1. Solution: Nonlinear Equations

1. Denote
$$G(x,y) = \begin{bmatrix} \frac{\partial g_1}{\partial x} & \frac{\partial g_1}{\partial y} \\ \frac{\partial g_2}{\partial x} & \frac{\partial g_2}{\partial y} \end{bmatrix}.$$
We seek a closed, bounded, and convex region, $D \in \Re^2$, for which
$$\begin{aligned} (x,y) \in D &\Rightarrow (g_1(x,y), g_2(x,y)) \in D \\ \lambda &:= \max_{(x,y)\in D} \|G\|_\infty < 1.0. \end{aligned}$$
See Atkinson, Theorem 2.9, page 105. (Note: any consistent matrix norm will suffice.)

2. Since $\frac{1}{\sqrt{2}} > \frac{2}{3}$, then $\forall (x,y) \in \Re^2$ we have
$$\begin{aligned} g_1(x,y) &> 0.0 \\ g_2(x,y) &> 0.0 \end{aligned}$$
Now,
$$G(x,y) = \begin{bmatrix} \frac{(x+y)}{\sqrt{2}\sqrt{1+(x+y)^2}} & \frac{(x+y)}{\sqrt{2}\sqrt{1+(x+y)^2}} \\ \frac{(x-y)}{\sqrt{2}\sqrt{1+(x-y)^2}} & \frac{-(x-y)}{\sqrt{2}\sqrt{1+(x-y)^2}} \end{bmatrix}.$$
and
$$\|G\|_\infty = \max\{\frac{\sqrt{2}|x+y|}{\sqrt{1+(x+y)^2}} \quad , \quad \frac{\sqrt{2}|x-y|}{\sqrt{1+(x-y)^2}}\} < 1.0$$
implies
$$\begin{aligned} |x+y| &< 1.0 \\ |x-y| &< 1.0. \end{aligned}$$
All requirements are satisfied if we define
$$D = \{(x,y) \ : \ x > 0.0, \ y > 0.0, \ \text{and } x+y < 1.0\}$$

3. Write the system as
$$F(x,y) = \begin{pmatrix} x - g_1(x,y) \\ y - g_2(x,y) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$
The Jacobian is given by
$$J(x,y) = I - G(x,y),$$
where $G(x,y)$ is defined as above. The iteration would be
$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} x_n \\ y_n \end{pmatrix} - J(x_n,y_n)^{-1}F(x_n,y_n)$$
For every $(x_0,y_0) \in D$, we have $\|G(x_0,y_0)\|_\infty < 1.0$, which implies $J(x_0,y_0)$ is nonsingular. However, we cannot guarantee that $(x_1,y_1) \in D$, without further restrictions.

2. Numerical quadrature

a. Trapezoidal rule:

$$\int_a^b f(x)dx = h\left[\tfrac{1}{2}f(x_0)+f(x_1)+f(x_2)+f(x_3)+f(x_4)+f(x_5)+\ldots+f(x_{n-1})+\tfrac{1}{2}f(x_n)\right]+O(h^2)$$

Simpson's rule:

$$\int_a^b f(x)dx = \frac{h}{3}[1f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+4f(x_5)+\ldots+4f(x_{n-1})+1f(x_n)]+O(h^4)$$

Richardson extrapolation of the trapezoidal rule gives

$$\frac{4\,T_h - T_{2h}}{3} =$$

$$= h\,[\ \ \tfrac{2}{3}f(x_0)+\tfrac{4}{3}f(x_1)+\tfrac{4}{3}f(x_2)+\tfrac{4}{3}f(x_3)+\tfrac{4}{3}f(x_4)+\tfrac{4}{3}f(x_5)+\ldots+\tfrac{4}{3}f(x_{n-1})+\tfrac{2}{3}f(x_n)-$$

$$-\tfrac{2}{3}\tfrac{1}{2}f(x_0) \qquad -\tfrac{2}{3}f(x_2) \qquad -\tfrac{2}{3}f(x_4) \qquad \ldots \qquad -\tfrac{2}{3}\tfrac{1}{2}f(x_n)] =$$

$$= \frac{h}{3}[1f(x_0)+4f(x_1)\ +2f(x_2)\ +4f(x_3)+2f(x_4)+4f(x_5)+\ldots\ +4f(x_{n-1})+1f(x_n)],$$

which agrees with Simpson's rule.

b. If one remembers Euler-MacLaurin's formula, the task is easy. With $\sum''$ meaning that the first and the last term is to be halved, it holds that

$$\int_a^b f(x)dx = h\sum_{i=0}^{n}{}'' f(x_i) - \frac{1}{12}h^2(f'(b)-f'(a)) - \frac{1}{168}h^4(f'''(b)-f'''(a)) - \ldots$$

The trapezoidal rule (with its $O(h^2)$ error) is obtained by ignoring all the correction terms following the sum in the right hand side. In order to get a formula that is accurate to $O(h^4)$, we just need to approximate $-\frac{1}{12}h^2(f'(b)-f'(a))$ to fourth order, i.e. the derivatives to second order accuracy. One-sided approximations, extending over three nodes

$$f'(a) = f'(x_0) = (-\frac{3}{2}f(x_0)\ \ +2f(x_1)\ \ \ -\frac{1}{2}f(x_2))/h + O(h^2)$$

$$f'(b) = f'(x_n) = (-\frac{1}{2}f(x_{n-2})+2f(x_{n-1})-\frac{3}{2}f(x_n))/h + O(h^2)$$

lead immediately to the desired result. The process can be extended to any order by just including additional terms from the Euler-MacLaurin expansion.

If one does not recall the Euler-MacLaurin expansion, here is another approach. To simplify the notation, consider just the correction around $x = a$; will be equivalent around $x = b$. Simpson's rule tells that

$$\int_a f(x)dx \quad = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + 4f(x_5) + \ldots] + O(h^4)$$

and

$$\int_{a+h} f(x)dx = \frac{h}{3}[\qquad\qquad f(x_1) + 4f(x_2) + 2f(x_3) + 4f(x_4) + 2f(x_4) + \ldots] + O(h^4).$$

Therefore

$$\int_a f(x)dx = \tfrac{1}{2}\int_a^{a+h} f(x)dx + \tfrac{1}{2}\int_a f(x)dx + \tfrac{1}{2}\int_{a+h} f(x)dx =$$

$$= \tfrac{1}{2}\int_a^{a+h} f(x)dx + \frac{h}{6}[f(x_0) + 5f(x_1) + 6\{f(x_2) + f(x_3) + f(x_4) + f(x_5) + \ldots\}] + O(h^4).$$

It now only remains to approximate $\int_a^{a+h} f(x)dx$ to order $O(h^4)$ based on the three node values $f(x_0)$, $f(x_1)$ and $f(x_2)$. Fitting a parabola through these, and integrating it will do the job. If one carries this out, the appropriate formula becomes

$$\int_a^{a+h} f(x)dx = \frac{h}{12}[5\,f(x_0) + 8\,f(x_1) - f(x_2)] + O(h^4).$$

For integration formulas of still higher orders, one could consider starting the equivalent procedure with higher order Newton-Cotes formulas.

As it happens, there are closed form expressions available for all the coefficients in the quadrature formulas of the type explored here (trapezoidal rule with end corrections). They are among the first quadrature formulas ever described in the literature, known as Gregory's formulas after James Gregory (1638-1675).

3. Interpolation / Approximation

a. $p_2(x) = 1\,\frac{(x-0)(x-2)}{(-1-0)(-1-2)} - 1\,\frac{(x+1)(x-2)}{(0+1)(0-2)} + 1\,\frac{(x+1)(x-0)}{(2+1)(2-0)} = x^2 - x - 1.$

b. Divided difference table: Interpolant:

x	y		
-1	1		
		$\frac{-1-1}{0-(-1)} = -2$	
0	-1		$\frac{1-(-2)}{2-(-1)} = 1$
		$\frac{1-(-1)}{2-0} = 1$	
2	1		

; $p_2(x) = 1 - 2(x+1) + 1(x-0)(x+1) = x^2 - x - 1.$

c. The overdetermined system to solve becomes $\begin{bmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$. Following the normal equations approach, we multiply from the left with the transpose of the coefficient matrix, which gives

$$\begin{bmatrix} 3 & 1 \\ 1 & 5 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \text{ with solution } a = \tfrac{2}{7},\ b = \tfrac{1}{7}.$$

d. Let the cubic on [-1,0] be $s_1(x) = ax^3 + bx^2 + cx + d$ and on [0,2] $s_2(x) = ex^3 + fx^2 + gx + h$. We obtain $s_1'(x) = 3ax^2 + 2bx + c,\ s_1''(x) = 6ax + 2b$, and $s_2'(x) = 3ex^2 + 2fx + g,\ s_2''(x) = 6ex + 2f$.

The conditions that need to be satisfied are:

Value at -1:	$-a + b - c + d = 1$	
Second derivative at -1:	$-6a + 2b = 0$	
Value at 0:	$d = -1,$	$h = -1$
Match first derivative at 0:	$c = g$	
Match second derivative at 0:	$2b = 2f$	
Value at 2:	$8e + 4f + 2g + h = 1$	
Second derivative at 2:	$12e + 2f = 0$	

We have here 8 equations in 8 unknowns. However, the simple structure allows a quick simplification down to a 2×2 system. One finds after not much algebra

$$a = \tfrac{1}{2},\ b = \tfrac{3}{2},\ c = -1,\ d = -1,\ e = -\tfrac{1}{4},\ f = \tfrac{3}{2},\ g = -1,\ h = -1.$$

4. Solution: Linear Algebra

1. The minimization problem yield the following linear least-squares problem

$$\begin{bmatrix} A \\ \lambda I \end{bmatrix} \underline{x} \simeq \begin{bmatrix} \underline{b} \\ \underline{0} \end{bmatrix}.$$

   The solution of this system is given by the normal equations

$$\begin{bmatrix} A^t & \lambda I \end{bmatrix} \begin{bmatrix} A \\ \lambda I \end{bmatrix} \underline{x} = \begin{bmatrix} A^t & \lambda I \end{bmatrix} \begin{bmatrix} \underline{b} \\ \underline{0} \end{bmatrix},$$

   which becomes

$$\left[A^t A + \lambda^2 I\right] \underline{x} = A^t \underline{b}.$$

2. Note that A^tA is positive semidefinite. If $\lambda > 0$, then $A^tA + \lambda^2 I$ is positive definite and, therefore, nonsingular. This guarantees a unique solution.
3. Denote the singular value decomposition of A by

$$A = U\Sigma V^*,$$

   where $U_{n\times n}$, $V_{n\times n}$ are unitary and $\Sigma_{n\times n} = \text{diag}\{\sigma_1, \sigma_2, \ldots, \sigma_n\}$, with $0 \le \sigma_1 \le \sigma_2 \le \ldots \le \sigma_n$.

The columns of U, which we denote by $\underline{u}_j$, are the left singular vectors of A, while the columns of V, which we denote by $\underline{v}_j$ are right singular vectors of A. Plugging this decomposition into the normal equations yields

$$\left[V\Sigma^*\Sigma V^* + \lambda^2\right] \underline{x} = \left[V\Sigma^* U^*\right] \underline{b}.$$

Expanding $\underline{b}$ in terms of the left singular vectors,

$$\underline{b} = \sum_{j=1}^{n} \beta_j \underline{u}_j, \qquad \text{where} \quad \beta_j = \underline{u}_j^* \underline{b},$$

yields

$$\underline{x}_\lambda = \sum_{j=1}^{n} \frac{\beta_j \sigma_j}{\lambda^2 + \sigma_j^2} \underline{v}_j$$

Denote the rank of A by r. If $r < n$, then we can rewrite the above expression as

$$\underline{x}_\lambda = \sum_{\sigma_j > 0} \frac{\beta_j \sigma_j}{\lambda^2 + \sigma_j^2} \underline{v}_j,$$

which yields

$$\lim_{\lambda \to 0} \underline{x} = \sum_{\sigma_j > 0} \frac{\beta_j}{\sigma_j} \underline{v}_j.$$

This is know as the minimal length least-squares solution.

5. Numerical ODE

a. The Taylor expansion of the ODE solution is

$$y(t+k)=y(t)+ky'(t)+\frac{k^2}{2}y''(t)+\frac{k^3}{6}y'''(t)+O(k^4)$$

Form the ODE $y'=f(t,y(t))$ follows by applying the chain rule that $y''=f_t+f_y y'=f_t+ff_y$. Substituting this into the equation above gives the scheme that was stated in the problem formulation:

$$y(t+k)=y(t)+kf+\frac{k^2}{2}(f_t+ff_y)+O(k^3)$$

In order to reach one order higher still, we need similarly to use the chain rule, the ODE, and also the product rule, to evaluate y''':

$$y'''=(f_t+ff_y)_t=f_{tt}+f_{ty}f+f_tf_y+f_yf\,f_y+ff_{yt}+ff_{yy}f,$$

and the scheme becomes

$$y(t+k)=y(t)+kf+\frac{k^2}{2}(f_t+ff_y)+\frac{k^3}{6}(ff_y^2+f^2f_{yy}+f_tf_y+2ff_{ty}+f_{tt})+O(k^4)$$

b. Taylor expansions of $d^{(1)}$ and $d^{(2)}$ around (t,y) give

$$d^{(1)}=kf(t,y),$$
$$d^{(2)}=kf(t+c\,k,y+a\cdot d^{(1)})=kf(t,y)+c\,k^2\,\frac{\partial f(t,y)}{\partial t}+a\,k^2\,f(t,y)\,\frac{\partial f(t,y)}{\partial y}+O(k^3),$$

and therefore

$$y(t+k)\quad=y(t)+b_1d^{(1)}+b_2d^{(2)}\quad=\quad y(t)+k\,(b_1+b_2)\,f+k^2(b_2c\,f_t+b_2a\,ff_y)+O(k^3).$$

Equating coefficients between this last expression and the Taylor scheme that was stated in the problem formulation (part a) gives the three compatibility conditions

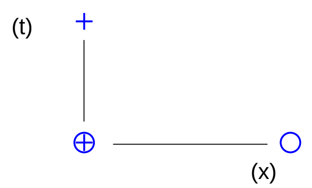
$$b_1+b_2=1,\ \ b_2\,c=\tfrac{1}{2},\ \ b_2\,a=\tfrac{1}{2}.$$

6. Solution: Numerical Solution of PDEs

1. For equation I, we have
$$\frac{u_j^{\ell+1}-u_j^\ell}{\Delta t} = b\frac{u_{j+1}^\ell - u_j^\ell}{\Delta x},$$
which becomes
$$u_j^{\ell+1} = (1-\frac{b\ \Delta t}{\Delta x})u_j^\ell + \frac{b\ \Delta t}{\Delta x}u_{j+1}^\ell.$$
For equation II, we have
$$\frac{u_j^{\ell+1}-u_j^\ell}{\Delta t} = \frac{u_{j+1}^\ell - 2u_j^\ell + u_{j-1}^\ell}{\Delta x^2},$$
which becomes
$$u_j^{\ell+1} = (1-\frac{2\Delta t}{\Delta x^2})u_j^\ell + \frac{\Delta t}{\Delta x^2}(u_{j+1}^\ell + u_{j-1}^\ell).$$
For equation III, we have
$$\frac{u_j^{\ell+1}-u_j^\ell}{\Delta t} = \frac{u_{j+1}^\ell - 2u_j^\ell + u_{j-1}^\ell}{\Delta x^2} + b\frac{u_{j+1}^\ell - u_j^\ell}{\Delta x},$$
which becomes
$$u_j^{\ell+1} = (1-(\frac{2\Delta t}{\Delta x^2}+\frac{b\ \Delta t}{\Delta x}))u_j^\ell + (\frac{\Delta t}{\Delta x^2}+\frac{b\ \Delta t}{\Delta x})u_{j+1}^\ell + \frac{\Delta t}{\Delta x^2}u_{j-1}^\ell.$$

2. Equation I

   Stencil : + time ○ first-order space

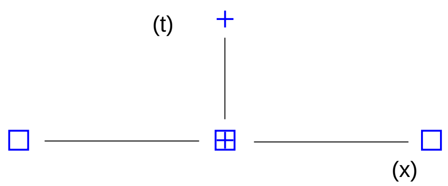


   Boundary Conditions

$$\begin{aligned} u(x,0) &= f(x) \qquad x \in [0,1] \\ u(0,t) &= g(t) \qquad t > 0. \end{aligned}$$

Equation II

Stencil: + time □ second-order space

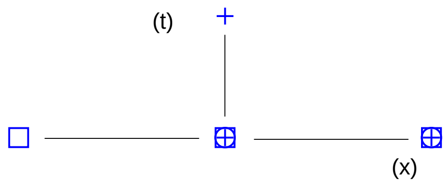


Boundary Conditions

$$
\begin{aligned}
u(x,0) &= f(x) \qquad x \in [0,1], \\
u(0,t) &= g_1(t) \qquad t > 0, \\
u(1,t) &= g_2(t) \qquad t > 0.
\end{aligned}
$$

Equation III

Stencil: + time ○ first-order space □ second-order space



Boundary conditions: Same as II.

3. For Von Neumann analysis, set $u_j^\ell = a^\ell e^{i\theta j}$ plug into the difference equation and simplify.

   Equation I

   $$\frac{a-1}{\Delta t} = b\frac{e^{i\theta}-1}{\Delta x}$$

   Solve for a to get

   $$a = (1 - \frac{b\Delta t}{\Delta x}) + \frac{b\Delta t}{\Delta x}e^{i\theta}.$$

   In the complex plane, the right side describes a circle, centered at $1 - \frac{b\Delta t}{\Delta x}$, of radius $\frac{b\Delta t}{\Delta x}$. Thus,

   $$|a| \leq 1.0 \Leftrightarrow \frac{b\Delta t}{\Delta x} \leq 1.0 \Leftrightarrow \Delta t \leq \frac{\Delta x}{b}$$

   Equation II

   $$\frac{a-1}{\Delta t} = \frac{e^{i\theta} - 2 + e^{-i\theta}}{\Delta x^2} = -\frac{4\sin^2\theta/2}{\Delta x^2}$$

   Solve for a to get

   $$a = (1 - \frac{4\Delta T}{\Delta x^2}\sin^2(\theta/2)).$$

   Stability is achieved if, for every $\theta \in [0, 2\pi)$, we have

   $$|a| \leq 1.0 \Leftrightarrow \frac{4\Delta t}{\Delta x^2} \leq 2.0 \Leftrightarrow \Delta t \leq \frac{\Delta x^2}{2}$$

4. Applying Von Neumann analysis to Equation III yields

   $$\begin{aligned} \frac{a-1}{\Delta t} &= \frac{e^{i\theta} - 2 + e^{-i\theta}}{\Delta x^2} + b\frac{e^{i\theta}-1}{\Delta x} \\ &= -\frac{4\sin^2(\theta/2)}{\Delta x^2} + b\frac{(\cos(\theta) - 1) + i\sin(\theta)}{\Delta x} \end{aligned}$$

   Solving for a and separating the real and complex parts and using the identities $\cos(\theta) = \cos^2(\theta/2) - \sin^2(\theta/2)$ and $\sin(\theta) = 2\sin(\theta/2)\cos(\theta/2)$ yields

   $$a = \left(1 - (\frac{4\Delta t}{\Delta x^2} + \frac{2b\Delta t}{\Delta x})\sin^2(\theta/2)\right) + i\left(\frac{2b\Delta t}{\Delta x}\sin(\theta/2)\cos(\theta/2)\right).$$

   Stability is guaranteed if $|a| \leq 1.0$ for all $\theta \in [0, 2\pi]$. This is complicated by the presence of real and imaginary parts.