CP315: Introduction to Scientific Computing

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1 Introduction

CP315 is a set of methods for solving mathematical problems with computers; fair enough - we will be using Maple and MatLab. Fundamental operations that are used: addition and multiplication. These are needed to evaluate a polynomial at a specific value. As we know, polynomials are basic objects in scientific computing $\rightsquigarrow$ efficient evaluation.

1.1 Polynomial Evaluation

Consider a general, fourth-degree polynomial:

$$P(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4$$

i. Find $P\left(\frac{1}{2}\right)$ naively requires substituting $\frac{1}{2}$ into $P(x) \rightsquigarrow 10$ multiplications and 4 additions comes to a total of 14 operations.

ii. Store powers of $\frac{1}{2}$ progressively $\rightsquigarrow$ 3 multiplications (from the powers) + 4 multiplications (from the coefficients) and 4 additions. The new total is 11 operations.

iii. *Horner's Method*: Rewrite $P(x)$ "backwards":

$$P(x) = c_0 + x(c_1 + x(c_2 + x(c_3 + x(c_4))))$$

This brings it down to 8 total operations.

Fact: A degree d polynomial can be a evaluated in d multiplications and d additions.

Portfolio Part 1: Implement Horner's Method in Maple and/or MatLab.

1.1.1 Variation on the Theme

Evaluate:

$$\begin{aligned} P(x) &= x^5 + x^8 + x^{11} + x^{14} \\ &= x^5(1 + x^3 + x^6 + x^9) \\ &= x^5(1 + x^3(1 + x^3 + x^6)) \\ &= x^5(1 + x^3(1 + x^3(1 + x^3))) \end{aligned}$$

We get a total of 6 multiplications by 3 additions, thus 9 operations.

Overview of Calculus

Theorem 1. *Intermediate Value Theorem*

If $f(x)$ is continuous in $[a,b]$ then $\forall$ y, such that, $f(a) \leq y \leq f(b)$ $\exists$ c, such that $a \leq c \leq b$ and $f(c) = y$.

***Corollary* 2.** *If $f(a), f(b) < 0$, then $\exists$ c, such that $f(c) = 0$. Where c is a root of $f(x) = 0$.*

Theorem 3. *Mean Value Theorem*

If $f(x)$ is differentiable in $[a,b]$ then $\exists$ c, such that $f'(c) = \frac{f(a) - f(b)}{b - a}$. Thus, there is a point where we will be able to calculate the slope at c.

***Corollary* 4.** *Rolle's Theorem*

If $f(x)$ is differentialable at $[a,b]$ then $\exists$ c, such that $a \leq c \leq b$ and $f'(c) = 0$.

Theorem 5. *Taylor's Theorem*

If $f(x)$ is $(k+1)$-differentiable in $[x_0, x]$, $\exists$ c, such that:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \ldots + \frac{f^{k+1}(x_0)}{(k+1)!}(x - x_0)^{k+1} + R$$

where $R = \frac{f^{(k+1)}(c)}{(k+1)!}(x - x_0)^{k+1}$, is the remainder. If we know $f(x_0)$, then we can find nearby values $f(x)$ as a polynomial of degree k.

Example 6. $f(x) = \sin(x)$. Find a degree-4 Taylor polynomial (approximation) about $x_0 = 0$.

$$P_4(x) = x - \frac{x^3}{6}$$

with a remainder is $R = \frac{x^5}{120}\cos(c)$. Now, we need to estimate the size of the remainder term:

$$|R| \leq \frac{|x|^5}{120}$$

If $|x| \leq 10^{-4}$ then $|R| \leq \frac{10^{-20}}{120}$. This tells us that for all numbers $\leq 10^{-4}$, R is close to zero and thus the Taylor approximation is accurate.

Theorem 7. *Mean Value Theorem for Integrals*

If f is continuous in $[a,b]$ and g is integrable in $[a,b]$ and does not change sign in $[a,b]$ then, $\exists$ c such that $a \leq c \leq b$ and

$$\int_a^b f(x)g(x)\mathrm{dx} = f(c)\int_a^b g(x)\mathrm{dx}$$

Note: *This helps because this result gives us a way to evaluate $\int f(x)g(x)$ - as there is no defined way to do this.*

2 Floating Point Representation of Real Numbers ($\mathbb{R}$)

IEEE 754 is a standard to model floating point arithmetic on a computer. The problem is that we have finite-precision memory locations to represent infinite-precision numbers, YIKES.

IEEE 754 is a set of **binary** representations of real numbers.

A floating point, or real, number has three parts:

1. Sign ($\pm$) - s
2. Mantissa (AKA significant digits) - m
3. Exponent - e

These three parts are stored in a word. There are three common precision types:

1. Single: 32 bits, (s: 1, m: 8, e: 23)
2. Double: 64 bits (s: 1, m: 11, e: 52)
3. Long-double: 80 bits, (s: 1, m: 15, e: 64)

Definition 8. *A normalized IEEE 754* ***floating point number*** *is the following:*

$$\pm 1.b_1 b_2 ... b_N \times 2^p$$

where p *is an M-bit binary number; where*

$$b_i \in \{0, 1\}, i = 1, ..., N$$

Example 9. 9 decimal and we want to convert to an IEEE FLP number.

$$\begin{aligned} 9 &\rightarrow 1001\,(\text{binary}) \\ +1 &\;.\; 001 \times 2^3 \\ N &= 3 \\ P &= 3 \end{aligned}$$

Multiplication by power of 2 $\equiv$ a shift.

Typical double precision parameters in C/MatLab: $M = 11$, $N = 52$.

Example 10. We want to represent 1.

$$\begin{aligned} 1 &\rightsquigarrow 0001 \\ +1 &\;.\; 0...0_{52} \times 2^0\,(52\,\text{zeroes}) \end{aligned}$$

What is the "next" number we can represent? The answer is: $+1.0...0_{51}1 \times 2^0 \rightsquigarrow 1 + 2^{-52}$, this is 51 zeroes.

Definition 11. *Machine epsilon,* $\mathrm{E_{mach}}$*, is the distance between* 1 *and the smallest FLP number greater than 1.*

***Remark* 12.** *For IEEE 754, double precision, we have* $\mathrm{E_{mach}} = 2^{52}$.

2.1 IEEE Nearest Rounding Rule

Example 13. 9.4 in decimal $\rightarrow 1001.\overline{0110}$

The binary representation of $0.4 \approx \frac{1}{2^2} + \frac{1}{2^3} + \frac{1}{2^6} + \frac{1}{2^7} + ... = \sum_{k=1}^{\infty} \left(\frac{1}{2^{4k+2}} + \frac{1}{2^{4k+3}} \right)$

We need to fit this precision number in 52 bits.

$$1.\underline{001}011001100110...0110\,\underline{0} \times 2^3$$

We have the three bits in the beginning following by 12 sets of 0110:

$$3\,\text{bits} + 12 \times 4\,\text{bits} = 51\,\text{bits}$$

RMR: Look at the 53rd bit to the right of the radix point: $\begin{cases} 1 \to \text{add 1 to bit 52} \\ 0 \to \text{do nothing} \end{cases}$

So in our example: 53rd bit is 1, so we add 1 to 52.

Thus, 9.4 is represented as:

$$+1.001\underline{0110}\,\mathbf{1} \times 2^3$$

which is actually $9.4 + 0.2 \times 2^{-49}$ in decimal.

Remark 14. The IEEE double precision number associated with 9.4 using RNR is:

$$fl(9.4) = 9.4 + 0.2 \times 2^{-49}$$

where 0.2×2^{-49} is the error.

Definition 15.

$$\begin{aligned} x_c &= \text{computed value of } x \\ \text{absolute error} &= |x_c - x| \\ \text{relative error} &= \frac{|x_c - x|}{|x|} \end{aligned}$$

***Remark* 16.** *Relative error in IEEE 754 is bounded by:*

$$\frac{|fl(x) - x|}{|x|} \leq \frac{1}{2} E_{\text{mach}}$$

2.2 Loss of Significant Digits

Example 17. $E_1 = \frac{1 - \cos(x)}{\sin^2(x)}$ and $E_2 = \frac{1}{1 + \cos(x)}$. $\therefore E_1 = E_2$ in exact arithmetic. Evaluate E_1 and E_2 numerically for $x = 1.000...$, $x = 0.100...$, $x = 0.010...$.

Remark 18. For values of $x < 10^{-5}$, E_1 losses signifcant digits. For $x < 10^{-8}$, E_1 has no correct significant digits. Well, we are subtracting numbers that are nearly equal.

Example 19. $x^2 + 9^{12}x - 3 = 0$, with $a = 1$, $b = 9^{12}$, $c = -3$.

$$\begin{aligned} \Delta &= \sqrt{b^2 - 4\text{ac}} \\ x &= \frac{-b \pm \Delta}{2a} \\ \oplus \rightsquigarrow \ x = & \frac{-b + b}{2a} = 0 \end{aligned}$$

But how?! We need to restructure the formula, using the conjugate quantity:

$$
\begin{aligned}
\frac{-b+\sqrt{\Delta}}{2a} &\times \left(\frac{-b+\sqrt{\Delta}}{-b+\sqrt{\Delta}}\right) \\
&= \frac{\Delta-b^2}{2a\left(b+\sqrt{\Delta}\right)^2} \\
&= \frac{-4\mathrm{ac}}{2a\left(b+\sqrt{\Delta}\right)} \\
&= \frac{-2c}{b+\sqrt{\Delta}}
\end{aligned}
$$

Note: This formula only applies for degree-2 polynomials.

3 Equation Solving

- We will explore iterative methods to locate solutions of $f(x)=0$
- Convergence, complexity

We are also going to look at three different methods of solving equations:

1. Bisection
2. Fixed-point
3. Newtons's method

3.1 Bisection Method

- We are looking to solve $f(x)=0$
- Means find r, st $f(r)=0$
- Existence of r: IVT

Steps:

1. Find $[a,b]$ st $f(a)\times f(b)<0$
2. Then, $\exists r\colon a<r<b$ st $f(r)=0$

Example 20. $f(x)=x^3+x-1$, we know $f(0)=-1,\ f(1)=1$ and thus:

$$\rightsquigarrow \exists r\in[0,1]\,\mathrm{st}\,f(r)=0$$

Also:

$$f\left(\frac{1}{2}\right)<0\rightsquigarrow f\left(\frac{1}{2}\right)\times f(1)<0\rightsquigarrow r\in\left[\frac{1}{2},1\right]$$

Next step in the interation:

$$f\left(\frac{1}{2}\right) > 0 \rightsquigarrow f(0) \times f\left(\frac{1}{2}\right) < 0 \rightsquigarrow r \in \left[0, \frac{1}{2}\right]$$

And thus we know:

$$f\left(\frac{1}{2}\right) < 0$$

We now know that $\frac{1}{2} < f\left(\frac{1}{2}\right) < 1$. We know can check the midpoint of $\left[\frac{1}{2}, 1\right]$ which is $\frac{3}{4}$. Next interation:

$$f\left(\frac{3}{4}\right) > 0 \rightsquigarrow r \in \left[\frac{1}{2}, \frac{3}{4}\right]$$

Portfolio Part 2: Implement Bisection Method in Maple and/or MatLab.

Algorithm 1

Bisection Method
Input: `f`, `a`, `b` st. $f(a) \times f(b) < 0$; tolerance (ϵ) - `e`
Output: approximate root `r`, in $[a, b]$, $f(r) = 0$

```
while (b-a)/2 > e do
     r=(a+b)/2
     if f(r)=0 then return r
     if f(a)*f(r) < 0
          b=r
          else
               a=r
     return (a+b)/2
```

Example 16 cont.

ϵ	#`while` step	approx `r`
10^{-4}	13	0.6823
10^{-5}	16	0.6823
10^{-6}	19	0.68232
10^{-7}	23	0.68232780

Definition 21. *An approximate solution is correct to* <u>*p decimal places*</u> *if the error*

$$|x_c - r| < \frac{1}{2} 10^{-p}$$

3.1.1 Error Analysis

- Start $[a, b]$
- After n bisection steps $[a_n, b_n]$

$$x_c = \frac{a_n + b_n}{2} \rightsquigarrow |x_c - r| < \frac{b-a}{2^{n+1}}$$

Question 22. *How many bisection steps are needed to compute a solution correct to 6 decimal places?*

Answer. *Error after n bisection steps: $\frac{1}{2^{n+1}}$ and thus*

$$\begin{aligned} \frac{1}{2^{n+1}} &< \frac{1}{2}10^{-6} \\ 10^6 &< 2^n \\ \log(10^6) &< \log(2^n) \\ 6 \times \log(10) &< n \times \log(2) \\ 6 &< n \times \log(2) \\ 19.9 &< n \end{aligned}$$

And thus we need 20 steps to compute 0.739085*.*

3.2 Fixed-Point Iteration

Definition 23. *r is a fixed point (fp) of a function $g(x)$, iff $g(r)=r$.*

Example 24. $g(x)=x^3$. We have three fixed points: $0, \pm 1$.

Observation. Finding a fp of $g(x) \Leftrightarrow$ solving the equation: $g(x) - x = 0$ where we can define $g(x) - x$ as $f(x)$.

Algorithm 2

FPI
Input: $f(x) = g(x) - x$, initial guess, x_0
Output: approximate solution of $f(x) = 0$, (ie. a fp of $g(x)$)

```
for i = 0..k
   x_{i+1}=g(x_i)
```

If the sequence x_0, x_1, x_2, ... converges to a value, r, then r is a fp of $g(x)$. For some j: $|x_{j+1} - x_j| < \mathrm{E}$.

Question 25. *Can any fct, $f(x)$ be written as $g(x) - x$?*

Answer. *Yes, and often in more ways than one.*

Example 26. $x^2 + x - 1 = 0$

$$x = 1 - x^3 \tag{1}$$

$$x = (1 - x)^{\frac{1}{3}} \tag{2}$$

$$x = \frac{1 + 2x^3}{1 + 3x^2} \tag{3}$$

Use fp iterations with $x_0 = 0.5$.

1. The interates flip-flop from 0 to 1, **no convergence**

2. The iterates converge to 0.6823 in 25 iterations

Explanation: $|g'(r) > 1, <1|$

Example 27.

$$\begin{aligned} g_1(x) = & -\frac{3}{2}x + \frac{5}{2} \quad \text{with } r = 1 \text{ and } |g_1'(1)| = \frac{3}{2} > 1 \\ g_2(x) = & -\frac{1}{2}x + \frac{3}{2} \quad \text{with } r = 1 \text{ and } |g_2'(1)| = \frac{1}{2} < 1 \end{aligned}$$

Thus, we have $x_{i+1} = g_1(x_i)$. Consider $g(x) \rightsquigarrow$

$$x_{i+1} - 1 = -\frac{3}{2}(x_i - 1)$$

denote by $e_i = |1 - x_i|$ then $e_{i+1} = \frac{3}{2} e_i \rightsquigarrow$ error increases, divergent.

Consider $g_2(x)$ with $x_{i+1} = g_2(x_i) \rightsquigarrow$

$$x_{i+1} - 1 = -\frac{1}{2}(x_i - 1)$$

then $e_{i+1} = \frac{1}{2} e_i$. 1

Definition 28. *Denote by e_i, the error at step i, of an iterative method.*

$$e_i = |r - x_i|$$

The method ***converges linearly*** *with rate, S, if:*

$$\lim_{i \to \infty} \frac{e_{i+1}}{e_i} = S$$

and $S < 1$.

Observation. *f-p iteration for $g_2(x)$ converges linearly with rate $S = \frac{1}{2}$.*

Theorem 29. *Assume g is differentiable.*

$$\begin{aligned} g(r) = & \quad r \qquad \text{and } r \text{ is an fp of } g \\ |g'(r)| = & \quad S < 1 \end{aligned}$$

Then, the fp iteration for g, conerges linearly with rate, S to r. For initial guesses, x_0, sufficiently close to r.

Example 30. $f(x) = x^3 + x - 1$ in the form of $g(x) = x$.

1. $g_1(x) = 1 - x^3$, now $|g_1'(x)| = 3x^2 \longrightarrow x = 0.6823 \longrightarrow >1$
2. $g_2(x) = (1 - x)^{\frac{1}{3}}$, now $|g_2'(x)| = \frac{1}{3}(1 - x)^{-\frac{2}{3}} + 1 \longrightarrow x = ... \longrightarrow <1 \qquad \therefore$ converges
3. $g_3(x) = \frac{1 + 2x^3}{1 + 3x^2}$, now $|g_3'(x)| = \frac{(6x^2)(1 + 3x^2) + (6x)(1 + 2x^3)}{(1 + 3x^2)^2} \longrightarrow x = ... \longrightarrow 0 < 1$ We have a linear convergence with rate, $S = 0$

3.2.1 Stopping Criteria for FPI

Where do we need to stop the iteration?

1. Bounded absolute error:

$$|x_{i+1} - x_i| < \mathrm{E}$$

2. Bounded relative error:

$$\frac{|x_{i+1}-x_i}{|x_{i+1}|}<\mathrm{E}$$

Example 31. $\begin{cases} g(x)=\frac{x+\frac{2}{x}}{2} \\ x_0=1 \end{cases}$. Set up FPI as $g(x)=x$.

$$g(\sqrt{2})=\frac{\sqrt{2}+\frac{2}{\sqrt{2}}}{2}=\sqrt{2}$$

3.2.2 Forward and Backward Error

Example 32. $f(x)=x^3-2x^2+\frac{4}{3}x-\frac{8}{27}$. Use the bisection method to compute a root with 6 correct significant digits. We have $f(0)\,f(1)<0$ and $f\left(\frac{2}{3}\right)=0$.

Observation. 16 steps $\rightsquigarrow$ 0.6666641. We cannot get the 6$^{\text{th}}$ digit correct.

IEEE double precision, there are many float point numbers within 10^{-5} of the correct root $r=\frac{2}{3}$.

Definition 33. *Suppose a function, f, with root r and $f(r)=0$. Also, x_a is an approximation to r computed by a root-finding method.*

Backwards error (BE): $|f(x_a)|$

Forward error (FE): $|r-x_a|$

BE amount by which we need to change $f(x)$ so that x_a is a solution. FE amount by which we need to change the approximate solution to make it correct.

***Remark* 34.** *The problem we encountered with the previous example is that the BE is near* $\mathrm{E}_{\text{mach}}=10^{-16}$ *and the FE* $\approx 10^{-5}$.

Definition 35. *Multiple Roots*

f, a differentiable function, with root r and $f(r)=0$ if

$$o=f(r)=f'(r)=f''(r)=\ldots=f^{(m-1)}(r)$$

and $f^{(m)}(r)\neq 0$. Then, f, has a root of multiplicity m, at r; where r is a multiple root of order m of f.

$$\begin{cases} m=1; r\,\text{single root} \\ m=2; r\,\text{double root} \\ m=3; r\,\text{triple root} \end{cases}$$

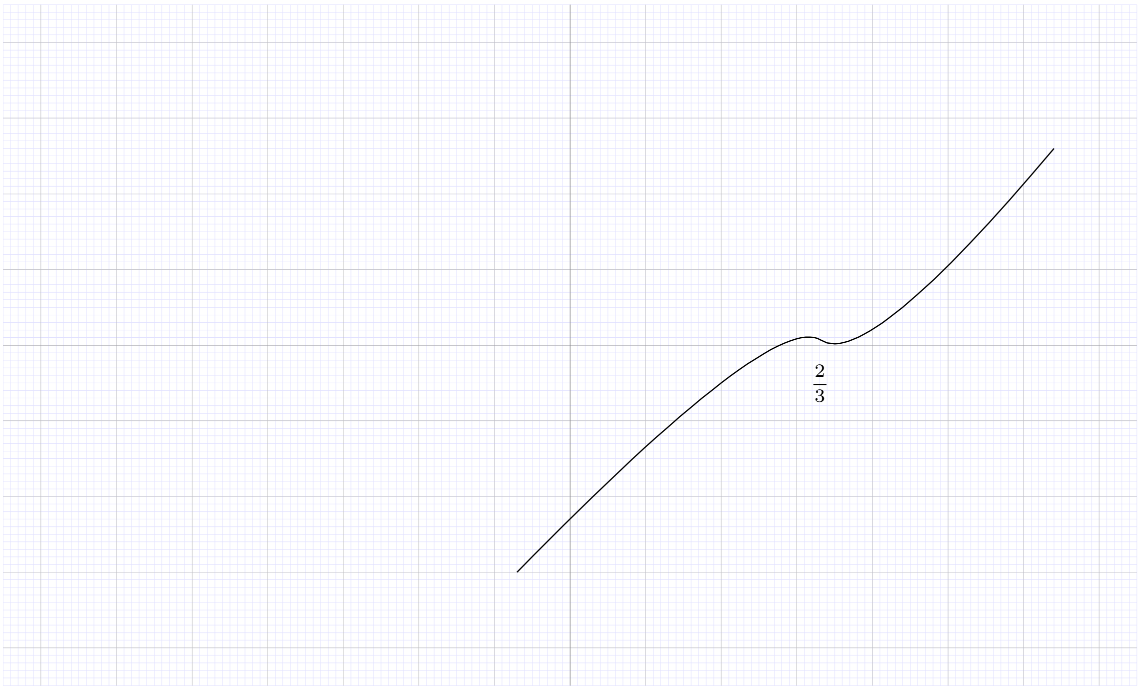
Example 36. $f(x)=x^2$, has a double root at $x=0$.

$$\begin{array}{ccc} f(0) & = & 0 \\ f'(0) & 2x|_{x=0} & =0 \\ f''(0) & = & 2\neq 0 \end{array}$$

Also, $f(x)=x^3$ has a triple root at $x=0$.

Geometric Intuition.

Graph of $f(x) = \left(x - \frac{2}{3}\right)^3$.



$\frac{2}{3}$ is a triple root. The graph is [supposed to be] flat around the triple root.

Consequence. Large disparity between BE and FE.

$$\mathrm{BE} \ll \mathrm{FE}$$

where BE is the vertical dimension and FE is the horizantal dimension.

Example 37. $f(x) = \sin(x) - x$ has a triple root at $r = 0$ and $x_a = 0.001$ is the approx. root. Compute BE and FE.

$$\begin{aligned} \text{BE:} \quad |r - x_a| &= 10^{-3} \\ \text{FE:} \quad |f(x_a)| &= |\sin(0.001) - 0.001| \\ &\approx 1.6667 \times 10^{-10} \end{aligned}$$

Stopping Criteria. Either make FE small or make BE small.

$$\text{Bisection:} \begin{cases} \text{BE: known} \\ \text{FE:} < \frac{b-a}{2} \end{cases}$$

> if abs(f(x_a)) < E then ...
> if abs($\frac{b-a}{2}$) < E then ...

$$\text{Fixed point:} \begin{cases} \text{BE: known} \\ \text{FE: not known} \end{cases}$$

3.2.3 Wilkinson Polynomial

$$\begin{aligned} W(x) &= (x-1)(x-2)\ldots(x-20) \\ &= \prod_{i=1}^{20} (x - i) \end{aligned}$$

It has 20 (simple) roots, $x = 1, ..., 20$. To compute numerical approximations to the roots of the expanded $W(x)$ is very hard. $W(x) = x^{20} \pm ...$

3.2.4 Sensitivity of Root Finding

A problem is called sensitive if small errors in the input (the eq. we are solving). This leads to large errors in the output (solution).

We need to measure how far a root is moved when the eq. is changed (perturbed).

Proposition 38. *Supposed, we change $f(x) \to f(x) + \epsilon\, g(x)$.*

Let Δ_r be the corresponding change to the root r.

$$f(r + \Delta_r) + \epsilon\, g(r + \Delta_r) = 0$$

D-d-d-d-d-drop the Taylor and neglect the higher order terms (H.O.T).

$$\Delta_r \approx -\frac{\epsilon\, g(r)}{f'(r)}$$

for $\epsilon \ll f'(r)$.

Example 39. Estimate the largest root of

$$P(x) = \left(\prod_{i=1}^{6} (x - i) \right) - 10^{-6} x^7$$

Get all emotional and used the sensitivity formula.

$$\begin{aligned} \epsilon &= -10^{-6} \\ g(x) &= x^7 \\ f(x) &= P(x) \end{aligned}$$

Now:

$$\Delta_r \approx \frac{\epsilon\, 6^7}{5!} = -2332.8\, \epsilon$$

and thus:

$$6 + \Delta_r = 6.0023$$

3.3 Newton's Method

Problem. Find a root of a fn, $f(x) = 0$.

The first thing we need to do is start with an initial guess of x_0. Draw the tangent line to f at x_0 and identify the point where the tangent intersects with the x-axis.

We can get the equation of the tangent line at $(x_0, f(x_0))$.

$$y - f(x_0) = f'(x_0)\,(x - x_0)$$

where $f'(x_0)$ is the slope. The intersection of the above equation and the x-axis $\rightsquigarrow y = 0$, we obtain:

$$x = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Algorithm 3

Input: $f(x)$, x_0 (initial guess)
Ouput: approximation to root r st $f(r)=0$
The way it would iterate:

$$x_{i+1}=x_i-\frac{f(x_i)}{f'(x_i)}$$

where $i=0,1,2,...$

Example 40. $f(x)=x^3+x-1$.

First compute $f'(x)=3x^2+1$. Newton iteration is:

$$\begin{aligned} x-\frac{f(x)}{f'(x)} &= x-\frac{x^3+x-1}{3x^2+1} \\ &= \frac{2x^3+1}{3x^2+1} \end{aligned}$$

Thus we have a generalized form: $x_{i+1}=\frac{2x_i^3+1}{3x_i^2+1}$ with $x_0=0.1$.

We can perform 6 iterations to give you the root with the correct 8 significant digits: 0.68232780.

Definition 41. *Denote e, as the error at step i:* $|r-x_i|$.

The iterative method converges quadratically $\Longleftrightarrow$

$$\lim_{i\to\infty}\frac{e_{i+2}}{e_i^2}=M$$

***Remark* 42.** *If* $f(r)=0$, *and* $f'(r)=0$, *then Newton's method converges quadratically to* r *and thus,* $M=\frac{f''(r)}{2f'(r)}$, *where* $\boldsymbol{M}$ *denotes the rate of convergence.*