IMPLEMENTING NEWTON'S METHOD

Kent M. Neuerburg

Abstract. Newton's Method, the recursive algorithm for computing the roots of an equation, is one of the most efficient and best known numerical techniques. The basics of the method are taught in any first-year calculus course. However, in most cases the two most important questions are often left unanswered. These questions are, "Where do I start?" and "When do I stop?" We give criteria for determining when a given value is a good starting value and how many iterations it will take to ensure that we have reached an approximate solution to within any predetermined accuracy.

Newton's Method. In his work *Of the Method of Fluxions and Infinite Series,* [3], Newton explains, by way of example, a recursive procedure for approximating roots of equations. This procedure is known to us today as Newton's Method and is a standard topic in every introductory Calculus course. Briefly, the technique, as presented in most Calculus texts, is as follows. Let f be a real valued function of one real variable that is continuous on $[a, b]$ and differentiable on (a, b). We compute a sequence of approximations to the zero of f via the recursive formula:

$$z_{i+1} = z_i - \frac{f(z_i)}{f'(z_i)}$$

where $z_0 \in (a, b)$ is chosen as a first approximation. Some texts go so far as to provide some criteria for convergence of this sequence. For example, in [2] we are told that a sufficient condition for convergence of Newton's Method to a zero of f is

$$\left| \frac{f(z)f''(z)}{[f'(z)]^2} \right| < 1$$

on an open interval containing the zero. Many Calculus texts go on to give examples in which this procedure fails to converge to a root. For example, the function $f(z) = z^{\frac{1}{3}}$ for which the sequence $\{z_i\}$ diverges for all $z_0 \neq 0$. Or the function $f(z) = -z^3 + 3z^2 - z + 1$ for which an initial approximation of $z_0 = 1$ yields $z_{2k} = 1$ and $z_{2k+1} = 0$ for all $k \in \mathbb{Z}^+$.

However, even though Newton's Method generally converges quickly to a root, students (and others, too) are generally left with the questions of

"How should one choose an initial approximation?" and "How many iterations will provide a good (meaning to within some predetermined accuracy) approximation to the root?" In other words,

"Where do I start?"

and

"When do I stop?"

Certainly, these are fundamental questions behind any algorithm. Providing the answers to these questions should help students appreciate the true power behind Newton's Method by "completing the process" in the sense that the student will now know how to begin and when to end the algorithm.

The answers to the above questions are provided through two key results, Theorem 2.2 and Theorem 3.2. Both of these theorems are stated without proof as their proofs require the development of many preliminary results. For a detailed development, the interested reader should consult [1].

2. Where to Start: Approximate Zeros. Let f be a differentiable function of one real variable. We begin the discussion of how to best pick an initial approximation to the root of an equation with the following definition.

Definition 2.1. We say that z is an approximate zero of f if the sequence given by $z_0 = z$ and $z_{i+1} = z_i - (f'(z_i))^{-1} f(z_i)$ is defined for all $i \in \mathbb{N}$ and there is a ξ such that $f(\xi) = 0$ with

$$|z_i - \xi| \leq \left(\frac{1}{2}\right)^{2^i - 1} |z - \xi|, \quad \text{for all } i \in \mathbb{N}.$$

We will call ξ the associated zero.

One should take the time to note how quickly the quantity on the right side of this inequality diminshes as i increases. If we take $|z - \xi| = 1$, then for $i = 1$, the right side of the inequality is $1/2$, for $i = 2$ we have $1/8$, for $i = 3$ it is down to $1/128$, at $i = 4$ the right side is $1/32768$, and by the time one gets to $i = 5$ the right side of the inequality is of the order of magnitude of 10^{-10}. This says the distance between the ith iterate of Newton's Method and the true zero, ξ, is rapidly approaching zero.

We next define an auxiliary quantity

$$\gamma(f, z) = \sup_{k \geq 2} \left| \frac{f'(z)^{-1} f^{(k)}(z)}{k!} \right|^{\frac{1}{k-1}}.$$

We are now prepared to state the following theorem.

<u>Theorem 2.2</u>. Suppose $f(\xi) = 0$ and $f'(\xi)^{-1}$ exists. If

$$|z - \xi| \leq \frac{3 - \sqrt{7}}{2\gamma}$$

for $\gamma = \gamma(f, z)$, then z is an approximate zero of f with associated zero ξ.

This theorem guarantees that all z in a certain domain containing ξ will act as approximate zeros for f. However, it does require us to already know a root ξ of $f(z) = 0$ in order to determine these approximate zeros. But if we know ξ already, why do we need z? We now resolve this dilemma.

3. When to Stop: Point Estimates for Approximate Zeros. We would like to develop a method of determining if a given z_0 is an approximate zero for $f(z) = 0$ from data available at the point z_0. We first define two additional quantities.

<u>Definition 3.1</u>. Let $f(z)$ be a differentiable function. Let

$$\beta(f, z) = |f'(z)^{-1} f(z)|,$$

and

$$\alpha(f, z) = \beta(f, z)\gamma(f, z).$$

We utilize these new quantities in the following result.

<u>Theorem 3.2</u>. There is a universal constant α_0 with the following property. If $\alpha(f, z) < \alpha_0$, then z is an approximate zero of f. Moreover, the distance from z to the associated zero is at most $2\beta(f, z)$.

In [1], we are told that we may take $\alpha_0 = 0.03$. In [4], the value $\alpha_0 = 0.130707$ is given. More recently, the value $\alpha_0 = \frac{1}{4}(13 - 3\sqrt{7}) \approx 0.15671$ is found in [5].

We may now use Theorem 3.2 together with the definition of approximate zero to determine the number of iterations of Newton's Method required to reach any predetermined accuracy.

Let us summarize the procedure. Suppose we are given a differentiable function $f(z)$ for which we want to find a root, ξ, with an expected level of accuracy of ϵ, then the steps are as follows.

Where do I start?

(1) Determine the functions $\gamma(f, z)$, $\beta(f, z)$, and $\alpha(f, z)$.
(2) Using the current best estimate of $\alpha_0 \approx 0.15671$, solve the inequality

$$\alpha(f, z) < \alpha_0$$

for z. This solution could be estimated graphically.

(3) Choose an approximate zero, z_0, from within the interval determined in step 2 above.

When do I stop?

(4) By Theorem 3.2, we know

$$|z_0 - \xi| < 2\beta(f, z_0) = B$$

so we have a bound for $|z_0 - \xi|$.

(5) By our definition of approximate zero, we know that

$$|z_i - \xi| \leq \left(\frac{1}{2}\right)^{2^i - 1} |z_0 - \xi|.$$

Combining this inequality with that from step 4 above we get

$$|z_i - \xi| \leq \left(\frac{1}{2}\right)^{2^i - 1} B.$$

We solve

$$\left(\frac{1}{2}\right)^{2^i - 1} B < \epsilon$$

for i in order to determine the number of iterations of Newton's Method required to obtain the expected accuracy, ϵ, of the root, ξ.

4. An Example. Newton's example in his *Of the Method of Fluxions and Infinite Series* is to approximate a root of the equation $y^3 - 2y - 5 = 0$.

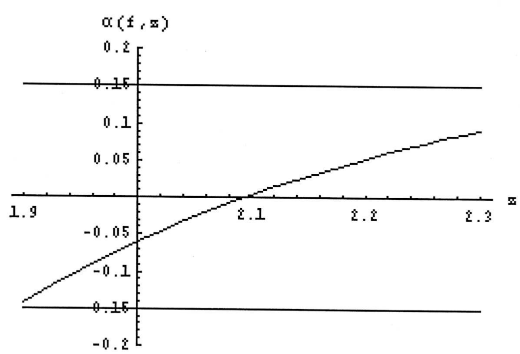

Fig. 1

After four iterations of his method, Newton gives the approximate root as $y = 2.09455148$. If we substitute this value into the expression $y^3 - 2y - 5$ we get (approximately) -0.0000000172. (Pretty close to zero!)

Let us try Newton's example. Let $f(z) = z^3 - 2z - 5$ and take $\epsilon = 10^{-8}$. Clearly, f has a zero near $z = 2$.

STEP 1. In order to apply Theorem 3.2, we observe that $f'(z) = 3z^2 - 2$, $f''(z) = 6z$, $f'''(z) = 6$, and $f^{(k)}(z) = 0$ for all $k \geq 4$. Computing (for z near 2) we have

$$\gamma(f, z) = \left| \frac{1}{3z^2 - 2} \cdot \frac{6z}{2!} \right|^{\frac{1}{2-1}} = \left| \frac{3z}{3z^2 - 2} \right|$$

$$\beta(f, z) = \left| \frac{1}{3z^2 - 2}(z^3 - 2z - 5) \right| = \left| \frac{z^3 - 2z - 5}{3z^2 - 2} \right|$$

$$\alpha(f, z) = \left| \frac{3z}{3z^2 - 2} \right| \left| \frac{z^3 - 2z - 5}{3z^2 - 2} \right| = \left| \frac{3z^4 - 6z^2 - 15z}{9z^4 - 12z^2 + 4} \right|.$$

STEP 2. Using the value $\alpha_0 = 0.15$, Theorem 3.2 guarantees that z will be an approximate zero of f if

$$\left| \frac{3z^4 - 6z^2 - 15z}{9z^4 - 12z^2 + 4} \right| < 0.15.$$

If we graph the function

$$\alpha(f, z) = \frac{3z^4 - 6z^2 - 15z}{9z^4 - 12z^2 + 4}$$

we see that the above inequality is easily satisfied for $1.9 < z < 2.3$.

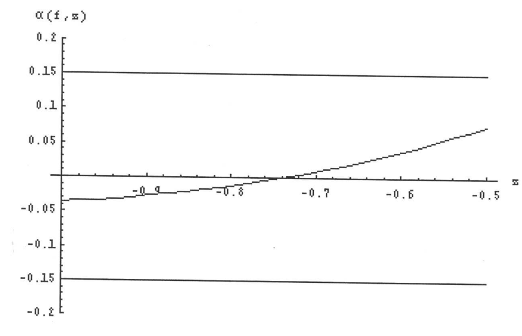

Fig. 2

STEP 3. Like Newton, we choose $z = 2$ as our first approximate zero. Note that $z = 2$ is within the interval $(1.9, 2.3)$ determined in step 2 above.

STEP 4. Again by Theorem 3.2, if ξ is the associated zero to our approximate zero, then we have

$$|z - \xi| < 2\beta(f, z) = 2\left|\frac{z^3 - 2z - 5}{3z^2 - 2}\right|.$$

At $z = 2$ we get

$$|2 - \xi| < 2\beta(f, 2) = 2\left|\frac{2^3 - 2 \cdot 2 - 5}{3 \cdot 2^2 - 2}\right| = 0.2.$$

STEP 5. According to our definition of approximate zero we will have

$$|z_i - \xi| \leq \left(\frac{1}{2}\right)^{2^i - 1} |z - \xi| \leq \left(\frac{1}{2}\right)^{2^i - 1} (0.2).$$

If our desire is to approximate ξ to within $\epsilon = 10^{-8}$ then we solve

$$\left(\frac{1}{2}\right)^{2^i - 1} (0.2) < 10^{-8}$$

for i to get $i \geq 5$. Hence, we will have the value of ξ to (at least) eight decimal places of accuracy after (at most) 5 iterations of Newton's Method. After five iterations we have $z_5 = 2.094551481542327$ which agrees with Newton's approximation to eight decimal places.

Since the roots of the previous example can be determined exactly by purely algebraic methods, let us consider a second example in which the roots are not so easily determined. Let $f(z) = \sin\left(z - \frac{\pi}{2}\right) - z$ and approximate to eight decimal places the root which lies in the interval $[-1, 0]$, see Fig. 3.

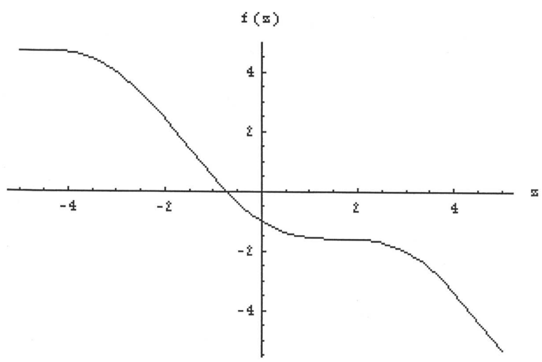

Fig. 3

STEP 1. In order to apply Theorem 3.2, we observe that $f'(z) = \cos\left(z - \frac{\pi}{2}\right) - 1$, $f''(z) = -\sin\left(z - \frac{\pi}{2}\right)$, $f'''(z) = -\cos\left(z - \frac{\pi}{2}\right)$, and $f^{(4)}(z) = \sin\left(z - \frac{\pi}{2}\right)$ and the pattern continues. Computing (for $-1 \leq z \leq -0.5$) we have

$$\gamma(f, z) = \left| \frac{\sin\left(z - \frac{\pi}{2}\right)}{2[\cos\left(z - \frac{\pi}{2}\right) - 1]} \right|$$

(the case $k = 2$ is the supremum for $-1 \leq z \leq -0.5$),

$$\beta(f, z) = \left| \frac{\sin\left(z - \frac{\pi}{2}\right) - z}{\cos\left(z - \frac{\pi}{2}\right) - 1} \right|,$$

and

$$\alpha(f, z) = \left| \frac{\sin\left(z - \frac{\pi}{2}\right)}{2[\cos\left(z - \frac{\pi}{2}\right) - 1]} \right| \cdot \left| \frac{\sin\left(z - \frac{\pi}{2}\right) - z}{\cos\left(z - \frac{\pi}{2}\right) - 1} \right|.$$

STEP 2. Using the value $\alpha_0 = 0.15$, Theorem 3.2 ensures that z will be an approximate zero of f if

$$\left|\frac{\sin\left(z-\frac{\pi}{2}\right)}{2[\cos\left(z-\frac{\pi}{2}\right)-1]}\right| \cdot \left|\frac{\sin\left(z-\frac{\pi}{2}\right)-z}{\cos\left(z-\frac{\pi}{2}\right)-1}\right| < 0.15.$$

If we graph the function

$$\alpha(f,z) = \left|\frac{\sin\left(z-\frac{\pi}{2}\right)}{2[\cos\left(z-\frac{\pi}{2}\right)-1]}\right| \cdot \left|\frac{\sin\left(z-\frac{\pi}{2}\right)-z}{\cos\left(z-\frac{\pi}{2}\right)-1}\right|$$

we see that the above inequality is easily satisfied for $-1 < z < -0.5$.

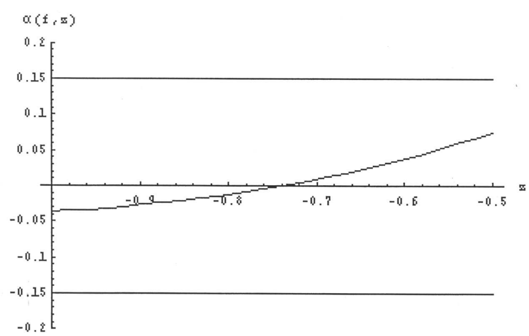

Fig. 4

STEP 3. In this case, we choose $z = -0.75$ as our first approximate zero. Note that $z = -0.75$ is within the interval $(-1, -0.5)$ determined in step 2 above.

STEP 4. Again by Theorem 3.2, if ξ is the associated zero to our approximate zero, then we have

$$|z - \xi| < 2\beta(f,z) = 2\left|\frac{\sin\left(z-\frac{\pi}{2}\right)-z}{\cos\left(z-\frac{\pi}{2}\right)-1}\right|.$$

At $z = -0.75$ we get

$$|-0.75 - \xi| < 2\beta(f, -0.75) = 2\left|\frac{\sin(-0.75 - \frac{\pi}{2}) - (-0.75)}{\cos(-0.75 - \frac{\pi}{2}) - 1}\right| \leq 0.1089.$$

<u>STEP 5</u>. According to our definition of approximate zero we will have

$$|z_i - \xi| \leq \left(\frac{1}{2}\right)^{2^i - 1} |z - \xi| \leq \left(\frac{1}{2}\right)^{2^i - 1} (0.1089).$$

Since we want to approximate ξ to within $\epsilon = 10^{-8}$, we need to solve

$$\left(\frac{1}{2}\right)^{2^i - 1} (0.1089) < 10^{-8}$$

for i. Doing so, we get $i \geq 5$. Hence, we will have the value of the true zero, ξ, to (at least) eight decimal places of accuracy after (at most) 5 iterations of Newton's Method.

5. Conclusion. In [1], Newton's Method is called the "'search algorithm' *sine qua non* of numerical analysis and scientific computation." As evidence of the speed and efficiency of Newton's Method, we observe that Newton's Method forms the basis of the **FindRoot** command in *Mathematica*, [6]. For such an efficient and effective algorithm, it is crucial that one has a well-defined condition for when to terminate the process. The above strategy provides exactly the information needed to determine the number of iterations of Newton's Method required to reach a predetermined level of accuracy based upon the function and initial approximation.

It should be noted that while we generally associate Newton's Method with approximating zeros of a function of one real variable, the above treatment immediately allows for $f\colon \mathbb{C} \to \mathbb{C}$. In fact, the results can be extended to systems of equations $f\colon \mathbb{C}^n \to \mathbb{C}^n$ and even to maps of Banach spaces $f\colon \mathbb{E} \to \mathbb{F}$. In these cases, we view $f'(z)$ as a continuous linear map which has an inverse. It is for this reason that we have adopted the notation

$$z_{i+1} = z_i - (f'(z_i))^{-1} f(z_i)$$

as opposed to the more traditional

$$z_{i+1} = z_i - \frac{f(z_i)}{f'(z_i)}.$$

In any setting, it is the simplicity, efficiency, and applicability of Newton's Method that ranks this technique amongst the great theorems of mathematics.

References

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Kent M. Neuerburg
Mathematics Department
Southeastern Louisiana University
Hammond, LA 70402
email: kneuerburg@selu.edu