D
if(nargout>2)
  D=diag(d);
end
```

When it is working this statement: `[L,d]=ldlK(11); norm(L*diag(d)*L'-ktbc(11))` should return `0`.

Question 10. *Matrix Symmetries:* A is an $N \times M$ matrix, C is a symmetric $M \times M$ matrix and x is a $N \times 1$ vector.

(1) What shape is $A^T CA$ and is it symmetric? Why or why not?
(2) What shape is $x^T A^T Ax$? Show that it is always greater than or equal to zero for all x? For what x will it be zero? (hint: Think proof by parentheses. What does Ax represent?)