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 $T - UV^{\mathrm{T}}$):

Woodbury-Sherman-Morrison
Inverse of $K = T - uv^{\mathrm{T}}$

$$K^{-1} = T^{-1} + \frac{T^{-1}uv^{\mathrm{T}}T^{-1}}{1 - v^{\mathrm{T}}T^{-1}u} \tag{21}$$

The proof multiplies the right side by $T - uv^{\mathrm{T}}$, and simplifies to I.
Problem 1.1.7 displays $T^{-1} - K^{-1}$ when the vectors have length $n = 4$:

$$v^{\mathrm{T}}T^{-1} = \text{row 1 of } T^{-1} = \begin{bmatrix} 4 & 3 & 2 & 1 \end{bmatrix} \quad 1 - v^{\mathrm{T}}T^{-1}u = 1 + 4 = 5.$$

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

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 $u(1) = 0$?

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

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:

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

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 $u_{\mathbf{part}}(x)$ and then the complete solution $u_{\mathbf{part}} + u_{\mathbf{null}}$.

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 $a \le x$, and $1-a$ for $a \ge x$):

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

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

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_4^{-1} in Figure 1.9 and T_4^{-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:

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

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

$$\int_{-\infty}^{\infty} g(x)\,\delta'(x)\,dx = -\int_{-\infty}^{\infty} (?)\,\delta(x)\,dx = (??) \text{ for smooth } g(x).$$

5 Construct $B = B_6$ and $[Q, E] = \mathsf{eig}(B)$ with $B(1,1) = 1$ and $B(6,6) = 1$. Verify that $E = \mathsf{diag}(e)$ with eigenvalues $2 * \mathsf{ones}(1,6) - 2 * \mathsf{cos}([0:5] * \mathsf{pi}/6)$ in e. How do you adjust Q to produce the (highly important) Discrete Cosine Transform with entries **DCT** $= \mathsf{cos}([.5:5.5]' * [0:5] * \mathsf{pi}/6)/\mathsf{sqrt}(3)$?

6 The free-fixed matrix $T = T_6$ has $T(1,1) = 1$. Check that its eigenvalues are $2 - 2\cos\left[(k - \frac{1}{2})\pi/6.5\right]$. The matrix $\mathsf{cos}([.5:5.5]' * [.5:5.5] * \mathsf{pi}/6.5)/\mathsf{sqrt}(3.25)$ should contain its unit eigenvectors. Compute $Q' * Q$ and $Q' * T * Q$.

7 The columns of the Fourier matrix F_4 are eigenvectors of the circulant matrix $C = C_4$. But $[Q, E] = \mathsf{eig}(C)$ 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 $2 - 2\cos\frac{k\pi}{n+1}$ of K_n add to the trace $2 + \cdots + 2$.

9 K_3 and B_4 have the same nonzero eigenvalues because they come from the same 4×3 backward difference Δ_-. Show that $K_3 = \Delta_-^{\mathrm{T}}\Delta_-$ and $B_4 = \Delta_-\Delta_-^{\mathrm{T}}$. The eigenvalues of K_3 are the squared **singular values** σ^2 of Δ_- 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 $A^2 = S\Lambda^2 S^{-1}$:

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

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

12 If A has $\lambda_1 = 2$ with eigenvector $x_1 = \left[\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right]$ and $\lambda_2 = 5$ with $x_2 = \left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]$, use $S\Lambda S^{-1}$ to find A. No other matrix has the same λ'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 $A + 2I = (\quad)(\quad)(\quad)^{-1}$.

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

(a) A is invertible (b) A is diagonalizable (c) S is invertible

15 The matrix $A = \left[\begin{smallmatrix} 3 & 1 \\ 0 & 3 \end{smallmatrix}\right]$ 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 $A^k = S\Lambda^k S^{-1}$ approaches the zero matrix as $k \to \infty$ if and only if every λ has absolute value less than ____. Which of these matrices has $A^k \to 0$?

$$A_1 = \begin{bmatrix} .6 & .4 \\ .4 & .6 \end{bmatrix} \quad \text{and} \quad A_2 = \begin{bmatrix} .6 & .9 \\ .1 & .6 \end{bmatrix} \quad \text{and} \quad A_3 = K_3.$$

1.5

19 If all $\lambda > 0$, show that $u^{\mathrm{T}}Ku > 0$ for *every* $u \neq 0$, not just the eigenvectors x_i. Write u as a combination of eigenvectors. Why are all "cross terms" $x_i^{\mathrm{T}}x_j = 0$?

$$u^{\mathrm{T}}Ku = (c_1x_1 + \cdots + c_nx_n)^{\mathrm{T}}(c_1\lambda_1x_1 + \cdots + c_n\lambda_nx_n) = c_1^2\lambda_1x_1^{\mathrm{T}}x_1 + \cdots + c_n^2\lambda_nx_n^{\mathrm{T}}x_n > 0$$

20 Without multiplying $A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 5 \end{bmatrix} \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$, 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:

$$H = \begin{bmatrix} \partial^2 f/\partial x^2 & \partial^2 f/\partial x\partial y \\ \partial^2 f/\partial y\partial x & \partial^2 f/\partial y^2 \end{bmatrix}.$$

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

$$P(u) = \frac{1}{2}u^{\mathrm{T}}Ku - u^{\mathrm{T}}f \quad \text{equals} \quad \frac{1}{2}(u - K^{-1}f)^{\mathrm{T}}K(u - K^{-1}f) - \frac{1}{2}f^{\mathrm{T}}K^{-1}f.$$

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

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 $[\,\boldsymbol{C^{-1}} \;\; \boldsymbol{A};\; \boldsymbol{A^{\mathrm{T}}} \;\; \_\_\_\_\,]$ 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 $\mathsf{chol}(M)$ constructed from $\mathsf{chol}(H)$ and $\mathsf{chol}(K)$?

1.6

3 A different A produces the circulant second-difference matrix $C = A^{\mathrm{T}}A$:

$$A = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \end{bmatrix} \quad \text{gives} \quad A^{\mathrm{T}}A = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}.$$

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

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

5 $u^{\mathrm{T}}Cu \geq 0$ means that $u_1^2 + u_2^2 + u_3^2 \geq u_1u_2 + u_2u_3 + u_3u_1$ for any u_1, u_2, u_3. A more unusual way to check this is by the Schwarz inequality $|v^{\mathrm{T}}w| \leq \|v\|\,\|w\|$:

$$|u_1u_2 + u_2u_3 + u_3u_1| \leq \sqrt{u_1^2 + u_2^2 + u_3^2}\,\sqrt{u_2^2 + u_3^2 + u_1^2}\,.$$

Which u's give *equality*? Check that $u^{\mathrm{T}}Cu = 0$ 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 $u^{\mathrm{T}}Ku$ with only one square. Find the pivots if $b = 5$.

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

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

We know that $u^{\mathrm{T}}Mu = (Bu)^{\mathrm{T}}(Bu) = (u_1 + 4u_2)^2 + (2u_1 + 5u_2)^2 + (3u_1 + 6u_2)^2$. Show how the three squares for $u^{\mathrm{T}}Ku = (Au)^{\mathrm{T}}(Au)$ 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 λ's. Find a vector u so that $u^{\mathrm{T}}A_1u < 0$.

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

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

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

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

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \boldsymbol{A}\boldsymbol{p}$$

for a probability vector $\boldsymbol{p}(t)$ (with nonnegative components that sum to 1). The matrix $\boldsymbol{A}$ 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 $\boldsymbol{p}_j$, and $a_{ij}\mathrm{d}t$ is approximately the probability for the state to change from j to i in a small time interval $\mathrm{d}t$. Given an initial probability distribution $\boldsymbol{p}(0)$, the solution is a matrix exponential $\quad \boldsymbol{p}(t) = e^{t\boldsymbol{A}}\boldsymbol{p}(0)$.

An example is the tridiagonal second difference matrix $\boldsymbol{A}$ with diagonals $1, -2, 1$, except that $\boldsymbol{A}_{11} = \boldsymbol{A}_{NN} = -1$. 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: $\mathrm{d}u/\mathrm{d}t = (\boldsymbol{A}/h^2)\, u$.

Another example is the matrix in the master equation for the the *bimolecular reaction*,

$$A + B \leftrightarrows C$$

where a molecule of A chemically combines with a molecule of B to form a molecule of C. The associated matrix is *not symmetric*:

$$\boldsymbol{A} = \begin{array}{c} \\ \textcircled{0} \\ \textcircled{1} \\ \textcircled{2} \\ \textcircled{3} \\ \textcircled{4} \end{array} \begin{array}{c} \begin{array}{ccccc} \textcircled{0} & \textcircled{1} & \textcircled{2} & \textcircled{3} & \textcircled{4} \end{array} \\ \begin{pmatrix} -16 & 1 & 0 & 0 & 0 \\ 16 & -10 & 2 & 0 & 0 \\ 0 & 9 & -6 & 3 & 0 \\ 0 & 0 & 4 & -4 & 4 \\ 0 & 0 & 0 & 1 & -4 \end{pmatrix} \end{array} \qquad (1)$$

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)

5 or 50 or 100

```
N = 5;   b = 0:N-1;  f = b.^2;  f = fliplr(f);  s = b+f;
A = spdiags([f' -s'  b'],[-1 0 1],N,N);  e = eig(full(A));
plot(e,'.')
```