18.303 Problem Set 2 Solutions

Problem 1 (5+5+5 points)

(a) We have $\langle x, x\rangle = x^*Bx > 0$ for $x \neq 0$ by definition of positive-definiteness. We have $\langle x, y\rangle = x^*By = (B^*x)^*y = (Bx)^*y = \overline{y^*(Bx)} = \overline{\langle y, x\rangle}$ by $B = B^*$.

(b) $\langle x, My\rangle = x^*BMy = \langle M^\dagger x, y\rangle = x^*M^{\dagger *}By$ for all x, y, and hence we must have $BM = M^{\dagger *}B$, or $M^{\dagger *} = BMB^{-1} \implies M^\dagger = (BMB^{-1})^* = (B^{-1})^*M^*B^*$. Using the fact that $B^* = B$ (and hence $(B^{-1})^* = B^{-1}$), we have $\boxed{M^\dagger = B^{-1}M^*B}$.

(c) If $M = B^{-1}A$ where $A = A^*$, then $M^\dagger = B^{-1}AB^{-1}B = B^{-1}A = M$. Q.E.D.

Problem 2: (5+5+(3+3+3)+5 points)

(a) As in class, let $u'([m + 0.5]\Delta x) \approx u'_{m+0.5} = \frac{u_{m+1}-u_m}{\Delta x}$. Define $c_{m+0.5} = c([m + 0.5]\Delta x)$. Now we want to take the derivative of $c_{m+0.5}u'_{m+0.5}$ in order to approximate $\hat{A}u$ at m by a center difference:

$$\hat{A}u\Big|_{m\Delta x} \approx \frac{c_{m+0.5}\left(\frac{u_{m+1}-u_m}{\Delta x}\right) - c_{m-0.5}\left(\frac{u_m-u_{m-1}}{\Delta x}\right)}{\Delta x}.$$

There are other ways to solve this problem of course, that are also second-order accurate.

(b) In order to approximate $\hat{A}u$, we did three things: compute u' by a center-difference as in class, multiply by $c_{m+0.5}$ at each point $m + 0.5$, then compute the derivative by another center-difference. The first and last steps are exactly the same center-difference steps as in class, so they correspond as in class to multiplying by D and $-D^T$, respectively, where D is the $(M + 1) \times M$ matrix

$$D = \frac{1}{\Delta x}\begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \\ & & & & -1 \end{pmatrix}.$$

The middle step, multiplying the $(M+1)$-component vector $\mathbf{u}'$ by $c_{m+0.5}$ at each point is just multiplication by a diagonal $(M + 1) \times (M + 1)$ matrix

$$C = \begin{pmatrix} c_{0.5} & & & \\ & c_{1.5} & & \\ & & \ddots & \\ & & & c_{M+0.5} \end{pmatrix}.$$

Putting these steps together in sequence, from right to left, means that $A = -D^TCD$

(c) In Julia, the `diagm(c)` command will create a diagonal matrix from a vector `c`. The function `diff1(M) = [ [1.0 zeros(1,M-1)]; diagm(ones(M-1),1) - eye(M) ]` will allow you to create the $(M + 1) \times M$ matrix D from class via `D = diff1(M)` for any given value of M. Using these two commands, we construct the matrix A from part (d) for $M = 100$ and $L = 1$ and $c(x) = e^{3x}$ via

```
L = 1
M = 100
D = diff1(M)
```

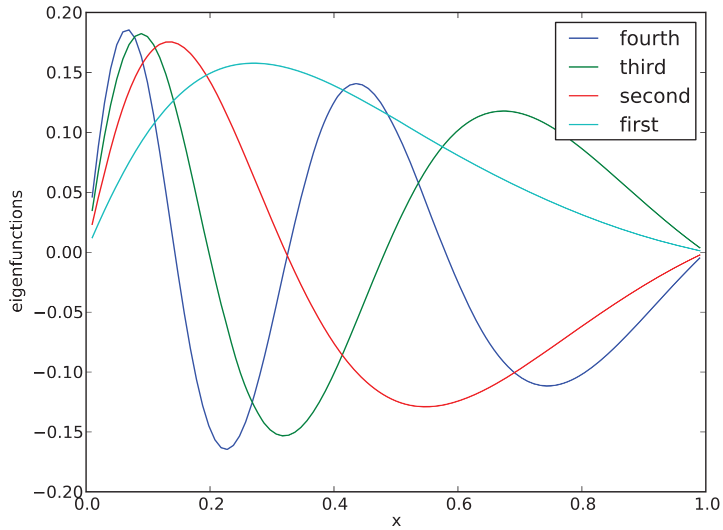

Figure 1: Smallest-$|\lambda|$ eigenfunctions of $\hat{A} = \frac{d}{dx}\left[c(x)\frac{d}{dx}\right]$ for $c(x) = e^{3x}$.

```
dx = L / (M+1)
x = dx*0.5:dx:L # sequence of x values from 0.5*dx to <= L in steps of dx
c(x) = exp(3x)
C = diagm(c(x))
A = -D' * C * D / dx^2
```

You can now get the eigenvalues and eigenvectors by `λ, U = eig(A)`, where λ is an array of eigenvalues and U is a matrix whose columns are the corresponding eigenvectors (notice that all the λ are < 0 since A is negative-definite).

(i) The plot is shown in Figure 1. The eigenfunctions look vaguely "sine-like"—they have the same number of oscillations as $\sin(n\pi x/L)$ for $n = 1, 2, 3, 4$—but are "squeezed" to the left-hand side.

(ii) We find that the dot product is $\approx 4.3 \times 10^{-16}$, which is zero up to roundoff errors (your exact value may differ, but should be of the same order of magnitude).

(iii) In the posted IJulia notebook for the solutions, we show a plot of $|\lambda_{2M} - \lambda_M|$ as a function of M on a log–log scale, and verify that it indeed decreases $\sim 1/M^2$. You can also just look at the numbers instead of plotting, and we find that this difference decreases by a factor of ≈ 3.95 from $M = 100$ to $M = 200$ and by a factor of ≈ 3.98 from $M = 200$ to $M = 400$, almost exactly the expected factor of 4. (For fun, in the solutions I went to $M = 1600$, but you only needed to go to $M = 800$.)

(d) In general, the eigenfunctions have the same number of nodes (sign oscillations) as $\sin(n\pi x/L)$, but the oscillations pushed towards the region of high $c(x)$. This is even more dramatic if we increase the $c(x)$ contrast. In Figure xxx, we show two examples. First, $c(x) = e^{20x}$, in which all of the functions are squished to the left where c is small. Second $c(x) = 1$ for $x < 0.3$ and 100 otherwise—in this case, the oscillations are at the left 1/3 where c is small, but the function is not zero in the right 2/3. Instead, the function is nearly constant where c is large. The reason for this has to do with the continuity of u: it is easy to see from the operator that cu' must be continuous for $(cu')'$ to exist, and hence the slope u' must decrease by a factor of

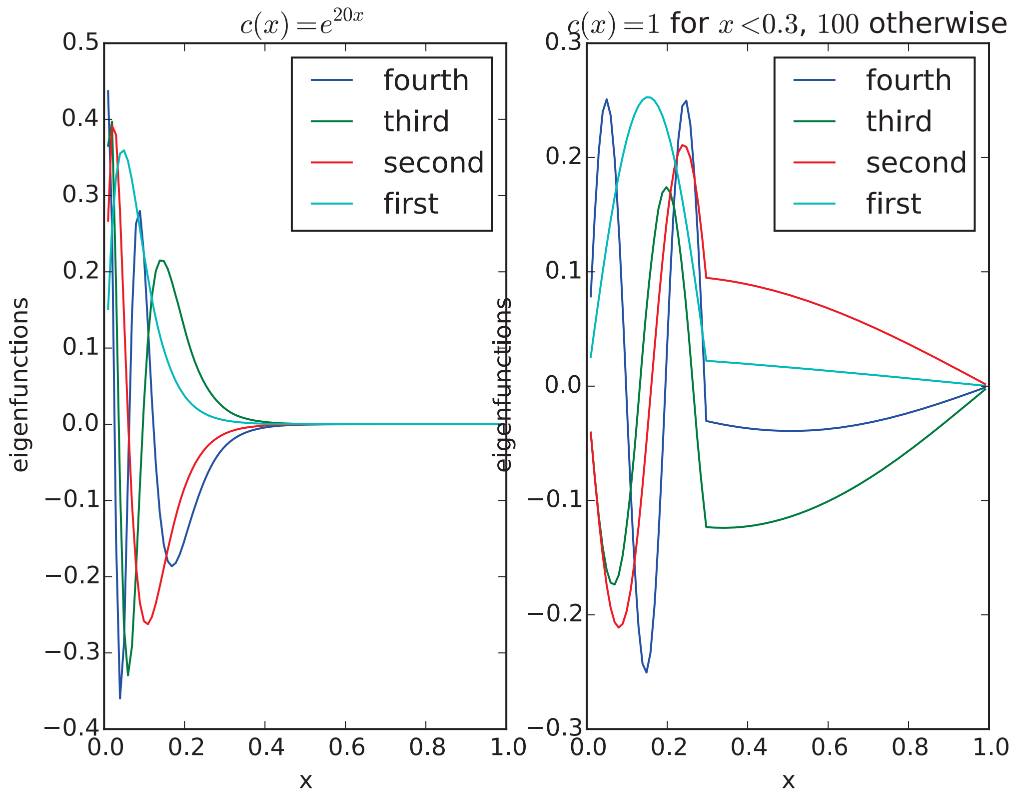

Figure 2: First four eigenfunctions of $\hat{A}u = (cu')'$ for two different choices of $c(x)$.

100 for $x > 0.3$, leading to a u that is nearly constant. (We will explore some of these issues further later in the semester.)

Problem 3: (5+5+5+5+5+5 points)

(a) The heat capacity equation tells us that $\frac{dT_n}{dt} = \frac{1}{c\rho a\Delta x}\frac{dQ_n}{dt}$, where dQ_n/dt is the rate of change of the heat in the n-th piece. The thermal conductivity equation tells us that dQ_n/dt, in turn, is equal to the sum of the rates q at which heat flows from $n+1$ and $n-1$ into n:

$$\frac{dT_n}{dt} = \frac{1}{c\rho a\Delta x}\frac{dQ_n}{dt} = \frac{1}{c\rho a\Delta x}\frac{\kappa a}{\Delta x}\left[(T_{n+1} - T_n) + (T_{n-1} - T_n)\right] = \alpha(T_{n+1} - T_n) + \alpha(T_{n-1} - T_n)$$

where $\boxed{\alpha = \frac{\kappa}{c\rho(\Delta x)^2}}$. The only difference for T_1 and T_N is that they have no heat flow $n-1$ and $n+1$, respectively, since the ends are insulated: $\frac{dT_1}{dt} = \alpha(T_2 - T_1)$ and $\frac{dT_N}{dt} = \alpha(T_{N-1} - T_N)$.

(b) We can obtain A in two ways. First, we can simply look directly at our equations above, which give $\frac{dT_n}{dt} = \alpha(T_{n+1} - 2T_n + T_{n-1})$ for every n except T_1 and T_N, and read off the corresponding rows of the matrix

$$\boxed{A = \alpha \begin{pmatrix} -1 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -1 \end{pmatrix}}.$$

Alternatively, we can write each of the above steps—differentiating T to get the rate of heat flow q to the left at each of the $N-1$ interfaces between the pieces, then taking the difference of the q's to get dT/dt, in matrix form, to write:

$$A = \frac{1}{c\rho a}\frac{1}{\Delta x}\underbrace{\begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \\ & & & & -1 \end{pmatrix}}_{D:\, N\times(N-1)} \kappa a \frac{1}{\Delta x}\underbrace{\begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \\ & & & & -1 \quad 1 \end{pmatrix}}_{-D^T:\,(N-1)\times N} = -\frac{\kappa}{c\rho}DD^T,$$

in terms of the D matrix from class (except with N reduced by 1), which gives the same A as above. As we will see in the parts below, this is indeed a second-derivative approximation, but with different boundary conditions—Neumann conditions—than the Dirichlet conditions in class.

By the way, it is interesting to consider $-DD^T$, compared to the $-D^TD$ we had in class. Clearly, $-DD^T$ is real-symmetric and negative semidefinite. It is *not*, however, negative definite, since D^T does not (and cannot) have full column rank (its rank must be $\leq$ the number of rows $N-1$, and in fact in class we showed that it has rank $N-1$).

(c) Ignoring the ends for the moment, for all the interior points we have $\frac{dT_n}{dt} = \frac{\kappa}{c\rho}\frac{T_{n+1}-2T_n+T_{n-1}}{\Delta x^2}$, which is exactly our familiar center-difference approximation for $\frac{\kappa}{c\rho}\frac{\partial^2 T}{\partial x^2}$ at the point n ($x = [n-0.5]\Delta x$). Hence, everywhere in the interior our equations converge to $\frac{\partial T}{\partial T} = \frac{\kappa}{c\rho}\frac{\partial^2 T}{\partial x^2}$, and thus $\boxed{\hat{A} = \frac{\kappa}{c\rho}\frac{\partial^2}{\partial x^2}}$.

(d) The boundary conditions are $\boxed{\frac{\partial T}{\partial x} = 0}$ at $x = 0, L$. The easiest way to see this is to observe that our heat flow q is really a first derivative, and zero heat flow at the ends means zero derivatives. That is, $q_{n+0.5} = \kappa a \frac{T_{n+1}-T_n}{\Delta x}$ is really an approximate derivative: $q_{n+0.5} \approx \kappa a \left.\frac{\partial T}{\partial x}\right|_{n+0.5} = \kappa a \left.\frac{\partial T}{\partial x}\right|_{n\Delta x}$, while the flows $q_{0.5}$ and $q_{N+0.5}$ to/from $n = 0$ and $n = N+1$ is zero, and hence $q_{0.5} = q_{N+0.5} = 0 \approx \kappa a \left.\frac{\partial T}{\partial x}\right|_{0,L}$.

Working backwards, consider $\hat{A}T = \frac{\partial^2 T}{\partial x^2} = T''$ (setting $\frac{\kappa}{c\rho} = 1$ for convenience) with these boundary conditions and center-difference approximations. We are given $T_n = T([n-0.5]\Delta x, t)$ for $n = 1, \ldots, N$. First, we compute $\left.\frac{\partial T}{\partial x}\right|_{n\Delta x} \approx T'_{n+0.5} = \frac{T_{n+1}-T_n}{\Delta x}$ for $n = 1, \ldots, N-1$ ($-D^T\mathbf{T}$ using the D above). Unlike the Dirichlet case in class, we *don't* compute $T'_{0.5}$ and $T'_{N+0.5}$, since these correspond to $\partial T/\partial x$ at $x = 0, L$, which are zero by the boundary conditions. Then, we compute our approximate 2nd derivatives $T''_n = \frac{T'_{n+0.5}-T'_{n-0.5}}{\Delta x}$

for $n = 1, \ldots, N$, where we let $T'_{0.5} = T'_{N+0.5} = 0$ ($D\mathbf{T}'$ using the D from above). This gives $T''_1 = \frac{T'_{1.5}-0}{\Delta x} = \frac{T_2 - T_1}{\Delta x^2}$, $T''_N = \frac{0 - T_{N-0.5}}{\Delta x} = \frac{-T_N + T_{N-1}}{\Delta x^2}$ at the endpoints, and $T''_n = \frac{(T_{n+1}-T_n)-(T_n - T_{n-1})}{\Delta x^2} = \frac{T_{n+1}-2T_n+T_{n-1}}{\Delta x^2}$ for $1 < n < N$, which are precisely the rows of our A matrix above.

(e) If $\kappa(x)$, then we get a different κ and α factor for each $T_{n+1} - T_n$ difference:

$$\frac{dT_n}{dt} = \alpha_{n+1/2}(T_{n+1} - T_n) + \alpha_{n-1/2}(T_{n-1} - T_n),$$

where $\alpha_{n+1/2} = \frac{\kappa_{n+1/2}}{c\rho(\Delta x)^2}$ and $\kappa_{n+1/2} = \kappa([n + 1/2]\Delta x)$. In the $N \to \infty$ limit, this gives $\boxed{\hat{A} = \frac{1}{c\rho}\frac{\partial}{\partial x}\kappa\frac{\partial}{\partial x}}$: we differentiated, multiplied by κ, differentiated again, and then divided by $c\rho$. (You weren't asked to handle the case where $c\rho$ is not a constant, so it's okay if you commuted $c\rho$ with the derivatives.)

(f) If we discretize to $T_{m,n} = T(m\Delta x, n\Delta y)$, the steps are basically the same except that we have to consider the heat flow in both the x and y directions, and hence we have to take differences in both x and y. In particular, suppose the thickness of the block is h. In this case, heat will flow from $T_{m,n}$ to $T_{m+1,n}$ at a rate $\frac{\kappa h \Delta y}{\Delta x}(T_{m,n} - T_{m+1,n})$ where $h\Delta y$ is the area of the interface between the two blocks. Then, to convert into a rate of temperature change, we will divide by $c\rho h \Delta x \Delta y$, where $h\Delta x \Delta y$ is the volume of the block. Putting this all together, we obtain:

$$\frac{dT_{m,n}}{dt} = \frac{\kappa}{c\rho}\left[\frac{T_{m+1,n} - 2T_{m,n} + T_{m-1,n}}{\Delta x^2} + \frac{T_{m,n+1} - 2T_{m,n} + T_{m,n+1}}{\Delta y^2}\right],$$

where the thing in $[\cdots]$ is precisely the five-point stencil approximation for ∇^2 from class. Hence, we obtain

$$\hat{A} = \frac{1}{c\rho}\nabla \cdot \kappa \nabla,$$

where for fun I have put the κ in the middle, which is the right place if κ is not a constant (you were not required to do this).