Coursework - foundations of numerical methods

(1) (a)

$$f(x) = \begin{cases} x-1, & x \geq 1 \\ 1-x, & x < 1 \end{cases}$$

In principle: Yes

In practice: you may have trouble if you try to implement the derivatives of f numerically

Justification: The Newton-Raphson method finds the root of a function by generating a sequence

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$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

p_n: root after n-th iteration

p_{n-1}: root after $(n-1)$st iteration

Such a sequence has been obtained from the Taylor expansion of a function $f(x)$ around the root p.

In general, for it to converge:

i) The initial guess p_0 should be near enough the root p (so that the powers of the Taylor expansion of $f(x)$ around the root can be neglected to a good approximation).

ii) The first and second derivatives of $f(x)$ should be continuous near the root. Such conditions come from the fact that $g'(x)$, with $g(x) = x - \frac{f(x)}{f'(x)}$, must be bounded in order to guarantee that the root is a stable fixed point of the above sequence (see Matthews + Fink, theorem 2.2 and section 2.4)

$f'(x)$ is discontinuous at the root. Hence, if $f(x)$ were non-linear the answer would be no.

However, $f(x)$ is Linear. Therefore, the Taylor expansion up to first order, around the root, is EXACT and it is not necessary to fulfill i) and ii) for the sequence to converge.

(note that $p = 1$ in our case).

If $p_0 > p$, $p_0 = p+\delta$ $\quad f'(p) = 1$ and

$$p = p+\delta - \frac{(p+\delta-1)}{1} = 1$$

If $p_0 < p$, $p_0 = p-\delta$ $\quad f'(p) = -1$

$$p = p-\delta + (1-p-\delta) = 1$$

(No assumption has been made about δ being large or small)

Exactly at the root the derivative is discontinuous and there would be trouble. Also if, instead of computing the derivatives analytically, one tried to implement them numerically using, e.g., forward, backward or centered difference formulae, depending on the increments and on the initial guess there could be further probs. due to this discontinuity (no need for that in practice though).

(b) Yes: $f(x)$ has a root at $f=1$, the initial guess is sufficiently close to such a value and the derivatives of f are continuous near the root

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(c) No: the initial guess is too large and the sequence generated by the method will approach $x \to \infty$.

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2) Cubic spline:

$$S_j(x) = a_j + b_j(x-x_j) + c_j(x-x_j)^2 + d_j(x-x_j)^3, \quad j=0,1,\dots,n-1$$

$$S'''_j(x) = 6d_j = \frac{6(c_{j+1}-c_j)}{3h_j}$$

Boundary conditions

(*) $S'''(x) \equiv 0$ in $[x_0, x_1] \Rightarrow 6d_0 = 0 \quad \therefore c_1 = c_0$

(**) $S'''(x) \equiv 0$ in $[x_{n-1}, x_n] \Rightarrow 6d_{n-1} = 0 \quad \therefore c_{n-1} = c_n$

(*) and (**) are equivalent to $c_0 - c_1 = 0$

$c_{n-1} - c_n = 0$,

respectively.

Recurrence relations seen in class

(derived from the continuity of the splines, their first and second derivatives at the nodes)

$$h_{j-1}c_{j-1} + 2(h_{j-1}+h_j)c_j + h_j c_{j+1} = \frac{3}{h_j}(a_{j+1}-a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1})$$

$j = 1, 2, \dots, n-1$

Let us now consider the tridiagonal system $A\vec{x} = \vec{b}$ with

$$A = \begin{bmatrix} 1 & -1 & 0 & \cdots & \cdots & 0 \\ h_0 & 2(h_0+h_1) & h_1 & \ddots & & \vdots \\ 0 & h_1 & 2(h_1+h_2) & \ddots & & 0 \\ \vdots & & \ddots & \ddots & \ddots & h_{n-1} \\ 0 & \cdots & \cdots & 0 & -1 & 1 \end{bmatrix}, \quad \vec{x} = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix},$$

$$\vec{b} = \begin{bmatrix} 0 \\ \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0) \\ \vdots \\ \frac{3}{h_{n-1}}(a_n - a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1} - a_{n-2}) \\ 0 \end{bmatrix}$$

Then

$$A\vec{x} = \begin{bmatrix} c_0 - c_1 \\ c_0 h_0 + 2(h_0 + h_1)c_1 + h_1 c_2 \\ c_1 h_1 + 2(h_1 + h_2)c_2 + h_2 c_3 \\ \vdots \\ c_{n-2} h_{n-2} + 2(h_{n-2} + h_{n-1})c_{n-1} + h_{n-1} c_n \\ c_{n-1} - c_n \end{bmatrix}$$

In general,

$$b_j = \begin{cases} 0, & \text{for } j = 0 \\ \frac{3}{h_j}(a_{j+1} - a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1}), & \text{for } j = 1, \dots, n-1 \\ 0, & \text{for } j = n \end{cases}$$

and

$$[A\vec{x}]_j = \begin{cases} c_j - c_{j+1}, & \text{for } j = 0 \\ h_{j-1} c_{j-1} + 2(h_{j-1} + h_j)c_j + h_j c_{j+1}, & \text{for } j = 1, \dots, n-1 \\ c_{j-1} - c_j, & \text{for } j = n \end{cases}$$

Hence

$[A\vec{x}]_j = b_j$ yields $\left.\begin{matrix} c_0 = c_1 \\ c_{n-1} = c_n \end{matrix}\right\}$ boundary conditions

and $h_{j-1} c_{j-1} + 2(h_{j-1} + h_j)c_j + h_j c_{j+1} = \frac{3}{h_j}(a_{j+1} - a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1})$, $j = 1, \dots, n-1$ (recurrence relation)

(4)

i	x_i	$f(x_i)$
0	-3	2
1	-2	0
2	1	3
3	4	1

$h_0 = x_1 - x_0 = 1$

$h_1 = x_2 - x_1 = 3$

$h_2 = x_3 - x_2 = 3$

$a_0 = f(x_0) = 2$

$a_1 = f(x_1) = 0$

$a_2 = f(x_2) = 3$

$a_3 = f(x_3) = 1$

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$$A = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 1 & 8 & 3 & 0 \\ 0 & 3 & 12 & 3 \\ 0 & 0 & -1 & 1 \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 0 \\ \underbrace{3+3\times 2}_{9} \\ \underbrace{-2-1\times 3}_{-5} \\ 0 \end{bmatrix}$$

$$\vec{c} = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix}$$

$c_0 = c_1$

$c_0 + 8c_1 + 3c_2 = 9$

$3c_1 + 12c_2 + 3c_3 = -5$

$c_2 = c_3$

$\Rightarrow$ $9c_1 + 3c_2 = 9$

$15c_2 + 3c_1 = -5$

$c_1 = c_0 = \frac{25}{21}$; $c_2 = c_3 = -\frac{4}{7}$ (checked with Mathematica)

Other coefficients:

$$b_0 = \frac{a_1 - a_0}{h_0} - \frac{h_0}{3}(2c_0 + c_1)$$

$$b_0 = -2 - \frac{1}{3} \cdot 3c_1 = -2 - c_1 = -\frac{67}{21}$$

$$b_1 = \frac{a_2 - a_1}{h_1} - \frac{h_1}{3}(2c_1 + c_2) = 1 - \left(2 \times \frac{25}{21} - \frac{4}{7}\right) = -\frac{17}{21}$$

$$b_2 = \frac{a_3 - a_2}{h_2} - \frac{h_2}{3}(2c_2 + c_3) = -\frac{2}{3} + \left(3 \times \frac{4}{7}\right) = \frac{22}{21}$$

$d_0 = d_2 = 0$

$d_1 = \frac{c_2 - c_1}{3 h_1} = \frac{-37}{189}$

Splines:

$$S(x) = \begin{cases} 2 - \frac{67}{21}(x+3) + \frac{25}{21}(x+3)^2 , & -3 \leq x < -2 \\ -\frac{17}{21}(x+2) + \frac{25}{21}(x+2)^2 - \frac{37}{189}(x+2)^3 , & -2 \leq x \leq 1 \\ 3 + \frac{22}{21}(x-1) + \frac{4}{7}(x-1)^2 , & 1 \leq x \leq 4 \end{cases}$$

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(3) Show that

$$\int_{x_0}^{x_4} f(x)\,dx \simeq \frac{2h}{45}\left[7 f(x_0) + 32 f(x_1) + 12 f(x_2) + 32 f(x_3) + 7 f(x_4)\right]$$

$h \equiv$ internodal spacing $\quad x_i - x_{i-1} = h \quad (i = 1, \dots, 4)$

Ansatz:

$f(x) \approx P_4(x)$ (fourth Lagrange interpolating polynomial)

(You can see you should use this ansatz from the above formula & from the discussions in class).

$$P_4(x) = \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)} f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)(x_1-x_4)} f(x_1)$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_3)(x-x_4)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)(x_2-x_4)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)(x-x_4)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)(x_3-x_4)} f(x_3)$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_2)(x-x_3)}{(x_4-x_0)(x_4-x_1)(x_4-x_2)(x_4-x_3)} f(x_4).$$

$$P_4(x) = \underbrace{\frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(-h)(-2h)(-3h)(-4h)}}_{24h^4} f(x_0) + \underbrace{\frac{(x-x_0)(x-x_2)(x-x_3)(x-x_4)}{h\,(-h)(-2h)(-3h)}}_{-6h^4} f(x_1)$$

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$$+ \underbrace{\frac{(x-x_0)(x-x_1)(x-x_3)(x-x_4)}{(2h)(h)(-h)(-2h)}}_{4h^4} f(x_2) + \underbrace{\frac{(x-x_0)(x-x_1)(x-x_2)(x-x_4)}{3h \cdot 2h \; h \; (-h)}}_{-6h^4} f(x_3)$$

$$+ \underbrace{\frac{(x-x_0)(x-x_1)(x-x_2)(x-x_3)}{(4h)(3h)(2h)(h)}}_{24h^4} f(x_4)$$

$$\int_{x_0}^{x_4} P_4(x)\,dx = \frac{f(x_0)}{24h^4} \overbrace{\int_{x_0}^{x_4} (x-x_1)(x-x_2)(x-x_3)(x-x_4)\,dx}^{I_0} +$$

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$$- \frac{f(x_1)}{6h^4} \overbrace{\int_{x_0}^{x_4} (x-x_0)(x-x_2)(x-x_3)(x-x_4)\,dx}^{I_1} +$$

$$+ \frac{f(x_2)}{4h^4} \overbrace{\int_{x_0}^{x_4} (x-x_0)(x-x_1)(x-x_3)(x-x_4)\,dx}^{I_2} +$$

$$- \frac{f(x_3)}{6h^4} \overbrace{\int_{x_0}^{x_4} (x-x_0)(x-x_1)(x-x_2)(x-x_4)\,dx}^{I_3}$$

$$+ \frac{f(x_4)}{24h^4} \underbrace{\int_{x_0}^{x_4} (x-x_0)(x-x_1)(x-x_2)(x-x_3)\,dx}_{I_4}$$

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Change of variable: $x = x_0 + ht$

$$I_0 = \int_{x_0}^{x_4} (x-x_1)(x-x_2)(x-x_3)(x-x_4)\,dx = h^5 \int_0^4 \underbrace{(t-1)(t-2)(t-3)(t-4)}_{t^4 - 10t^3 + 35t^2 - 50t + 24}\,dt$$

$$I_0 = \frac{112}{15} h^5 \Rightarrow \frac{f(x_0)}{24h^4} I_0 = \frac{14}{45} h\, f(x_0)$$

$$I_1 = \int_{x_0}^{x_4} (x-x_0)(x-x_2)(x-x_3)(x-x_4)\,dx = h^5 \int_0^4 t(t-2)(t-3)(t-4)\,dt =$$

$$= -\frac{128}{15} h^5 \Rightarrow -\frac{f(x_1) I_1}{6h^4} = \frac{64}{45} h\, f(x_1)$$

$$I_2 = \int_{x_0}^{x_4} (x-x_0)(x-x_1)(x-x_3)(x-x_4)\,dx = h^5 \int_0^4 t(t-1)(t-3)(t-4)\,dt =$$

$$= \frac{32}{15} h^5 \Rightarrow \frac{f(x_2) I_2}{4h^4} = \frac{8}{15} h\, f(x_2)$$

$$I_3 = \int_{x_0}^{x_4} (x-x_0)(x-x_1)(x-x_2)(x-x_4)\,dx = h^5 \int_0^4 t(t-1)(t-2)(t-4)\,dt =$$

$$= -\frac{128 h^5}{15} \Rightarrow -\frac{f(x_3) I_3}{6h^4} = \frac{64}{45} h f(x_3)$$

$$I_4 = \int_{x_0}^{x_4} (x-x_0)(x-x_1)(x-x_2)(x-x_3)\,dx = h^5 \int_0^4 t(t-1)(t-2)(t-3)\,dt$$

$$= \frac{112 h^5}{15} \Rightarrow \frac{f(x_4) I_4}{24 h^4} = h \times \frac{14}{45} f(x_4)$$

$$\int_{x_0}^{x_4} P_4(x)\,dx = h\left(\frac{14}{45} f(x_0) + \frac{64}{45} f(x_1) + \frac{8}{15} f(x_2) + \frac{64}{45} f(x_3) + \frac{14}{45} f(x_4)\right]$$

$$= \frac{2h}{45}\left[7f(x_0) + 32 f(x_1) + 12 f(x_2) + 32 f(x_3) + 7 f(x_4)\right]$$

Application

$$\int_0^2 e^{2x} \sin 3x \, dx$$

$x_0 = 0$ Internodal spacing: $\frac{2}{4} = 1/2$

$x_4 = 2$

Hence:

$x_1 = 1/2$

$x_2 = 1$

$x_3 = 3/2$

(*) Approximation derived:

$$\int_0^2 e^{2x} \sin 3x\,dx \simeq \frac{1}{45}\Big[\underbrace{7 \cdot e^0 \sin(0)}_{=0} + 32\, e \sin\left(\tfrac{3}{2}\right) + 12\, e^2 \sin(3) + 32\, e^3 \sin(9/2) + 7\, e^4 \sin(6)\Big] = -14.129$$

(computation performed using 5-digit rounding arithmetic)

Absolute error: 0.085002

Relative error: 0.0059802

(*) Simpson's composite method:

(4 ≡ number of subintervals) $\frac{n}{2} = 4 \Rightarrow n = 8$ $h = \frac{2}{8} = \frac{1}{4}$

number of subintervals

$$\int_0^2 f(x)\,dx = \sum_{j=1}^{n/2} \left\{ \frac{h}{3}\left[f(x_{2j-2}) + 4 f(x_{2j-1}) + f(x_{2j}) \right] \right\}$$

$x_0 = 0,\ x_1 = 1/4,\ x_2 = 1/2, \dots$ $(x_i = x_0 + ih)$

$$\int_0^2 f(x)\,dx = \int_0^2 e^{2x} \sin 3x\,dx \simeq \sum_{j=1}^{4} \left\{ \frac{1}{12}\left[f(x_{2j-2}) + 4 f(x_{2j-1}) + f(x_{2j}) \right] \right\} = \frac{1}{12}\Big[f(x_0) + 4 f(x_1) + f(x_2) + f(x_2) + 4 f(x_3) + f(x_4) + f(x_4) + 4 f(x_5) + f(x_6) + f(x_6) + 4 f(x_7) + f(x_8) \Big]$$

$$= \frac{1}{12}\Big[\underbrace{e^0 \sin(0)}_{0} + 4 e^{1/2} \sin(3/4) + 2\, e \sin(3/2) + 4 e^{3/2} \sin(9/4) +$$

$2e^{2}\sin(3) + 4e^{5/2}\sin\left(\frac{15}{4}\right) + 2e^{3}\sin(9/2) + 4e^{7/2}\sin\left(\frac{21}{4}\right)$

$+ e^{4}\sin(6)\Big] = -14.1833$

(5-digit rounding arithmetic)

(*) Absolute error: 0.030636

Relative error: 0.0021553

Conclusion: the composite Simpson method is around 3 times more accurate than the approximation which has been derived. This could have been estimated from the specific error formulae for both cases, and is expected due to the fact that, in the composite Simpson's method case, one is taking a finer grid.

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(4)

Inputs: length of steps: Δl
total number of steps: n
"Seed" for random-number generator: iseed
(optional, depends on how one generates such numbers)

Outputs: ns (number of steps walked towards the south)
nn (" " " " north)
nw (" " " " " west)
ne (east)

Total lengths walked:
South: $l_s = n_s * \Delta l$
north: $l_n = n_n * \Delta l$
east: $l_e = n_e * \Delta l$ (they will be calculated in
west: $l_w = n_w * \Delta l$ in Step 9)

Step 1 : (initialize ns, nn, nw, ne)

ns = 0
nn = 0
nw = 0
ne = 0

Step 3 For i = 1, .., n do steps 4 – 8

Step 4 itest = ran(iseed) (generates a uniformly distributed random number from 0 to 1).

Step 5 If itest ≤ 0.25 then
ns = ns + 1
else
Step 6 If itest ≤ 0.5 then
nn = nn + 1
else
Step 7 If itest ≤ 0.75 then
nw = nw + 1

else

Step 8 $n_e = n_e + 1$

Step 9 $l_s = n_s * \Delta e$ (computes total length walked by the animal)

$l_n = n_n * \Delta e$

$l_w = n_w * \Delta e$

3 $l_e = n_e * \Delta e$

Step 10 write ('number of steps to the north') nn
write ('number of steps to the south') ns
write ('number of steps to the east') ne
write ('number of steps to the west') nw

Step 11 write ('total length to the north') ln
write ('total length to the south') ls
write ('total length to the west') lw
write ('total length to the east') le

Step 12 Stop
end

(20)

5) In order to generate a random number between 0 and 1 obeying p(x) from a uniformly distributed random number we should

i) Generate a uniformly distributed random number y between 0 and 1:

2 $y = ran(iseed)$ (syntax may change depending on the language)

ii) Compute the random number x(y) so that

8 $x(y) = F^{-1}(y)$, with

$$F = \int_0^x p(t)dt$$

In our case,

$$y = \int_0^x p(t)\,dt = \frac{4}{\pi}\int_0^x \frac{dt}{1+t^2} = \frac{4}{\pi}\operatorname{Arctan}(x)$$

Hence we should compute

$$x = \tan\left(\frac{\pi y}{4}\right)$$

from the numbers generated in i), and give x as the output

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