Math 104A - Intro to Numerical Analysis

Root finding

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Introduction

Introduction

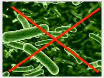
Introduction to Numerical analysis

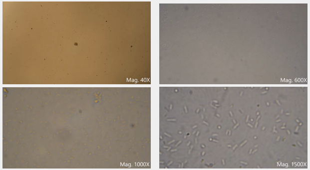
Some analogy and what we will learn

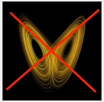
Goal

$$\begin{cases} x_t = y - x, \\ y_t = -xz + \frac{1}{9}x - y, \\ z_t = xy - 2z, \\ x(0) = 1, y(0) = 1, z(0) = 1 \end{cases}$$

Tool







(x(t), y(t), z(t))=(NaN, NaN, NaN)

(x(t), y(t), z(t))=(0,0,0)

(x(t), y(t), z(t))=(0.893,1.26,2.22)

(x(t), y(t), z(t))=(1.2e10,2.5e-7, 5.332)

Interpret

Is it supposed to be this way? How can I tell this is what I am looking for?

Which one is correct? How can I trust the result?

- What tools are available for a specific problem? → Methods (Tool; microscopes)
- How reliable are they? Convergence, order of accuracy, etc. (Tool; knowledge on microscopes)
- What to be careful of? Wisdom, general knowledge, etc. (Interpret)
- Different aspects are waiting: abstract, beautiful, artistic, etc.

Root Finding

Root Finding

Problem of interest

Problem of interest

Find x such that $f(x) = 0$.

In many applications, finding a solution of an equation $f(x) = 0$ is a necessary sub-problem to move on to the next step, or even the main problem.

- $x - \tan(x) = 0$ (diffraction of light)
- $x - a\sin(x) = b$, where a, b take various values (planetary orbits)
- A quintic equation (i.e. polynomial of degree 5) with quite complicated coefficients as a subproblem in a materials science problem.
- And many more.

In many cases, exact solutions are not known, but we can find them approximately.

- No general solution involving only elementary operations to $p(x) = 0$ for $p \in \Pi_n$ ($n \geq 5$): Abel–Ruffini (1824).
- **Notation**: $\Pi_n := \{a_n x^n + \cdots + a_1 x + a_0 \ : \ a_i \in \mathbb{R}, 0 \leq i \leq n\}$, where $n \geq 0$, normally called the set of "polynomials of degree at most n."

Equation and energy (Aside)

- In many applications, the problem can be posed as minimizing an energy (cost or objective etc depending on the context).
- Minimum occurs at critical points, i.e., when the derivative vanishes.
- $E'(x) = 0$ becomes the central problem (i.e., set $f \leftarrow E'$).
- The opposite direction is also useful: model using an equation, find an energy, and minimize it.

Example: If our problem comes from minimizing the energy $E(x) = \frac{1}{2}(2x-4)^2$, we need to solve the equation

$$0 = E'(x) = 4x - 8 =: f(x)$$

Exercise: Can you go backwards from an equation you want to solve?

- Real problems are high dimensional, 1D problems shares some basic intuition.
- **Bottom line**: What we are doing is more than finding root for Cal1 functions.
- **Subjective Question**: Suppose you have observed many time that this works nicely. What would you name it?

Root Finding

Bisection Method

Bisection Method

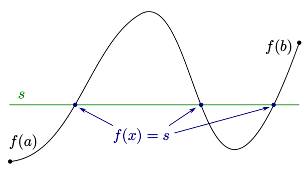
Recall the Intermediate Value Theorem from Calculus.

Theorem

Let $f : [a, b] \to \mathbb{R}$ be a continuous function and let $m = \min_{a \leq t \leq b} f(t)$ and $M = \max_{a \leq t \leq b} f(t)$. If $m \leq s \leq M$, there exist $x \in [a, b]$ such that $f(x) = s$.

Proof.

Resort to intuition.



- A rigorous treatment involves *completeness* of real numbers. If interested, look at typical textbook of "introductory mathematical analysis" or "advanced calculus."

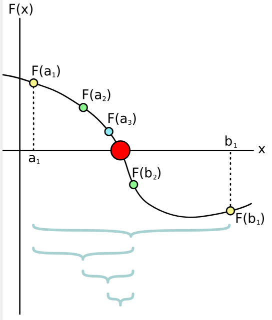
Corollary (Root finding version)

Let $f : [a, b] \to \mathbb{R}$ be a continuous function. If $f(a)f(b) \leq 0$, there exist $\xi \in [a, b]$ such that $f(\xi) = 0$.

Bisection Method

Given a function $f \in C[a, b]$, generate a sequence of intervals $[a_0, b_0] = [a, b], [a_1, b_1], [a_2, b_2], \cdots$ so that $f(a_n)f(b_n) \leq 0$ and one end point of n–th interval is the midpoint of the previous one.

A dynamic example due to El Mostafa Kalmoun, Ioan



- **Notation**: $C[a, b]$ is the collection of all continuous functions defined on $[a, b]$.

Theorem (Convergence and Error)

Suppose the bisection method is applied to a continuous function $f : [a, b] \to \mathbb{R}$ *(*$f(a)f(b) \leq 0$*). Let* $[a_0, b_0] = [a, b], [a_1, b_1], [a_2, b_2], \cdots$ *be the intervals generated by the method and let* $c_n = (a_n + b_n)/2$ *be the midpoint of* $[a_n, b_n]$*. Then* $\lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n = \lim_{n\to\infty} c_n = \xi$*, where* $\xi \in [a, b]$ *satisfies* $f(\xi) = 0$*. Furthermore,*

$$|c_n - \xi| \leq 2^{-(n+1)}(b - a)$$

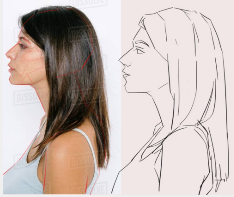
Proof.

Board work. □

Root Finding

Newton's Method

Idea: "sketch" the function → **A dynamic example**



Task: Devise the Newton's method. → Board work

Another derivation: Taylor expansion (works better in high dimensions)

1. Let ξ is a root, i.e., $f(\xi) = 0$.
2. Expand $f(\xi)$ around the current position, say, x_n.
3. Take the linear approximation, namely, ignore the second order term or higher
4. Solve for ξ, but call it x_{n+1}.

1. Pretending to know the answer is the start of all magic.
2. Assume you are close to the root, but not quite. You can only access $f'(x_n)$, but not $f'(\xi)$. So, where would you expand the series?
3. This is the key step. You have traded accuracy for simplicity.
4. This will alter the location of the solution. But that's our best guess.

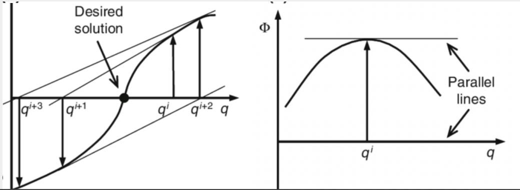
Newton's Method

Good things

- Newton's method finds the root in a few iterations (if it does).
- It motivates many other methods.
- It bears rich interpretations and connections with other concepts.

Bad things

- Newton's method costs a lot computationally. (It is actually slower than many other methods in wall-clock time.)
- It may diverge. A good initial guess is vital.



- Newton's method: Given x_0, $x_{n+1} = x_n - f(x_n)/f'(x_n)$, $(n \geq 0)$.

Newton's Method - Error analysis

Theorem

Suppose f'' is continuous and let ξ be a simple zero of f. If Newton's method is implemented with a starting value x_0 that is sufficiently close to ξ, then, it converges to ξ. Furthermore, there is a neighborhood I of ξ, i.e. $I \ni \xi$, and a constant $C > 0$ such that if $x_0 \in I$, then for all $n \geq 0$ $x_n \in I$ and

$$|x_{n+1} - \xi| \leq C|x_n - \xi|^2$$

Proof.

Board work. □

- This property is called *quadratic convergence*.
- **Terminology**: A neighborhood is always meant to be an open interval.

Theorem (Global convergence for convex functions)

Suppose $f \in C^2(\mathbb{R})$ is increasing and convex, and has a zero. Then, the zero is unique, and the Newton's method converges to it for any starting value.

Proof.

Board work. $\square$

- **Question**: Is this contradictory to possible divergence previously mentioned?
- **Subjective question**: How would you summarize the convergence of Newton's method? If too long, it wouldn't help much. If too short, it may be misleading.

Example (Square root)

Devise an algorithm to find $\sqrt{a}$ ($a > 0$) using Newton's method.
And write a program that implements your algorithm.

Root Finding

Secant Method

Motivation: What if we replace $f'(x_n)$ with something simpler?

Secant Method

Given $x_0, x_1 \in \mathbb{R}$, compute

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

- The big fraction is an approximation of $1/f'(x_n)$
- (Aside) Counterpart of the secant method in a higher dimensional setting is called *quasi-Newton* method, where the derivative is replaced by its approximations.
- Users must feed two initial guesses.

Error of Secant Method

(Assuming there is no technical difficulties) The convergence of the secant method is *superlinear*. More specifically,

$$|x_{n+1} - \xi| \sim C|x_n - \xi|^{\phi_0}, \tag{1}$$

where $\phi_0 = (1 + \sqrt{5})/2$ is the golden ratio and $C > 0$.

Proof.

Board work. $\square$

Exercise

Argue that the secant method is superior than Newton's method.
Hint: Take into account the c____!

- (Notation) Here, (1) means $e_{n+1}/(Ce_n^{\phi_0}) \to 1$ as $n \to \infty$, where $e_n := |x_n - \xi|$.
- Does this exercise even make sense?

Root Finding

Fixed Points and Functional Iterations

Fixed Points and Functional Iterations

Goal of the section: Develop a general framework to which many root finding methods belong.

Fixed point/Functional/Picard iterations

Given $F : \mathcal{D} \to \mathcal{D}$ ($\mathcal{D}$ is some suitable domain), choose x_0, and compute

$$x_{n+1} = F(x_n).$$

Quick Question: Does the Newton's method fit this framework?

Definition (Fixed point)

$x \in \mathcal{D}$ is called a *fixed point* of the function $F : \mathcal{D} \to \mathcal{D}$ if $F(x) = x$.

Definition (Contraction/Contractive mapping)

A function $F : \mathcal{D} \to \mathcal{D}$ is called *contractive* or a *contractive mapping/contraction* if there is $\lambda \in [0, 1)$ such that $|F(x) - F(y)| \leq \lambda |x - y|$.

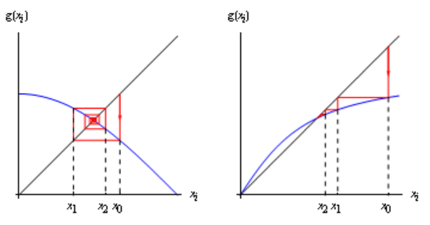
Theorem (Contraction Mapping Theorem)

Let $\mathcal{D}$ be a closed subset of $\mathbb{R}$. If $F : \mathcal{D} \to \mathcal{D}$ is a contraction, then it has a unique fixed point. Moreover, this fixed point is the limit of the functional iteration starting with any initial guess.

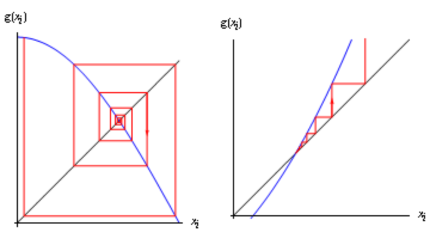
Proof) Board work.

- λ must be strictly less than 1. If $\lambda = 1$ is allowed, the next theorem is not true. **Exercise**: come up with such an example (cubic connecting (-1,1), (0,0), (1,-1); start with integrating $x^2 - 1$)
- The contraction mapping theorem is a powerful tool since F can be highly non-linear as long as the function is contractive.

Illustration of Picard iterations.



(A) Convergent case



- The slope near the point of intersection determines the behavior. If the slope<1, the function is contractive on some closed interval. Otherwise, it may be impossible to fit it into the theorem.