1.

a) Make a graph of the boundary of the absolute stability region for the Runge-Kutta RK4 method on page 24.

b) Apply the RK4 method to $u' = 30u(1-u)$ with u(0) = 0.1 on the interval $0 \le t \le 2$. Use 14, 17 and 25 steps. For each run graph the numerical solution and the exact solution on the same plot.

c) Explain the previous sequence of graphs in terms of the ODE and the plot from part a. Your answer should contain a quantitative explanation for why the transiton occurs at the value of h you observe.

Solution, part a:
The RK4 method applied to $u' = \lambda u$ becomes

$$u_{i+1} = R(z)u_i$$

where $R(z) = 1 + z + z^2/2 + z^3/3! + z^4/4!$. The boundary of the stability region is therefore those values of z such that $|R(z)| = 1$. The worksheet has a graph of this region.

Solution, part b:
See worksheet.

Solution, part c:
The exact solution of the IVP is

$$u(t) = \frac{1}{1 + 9e^{-30t}}.$$

As $t \to \infty$, $u(t) \to 1$. We can write $u(t) = 1 + w(t)$ where w is a small perturbation for large values of t. Inserting this into the ODE we find

$$w' = 30(1+w)(-w) = -30w - 30w^2.$$

When w is close to 0, we can ignore the w^2 term and we find that

$$w' \approx -30w.$$

That is, w is a transient with large exponential decay. To accurately capture it with RK4, and not experience instability, we need to pick a time step such that $z = -30h$ lies in the absolute stability region. From the graph of the absolute stability region in part a, we see that this requires $-3 < -30h$. Since $h = 2/M$, where M is the number of time steps, this condition becomes $2/M < 1/10$, or $M > 20$. The unusual behaviour observed for $M = 14$ and $M = 17$ are a consequence of the violation of z laying in the absolute stability region.

2. The θ-method for finite difference solutions of ODEs is

$$u_{n+1} = u_n + h[\theta f_{n+1} + (1-\theta) f_n]$$

where $\theta \in [0,1]$.

a) Compute the order of convergence of this method. Hint: it depends on θ.

b) Numerically graph the boundary of the absolute stability region for $\theta = 1/4$.

c) Show that the method is A-stable if and only if $\theta \geq 1/2$.

d) Bonus: Analytically compute the boundary of the absolute stability region for $\theta = 1/4$

Solution, part a:
Let u be a solution of $u' = f(t,u)$. We have

$$\begin{aligned} u(t_n+h) &= u(t_n) + u'(t_n)h + u''(t_n)\frac{h^2}{2} + u'''(t_n)\frac{h^3}{6} + O(h^4) \\ u'(t_n+h) &= u'(t_n) + u''(t_n)h + u'''(t_n)\frac{h^2}{2} + O(h^3). \end{aligned} \tag{1}$$

Subsituting u into the differential form of the finite difference scheme we find

$$\begin{aligned} \frac{u(t_n+h)-u(t_n)}{h} - \theta u'(t_n+h) - (1-\theta)u'(t_n) &= u'(t_n) + u''(t_n)\frac{h}{2} + u'''(t_n)\frac{h^2}{6} \\ &\quad - \theta\left[u'(t_n) + u''(t_n)h + u'''(t_n)\frac{h^2}{2}\right] \\ &\quad - (1-\theta)u'(t_n) + O(h^3) \\ &= u''(t_n)\left[\frac{1}{2}-\theta\right]h + u'''(t_n)\left[\frac{1}{6}-\frac{\theta}{2}\right]h^2 + O(h^3). \end{aligned} \tag{2}$$

Thus the scheme is $O(h)$ unless $\theta = 1/2$, in which case it is $O(h^2)$.

Solution, part b:
The stability polynomial for this scheme comes from subsituting $u_{n+1} = \rho$, $u_n = 1$ and $f(t,u) = \lambda u$. That is

$$\rho = 1 + z(\theta\rho + (1-\theta))$$

so

$$p(\rho) = (1-\theta z)\rho - (1 + z(1-\theta)).$$

The root of this polynomial is

$$\rho = \frac{1+(1-\theta)z}{1-\theta z}.$$

Solving for z instead we find

$$z = \frac{\rho-1}{\theta\rho+(1-\theta)} = \frac{\rho-1}{1+\theta\rho-1}$$

The worksheet contains a plot of z for $\rho = e^{is}$ with $0 \leq s \leq 2\pi$.

Solution, part c:
Notice that $|\rho| = 1$ if and only if

$$|1 + (1-\theta)z|^2 = |1 - \theta z|^2$$

which is equivalent to

$$1 + (1-\theta)(z + \overline{z}) + (1-\theta)^2|z|^2 = 1 - \theta(z + \overline{z}) + \theta^2|z|^2.$$

This last equation is the same as

$$2\Re(z) + (1 - 2\theta)|z|^2 = 0$$

or

$$2\Re(z) = (2\theta - 1)|z|^2.$$

Setting $a = 1/(2\theta - 1)$, and writing $z = x + iy$, this equation becomes

$$(x-a)^2 + y^2 = a^2,$$

i.e. the circle of radius $|a|$ centered at $x = a$, $y = 0$.

To determine if the scheme is A-stable, we need to determine if the left half plane lies in the stability region. Moreover, when $z = -1$, the root of the stability polynomial is

$$\rho = \frac{\theta}{1+\theta}$$

which has norm less than 1. So part of the negative real axis is always in the absolute stability region. Thus the absolute stability region contains the left half plane if and only if the boundary of the absolute stability region is contained in the region $\Re(z) \geq 0$.

When $\theta < 1/2$, $a < 0$ and the boundary of the stability region includes $x = a$, $y = 0$, a point in the left half plane. So the scheme is not A-stable. On the other hand, if $\theta \geq 1/2$ the boundary of the stability region is a circle contained in the region $\Re(z) \geq 0$ (or the y-axis when $\theta = 1/2$). Thus for $\theta \geq 1/2$ the scheme is A-stable.

Solution, part d:
When $\theta = 1/4$, the above analysis shows the boundary of the stability region is the circle of radius 2 centered at $x = -2$, $y = 0$.

3. Newton's method can be used to solve

$$f(x) = 0$$

where $x \in \mathbb{R}^n$ and $f(x) \in \mathbb{R}^n$. Starting from an initial guess x_k,

$$x_{k+1} = x_k - Df(x_k)^{-1} f(x_k).$$

Here, $Df(x)$ is the Jacobian matrix

$$Df_{ij} = \frac{\partial f_i}{\partial x_j}$$

Implement Newton's method for systems. Your function should take as arguments f, Df and x_0 (an initial guess). It should terminate whenever either

- $|f(x)|_\infty$ is less than a specified tolerance
- $|f(x)|_\infty$ is less than a sepcified fraction of $|f(x_0)|_\infty$.

These tolerances should be specified with optional arguments as used in your language of choice, with values of 10^{-8} as the default.

Your function should return the estimated root and, as a diagnostic, the number of iterations needed to find the root.

Test your code against solving the simultaneous equations $x^2 + y^2 = 1$ and $x = y$ starting from $x = 0$, $y = 3$. Report the root found and the number of iterations needed to find it.

Solution:
See worksheet.

4. The energy for the heat equation $u_t = u_{xx}$ for $0 \le x \le 1$ is

$$E(t) = \frac{1}{2}\int_0^1 (u_x(x,t))^2\,dx.$$

a) Assuming that at $x = 0$ and at $x = 1$ u satisfies either a homogeneous Dirichlet condition or a homogeneous Neumann condition, show that

$$\frac{d}{dt}E(t) \le 0.$$

Hint: Take a time derivative, use the PDE, and integrate by parts.

b) Conclude that the only solution of $u_t = u_{xx}$ with $u = 0$ at $t = 0$, and at $x = 0$ and $x = 1$ is the zero solution.

Solution, part a:
From integration by parts and applying the heat equation,

$$\begin{aligned}
\frac{d}{dt}E(t) &= \int_0^1 u_x(x,t)u_{tx}(x,t)\,dx \\
&= \int_0^1 u_x(x,t)\frac{d}{dx}u_t(x,t)\,dx \\
&= -\int_0^1 u_x x(x,t)u_t(x,t)\,dx + u_x u_t|_{x=0}^1 \\
&= -\int_0^1 u_t(x,t)u_t(x,t)\,dx + u_x u_t|_{x=0}^1
\end{aligned} \tag{3}$$

At an endpoint where a homogeneous Neuman condition holds, $u_x = 0$, so $u_x u_t = 0$. On the other hand, at an endpoint where a homogeneous Diriclhet condition holds, $u_t = 0$ and $u_x u_t = 0$. Thus there are no contributions from the boundary terms and we find

$$\frac{d}{dt}E(t) = -\int_0^1 u_t(x,t)u_t(x,t)\,dx \le 0.$$

Solution, part b:

Suppose we start with initial data $u = 0$. Then the initial energy is zero as well. But energy decreases in time and is non-negative. So $E(t) = 0$ for all t. This implies $u_x = 0$ for all x and t. So x is constant at each time, and from the boundary conditions we conclude $u = 0$ everywhere.

5. The backwards heat equation reads

$$u_t = -u_{xx},$$

so all that differs is a sign on the right-hand side. But this sign makes all the difference.

We will work with this equation for $0 \le x \le 1$ and $0 \le t \le 1$, and with homogeneous Dirichlet boundary conditions, so $u = 0$ at $x = 0$ and $x = 1$.

a) Show that

$$v(t) = \sin(k\pi x)e^{k^2\pi^2 t}$$

is a solution of the PDE and the boundary conditions.

b) For each $\epsilon > 0$, find a solution of the PDE and boundary conditions that satisfies $|u(0,x)| < \epsilon$ at each x, but $|u(1,x)| \ge 1$ at some x.

c) Suppose you wish to find the solution u of the backwards heat equation with initial condition u_0. But you don't know u_0 exactly, you know $\hat{u}_0$, and that $|u_0(x) - \hat{u}_0(x)| < 10^{-47}$ at every x. So you solve the backwards heat equation for $\hat{u}$ instead. Find an L such that $|u(x,1) - \hat{u}(x,1)| < L$ for all x, or explain why no such L exists.

Solution, part a:
Evidently $v_t(x,t) = (k^2\pi^2)v$ and $v_{xx} = -(k^2\pi^2)v$. So $v_t = -v_{xx}$.

Solution, part b:
Let $\epsilon > 0$. Pick a natural number k such that $e^{k^2\pi^2} > 1/\epsilon$. Observe that

$$u(x,t) = \epsilon \sin(k\pi x)e^{k^2\pi^2 t}$$

solves the backwards heat equation (by part a), and satisfies $|u| \le \epsilon$ at $t = 0$. But at $t = 1$ there is a choice of x such that $|\sin(k\pi x)| = 1$, and at that point,

$$|u(x,t)| = \epsilon e^{k^2\pi^2} > 1$$

by our choice of k.

Solution, part c:
No such L exists. There is nothing special about the number 1 in the previous argument. For any $\epsilon > 0$ there is a solution of the backwards heat equation that satisfies $|u| \le \epsilon$ at $t = 0$ but such that $|u| \ge L$ at $t = 1$ This applies when $\epsilon = 10^{-43}$. So in effect, if there is any

error in our estimate of the initial data, we have no estimate whatsoever for the value of the solution at $t = 1$.

6. Implement the explict method for solving the heat equation with right-hand side function

$$u_t = u_{xx} + f$$

on $0 \le x \le 1$ and $0 \le t \le T$. You function should have the following signature:

forcedheat(f,u0,N,M)

where

- $f(x,t)$ is a function and provedes the desired forcing term
- $u0(x)$ is a function and provides the desired initial condition.
- $N+1$ is the number of interior spatial steps
- M is the number of time steps

It should return (x,t,u) where x is an array of grid coordinates that includes 0 and 1, t is a vector of t coordinates that includes 0 and T, and where u is an $(N+2)\times(M+1)$ matrix where column j encodes the solution at time t_j.

Test your code as follows

- Compute what f is if the solution is $u(t,x) = \sin(t)x(1-x)$.
- Now, working on $0 \le x \le 1$ and $0 \le t \le 2\pi$ compute solutions with this forcing term and compare your solution with the exact solution. By working with various grid sizes, confirm that your code has the expected order of convergence.

Solution:
If $u = \sin(t)x(1-x)$ then

$$u_t = \cos(t)x(1-x)$$

and

$$u_{xx} = -2\sin(t).$$

Thus

$$f = u_t - u_{xx} = \cos(t)x(1-x) + 2\sin(t).$$

For convergence analysis, see the worksheet.