COMP116 – Work Sheet Three – Solutions

Associated Module Learning Outcomes

1. basic understanding of the range of techniques used to analyse and reason about computational settings.
2. Ability to apply basic rules to differentiate commonly arising functions.

Question 1: Derivatives and Critical Points

For each of the following Real valued functions $f : \mathbb{R} \to \mathbb{R}$ describe:

a. Its **first** derivative with respect to x, i.e. $f'(x)$.

b. Whether after some **fixed** number, k say, repeatedly finding the derivative produces no change. e.g. if $f(x) = 3$, then $f'(x) = 0$ and $f''(x) = 0$, so in this case $k = 2$.

c. Comment on the **critical** points of $f(x)$. Note you are **not** asked to compute these only to give an informal justification as to whether these exist, are minima or maxima, indeterminate, etc.

1. $f(x) = x^2 + 2x - 8$.
2. $f(x) = x^3/3 \ + \ x \ + \ 10$.
3. $f(x) = \frac{x^2-5x+6}{x-2}$.
4. $f(x) = \sqrt{x}$.
5. $f(x) = 1/x^2$.
6. $f(x) = \sin^2(x) + \cos^2(x) + x^2$.
7. $f(x) = \sin(x^2) + \cos(x^2) + x^2$.
8. $f(x) = \exp(x \log x)$ (recall that $\log$ is Natural, i.e. base e unless explicitly stated to be otherwise).

Answers:

1. $f'(x) = 2x + 2$ with a single critical point (at $x = -1$) which is a **minimum** ($f''(x) = 2$ and positive). Since $f'''(x) = 0$ there are no further derivatives (i.e. **different** functions).

2. $f'(x) = x^2 + 1$, however, this function has **no Real-valued** critical points. As with (1) there are only a finite number of times $f(x)$ can be differentiated before reaching 0.

3. The key point to notice is that $x^2 - 5x + 6 = (x-2)(x-3)$ so that $f(x) = x - 3$. As $f'(x) = 1$ there are no critical points.

4. $f'(x) = 0.5/\sqrt{x}$. There are no critical points but unlike the previous examples this can be differentiated infinitely often with different functions arising.

5. $f'(x) = -2/x^3$. Again there are no critical points and like (4) this can be differentiated infinitely often with different functions arising. Denoting by $f^k(x)$ the result after k so that $f^1(x) \equiv f'(x)$, $f^2(x) \equiv f''(x)$ etc $f^k(x) = (k+1)!/x^{k+1}$.

6. As with example (3), see if there are "obvious" simplifications possible. Here, since $\sin^2(x) + \cos^2(x) = 1$ for every x, we get $f(x) \equiv x^2$ with $f'(x) = 2x$, a single critical point ($x = 0$) which is a minimum. Only finitely many differentations are possible before reaching 0.

7. Combining trigonomentric and chain rules gives $f'(x) = 2x\cos(x^2) - 2x\sin(x^2) + 2x$. The function $f(x)$ has infinitely many critical points (mixing minima with maxima) and arising from the periodic behaviour of $\sin$ and $\cos$. It also may be differentiatied infinitely often.

8. Again, using the chain, product (for $x\log x$), $\exp$ and $\log$ rules we have $f'(x) = \exp(x\log x)(1 + \log x)$. Although $\exp(y) > 0$ for all y the term $1 + \log x$ is 0 when $x = 1/e$. This is the only critical point and a minimum. This function is, again, infinitely differentiable.

Question 2 – Roots Revisited

A very basic method for discovering a root of a polynomial function was discussed in the first worksheet. An informal realization of the approach outlined would be

Algorithm 1 Simple root-finding method for polynomials with coefficients in $\mathbb{R}$

Input: $p(x) \in \mathbb{R}[X]$; $a, b \in \mathbb{R}$ with $p(a) < 0$ and $p(b) > 0$
Input: $MAX \in \mathbb{N}$; $\varepsilon \in \mathbb{R}$ with $\varepsilon > 0$;
$\{MAX$ is a "cut-off" to prevent indefinite looping; ε a "tolerance" threshold.$\}$
$low := a$; $high := b$; $k := 0$;
repeat
  $x := (low + high)/2$; {Find value in "middle", i.e. average of $\{low, high\}$.}
  if $p(x) < 0$ **then**
    $low := x$;
  else if $p(x) \geq 0$ **then**
    $high := x$;
  end if
  $k := k + 1$;
until $|p(x)| \leq \varepsilon$ or $k > MAX$
return x;

Algorithm 1 uses a simple "binary search" (if you have not met "binary search" already in Year 1, then you will certainly be introduced to it on COMP108: this is one of the most basic and effective data searching techniques). It can (provided suitable initial values a and b are identified) be applied as an approach to (try and) find not only roots of polynomials but also so-called "zeros" of arbitrary Real valued functions, i.e. for $f : \mathbb{R} \to \mathbb{R}$, values c with which $f(c) = 0$.

Following the discovery of Differential Calculus in the 17th Century, rather more sophisticated techniques were developed. One of these (the Newton–Raphson method) is still widely taught. As with the binary search technique in Algorithm 1 this can be adapted to arbitrary functions (subject to some technical conditions). Another very powerful general method is Halley's Method mentioned briefly in the first worksheet.

Halley's Method is presented in Algorithm 2.

One required property of $f(x)$ in order to use Halley's Method to find zeros of f is that not only is $f'(x)$ (the first derivative of f) well-defined but also $f''(x)$ (its second derivative). Depending on how the transitions from x_0 to x_1 through to x_k develop this *might* lead to complications, although it should be noted that it is *not* required that $f'(x)$ and $f''(x)$ are well defined for every $x \in \mathbb{R}$.

Algorithm 2 Halley's Method for finding roots of $f(x)$

Input: $f : \mathbb{R} \rightarrow \mathbb{R}$; {e.g. could be name of an implemented function.}
Input: $x_0 \in \mathbb{R}$; {An initial guess for $f(x_0) = 0$.}
Input: $MAX \in \mathbb{N}$; $\varepsilon \in \mathbb{R}$ with $\varepsilon > 0$;
{MAX is a "cut-off" to prevent indefinite looping; ε a "tolerance" threshold.}
$k := 0$;
repeat

$$x_{k+1} \;:=\; x_k \;-\; \frac{2f(x_k)f'(x_k)}{2(f'(x_k))^2 - f(x_k)f''(x_k)}$$

   $k := k + 1$;
until $|f(x_k)| \leq \varepsilon$ or $k > MAX$
return x_k;

One significant advantage of Halley's Method for high-degree polynomials is that, unlike a number of methods, it does not require the computation of *square roots*, i.e. functions of the form $\sqrt{f(x)}$. This can be especially useful, in comparison with techniques such as Laguerre's (module textbook, pages 156-7), when dealing with polynomial functions.

a. Suppose $f(x) = \frac{\cos(5x+1)}{x+5}$.

   VERY IMPORTANT: Measures are in **radians** and not degrees.

   1. Why is it sufficient to consider *only* the behaviour of $\cos(5x+1)$ when seeking zeros of $f(x)$?
   2. Using $a = -1$ (so that $\cos(5a + 1) \sim -0.654$) and $b = 1$ (with $\cos(5b+1) \sim 0.96$) what are the first **five** values found for $\cos(5x+1)$ using the method of Algorithm 1?
   3. Now use Halley's Method to compute the first three values using an initial guess $x_0 = 0$, i.e. $(-1+1)/2$.
   4. If x_{binary} is the value discovered by Algorithm 1 and x_{halley} that found with Algorithm 2, which of these describes a "better zero" of $f(x)$, i.e. which of $\{|f(x_{binary})|, |f(x_{halley})|\}$ is smaller (closest to 0)?

Answers

1. Whether $\frac{\cos(5x+1))}{x+5} = 0$ is dependent only on $\cos(5x+1) = 0$ irrespective (assuming $x \neq -5$) of the value of $x+5$.

Table 1: Bisection Method zero search case

a	b	m	$\cos(5m+1)$
-1	1	0	0.54
-1	0	-0.5	0.071
-1	-0.5	-0.75	-0.92
-0.75	-0.5	-0.625	-0.526
-0.625	-0.5	-0.5625	-0.234

2. This very small example illustrates one problem with the Bisection Approach: an actual root of $\cos(5x+1)$ is $x \sim -0.514$ (radians). Although the case -0.5 produces the best approximation to this root it will take some further iterations to come close to it depending on the precision required. The problem is that when the upper estimate (b) is already close to a zero the lower estimate (a) is still some distance away: this is what has happened when $b = m = -0.5$, $f(b) > 0$, $|f(b)| < 0.072$, but $f(a) < 0$ with $|f(a)| > 0.526$.
3. Halley's method discovers the next x using

$$\begin{array}{rcl} f(x) & = & \cos(5x+1) \\ f'(x) & = & -5\sin(5x+1) \\ f''(x) & = & -25\cos(5x+1) \end{array}$$

Notice that

$$\begin{array}{rcl} f(x)f'(x) & = & -5\cos(5x+1)\sin(5x+1) \\ (f'(x))^2 & = & 25\sin^2(5x+1) \\ f(x)f''(x) & = & -25\cos^2(5x+1) \end{array}$$

So that successive approximations are found by iterating

$$x_k + \frac{10\cos(5x+1)\sin(5x+1)}{50\sin^2(5x+1) + 25\cos^2(5x+1)} \equiv x_k + \frac{10\cos(5x+1)\sin(5x+1)}{25(1+\sin^2(5x+1)}$$

(Again using the relation $\sin^2(x) + \cos^2(x) = 1$). Simplifying further gives the final form to be iterated as,

$$x_{k+1} = x_k + \frac{2}{5}\left(\frac{\cos(5x+1)\sin(5x+1)}{1+\sin^2(5x+1)}\right)$$

Table 2: Halley's Method zero search case

k	x_k	x_{k+1}	$\lvert\cos(5x_{k+1}+1)\rvert$
0	0	0.106	0.041
1	0.106	0.114	0.0008
2	0.114	0.114	0.0008

Applying Halley's method with initial guess $x_0 = 0$ Notice this converges to a zero (0.1142) "quickly".

d. We find $x_{binary} \sim -0.5625$ and, after sufficiently many further iterations will hone in on the zero -0.514. In contrast, $x_{halley} \sim 0.114$: a different zero of $\cos(5x+1)$ and discovered after fewer iterations.

b. For the degree 5 polynomial

$$p(x) = x^5 + 2x^4 - 11x^3 - 22x^2 + 30x + 60$$

1. Carry out the same comparison (again with 5 iterations) of Algorithm 1 and Algorithm 2, this time for the degree 5 polynomial $p(x)$. Use $a = -2.7$ (with $p(a) \sim -2.068$) and $b = 0$ (so that $p(b) = 60$) in Algorithm 1 and $x_0 = -1.35$ (i.e. $(-2.7+0)/2$) in Algorithm 2.
2. Which of the two seems to converge to a root of $p(x)$ more quickly?
3. Do Algorithm 1 and Algorithm 2 seem to converge to the *same* root?

Solutions:

1. Using Algorithm 1.

Table 3: Bisection Method Polynomial Root search

a	b	m	$p(m)$
-2.7	0	-1.35	8.628
-2.7	-1.35	-2.025	-0.0427
-2.025	-1.35	-1.688	2.214
-2.025	-1.688	-1.856	0.572
-2.025	-1.856	-1.94	0.166
-2.025	-1.94	-1.98	0.045

In this case we see a similar problem to that observed in the $\cos(5x+1)$ example: an actual root is $x = -2$ which a value (-2.025) close to this is found quickly. However given the disparity between a and b the next stages move away from this root.

With Halley's method we find:

$$\begin{aligned} p(x) &= x^5 + 2x^4 - 11x^3 - 22x^2 + 30x + 60 \\ p'(x) &= 5x^4 + 8x^3 - 33x^2 - 44x + 30 \\ p''(x) &= 20x^3 + 24x^2 - 66x - 44 \end{aligned}$$

Leading to,

$$\begin{aligned} p(x)p'(x) &= (x^5 + 2x^4 - 11x^3 - 22x^2 + 30x + 60)(5x^4 + 8x^3 - 33x^2 - 44x + 30) \\ (p'(x))^2 &= (5x^4 + 8x^3 - 33x^2 - 44x + 30)^2 \\ p(x)p''(x) &= (x^5 + 2x^4 - 11x^3 - 22x^2 + 30x + 60)(5x^4 + 8x^3 - 33x^2 - 44x + 30) \end{aligned}$$

and

Table 4: Halley's Method Polynomial roots

k	x_k	x_{k+1}	$\lvert p(x_k)\rvert$
0	-1.35	1.789050709692225	8.628104062499997
1	-1.789050709692225	1.9594126779330223	1.062502901033703
2	-1.9594126779330223	1.998813215491566	0.1017902028870985
3	-1.998813215491566	1.9999999514789264	0.0023904922205915113
4	-1.9999999514789264	1.9999999999999998	$9.704217518446967 \times 10^{-8}$
5	-1.9999999999999998	2.0000000000000018	$3.552713678800501 \times 10^{-15}$

Halley's method in this example has (when $k = 3$) come very close to identifying the root $x = -2$. The estimation improves so that by $k = 5$ the value identified differs from -2 by under 10^{-15}. Notice that (unlike the $\cos(5x + 1)$ case) this is the same root discovered by the bisection method.