18.303 Problem Set 2 Solutions

Problem 1: (10+10)

Consider a finite-difference approximation for the second derivative of the form:

$$u''(x) \approx \frac{a \cdot u(x+2\Delta x) + b \cdot u(x+\Delta x) + c \cdot u(x) + b \cdot u(x-\Delta x) + a \cdot u(x-2\Delta x)}{d \cdot (\Delta x)^2}.$$

(a) Plugging in the Taylor expansions (for $k = 1, 2$)

$$u(x \pm k\Delta x) = u(x) \pm k\Delta x\, u'(x) + (k\Delta x)^2 \frac{u''(x)}{2} \pm (k\Delta x)^3 \frac{u'''(x)}{3!} + \cdots,$$

we immediately find that all of the *odd*-order terms cancel, while the *even*-order terms add, yielding an expression

$$u''(x) \approx \frac{c_0}{\Delta x^2} u(x) + c_2 u''(x) + c_4 u''''(x) \cdot \Delta x^2 + c_6 u^{(6)}(x) \Delta x^4 + \cdots,$$

for some coefficients c_n in terms of $\{a, b, c, d\}$, and we wish to satisfy the equations $c_0 = 0$, $c_2 = 1$, and $c_4 = 0$. This gives us only 3 equations in 4 unknowns, so the system is underdetermined; that is because we can multiply numerator and denominator by our expression by any constant and get an equivalent expression. So, we can freely choose $\boxed{d = 1}$ (or any other value). This leads to the 3 equations:

$$c_0 = 0 = 2a + 2b + c \implies c = -2(a+b)$$

$$c_2 = 1 = 4a + b \implies b = 1 - 4a$$

$$c_4 = 0 = \frac{2}{4!}(16a + b) \implies 16a + (1 - 4a) = 0 \implies \boxed{a = -\frac{1}{12}, b = \frac{4}{3}, c = -\frac{15}{6}}.$$

Alternatively, multiplying numerator and deminator by 12, we obtain $\boxed{a = -1, b = 16, c = -30, d = 12}$.

(b) Figure 1 plots the error $|u''(1) + \sin(x)|$ for $u(x) = \sin(x)$ versus Δx on a log–log scale, along with the line Δx^4 for comparison, and we can see that the error is indeed (asymptotically) parallel to Δx^4. The corresponding code is:

```
dx = logspace(-4,1,50);
x = 1;
u = @(x) sin(x);
upp = (-u(x+2*dx)+16*u(x+dx)-30*u(x)+16*u(x-dx)-u(x-2*dx)) ./ (12*dx.^2);
loglog(dx, abs(upp + sin(x)), 'r.-', dx, dx.^4, 'k--')
xlabel('{\Delta}x')
legend('|error|', '{\Delta}x^4', 'Location', 'NorthWest')
```

Problem 2: (10+10)

Here, we consider inner products $\langle u, v \rangle$ on some vector space of complex-valued functions and the corresponding adjoint $\hat{A}^*$ of linear operators $\hat{A}$, where the adjoint is defined, as in class, by whatever satisfies $\langle u, \hat{A}v \rangle$ for all u and v. Usually, $\hat{A}^*$ is obtained from $\hat{A}$ by some kind of integration by parts. In particular, suppose V consists of functions[1] $u(x)$ on $x \in [0, L]$ with *periodic* boundary conditions $u(0) = u(L)$ as in pset 1, and define the inner product $\langle u, v \rangle = \int_0^L \overline{u(x)} v(x) dx$ as in class.

[1] As mentioned in class, we technically need to restrict ourselves to a Sobolev space of u where $\langle u, \hat{A}u \rangle$ is defined and finite, i.e. we are implicitly assuming that u is sufficiently differentiable and not too divergent, etcetera, but for the most part we will pass over such technicalities in 18.303 (which are important for rigorous proofs, but only serve to exclude counter-examples that have no physical relevance).

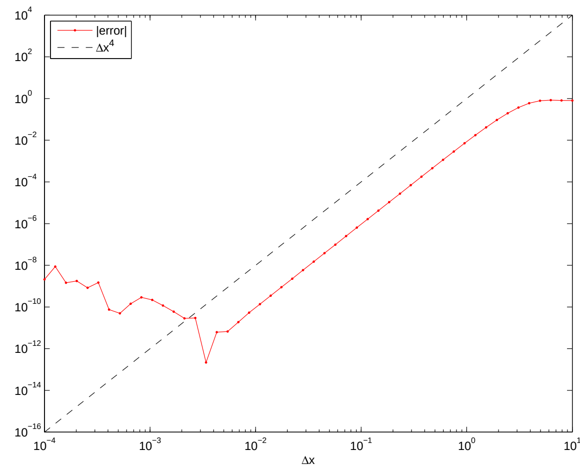

Figure 1: Plot of the error $|u''(1) + \sin(x)|$ for $u(x) = \sin(x)$ in our 4th-order accurate u'' approximation from problem 1(a), along with Δx^4 for reference, to verify the 4th-order convergence. Note that when the error becomes sufficiently small, it ceases to improve because we reach the limits of the computer arithmetic accuracy (and it starts to get worse for smaller Δx, because roundoff errors worsen).

(a) As in class, we integrate by parts:

$$\begin{aligned}\langle u, \hat{A}v\rangle &= -\int_0^L \bar{u}(cv')'dx = -\bar{u}cv'\big|_0^L + \int_0^L \overline{cu'}v'dx = \left(\overline{cu'}v - \bar{u}cv'\right)\Big|_0^L - \int_0^L \overline{(cu')'}v\,dx \\ &= \langle \hat{A}u, v\rangle + \left(\overline{cu'}v - \bar{u}cv'\right)\Big|_0^L.\end{aligned}$$

So, $\hat{A}$ is self-adjoint as long as the boundary terms vanish. For periodic boundaries, $\overline{cu'}v - \bar{u}cv'$ will *not* vanish when evaluated at $x = 0$ and L individually, but will give *equal* values at the two endpoints and hence the boundary terms *cancel*. v and $\bar{u}$ are clearly equal at the two boundaries. The simplest case is if c is periodic [$c(0) = c(L)$], in which case you can assume that u' and v' are periodic as well as the endpoints cancel; you were told via email that it was acceptable to assume this. More generally, we have to more careful about what function space we are considering. One can be very sophisticated about this, but at the level of 18.303 it is sufficient to suppose that, for $(cu')'$ to be defined on a periodic domain (where you imagine $x = 0$ and $x = L$ to be connected into a circle), we must require that u be continuous (for u') and that cu' be continuous (for $(cu')'$) on the *periodic* domain, and hence restrict ourselves to functions where cu' is periodic. (A more sophisticated treatment would look at Sobolev spaces and weak derivatives, but this is too fancy for now.)

Examining the intermediate term in the above expression, after integrating by parts *once*, we find as in class that

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

so $\hat{A}$ is certainly at least positive semi-definite. However, it is *not* positive *definite*, since the function $u(x) = 1$ (or any nonzero constant) is periodic and $\neq 0$ but gives $\langle u, \hat{A}u\rangle = 0$. (In class for Dirichlet boundary conditions, this function was not allowed.)

(b) We are given $\hat{B}$ where $v = \hat{B}u$ is $v(x) = \int_0^L G(x,x')u(x')dx'$. Then

$$\begin{aligned}
\langle u, \hat{B}v\rangle &= \int_0^L \overline{u(x)} \left[\hat{B}v\Big|_x \right] dx \\
&= \int_0^L \overline{u(x)} \left[\int_0^L G(x,x')v(x')dx' \right] dx \\
&= \int_0^L \overline{\left[\int_0^L \overline{G(x,x')}u(x)dx \right]} v(x')dx' \\
&= \int_0^L \overline{\left[\int_0^L \overline{G(x',x)}u(x')dx' \right]} v(x)dx \\
&= \langle \hat{B}^* u, v\rangle,
\end{aligned}$$

where in the third line we have exchanged the order of the integrals, in the fourth line we have swapped the x and x' labels (since both are just integration variables we can rename them as needed), and in the fifth line we have defined

$$\hat{B}^* u\Big|_x = \int_0^L \overline{G(x',x)}u(x')dx'.$$

By inspection, $\hat{B} = \hat{B}^*$ if

$$\boxed{\overline{G(x',x)} = G(x,x')}$$

for all $x, x' \in [0, L]$. (Notice that this is reminiscent of the condition for a matrix A to be self-adjoint under the usual dot product: $\overline{A_{nm}} = A_{mn}$. This is no coincidence, and is something we will come back to later in 18.303: such an integral operator $\hat{B}$ is directly analogous to multiplying by a dense matrix.)

Problem 2: (5+5+5+5+(5+5+5))

(a) The equation for u''_m in the interior of the domain is the same as before. The only changes are to the boundary terms

$$u''_1 = \frac{u_2 - 2u_1 + u_0}{\Delta x^2} = \frac{u_2 - 2u_1 + u_M}{\Delta x^2},$$

$$u''_M = \frac{u_{M+1} - 2u_M + u_{M-1}}{\Delta x^2} = \frac{u_1 - 2u_M + u_{M-1}}{\Delta x^2},$$

so that we approximate $-\frac{d^2}{dx^2}$ by the matrix

$$A = \frac{1}{\Delta x^2}\begin{pmatrix}
2 & -1 & & & & -1 \\
-1 & 2 & 1 & & & \\
 & 1 & -2 & 1 & & \\
 & & \ddots & \ddots & \ddots & \\
 & & & -1 & 2 & -1 \\
-1 & & & & -1 & 2
\end{pmatrix},$$

which only differs from the Dirichlet A by the -1 factors in the upper-right and lower-left corners.

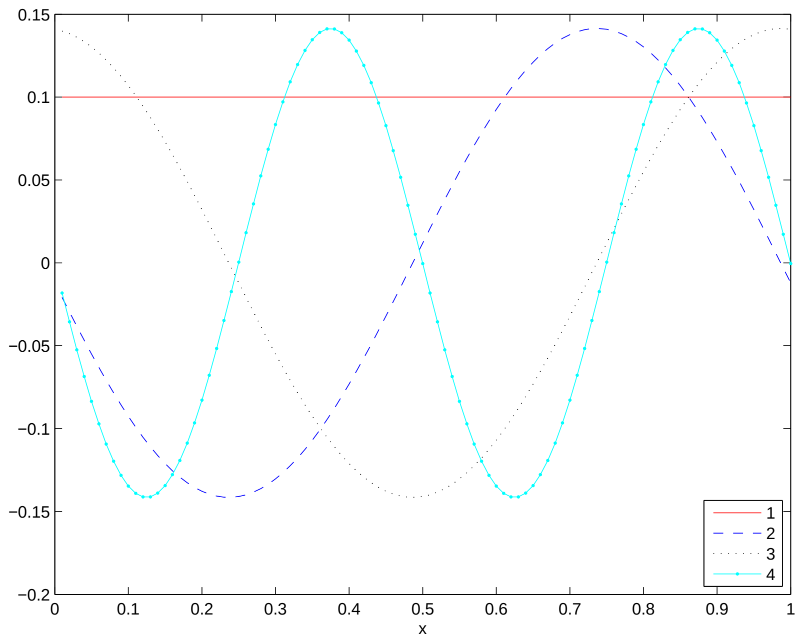

Figure 2: First four eigenvectors of the finite-difference approximation of $-d^2/dx^2$ with periodic boundary conditions.

(b) Matlab code to construct this A is simply:

```
L=1; M=100;
dx = L/M; D = diff1(M); A = D'*D / dx^2;
A(1,M) = -1/dx^2; A(M,1) = -1/dx^2;
```

(c) The eigenvalues indeed start at 0 and increase from there, so they are all non-negative; the first few returned by Matlab are 0, 39.4654, 39.4654, 157.7060, 157.7060, 354.2550, 354.2550, and so on, so that the nonzero eigenvalues are all of multiplicity 2 [with one exception: the 100th eigenvalue is *not* repeated, for reasons explained below]. The difference between these and $(2\pi n/L)^2$ for $n = 0, 1, 2, 3$ is $0, -0.0130, -0.0130, -0.2077, -0.2077, -1.0508, -1.0508$, respectively (corresponding to a *fractional* error of about 0.0003, 0.005, and 0.02 for $n = 1, 2, 3$).

(d) The first four eigenvectors are plotted in figure 2. As predicted analytically, the first eigenfunction is a constant, the second two are sinusoids where L is one period ($\pi/2$ out of phase), and the next one is a sinusoid where L is two periods. Note that the normalizations are different from those you probably chose in pset 1, but of course the normalization is arbitrary. Furthermore, Matlab need not return sin and cos—it can return any linear combination of these (since they share the same eigenvalue), corresponding to sine and cosine of $\frac{2\pi n}{L}x - \phi$ for an arbitrary phase shift ϕ.

(e) Get the eigenvectors *and* eigenvalues by [V,S]=eig(A); (the columns of V are the eigenvectors, and S is a diagonal matrix of eigenvalues). Again, make sure these are sorted in order of λ by using the commands: [lambda,i]=sort(diag(S)); and V = V(:,i); Now, plot the first few eigenvectors by the command x=linspace(0,L,M+1); x=x(2:end); plot(x,V(:,1),'r-', x,V(:,2), 'b–', x,V(:3),'k:', x,V(:4),'c.-'); legend('1','2','3','4'); xlabel('x'); ylabel('eigenfunctions') ...do they match your predictions from pset 1?

(f) Exact solutions

(i) Plugging in $u_m = e^{ikm\Delta x}$, we obtain

$$\begin{aligned} \lambda e^{ikm\Delta x} &= \frac{-u_{m+1} + 2u_m - u_{m-1}}{\Delta x^2} = \frac{e^{ikm\Delta x}}{\Delta x^2}\left(-e^{ik\Delta x} + 2 - e^{-ik\Delta x}\right) \\ &= \frac{2e^{ikm\Delta x}}{\Delta x^2}\left[1 - \cos(k\Delta x)\right] = \frac{4e^{ikm\Delta x}}{\Delta x^2}\sin^2(k\Delta x/2), \end{aligned}$$

where we have used the identies $e^{i\theta} + e^{-i\theta} = \cos\theta$ and $1 - \cos\theta = 2\sin^2(\theta/2)$ to simplify the equations. The main point is that $e^{ikm\Delta x}$ cancels on both sides—we satisfy the eigenequation! However, we must also satisfy the periodic boundary conditions $u_0 = u_M$, which gives

$$1 = e^{ikM\Delta x} \implies \boxed{k = \frac{2\pi n}{M\Delta x} = \frac{2\pi n}{L}}$$

for $n = 0, 1, 2, \ldots$.

This seems like an infinite number of solutions, but most of them are redundant, since $e^{i\frac{2\pi(n+M)}{M\Delta x}m\Delta x} = e^{i\frac{2\pi n}{M\Delta x}m\Delta x}e^{i2\pi nm} = e^{i\frac{2\pi n}{M\Delta x}m\Delta x}$ for all m, so n and $n + M$ give the same vector u_m. Hence we only need to consider $n = 0, 1, 2, \ldots, M - 1$ (for example).

(ii) Solving for λ, we obtain

$$\lambda = \left[\frac{2}{\Delta x}\sin(k\Delta x/2)\right]^2 .$$

and hence

$$\boxed{\lambda_n = \left[\frac{2}{\Delta x}\sin\left(\frac{\pi n\Delta x}{L}\right)\right]^2 = \left[\frac{2}{\Delta x}\sin\left(\frac{\pi n}{M}\right)\right]^2 .}$$

Note that, as above, n and $n + M$ give the same λ. Also, n and $M - n$ give the same value, so all of the eigenvalues are doubly repeated except for $n = 0$ and $n = M/2$ (fo even M). So, we only need to consider $n = 0, \ldots, \frac{M}{2}$ to get the distinct eigenvalues.

We could check these one by 1 in Matlab, but let's just check them all at once, using the fact that most of the eigenvalues are repeated so that we only have to check every other eigenvalue. The $n = 0$ eigenvalue is $\lambda_0 = 0$, and we already noticed that this was exact. The maximum fractional (relative) error in the remaining eigenvalues is given by the command `max(abs(lambda(2:2:end) - (2/dx * sin(pi*[1:M/2]'/M)).^2) ./ lambda(2:2:end))`, which prints 1.6724e-13: the remaining eigenvalues match our prediction to about 13 significant digits.

(iii) Consider a fixed value of n and what happens to λ_n as $M \to \infty$ (i.e. $\Delta x \to 0$). Taylor expanding sine, we find

$$\begin{aligned} \lambda_n &= \left[\frac{2}{\Delta x}\sin\left(\frac{\pi n\Delta x}{L}\right)\right]^2 = \left[\frac{2}{\Delta x}\left\{\frac{\pi n\Delta x}{L} - \frac{1}{6}\left(\frac{\pi n\Delta x}{L}\right)^3 + \cdots\right\}\right]^2 \\ &= \left[\frac{2\pi n}{L} - \frac{1}{3}\left(\frac{\pi n}{L}\right)^3\Delta x^2 + \cdots\right]^2 = \left(\frac{2\pi n}{L}\right)^2 - \frac{4\pi n}{3L}\left(\frac{\pi n}{L}\right)^3\Delta x^2 + \cdots , \end{aligned}$$

which matches the exact $(2\pi n/L)^2$ formula plus an error term $\sim \Delta x^2$.