Numerical Analysis

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Let $f \in C[a,b]$ and $f(a)f(b) < 0$, then f must have a zero in $[a,b]$.
Bisection method: Calculate $c = (a+b)/2$.

- if $f(a)f(c) < 0$, f has a zero in $[a,c]$.
- if $f(a)f(c) > 0$, i.e., $f(b)f(c) < 0$, f has a zero in $[c,b]$.
- if $f(a)f(c) = 0$, then $f(c) = 0$ and a zero has been found. However, it is quite unlikely that $f(c)$ ill be zero in the computer because of roundoff errors. Thus, the stopping criterion should not be whether $|f(c)| = 0$. A reasonable tolerance must be allowed, such as $|f(c)| < \epsilon$.

Thus the root must be in $[a,c]$ or $[c,b]$. These interval length are the one half of $[a,b]$. Repeating this process, the root locates in an interval, which length is very small. Thus the bisection method is also known as the method of interval halving.

To analyze the bisection method, let us denote the successive intervals that arise in the process by $[a_0, b_0]$, $[a_1, b_1]$, and so on. Here are some observations

$$a_0 \leq a_1 \leq a_2 \leq \cdots \leq b_0$$

$$b_0 \geq b_1 \geq b_2 \geq \cdots \geq a_0$$

$$b_{n+1} - a_{n+1} = \frac{1}{2}(b_n - a_n) \quad (n \geq 0)$$

Repeating the above formula,

$$b_n - a_n = 2^{-n}(b_0 - a_0)$$

Thus

$$\lim_{n\to\infty} b_n - \lim_{n\to\infty} a_n = 0$$

Bisection Method

Let

$$r = \lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n$$

By taking a limit of the inequality $0 \geq f(a_n)f(b_n)$, we obtain $0 \geq |f(r)|^2$, whence $f(r) = 0$.
Suppose that at a certain stage in the process, the interval $[a_n, b_n]$ has just been defined. If the process is now stopped, the root is certain to lie in this interval. The best estimate of the root at this stage is not a_n or b_n but the midpoint of the interval: $c_n = (a_n + b_n)/2$. The error is then bound

$$|r - c_n| \leq \frac{1}{2}|b_n - a_n| \leq 2^{-(n+1)}(b_0 - a_0)$$

Exercises: P.62

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Newton's Method

This is also called the Newton-Raphson iteration. Let r be a zero of f and let x be an approximation to r. If f'' exists and is continuous, then by Taylor's Theorem

$$0 = f(r) = f(x+h) = f(x) + hf'(x) + O(h^2)$$

where $h = r - x$. If h is small (that is, x is near r), then it is reasonable to ignore the $O(h^2)$-term and solve the remaining equation for h. Therefore, the result is $h = -f(x)/f'(x)$. If x is an approximation to r, then $x - f(x)/f'(x)$ should be a better approximation to r. Newton's method begins with an estimate x_0 of r and then defines inductively

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

The graphic explanation of the Newton iteration.

To analyze the errors in Newton's method. By errors, we mean the quantities

$$e_n = x_n - r$$

Let us assume that f'' is continuous and r is a simple zero of f, so that $f(r) = 0 \neq f'(r)$. From the definition of the Newton iteration,

$$e_{n+1} = x_{n+1} - r = x_n - \frac{f(x_n)}{f'(x_n)} - r = \frac{e_n f'(x_n) - f(x_n)}{f'(x_n)}$$

By Tayor's Theorem, we have

$$0 = f(r) = f(x_n - e_n) = f(x_n) - e_n f'(x_n) + \frac{1}{2} e_n^2 f''(\xi_n)$$

where ξ_n is a number between x_n and r. From this equation, we have

$$e_n f'(x_n) - f(x_n) = \frac{1}{2} f''(\xi_n) e_n^2$$

Thus

$$e_{n+1} = \frac{1}{2}\frac{f''(\xi_n)}{f'(x_n)}e_n^2 \approx \frac{1}{2}\frac{f''(r)}{f'(r)}e_n^2 = Ce_n^2$$

This equation tells us that e_{n+1} is roughly a constant times e_n^2. This desirable state of affairs is called quadratic convergence.

We want to establish the convergence of the method. the idea of the proof is simple: If e_n is small and if the factor $\frac{1}{2}\frac{f''(r)}{f'(r)}$ is not too large, then e_{n+1} will be smaller than e_n. Define

$$c(\delta) = \frac{1}{2}\max_{|x-r|\leq\delta}|f''(x)| / \min_{|x-r|\leq\delta}|f'(x)| \quad (\delta > 0)$$

We select δ small enough to be sure that the denominator is positive, and then if necessary we decrease δ so that $\delta c(\delta) < 1$. Having fixed δ, set $\rho = \delta c(\delta)$.

Newton's Method

Suppose that we start the Newton iteration with a point x_0 satisfying $|x_0 - r| \leq \delta$. Then $|e_0| \leq \delta$ and $|\xi_0 - r| \leq \delta$. Hence by the definition of $c(\delta)$, we have

$$\frac{1}{2}|f''(\xi_0)/f'(x_0)| \leq c(\delta)$$

Therefore,

$$|x_1 - r| = |e_1| \leq e_0^2 c(\delta) \leq |e_0|\delta c(\delta) = e_0\rho < |e_0| \leq \delta$$

This shows that the next point, x_1, also lies within δ units of r. Hence the argument can be repeated, with the results

$$|e_1| \leq \rho|e_0|$$

$$|e_2| \leq \rho|e_1| \leq \rho^2|e_0|$$

$$|e_3| \leq \rho|e_2| \leq \rho^3|e_0|$$

In general, we have $|e_n| \leq \rho^n|e_0|$. Since $0 \leq \rho < 1$, we have $\lim_{n\to\infty} \rho^n = 0$ and so $\lim_{n\to\infty} e_n = 0$.

Let f'' be continuous and let r be a simple zero of f. Then there is a neighborhood of r and a constant C such that if Newton's method is started in that neighborhood, then the successive points become steadily closer to r, and satisfy

$$|x_{n+1} - r| \le C|x_n - r|^2 \quad (n \ge 0)$$

If f belongs to $C^2(R)$, is increasing, is convex, and has a zero, then the zero is unique, and the Newton iteration will converge to it from any starting point.

Proof Recall that a function f is convex if $f''(x) > 0$ for all x. Since f is increasing, $f' > 0$ on R. By $e_{n+1} = \frac{1}{2}\frac{f''(\xi_n)}{f'(x_n)}e_n^2$, $e_{n+1} > 0$. Thus, $x_n > r$ for $n \geq 1$. Since f is increasing, $f(x_n) > f(r) = 0$. By $e_{n+1} = e_n - \frac{f(x_n)}{f'(x_n)}$, $e_{n+1} < e_n$. Thus, the sequences $\{e_n\}$ and $\{x_n\}$ are decreasing and bounded below (by 0 and r, respectively). Therefore, the limits $e^* = \lim_{n\to\infty} e_n$ and $x^* = \lim_{n\to\infty} x_n$ exist. We have $e^* = e^* - f(x^*)/f'(x^*)$, whence $f(x^*) = 0$ and $x^* = r$.

Newton's Method

The equation $G(x, y) = 0$ gives implicitly the definition of y as a function of x. This function can be solved by the Newton's iteration

$$y_{n+1} = y_n - \frac{G(x, y_n)}{\frac{\partial G}{\partial y}(x, y_n)}$$

Newton's Method

Solve a pais of equations involving two variables

$$\begin{cases} f_1(x_1, x_2) = 0 \\ f_2(x_1, x_2) = 0 \end{cases}$$

Linearize the systems

$$\begin{cases} 0 = f_1(x_1 + h_1, x_2 + h_2) \approx f_1(x_1, x_2) + h_1 \frac{\partial f_1}{\partial x_1} + h_2 \frac{\partial f_1}{\partial x_2} \\ 0 = f_2(x_1 + h_1, x_2 + h_2) \approx f_2(x_1, x_2) + h_1 \frac{\partial f_2}{\partial x_1} + h_2 \frac{\partial f_2}{\partial x_2} \end{cases}$$

and solve for h_1 and h_2

$$\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = -J^{-1} \begin{pmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{pmatrix}$$

where J is the Jacobi matrix

$$\begin{pmatrix} \partial f_1 / \partial x_1 & \partial f_1 / \partial x_2 \\ \partial f_2 / \partial x_1 & \partial f_2 / \partial x_2 \end{pmatrix}$$

The Newton's method is

$$\begin{pmatrix} x_1^{(k+1)} \\ x_2^{(k+1)} \end{pmatrix} = \begin{pmatrix} x_1^{(k)} \\ x_2^{(k)} \end{pmatrix} + \begin{pmatrix} h_1^{(k)} \\ h_2^{(k)} \end{pmatrix}$$

where the linear system

$$J|_{(x_1^{(k)}, x_2^{(k)})} \begin{pmatrix} h_1^{(k)} \\ h_2^{(k)} \end{pmatrix} = -\begin{pmatrix} f_1(x_1^{(k)}) \\ f_2(x_2^{(k)}) \end{pmatrix}$$

is solved using Gaussian elimination.
More larger systems involving many variables

$$f_i(x_1, \cdots, x_n) = 0 \quad (1 \le i \le n)$$

can be written as

$$F(X) = 0$$

by letting $X = (x_1, \cdots, x_n)^T$ and $F = (f_1, \cdots, f_n)^T$.

Newton's Method

Linearizing the nonlinear equation, one has

$$0 = F(X + H) \approx F(X) + F'(X)H$$

where $H = (h_1, \cdots, h_n)^T$ and $F'(X)$ is the $n \times n$ Jacobi matrix with elements $\partial f_i / \partial x_j$. H can then be solved by

$$H = -F'(X)^{-1} F(X)$$

Hence the Newton's iteration to solve the the nonlinear equation $F(X) = 0$ is

$$X^{(k+1)} = X^{(k)} + H^{(k)}$$

where

$$F'(X^{(k)})H^{(k)} = -F(X^{(k)})$$

Secant Method

If the first derivative $f'(x_n)$ is approximated by

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

the Newton's iteration becomes

$$x_{n+1} = x_n - f(x_n)\left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}\right] \quad (n \geq 1)$$

which is called the secant method (iteration) to solve $f(x) = 0$. The geometric interpretation of secant method is using a secant line to replace the tangent line.

Define the error $e_n = x_n - r$,

$$\begin{aligned} e_{n+1} &= x_{n+1} - r = \frac{f(x_n)e_{n-1} - f(x_{n-1})e_n}{f(x_n) - f(x_{n-1})} \\ &= \left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}\right]\left[\frac{f(x_n)/e_n - f(x_{n-1})/e_{n-1}}{x_n - x_{n-1}}\right] e_n e_{n-1} \end{aligned}$$

By Taylor's theorem,

$$f(x_n) = f(r + e_n) = f(r) + e_n f'(r) + \frac{1}{2}e_n^2 f''(r) + O(e_n^3)$$

which gives

$$f(x_n)/e_n = f'(r) + \frac{1}{2}e_n f''(r) + O(e_n^2)$$

Thus,

$$f(x_n)/e_n - f(x_{n-1})/e_{n-1} = \frac{1}{2}(e_n - e_{n-1})f''(r) + O(e_{n-1}^2)$$

Since $x_n - x_{n-1} = e_n - e_{n-1}$,

$$\frac{f(x_n)/e_n - f(x_{n-1})/e_{n-1}}{x_n - x_{n-1}} \approx \frac{1}{2}f''(r)$$

Hence

$$e_{n+1} \approx \frac{1}{2}\frac{f''(r)}{f'(r)}e_n e_{n-1} = Ce_n e_{n-1}$$

To discover the order of convergence of the secant method, we postulate the asymptotic relationship

$$|e_{n+1}| \sim A|e_n|^\alpha$$

Substituting this relationship to the above result,

$$A|e_n|^\alpha \approx C|e_n|A^{-1/\alpha}|e_n|^{1/\alpha}$$

i.e.,

$$A^{1+1/\alpha}C^{-1} \sim |e_n|^{1-\alpha+1/\alpha}$$

We thus $1 - \alpha + 1/\alpha = 0$, or $\alpha = (1 + \sqrt{5})/2 \approx 1.62$.

Hence the secant method's rate of convergence is superlinear (that is, better than linear).

$$A = C^{1/(1+1/\alpha)} = C^{\alpha-1} = C^{0.62} = \left[\frac{f''(r)}{2f'(r)}\right]^{0.62}$$

With A is just given, we finally have for the secant method

$$|e_{n+1}| \approx A|e_n|^{(1+\sqrt{5})/2}$$

Since $(1+\sqrt{5})/2 \approx 1.62 < 2$, the rapidity of convergence of the secant method is not as good as Newton's method but better than the bisection method. However, each step of the secant method requires only one new function evaluation, while each step of the Newton algorithm requires two function evaluations, namely $f(x)$ and $f'(x)$.

Exercises: P.79

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Fixed points and Functional Iteration

The iteration

$$x_{n+1} = F(x_n) \quad (n \geq 0)$$

which is called functional iteration. In Newton's iteration

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

If the functional iteration is convergent, its limit satisfies

$$x = F(x)$$

which is called the fixed point of the function F.
A mapping (or function) F is said to be contractive if there exists a number λ less than 1 such that

$$|F(x) - F(y)| \leq \lambda |x - y|$$

for all x and y in the domain of F.

Let F be a contractive mapping of a closed set $C \subset R$ into C. Then F has a unique fixed point. Moreover, this fixed point is the limit of every sequence obtained from $x_{n+1} = F(x_n)$ with any starting point $x_0 \in C$.
Proof. First

$$|x_n - x_{n-1}| = |F(x_{n-1}) - F(x_{n-2})| \leq \lambda |x_{n-1} - x_{n-2}| \leq \cdots \leq \lambda^{n-1} |x_1 - x_0|$$

Thus the sequence $\{x_n\}$ is a Cauchy sequence, is thus convergent with a limit s. Taking the limit of $x_{n+1} = F(x_n)$, we know that the limit x is a fixed point of F. Moreover the fixed point of F is unique since F is contractive.

Now we want to analyze of the errors. Let $e_n = x_n - s$,

$$e_{n+1} = x_{n+1} - s = F(x_n) - F(s) = F'(\xi_n)(x_n - s) = F'(\xi_n)e_n$$

We assume that

$$F^{(k)}(s) = 0, \quad 1 \leq k \leq q-1, \quad F^{(q)}(s) \neq 0$$

$$e_{n+1} = F(x_n) - F(s) = F(s + e_n) - F(s) = \frac{1}{q!} e_n^q F^{(q)}(\xi_n)$$

and therefore

$$\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^q} = \frac{1}{q!} e_n^q F^{(q)}(s)$$

and thus the order of convergence is q.

For the Newton's iteration, $F'(s) = 0$ and $F''(s) \neq 0$ and then $q = 2$

$$e_{n+1} = \frac{1}{2} F''(\xi_n) e_n^2$$

Exercises: P.85

1,4(a)(b),10,23(a)(b)