Mathematics 3BA1

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Root Finding I

We are trying to find an x such that

$$f(x) = 0$$

for non-linear f, which we know how to compute.

We shall assume:

- that f is differentiable,
- and that that the root is simple (i.e. $f'(x) \neq 0$ at root). We shall let x^* denote the root: $f(x^*) = 0$ (and $f'(x^*) \neq 0$).

Root Finding II

There are two broad classes of iterative techniques:

1. Intervals: we attempt to bracket the root in an interval and then shrink the interval around the root until the desired accuracy is reached.
   1. Bisection
   2. Regula Falsi
   3. Secant
2. Points: we take a single guess and try to move it closer to the root
   1. Newton-Raphson
   2. Fixed-Point iteration

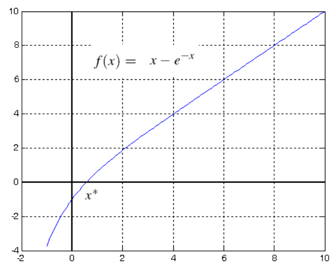
Root Finding: An example

We will find that most interval techniques are safe, but slow, while point techniques tend to be faster, but run the risk of diverging.

In the sequel, we shall use the following running example:

$$f(x) = x - e^{-x}$$

and search for the root $f(x^*) = 0$.



Generating initial guesses

- One technique is to plot the graph of the function. In this case, we note that we are in fact solving $x = e^{-x}$, and so it is easiest to plot e^{-x} and x and to see where they intersect.
- Another technique is to tabulate values and look for a change in sign (this technique is easier to automate than the graphing one).
  If we do that for our example, we will discover that a root lies between 0.5 and 0.6: For $x - e^{-x}$, we have $0.5 < x^* < 0.6$.

Interval Techniques: Bisection I

Bisection.
Given an initial interval, we determine subsequent intervals by finding the mid-point, evaluating f at that point, and then producing a new interval with the mid-point as one end, and the original end-point where f has a different sign at the other end.
Given interval $[x_{n-1}, x_n]$, $\text{sign}(f(x_{n-1})) \neq \text{sign}(f(x_n))$ we compute

$$x_{n+1} = \frac{x_{n-1} + x_n}{2}$$

If $\text{sign}(f(x_{n+1})) = \text{sign}(f(x_n))$ then the new interval is $[x_{n-1}, x_{n+1}]$, otherwise it is $[x_n, x_{n+1}]$.

Interval Techniques: Bisection II

- This technique is robust: if the starting interval encloses the root, then all subsequent intervals will.
- It is slow: the interval size (accuracy of result) halves at each iteration.

  Consider the starting interval $[0.5, 0.6]$, of size 10^{-1}, or about 2^{-3}. To get to an interval of width approximately 10^{-6} (IEEE Single precision) we need about 17 iterations. see `matlab/Bissection.xls`

As a general principle, we hope to find that we can get faster algorithms, by making more use of the information we have about f. The bisection technique only makes use of the sign of $f(x)$.

Interval Techniques: Regula Falsi I

Regula Falsi.
The Regula Falsi technique exploits knowledge about the approximate slope of the function around the root to improve the next guess.
Given interval $[x_{n-1}, x_n], \text{sign}(f(x_{n-1})) \neq \text{sign}(f(x_n))$, we can determine two points as $(x_{n-1}, f(x_{n-1}))$ and $(x_n, f(x_n))$. We determine the equation of the straight-line between them as :

$$\frac{y - f(x_n)}{x - x_n} = \frac{f(x_{n-1}) - f(x_n)}{x_{n-1} - x_n}$$

The next interval end-point ($x = x_{n+1}$) is where this line intersects the x-axis ($y = 0$):

$$x_{n+1} = x_n - \frac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}$$

Once we have computed x_{n+1} in this way, we determine the new interval exactly as we did for the bisection method.

Interval Techniques: Regula Falsi II

- This method is robust,
- but is still slow.

Interval Techniques: Secant I

Secant.
The secant method uses the same formula as Regula Falsi, but it does not attempt to keep the interval surrounding the root. Instead the new interval is $[x_n, x_{n+1}]$, regardless of the signs of the functions at those points.

- The secant method converges faster than Regula Falsi, when it converges at all.
- It is not robust. A key idea is to use the robust (but slow) techniques to improve initial guesses to the point were the faster, less robust techniques can be safely used. Usually this point occurs where we are close enough to the root that the function is *well-behaved* with no great changes in value or slope.

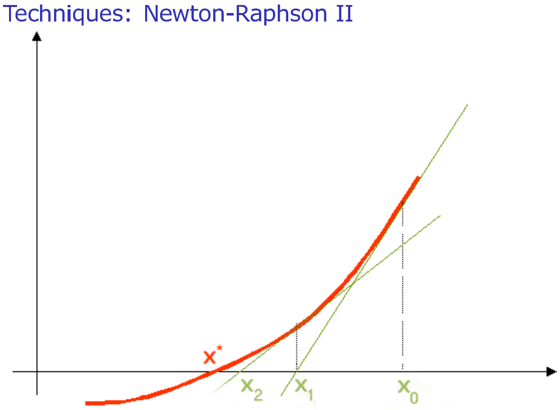
Point Techniques: Newton-Raphson I

Newton-Raphson method.
Let r be the root of a non-linear equation $f(x) = 0$. Starting from an initial guess r_0, the sequence defined as:

$$r_{n+1} = r_n - \frac{f(r_n)}{f'(r_n)}$$

is converging toward r. Using a computer, you use a *for* loop until the iteration n such as r_n is close enough to r (i.e. depending of the accuracy required).

Point Techniques: Newton-Raphson II



Point Techniques: Newton-Raphson III

- This method is very fast, and quickly reaches a solution, if it converges.
- However it is not completely robust.
- When it does converge, it is very fast, typically doubling the number of significant digits in the answer with each iteration.

Points Techniques: Fixed Point Iteration I

Fixed Point Iteration.
Instead of trying to find the root x^* of the function f (e.g. $f(x^*) = 0$), we define a function $\varphi(x)$ such that $\varphi(x^*) = x^*$. We simply start with our initial guess x_0 and repeatedly apply φ:

$$x_{n+1} = \varphi(x_n)$$

We generate a series we hope converges to the solution x^*:

$$x_0, \varphi(x_0), \varphi(\varphi(x_0)), \varphi^3(x_0), \varphi^4(x_0), \ldots \to x^*$$

Points Techniques: Fixed Point Iteration II

1. First example, consider :

$$\varphi_1(x) = e^{-x}$$

So we are solving $x = e^{-x}$, which as we have already observed, is equivalent to solving $x - e^{-x} = 0$.
If we try this with $x_0 = 0.5$ we see that it converges to the required result, but quite slowly.

2. As another example, consider

$$\varphi_2(x) = -\ln x$$

We show that the solution to $-\ln x = x$ is the same as that for $x - e^{-x} = 0$ by plugging this value in: it into the equation for f:

$$\begin{aligned} f(-\ln x) &= -\ln x - e^{-(-\ln x)} \\ &= -\ln x - e^{\ln x} \\ &= -\ln x - x \end{aligned}$$

Points Techniques: Fixed Point Iteration III

If x^* is a solution to $-\ln x - x = 0$, then it means that $x^* = -\ln x^*$, and it is a solution to $f(-\ln x) = 0$ as we have just shown, so

$$f(-\ln x^*) = 0 = f(x^*) \qquad \textbf{and} \qquad x^* = -\ln x^*$$

However, if we try this fixed-point equation with $x_0 = 0.5$, we find that the values rapidly diverge.

3. Finally, we note that Newton-Raphson can be formulated as a a fixed point iteration: assume that $f(x^*) = 0$. Then, if

$$\varphi_3(x) = x - \frac{f(x)}{f'(x)}$$

Points Techniques: Fixed Point Iteration IV

we see that:

$$\begin{aligned} \varphi_3(x^*) = & \quad \text{“defn.}\varphi_3\text{“} \\ & x^* - \frac{f(x^*)}{f'(x^*)} \\ = & \quad \text{“}x^* \text{ is a root of } f\text{, root is simple, so } f'(x^*) \neq 0\text{”} \\ & x^* - \frac{0}{f'(x^*)} \\ = & \quad \text{“clean up”} \\ & x^* \end{aligned}$$

We have shown that $\varphi_3(x^*) = x^*$, i.e. that it is a fixed point of φ_3.

Points Techniques: Fixed Point Iteration V

Is there a general theory that predicts if and how fast these fixed-points converge ?