UNIVERSITY OF NEW SOUTH WALES
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MATH2089 Numerical Methods and Statistics
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Numerical Methods Tutorial – Week 4 Solutions

1. For each of the following expressions, what is the "Big O" $O()$ and what is "Little o" $o()$, as $h \to 0$

   (a) $f_1(h) = 945.2h^2 - 27.6h$
   (b) $f_2(h) = 3.5h^2 + 26.7\sqrt{h}$

   Answer As h gets smaller the definitions are

   $$\alpha = o(h^k) \iff \lim_{h\to 0} \frac{\alpha}{h^k} = 0, \qquad \beta = O(h^k) \iff \lim_{h\to 0} \frac{\beta}{h^k} = K$$

   for some non-zero finite constant K. Thus, as $h \to 0$

   (a) $f_1(h) = 945.2h^2 - 27.6h = O(h)$ and $f_1(h) = o\left(h^\lambda\right)$ for $\lambda \in (0,1)$ or $f_1(h) = o(1)$.
   (b) $f_2(h) = 3.5h^2 + 26.7\sqrt{h} = O\left(h^{\frac{1}{2}}\right)$ and $f_2(h) = o\left(h^\lambda\right)$ for $\lambda \in (0, \frac{1}{2})$. It is also true that $f_2(h) = o(1)$.

2. (a) Give at least two examples of functions of n which are $o(n)$ as $n \to \infty$.
   Answer Little "o" terms are smaller as n gets larger, or from the definition

   $$\alpha = o\left(n^k\right) \iff \lim_{n\to\infty} \frac{\alpha}{n^k} = 0.$$

   Thus $3.6\sqrt{n}$ and $17.6\log(n)$ are $o(n)$ as $n \to \infty$

   (b) Give at least two functions of n that are $O(n^k)$ for a positive integer k.
   Answer "Big O" terms are of the same size as n gets larger, or from the definition

   $$\alpha = O\left(n^k\right) \iff \lim_{n\to\infty} \frac{\alpha}{n^k} = K$$

   for some non-zero constant K. Thus $\alpha = 34.56n^k + 234.901n^{k-1} = O(n^k)$ and $\beta = -\sqrt{2}n^k + 43.5n^{\frac{k}{2}} = O(n^k)$ as $n \to \infty$.

3. The central difference approximation of $O(h^2)$ to the second derivative is

   $$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2).$$

   (a) Use Taylor expansions of $O(h^4)$ to both $f(x+h)$ and $f(x-h)$ to derive this formula.
   (b) The rounding error in calculating the difference approximation is $O\left(\frac{\epsilon}{h^2}\right)$. Estimate the optimal value of h that will minimize the sum of the rounding error and the $O(h^2)$ truncation error.

   Answer

(a) Taylor series expansion of $O(h^4)$ are

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(x) + O(h^4), \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(x) + O(h^4). \end{aligned}$$

Adding these two equations gives

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + O(h^4).$$

Rearranging gives

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2),$$

as $O(h^4)/h^2 = O(h^2)$.

(b) The sum of the rounding error in calculating the approximation on the computer and the truncation error is

$$E(h) = \frac{K_1 \epsilon}{h^2} + K_2 h^2$$

where $K_1 > 0$ and $K_2 > 0$ are constants. A stationary point of $E(h)$ satisfies

$$E'(h) = -\frac{2K_1\epsilon}{h^3} + 2K_2 h = 0 \Longrightarrow h^4 = \frac{K_1\epsilon}{K_2} \Longrightarrow h = O(\epsilon^{1/4}).$$

Moreover $E''(h) = 6K_1\epsilon/h^4 + 2K_2 > 0$, so this stationary point corresponds to a (local) minimum.

Thus the optimal step size h to use in this finite difference approximation of the second derivative is

$$h^* \approx \epsilon^{1/4} = \left(2 \times 10^{-16}\right)^{1/4} \approx 1.2 \times 10^{-4}.$$

4. Let $f(x) = x^3 - 6x^2 + 11x - 6$.

(a) Prove that f has at least one zero on the interval $[0, 4]$.

(b) Is this zero unique?

Answer

(a) The function f is a polynomial, so is continuous on the whole of $\mathbb{R}$. As $f(0) = -6$ and $f(4) = 6$, so $f(0)f(4) < 0$, which implies there exists at least one zero of f on the interval $[0, 4]$.

(b) A sufficient condition for the zero to be unique is that the function f is either strictly increasing, $f'(x) > 0$ for all $x \in (0, 4)$, or strictly decreasing, $f'(x) < 0$ for all $x \in (0, 4)$. Here $f'(x) = 3x^2 - 12x + 11$, so $f'(0) = 11$ and $f'(4) = 11$. However these are just the end points, and $f'(2) = -1$, so f is neither strictly increasing nor strictly decreasing (see the plot in Figure 1). In fact f has three zeros on the interval $[0, 4]$ as $f(x) = (x-1)(x-2)(x-3)$.

5. Consider the function

$$f(x) = \begin{cases} -e^{x+1} & \text{if } x < 0; \\ x^2 - x + \frac{1}{2} & \text{otherwise.} \end{cases}$$

(a) Does f have a zero on $[-1, 1]$?

(b) **[H]**Write an anonymous function `func` to calculate f for a vector of inputs `x`.
Hint: What do the following MATLAB commands produce

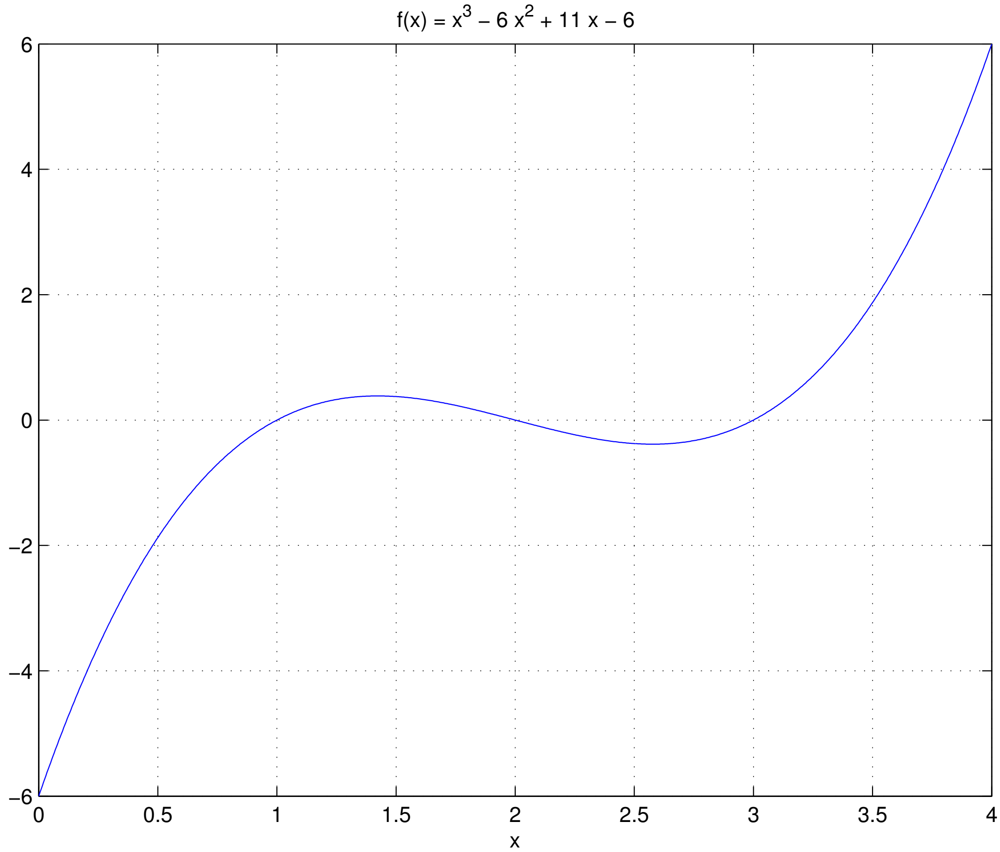

Figure 1: Plot of $f(x) = x^3 - 6x^2 + 11x - 6$ on $[0, 4]$

```
x = linspace(-1, 1, 11)
ans1 = x < 0
ans2 = x >= 0
```

(c) Plot the function f over $[-2, 2]$ using a grid on 2001 equally spaced points.

Answer

(a) For this function $f(-1) = -e^0 = -1$, and $f(1) = 1/2$, so $f(-1)f(1) < 0$. However f is **not** continuous on $[-1, 1]$, with a discontinuity at $x = 0$ as $\lim_{x\to 0^-} f(x) = -e$ and $\lim_{x\to 0+} f(x) = 1/5$ are not equal (see the first plot in Figure 2) where the definition of f changes. Thus we cannot conclude anything from the fact that $f(-1)$ and $f(1)$ are of opposite sign. In fact f does not have any zeros on $[-1, 1]$.

(b) An anonymous function for f is

```
f = @(x)  -exp(x+1).*(x<0) + (x.^2 - x + 1/2).*(x>=0);
```

As MATLAB creates a plot by joining points with straight lines,

```
f = @(x)  -exp(x+1).*(x<0) + (x.^2 - x + 1/2).*(x>=0);
x = linspace(-2, 2, 2001);
plot(x, f(x))
```

produces a plot with a line joining the discontinuity (see the second plot in Figure 2). As MATLAB does not plot `NaN`, this can be used to create a correct plot of the function (the first plot in Figure 2)

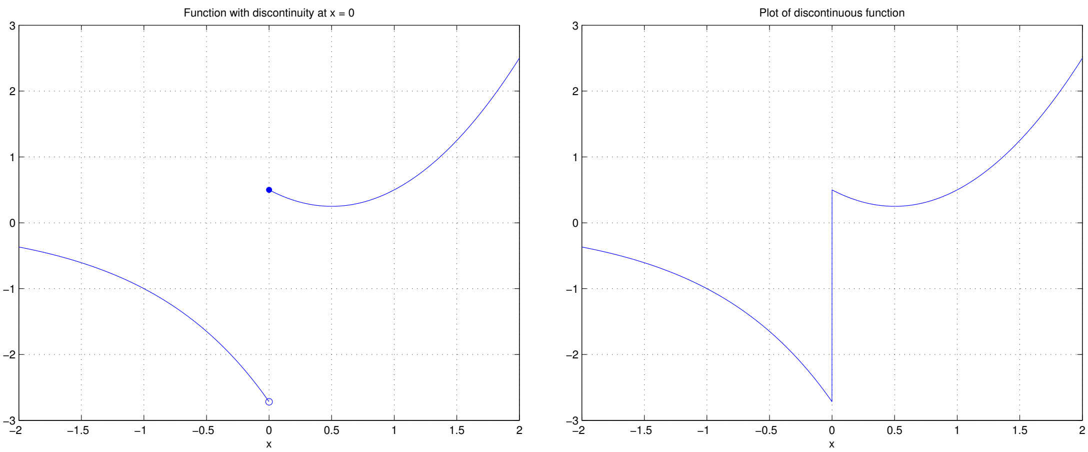

Figure 2: Plot of $f(x)$ on $[-2, 2]$

```
f = @(x)  -exp(x+1).*(x<0) + (x.^2 - x + 1/2).*(x>=0);
x = linspace(-2, 2, 2001); % Need 2001 points not 2000 for next step
i0 = find(x == 0)          % Find index of element of x equal to 0
F = f(x);
F(i0) = NaN;
plot(x, F, -eps, f(-eps), 'o', 0, f(0), '.');
grid on
```

6. You want to calculate $a^{\frac{1}{3}}$ where $a > 1$ on a computer using only the basic arithmetic operations of addition, subtraction, multiplication and division.

(a) Write this problem in the form of finding a zero to a **cubic** polynomial $p(x) = 0$.

(b) Show that there exists at least one zero of p on $[1, a]$.

(c) Show that there exists at most one zero of p on $[1, a]$.

(d) Consider using Newton's method to solve $p(x) = 0$.

i. Show that the iterates can be written as

$$x_{k+1} = \frac{1}{3}\left(2x_k + \frac{a}{x_k^2}\right).$$

ii. What other information does Newton's method require?

iii. The errors in the iterates are $e_k = |x^* - x_k|$ where $x^* = a^{\frac{1}{3}}$. If $e_4 = 2 \times 10^{-4}$, estimate e_5. What if $e_4 = 2 \times 10^{-10}$?

Answer

(a) Calculating $x = a^{\frac{1}{3}}$ is equivalent to finding a zero of the polynomial $p(x) = x^3 - a$.

(b) As p is a polynomial it is continuous on any subset of $\mathbb{R}$, in particular on $[1, a]$. As $a > 1$, $p(1) = 1 - a < 0$ and $p(a) = a^3 - a = a(a^2 - 1) > 0$, so $p(1)p(a) < 0$, implying there exists at least one zero of p on $[1, a]$.

(c) The derivative of p is $p'(x) = 3x^2 > 0$ for all $x \in [1, a]$, so p is strictly increasing on $[1, a]$. Thus p has at most one zero on $[1, a]$.

(d) Newton's method is

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} = x_k - \frac{x_k^3 - a}{3x_k^2} = \frac{1}{3}\left(2x_k + \frac{a}{x_k^2}\right).$$

Newton's method requires a starting point (initial guess) x_1.

(e) As the root x^* is a simple root ($p(x^*) = 0$, $p'(x^*) \neq 0$) Newton's method converges at a second order rate (order of convergence $\nu = 2$). Thus

$$e_{k+1} \approx e_k^\nu \implies e_5 \approx e_4^2 = \left(2 \times 10^{-4}\right)^2 = 4 \times 10^{-8}.$$

If $e_4 = 2 \times 10^{-10}$, then $e_5 \approx e_4^2 = 4 \times 10^{-20}$. However if these quantities are calculated on a computer using double precision arithmetic, then rounding error will affect the calculations so $e_5 > \epsilon = 2 \times 10^{-16}$.

7. For the function $f(x) = (x-1)^3$

(a) What is the zero of f and what is its multiplicity?
Answer The derivatives of f are $f'(x) = 3(x-1)^2$, $f''(x) = 6(x-1)$ and $f''(x) = 6$. The zero of f is $x^* = 1$, where

$$f(1) = 0, \quad f'(1) = 0, \quad f''(1) = 0, \quad f'''(1) = 6,$$

so the root has multiplicity 3.

(b) Give an initial bracket on a zero?
Answer As f is continuous on $\mathbb{R}$ and

$$f(0) = (-1)^3 = -1 < 0, \qquad f(2) = (2-1)^3 = 1 > 0$$

the interval $[0, 2]$ brackets a root of f.

(c) Perform 2 iterations of Newton's method starting from $x^{(1)} = 2$.
Answer Newton's method is

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}.$$

Using the starting point $x_1 = 2$ and arranging the values in a table gives

k	x_k	$f(x_k)$	$f'(x_k)$
1	2	1	3
2	$\frac{5}{3}$	$\frac{8}{27}$	$\frac{4}{3}$
3	$\frac{13}{9}$		

Note that you were only asked for two iterations.

(d) A MATLAB implementation of Newton's method produced

k	e(k)	e(k+1)/e(k)	e(k+1)/e(k)^2	e(k+1)/e(k)^3
1	1.00e+00	6.67e-01	6.67e-01	6.67e-01
2	6.67e-01	6.67e-01	1.00e-00	1.50e+00
3	4.44e-01	6.67e-01	1.50e+00	3.38e+00
4	2.96e-01	6.67e-01	2.25e+00	7.59e+00
5	1.98e-01	6.67e-01	3.38e+00	1.71e+01
6	1.32e-01	6.67e-01	5.06e+00	3.84e+01
7	8.78e-02	6.67e-01	7.59e+00	8.65e+01
8	5.85e-02	6.67e-01	1.14e+01	1.95e+02
9	3.90e-02	6.67e-01	1.71e+01	4.38e+02
10	2.60e-02			

Is the rate of convergence what you expect for Newton's method?

Answer If $f(x^*) = 0$ and $f'(x^*) \neq 0$ (ie x^* is a simple root) and x_1 is sufficiently close to x^*, then Newton's method will converge to x^* and the rate of convergence will be quadratic (order of convergence 2).

Here the root x^* is not a simple root as $f'(x^*) = 0$, so you do not get quadratic convergence. This is confirmed by the values in the table, where `e(k)` is going to zero (convergence), `e(k+1)/e(k)` is converging to $\beta = 0.667 \in (0, 1)$ (linear convergence with rate β), and the last two columns are growing (order of convergence is less than 2 and 3 respectively).

8. Consider using fixed point iteration to find a zero of $f(x) = 2x - \cos(x)$.

   (a) Prove that $f(x)$ has a unique zero $[0, 1]$.

   Answer As f is continuous and $f(0) = -1 < 0$ and $f(1) = 2 - \cos(1) > 0$, there exists at least one zero of f on $[0, 1]$.

   As $f'(x) = 2 + \sin(x) > 0$ for all $x \in [0, 1]$, f is strictly increasing, so there exists at most one zero of f on $[0, 1]$.

   Combining these two results shows that f has a unique zero on $[0, 1]$.

   (b) Pose this as a fixed point problem $x = g(x)$ (there is one obvious and one slightly less obvious way).

   Answer Equivalent fixed point forms are

   $$f(x) = 2x - \cos(x) = 0 \iff x = \frac{\cos(x)}{2} \iff x = \cos^{-1}(2x).$$

   (c) Prove that your fixed point iteration will converge for any starting point in $[0, 1]$.

   Answer Using the form $x = g(x) = \cos(x)/2$ gives

   $$g'(x) = \frac{-\sin(x)}{2} \Longrightarrow |g'(x)| \leq K = \frac{1}{2} < 1 \text{ for all } x.$$

   Thus fixed point iteration $x_{k+1} = g(x_k)$ converges for any starting point!

   (d) Perform 2 iterations of fixed point iteration starting from $x^{(1)} = 1/2$.

   Answer Starting from $x_1 = \frac{1}{2}$, the midpoint of the interval bracketing a zero, fixed point iteration using $g(x) = \cos(x)/2$ gives (with numbers rounded to 4 decimal places)

k	x_k	$g(x_k)$
1	0.5	$\cos(0.5)/2$
2	0.4387	$\cos(0.4837)/2$
3	0.4526	

   (e) Write a simple MATLAB script to implement fixed point iteration. (**Hint:** Look at the script `nlog2n.m` discussed in lectures.)

   Answer

9. For each of the tables of errors $e^{(k)} = |x^* - x^{(k)}|$ below, answer the following questions

   (a) Is the method converging?

   (b) What is the order of convergence (linear, superlinear, quadratic)?

   (c) Can you trust the last few values?

   - Method 1

k	e(k)	e(k+1)/e(k)	e(k+1)/e(k)^2	e(k+1)/e(k)^3
1	7.41e-02	1.15e-01	1.56e+00	2.10e+01
2	8.53e-03	8.41e-03	9.86e-01	1.16e+02
3	7.18e-05	7.41e-05	1.03e+00	1.44e+04
4	5.32e-09	7.34e-09	1.38e+00	2.60e+08
5	3.91e-17			

Answer

- As $e^{(k)} = |x^{(k)} - x^*| \to 0$, the iterates are converging.
- As $e^{(k+1)}/e^{(k)} \to 0$ the rate of convergence is superlinear (order of convergence $\nu > 1$).
- As $e^{(k+1)}/e^{(k)^2} \to K$, where $0 < K < \infty$, the rate of convergence is quadratic (order of convergence $\nu = 2$). This is confirmed by noting that $e^{(k+1)} \approx e^{(k)^2}$ in the first column.
- As $e^{(k+1)}/e^{(k)^3} \to \infty$ the order of convergence $\nu < 3$.
- As $e^{(5)} < \epsilon \approx 2 \times 10^{-16}$ (ϵ is the relative machine precision), this value may have been corrupted by rounding errors on the computer. This will also affect the ratios in row 4 of the table.

• Method 2

k	e(k)	e(k+1)/e(k)	e(k+1)/e(k)^2	e(k+1)/e(k)^3
1	1.00e-01	1.49e-01	1.49e+00	1.49e+01
2	1.49e-02	8.24e+00	5.52e+02	3.69e+04
3	1.23e-01	1.31e-01	1.07e+00	8.66e+00
4	1.61e-02	2.26e+01	1.40e+03	8.68e+04
5	3.65e-01	4.29e-01	1.18e+00	3.23e+00
6	1.57e-01	3.05e-01	1.95e+00	1.24e+01
7	4.78e-02	6.31e+00	1.32e+02	2.76e+03
8	3.01e-01	3.42e-01	1.14e+00	3.77e+00
9	1.03e-01	5.07e-02	4.92e-01	4.78e+00
10	5.23e-03	4.21e+01	8.04e+03	1.54e+06
11	2.20e-01	4.12e-01	1.88e+00	8.53e+00
12	9.07e-02	3.53e-01	3.89e+00	4.29e+01
13	3.20e-02	2.63e+00	8.21e+01	2.57e+03
14	8.40e-02	5.58e-01	6.65e+00	7.91e+01
15	4.69e-02	1.29e+00	2.76e+01	5.88e+02
16	6.07e-02	2.34e+00	3.85e+01	6.33e+02
17	1.42e-01	1.54e-01	1.09e+00	7.67e+00
18	2.19e-02	4.78e+00	2.18e+02	9.95e+03
19	1.05e-01	7.19e-02	6.87e-01	6.56e+00
20	7.53e-03			

Answer

- As $e^{(k)} = |x^{(k)} - x^*| \not\to 0$, the iterates are **not** converging. In this case you do not need to consider the other columns.

• Method 3

k	e(k)	e(k+1)/e(k)	e(k+1)/e(k)^2	e(k+1)/e(k)^3
1	1.76e-01	1.84e+00	1.05e+01	5.95e+01
2	3.24e-01	2.91e-01	8.96e-01	2.77e+00
3	9.41e-02	1.41e+00	1.50e+01	1.59e+02
4	1.33e-01	8.86e-02	6.67e-01	5.03e+00

5	1.18e-02	9.82e-02	8.35e+00	7.11e+02
6	1.15e-03	1.26e-02	1.09e+01	9.43e+03
7	1.45e-05	1.20e-03	8.24e+01	5.68e+06
8	1.74e-08	1.50e-05	8.64e+02	4.98e+10
9	2.60e-13	1.50e-04	5.77e+08	2.22e+21
10	3.91e-17			

Answer

- As $e^{(k)} = |x^{(k)} - x^*| \to 0$, the iterates are converging.
- As $e^{(k+1)}/e^{(k)} \to 0$ the rate of convergence is superlinear (order of convergence $\nu > 1$).
- As $e^{(k+1)}/{e^{(k)}}^2 \to \infty$, the order of convergence $\nu < 2$.
- As $e^{(k+1)}/{e^{(k)}}^3 \to \infty$ the order of convergence $\nu < 3$.
- As $e^{(10)} < \epsilon \approx 2 \times 10^{-16}$, this value may have been corrupted by rounding errors on the computer. This will also affect the ratios in row 9 of the table.