Homework 4
Due: May 21, 2021

1. Consider solving the following heat equation with "linked" boundary conditions

$$\begin{cases} u_t = \frac{1}{2}u_{xx} \\ u(0,t) = su(1,t) \\ u_x(0,t) = u_x(1,t), \\ u(x,0) = \eta(x), \end{cases}$$

where $s \neq -1$. Recall that the MOL discretization with the standard second-order stencil can be written as

$$U'(t) = \frac{1}{2h^2}AU(t) + \begin{bmatrix} \frac{U_0(t)}{2h^2} \\ \vdots \\ \frac{U_{m+1}(t)}{2h^2} \end{bmatrix}, \quad A = \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 \end{bmatrix}.$$

The first boundary condition is naturally enforced via $U_0(t) = sU_{m+1}(t)$. Show that if we suppose

$$\frac{U_1(t) - U_0(t)}{h} = \frac{U_{m+1}(t) - U_m(t)}{h},$$

then the MOL system becomes

$$U'(t) = \frac{1}{2h^2}BU(t), \quad B = \begin{bmatrix} -2 + \frac{s}{1+s} & 1 & & & & \frac{s}{1+s} \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ \frac{1}{1+s} & & & & 1 & -2 + \frac{1}{1+s} \end{bmatrix}. \tag{1}$$

Solution.

Rearranging yields

$$\begin{aligned} U_1 - U_0 &= -2U_0 + U_1 + U_0 \\ &= -2U_0 + U_1 + \frac{s}{1+s}(1+s)U_{m+1} \\ &= -2U_0 + U_1 + \frac{s}{1+s}(U_0 + U_{m+1}) \\ &= (-2 + \frac{s}{1+s})U_0 + U_1 + \frac{s}{1+s}U_{m+1} \end{aligned}$$

which is the first row of B. The last row becomes

$$\begin{aligned}
U_m - U_{m+1} &= U_0 - U_1 \\
&= (2 - \frac{s}{1+s})U_0 - U_1 - \frac{s}{1+s}U_{m+1} \\
&= (2 - \frac{s}{1+s})U_0 - (U_{m+1} - U_m + U_0) - \frac{s}{1+s}U_{m+1} \\
&= \frac{1}{1+s}U_0 + U_m - (\frac{1+2s}{1+s})U_{m+1} \\
&= \frac{1}{1+s}U_0 + U_m - (\frac{2+2s-1}{1+s})U_{m+1} \\
&= \frac{1}{1+s}U_0 + U_m + (-2 + \frac{1}{1+s})U_{m+1}
\end{aligned}$$

2. Apply the backward Euler method to (1) to give

$$\left(I - \frac{k}{2h^2}B\right)U^{n+1} = U^n, \quad U^n = \begin{bmatrix} U_1^n \\ U_2^n \\ \vdots \\ U_m^n \end{bmatrix}, \tag{2}$$

and write a routine to solve the system (1) with initial condition

$$\eta(x) = e^{-20(x-1/2)^2},$$

using $k = h$ and $h = 0.001$ with $s = 2$. Plot the solution at times $t = 0.001, 0.01, 0.1$. Note: One could use trapezoid to solve this problem but it wouldn't preserve some important features that we care about. See the last extra credit problem.

Solution.

The backward Euler has the form

$$\begin{aligned} U^{n+1} &= U^n + kf(U^{n+1}) = U^n + \frac{k}{2h^2}BU^{n+1} \\ U^{n+1} &= \left(I - \frac{k}{2h^2}B\right)^{-1} U^n \end{aligned}$$

We implement this in `backward_euler`. See Figure 1.

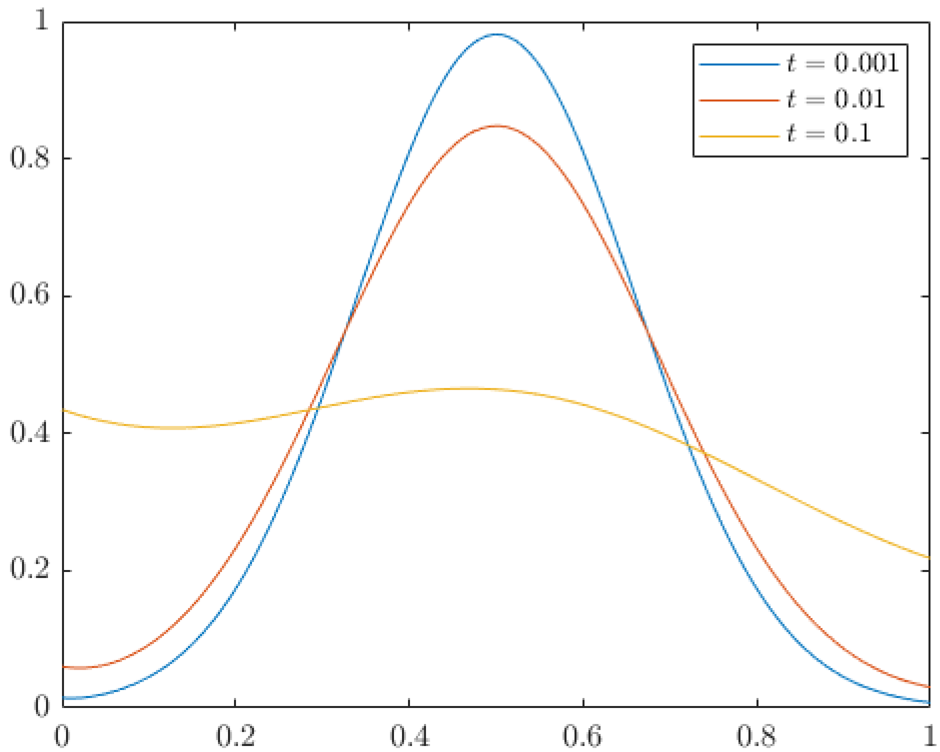

Figure 1: Solution of the heat equation using backward Euler

3. In the next two problems you will use the heat equation to assist with a statistics problem.

   - Consider data points $X_1, X_2, \ldots, X_N, \ldots$ each being a real number arising from a repeated experiment. We may want to know what probability distribution (if any) they come from. One way of coming up with an approximation to the density is to use

$$\frac{1}{N} \sum_{j=1}^{N} \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{(x - X_j)^2}{2t}\right), \quad t > 0. \tag{3}$$

     Use normally distributed random data (`X = randn(n)` in `Julia`, `X = randn(n,1)` in `Matlab` and `X = numpy.random.randn(n,1)` in `Python`) with $n = 10000$ and plot this function for $t = 0.001, 0.01, 0.1, 1, 10$ and compare it with the true probabilty density function for the data: $\rho(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$. Visually, which "time" t gives the best approximation?

     Note: The solution of the heat equation $u_t = \frac{1}{2} u_{xx}$ with initial condition $u(x, 0) = \delta(x)$ where δ is the standard Dirac delta function is given by $u(x, t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right)$. So (3) can be seen as the solution of $u_t = \frac{1}{2} u_{xx}$ with

$$u(x, 0) = \frac{1}{N} \sum_{j=1}^{N} \delta(x - X_j).$$

   - The previous approach works well if the underlying distribution is smooth and decays exponentially in both directions. But there physical situations within cell biology, in particular, where the density should only be non-zero on a finite interval $[0, 1]$ and satisfy some natural boundary conditions:

$$\rho(0) = s\rho(1), \quad \rho'(0) = \rho'(1).$$

     An example of such a function for $s = 2$ is given by

$$\rho(x) = -\frac{2}{3}x + \frac{4}{3} + \frac{1}{2}\sin(2\pi x).$$

     Code to generate $X_1, X_2, \ldots, X_N, \ldots$ with this probability density in our three languages is given at the end of the homework. Repeat the calculation in the prevous part with this data, $X_1, X_2, \ldots$.

Solution.

Clearly $t = 0.01$ gives the best approximation for the first distribution.

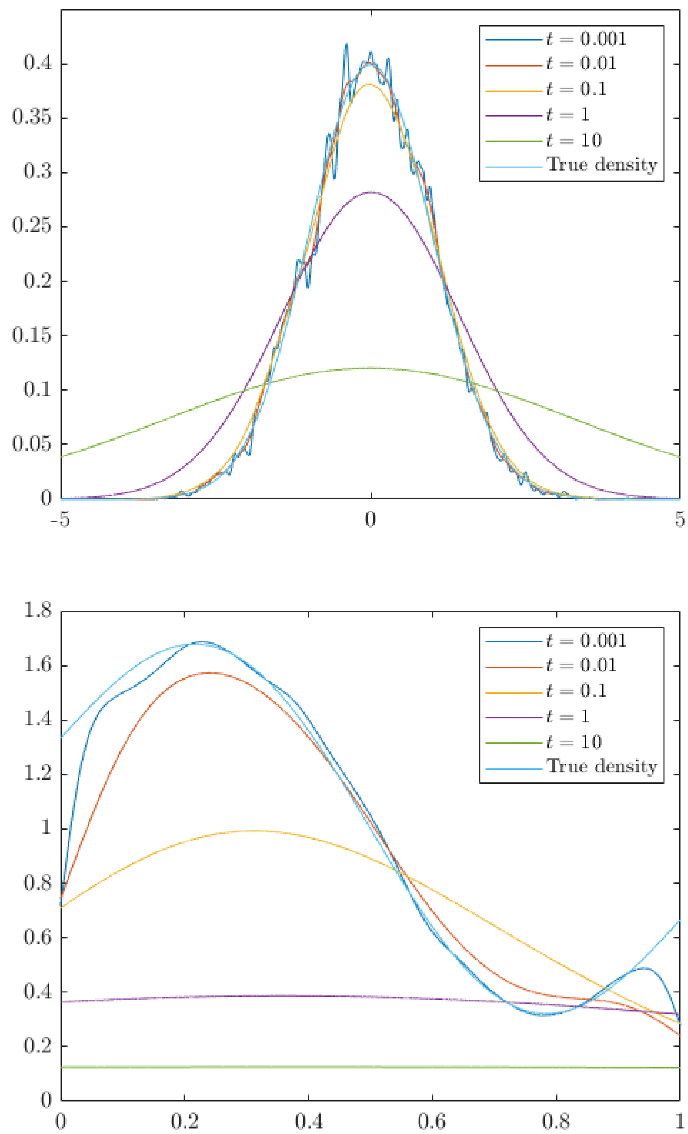

Figure 2: Approximations using normal distributions.

4. Consider binning data $X_1, X_2, \ldots, X_N$, $X_j \in (0,1)$ as follows:

   - Find Y_i so that Y_i is the number of data points X_j that lie in the interval $[ih, (i+1)h) = [x_i, x_{i+1})$.
   - Set $U_i^0 = \frac{Y_i}{hN}$.

   With $N = m$, $h = 0.0001$, $k = 10h$, $s = 2$, generate $X_1, \ldots, X_N$ using the `prand` function, and bin the data to get the initial condition U_i^0, $i = 1, 2, \ldots, m$ for the MOL discretization (1). Solve with this initial condition using your code from **Problem 2** to times $t = 0.001, 0.01, 0.1$. Compare with Part 2 of Problem 3.

Solution.

Clearly this method works better than that used in part 2 of problem 3.

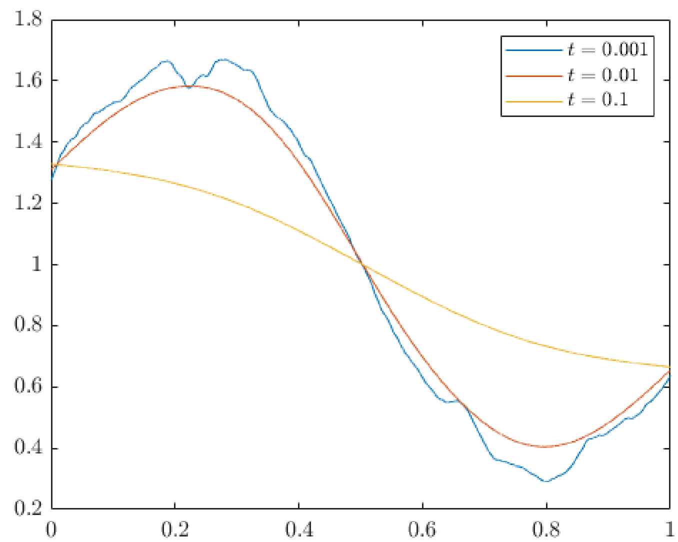

Figure 3: Approximation of binned data

5. Suppose the following is true: For $s > 0$, if y is a vector with non-negative entries and $\left(I - \frac{k}{2h^2}B\right)x = y$ then x has non-negative entries.

   For $s > 0$, establish the following:

   - $\begin{bmatrix}1 & 1 & \cdots & 1\end{bmatrix} B = 0$ and therefore $\sum_j U_j^n = \sum_j U_j^0$ for all n.
   - Show that (2) is Lax-Richtmeyer stable in the 1-norm, $\|u\|_1 = h\sum_{i=1}^m |u_i|$.

   Solution.

   $\begin{bmatrix}1 & 1 & \cdots & 1\end{bmatrix} B$ is the column sum of B, which is always 0. Taking dot product between y and 1-vector

$$\begin{bmatrix}1 & 1 & \cdots & 1\end{bmatrix}\left(I - \frac{k}{2h^2}B\right)x = \begin{bmatrix}1 & 1 & \cdots & 1\end{bmatrix} y$$
$$\sum_j x_j = \sum_j y_j$$

   Since $\left(I - \frac{k}{2h^2}B\right)U^1 = U^0$, we have $\sum_j U_j^1 = \sum_j U_j^0$. Applying this relation iteratively to $U^1, \ldots, U^{n-1}$, we have

$$\sum_j U_j^n = \sum_j U_j^0$$
$$h\sum_j |U_j^n| = h\sum_j |U_j^0|$$
$$\|U^n\|_1 = \|U^0\|_1$$

   We know that

$$\|U^n\|_1 = \|B(k)^n U^0\|_1$$

   where $B(k) = (I - \frac{k}{2h^2}B)^{-1}$. Then it must be true that

$$\|B(k)^n U^0\|_1 = \|U^0\|_1 \tag{4}$$

   for U^0 with non-negative entries. Suppose V^0 has non-positive entries, since $-V^0$ has non-negative entries

$$\|B(k)^n V^0\|_1 = \|V^0\|_1 \tag{5}$$

   Adding (4) and (5) and letting $W^0 = U^0 + V^0$

$$\|B(k)^n W^0\|_1 = \|W^0\|_1$$

   Since W^0 can be any vector, we prove that (2) is Lax-Richtmeyer stable.

6. A challenge (extra credit): For $s > 0$, establish:

   - If y is a vector with non-negative entries and $\left(I - \frac{k}{2h^2}B\right)x = y$ then x has non-negative entries.

   Note that this shows that if $\sum_j U_j^0 = 1$ then at each step n we can interpret U_j^n as the evolution of a probability distribution.

   Solution.

   Since the eigenvalues of $I - \frac{k}{2h^2}B$ are in $\left[1 + \frac{k}{h^2} - \frac{ks}{2h^2(1+s)}, 1 + \frac{k}{h^2}\right]$, we have $I - \frac{k}{2h^2}B \geq 0$, thus $B(k) = (I - \frac{k}{2h^2}B)^{-1} \geq 0$. Since $y \geq 0$, $x = B(k)y \geq B(k)0 = 0$.