Nonlinear Equations

Open Methods

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References

- S. Chapra and R. Canale, Numerical Methods for Engineers
- A. Greenbaum and T. Chartier, Numerical Methods: Design, Analysis, and Computer Implementation of Algorithms
- M. Heath, Scientific Computing: An Introductory Survey
  The interactive educational modules* associated with "nonlinear equations" provide a very nice "feel" for how all the methods considered in class work.

*http://www.cse.illinois.edu/iem/

Contents

Thus far, we have looked at “closed methods” like bisection and regula falsi.

We call them “closed” since the solution is *enclosed or confined* to an interval that keeps shrinking with more iteration

We are now ready to consider “open methods” which abandon the safety of knowing the solution is never lost, for the promise of much faster convergence.

- Fixed Point Iteration
- Newton’s Method
- Secant Method

Introduction

- Bisection and Regula Falsi were bracketing or closed methods
- The solution was always contained within the interval, and convergence was guaranteed
- Open methods start with an initial guess – not an interval – and seek to improve that guess
- Convergence is not guaranteed: frequently, the iterates diverge away from the true solution
- But when the method does converge, it often converges much faster than closed methods

Fixed Point Iteration

- Involves rewriting $f(x) = 0$ as $x = g(x)$
- Examples:

$$\begin{aligned} f(x) = x^2 - 4x + 3 = 0 \quad &\implies x &= \frac{x^2+3}{4} \\ f(x) = \sin(x) = 0 \quad &\implies x &= \sin(x) + x \end{aligned}$$

- Starting with an initial guess x_0, it involves iterating

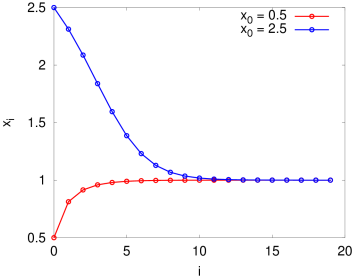
$$x_{i+1} = g(x_i)$$

Example

- Consider solving with initial guess $x_0 = 0.5$, the equation

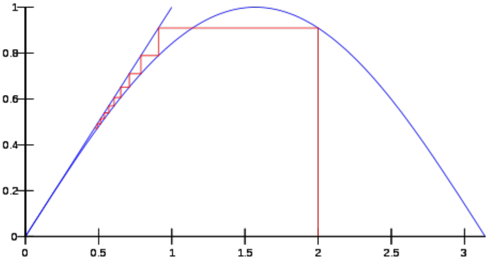
$$x = \frac{x^2 + 3}{4}$$

- The solutions to the original quadratic equation $f(x) = x^2 - 4x + 3 = 0$ are 3 and 1.



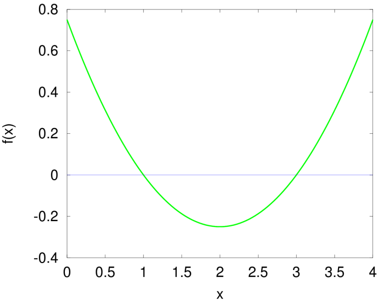
Fixed Point Iteration

- Why does this method work? Graphically,[†]

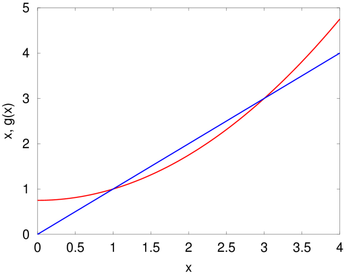


[†]wikipedia.org, solving $x = \sin(x)$

Our Example

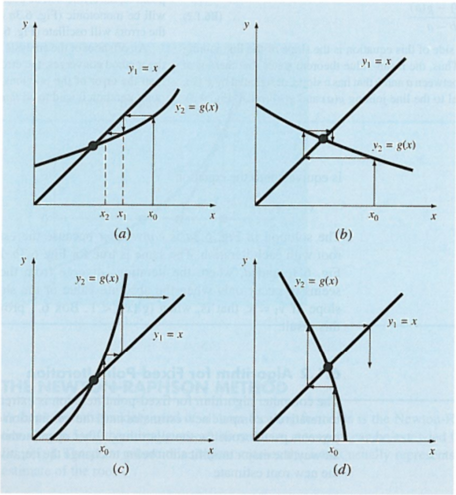


0.8
0.6
0.4
0.2
0
-0.2
-0.4
f(x)
0
0.5
1
1.5
2
2.5
3
3.5
4
x



5
4
3
2
1
0
x, g(x)
0
0.5
1
1.5
2
2.5
3
3.5
4
x

Convergence



‡

‡Chapra and Canale

Convergence

- When it converges, it converges linearly
- It only converges, if $|g'(x)| < 1$ in region of interest.
- Proof: Each iteration is:

$$x_{i+1} = g(x_i) \tag{1}$$

If x^* is the solution, then

$$x^* = g(x^*) \tag{2}$$

Subtracting the two equations:

$$x^* - x_{i+1} = g(x^*) - g(x_i) \tag{3}$$

Proof Continued

- The "derivative" mean-value theorem[§] says that given a function $g(x)$ differentiable over an interval $a \le x \le b$, then there exists $\xi \in [a, b]$, such that

$$g'(\xi) = \frac{g(b) - g(a)}{b - a}$$

- We use this theorem by setting $a = x_i$ and $b = x^*$ to get

$$g(x^*) - g(x_i) = (x^* - x_i)\ g'(\xi), \quad \xi \in [x_i, x^*] \tag{4}$$

- Using this in eqn. 3, we get

$$x^* - x_{i+1} = (x^* - x_i)\ g'(\xi) \tag{5}$$

[§] http://en.wikipedia.org/wiki/Mean_value_theorem

Proof Continued

- If the true absolute error at iteration i is defined as $E_{t,i} = x^* - x_i$, we have

$$E_{t,i+1} = g'(\xi)\ E_{t,i}$$

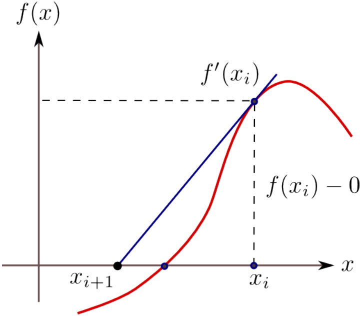
- Thus if $|g'(x)| < 1$ in the interval $[x_0, x^*]$, them the error decays and approaches zero.

Newton-Raphson Method

- Often simply called "Newton's Method"
- Thomas Simpson (of the namesake rule) first described a root-finding algorithm that was both iterative and involved derivatives
- The actual relation we currently call Newton-Raphson method was developed by Joseph Raphson
- There are many such "who-gets-the-credit" discoveries associated with Newton, including calculus (Leibnitz), and inverse square law of gravitation (Hooke).

Newton's Method

- Graphical Idea: Draw tangent at current position and use the intersection with the x-axis as the next iterate



$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}} \implies \boxed{x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}}$$

Example

- Skydiver jumping example

$$f(x) = \frac{a}{\sqrt{x}} \tanh\left(b\sqrt{x}\right) - 10 = 0,$$

  with $a = 26.1916$ and $b = 7.4833$

- The derivative is

$$\frac{df}{dx} = \frac{1}{2}\left(\frac{ab\ \mathrm{sech}^2(b\sqrt{x})}{x} - \frac{a\tanh(b\sqrt{x})}{x^{3/2}}\right)$$

Convergence

- Newton's method doesn't always converge, but when it does, it is extremely fast!

i	x_i	e_a	e_t
0	10.0000		45.77
1	5.8527	70.86	14.68
2	6.7462	13.24	1.66
3	6.8586	1.64	0.02
4	6.8600	0.02	0.00
5	6.8600	0.00	0.00

Convergence: Derivation

- Consider an alternate derivation of Newton's method from Taylor series around x_i

$$f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{f''(\xi)}{2}(x - x_i)^2$$

- If we truncate after the linear term, we get

$$f(x) \approx f(x_i) + f'(x_i)(x - x_i)$$

- We want to find x for which $f(x)$ above is zero, and set that $x = x_{i+1}$ as the next iterate

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i) \tag{6}$$

- This can be solved to obtain Newton's method formula

Convergence: Derivation

- Let x^* be the true root. Expand $f(x^*)$ around x_i

$$f(x^*) = 0 = f(x_i) + f'(x_i)(x^* - x_i) + \frac{f''(\xi)}{2}(x^* - x_i)^2 \quad (7)$$

  where $\xi \in [x_i, x^*]$
- Subtract 6 from 7

$$0 = f'(x_i)(x^* - x_{i+1}) + \frac{f''(\xi)}{2}(x^* - x_i)^2$$

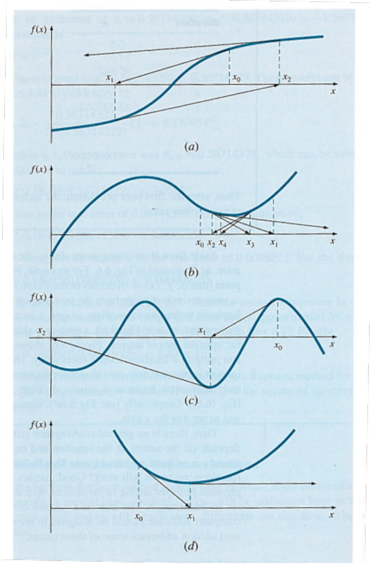
- If $E_{t,i} = x^* - x_i$, then

$$0 = f'(x_i)E_{t,i+1} + \frac{f''(\xi)}{2}E_{t,i}^2$$

Convergence: Derivation

- This implies
$$E_{t,i+1} = -\frac{f''(\xi)}{2f'(x_i)} E_{t,i}^2$$
- Error decays quadratically, once the estimate is close enough to the true solution
- Divergence can be understood in terms of the criteria for fixed point iteration $x_{i+1} = g(x_i)$
- Newton's method is a fixed point iteration with $g(x) = x - f(x)/f'(x)$
- So if $|g'(x)| < 1$ between x_0 and x^* will converge
- However this condition may be hard to check since x^* is not known ahead of time

Convergence: Failures



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¶Chapra and Canale

What if $f^{'}(x^*) = 0$?

- If $f^{'}(x^*) = 0$, it does *not necessarily* mean that Newton's method will fail.
- Consider $f(x) = x^2$, for example, for which $x^* = 0$, but $f'(x) = 2x$ which is also zero at $x^* = 0$.
- In fact for this case, we can easily see what would happen

  $$x_{i+1} = x_i - \frac{x_i^2}{2x_i} = \frac{1}{2}x_i$$

  Regardless of where you start with x_0, you would reduce the error each step by a factor of 2, *instead of squaring the error*.
- Indeed, for multiple roots $f^{'}(x^*) = 0$, and the convergence of Newton's method become linear, instead of quadratic.

Secant Method

- Tries to circumvent the evaluation of the derivative (which may be nontrivial for some complex functions)
- Use the approximation

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

  in Newton's method
- This leads to the following formula for the secant method

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

Secant Method: Example

- On the skydiver example with $x_0 = 12$ and $x_1 = 10$:

i	x_i	e_a	e_t
1	10.0000		45.77
2	5.2401	90.84	23.61
3	7.4123	29.31	8.05
4	6.9594	6.51	1.45
5	6.8540	1.54	0.09
6	6.8601	0.09	0.00
7	6.8600	0.00	0.00

Secant Method

- Not a fixed point method
- Can be modified to estimate the derivative as:

  $$f'(x_i) \approx \frac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i}$$

  instead of using arbitrary points
- Convergence can be shown to be $(1 + \sqrt{5})/2 = 1.618$ (golden ratio)

Open v/s Closed Methods

- Open Methods are usually faster (FP iteration: 1, Secant: 1.62, Newton: 2)
- Closed methods are guaranteed to converge
- Closed methods usually require more work to provide initial interval
- Open Methods can be used to solve for multiple roots $f(x) = (x-1)^2 = 0$, where there is no change of sign near the root