1. a. The points \( \{x_{n+1}, 0\}, \{x_n, f_n\}, \{x_{n-1}, f_{n-1}\} \) should be co-linear. Say they lie on the line \( ax + y = \beta \). This gives the relations

\[
\begin{align*}
ax_{n+1} + 0 &= \beta \\
ax_n - tf_n &= \beta \\
ax_{n-1} + tf_{n-1} &= \beta
\end{align*}
\]

Eliminating \( \alpha \) and \( \beta \) gives

\[
x_{n+1} = \frac{x_n - x_{n-1}}{f_n - f_{n-1}} = x_n - f_n \frac{x_n - x_{n-1}}{f_n - f_{n-1}}.
\]

(1)

b. Denote the root \( \xi, \) i.e. \( x_k = \xi + \epsilon_k, \) \( k = 0, 1, 2, \ldots \) Taylor expanding around the root gives

\[
f_k = f(\xi + \epsilon_k) = f(\xi) + \frac{1}{2} f''(\xi) \epsilon_k + \ldots
\]

Substitution into (1) gives, after simple algebra

\[
\epsilon_{n+1} = \frac{1}{2} \frac{f''(\xi)}{f'(\xi)} \epsilon_n \epsilon_{n-1} + \{ \text{smaller terms} \}.
\]

(2)

Given that the successive errors are getting smaller, only the first term on the right can balance the one on the left. Hence

\[
\epsilon_{n+1} = \frac{1}{2} \frac{f''(\xi)}{f'(\xi)} \epsilon_n \epsilon_{n-1} + \{ \text{smaller terms} \}.
\]

We drop the \{ smaller terms \} and set \( c_1 = \frac{1}{2} \frac{f''(\xi)}{f'(\xi)}. \) Equation (2) can then be written

\[
c_1 \epsilon_{n+1} = c_1 \epsilon_n \cdot c_1 \epsilon_{n-1}. \]

After taking logs, this becomes

\[
d_{n+1} = d_n + d_{n-1}
\]

(3)

where \( d_k = \ln(c \epsilon_k). \) The recursion relation (3) is easiest solved by its characteristic equation

\[
r^2 - r - 1 = 0,
\]

with roots \( r_{1,2} = \frac{1 \pm \sqrt{5}}{2}. \) The growing solution to (3) is therefore

\[
d_n = c_2 \left( \frac{\sqrt{5} + 1}{2} \right)^n,
\]

and we get

\[
\ln(c \epsilon_n) = c_2 \left( \frac{\sqrt{5} + 1}{2} \right)^n \ln(c_1 \epsilon_{n-1}) = \ln((c_1 \epsilon_{n-1})^{(\sqrt{5} + 1)/2}),
\]

and the result follows.

c. Given that the points \( \{x_{n+1}, y_{n+1}, 0\} \) and \( \{x_k, y_k, f_k\}, \) \( k = n, n-1, n-2 \) all lie on the first plane, we have

\[
\begin{align*}
ax_{n+1} + \beta y_{n+1} + 0 &= \gamma \\
ax_n + \beta y_n + f_n &= \gamma \\
ax_{n-1} + \beta y_{n-1} + f_{n-1} &= \gamma \\
ax_{n-2} + \beta y_{n-2} + f_{n-2} &= \gamma
\end{align*}
\]

Subtracting the top equation from the remaining ones gives

\[
\begin{bmatrix}
ax_{n+1} \\
x_{n-1} - x_{n+1} \\
x_{n-2} - x_{n+1}
\end{bmatrix} + \beta
\begin{bmatrix}
y_{n+1} - y_{n+1} \\
y_{n-1} - y_{n+1} \\
y_{n-2} - y_{n+1}
\end{bmatrix}
+ \begin{bmatrix}
f_n \\
f_{n-1} \\
f_{n-2}
\end{bmatrix} = \begin{bmatrix} 0 \\
0 \\
0 \end{bmatrix}.
\]

(4)

Similarly for the second plane

\[
\begin{bmatrix}
x_{n+1} - x_{n+1} \\
x_{n-1} - x_{n+1} \\
x_{n-2} - x_{n+1}
\end{bmatrix} + \delta
\begin{bmatrix}
y_{n+1} - y_{n+1} \\
y_{n-1} - y_{n+1} \\
y_{n-2} - y_{n+1}
\end{bmatrix}
+ \begin{bmatrix}
g_n \\
g_{n-1} \\
g_{n-2}
\end{bmatrix} = \begin{bmatrix} 0 \\
0 \\
0 \end{bmatrix}.
\]

(5)

The relations (4) and (5) show that only two of the four different vectors that appear in their left hand sides can be independent. Hence, the two determinants in the hint for the problem must both be zero.
Numerical Quadrature

2. Consider the singular integral $I := \int_0^1 r^{-\alpha} dr$, for $0 < \alpha < 1$.

a. Since the integrand is concave, the right-hand rule satisfies the following bound,

$$I_R := \sum_{j=1}^{N} h(jh)^{-\alpha} \leq I$$

where $h = 1/N$. This same rule can be viewed as a left-hand rule for the integral on the interval $(h, 1 + h)$ which yields the bound

$$\int_h^{1+h} r^{-\alpha} dr \leq I_R$$

Use this information to develop a bound on the error $E_R = |I - I_R|$. Find a simple lower bound on the error.

The two bounds above yield

$$0 \leq I - I_R \leq I - \int_h^{1+h} r^{-\alpha} dr \leq \int_0^h r^{-\alpha} dr - \int_1^{1+h} r^{-\alpha} dr \leq \frac{1}{1-\alpha}((1+h)^{1-\alpha} - ((1+h)(1-\alpha) - 1)) \leq \frac{1}{1-\alpha} h^{1-\alpha}$$

For a lower bound on the error, we have the error in the first interval

$$|I - I_R| \geq \int_0^h r^{-\alpha} - h^{1-\alpha} = \frac{\alpha}{1-\alpha} h^{1-\alpha}.$$ 

b. Use the same technique to develop an upper bound on the error for the midpoint rule.

$$I_M := \sum_{j=1}^{N} h((j - \frac{1}{2})h)^{-\alpha}$$

Shift to the left by $\frac{h}{2}$ and subtract the part of the rule to the left of the origin to get

$$I_M - \left(\frac{h}{2}\right)^{1-\alpha} \leq I$$

Shift to the right by $\frac{h}{2}$ to get the bound

$$\int_{\frac{h}{2}}^{1+\frac{h}{2}} \leq I_M$$
Putting this together we have

\[- (\frac{h}{2})^{1-\alpha} \leq I - I_M \leq \int_0^{\frac{h}{2}} - \int_1^{1+\frac{h}{2}} \leq \frac{1}{1-\alpha}((\frac{h}{2})^{1-\alpha} - ((1 + \frac{h}{2})^{1-\alpha} - 1)) \leq \frac{1}{1-\alpha}(\frac{h}{2})^{1-\alpha}\]

Choosing the larger of the two extremes yields

\[|I - I_M| \leq \frac{1}{1-\alpha}(\frac{h}{2})^{1-\alpha}\]

c. Let \(f(r) \in C^4\). Find a transformation on the problem that allows the use of standard quadrature rules for the integral

\[\int_0^1 r^{-\alpha} f(r)dr\]

Write the error bounds for the composite trapezoidal rule on the transformed integral. What transformation assures \(O(h^2)\) convergence.

Consider the transformation \(r = s^k\). This yields

\[\int_0^1 r^{-\alpha} f(r)dr = \int_0^1 s^{(1-\alpha)k-1} f(s^k)ds\]

For \(k > \frac{1}{1-\alpha}\), the integrand, \(F(s) = s^{(1-\alpha)k-1} f(s^k)\) is bounded. The composite trapezoidal rule has error bound

\[|I - I_T| \leq \frac{h^2}{12} \|F''\|_{\infty}\]

If we choose \(k = \frac{3}{1-\alpha}\), then \(F(s) = s^2 f(s^k)\). This yields

\[F'(s) = 2sf(s^k) + ks^{1+k} f'(s^k)\]

\[F''(s) = 2f(s^k) + 2ks^k f'(s^k) + k(k+1)s^k f'(s^k) + k^2 s^{2k} f''(s^k)\]

Since \(f \in C^4\), we know that \(\|F''\|_{\infty}\) is bounded.
Interpolation/approximation

a) Consider a function \( f(x) \) sampled at \( x = 0, 1, 2, 3 \) with the values \( f(0) = 0, \ f(1) = 1, \ f(2) = 0 \) and, \( f(3) = -1 \). Find the 3rd degree polynomial that fits the data.

Solution.
Using the Lagrange interpolants
\[
    l_i(x) = \prod_{j=0, j \neq i}^{N} \frac{(x - x_j)}{(x_i - x_j)}
\]
we can write the interpolating polynomial as
\[
    p(x) = \sum_{i=0}^{3} f(x_i) l_i(x) = l_1(x) - l_3(x) = \frac{x(x-2)(x-3)}{2} - \frac{x(x-1)(x-2)}{3 \times 2} = \frac{x^3 - 6x^2 + 8x}{3}.
\]

Using B-splines we can piecewise interpolate the data \( s_0, \ldots, s_N \) given at \( x = 0, \ldots, N \) by
\[
    s(x) = \sum_{k=0}^{N} B^{(m)}(x - k) s_k \quad (1)
\]
with the B-splines of order \( m + 1 \) given by
\[
    B^{(m)}(x) = \sum_{l=0}^{m+1} (-1)^l \binom{m+1}{l} \frac{(x + (m + 1)/2 - l)^m}{m!} \quad (2)
\]
and \( x^m_+ \) is defined as \( x^m \) for \( x > 0 \) and zero for \( x \leq 0 \).

b) Using the properties of B-splines, relate the smoothness of \( s(x) \) in (1)
to the integer $m$ in the (2). In other words, for a given $m$, what’s the differentiability of $s(x)$?

**Solution.**

Using the smoothness at the knots imposed by spline interpolation, we get the following table:

<table>
<thead>
<tr>
<th>$m$</th>
<th>Spline interpolation</th>
<th>Smoothness of $s(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m = 0$</td>
<td>constant</td>
<td>Discontinuous</td>
</tr>
<tr>
<td>$m = 1$</td>
<td>linear</td>
<td>Continuous</td>
</tr>
<tr>
<td>$m = 2$</td>
<td>quadratic</td>
<td>Differentiable</td>
</tr>
<tr>
<td>$m = 3$</td>
<td>cubic</td>
<td>Twice differentiable</td>
</tr>
<tr>
<td>$\vdots$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m = k$</td>
<td></td>
<td>$s(x) \in C^{k-1}(\mathbb{R})$</td>
</tr>
</tbody>
</table>

c) Write down the expression and draw a picture of the B-spline used for piecewise linear interpolation of a data set.

**Solution.** We have that

$$B^{(1)}(x) = \sum_{l=0}^{2} (-1)^l \binom{2}{l} (x + 1 - l)_+$$

where the first term is given by

$$(x + 1)_+ = \begin{cases} 
0, & x \leq -1 \\
1 + x, & x > -1 
\end{cases}$$

the second term is given by

$$-2x_+ = \begin{cases} 
0, & x \leq 0 \\
-2x, & x > 0 
\end{cases}$$

and the third term is given by

$$(x - 1)_+ = \begin{cases} 
0, & x \leq 1 \\
x - 1, & x > 1 
\end{cases}$$
Hence,

\[ B^{(1)}(x) = \begin{cases} 
0, & x \leq -1 \\
1 + x, & -1 < x \leq 0 \\
1 + x - 2x = 1 - x, & 0 < x \leq 1 \\
1 + x - 2x + x - 1 = 0, & x > 1 
\end{cases} = \begin{cases} 
1 - |x|, & |x| < 1 \\
0, & |x| \geq 1 
\end{cases}, \]

that is, the "tent function".

---

d) Compute the Fourier transform of a function obtained by piecewise linear spline interpolation of a data set, and show that it decays as \( O(\omega^{-2}) \).

**Hint:** You can use that if \( g(x) \) is real and even, then its Fourier transform

\[ \hat{g}(\omega) = \int_{-\infty}^{\infty} g(x) e^{2\pi i \omega x} \, dx = 2 \text{Re} \left( \int_{0}^{\infty} g(x) e^{2\pi i \omega x} \, dx \right). \]

**Solution.** We have that

\[ \hat{s}(\omega) = \sum_{k=0}^{N} s_k \int_{-\infty}^{\infty} B^{(1)}(x - k) e^{2\pi i \omega x} \, dx = \sum_{k=0}^{N} s_k e^{2\pi i \omega k} \int_{-\infty}^{\infty} B^{(1)}(t) e^{2\pi i \omega t} \, dt. \]
Using the hint and the expression for $B^{(1)}(x)$ we have that

$$\widehat{B^{(1)}}(\omega) \equiv \int_{-\infty}^{\infty} B^{(1)}(t)e^{2\pi i \omega t} dt = 2\text{Re} \left( \int_{0}^{1} (1-t)e^{2\pi i \omega t} dt \right)$$

where

$$\int_{0}^{1} (1-t)e^{2\pi i \omega t} dt = \left[ \frac{(1-t)e^{2\pi i \omega t}}{2\pi i \omega} \right]_{0}^{1} + \frac{1}{2\pi i \omega} \int_{0}^{1} e^{2\pi i \omega t} dt$$

$$= -\frac{1}{2\pi i \omega} + \frac{1}{2\pi i \omega} \left[ \frac{e^{2\pi i \omega t}}{2\pi i \omega} \right]_{0}^{1}$$

$$= -\frac{1}{2\pi i \omega} - \frac{1}{4\pi^2 \omega^2} (e^{2\pi i \omega} - 1).$$

The real part of (3) is given by

$$-\frac{1}{4\pi^2 \omega^2} (\cos 2\pi \omega - 1) = \frac{\sin^2 \pi \omega}{2\pi^2 \omega^2}$$

and hence $\widehat{B^{(1)}}(\omega) = \frac{\sin^2 \pi \omega}{\pi^2 \omega^2}$ which decays as $\frac{1}{\omega^2}$. 


**Linear algebra:**

4. **a.** We modify the system \( Ax = b \) to \( (U^*AU)^*x = U^*b \) where \( U \) is the DFT (discrete Fourier transform) matrix. The matrix \( U^*AU \) is then diagonal, and it will cost one FFT to obtain its elements. Likewise, it will take one FFT to compute \( U^*b \) and finally one more FFT to extract \( x \) from \( U^*x \). With each FFT costing \( O(N \log N) \) operations, this will also become the estimate for the total cost.

**b.** Unpivoted Gaussian elimination for a banded system will produce banded \( L \) and \( U \) factors at a cost of \( O(1) \) operations for each row/column of \( U \) and \( L \). For each of the two beck substitutions, the cost will again be \( O(1) \) operations for each computed entry. The total cost will therefore be \( O(N) \) operations.

**c.** We can interchange rows and columns in \( A \) so that its structure instead becomes

\[ A' = \begin{bmatrix}
\vdots & \vdots & \vdots & \vdots \\
\ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots \\
\end{bmatrix}. \]

By elementary row operations, we can modify each of the diagonal \( 2 \times 2 \) blocks to purely diagonal form. Using the top \( N-2 \) equations, we can next eliminate all entries in the last two rows - up to their last two columns. We then diagonalize the bottom right \( 2 \times 2 \) block, and then use the last two rows to eliminate all remaining entries of the last two columns. We have after that a purely diagonal system to solve. Each of the major steps described (diagonalizing the top left \( (N-2) \times (N-2) \) block, eliminating the last two rows and eliminating the last two columns) takes only \( O(N) \) operations. Hence, this will also be the overall cost.

Alternatively, one can note that the system takes the form of a tridiagonal matrix with two extra full rows and columns appended. The system can be solved as a tridiagonal system plus use of Woodbury's formula, each requiring \( O(N) \) operations.
ODEs

a) Derive the coefficients for the backward differentiation formula

\[ c_0 u_{n+1} + c_1 u_n + c_2 u_{n-1} = f(t_{n+1}, u_{n+1}) \]

that result in a 2nd order method for solving the ODE \( u' = f(t, u) \).

Solution.

The formula should hold for \( \{ u = 1, f = 0 \} \), \( \{ u = t, f = 1 \} \), and \( \{ u = t^2, f = 2t \} \) which, for \( t_{n-1} = -k \), \( t_n = 0 \) and \( t_{n+1} = k \), gives the system

\[
\begin{align*}
    c_0 + c_1 + c_2 &= 0 \\
    k(c_0 - c_2) &= 1 \\
    k^2(c_0 + c_2) &= 2k
\end{align*}
\]

with the solution \( c_0 = \frac{3}{2k}, c_1 = -2/k \) and \( c_2 = \frac{1}{2k} \).

b) Show that the scheme derived in a) is convergent.

Solution.

To establish convergence we need to confirm

- consistency (OK, since our scheme is 2nd order accurate), and
- stability.

To show stability, we need to check the root condition. The characteristic equation is given by

\[
\frac{3r^2}{2} - 2r + \frac{1}{2} = 0
\]

with the roots \( r = 1 \) and \( r = 1/3 \). These roots are within the unit circle, and since there is no double root on the unit circle, the root condition is satisfied and the scheme is stable.
Consider a stiff linear system of ODEs of the form

$$\frac{d\mathbf{u}}{dt} = A\mathbf{u}, \ \mathbf{u}(0) = \mathbf{u}_0$$  \hspace{1cm} (1)$$

where $A$ is a negative definite matrix.

c) Explain what is meant by a stiff system.

Solution.
There is no strict definition, but we can think of stiff ODEs as something like

- "the numerical solution requires a significant reduction in step size to achieve stability", or
- "the ratio of the largest and smallest eigenvalues of the linear system is large", or
- "the system contains both rapidly and slowly decaying modes".

d) By studying the stability domain of the scheme derived in a), determine if this scheme is suitable for solving (1).

Hint: You don’t have to derive the entire stability domain. It suffices to establish stability for the part of the complex plane that is relevant for the system in (1).

Solution.
Since $A$ is negative definite and therefore has only negative eigenvalues, it suffices to investigate stability for the test equation $u’ = -\lambda u$ where $\lambda > 0$.

Applying our scheme to this test equation with time step $k$ gives us

$$\frac{3}{2k}u_{n+1} - \frac{2}{k}u_n + \frac{u_{n-1}}{2k} = -\lambda u_{n+1}.$$
We set \( \mu \equiv k \lambda \) which gives the characteristic equation
\[
r^2 - \frac{4r}{3 + 2\mu} + \frac{1}{3 + 2\mu} = 0
\]
with the solution
\[
r = \frac{2 \pm \sqrt{1 - 2\mu}}{3 + 2\mu}.
\]

In order to see if \(|r| \leq 1\), we distinguish two cases:

- \( 0 \leq \mu \leq 1/2 \): Then the numerator is real and bounded by 3, and hence \(|r| \leq \frac{3}{3+2\mu} \leq 1\).

- \( \mu > 1/2 \): The numerator is complex valued and \( r \) can be written as
\[
r = \frac{2 \pm i\sqrt{2\mu - 1}}{3 + 2\mu}.
\]

Then
\[
|r|^2 = \frac{4 + 2\mu - 1}{(3 + 2\mu)^2} = \frac{1}{3 + 2\mu} < 1.
\]

Hence, since \(|r| \leq 1\) for the test equation, the scheme is stable for all negative eigenvalues, and therefore the scheme is suitable for the problem.
PDEs Consider the wave equation

\[ u_{tt} = c u_{xx}, \quad x \in [0, 1], \; t > 0, \]

with initial conditions \( u(x, 0) = f(x), \; u_t(x, 0) = g(x), \) and boundary conditions \( u(0, t) = u(1, t) = 0, \) for \( t > 0. \) Let \( \Delta x = 1/N \) and define the mesh \((x_k, t_\ell) = (k\Delta x, \ell\Delta t).\) Let \( u_k^\ell \) approximate \( u(x_k, t_\ell).\) Use von Neumann analysis to determine the relationship between \( \Delta t \) and \( \Delta x \) for which the following scheme is stable:

\[
\frac{u_k^{\ell+1} - 2u_k^\ell + u_k^{\ell-1}}{\Delta t^2} = c \frac{u_{k+1}^\ell - 2u_k^\ell + u_{k-1}^\ell}{\Delta x^2}.
\]

Justify your answer.

Solution Using von Neumann analysis we set \( u_k^\ell = a^\ell e^{ik\theta} \) and plug into the difference formula to determine the amplification factor, \( a.\) This yields

\[
a - 2 + 1/a = c \left( \frac{\Delta t}{\Delta x} \right)^2 (e^{i\theta} - 2 + e^{-i\theta}) = -4c \left( \frac{\Delta t}{\Delta x} \right)^2 \sin(\theta/2)^2
\]

Let \( s = \sin(\theta/2) \) and \( \lambda = \left( \frac{\Delta t}{\Delta x} \right).\) This yields the following equation for \( a:\)

\[
a^2 - (2 - 4c\lambda^2 s^2)a + 1 = 0
\]

Solving for \( a \) yields:

\[
a = (1 - 2c\lambda^2 s^2) \pm \sqrt{(1 - 2c\lambda^2 s^2)^2 - 1}
\]

i. For \( 0 < 2c\lambda^2 s^2 < 2.0 \) the roots are complex with modulous 1.0.

ii. For \( 0 = 2c\lambda^2 s^2, \) \( a = 1.0 \) is the only root while for \( 2c\lambda^2 s^2 = 2.0 \) \( a = -1 \) is the only root.

iii. For \( 2c\lambda^2 s^2 > 2.0 \) there is a root with \( a > 1.0.\)

Since we want \( a \leq 1.0 \) for all \( \theta, \) and if \( |a| = 1 \) we want a simple root, we have the condition:

\[
\lambda < \frac{1}{\sqrt{c}} \quad \text{or} \quad \Delta t < \frac{\Delta x}{\sqrt{c}}
\]