Numerical analysis, week 10: Approximating roots of nonlinear equations

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The main task is to solve nonlinear equations $f(x) = 0$, e.g. $f(x) = e^x - 3x - 1$ which doesn't have an analytic solution (compare with a linear equation $f(x) = ax + b$).

1 Bisection method

1. $f : [a, b] \to \mathbb{R}$ continuous. Suppose $f(a) f(b) < 0$. By mean value theorem: $\exists \alpha \in (a, b)$ s.t. $f(\alpha) = 0$.
2. **The bisection method**:
   (a) Start with $[a_0, b_0] = [a, b]$
   (b) repeat:
      i. $m_i = \frac{a_i + b_i}{2}$
      ii. if $f(m_i) = 0$ then $\alpha = m_i$ (finish)
      iii. else if $f(a_i) f(m_i) < 0$: $a_{i+1} = a_i, b_{i+1} = m_i$
      iv. else $a_{i+1} = m_i, b_{i+1} = b_i$
3. At each step we have $|\alpha - m_n| \leq \frac{b-a}{2^{n+1}}$
4. Example: $f(x) = x^2 - 2$ on $[1, 2]$. (clearly $\alpha = \sqrt{2}$ but we will want to compute using

only basic arithmetic operations).

n	a_n	b_n	m_n	$f(a_n)$	$f(b_n)$	$f(m_n)$
0	1	2	1.5	-1	2	0.25
1	1	1.5	1.25	-1	0.25	-0.4375
2	1.25	1.5	1.375	-0.4375	0.25	-0.109375
3	1.375	1.5	1.4375	-0.109375	0.25	0.0640625
4	1.375	1.4375	1.40625	-0.109375	0.0640625	-0.0224609
5	1.40625	1.4375	1.421875	-0.0224609	0.0640625	0.0217285
6	1.40625	1.421875	1.4140625	-0.0224609	0.0217285	-0.0004272
7	1.4140625	1.421875	1.41796875	-0.0004272	0.0217285	0.010635376
8	1.4140625	1.41796875	1.416015625	-0.0004272	0.010635376	0.00510025

So the convergence to $\alpha \approx 1.4142$ is slow.

5. Define $e_n = \alpha - m_n$, then

$$\begin{aligned} |e_n| &\leq \frac{b-a}{2^{n+1}} \\ |e_{n+1}| &\approx \frac{1}{2}|e_n| \qquad \text{(in fact this is not as simple...)} \end{aligned}$$

Definition 1. Suppose $e_n \to 0$. The **order of convergence** of a method is at least p if $|e_{n+1}| \leq C|e_n|^p$, and equal to p if

$$0 < \lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^p} < \infty.$$

So, the bisection method has (sometimes) order of convergence=1 (also called *linear convergence*).

2 Newton's method

The idea is to approximate the function at the current estimate x_n by its tangent line, and take the next estimate to be the intersection of this line with the x axis.

So if $f'(x_n) \neq 0$, the line $\ell(x) = f(x_n) + f'(x_n)(x - x_n)$ has the root

$$\ell(x_{n+1}) = 0 \Rightarrow x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \quad n = 0, 1, 2, \ldots. \tag{1}$$

This is the Newton's method.

Continuing with our previous example $f(x) = x^2 - 2$ and applying the Newton's method with $x_0 = 1.5$ we obtain

n	x_n	$f(x_n)$	$f'(x_n)$
0	1.5	0.25	3.00
1	1.41666	0.0069444	2.8332
2	1.4142089	-1.3107*10^{-3}	2.8284178
3	1.41467230	$1.2977 * 10^{-3}$	2.829344
4	1.414213642	2.2647*10^{-7}	2.828427

so the convergence now is very fast (in fact we will see later that whenever $f'(\alpha) \neq 0$ we have $p = 2$, or *quadratic convergence*).

3 Fixed point iteration

A fixed point iteration is a method of the form

$$x_{n+1} = g(x_n)$$

for some continuous (later, continuously differentiable) function g. For Newton's method: $g(x) = x - \frac{f(x)}{f'(x)}$.Clearly if $x_n \to \beta$ then $g(\beta) = \beta = \beta - \frac{f(\beta)}{f'(\beta)}$ and so $f(\beta) = 0$.

This is not the single possible fixed point iteration for finding a zero of $f(x)$. For example: $g(x) = x + f(x)$ or $g(x) = x + \phi(x) f(x)$. At this point it is not obvious whether any of these iterations should converge.

Definition 2. α is called the fixed point of $g(x)$ if $g(\alpha) = \alpha$.

Definition 3. The fixed point iteration $x_{n+1} = g(x)$ is called consistent with $f(x) = 0$ if a fixed point of g is also a zero of f.

Theorem 1. *If $g : [a, b] \to [a, b]$ is continuous, then it has a fixed point in $[a, b]$.*

Proof. Define $h(x) = g(x) - x$, then unless $g(a) = a$ we must have $h(a) < 0$. Analogously, unless $g(b) = b$ we must have $h(b) > 0$. Overall, h must have a zero in $[a, b]$. $\square$

Theorem 2. *Let $g : [a, b] \to [a, b]$ be continuous in $I = [a, b]$, and suppose $|g'(x)| \leq K < 1$ for $x \in I$. Then g has a unique fixed point in I, and the fixed point iteration will converge to it for any $x_0 \in I$.*

Proof. We already know g has a fixed point, let us show uniqueness. If α, β are two fixed points then

$$|\alpha - \beta| = |g(\alpha) - g(\beta)| \leq K|\alpha - \beta| < |\alpha - \beta|,$$

a contradiction. Now, for every n we have $g(x_n) \in I$.

$$\begin{aligned} |x_{n+1} - \alpha| &= |g(x_n) - g(\alpha)| = |g'(c_n)| \, |x_n - \alpha| \leq K \, |x_n - \alpha| \\ &\leq K^n \, |x_0 - \alpha| \to 0 \qquad (K < 1), \end{aligned}$$

and we conclude that $x_n \to \alpha$. ☐

Remark 1. In the condition of theorem 2, the condition $g : [a, b] \to [a, b]$ may be replaced by $g : \mathbb{R} \to \mathbb{R}$ (or semi-infinite intervals $[a, \infty)$ or $(-\infty, b]$, while the global bound on the derivative may be replaced by Lipschitz continuity: $|g(x) - g(y)| \leq K |x - y|$ for $K < 1$ (this is weaker than everywhere differentiable or continuously differentiable, e.g. $g(x) = |x|$ is Lipschitz continuous).

Instead of requiring some global information of g, it is also possible to show convergence to a fixed point αstarting with a sufficiently close initial guess, provided $|g'(\alpha)| < 1$ and the derivative of g is continuous in a neighborhood of α.

Theorem 3. *Let $g \in C^1$ on an open interval I containing the fixed point α, with $|g'(\alpha)| < 1$. Then $\exists \epsilon > 0$ s.t. for every $|x_0 - \alpha| < \epsilon$ the iteration $x_{n+1} = g(x_n)$ converges to α.*

Proof. Since $g(x)$ is continuous and $|g'(\alpha)| < 1$, there exists an interval $I_\epsilon = [\alpha - \epsilon, \alpha + \epsilon]$ containing α such that $|g'(x)| \leq K < 1$ for $x \in I_\epsilon$. Now if $x_n \in I_\epsilon$ then

$$|x_{n+1} - \alpha| = |g(x_n) - g(\alpha)| = |g'(c_n)| \, |x_n - \alpha| < |x_n - \alpha| \leq \epsilon, \quad c_n \in I_\epsilon,$$

therefore $x_{n+1} \in I_\epsilon$. This shows $g : I_\epsilon \to I_\epsilon$ and $\max_{x \in I_\epsilon} |g'| < 1$. The proof is finished by applying theorem 2. ☐

4 Estimating order of convergence

Recall Definition 1 of order of convergence.

Theorem 4. *Let α be a fixed point of $g(x)$ which is $p \geq 1$ times continuously differentiable in an (open) neighborhood of α.*

1. *If $p = 1$ and $0 < |g'(\alpha)| < 1$ then the fixed point iteration converges with order* 1.
2. *If $p \geq 2$ and $g'(\alpha) = \cdots = g^{(p-1)}(\alpha)$ while also $g^{(p)}(\alpha) \neq 0$ for then the fixed point iteration converges with order p.*

Proof. Taylor expansion up to order p gives

$$\begin{aligned} x_{n+1} = g\left(x_n\right) &= g\left(\alpha\right) + \frac{g^{(p)}\left(\xi_n\right)}{p!}\left(x_n - \alpha\right)^p \\ \left|\frac{x_{n+1}-\alpha}{\left(x_n-\alpha\right)^p}\right| &= \left|\frac{g^{(p)}\left(\xi_n\right)}{p!}\right|, \quad \xi_n \text{ between } x_n, \alpha \end{aligned}$$

Since $g^{(p)}$ is continuous, taking the limit $x_n \to \alpha$ (we know the iteration converges by theorem 3 as in both cases $\left|g'\left(\alpha\right)\right| < 1$) we conclude

$$\lim_{n\to\infty}\left|\frac{x_{n+1}-\alpha}{\left(x_n-\alpha\right)^p}\right| = \frac{1}{p!}\left|g^{(p)}\left(\alpha\right)\right| \neq 0.$$

Therefore in both cases the order of convergence is p by definition. □

5 Newton's method - convergence analysis

1. If α is a simple root, i.e. $f\left(\alpha\right) = 0, f'\left(\alpha\right) \neq 0$, and also $f''\left(\alpha\right) \neq 0$, then the Newton method converges with order=2:

$$\begin{aligned} & g(x) = x - \tfrac{f(x)}{f'(x)} \\ & g'(x) = 1 - \tfrac{(f'(x))^2 - f(x)f''(x)}{(f'(x))^2} = \tfrac{f(x)f''(x)}{(f'(x))^2} \Rightarrow g'(\alpha) = 0, \\ & g''(x) = \tfrac{(f'(x)f''(x) + f(x)f''(x))(f'(x))^2 - 2f'(x)f(x)(f''(x))^2}{(f'(x))^4} \\ & \underset{f(\alpha)=0}{\Rightarrow} g''(\alpha) = \tfrac{f''(\alpha)}{f'(\alpha)} \neq 0 \end{aligned}$$

   If $f''\left(\alpha\right) = 0$ (but still $f'\left(\alpha\right) \neq 0$) the order is larger than 2.

2. If α is a double root (i.e. $f\left(\alpha\right) = f'\left(\alpha\right) = 0$), we have linear convergence, since in this case $g'\left(\alpha\right) = \lim_{x\to\alpha} g'\left(x\right) = \cdots = \frac{1}{2}$.

For higher multiplicity roots one can use Modified Newton's method:

$$x_{n+1} = x_n - m\frac{f\left(x_n\right)}{f'\left(x_n\right)}$$

where m is the multiplicity.

Alternatively, if the multiplicity is unknown, one can use $u\left(x\right) = \frac{f(x)}{f'(x)}$. α is a simple root of $u\left(x\right)$ (check!), and therefore Newton's method with u will converge $\underline{\text{quadratically}}$.

6 Examples

Example 1. Consider the equation

$$2x - \cos x = 0$$

1. Prove that the equation above has a unique solution $\alpha \in \left(0, \frac{\pi}{2}\right)$.
2. Let $g(x) = \cos x - x$. Does the iteration $x_{n+1} = g(x_n)$ converge to α for every $x_0 \in \left[0, \frac{\pi}{2}\right]$?
3. Let $h(x) = \frac{1}{2}\cos x$. Does the iteration
$$x_{n+1} = h(x_n)$$
converge to α for every $x_0 \in \left[0, \frac{\pi}{2}\right]$? If so, what is the order of convergence?

Solution. Let $f(x) = 2x - \cos x$.

1. $f(0) = -1 < 0, f\left(\frac{\pi}{2}\right) = \pi > 0$, apply mean value theorem. Furthermore $f'(x) > 0$ and therefore the solution is unique.
2. $f(\alpha) = 2\alpha - \cos\alpha = 0$ and so $\alpha = \cos\alpha - \alpha = g(\alpha)$, i.e. α is a fixed point of g (so the iteration is consistent). Furthermore, $g'(x) = -\sin x - 1 < -1$, therefore the iteration will diverge for every initial guess: indeed,
$$|x_{n+1} - \alpha| = |g(x_n) - g(\alpha)| = |g'(c)|\,|x_n - \alpha| > |x_n - \alpha|.$$
3. We immediately check that $h(\alpha) = \alpha$ so the iteration is consistent. $h'(x) = -\frac{1}{2}\sin x$ and so $|h'(x)| < 1$ for all $x \in \left[0, \frac{\pi}{2}\right]$, thus the iteration will converge. Furthermore, $0 < |h'(\alpha)| < 1$ and therefore the order of convergence is 1.

Example 2. Consider the equation $\ln x + x = 0$.

1. Show there is a unique solution $\alpha \in \left[\frac{1}{3}, 1\right]$.
2. Show that for every $x_0 \in \left[\frac{1}{3}, 1\right]$ the iteration $x_{n+1} = e^{-x_n}$ converges to α. What is the order of convergence?
3. Find another iteration which convergence for x_0 sufficiently close to α with order 2. Prove that the order is indeed 2.

Solution.

Example 3. Approximating the root of $f(x) = x - e^{-x}$.

1. There is a root $\alpha \in (0,1)$ since $f(0)\,f(1) = -\left(1 - \frac{1}{e}\right) < 0$.
2. The fixed point iteration $x_{n+1} = g(x_n) = e^{-x_n}$ is consistent (check!), while also $g([0,1]) \subset \left[\frac{1}{e}, 1\right] \subset [0,1]$ (check).
3. $|g'(x)| = |e^{-x}| < 1$ for $x \in [a,1]$ with any $0 < a < \frac{1}{e}$. So for any $x_0 \in (0,1)$ the iteration will converge to α (which is also the unique fixed point).

Solution.

Example 4. For $f \in C^1$ with $f(\alpha) = 0$ and $f'(\alpha) \neq 0$, find the order of convergence of Steffensen method

$$x_{n+1} = x_n - \frac{f(x_n)}{h(x_n)}, \quad h(x) = \frac{f(x + f(x)) - f(x)}{f(x)} = \frac{f(x + f(x))}{f(x)} - 1.$$

Solution.

Example 5. We would like to approximate a cubic root $\alpha = a^{1/3}$ by the fixed point iteration $x_{n+1} = g\left(x_n\right)$ with

$$g(x) = Ax + B\frac{a}{x^2} + C\frac{a^2}{x^5}.$$

Find A, B, C to obtain maximal possible order of convergence.

Solution.

Example 6. What is the order of convergence of the fixed point iteration $x_{n+1} = g\left(x_n\right)$ with

$$g(x) = x\frac{x^2 + 3a}{3x^2 + a},$$

for approximating the root of $f\left(x\right) = x^2 - a = 0$?

Solution.

7 Stability of multiple roots

The problem of finding multiple roots of nonlinear equations is inherently unstable (that is why, in particular, Newton's method fails to converge quadratically). To explain this phenomenon in more detail, consider Taylor expansion around a root:

$$f(x_n) = \underbrace{f(\alpha)}_{=0} + e_n f'(\xi_n).$$

Now suppose we compute $\tilde{f}(x_n) = f(x_n) + \Delta f_n$ (for example, in a floating point arithmetic). Even when $\tilde{f}(x_n) = 0$ (so as far as any algorithm is concerned, we have found a root), still

$$|e_n| = \left| \frac{\Delta f_n}{f'(\xi_n)} \right|$$

so when $f'(\xi_n) \approx 0$ we may have large error in the solution.

As a result, a reasonable **stopping criterion** for the various iterative methods is

$$\left| \frac{f(x_n)}{f'(x_n)} \right| \approx \left| \frac{f(x_n)}{\frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}} \right| < \epsilon$$

instead of, say $|f(x_n)| < \epsilon$.

What about multiple roots? If α is a root of multiplicity $p \geq 2$, then proceeding by Taylor expansion as before, we get

$$f(x_n) = \frac{e_n^p}{p!} f^{(p)}(\xi_n) \Longrightarrow |e_n| = \left| \frac{p! \Delta f_n}{f^{(p)}(\xi_n)} \right|^{1/p}.$$

The loss of accuracy may be significant: if $f(x_n)$ is computed with D digits, the accuracy of the root α is only $\lfloor \frac{D}{p} \rfloor$ digits.