Numerical Methods

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Contents

Preliminaries

Before this course, you need to be familiar with

- Calculus I
- Calculus II: especially Sequences and Series
- Linear Algebra
  1. Vectors, norm, dot product
  2. Linear Independence and Dependence
  3. Span, subspace, bases, dimension of a subspace/vector space
  4. Properties of orthogonal or orthonormal sets/bases; Gram-Schmidt algorithm
  5. Matrix multiplication; Determinant; Inverse
  6. Solving linear equations: algorithm, existence and uniqueness.
  7. Projections; Least square
  8. Eigenvalues and Eigenvectors
  9. SVD

Notations

- $\{x|$ descriptions of $x\}$ is the set of all x that meets the description after the ":" sign. For example, $\{x|x^2-1<0\}$ is the set of all number x such that $x^2-1<0$. We can solve this inequality further and see that $\{x|x^2-1<0\}=(-1,1)$

  Remark: Some books use colon instead of verticle bar as $\{x:$ descriptions of $x\}$

- $\in$: belongs to/is contained in. For example, $a \in \{x|x^2-1<0\}$ means that a is a number satisfying $a^2-1<0$.
- s.t.: such that

Chapter 1

Solving nonlinear equations

If you recall the equations that you are able to solve, you would realize that there are very few. You know how to solve $x^2 - x - 1 = 0$ using the famous quadratic formula, but have you ever wondered formulas for finding roots of polynomials whose degree is higher than 2? Unfortunately, even as simple as a polynomial equation $x^5 - x - 1 = 0$, a math Ph.D feels hopeless to find an exact answer by hand (so you shouldn't feel bad). In fact, there are no formula for polynomials of degree bigger than 4. Equations like $\cos x = x$? does not have a closed form solution either.

When we need to solve nonlinear equations that frequently occur in every aspect of sciences and applications, we use iterative methods.

1.1 Bisection Method

This is a simple, yet efficient method that can be covered in Calculus I as an application of the Intermediate Value Theorem (IVT).

Theorem 1.1 (Intermediate Value Theorem)**.** *If $f(x)$ is continuous on $[a, b]$, then for any m that is in between $f(a)$ and $f(b)$, there exists a number $c \in [a, b]$ such that $f(c) = m$.*

Take $f(x) = x^5 - x - 1$ as an example, whose graph is shown on the left of Figure 1.1. Since $f(1) = -1 < 0$ and $f(1.5) \approx 5.09 > 0$, then by IVT, there is $c \in [1, 1.5]$ such that $f(c) = 0$ and this c is exactly the root that we are looking for.

To have a more precise estimate of c, we evaluate f at the middle point $\dfrac{1 + 1.5}{2} = 1.25$. $f(1.25) \approx 0.8 > 0$. By IVT again, we conclude that the root $c \in [1, 1.25]$. We can keep bisecting the interval and eventually find the root to a sufficient precision. See Figure 1.1.

Note that the key of this Bisection method are:

1. The function needs to be continuous.
2. One needs to be given initial points a, b such that $f(a)f(b) < 0$.

1.2 Newton's Method

Newton's method is a little more sophisticated: it involves derivatives, but it is still Calc I material. This is usually how a calculator or a computer finds a root.

If we are to find the root of $y = f(x)$, we start with a random initial guess x_1. Consider the the tangent line to the curve $y = f(x)$, at $P_0 = (x_0, f(x_0))$. The idea behind Newton's method

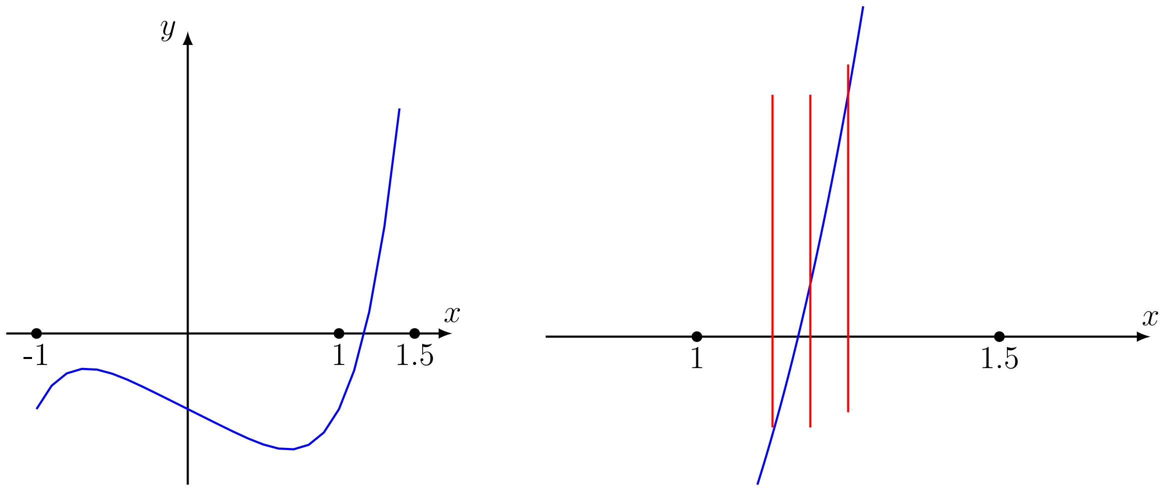

Figure 1.1: Bisection Method

is linearization. Since the tangent line (linearization of f) is close to f, then its x-intercept, x_2, is close to the x-intercept of the curve $y = f(x)$. We can easily find x_2.

The tangent line at the point $(x_0, f(x_0))$ is

$$y - f(x_0) = f'(x_0)(x - x_0).$$

Plugging in $y = 0$ to solve for the x-intercept:

$$0 - f(x_0) = f'(x_0)(x - x_0) \Longrightarrow x = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

So $x_1 = x_0 - \dfrac{f(x_0)}{f'(x_0)}$. We use x_1 as the next approximation and keep repeating this process, as shown in Figure 1.2, where we gain this iteration formula

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, k \geq 0 \tag{1.1}$$

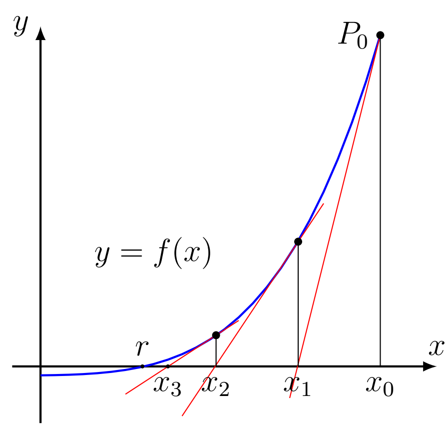

Figure 1.2: Newton's method

Example 1.2. Use Newton's method to approximate $\sqrt{2}$.

Let $f(x) = x^2 - 2$, which makes $\sqrt{2}$ a root of $f(x)$. $f'(x) = 2x$. Let $x_0 = 4$.

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

$x_1 = 2 + 1/4 = 9/4$
$x_2 = 9/8 + 4/9 = 113/72$
...

The two drawbacks of the Newton's method are: (1) It requires the knowledge of the derivative function; (2) It may not converge if you have an unlucky initial guess x_0. For example, if one picks $x_1 = 0$ for finding root of $y = x^5 - x - 1$, the sequence will not converge to the root (try to draw tangent lines on your own). However, we do have convergence if the initial guess is close enough.

Theorem 1.3 ([1, Theorem 4.3.1])**.** *If the second derivative of $f(x)$ is continuous, and x_0 is sufficiently close to a root r of f, then Newton's method converges to r and ultimately the convergence rate is quadratic.*

The next section introduces the secant method which is Newton's method without requiring derivatives.

1.3 Secant Method

The secant method is defined by taking $f'(x_n)$ to be

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

So the iteration formula for the secant method is:

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

1.4 Fixed point methods

x is called a fixed point of $\varphi(x)$ if $\varphi(x) = x$.

Example 1.4. Find fixed point of $\varphi(x) = x^2$.

This is to solve $x = x^2 \Longrightarrow x(x-1) = 0 \Longrightarrow x = 1, 0$

What about finding fixed points of $\varphi(x) = e^{-x}$ since we can't solve $e^{-x} = x$ by hand anymore? A common way is to iterate using the formula

$$x_{k+1} = \varphi(x_k), \qquad k \geq 0$$

which in this example will be $x_0 = 0, x_1 = \varphi(x_0) = 1, x_2 = \varphi(x_1) = e^{-1}, ...$

Finding the fixed point of $\varphi(x)$ is equivalent to finding the root of $\varphi(x) - x$, which means we can always use Newton's method to find a fixed point. Using the same example, we let

$f(x) = e^{-x} - x$, then $f'(x) = -e^{-x} - 1$. So the Newton' iteration is $x_{k+1} = x_k + \dfrac{e^{-x_k} - x_k}{e^{-x_k} + 1}$. Still letting $x_0 = 0$, we have $x_1 = 0 + 1/2 = 1/2$, which is already a better approximation than the fixed point iteration.

Theorem 1.5. *Assume $\varphi \in C^1$ and $|\varphi'(x)| < 1$ in some interval $[r - \delta, r + \delta]$ where r is a fixed point of φ. If $x_0 \in [r - \delta, r + \delta]$ and we use iteration $x_{k+1} = \varphi(x_k)$, then $\lim\limits_{k\to\infty} x_k = r$.*

Proof. See page 95 of [1]. □

Newton's method (**??**) can be considered as a fixed point iteration. To be specific, (**??**) is equivalent to $x_{k+1} = \varphi(x_k)$ with $\varphi(x) = x - \dfrac{f(x)}{f'(x)}$. We can apply Theorem 1.5 to pick a good initial point for Newton's method.

Example 1.6. We are trying to use Newton's method to find the root of $f(x) = x^3 - 1$. The Newton's iteration is $x_{k+1} = \varphi(x_k)$, where $\varphi(x) = x - \dfrac{f(x)}{f'(x)} = x - \dfrac{x^3 - 1}{3x^2} = \dfrac{2}{3}x + \dfrac{1}{3x^2}$. $\varphi'(x) = \dfrac{2}{3} - \dfrac{2}{3}x^{-3}$.

$$|\varphi'(x)| < 1 \Longrightarrow \left|\frac{2}{3} - \frac{2}{3}x^{-3}\right| < 1 \Longrightarrow |\frac{1}{x^3} - 1| < \frac{3}{2} \Longrightarrow -\frac{3}{2} < \frac{1}{x^3} - 1 < \frac{3}{2} \Longrightarrow x^3 > \frac{2}{5} \text{ or } x^3 < -2$$

We can pick x_0 from the interval $(\left(\dfrac{2}{5}\right)^{1/3}, 2 - \left(\dfrac{2}{5}\right)^{1/3})$. Notice that the interval has to be centered around 1.

Remark 1.7. Note that Theorem 1.5 is only a sufficient condition. Even if $|\varphi'(x_0)| < 1$, x_0 can be still a fine initial point. For example, any x_0 can work in Example 1.6.

Chapter 1 Exercises

* means extra credit problems

1 Use Newton's method to approximate $\sqrt{2}$. Let $x_0 = 1$. Compute 2 iterates only.

2 Prove that Newton's method will converge to 0 given any initial value x_0 if we are solving $x^2 = 0$.

3 Write down the first three iterates of the secand method for solving $x^2 - 3 = 0$, starting with $x_0 = 0$ and $x_1 = 1$.

4 We can compute 1/3 by solving $f(x) = 0$ with $f(x) = x^{-1} - 3$.

   (a) Write down the Newton iteration for this problem, and compute by hand the first 2 Newton iterates for approximating 1/3, starting with $x_0 = 0.5$.

   (b) What happens if you start with $x_0 = 1$?

   (c) *In the case of (b), show that the iterates $x_k \to -\infty$ as $k \to \infty$.

(d) Use the theory of fixed point iteration to determine an interval about 1/3 from which Newton's method will converge to 1/3.

5 Let function $\varphi(x) = (x^2 + 4)/5$.

(a) Find the fixed point(s) of $\varphi(x)$.

(b) Would the fixed point iteration, $x_{k+1} = \varphi(x_k)$, converge to a fixed point in the interval $[0, 2]$ for all initial gueses $x_0 \in [0, 2]$?

(c) *Find a function $f(x)$ such that its Newton iterations are $x_{k+1} = \varphi(x_k)$. (Hint: You need to solve a separable differential equation (Calc II material))

6 Compare Bisection method and Newton's method. List their pros and cons. Think of a way to combine Bisection method and Newton's method to overcome the drawbacks of the Newton's method.

Bibliography

[1] Anne, Greenbaum, and Timothy P. Chartier. *Numerical methods: design, analysis, and computer implementation of algorithms*. Princeton University Press, 2012.