Chapter 2
Rootfinding

Given a function $f(x)$, a root is a number r satisfying $f(r) = 0$. For example, for $f(x) = x^2 - 3$, the roots are $r = \pm\sqrt{3}$. We want to find the roots of a general function $f(x)$ using a computer.

The bisection method

Suppose we find an interval $[a,b]$ such that $f(a)$ and $f(b)$ have opposite sign (for example $f(a) < 0$ and $f(b) > 0$). Then, by the intermediate value theorem[1], $f(x)$ has a root in $[a,b]$. Next we consider the midpoint $x_0 = \frac{1}{2}(a+b)$. The root r is contained in either the left subinterval or the right subinterval. To determine which one, we compute $f(x_0)$. Then repeat. The rootfinding by this rather simple idea is called the bisection method.

Example 1. Let us find a root of $f(x) = x^2 - 3$. We note that $f(1) = -2$ and $f(2) = 1$. Indeed, there is a root $r = \sqrt{3} = 1.73205\ldots$ on the interval $[1,2]$.

n	a_n	b_n	x_n	$f(x_n)$	$\lvert r - x_n \rvert$
0	1	2	1.5	−0.75	0.2321
1	1.5	2	1.75	0.0625	0.0179
2	1.5	1.75	1.625	−0.3594	0.1071
3	1.625	1.75	1.6875	−0.1523	0.0446
4	1.6875	1.75	1.71875	−0.0459	0.0133

The bisection method is implemented as follows (we assume $f(a) \cdot f(b) < 0$).

Step 1 $\quad n = 0$, $a_0 = a$, $b_0 = b$
Step 2 $\quad x_n = \frac{1}{2}(a_n + b_n)$ $\quad$ % current estimate of the root

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Step 3 if $f(x_n) \cdot f(a_n) < 0$, then $a_{n+1} = a_n$, $b_{n+1} = x_n$
Step 4 else $a_{n+1} = x_n$, $b_{n+1} = b_n$
Step 5 set $n = n+1$ and go to Step 2

When to stop? There are three stopping criterions:

$$|b_n - a_n| < \varepsilon, \qquad |f(x_n)| < \varepsilon, \qquad n = n_{\max}.$$

Suppose we find a root x_n. The error is estimated as

$$|r - x_n| \le \frac{1}{2}|b_n - a_n| = \left(\frac{1}{2}\right)^2 |b_{n-1} - a_{n-1}| = \cdots = \left(\frac{1}{2}\right)^{n+1} |b_0 - a_0|.$$

Example 2. In the above example, how large n is needed to ensure that the error is less than 10^{-3}? We have

$$|r - x_n| \le \left(\frac{1}{2}\right)^{n+1} |b_0 - a_0| \le 10^{-3},$$

where $a_0 = 1$, $b_0 = 2$. Since $2^{10} = 1024 \approx 10^3$, we can say $n \ge 9$.

Fixed-point iteration

Suppose $f(x) = 0$ is equivalent to $x = g(x)$. Then, r is a root of $f(x)$ only if r is a fixed point of $g(x)$. The fixed-point iteration is the method of solving $x = g(x)$ by computing $x_{n+1} = g(x_n)$ with some initial guess x_0.

Example 3. To obtain the positive root of $f(x) = x^2 - 3 = 0$, we can rewrite the equation as

$$x = g_1(x) = \frac{3}{x}, \qquad x = g_2(x) = x - (x^2 - 3), \qquad x = g_3(x) = x - \frac{1}{2}(x^2 - 3).$$

Recall $r = \sqrt{3} = 1.73205\ldots$. Let us start the fixed-point iteration with $x_0 = 1.5$.

	Case 1	Case 2	Case 3
n	x_n	x_n	x_n
0	1.5	1.5	1.5
1	2	2.25	1.875
2	1.5	0.1875	1.6172
3	2	3.1523	1.8095
4	1.5	−3.7849	1.6723
5	2	−15.1106	1.7740

We see that Case 3 converges whereas Case 1 and Case 2 diverge. We have to choose a good $g(x)$.

Theorem 1. *Assume that x_0 is sufficiently close to r and let $k = |g'(r)|$. Then fixed-point iteration converges if and only if $k < 1$.*

To understand the above theorem, we consider

$$|r - x_{n+1}| = |g(r) - g(x_n)| \sim |g'(r)|\,|r - x_n|,$$

where we used the Taylor expansion $g(x_n) = g(r) + g'(r)(x_n - r) + \cdots$. We have

$$|r - x_{n+1}| \sim k|r - x_n| \sim k^2|r - x_{n-1}| \sim \cdots \sim k^{n+1}|r - x_0|.$$

The right-hand side of the above equation goes to zero if $k < 1$.

We have $|r - x_{n+1}| \sim k|k - x_n|$. This is called linear convergence and k is called the asymptotic error constant. The bisection method also converges linearly with $k = 1/2$.

Example 4. Let us calculate k for Cases 1, 2, and 3 in the above example.

$$\begin{aligned} g_1'(x) &= -\tfrac{3}{x^2}. \qquad \therefore k = |g_1'(r)| = 1. \\ g_2'(x) &= 1 - 2x. \qquad \therefore k = |g_2'(r)| = 2.4641. \\ g_3'(x) &= 1 - x. \qquad \therefore k = |g_3'(r)| = 0.73205. \qquad \leftarrow \text{ converge} \end{aligned}$$

Newton's method

Suppose we want to find a root r of a smooth function $y = f(x)$. We take a point x_n which is close to r. The tangent line at x_n is expressed as

$$y = f'(x_n)(x - x_n) + f(x_n).$$

Let the x-intercept of the line (the root of the tangent line) denote x_{n+1}. At $x = x_{n+1}$ we have

$$0 = f'(x_n)(x_{n+1} - x_n) + f(x_n). \qquad \therefore \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

Next we consider the tangent line of $f(x)$ at $x = x_{n+1}$. By repeating this procedure, the points $x_n, x_{n+1}, \ldots$ approach r. For x_{n+1} sufficiently close to r, we can understand Newton's method with the Taylor series as

$$\underbrace{f(x_{n+1})}_{\approx 0} = f(x_n) + f'(x_n)(x_{n+1} - x_n) + \underbrace{\cdots}_{\approx 0}. \tag{2.1}$$

The next example shows that Newton's method has rapid convergence.

Example 5. For $f(x) = x^2 - 3$, we obtain

$$x_{n+1} = x_n - \frac{x_n^2 - 3}{2x_n}.$$

n	x_n	$f(x_n)$	$\lvert r - x_n\rvert$
0	1.5	−0.75	0.23205081
1	1.75	0.0625	0.01794919
2	1.73214286	0.00031888	0.00009205
3	1.73205081	0.00000001	0.00000001

We see that Newton's method is a fixed point iteration by writing

$$x_{n+1} = g(x_n), \qquad g(x) = x - \frac{f(x)}{f'(x)}.$$

We have

$$g'(r) = 1 - \left.\frac{f'(x)^2 - f(x)\cdot f''(x)}{f'(x)^2}\right|_{x=r} = 0.$$

This implies that Newton's method converges faster than linearly. In fact, it has quadratic convergence: $|r - x_{n+1}| \le C|r - x_n|^2$.

$$\because \quad r - x_{n+1} = g(r) - g(x_n) = g(r) - \left[g(r) + \underbrace{g'(r)}_{=0}(x_n - r) + O\left((x_n - r)^2\right)\right].$$

Let us summarize rootfinding methods.

method	rate of convergence	cost per step
bisection	linear , $k = \frac{1}{2}$	$f(x_n)$
fixed-point iteration	linear , $k = \lvert g'(r)\rvert$	$g(x_n)$
Newton	quadratic	$f(x_n), f'(x_n)$

The bisection method is guaranteed to converge if the initial interval contains a root; the other methods are sensitive to the choice of x_0.

Rootfinding for nonlinear systems

Using Newton's method, let us find roots of

$$\begin{cases} f(x,y) = 0, \\ g(x,y) = 0. \end{cases}$$

For given (x_n, y_n), we want to find (x_{n+1}, y_{n+1}). Recalling (2.1), we consider the Taylor series:

$$\underbrace{f(x_{n+1}, y_{n+1})}_{\approx 0} = f(x_n, y_n) + \frac{\partial f}{\partial x}(x_n, y_n)(x_{n+1} - x_n) + \frac{\partial f}{\partial y}(x_n, y_n)(y_{n+1} - y_n) + \underbrace{\cdots}_{\approx 0},$$

$$\underbrace{g(x_{n+1}, y_{n+1})}_{\approx 0} = g(x_n, y_n) + \frac{\partial g}{\partial x}(x_n, y_n)(x_{n+1} - x_n) + \frac{\partial g}{\partial y}(x_n, y_n)(y_{n+1} - y_n) + \underbrace{\cdots}_{\approx 0}.$$

Thus we obtain

$$A_n (\mathbf{x}_{n+1} - \mathbf{x}_n) = -\mathbf{f}_n,$$

where we introduced

$$A_n = \left. \begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix} \right|_{(x_n, y_n)}, \qquad \mathbf{x}_n = \begin{pmatrix} x_n \\ y_n \end{pmatrix}, \qquad \mathbf{f}_n = \begin{pmatrix} f(x_n, y_n) \\ g(x_n, y_n) \end{pmatrix}.$$

The matrix A_n is called the Jacobian matrix. We then obtain

$$\mathbf{x}_{n+1} = \mathbf{x}_n - A_n^{-1} \mathbf{f}_n.$$

Example 6. Let us consider $f(x,y) = x^3 + y - 1$, $g(x,y) = y^3 - x + 1$. In this case, we obtain

$$A_n = \begin{pmatrix} 3x_n^2 & 1 \\ -1 & 3y_n^2 \end{pmatrix}, \qquad \mathbf{f}_n = \begin{pmatrix} x_n^3 + y_n - 1 \\ y_n^3 - x_n + 1 \end{pmatrix}.$$

Let us plot $f = 0$, $g = 0$ using Matlab. The system has the root at $(x,y) = (1,0)$.

```
f='x^3+y-1';
g='y^3-x+1';
p1=ezplot(f);
set(p1,'Color','red')
hold on
p2=ezplot(g);
set(p2,'Color','blue')
legend(f,g)
title('')
hold off
```