Homework 2 in 18.085

Due: Thursday, Sept 18

The first problems come from Section 1.4–5–6 of the CSE text. For this week (but not forever) I have reproduced them here. The last questions come from a paper in preparation on Master Equations.

1.4    7, 9, 11
1.5    9 (and find the eigenvalues by Matlab), 20
1.6    3, 9

Master Equations

(Outlined in red)
Here is one of the most useful formulas in linear algebra (it extends to $T - U V^T$):

**Woodbury-Sherman-Morrison**

Inverse of $K = T - uv^T$

$$K^{-1} = T^{-1} + \frac{T^{-1}uv^TT^{-1}}{1 - v^TT^{-1}u}$$  \hspace{1cm} (21)

The proof multiplies the right side by $T - uv^T$, and simplifies to $I$.

Problem 1.1.7 displays $T^{-1} - K^{-1}$ when the vectors have length $n = 4$:

$$v^TT^{-1} = \text{row 1 of } T^{-1} = [4 \ 3 \ 2 \ 1] \quad 1 - v^TT^{-1}u = 1 + 4 = 5.$$  \hspace{1cm}

For any $n$, $K^{-1}$ comes from the simpler $T^{-1}$ by subtracting $w^Tw/(n+1)$ with $w = n^{-1}$.

**Problem Set 1.4**

1. For $-u'' = \delta(x - a)$, the solution must be linear on each side of the load. What four conditions determine $A, B, C, D$ if $u(0) = 2$ and $u(1) = 0$?

   $$u(x) = Ax + B \quad \text{for} \quad 0 \leq x \leq a \quad \text{and} \quad u(x) = Cx + D \quad \text{for} \quad a \leq x \leq 1.$$

2. Change Problem 1 to the free-fixed case $u'(0) = 0$ and $u(1) = 4$. Find and solve the four equations for $A, B, C, D$.

3. Suppose there are two unit loads, at the points $a = \frac{1}{3}$ and $b = \frac{2}{3}$. Solve the fixed-fixed problem in two ways: First combine the two single-load solutions. The other way is to find six conditions for $A, B, C, D, E, F$:

   $$u(x) = Ax + B \quad \text{for} \quad x \leq \frac{1}{3}, \quad Cx + D \quad \text{for} \quad \frac{1}{3} \leq x \leq \frac{2}{3}, \quad Ex + F \quad \text{for} \quad x \geq \frac{2}{3}.$$

4. Solve the equation $-d^2u/dx^2 = \delta(x - a)$ with fixed-free boundary conditions $u(0) = 0$ and $u'(1) = 0$. Draw the graphs of $u(x)$ and $u'(x)$.

5. Show that the same equation with free-free conditions $u'(0) = 0$ and $u'(1) = 0$ has no solution. The equations for $C$ and $D$ cannot be solved. This corresponds to the singular matrix $B_n$ (with 1, 1 and $n, n$ entries both changed to 1).

6. Show that $-u'' = \delta(x - a)$ with periodic conditions $u(0) = u(1)$ and $u'(0) = u'(1)$ cannot be solved. Again the requirements on $C$ and $D$ cannot be met. This corresponds to the singular circulant matrix $C_n$ (with 1, $n$ and $n, 1$ entries changed to 1).

7. A difference of point loads, $f(x) = \delta(x - \frac{1}{3}) - \delta(x - \frac{2}{3})$, does allow a free-free solution to $-u'' = f$. Find infinitely many solutions with $u'(0) = 0$ and $u'(1) = 0$.

8. The difference $f(x) = \delta(x - \frac{1}{3}) - \delta(x - \frac{2}{3})$ has zero total load, and $-u'' = f(x)$ can also be solved with periodic boundary conditions. Find a particular solution $u_{\text{part}}(x)$ and then the complete solution $u_{\text{part}} + u_{\text{null}}$. 
9 The distributed load \( f(x) = 1 \) is the integral of loads \( \delta(x-a) \) at all points \( x = a \). The free-fixed solution \( u(x) = \frac{1}{2}(1 - x^2) \) from Section 1.3 should then be the integral of the point-load solutions \( (1 - x) \) for \( a \leq x \), and \( 1 - a \) for \( a \geq x \): 

\[
 u(x) = \int_0^x (1-x) \, da + \int_x^1 (1-a) \, da = (1-x)x + (1-\frac{1^2}{2}) - (x-\frac{x^2}{2}) = \frac{1}{2} - \frac{1}{2}x^2. \text{ YES!}
\]

Check the fixed-fixed case \( u(x) = \int_0^x (1-x)a \, da + \int_x^1 (1-a)x \, da = \ldots \).

10 If you add together the columns of \( K^{-1} \) (or \( T^{-1} \)), you get a “discrete parabola” that solves the equation \( Ku = f \) (or \( Tu = f \)) with what vector \( f \)? Do this addition for \( K^{-1} \) in Figure 1.9 and \( T^{-1} \) in Figure 1.10.

Problems 11–15 are about delta functions and their integrals and derivatives.

11 The integral of \( \delta(x) \) is the step function \( S(x) \). The integral of \( S(x) \) is the ramp \( R(x) \). Find and graph the next two integrals: the quadratic spline \( Q(x) \) and the cubic spline \( C(x) \). Which derivatives of \( C(x) \) are continuous at \( x = 0 \)?

12 The cubic spline \( C(x) \) solves the fourth-order equation \( u'''' = \delta(x) \). What is the complete solution \( u(x) \) with four arbitrary constants? Choose those constants so that \( u(1) = u''(1) = u(-1) = u''(-1) = 0 \). This gives the bending of a uniform simply supported beam under a point load.

13 The defining property of the delta function \( \delta(x) \) is that 

\[
 \int_{-\infty}^{\infty} \delta(x) \, g(x) \, dx = g(0) \quad \text{for every smooth function } g(x).
\]

How does this give “area = 1” under \( \delta(x) \)? What is \( \int \delta(x-3) \, g(x) \, dx \)?

14 The function \( \delta(x) \) is a “weak limit” of very high, very thin square waves \( SW \): 

\[
 SW(x) = \frac{1}{2h} \quad \text{for } |x| \leq h \quad \text{has} \quad \int_{-\infty}^{\infty} SW(x) \, g(x) \, dx \to g(0) \quad \text{as } h \to 0.
\]

For a constant \( g(x) = 1 \) and every \( g(x) = x^n \), show that \( \int SW(x)g(x) \, dx \to g(0) \). We use the word “weak” because the rule depends on test functions \( g(x) \).

15 The derivative of \( \delta(x) \) is the doublet \( \delta'(x) \). Integrate by parts to compute 

\[
 \int_{-\infty}^{\infty} g(x) \, \delta'(x) \, dx = -\int_{-\infty}^{\infty} (\text{?}) \, \delta(x) \, dx = (??) \quad \text{for smooth } g(x).
\]
1.5 Eigenvalues and Eigenvectors

5 Construct $B = B_0$ and $[Q, E] = \text{eig}(B)$ with $B(1, 1) = 1$ and $B(6, 6) = 1$. Verify that $E = \text{diag}(e)$ with eigenvalues $2 \times \text{ones}(1, 6) - 2 \times \cos([0 : 5] \times \pi/6)$ in $e$. How do you adjust $Q$ to produce the (highly important) Discrete Cosine Transform with entries $\text{DCT} = \cos([.5 : 5.5]' \times [0 : 5] \times \pi/6)/\sqrt{2}$?

6 The free-fixed matrix $T = T_6$ has $T(1, 1) = 1$. Check that its eigenvalues are $2 - 2 \cos[(k - 1)/6]\pi/6.5]$. The matrix $\cos([.5 : 5.5]' \times [.5 : 5.5] \times \pi/6.5)/\sqrt{2}$ should contain its unit eigenvectors. Compute $Q' \times Q$ and $Q' \times T \times Q$.

7 The columns of the Fourier matrix $F_4$ are eigenvectors of the circulant matrix $C = C_F$. But $[Q, E] = \text{eig}(C)$ does not produce $Q = F_4$. What combinations of the columns of $Q$ give the columns of $F_4$? Notice the double eigenvalue in $E$.

8 Show that the $n$ eigenvalues $2 - 2 \cos[\frac{2\pi}{n+1}]$ of $K_n$ add to the trace $2 + \cdots + 2$.

9 $K_3$ and $B_3$ have the same nonzero eigenvalues because they come from the same 4×3 backward difference $\Delta_n$. Show that $K_3 = \Delta_n\Delta_n$ and $B_3 = \Delta_n\Delta_n^T$. The eigenvalues of $K_3$ are the squared singular values $\sigma^2$ of $\Delta_n$ in 1.7.

Problems 10–23 are about diagonalizing $A$ by its eigenvectors in $S$.

10 Factor these two matrices into $A = S\Lambda S^{-1}$. Check that $A^2 = SA^2S^{-1}$:

\[
A = \begin{bmatrix} 1 & 2 \\ 0 & 3 \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix}.
\]

11 If $A = S\Lambda S^{-1}$ then $A^{-1} = (\text{ })^T(\text{ })^T(\text{ })^T$. The eigenvectors of $A^3$ are (the same columns of $S$)(different vectors).

12 If $A$ has $\lambda_1 = 2$ with eigenvector $x_1 = [1]^T$ and $\lambda_2 = 5$ with $x_2 = [1]^T$, use $S\Lambda S^{-1}$ to find $A$. No other matrix has the same $\lambda$'s and $x$'s.

13 Suppose $A = S\Lambda S^{-1}$. What is the eigenvalue matrix for $A + 2I$? What is the eigenvector matrix? Check that $A + 2I = (\text{ })(\text{ })(\text{ })^{-1}$.

14 If the columns of $S$ ($n$ eigenvectors of $A$) are linearly independent, then

(a) $A$ is invertible \hspace{1cm} (b) $A$ is diagonalizable \hspace{1cm} (c) $S$ is invertible

15 The matrix $A = \begin{bmatrix} 3 & 1 \\ 3 & 3 \end{bmatrix}$ is not diagonalizable because the rank of $A - 3I$ is ____. $A$ only has one line of eigenvector. Which entries could you change to make $A$ diagonalizable, with two eigenvectors?

16 $A^k = SA^kS^{-1}$ approaches the zero matrix as $k \to \infty$ if and only if every $\lambda$ has absolute value less than ____. Which of these matrices has $A^k \to 0$?

\[
A_1 = \begin{bmatrix} .6 & .4 \\ .4 & .6 \end{bmatrix} \quad \text{and} \quad A_2 = \begin{bmatrix} .6 & .9 \\ .1 & .6 \end{bmatrix} \quad \text{and} \quad A_3 = K_3.
\]
19. If all $\lambda > 0$, show that $u^T Ku > 0$ for every $u \neq 0$, not just the eigenvectors $x_i$. Write $u$ as a combination of eigenvectors. Why are all “cross terms” $x_i^T x_j = 0$?

\[ u^T Ku = (c_1 x_1 + \cdots + c_n x_n)^T (c_1 \lambda_1 x_1 + \cdots + c_n \lambda_n x_n) = c_1^2 \lambda_1 x_1^T x_1 + \cdots + c_n^2 \lambda_n x_n^T x_n > 0 \]

20. Without multiplying $A = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$, find

(a) the determinant of $A$  
(b) the eigenvalues of $A$  
(c) the eigenvectors of $A$  
(d) a reason why $A$ is symmetric positive definite.

21. For $f_1(x, y) = \frac{1}{4}x^4 + x^2y + y^2$ and $f_2(x, y) = x^3 + xy - x$ find the second derivative (Hessian) matrices $H_1$ and $H_2$:

\[
H = \begin{bmatrix}
\frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\
\frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2}
\end{bmatrix}
\]

$H_1$ is positive definite so $f_1$ is concave up (= convex). Find the minimum point of $f_1$ and the saddle point of $f_2$ (look where first derivatives are zero).

22. The graph of $z = x^2 + y^2$ is a bowl opening upward. The graph of $z = x^2 - y^2$ is a saddle. The graph of $z = -x^2 - y^2$ is a bowl opening downward. What is a test on $a, b, c$ for $z = ax^2 + 2bxy + cy^2$ to have a saddle at $(0, 0)$?

23. Which values of $c$ give a bowl and which give a saddle point for the graph of $z = 4x^2 + 12xy + cy^2$? Describe this graph at the borderline value of $c$.

24. Here is another way to work with the quadratic function $P(u)$. Check that

\[
P(u) = \frac{1}{2}u^T Ku - u^T f \quad \text{equals} \quad \frac{1}{2} \left( u - K^{-1} f \right)^T K \left( u - K^{-1} f \right) - \frac{1}{2} f^T K^{-1} f.
\]

The last term $-\frac{1}{2} f^T K^{-1} f$ is $P_{\min}$. The other (long) term on the right side is always ____. When $u = K^{-1} f$, this long term is zero so $P = P_{\min}$.

25. Find the first derivatives in $f = \partial P / \partial u$ and the second derivatives in the matrix $H$ for $P(u) = u_1^2 + u_2^2 - c(u_1^2 + u_2^2)^4$. Start Newton’s iteration (21) at $u^0 = (1, 0)$. Which values of $c$ give a next vector $u^1$ that is closer to the local minimum at $u^* = (0, 0)$? Why is $(0, 0)$ not a global minimum?

26. Guess the smallest 2, 2 block that makes $\begin{bmatrix} C^{-1} & A \\ A^T & \end{bmatrix}$ semidefinite.

27. If $H$ and $K$ are positive definite, explain why $M = \begin{bmatrix} H & 0 \\ 0 & K \end{bmatrix}$ is positive definite but $N = \begin{bmatrix} K & K \\ K & K \end{bmatrix}$ is not. Connect the pivots and eigenvalues of $M$ and $N$ to the pivots and eigenvalues of $H$ and $K$. How is $\text{chol}(M)$ constructed from $\text{chol}(H)$ and $\text{chol}(K)$?
3 A different $A$ produces the circulant second-difference matrix $C = A^T A$:

$$
A = \begin{bmatrix}
1 & -1 & 0 \\
0 & 1 & -1 \\
-1 & 0 & 1
\end{bmatrix}
$$

gives $A^T A = \begin{bmatrix}
2 & -1 & -1 \\
-1 & 2 & -1 \\
-1 & -1 & 2
\end{bmatrix}$.

How can you tell from $A$ that $C = A^T A$ is only semidefinite? Which vectors solve $Au = 0$ and therefore $Cu = 0$? Note that $\text{chol}(C)$ will fail.

4 Confirm that the circulant $C = A^T A$ above is semidefinite by the pivot test. Write $u^T Cu$ as a sum of two squares with the pivots as coefficients. (The eigenvalues 0, 3, 3 give another proof that $C$ is semidefinite.)

5 $u^T Cu \geq 0$ means that $u_1^2 + u_2^2 + u_3^2 \geq u_1 u_2 + u_2 u_3 + u_3 u_1$ for any $u_1, u_2, u_3$. A more unusual way to check this is by the Schwarz inequality $|v^T w| \leq \|v\| \|w\|$:

$$
|u_1 u_2 + u_2 u_3 + u_3 u_1| \leq \sqrt{u_1^2 + u_2^2 + u_3^2} \sqrt{u_2^2 + u_3^2 + u_1^2}.
$$

Which $u$'s give equality? Check that $u^T Cu = 0$ for those $u$.

6 For what range of numbers $b$ is this matrix positive definite?

$$
K = \begin{bmatrix}
1 & b \\
b & 4
\end{bmatrix}.
$$

There are two borderline values of $b$ when $K$ is only semidefinite. In those cases write $u^T Ku$ with only one square. Find the pivots if $b = 5$.

7 Is $K = A^T A$ or $M = B^T B$ positive definite (independent columns in $A$ or $B$)?

$$
A = \begin{bmatrix}
1 & 2 \\
2 & 4 \\
3 & 6
\end{bmatrix} \quad B = \begin{bmatrix}
1 & 4 \\
2 & 5 \\
3 & 6
\end{bmatrix}
$$

We know that $u^T Mu = (Bu)^T (Bu) = (u_1 + 4u_2)^2 + (2u_1 + 5u_2)^2 + (3u_1 + 6u_2)^2$.

Show how the three squares for $u^T Ku = (Au)^T (Au)$ collapse into one square.

Problems 8–16 are about tests for positive definiteness.

8 Which of $A_1, A_2, A_3, A_4$ has two positive eigenvalues? Use the tests $a > 0$ and $ac > b^2$, don’t compute the $\lambda$'s. Find a vector $u$ so that $u^T A_1 u < 0$.

$$
A_1 = \begin{bmatrix}
5 & 6 \\
6 & 7
\end{bmatrix} \quad A_2 = \begin{bmatrix}
-1 & -2 \\
-2 & -5
\end{bmatrix} \quad A_3 = \begin{bmatrix}
1 & 10 \\
10 & 100
\end{bmatrix} \quad A_4 = \begin{bmatrix}
1 & 10 \\
10 & 101
\end{bmatrix}.
$$

9 For which numbers $b$ and $c$ are these matrices positive definite?

$$
A = \begin{bmatrix}
1 & b \\
b & 9
\end{bmatrix} \quad A = \begin{bmatrix}
2 & 4 \\
4 & c
\end{bmatrix}.
$$

With the pivots in $D$ and multiplier in $L$, factor each $A$ into $LDL^T$. 
Master Equations

Gilbert Strang and Shev Macnamara

Master equations are blessed with an impressive name. They are linear differential equations
\[
\frac{dp}{dt} = Ap
\]
for a probability vector \( p(t) \) (with nonnegative components that sum to 1). The matrix \( A \) has special structure: nonnegative off-diagonals, and zero column sum. The master equation governs the continuous time evolution of the probability distribution of a Markov process with discrete states. The probability of being in state \( j \) is given by \( p_j \), and \( a_{ij}dt \) is approximately the probability for the state to change from \( j \) to \( i \) in a small time interval \( dt \). Given an initial probability distribution \( p(0) \), the solution is a matrix exponential \( p(t) = e^{tA}p(0) \).

An example is the tridiagonal second difference matrix \( A \) with diagonals \( 1, -2, 1 \), except that \( A_{11} = A_{NN} = -1 \). This is minus the graph Laplacian on a line of nodes. Finite difference approximations to the heat equation with Neumann boundary conditions use the same matrix: \( du/dt = (A/h^2)u \).

Another example is the matrix in the master equation for the the bimolecular reaction,
\[
A + B \rightleftharpoons C
\]
where a molecule of \( A \) chemically combines with a molecule of \( B \) to form a molecule of \( C \). The associated matrix is not symmetric:
\[
A = \begin{pmatrix}
0 & 1 & 2 & 3 & 4 \\
-16 & 1 & 0 & 0 & 0 \\
16 & -10 & 2 & 0 & 0 \\
0 & 9 & -6 & 3 & 0 \\
0 & 0 & 4 & -4 & 4 \\
0 & 0 & 0 & 1 & -4
\end{pmatrix}
\]

There is always a directed graph associated with a master equation, which helps to find the matrix – an explanation of the graph and the matrix is coming in a moment. In the mean time, MATLAB makes this example (\( N = 5 \) here, but you will try larger examples!):

(a) Choose a diagonal matrix \( D \) so that \( DAD^{-1} \) is symmetric. This shows that \( A \) has real eigenvalues.
(b) Plot the eigenvalues that come from this MATLAB code (to see numerical instability at work)

\[
N = 10; \quad b = 0:N-1; \quad f = b.^2; \quad f = fliplr(f); \quad s = b+f; \\
A = spdiags([f' -s' b'], [-1 0 1], N,N); \quad e = eig(full(A)); \\
plot(e,’.’)
\]