Please submit your solutions to the following problems on Gradescope by **10pm** on the due date. Collaboration is encouraged, however, you must write up your solutions individually.

1) Differential Operators. Consider the linear differential operator defined by

$$[Lu](x) = u'(x) + x\,u(x), \qquad u \in \mathcal{C}^1[-1,1].$$

(a) Describe the null-space of L, that is, find all solutions to $Lu = 0$.

Solution: The nullspace of L is the set of solutions to the homogeneous equation $Lu = u'(x) + xu(x) = 0$. Multiplying both sides of the equation by the integrating factor $\exp(x^2/2)$, we find that the left-hand side is equal to

$$e^{x^2/2}\left(u'(x) + xu(x)\right) = (e^{x^2/2}u(x))'.$$

Integrating directly on both sides and solving for the unknown function $u(x)$, we obtain

$$u(x) = Ce^{-x^2/2}, \qquad \text{where} \qquad C = \text{integration constant}.$$

This means that the Gaussian $e^{-x^2/2}$ is a basis for the one-dimensional nullspace of L.

Now, apply a boundary condition $u(-1) = 0$ and restrict the domain of L to the subspace of continuously differentiable functions that satisfy this boundary condition.

(b) Calculate the adjoint of L, that is, find $L^\dagger$ such that $\int_{-1}^1 v(x)[Lu](x)\,dx = \int_{-1}^1 u(x)[L^\dagger v](x)$ holds for any $u, v \in \mathcal{C}^1[-1,1]$ satisfying $u(-1) = 0$ and $v(1) = 0$. Does $L^\dagger L = LL^\dagger$?

Solution: We can calculate the adjoint of L by integrating-by-parts once. Then,

$$\begin{aligned}\int_{-1}^1 v(x)\left[u'(x) + xu(x)\right]\,dx &= \int_{-1}^1 v(x)u'(x)\,dx + \int_{-1}^1 v(x)xu(x)\,dx \\ &= u(1)v(1) - u(-1)v(-1) - \int_{-1}^1 v'(x)u(x)\,dx + \int_{-1}^1 xv(x)u(x)\,dx \\ &= \int_{-1}^1 \left[-v'(x) + xv(x)\right]u(x)\,dx.\end{aligned}$$

Notice that the boundaries terms from integration-by-parts vanish because of the restrictions $u(-1) = 0$ and $v(1) = 0$ on the domains of L and $L^\dagger$, respectively.

The product of the operator and its adjoint is a second-order differential operator

$$\begin{aligned}[L^\dagger Lu](x) = \left[-\frac{d}{dx} + x\right]\left[\frac{d}{dx} + x\right]u(x) &= -u''(x) - (xu(x))' + xu'(x) + x^2u(x) \\ &= -u''(x) + (x^2 - 1)u(x).\end{aligned}$$

Switching the order of the products, we obtain a different differential operator

$$\begin{aligned}[LL^\dagger u](x) = \left[\frac{d}{dx} + x\right]\left[-\frac{d}{dx} + x\right]u(x) &= -u''(x) + (xu(x))' - xu'(x) + x^2u(x) \\ &= -u''(x) + (x^2 + 1)u(x).\end{aligned}$$

Therefore, $L^\dagger L \neq LL^\dagger$: we say that L is a *non-normal* differential operator. The eigenvectors of non-normal operators do not form an orthogonal basis for $L^2(-1,1)$.

(c) Calculate the inverse of L, that is, find an integral operator K such that $Lu = f$ if and only if $u = Kf$. (Hint: use the method of integrating factors from 18.03.)

Solution: Multiplying both sides of $Lu = f$ by the integrating factor $\exp(x^2/2)$ as in part (a), we integrate both sides from $y = -1$ to $y = x$ and apply the boundary condition $u(-1) = 0$ to obtain

$$e^{x^2/2}u(x) = \int_{-1}^{x} e^{y^2/2} f(y)\, dy.$$

Multiplying both sides by $e^{-x^2/2}$ to solve for $u(x)$, we arrive at the expression

$$u(x) = e^{-x^2/2} \int_{-1}^{x} e^{y^2/2} f(y)\, dy.$$

Therefore, the inverse of L is the integral operator $[Kf] = e^{-x^2/2} \int_{-1}^{x} e^{-y^2/2} f(y)dy$.

2) Central Differences. The `hw1.jl` notebook on the course repository may be helpful for the computational components of this exercise (`https://github.com/mitmath/18303/`).

(a) Show that the centered difference formula (see Lecture 3 notes) approximates $u'(x)$ with accuracy proportional to h^2 if $u(x)$ has three continuous derivatives.

Solution: If $u(x)$ has three continuous derivatives, then a third-order Taylor expansion around grid point x_k gives (for some $-1 \leq \xi_+ \leq 1$) a formula for $u(x_{k+1}) = u(x+h)$,

$$u(x+h) = u(x_k) + u'(x_k)h + \frac{1}{2}u''(x_k)h^2 + \frac{1}{6}u'''(\xi_+)h^3.$$

Similarly, we obtain (for some $-1 \leq \xi_- \leq 1$) a formula for $u(x_{k-1}) = u(x-h)$,

$$u(x-h) = u(x_k) - u'(x_k)h + \frac{1}{2}u''(x_k)h^2 - \frac{1}{6}u'''(\xi_-)h^3.$$

Taking the difference of the two formulas, dividing by $2h > 0$, and solving for $u'(x_k)$, we obtain

$$u'(x_k) = \frac{u(x+h) - u(x-h)}{2h} + \frac{h^2}{3}(u'''(\xi_+) + u'''(\xi_-)).$$

Since $u'''(x)$ is continuous on $[-1, 1]$ it achieves a maximum on that interval and the last term on the left is bounded by a constant proportional to h^2. We have the bound

$$\left| u'(x_k) - \frac{u(x+h) - u(x-h)}{2h} \right| \leq \frac{2M}{3}h^2, \qquad \text{where} \qquad M = \max_{-1 \leq y \leq 1} |u'''(y)|.$$

(b) Derive a fourth-order accurate centered difference formula to approximate $u'(x)$ from samples $u(x-2h), u(x-h), u(x), u(x+h), u(x+2h)$ with grid spacing $h > 0$.

Solution: Supposing that $u(x)$ has five continuous derivatives, we can develop Taylor expansions of the samples around the central point x. For $x + h$, we have

$$u(x+h) = u(x) + u'(x)h + \frac{1}{2}u''(x)h^2 + \frac{1}{6}u'''(x)h^3 + \frac{1}{24}u^{(4)}(x)h^4 + \frac{1}{120}u^{(5)}(\xi_{+h})h^5,$$

while for $x - h$, we have

$$u(x-h) = u(x) - u'(x)h + \frac{1}{2}u''(x)h^2 - \frac{1}{6}u'''(x)h^3 + \frac{1}{24}u^{(4)}(x)h^4 - \frac{1}{120}u^{(5)}(\xi_{-h})h^5.$$

Taking the difference of the two formulas as before, we calculate the difference

$$u(x+h) - u(x-h) = 2u'(x)h + \frac{1}{3}u'''(x)h^3 + \frac{1}{120}\left(u^{(5)}(\xi_{+h}) - u^{(5)}(\xi_{-h})\right)h^5.$$

Now, the key idea is to improve the order of accuracy by incorporating the extra samples to eliminate the h^3 term. Taking the difference $u(x+2h) - u(x-2h)$ and repeating the Taylor series argument above, we find that

$$u(x+2h) - u(x-2h) = 2u'(x)(2h) + \frac{1}{3}u'''(x)(2h)^3 + \frac{1}{120}\left(u^{(5)}(\xi_{+2h}) - u^{(5)}(\xi_{-2h})\right)(2h)^5.$$

If we multiply the first difference $(u(x+h) - u(x-h))$ by $2^3 = 8$ and subtract the new difference $(u(x+2h) - u(x-2h))$, we cancel the h^3 term and obtain

$$8\left(u(x+h) - u(x-h)\right) - \left(u(x+2h) - u(x-2h)\right) = 12u'(x)h + \mathcal{O}(h^5).$$

The notation $\mathcal{O}(h^5)$ is used here as a shorthand for the term proportional to h^5. Solving for $u'(x)$ by dividing by $12h$, we obtain the fourth-order accurate approximation

$$u'(x) = \frac{-u(x+2h) + 8u(x+h) - 8u(x-h) + u(x-2h)}{12h} + \mathcal{O}(h^4).$$

An error bound can be calculated explicitly, using $M = \max_{-1\leq y\leq 1}|u^{(4)}(y)|$, as

$$\left|u'(x) - \frac{-u(x+2h) + 8u(x+h) - 8u(x-h) + u(x-2h)}{12h}\right| \leq \frac{M}{18}h^4.$$

However, this error bound may not hold where $u(x)$ is not sufficiently smooth and the Taylor formulas with remainder term are not valid! See numerical experiments below.

(c) For parts (a) and (b), what are the corresponding difference matrices representing differentiation on a grid of n equispaced points (with spacing $h = 1/(n+1)$) on the periodic interval $[0, 1)$? What can you say about the pattern of nonzero entries?

Solution: The second-order and fourth-order differences approximate $u'(x_k)$ by linear combinations of samples of $u(x)$ at the adjacent two and four, respectively, grid points. The second-order matrix is skew-symmetric, meaning that $A = -A^T$, constant along each diagonal, and is tridiagonal except for two nonzero corner entries corresponding to periodic boundary conditions. The fourth-order matrix is also skew symmetric, constant along each diagonal, and is pentadiagonal except for three nonzero entries in each corner corresponding to the periodic boundary conditions. See `hw1_soln.jl` for the construction and visualization of the second- and fourth-order difference matrices.

(d) Use the matrices in part (c) to approximate the derivatives of the functions $\sin(2\pi x)$, $\cos(\pi(x-0.5))$, and $\sqrt{(1+\cos(2\pi x))^3}$ on an equispaced grid of $n = 500$ points on the periodic interval $[0,1)$. Plot the error in your approximation of the derivative at each grid point and then plot the maximum absolute error on grids with $n = 100, 200, 300, \ldots, 10^4$ (use a logarithmic scale for both axes). Can you explain the behavior of the error for each function (e.g., why proportional to h^2, h^4, etc.)?

Solution: See `hw1_soln.jl` for the numerical experiments and plots. The first function is infinitely-differentiable and periodic on the unit interval so that second- and fourth-order difference approximations converge at rates of h^2 and h^4, respectively. The second function is infinitely differentiable on $[-1,1)$, but not periodic. In effect, it is not differentiable at the point $x=-1$ on the periodic interval so the difference approximation does not converge there. The final function has only two continuous derivatives at $x=\pm 1/2$ and is not three times differentiable there. However, numerical experiments reveal that both second- and fourth-order approximations still converge at a rate proportional to h^2 there. One can explain the persistence of h^2 convergence by replacing the Lagrange form of the remainder in the Taylor series arguments (see parts (a) and (b)) with a more general integral form of the remainder that requires only the *absolutely continuity* of $u''(x)$, which holds in this case.

3) Method of Characteristics. Consider the first-order linear PDEs with form

$$\partial_t u(x,t) + b(x)\,\partial_x u(x,t) + c\,u(x,t) = 0, \qquad \text{where} \qquad u(x,0) = g(x).$$

(a) Find the characteristic curves for $b(x) = x^2$ and plot them in the (x,t)-plane.

Solution: When $b(x) = x^2$, the characteristic curves with parametrization $(x(s), t(s)$ are defined by the ordinary differential equations

$$\frac{dt}{ds} = 1, \qquad \text{and} \qquad \frac{dx}{ds} = x^2.$$

Integrate the first equation directly to obtain $t(s) = s + t(0) = s$, since $t(0) = 0$. The second equation can be solved with separation of variables, yielding $x(s) = 1/(x_0^{-1} - s)$ if $x(0) = x_0 \neq 0$ and $x(s) = 0$ if $x(0) = x_0 = 0$. Substituting $t(s) = s$, we have

$$x(t) = x_0/(1 - x_0 t), \qquad 0 \le t < 1/x_0.$$

Note that when $x_0 > 0$, the characteristic curves "blow-up" in finite time because there is a vertical asymptote at $t = 1/x_0$. The rate-of-change in the x-coordinate increases quadratically as x increases, leading to this finite-time instability. When $x_0 < 0$, $x(t)$ decreases in magnitude and the characteristics tend toward the origin, with $\lim_{t\to\infty} x(t) = 0$. See `hw1_soln.jl` for plots of the characteristic curves $(x(s), t(s))$.

(b) Given initial condition $g(x) = \exp(-100(x-0.5)^2)$, write down a solution $u(x,t)$ when $c = 0$. Is the solution unique? How does the solution change if $c = 1$?

Solution: The behavior of the solution along a characteristic curve is governed by the third ordinary differential equation:

$$\frac{du}{ds} = \frac{\partial u}{\partial x}\frac{dx}{ds} + \frac{\partial u}{\partial t}\frac{dt}{ds} = -cu, \qquad \text{where} \qquad u(0) = u_0.$$

The solution to this ODE is given by the exponential function, $u(s) = u_0 e^{-cs}$. Substituting the characteristic formulas for $x(s)$ and $t(s)$ into this solution, we find that

$$u(x(s), t(s)) = u_0(x_0, 0)e^{-cs} = g(x/(1 + tx))e^{-ct}.$$

Note that the third equality is derived by solving for x in terms of x_0 and substituting.

When $c = 0$, the initial values of $u(x_0, 0) = g(x_0)$ are simply transported along the characteristic curves. With the given Gaussian initial condition centered at $x_0 = 1/2$, the Gaussian will stretch out and transport rapidly to the right. When $c = 1$, the solution decays exponentially with rate c along the characteristic curves, leading to a loss of amplitude in the Gaussian during transport.

(c) Use a forward Euler approximation in time and a second-order centered difference in space to approximate $u(x, t)$ on the periodic interval $x \in [0, 1)$ from time $t = 0$ to $t = 1$. Use time step $h_t = 0.01$ and spatial grid of length 200. How does your numerical solution compare to the exact solution in part (b) for the case $c = 0$? How does it compare with the forward difference spatial discretization provided in `hw1.jl`?

Solution: See `hw1_soln.jl` for the numerical experiments.