18.303 Problem Set 1 Solutions

Problem 1: \((5+(2+2+2+2)+(10+5))\) points

Note that I don’t expect you to rederive basic linear-algebra facts. You can use things derived in 18.06, like the existence of an orthonormal diagonalization of Hermitian matrices.

(a) Since it is Hermitian, \(B\) can be diagonalized: \(B = QAQ^*\), where \(Q\) is the matrix whose columns are the eigenvectors (chosen orthonormal so that \(Q^{-1} = Q^*\)) and \(\Lambda\) is the diagonal matrix of eigenvalues. Define \(\sqrt{\Lambda}\) as the diagonal matrix of the (positive) square roots of the eigenvalues, which is possible because the eigenvalues are > 0 (since \(B\) is positive-definite). Then define \(\sqrt{B} = Q\sqrt{\Lambda}Q^*\), and by inspection we obtain \((\sqrt{B})^2 = B\). By construction, \(\sqrt{B}\) is positive-definite and Hermitian.

It is easy to see that this \(\sqrt{B}\) is unique, even though the eigenvectors \(X\) are not unique, because any acceptable transformation of \(Q\) must commute with \(\Lambda\) and hence with \(\sqrt{\Lambda}\). Consider for simplicity the case of distinct eigenvalues: in this case, we can only scale the eigenvectors by (nonzero) constants, corresponding to multiplying\(Q\) on the right by a diagonal (nonsingular) matrix \(D\). This gives the same \(B\) for any \(D\), since \(QDA(QD)^{-1} = QADD^{-1}Q^{-1} = Q\Lambda Q^{-1}\) (diagonal matrices commute), and for the same reason it gives the same \(\sqrt{B}\). For repeated eigenvalues \(\lambda\), \(D\) can have off-diagonal elements that mix eigenvectors of the same eigenvalue, but \(D\) still commutes with \(\Lambda\) because these off-diagonal elements only appear in blocks where \(\Lambda\) is a multiple \(\lambda I\) of the identity (which commutes with anything).

(b) Solutions:

(i) From 18.06, \(B^{-1}A\) is similar to \(C = MB^{-1}AM^{-1}\) for any invertible \(M\). Let \(M = B^{1/2}\) from above. Then \(C = B^{-1/2}AB^{-1/2}\), which is clearly Hermitian since \(A\) and \(B^{-1/2}\) are Hermitian. (Why is \(B^{-1/2}\) Hermitian? Because \(B^{1/2}\) is Hermitian from above, and the inverse of a Hermitian matrix is Hermitian.)

(ii) From 18.06, similarity means that \(B^{-1}A\) has the same eigenvalues as \(C\), and since \(C\) is Hermitian these eigenvalues are real.

(iii) No, they are not (in general) orthogonal. The eigenvectors \(Q\) of \(C\) are (or can be chosen) to be orthonormal \((Q^*Q = I)\), but the eigenvectors of \(B^{-1}A\) are \(X = M^{-1}Q = B^{-1/2}Q\), and hence \(X^*X = Q^*B^{-1/2}Q \neq I\) unless \(B = I\).

(iv) Note that there was a typo in the pset. The \texttt{eigvals} function returns only the eigenvalues; you should use the \texttt{eig} function instead to get both eigenvalues and eigenvectors, as explained in the Julia handout.

The array \texttt{lambda} that you obtain in Julia should be purely real, as expected. (You might notice that the eigenvalues are in somewhat random order, e.g. \(-8.11, 3.73, 1.65, -1.502, 0.443\). This is a side effect of how eigenvalues of non-symmetric matrices are computed in standard linear-algebra libraries like LAPACK.) You can check orthogonality by computing \(X^*X\) via \texttt{X'*X}, and the result is not a diagonal matrix (or even close to one), hence the vectors are not orthogonal.

(v) When you compute \(C = X^*BX\) via \texttt{C=X'*B*X}, you should find that \(C\) is nearly diagonal: the off-diagonal entries are all very close to zero (around \(10^{-15}\) or less). They would be \textit{exactly} zero except for roundoff errors (as mentioned in class, computers keep only around 15 significant digits). From the definition of matrix multiplication, the entry \(C_{ij}\) is given by the \(i\)-th row of \(X^*\) multiplied by \(B\), multiplied by the \(j\)-th column of \(X\). But the \(j\)-th column \(X\) is the \(j\)-th eigenvector \(x_j\), and the \(i\)-th row of \(X^*\) is \(x_i^*\). Hence \(C_{ij} = x_i^*Bx_j\), which looks like a dot product but with \(B\) in the middle. The fact that \(C\)
is diagonal means that $x_i^* B x_j = 0$ for $i \neq j$, which is a kind of orthogonality relation.

[In fact, if we define the inner product $(x, y) = x^* B y$, this is a perfectly good inner product (it satisfies all the inner-product criteria because $B$ is positive-definite), and we will see in the next pset that $B^{-1} A$ is actually self-adjoint under this inner product. Hence it is no surprise that we get real eigenvalues and orthogonal eigenvectors with respect to this inner product.]

(c) Solutions:

(i) If we write $x(t) = \sum_{n=1}^4 c_n(t) x_n$, then plugging it into the ODE and using the eigenvalue equation yields

$$\sum_{n=1}^4 [\ddot{c}_n - 2\dot{c}_n - \lambda_n c_n] x_n = 0.$$  

Using the fact that the $x_n$ are necessarily orthogonal (they are eigenvectors of a Hermitian matrix for distinct eigenvalues), we can take the dot product of both sides with $x_m$ to find that $\ddot{c}_n - 2\dot{c}_n - \lambda_n c_n = 0$ for each $n$, and hence

$$c_n(t) = \alpha_n e^{(1+\sqrt{1+\lambda_n})t} + \beta_n e^{(1-\sqrt{1+\lambda_n})t}$$

for constants $\alpha_n$ and $\beta_n$ to be determined from the initial conditions. Plugging in the initial conditions $x(0) = a_0$ and $x'(0) = b_0$, we obtain the equations:

$$\sum_{n=1}^4 (\alpha_n + \beta_n) x_n = a_0,$$

$$\sum_{n=1}^4 ([\alpha_n + \beta_n] + \sqrt{1+\lambda_n}[\alpha_n - \beta_n]) x_n = b_0.$$

Again using orthogonality to pull out the $n$-th term, we find

$$\alpha_n + \beta_n = \frac{x_n^* a_0}{\|x_n\|^2}$$

$$[\alpha_n + \beta_n] + \sqrt{1+\lambda_n}[\alpha_n - \beta_n] = \frac{x_n^* b_0}{\|x_n\|^2} \implies \alpha_n - \beta_n = \frac{x_n^* (b_0 - a_0)}{\|x_n\|^2 \sqrt{1+\lambda_n}}$$

(note that we were not given that $x_n$ were normalized to unit length, and this is not automatic) and hence we can solve for $\alpha_n$ and $\beta_n$ to obtain:

$$x(t) = \sum_{n=1}^4 \left[ x_n^* a_0 + \frac{x_n^* (b_0 - a_0)}{\sqrt{1+\lambda_n}} \right] e^{(1+\sqrt{1+\lambda_n})t} + \left[ x_n^* a_0 + \frac{x_n^* (b_0 - a_0)}{\sqrt{1+\lambda_n}} \right] e^{(1-\sqrt{1+\lambda_n})t} \frac{x_n}{2\|x_n\|^2}.$$  

(ii) After a long time, this expression will be dominated by the fastest growing term, which is the $e^{(1+\sqrt{1+\lambda_n})t}$ term for $\lambda_4 = 24$, hence:

$$x(t) \approx \left[ x_4^* a_0 + \frac{x_4^* (b_0 - a_0)}{5} \right] e^{6t} \frac{x_4}{2\|x_4\|^2}.$$  

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Problem 2: \(((5+5+10)+5+5\) points)

(a) Suppose that we change the boundary conditions to the \textit{periodic} boundary condition \(u(0) = u(L)\).

(i) As in class, the eigenfunctions are sines, cosines, and exponentials, and it only remains to apply the boundary conditions. \(\sin(kx)\) is periodic if \(k = \frac{2\pi n}{L}\) for \(n = 1, 2, \ldots\) (excluding \(n = 0\) because we do not allow zero eigenfunctions and excluding \(n < 0\) because they are not linearly independent), and \(\cos(kx)\) is periodic if \(n = 0, 1, 2, \ldots\) (excluding \(n < 0\) since they are the same functions). The eigenvalues are \(-k^2 = -(2\pi n/L)^2\).

\(e^{kx}\) is periodic only for imaginary \(k = i\frac{2\pi n}{L}\), but in this case we obtain \(e^{i\frac{2\pi n}{L}x} = \cos(2\pi nx/L) + i\sin(2\pi nx/L)\), which is not linearly independent of the sine and cosine eigenfunctions above. Recall from 18.06 that the eigenvectors for a given eigenvalue form a vector space (the null space of \(A\)). Alternatively, it is acceptable to start with exponentials and call our eigenfunctions \(e^{i\frac{2\pi n}{L}x}\) for all integers \(n\), in which case we wouldn’t give sine and cosine eigenfunctions separately.

Similarly, \(\sin(\phi + 2\pi nx/L)\) is periodic for any \(\phi\), but this is not linearly independent since \(\sin(\phi + 2\pi nx/L) = \sin(\phi)\cos(2\pi nx/L) + \cos(\phi)\sin(2\pi nx/L)\).

[Several of you were tempted to also allow \(\sin(m\pi x/L)\) for odd \(m\) (not just the even \(m\) considered above). At first glance, this seems like it satisfies the PDE and also has \(u(0) = u(L) = 0\). Consider, for example, \(m = 1\), i.e. \(\sin(\pi x/L)\) solutions. This can’t be right, however; e.g. it is not orthogonal to \(1 = \cos(0x)\), as required for self-adjoint problems. The basic problem here is that if you consider the periodic extension of \(\sin(\pi x/L)\), then it doesn’t actually satisfy the PDE, because it has a slope discontinuity at the endpoints. Another way of thinking about it is that periodic boundary conditions arise because we have a PDE defined on a torus, e.g. diffusion around a circular tube, and in this case the choice of endpoints is not unique—we can easily redefine our endpoints so that \(x = 0\) is in the “middle” of the domain, making it clearer that we can’t have a kink there. (This is one of those cases where to be completely rigorous we would need to be a bit more careful about defining the domain of our operator.)]

(ii) No, any solution will not be unique, because we now have a nonzero nullspace spanned by the constant function \(u(x) = 1\) (which is periodic): \(\frac{d}{dx} 1 = 0\). Equivalently, we have a 0 eigenvalue corresponding to \(\cos(2\pi nx/L)\) for \(n = 0\) above.

(iii) As suggested, let us restrict ourselves to \(f(x)\) with a convergent Fourier series. That is, as in class, we are expanding \(f(x)\) in terms of the eigenfunctions:

\[
f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i\frac{2\pi n}{L}x}.
\]

(You could also write out the Fourier series in terms of sines and cosines, but the complex-exponential form is more compact so I will use it here.) Here, the coefficients \(c_n\), by the usual orthogonality properties of the Fourier series, or equivalently by self-adjointness of \(A\), are \(c_n = \frac{1}{L} \int_{0}^{L} e^{-i\frac{2\pi n}{L}x} f(x)dx\).

In order to solve \(\frac{d^2 u}{dx^2} = f\), as in class we would divide each term by its eigenvalue \(-(2\pi n/L)^2\), but we can only do this for \(n \neq 0\). Hence, we can only solve the equation if the \(n = 0\) term is absent, i.e. \(c_0 = 0\). Applying the explicit formula for \(c_0\), the equation is
solvable (for \( f \) with a Fourier series) if and only if:

\[
\int_0^L f(x) \, dx = 0.
\]

There are other ways to come to the same conclusion. For example, we could expand \( u(x) \) in a Fourier series (i.e. in the eigenfunction basis), apply \( \frac{d^2}{dx^2} \), and ask what is the column space of \( \frac{d^2}{dx^2} \)? Again, we would find that upon taking the second derivative the \( n = 0 \) (constant) term vanishes, and so the column space consist of Fourier series missing a constant term.

The same reasoning works if you write out the Fourier series in terms of \( \sin \) and \( \cos \) sums separately, in which case you find that \( f \) must be missing the \( n = 0 \) cosine term, giving the same result.

(b) No. For example, the function \( 0 \) (which must be in any vector space) does not satisfy those boundary conditions. (Also adding functions doesn’t work, scaling them by constants, etcetera.)

(c) We merely pick any twice-differentiable function \( q(x) \) with \( q(L) - q(0) = -1 \), in which case \( u(L) - u(0) = \left( v(L) - v(0) \right) + \left( q(L) - q(0) \right) = 1 - 1 = 0 \) and \( u \) is periodic. Then, plugging \( v = u - q \) into \( \frac{d^2}{dx^2} v(x) = f(x) \), we obtain

\[
\frac{d^2}{dx^2} u(x) = f(x) + \frac{d^2 q}{dx^2},
\]

which is the (periodic-\( u \)) Poisson equation for \( u \) with a (possibly) modified right-hand side.

For example, the simplest such \( q \) is probably \( q(x) = x/L \), in which case \( \frac{d^2 q}{dx^2} = 0 \) and \( u \) solves the Poisson equation with an unmodified right-hand side.

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

We are using a difference approximation of the form:

\[
u'(x) \approx \frac{-u(x + 2\Delta x) + c \cdot u(x + \Delta x) - c \cdot u(x - \Delta x) + u(x - 2\Delta x)}{d \cdot \Delta x}.
\]

(a) First, we Taylor expand:

\[
u(x + \Delta x) = \sum_{n=0}^{\infty} \frac{u^{(n)}(x)}{n!} \Delta x^n.
\]

The numerator of the difference formula flips sign if \( \Delta x \to -\Delta x \), which means that when you plug in the Taylor series all of the even powers of \( \Delta x \) must cancel! To get 4th-order accuracy, the \( \Delta x^3 \) term in the numerator (which would give an error \( \sim \Delta x^2 \)) must cancel as well, and this determines our choice of \( c \): the \( \Delta x^3 \) term in the numerator is

\[
\frac{u'''(x)}{3!} \Delta x^3 \left[ -2^3 + c + c - 2^4 \right],
\]

and hence we must have \( c = 2^3 = 8 \). The remaining terms in the numerator are the \( \Delta x \) term and the \( \Delta x^5 \) term:

\[
u'(x) \Delta x \left[ -2 + c + c - 2 \right] + \frac{u^{(5)}(x)}{5!} \Delta x^5 \left[ -2^5 + c + c - 2^5 \right] = 12u'(x) \Delta x - 2 \frac{5}{3} u^{(5)}(x) \Delta x^5 + \cdots.
\]

Clearly, to get the correct \( u'(x) \) as \( \Delta x \to 0 \), we must have \( d = 12 \). Hence, the error is approximately \( -\frac{1}{120} \Delta x^4 \), which is \( \sim \Delta x^4 \) as desired.
Figure 1: Actual vs. predicted error for problem 1(b), using fourth-order difference approximation for $u'(x)$ with $u(x) = \sin(x)$, at $x = 1$.

(b) The Julia code is the same as in the handout, except now we compute our difference approximation by the command: $d = (-\sin(x+2*dx) + 8*\sin(x+dx) - 8*\sin(x+dx) + \sin(x-2*dx)) / (12 * dx)$; the result is plotted in Fig. 1. Note that the error falls as a straight line (a power law), until it reaches $\sim 10^{-15}$, when it starts becoming dominated by roundoff errors (and actually gets worse). To verify the order of accuracy, it would be sufficient to check the slope of the straight-line region, but it is more fun to plot the actual predicted error from the previous part, where $\frac{d^5}{dx^5} \sin(x) = -\cos(x)$. Clearly the predicted error is almost exactly right (until roundoff errors take over).