One dimensional root finding

Given a function $f\colon \mathbf{R} \to \mathbf{R}$ the *one dimensional root finding* problem is to find $x \in \mathbf{R}$ with $f(x) = 0$. If we want to find x such that $f(x) = a$ we can reduce this to finding the root of $g(x) = f(x) - a$. In particular this can be used to find the inverse of a function at a given value.

There is no general algoritm for finding roots. The first thing to do is plot a graph of the function to see where the problematic roots might occur.

To find a root you need to have one or more initial guesses, a way to improve these, and a criterion for when to stop.

Initial Guess(s)

Knowing something about the function is crucial for deciding on where to start looking. This is why you should plot the function as the first step.

If a function is continuous and $f(x_0)$ and $f(x_1)$ have different signs then the Intermediate Value Theorem guarentees there is a root between x_0 and x_1. These values *bracket* the root.

Improving Guesses

There are many algorithms for improving initial guesses of roots.

Bisection

Given $x_0 < x_1$ that bracket the root, the bisection method uses $x_2 = (x_0 + x_1)/2$ to get a tighter bracket. Either x_0 and x_2 or x_2 and x_1 bracket the root. This method sure but slow. It improves the solution by only one binary digit with each step.

Secant

Given x_0 and x_1, not necessarily bracketing the root, the secant method uses root of the line through $(x_0, f(x_0))$ and $(x_1, f(x_1))$ as the next approximation.

The line is $y = m(x - x_0) + y_0$ where $m = (y_1 - y_0)/(x_1 - x_0)$ and $y_j = f(x_j)$, $j = 0, 1$ so $y = 0$ when $x = x_0 - y_0/m$. A simple calculation shows $x = (x_0 y_1 - x_1 y_0)/(y_1 - y_0)$.

It has faster convergence than the bisection method. If Δx is the difference of the previous guesses, the difference of the next guesses is approximately $(\Delta x)^{1.6}$. This is called convergence of order 1.6. Of course this is only useful if $\Delta x < 1$.

False Position (Regula Falsi)

Given $x_0 < x_1$ that bracket the root, use the secant method but take the guesses that keep the root bracketed. In some cases this can be slower than bisection.

Newton-Raphson

This requires only one initial guess, x_0, and approximates the function by the line tangent to the function at x_0: $y = f(x_0) + f'(x_0)(x - x_0)$ so $y = 0$ when $x = x_0 - y_0/f'(x_0)$ where $y_0 = f(x_0)$.

Things can go seriously wrong with this method, but when the derivative is monotone in a neighborhood of the root it has convergence of order 2.

This method requires computing the derivative of f. A modification of the method is to compute the derivative once and use that in subsequenct approximations.

Parabolic

Given three guesses, x_j, $j = 0, 1, 2$, there is a unique parabola $x = a + by + cy^2$ through the points $(x_j, f(x_j))$, $j = 0, 1, 2$. The next guess is the value a. There is also a unique parabola $y = a + bx + cx^2$ through the three points but there may be no solution for $y = 0$.

Convergence Criteria

If the derivative at the root of f, x, is not 0 then the best criteria is simple: are the next floating point numbers less than and greater than x a worse approximation? This is the best possible floating point approximation. It is also the best possible approximation if $f'(x) = 0$ and $f(x) = 0$.

If this is too slow, then the algorithm can be stopped when the number of iterations exceeds the computational budget.