# APPM 5600 - Homework 2

Eappen Nelluvelil

September 10, 2021

1. Which of the following iterations will converge to the indicated fixed point $x_*$ (provided $x_0$ is sufficiently close to $x_*$)? If it does converge, give the order of convergence; for linear convergence, give the rate of linear convergence.

   (a) $x_{n+1} = -16 + 6x_n + \frac{12}{x_n}$, $x_* = 2$.
   Let $g$ be defined by $g(x) = -16 + 6x + \frac{12}{x}$. The first derivative of $g$ is given by

   $$g'(x) = 6 + \frac{12}{x^2}.$$

   We can perform a first-order Taylor expansion of $g$ centered at 2 as follows:

   $$\begin{aligned} g(x) &= g(2) + g'(\xi_x)(x-2) \\ &= 2 + \left(6 + \frac{12}{\xi_x^2}\right)(x-2), \end{aligned}$$

   where $\xi_x$ is a number between $x$ and 2. Evaluating the above Taylor expansion at $x_n$, we see that

   $$x_{n+1} = 2 + \left(6 + \frac{12}{\xi_x^2}\right)(x_n - 2) \Rightarrow \left|\frac{x_{n+1}-2}{x_n-2}\right| = \left|6 + \frac{12}{\xi_x^2}\right|.$$

   On the interval $[1.8, 2.5]$, the quantity $\left|6 + \frac{12}{\xi_x^2}\right|$ is minimized at $\xi_x = 2.5$, with the minimum being 7.92. Since $\min_{x\in[1.8,2.5]} \left|6 + \frac{12}{\xi_x^2}\right|$ is greater than 1, the fixed point iteration cannot converge to $x^*$ for any $x$ in the interval $[1.8, 2.5]$, other than for the fixed point.

   (b) $x_{n+1} = \frac{2}{3}x_n + \frac{1}{x_n^2}$, $x_* = 3^{1/3}$.
   Our fixed point iteration is $x_{n+1} = g(x_n)$, where $g(x) = \frac{2}{3}x + \frac{1}{x^2}$. The derivative of $g$ is given by

   $$g'(x) = \frac{2}{3} - \frac{2}{x^3}.$$

   Consider the interval $[a, b] = [1, 2]$. We see that $g(a) = \frac{2}{3} + 1 = \frac{5}{3}$, which is greater than $a$ and less than $b$, and $g(b) = \frac{4}{3} + \frac{1}{4} = \frac{16}{12} + \frac{3}{12} = \frac{19}{12}$, which is greater than $a$ and less than $b$. Furthermore, for every $x \in [a, b]$, $a \leq g(x) \leq b$, i.e., $g([a, b]) \subset [a, b]$. On the interval $[a, b]$, $g'$ is a positive and decreasing function, and

   $$\begin{aligned} \max_{x\in[a,b]} |g'(x)| &= |g'(b)| \\ &= \frac{2}{3} - \frac{1}{4} \\ &= \frac{5}{12} \\ &< 1. \end{aligned}$$

Thus, by the contraction mapping theorem, the iteration will converge to $x_* = 3^{1/3}$.
The order of convergence is quadratic, which can be seen by taking a second-order Taylor expansion of $g$ centered at $x_*$. The second derivative of $g$ is given by

$$g''(x) = -\frac{6}{x^4}.$$

Then, we have that

$$\begin{aligned} g'(x) &= g(x_*) + g'(x_*)(x - x_*) + \frac{g''(\xi_x)}{2}(x - x_*)^2 \\ &= x_* + \frac{g''(\xi_x)}{2}(x - x_*)^2, \end{aligned}$$

where $\xi_x$ is a number between $x$ and $x_*$. In addition, we have used the fact that $g'(x_*) = 0$. Evaluating this Taylor expansion at $x_n$, we have that

$$\begin{aligned} g(x_n) = x_* + \frac{g''(\xi_x)}{2}(x_n - x_*)^2 &\Rightarrow x_{n+1} = x_* + \frac{g''(\xi_x)}{2}(x_n - x_*)^2 \\ &\Rightarrow \frac{x_{n+1} - x_*}{(x_n - x_*)^2} = \frac{g''(\xi_x)}{2}, \end{aligned}$$

where $\xi_x$ is a number between $x_n$ and $x_*$. We can then take the limit of the absolute value of both sides, letting $n \to \infty$, and we obtain that

$$\begin{aligned} \lim_{n\to\infty} \left| \frac{x_{n+1} - x_*}{(x_n - x_*)^2} \right| &= \lim_{n\to\infty} \left| \frac{g''(\xi_x)}{2} \right| \\ &= \left| \frac{g''(x_*)}{2} \right| \\ &= \frac{3}{3^{4/3}} \\ &= 3^{-1/3}, \end{aligned}$$

where we used the fact that the $x_n$'s converge to $x_*$ as $n \to \infty$.

(c) $x_{n+1} = \frac{12}{1+x_n}$, $x_* = 3$.
Our fixed point iteration is $x_{n+1} = g(x_n)$, where $g(x) = \frac{12}{1+x}$. The derivative of $g$ is given by

$$g'(x) = -\frac{12}{(1+x)^2}.$$

Consider the interval $[a, b] = [2.5, 4]$. We see that $g(a) = \frac{24}{7}$, which is greater than $a$ and less than $b$. We also see that $g(b) = 3$, which is greater than $a$ and less than $b$. Furthermore, for every $x \in [a, b]$, $a \le g(x) \le b$, i.e., $g([a, b]) \subset [a, b]$. On the interval $[a, b]$, $g'$ is a negative and increasing function, and we see that

$$\begin{aligned} \max_{x\in[a,b]} |g'(x)| &= |g'(a)| \\ &= \left| -\frac{12}{\left(1 + \frac{7}{2}\right)^2} \right| \\ &= \frac{48}{49} \\ &< 1. \end{aligned}$$

Thus, by the contraction mapping theorem, the iteration will converge to $x_* = 3$.

The order of convergence is linear, which can be seen by taking a first-order Taylor expansion of $g$ centered at $x_*$:

$$g(x) = g(x_*) + g'(\xi_x)(x - x_*),$$

where $\xi_x$ is a number between $x$ and $x_*$. Evaluating this Taylor expansion at $x_n$, we have that

$$\begin{aligned} g(x_n) = x_* + g'(\xi_x)(x_n - x_*) &\Rightarrow x_{n+1} = x_* + g'(\xi_x)(x_n - x_*) \\ &\Rightarrow \frac{x_{n+1} - x_*}{x_n - x_*} = g'(\xi_x), \end{aligned}$$

where $\xi_x$ is a number between $x_n$ and $x_*$. We can then take the limit of the absolute value of both sides, letting $n \to \infty$, and we obtain that

$$\begin{aligned} \lim_{n\to\infty} \left| \frac{x_{n+1} - x_*}{x_n - x_*} \right| &= \lim_{n\to\infty} |g'(\xi_x)| \\ &= |g'(x_*)| \\ &= \left| -\frac{12}{(1+3)^2} \right| \\ &= \left| \frac{12}{16} \right| \\ &= \frac{3}{4} \\ &< 1. \end{aligned}$$

Thus the rate of linear convergence for this iteration is $\frac{3}{4}$.

2. In laying water mains, utilities must be concerned with the possibility of freezing. Although soil and weather conditions are complicated, reasonable approximations can be made on the basis of the assumption that soil is uniform in all directions. In that case, the temperature in degrees Celsius $T(x,t)$, at a distance $x$ (in meters) below the surface and $t$ seconds after the beginning of a cold snap, approximately satisfies

$$\frac{T(x,t) - T_s}{T_i - T_s} = \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right),$$

where $T_s$ is the constant temperature during a cold period, $T_i$ is the initial soil temperature before the cold snap, $\alpha$ is the thermal conductivity (in meters$^2$ per second), and

$$\operatorname{erf}(t) = \frac{2}{\sqrt{\pi}} \int_0^t \exp\left(-s^2\right) ds.$$

Assume that $T_i = 20$ [degrees Celsius], $T_s = -15$ [degrees Celsius], and $\alpha = 0.138 \cdot 10^{-6}$ [meters$^2$ per second]. For parts (II) and (III), run your experiments with a tolerance of $\epsilon = 10^{-13}$.

(a) We want to determine how deep a water main should be buried so that it will only freeze after 60 *days* exposure at this constant surface temperature. Formulate the problem as a root finding problem $f(x) = 0$. What is $f$ and $f'$? Plot the function $f$ on $[0, \overline{x}]$, where $\overline{x}$ is chosen so that $f(\overline{x}) > 0$.

**Note**: See attached code and plots.

Here, $f$ is the function $T(x, t = 60\,\text{days}) = T(x)$, which is given by

$$f(x) = T(x) = (T_i - T_s)\left(\frac{2}{\sqrt{\pi}} \int_0^{x_f} \exp\left(-s^2\right) ds\right) + T_s,$$

where $x_f = \frac{x}{2\sqrt{\alpha t_f}}$ and $t_f = 5184000$ [seconds]. The derivative of $f$ is given by

$$\begin{aligned} f'(x) = T'(x) &= (T_i - T_s)\left(\frac{2}{\sqrt{\pi}}\exp\left(-\frac{x^2}{4\alpha t_f}\right)\frac{1}{2\sqrt{\alpha t_f}}\right) \\ &= (T_i - T_s)\left(\frac{1}{\sqrt{\pi\alpha t_f}}\exp\left(-\frac{x^2}{4\alpha t_f}\right)\right). \end{aligned}$$

The goal is to then find a root of $f$ via a root-finding technique.

(b) Compute an approximate depth using the bisection method with starting values $a_0 = 0$ [meters] and $b_0 = \overline{x}$ [meters].

We take $\overline{x}$ to be $1$ because $f(\overline{x}) > 0$. Applying the bisection method with the above parameters, we find an approximate depth of $0.6769618544819309$ meters.

(c) Compute an approximate depth using Newton's method with starting value $x_0 = 0.01$ [meters]. What happens if you start with $x_0 = \overline{x}$? Which is your preferred method and why?

Applying Newton's method with the above parameters and $x_0 = 0.01$ [meters], we find an approximate depth of $0.6769618544819355$ meters in $14$ iterations. If Newton's method is applied with the same parameters and $x_0 = \overline{x}$ [meters], the method returns an approximate depth of $0.6769618544819372$ meters in $14$ iterations.

I prefer Newton's method over the bisection method because Newton's method converges to an approximate root of $T$ in far fewer iterations, especially if the initial iterate is close enough to the root of $T$.

3. Consider applying Newton's method to a real cubic polynomial.

(a) In the case that the polynomial has three distinct real roots, $x = \alpha$, $x = \beta$, and $x = \gamma$, show that the starting guess $x_0 = \frac{1}{2}(\alpha + \beta)$ will yield the root $\gamma$ in one step.

Suppose $f$ is a real cubic polynomial whose roots are distinct and are given by $\alpha$, $\beta$, and $\gamma$. We can write $f$ as

$$\begin{aligned} f(x) &= (x-\alpha)(x-\beta)(x-\gamma) \\ &= \left(x^2 - \beta x - \alpha x + \alpha\beta\right)(x-\gamma) \\ &= \left(x^2 - (\alpha+\beta)x + \alpha\beta\right)(x-\gamma) \\ &= x^3 - \gamma x^2 - (\alpha+\beta)x^2 + (\alpha+\beta)\gamma x + \alpha\beta x - \alpha\beta\gamma \\ &= x^3 - (\alpha+\beta+\gamma)x^2 + (\gamma(\alpha+\beta)+\alpha\beta)x - \alpha\beta\gamma \end{aligned}$$

and

$$f'(x) = 3x^2 - 2(\alpha+\beta+\gamma)x + (\gamma(\alpha+\beta)+\alpha\beta).$$

The first iteration of Newton's method is given by

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)},$$

which is given by

$$
\begin{aligned}
x_1 &= \frac{1}{2}(\alpha+\beta) - \frac{\left(\frac{1}{2}(\alpha+\beta)-\alpha\right)\left(\frac{1}{2}(\alpha+\beta)-\beta\right)\left(\frac{1}{2}(\alpha+\beta)-\gamma\right)}{3\left(\frac{1}{2}(\alpha+\beta)\right)^2 - 2(\alpha+\beta+\gamma)\left(\frac{1}{2}(\alpha+\beta)\right) + (\gamma(\alpha+\beta)+\alpha\beta)} \\
&= \frac{1}{2}(\alpha+\beta) + \frac{\frac{1}{4}(\beta-\alpha)^2\left(\frac{1}{2}(\alpha+\beta)-\gamma\right)}{\frac{-\alpha^2-2\alpha\beta-\beta^2+4\alpha\beta}{4}} \\
&= \frac{1}{2}(\alpha+\beta) + \frac{(\beta-\alpha)^2\left(\frac{1}{2}(\alpha+\beta)-\gamma\right)}{-\alpha^2+2\alpha\beta-\beta^2} \\
&= \frac{1}{2}(\alpha+\beta) + \frac{(\beta-\alpha)^2\left(\frac{1}{2}(\alpha+\beta)-\gamma\right)}{-(\beta-\alpha)^2} \\
&= \frac{1}{2}(\alpha+\beta) - \frac{1}{2}(\alpha+\beta) + \gamma \\
&= \gamma,
\end{aligned}
$$

as desired.

(b) Give a heuristic, e.g., geometric, argument showing that if two roots coincide (say $\beta = \gamma$), there is precisely one starting guess $x_0$ (other than the double root) for which Newton will fail, and that this one separates the basins of attraction for the distinct roots.

Recall that Newton's method is a fixed point iteration, i.e., we are trying to find an $\alpha$ such that $\alpha = g(\alpha)$, where $g(x) = x - \frac{f(x)}{f'(x)}$ and $\alpha$ is a root of $f$. The interval around $\alpha$ for which $g$ is a contraction is called the basin of convergence for $\alpha$.

A cubic that has three real roots, with two roots having multiplicity two, has the property that its first derivative is zero at the double root.

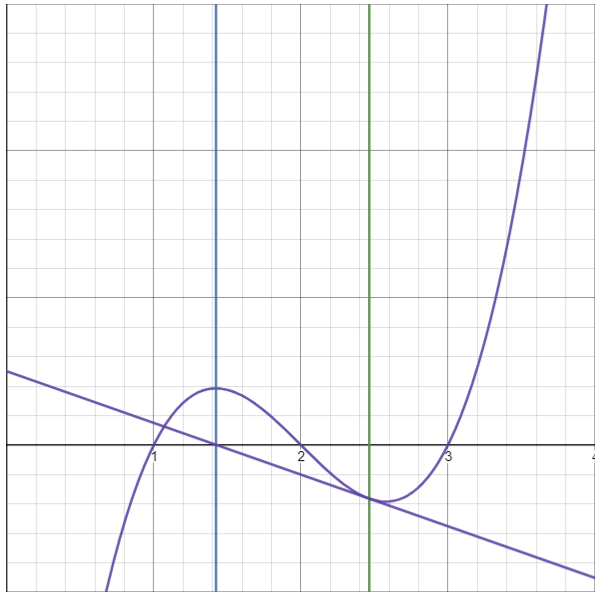
The derivative of $f$, assuming that $\alpha = \beta$, is given by

$$
f'(x) = 3x^2 - 2(2\alpha+\gamma)x + \left(2\alpha\gamma + \alpha^2\right).
$$

The first derivative $f'$ has two roots, one at the double root $\alpha = \beta$ and another point $x^0$. Newton's method will fail if the initial iterate is $x^0$ as $\frac{f(x^0)}{f'(x^0)}$ is undefined. Furthermore, this is the only initial starting point for which Newton's method will fail in this case. This is because it is not possible to pick another initial iterate such that the tangent line of $f$ at this iterate crosses the $x$-axis at $x^0$, which would cause the Newton iteration to fail.

(c) Extend the argument in part (II) to the case when all three roots again are distinct. Explain why there are now infinitely many starting guesses $x_0$ for which the iteration will fail.

Suppose that $f$ is a cubic polynomial with three real and distinct roots. As before, $f'$ has two roots, but now, its roots do not coincide with the roots of $f$. Newton's method fails at the roots of $f'$, but it is possible to arrive at these roots even if the initial Newton iterate is not one of the roots of $f'$. Consider the cubic $f(x) = (x-1)(x-2)(x-3)$:




One of the roots of $f'$ is located approximately at $x = 1.42264973081$, indicated by the vertical blue line. If the initial Newton iterate is approximately $2.465$, i.e., $x^0 \approx 2.465$, the tangent line of $f$ at $x^0$ will pass through $x = 1.42264973081$, at which the next Newton iteration fails. However, it is possible to find another initial iterate that produces $2.465$ (indicated by the vertical green line) as the next iterate, which leads to the eventual failure to Newton's method. This process can be repeated ad infinitum, which implies that there are infinitely many initial iterates that will cause Newton's method to eventually fail when trying to find the roots of the above cubic, and in fact, any cubic with real, distinct roots.

4. The sequence $x_k$ produced by Newton's method is quadratically convergent to $x_*$ with $f(x_*) = 0$, $f'(x_*) \neq 0$, and $f''(x)$ continuous at $x_*$.

   Let $f(x) = (x - x_*)^p \, q(x)$, with $p$ being a positive integer, $q$ twice continuously differentiable, and $q(x_*) \neq 0$. (**Note**: $f'(x_*) = 0$.) In the following sub-problems, for $x_k$, let $f_k = f(x_k)$ and $e_k = |x_* - x_k|$.

   (a) Prove that Newton's method converges linearly for $f(x)$.

   To show that Newton's method converges linearly for $f$, we have to show that there exists a constant $C$ such that $C \in (0, 1)$ and for all $k \geq 0$,

$$|x_* - x_{k+1}| \leq C\,|x_* - x_k| \iff \left|\frac{x_{k+1} - x_*}{x_k - x_*}\right| \leq C.$$

   The first derivative of $f$ is given by

$$f'(x) = p\,(x - x_*)^{p-1}\, q(x) + (x - x_*)^p\, q'(x)\,.$$

   Then, the Newton iteration is given by

$$\begin{aligned} x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} &\Rightarrow x_{k+1} = x_k - \frac{(x_k - x_*)^p\, q(x_k)}{p\,(x_k - x_*)^{p-1}\, q(x_k) + (x_k - x_*)^p\, q'(x_k)} \\ &\Rightarrow x_{k+1} = x_k - \frac{(x_k - x_*)\, q(x_k)}{pq(x_k) + (x_k - x_*)\, q'(x_k)}. \end{aligned}$$

Subtracting $x_*$ from both sides and taking absolute values, we see that

$$\begin{aligned}\left|x_{k+1}-x_k\right| &= \left|x_k - x_* - \frac{(x_k - x_*)\, q(x_k)}{pq(x_k) + (x_k - x_*)\, q'(x_k)}\right| \\ &= \left|x_k - x_*\right| \left|1 - \frac{q(x_k)}{pq(x_k) + (x_k - x_*)\, q'(x_k)}\right|\end{aligned}$$

Dividing both sides by $|x_k - x_*|$ and taking the limit as $k \to \infty$, we see that

$$\begin{aligned}\lim_{k\to\infty}\left|\frac{x_{k+1}-x_*}{x_k - x_*}\right| &= \lim_{k\to\infty}\left|1 - \frac{q(x_k)}{pq(x_k) + (x_k - x_*)\, q'(x_k)}\right| \\ &= \lim_{k\to\infty}\left|1 - \frac{q(x_k)}{pq(x_k)}\right| \\ &= \left|1 - \frac{q(x_*)}{pq(x_*)}\right| \\ &= \left|1 - \frac{1}{p}\right| \\ &< 1\end{aligned}$$

because $p$ is a positive integer and $x_k$ converges to $x_*$ as $k \to \infty$. Thus, Newton's method converges linearly for $f$.

(b) Consider the modified Newton iteration defined by

$$x_{k+1} = x_k - p\frac{f_k}{f'_k}.$$

Prove that if $x_k$ converges to $x_*$, then the rate of convergence is quadratic, i.e., show that

$$|e_{k+1}| \leq C\,|e_k|^2$$

for some positive constant $C$ as $x_k \to x_*$.

Using the Newton iteration from earlier, we see that the modified Newton iteration is given by

$$x_{k+1} = x_k - p\frac{(x_k - x_*)\, q(x_k)}{pq(x_k) + (x_k - x_*)\, q'(x_k)}.$$

Subtracting $x_*$ from both sides and taking absolute values, we see that

$$\begin{aligned}\left|x_{k+1}-x_*\right| &= \left|x_k - x_* - p\frac{(x_k - x_*)\, q(x_k)}{pq(x_k) + (x_k - x_*)\, q'(x_k)}\right| \\ &= \left|\frac{(x_k - x_*)^2}{x_k - x_*} - p\frac{(x_k - x_*)^2\, q(x_k)}{(x_k - x_*)\left(pq(x_k) + (x_k - x_*)\, q'(x_k)\right)}\right| \\ &= \left|(x_k - x_*)^2\right| \left|\frac{1}{x_k - x_*} - p\frac{q(x_k)}{(x_k - x_*)\left(pq(x_k) + (x_k - x_*)\, q'(x_k)\right)}\right| \\ &= \left|(x_k - x_*)^2\right| \left|\frac{pq(x_k) + (x_k - x_*)\, q'(x_k) - pq(x_k)}{(x_k - x_*)\left(pq(x_k) + (x_k - x_*)\, q'(x_k)\right)}\right| \\ &= \left|(x_k - x_*)^2\right| \left|\frac{q'(x_k)}{\left(pq(x_k) + (x_k - x_*)\, q'(x_k)\right)}\right|.\end{aligned}$$

Dividing both sides by $|x_k - x_*|^2$ and taking the limit as $k \to \infty$, we see that

$$\begin{aligned}\lim_{k\to\infty}\left|\frac{x_{k+1}-x_*}{(x_k-x_*)^2}\right| &= \lim_{k\to\infty}\left|\frac{q'(x_k)}{(pq(x_k)+(x_k-x_*)\,q'(x_k))}\right| \\ &= \left|\frac{q'(x_*)}{pq(x_*)}\right|,\end{aligned}$$

where we have used the fact that $x_k$ converges to $x_*$ as $k \to \infty$. Thus, the modified Newton iteration converges quadratically for $f$.

(c) Write MATLAB codes for both Newton and modified Newton methods. Apply these to the function

$$f(x) = (x-1)^5 \exp(x)$$

and compare the results. Use $x_0 = 0$ as a starting point. I would like this in the form of two tables, one for Newton and one for modified Newton. Each of these should have two columns, the first for the iterates $x_k$ and the second for the error $e_k = |x_k - x_*|$. Use `format long e` or equivalent formatting. Do enough iterations in each code to assure a relative error of $10^{-15}$ in the approximate solution $x$. Plot $k$ vs $e_k$. Comment about the plots vs. the theory.

**Note**: See attached code and plots.

In the attached plots, we see that when Newton's method is applied to $f$, Newton's method takes $149$ iterations (starting from an initial iterate of 0) to converge to a root of $f$. When viewing the plot of $k$ vs. the logarithm of the relative error between the Newton iterates and the root $x_* = 1$, where $k$ is the iteration counter, the resulting plot appears linear, which agrees with the theoretical result that was proved in (4a).

On the other hand, when the modified Newton applied is applied to $f$ with an initial iterate of $0$, the modified Newton method takes $6$ iterates to converge to a root of $f$. Furthermore, when viewing the plot of $k$ vs. the logarithm of the relative error between the modified Newton iterates and $x_* = 1$ , the resulting plot shows quadratic behavior, which agrees with the theoretical result that was proved in (4b).