Numerical Methods :: Nonlinear equations

Nonlinear equations

Consider the problem of finding solutions of

$$f(x) = 0$$

for some given function f. Such solutions are referred to as roots of the equation, or zeros of the function.

Fixed-point iteration

Rewrite $f(x) = 0$ as

$$x = g(x).$$

Guess $x = x_0$ and iterate according to

$$x_{k+1} = g(x_k), \quad k = 0, 1, \ldots$$

If $\lim_{k\to\infty} x_k = s$ and g is continuous, then $s = g(s)$. The point s is called a fixed point of g.

Fixed-point iteration

Example 7.1

Suppose we do not know the formula for solving
$x^2 - 3x + 1 = 0$.

We can write this as $f(x) = 0$, where $f(x) = x^2 - 3x + 1$.
Then we can rewrite as

$$x = \frac{1}{3}(x^2 + 1) \quad \text{or} \quad x = 3 - \frac{1}{x},$$

which yield the iteration formulae

$$x_{k+1} = \frac{1}{3}(x_k^2 + 1) \quad \text{or} \quad x_{k+1} = 3 - \frac{1}{x_k}.$$

Fixed-point iteration

Starting at $x_0 = 1$, the first iteration formula produces the sequence

$$1,\, 0.6667,\, 0.4815,\, \ldots,\, 0.3820.,$$

while the second produces the sequence

$$1,\, 2,\, 2.5,\, \ldots,\, 2.6180,$$

which converge to the two roots of $f(x) = 0$.

However, other initial guesses, such as $x_0 = 3$ or $x_0 = 0$ are not successful.

Fixed-point iteration

Theorem 7.2

Let $x = s$ be a solution of $x = g(x)$ and suppose that the function g has a continuous derivative in some interval I containing s and that $|g'(x)| \leq G < 1$ in I. Then the iteration $x_{k+1} = g(x_k)$ converges for any initial x_0 in I and $\lim_{k\to\infty} x_k = s$.

Proof.

We use Taylor's theorem about $x = s$ to show that

$$|x_k - s| \leq G|x_{k-1} - s| \leq G^2|x_{k-2} - s| \leq \cdots \leq G^k|x_0 - s|.$$

When $G < 1$, $G^k \to 0$ as $k \to \infty$, hence the iteration converges with $x_k \to s$ as $k \to \infty$. $\square$

Newton iteration

Suppose $f(x)$ can be approximated near x_k by a truncated Taylor series. Then

$$f(x_{k+1}) \approx f(x_k) + f'(x_k)(x_{k+1} - x_k).$$

We want $f(x_{k+1}) = 0$, hence

$$\begin{aligned} f(x_k) + f'(x_k)(x_{k+1} - x_k) &= 0 \\ \Rightarrow x_{k+1} &= x_k - \frac{f(x_k)}{f'(x_k)}. \end{aligned}$$

Newton iteration

Example 7.3

Consider the cubic

$$f(x) = x^3 - 4 = 0.$$

Newton iteration is given by

$$x_{k+1} = x_k - \frac{x_k^3 - 4}{3x_k^2}$$

Newton iteration

Starting at $x_0 = 2$, we obtain the sequence

$$2,\ 1.6667,\ 1.5911,\ 1.5874.$$

Only three iterations were necessary to obtain four decimal place accuracy in this example.

Our Newton iteration is equivalent to fixed-point iteration with $g(x) = x - (x^3 - 4)/(3x^2)$. Notice that $g'(x)$ is zero near the root, hence G^k rapidly becomes small ($|g'(x)| \leq G$) and convergence is fast.

Convergence

Theorem 7.4

If $f(x)$ is thrice differentiable and f' and f'' are not zero at a root s of $f(x) = 0$, then for initial x_0 sufficiently close to s, the rate of convergence of Newton's method is quadratic.

Proof.

We use an additional term in Taylor's theorem about $x = s$ to show that

$$|x_{k+1} - s| = |g(x_k) - g(s)| = \frac{1}{2}|g''(t)(x_k - s)^2| \leq \frac{1}{2}M|x_k - s|^2,$$

where $g(x) = x - f(x)/f'(x)$ and $|g''(x)| < M$ on the interval around the root. $\square$

Termination

Example 7.5

Reconsider the cubic

$$f(x) = x^3 - 4 = 0.$$

whose Newton iteration is given by

$$x_{k+1} = x_k - \frac{x_k^3 - 4}{3x_k^2}$$

To terminate, we can try

```
if abs(xNew - x) < tol, break, end
```

Termination

Various termination criteria are possible. Depending on the problem, we could choose:

- an absolute test on the iterates, $|x_{k+1} - x_k| < \epsilon$, or
- a relative test on the iterates, $|x_{k+1} - x_k| < \epsilon |x_k|$, or
- an absolute test on the residual, $|f(x_k)| < \epsilon$, or
- a relative test on the residual, $|f(x_k)| < \epsilon |f(x_0)|$.

Depending on the circumstances, any of these may be misleading or even fail. You need to choose a termination condition that is suitable for your problem.

No Derivative, No Problems

Sometimes the derivative $f'(x)$ is unavailable (perhaps the function is calculated by some 'black box' software). In that case, we can use a finite difference approximation to the derivative, such as those we derived earlier. For example,

$$f'(x) \approx \frac{f(x+h) - f(x)}{h},$$

where h is about 10^{-6} to 10^{-8}.

No Derivative, No Problems

Example 7.6

Use Newton's method to find a solution of

$$\exp(\sin(x^2 - 3x + 2) - x) = 1.$$

In this case, the residual is

$$f(x) = \exp(\sin(x^2 - 3x + 2) - x) - 1.$$

Using a finite difference approximation for $f'(x)$ and starting at $x_0 = 1$, we converge to $x = 0.57272914$.

Nonlinear systems

The simplest nonlinear system consists of two nonlinear equations in two variables:

$$f(x, y) = 0$$
$$g(x, y) = 0$$

A solution to this system consists of those values of x and y that satisfy both equations simultaneously. Newton iteration can be adapted to find such solutions.

Newton iteration of two equations

Example 7.7

Suppose we wish to solve the nonlinear system

$$\begin{aligned} f(x,y) &= x^2 - xy^2 - xy - 1 = 0, \\ g(x,y) &= y^2 + x^3 + xy - 3 = 0. \end{aligned}$$

Try guessing $(x,y) = (1,0)$. We find $f(1,0) = 0$ and $g(1,0) = -2$. This is not a solution, because a solution must satisfy both equations.

Newton iteration of two equations

Try to find a better solution by modifying the original guess as $(x, y) = (1 + \Delta x, \Delta y)$, where Δx and Δy are small. Ignoring the very small nonlinear terms (such as Δx^2, Δy^2, $\Delta x \Delta y$, and so on), we obtain

$$\begin{aligned} f(1 + \Delta x, \Delta y) &\approx 2\Delta x - \Delta y, \\ g(1 + \Delta x, \Delta y) &\approx 3\Delta x + \Delta y - 2, \end{aligned}$$

We want $f(1 + \Delta x, \Delta y) = g(1 + \Delta x, \Delta y) = 0$, hence we obtain a linear system

$$\begin{bmatrix} 2 & -1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = -\begin{bmatrix} 0 \\ -2 \end{bmatrix}.$$

Newton iteration of two equations

Solving the linear system yields $(\Delta x, \Delta y) = (2/5, 4/5)$. The new guess is thus $(x_1, y_1) = (1 + \Delta x, \Delta y) = (7/5, 4/5)$.

We can continue this process by searching for an even better guess $(x, y) = (x_1 + \Delta x, y_1 + \Delta y)$. We approximate f and g as before, obtaining

$$\begin{aligned}
f(x_1 + \Delta x, y_1 + \Delta y) &\approx (x_1^2 - x_1 y_1^2 - x_1 y_1 - 1) \\
&\quad + (2x_1 - y_1^2 - y_1)\Delta x + (-2x_1 y_1 - x_1)\Delta y, \\
g(x_1 + \Delta x, y_1 + \Delta y) &\approx (y_1^2 + x_1^3 + x_1 y_1 - 3) \\
&\quad + (3x_1^2 + y_1)\Delta x + (x_1 + 2y_1)\Delta y.
\end{aligned}$$

Newton iteration of two equations

Setting $f(x_1 + \Delta x, y_1 + \Delta y) = g(x_1 + \Delta x, y_1 + \Delta y) = 0$ yields

$$\begin{bmatrix} 2x_1 - y_1^2 - y_1 & -2x_1y_1 - x_1 \\ 3x_1^2 + y_1 & x_1 + 2y_1 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = - \begin{bmatrix} f_1 \\ g_1 \end{bmatrix},$$

where

$$\begin{aligned} f_1 &= f(x_1, y_1) = x_1^2 - x_1y_1^2 - x_1y_1 - 1 \\ g_1 &= g(x_1, y_1) = y_1^2 + x_1^3 + x_1y_1 - 3. \end{aligned}$$

We again solve for $(\Delta x, \Delta y)$ and hence find a new guess $(x_1 + \Delta x, y_1 + \Delta y)$. And so on...

Newton iteration of two equations

Suppose $f(x,y)$ and $g(x,y)$ can be approximated near (x_k, y_k) by truncated multivariable Taylor series. Then

$$f(x_{k+1}, y_{k+1}) \approx f(x_k, y_k) + \left.\frac{\partial f}{\partial x}\right|_{x_k, y_k} \Delta x + \left.\frac{\partial f}{\partial y}\right|_{x_k, y_k} \Delta y,$$

$$g(x_{k+1}, y_{k+1}) \approx g(x_k, y_k) + \left.\frac{\partial g}{\partial x}\right|_{x_k, y_k} \Delta x + \left.\frac{\partial g}{\partial y}\right|_{x_k, y_k} \Delta y,$$

where $\Delta x = x_{k+1} - x_k$ and $\Delta y = y_{k+1} - y_k$.

Newton iteration of two equations

We want $f(x_{k+1}, y_{k+1}) = 0$ and $g(x_{k+1}, y_{k+1}) = 0$, hence

$$f(x_k, y_k) + \left.\frac{\partial f}{\partial x}\right|_{x_k, y_k} \Delta x + \left.\frac{\partial f}{\partial y}\right|_{x_k, y_k} \Delta y = 0,$$
$$g(x_k, y_k) + \left.\frac{\partial g}{\partial x}\right|_{x_k, y_k} \Delta x + \left.\frac{\partial g}{\partial y}\right|_{x_k, y_k} \Delta y = 0,$$

which can be written as a linear system

$$\begin{bmatrix} \left.\frac{\partial f}{\partial x}\right|_{x_k, y_k} & \left.\frac{\partial f}{\partial y}\right|_{x_k, y_k} \\ \left.\frac{\partial g}{\partial x}\right|_{x_k, y_k} & \left.\frac{\partial g}{\partial y}\right|_{x_k, y_k} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = - \begin{bmatrix} f(x_k, y_k) \\ g(x_k, y_k) \end{bmatrix}.$$

The matrix on the left hand side is the Jacobian $\boldsymbol{J}_k$.

Newton iteration of two equations

Assuming this system can be solved for Δx and Δy, the new iterates can be found using

$$x_{k+1} = x_k + \Delta x,$$
$$y_{k+1} = y_k + \Delta y.$$

Newton iteration of two equations

Example 7.8

Suppose we wish to solve the nonlinear system

$$\begin{aligned} f(x, y) &= x^2 + y^2 - 2 = 0, \\ g(x, y) &= y - \cos x = 0. \end{aligned}$$

Newton iteration is given by

$$\begin{aligned} x_{k+1} &= x_k + \Delta x, \\ y_{k+1} &= y_k + \Delta y, \end{aligned}$$

$$\begin{bmatrix} 2x_k & 2y_k \\ \sin x_k & 1 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = - \begin{bmatrix} x_k^2 + y_k^2 - 2 \\ y_k - \cos x_k \end{bmatrix}.$$

Newton iteration of two equations

Let $\boldsymbol{x}_k = [x_k, y_k]^T$ and $\Delta\boldsymbol{x} = [\Delta x_k, \Delta y_k]^T$. Then the iteration formulae are

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \Delta\boldsymbol{x}, \quad \boldsymbol{J}_k \Delta\boldsymbol{x} = -\boldsymbol{r}_k.$$

where $\boldsymbol{r}_k = [f(x_k, y_k), g(x_k, y_k)]^T$.

Although you would not compute the inverse of the Jacobian, the above formulae can also be written as

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \boldsymbol{J}_k^{-1}\boldsymbol{r}_k,$$

which is analogous to the single variable formula

$$x_{k+1} = x_k - [f'(x_k)]^{-1} f(x_k).$$

General Newton iteration

A system of n nonlinear equations can be written as

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0},$$

where $\boldsymbol{f}$ and $\boldsymbol{x}$ are vectors of length n.

The Newton iteration formulae for such a system are

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \Delta\boldsymbol{x}, \quad \boldsymbol{J}_k \Delta\boldsymbol{x} = -\boldsymbol{f}_k.$$

where $\boldsymbol{f}_k = \boldsymbol{f}(\boldsymbol{x}_k)$ and the elements of the Jacobian are

$$J_{ij} = \frac{\partial f_i}{\partial x_j}.$$

General Newton iteration

Start with an initial guess $\boldsymbol{x}_0$. Continue iteration until

- $\|\boldsymbol{x}_{k+1} - \boldsymbol{x}_k\| < \epsilon$, or
- $\|\boldsymbol{f}(\boldsymbol{x}_k)\| < \epsilon$,

where ϵ is the tolerance. As for the single variable case, it is also possible to rewrite the above in terms of relative magnitude.

Aside: Newton Fractals

Consider solving $f(z) = z^4 - 1 = 0$ over the complex plane using Newton's method. The roots are:

$$1, -1, i, -i$$

and every starting point $z_0 \in \mathbb{C}$ will eventually converge to one of these roots.

Newton's method over $\mathbb{C}$ works exactly as it does over $\mathbb{R}$:

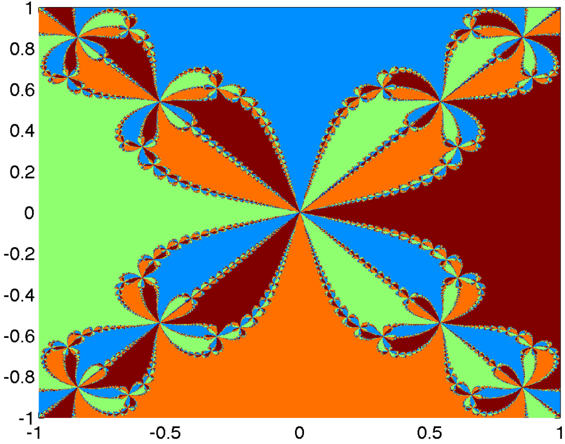
$$\begin{aligned} z_{k+1} &= z_k - \frac{f(z_k)}{f'(z_k)} \\ &= z_k - \frac{z^4 - 1}{4z^3} \end{aligned}$$

Obviously starting points near 1 converge to the root $1 + 0i$, and similarly for the other roots.

What happens at the boundaries between regions?

Aside: Newton Fractals

The boundaries dividing basins of attraction for each z_0 turn out to be quite interesting!



Points coloured by the root which they eventually converge to.
Many other fractals possible, depending on the choice of $f(z)$!

Aside: Newton Fractals

For more information:

- Simon Tatham. *Fractals derived from Newton-Raphson*. `http://www.chiark.greenend.org.uk/~sgtatham/newton/`
- Johannes Rueckert. *Newton's Method as a Dynamical System* (PhD thesis). `http://www.math.stonybrook.edu/cgi-bin/thesis.pl?thesis06-1`