18.303 Problem Set 2 Solutions

Problem 1: (10+10 points)

(a) For any $u, v \in V$, we integrate by parts as in class to obtain $\langle u, \hat{A}v\rangle = -\int_0^L \bar{u}v'' = -\bar{u}v'|_0^L + \int_0^L \overline{u'}v' = -\bar{u}v'|_0^L + \overline{u'}v\big|_0^L - \int_0^L \overline{u''}v = \langle \hat{A}u, v\rangle$, where in the last step we used the fact that the boundary terms are zero via the boundary conditions:

$$\bar{u}v'|_0^L = \overline{u(L)}v'(L) - \overline{u(0)}v'(0) = \overline{u(L)}v'(L) - \overline{e^{i\phi}u(L)}e^{i\phi}v'(L) = 0,$$

and similarly for the $\overline{u'}v\big|_0^L$ term; hence $\hat{A} = \hat{A}^*$.

To check definiteness, as in class we integrate by parts only once to obtain

$$\langle u, \hat{A}u\rangle = \int_0^L |u'(x)|^2 \, dx \geq 0,$$

so we clearly have $\hat{A} \succeq 0$ (positive semidefinite). To get $\hat{A} \succ 0$ (positive-definite), we need to show that $\langle u, \hat{A}u\rangle > 0$ for $u \neq 0$. The integral above is only zero if $u'(x) = 0$, in which case u is a constant. And the only way a nonzero constant can satisfy the boundary conditions is if $e^{i\phi} = 1$, i.e. $\phi = 2\pi\ell$ for some integer ℓ. So, $\hat{A} \succ 0$ if and only if $\phi \neq 2\pi\ell$.

This is consistent with what we found in problem 3(a) of pset 1, where we looked at the operator $-\hat{A}$ with the same boundary conditions. The fact that $\hat{A} = \hat{A}^*$ implies that the eigenvalues of $\hat{A}$ (and $-\hat{A}$) are real and that the eigenfunctions are orthogonal, both of which were true for the explicit solutions $u_n = e^{i\frac{2\pi n}{L}x - i\frac{\phi}{L}x}$ and $\lambda_n = -\frac{1}{L^2}(2\pi n - \phi)^2$. The fact that $\hat{A} \succ 0$ for $\phi \neq 2\pi\ell$ implies that the eigenvalues of $-\hat{A}$ are < 0 for these ϕ, whereas $\lambda_\ell = 0$ if $\phi = 2\pi\ell$, which is also what we found in pset 1.

(b) We already showed that $-\frac{d^2}{dx^2}$ is self-adjoint. It is also trivially true that $(\hat{B}+\hat{C})^* = \hat{B}^* + \hat{C}^*$ by definition of the adjoint and by linearity, since $\langle u, (\hat{B} + C)v\rangle = \langle u, \hat{B}v\rangle + \langle u, \hat{C}v\rangle = \langle \hat{B}^*u, v\rangle + \langle \hat{C}^*u, v\rangle = \langle (\hat{B}^* + \hat{C}^*)u, v\rangle$. So, the sum of two Hermitian operators is Hermitian, and hence we just need to show that $q(x)$ is Hermitian. But this is also trivial since q is real: $\langle u, qv\rangle = \int \bar{u}qv = \int \overline{qu}v = \langle qu, v\rangle$. Hence $\hat{A} = -\frac{d^2}{dx^2} + q(x)$ is Hermitian.

If we take the operator $\hat{A} - q_0$, we can easily see that it is positive semidefinite:

$$\begin{aligned} \langle u, (\hat{A} - q_0)u\rangle &= \langle u, -u''\rangle + \langle u, (q - q_0)u\rangle \\ &= \int |u'|^2 + \int (q - q_0)|u|^2 \geq 0, \end{aligned}$$

where we have integrated by parts from above, and used the fact that $q(x) - q_0 \geq 0$ everywhere. Hence the eigenvalues of $\hat{A} - q_0$ are ≥ 0. But this means that the eigenvalues of $\hat{A}$ are $\geq q_0$, since for any eigensolution $\hat{A}u = \lambda u$ we have $(\hat{A} - q_0)u = (\lambda - q_0)u$ and hence $\lambda - q_0 \geq 0$. (Adding a constant to an operator just shifts the eigenvalues by a constant, just like adding a multiple of the identity matrix in 18.06.)

Problem 2: (10 points)

Proof:

$$\langle \mathbf{x}, B^{-1}A\mathbf{y}\rangle_B = \mathbf{x}^*B(B^{-1}A\mathbf{y}) = \mathbf{x}^*A\mathbf{y} = \mathbf{x}^*AB^{-1}B\mathbf{y} = (B^{-1}A\mathbf{x})^*B\mathbf{y} = \langle B^{-1}A\mathbf{x}, \mathbf{y}\rangle_B,$$

where we have used the fact that $(B^{-1})^* = (B^*)^{-1} = B^{-1}$ (reviewed in pset 1).

Problem 3: (5+5+5+5+10 points)

(a) Discretizing $\frac{d^2}{dx^2}$ with center differences leads to the matrix $-D^T D$, exactly as in class. To discretize $c\frac{d^2u}{dx^2}$, we just need to multiply the second derivative u''_m at each point m by $c_m = c(m\Delta x)$. This corresponds to multiplying on the left by the $M \times M$ diagonal matrix

$$C = \begin{pmatrix} c_1 & & & & \\ & c_2 & & & \\ & & \ddots & & \\ & & & c_{M-1} & \\ & & & & c_M \end{pmatrix}$$

to obtain $A = -CD^T D$.

(b) Following problem 2, we choose the inner product $\langle \mathbf{x}, \mathbf{y} \rangle_{C^{-1}} = \mathbf{x}^* C^{-1} \mathbf{y}$, which is valid because C is (obviously) real-symmetric and positive-definite (its eigenvalues are $c_m > 0$). Then, from problem 2, A is self-adjoint with respect to this inner product, so the eigenvalues are real. Furthermore, $\langle \mathbf{x}, A\mathbf{x} \rangle_{C^{-1}} = -\mathbf{x}^* D^T D \mathbf{x} < 0$ (using the fact, proved in class, that $-D^T D$ is negative-definite) so the eigenvalues are negative.

(c) See solutions notebook.

(d) See solutions notebook.

(e) In class, we had $u_0 = u_{M+1} = 0$, with $(M+1)\Delta x = L$. Now, we will want to write $u(0)$ in terms of $u(L)$, so we want $u_M = u(L)$ as one of our degrees of freedom, and set $\boxed{M\Delta x = L}$ (i.e. the definition of Δx changes!). In this case we get $u_0 = e^{i\phi} u_M$, and the first row of our second-derivative approximation becomes

$$u''_1 \approx \frac{u_2 - 2u_1 + u_0}{\Delta x^2} = \frac{u_2 - 2u_1 + e^{i\phi} u_M}{\Delta x^2}.$$

To get the last row, i.e. u''_M, we need an equation for u_{M+1}. If we think of the whole function as living "in a loop," i.e. $u(x) = e^{i\phi} u(x + L)$, then we would get $u_{M+1} = e^{-i\phi} u_1$. However, the boundary condition that was explicitly supplied was $u'(0) = e^{i\phi} u'(L)$. If we discretize this as

$$\frac{u_1 - u_0}{\Delta x} = e^{i\phi} \frac{u_{M+1} - u_M}{\Delta x}$$

and cancel $u_0 = e^{i\phi} u_M$ from both sides, we still get $\boxed{u_{M+1} = e^{-i\phi} u_1}$, in which case the equation for the last row becomes

$$u''_M \approx \frac{u_{M+1} - 2u_M + u_{M-1}}{\Delta x^2} = \frac{e^{-i\phi} u_1 - 2u_M + u_{M-1}}{\Delta x^2}.$$

Writing this all out in matrix form, we get

$$\boxed{A = \frac{1}{\Delta x^2} \begin{pmatrix} c_1 & & & & \\ & c_2 & & & \\ & & \ddots & & \\ & & & c_{M-1} & \\ & & & & c_M \end{pmatrix} \begin{pmatrix} -2 & 1 & & & e^{i\phi} \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ e^{-i\phi} & & & 1 & -2 \end{pmatrix}}.$$

Notice that the second matrix is our usual 2nd-derivative matrix except with $e^{\pm i\phi}$ in the corners (which makes it still Hermitian but no longer real!).