Root Finding - Newton Method and Secant Method

Root finding iterative methods are all centered around nonlinear equations; note that linear equations are much easier to solve. The next two methods both center around the idea of using a good, approximate line to find an exact root.

Example 1. $f(x) = 2 - x^2$

Remark. So the roots are $\pm\sqrt(2)$. We can find the equations of the tangent line at the integers near them to start to approximate those roots. For instance, $f'(x) = -2x$, so the equation of the tangent line at $x = 1$ is $y - 1 = (-2)(x - 1)$ or $y = -2x + 3$. Since that line has a root at $\frac{3}{2}$, we use $\frac{3}{2}$ as a better guess than 1 for the root.

The formula for Newton's Method is:

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

Question 2. Can you derive the Newton's Method formula from the equation of a tangent line?

Remark. If we start with the form of the tangent line $y - y_0 = f'(x_0)(x - x_0)$, it is the root x that we are solving for and we know that $y = f(x) = 0$ at a root. So we have:

$$\begin{aligned} 0 - y_0 &= f'(x_0)(x - x_0) \\ -\frac{y_0}{f'(x_0)} &= x - x_0 \\ x &= x_0 - \frac{y_0}{f'(x_0)}. \end{aligned}$$

Changing the notation from x_0 to x_i, x to x_{i+1}, and y_0 to $f(x_i)$ gives the Newton's Method formula.

Algorithm 1 Newton's Method

Input: A function f, its derivative f', an initial guess x_0, number of iterations n
for $i = 0, \ldots, n-1$ **do**
  $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$
Return x_n

Example 3. Apply two steps of Newton's Method to $f(x) = 3x^2 - 6x$ with initial guess $x = 3$.

Remark. We begin with finding $f'(x) = 6x - 6$. Then you can either evaluate each function at the starting point and then substitute into the formula, OR simplify the formula and plug the initial guess into the simplified form. I demonstrate both ways.

1. No simplifying. Then $f(3) = 3(9) - 6(3) = 9$ and $f'(3) = 6(3) - 6 = 12$, so $x_1 = 3 - \frac{9}{12} = 3 - \frac{3}{4} = \frac{9}{4}$. Since $f(\frac{9}{4}) = 3(\frac{9}{4})^2 - 6(\frac{9}{4}) = \frac{3(9^2)-6(9)(4)}{4^2} = \frac{27}{16}$ and $f'(\frac{9}{4}) = 6(\frac{9}{4}) - 6 = \frac{15}{2}$, we have $x_2 = \frac{9}{4} - \frac{\frac{27}{16}}{\frac{15}{2}} = \frac{81}{40}$ or 2.025.

2. Simplified. Then the formula for this function is $x_{i+1} = x_i - \frac{3x_i^2 - 6x_i}{6x_i - 6}$. Simplifying, we get $x_i - \frac{x_i^2 - 2x_i}{2x_i - 2} = \frac{2x_i^2 - 2x_i - x_i^2 + 2x_i}{2x_i - 2} = \frac{x_i^2}{2x_i - 2}$. For x_1, we get $x_1 = \frac{9}{2(3)-2} = \frac{9}{4}$. Then $x_2 = \frac{(\frac{9}{4})^2}{2(\frac{9}{4})-2} = \frac{81}{40}$ or 2.025.

Question 4. When can you not use Newton's Method at all?

Remark. If at any point you encounter $f'(x_i) = 0$, the method will fail. Often this is avoidable by choosing a new initial guess x_0. It also doesn't work for any function whose derivative is unknown - see the next method.

Question 5. How fast does Newton's Method converge?

Remark. Recall that the rate of convergence, i.e. linear, depends on the error term $e_i = |r - x_i|$. This expression, combined with the fact we're already using the derivative, gives us the idea to look at the Taylor polynomial for f (check out the similarities with the terms below).

We assume that $f(x)$ is twice continuously differentiable, meaning $f''(x)$ exists and is continuous. Then there exists a c_i between x_i and r where

$$f(r) = f(x_i) + (r - x_i)f'(x_i) + \frac{(r - x_i)^2}{2}(f''(c_i)).$$

We again know that $f(r)$ should be zero. If $f'(x_i) \neq 0$ (and that's a big if, we'll come back to that momentarily), we have:

$$\begin{aligned}
0 &= f(x_i) + (r - x_i)f'(x_i) + \frac{(r - x_i)^2}{2}(f''(c_i)) \\
-f(x_i) &= (r - x_i)f'(x_i) + \frac{(r - x_i)^2}{2}(f''(c_i)) \\
\frac{-f(x_i)}{f'(x_i)} &= r - x_i + \frac{(r - x_i)^2}{2f'(x_i)}(f''(c_i)) \\
x_i - \frac{f(x_i)}{f'(x_i)} - r &= \frac{(r - x_i)^2}{2f'(x_i)}(f''(c_i))
\end{aligned}$$

Note that the first two terms on the left are the formula for Newton's method, and thus combine to x_{i+1}. That means we have

$$x_{i+1} - r = \frac{(r - x_i)^2}{2f'(x_i)}(f''(c_i)).$$

Introducing absolute values gives

$$|x_{i+1} - r| = |\frac{(r - x_i)^2}{2f'(x_i)}(f''(c_i))|$$
$$e_{i+1} = e_i^2|\frac{f''(c_i)}{2f'(x_i)}|,$$

and in the limit, $e_{i+1} \approx e_i^2 M$ where $M = |\frac{f''(r)}{2f'(r)}|$.

This means that not only is $\lim_{i\to\infty} \frac{e_{i+1}}{e_i} = S = 0 < 1$ satisfied, we have something stronger: $\lim_{i\to\infty} \frac{e_{i+1}}{e_i^2} = |\frac{f''(r)}{2f'(r)}|$. This limit is the definition of *quadratic convergence*, which holds for any finite value of the limit.

However, that is only true when $f'(r) \neq 0$, which holds for simple roots. At a repeated root, Newton's method will only converge linearly, which puts it in the same category as those previously studied (Bisection and Fixed Point Iteration). The S value for a multiple root is $S = \frac{m-1}{m}$ where m is the *multiplicity* of the root, that is, the number of times the root appears. An example with repeated roots is $f(x) = (x-2)^4$, whose only root 2 has multiplicity 4, and where $S = \frac{3}{4}$.

Definition 6. Let e_i denote the error after step i of an iterative method. The iteration is *quadratically convergent* if

$$M = \lim_{i\to\infty} \frac{e_{i+1}}{e_i^2} < \infty.$$

Theorem 7. *Let $f(x)$ be twice continuously differentiable and let r be an element of the domain such that $f(r) = 0$. If $f'(r) \neq 0$, Newton's Method is locally and quadratically convergent to r, and $e_{i+1} \approx e_i^2 \left|\frac{f''(r)}{2f'(r)}\right|$. If $f'(r) = 0$, Newton's Method is locally and linearly convergent to r,and $e_{i+1} \approx e_i \left(\frac{m-1}{m}\right)$ where m is the multiplicity of the root.*

Secant Method

Well, before you learned about tangent lines... you learned about secant lines!

That's really the idea in this last method: replace the derivative with slope between two points. One downside to this idea: you now need two different initial guesses.

Algorithm 2 Secant Method

Input: A function f, initial guesses x_0 and x_1, number of iterations n
for $i = 1, \ldots, n$ **do**
  $x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$
Return x_{n+1}

Example 8. Apply the first step of the Secant Method to $f(x) = (x-1)(x-2)(x-5)$ with initial guesses $x_0 = 3$ and $x_1 = 4$.

Since $f(3) = 2(1)(-2) = -4$ and $f(4) = 3(2)(-1) = -6$, we have $x_2 = 4 - \frac{(-6)(4-3)}{-6-(-2)} = 4 + \frac{6}{-2} = 4 - 3 = 1$. This is a root, since $f(1) = (0)(-2)(-5) = 0$. But interestingly, it wasn't either of the roots closest to our two initial guesses! Different initial guesses will lead to other roots (for instance, 3 and 6 will converge to 5, and 2.5 and 3 will lead to 2).

How fast is the Secant Method? For simple roots, we observe superlinear convergence.

Definition 9. Let e_i denote the error after step i of an iterative method. The iteration is *superlinearly convergent* if

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

for some $1 < \alpha < 2$.

Just as a note - this limit is really generalizing all of what we're looking for with rates of convergence. When $\alpha = 1$, that's linear convergence. Similarly, $\alpha = 2$ is quadratic, $\alpha = 3$ is cubic, and so on. We are always interested in $\alpha > 0$

To find such an α, we start with the fact that for simple roots ($f'(r) \neq 0$), a very similar argument to Newton's Method gives that $e_{i+1} \approx \left|\frac{f''(r)}{2f'(r)}\right| e_i e_{i-1}$. For legibility, let $M = \left|\frac{f''(r)}{2f'(r)}\right|$.

To evaluate the limit $\lim_{i\to\infty} \frac{e_{i+1}}{e_i^\alpha} = S$, we're looking to find S and α such that $e_{i+1} \approx S e_i^\alpha$. Using our approximations together, we have $S e_i^\alpha = M e_i e_{i-1}$. Thus:

$$\begin{aligned} S e_i^\alpha &\approx M e_i e_{i-1} \\ e_i^{\alpha-1} &\approx \frac{M}{S} e_{i-1} \\ e_i &\approx \frac{M}{S}^{\frac{1}{\alpha-1}} e_{i-1}^{\frac{1}{\alpha-1}}. \end{aligned}$$

A direct comparison to $e_{i+1} \approx S e_i^\alpha$ gives that $S = \frac{M}{S}^{\frac{1}{\alpha-1}}$ (so $S = \left|\frac{f''(r)}{2f'(r)}\right|^{\alpha-1}$) and $\alpha = \frac{1}{\alpha-1}$. Therefore the α for the Secant Method is $\frac{1+\sqrt{5}}{2}$. Ever seen that number before???

So at the end of the day, for simple roots, the fastest convergence is Newton's Method, but that requires the derivative. Evaluating the Secant Method's formula is often faster that the Newton's Method formula per step, and is still superlinear (so it should converge faster than Bisection and FPI). Only the Bisection Method is guaranteed to converge; the others require "good" guesses.

One other note: the fact that the Bisection Method brackets the root is also an advantage. It gives you a sense of zooming in on the root and at every step you gain knowledge about the root. By contrast, Newton's Method and the Secant Method do NOT bracket the root, but there do exist modifications that can be made to the Secant Method so that it will.