18.335 / 6.7310 Introduction to Numerical Methods

Course Overview

- handouts, syllabus, psets, etc.
  - Canvas + Piazza + Gradescope
  - github.com/mitmath/18335

- Optional Julia tutorial this Friday (Feb. 7) 4-5:30 pm @ 2-190
- Parallel courses this semester (by Prof. Johnson)
  : 18.S190 Interdisciplinary Numerical Methods

Numerical analysis:

Fast algorithms for approximately solving the problem of "continuous math" } math + time + accuracy

Example: nonlinear equations

$f: \mathbb{R} \to \mathbb{R}$, f is continuous

Find $f(x) = 0$

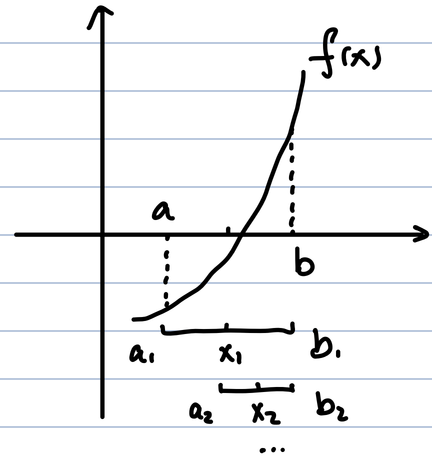
- f is a general polynomial of degree ≥ 5:

  no root formula using $+, -, \times, \div, \sqrt[n]{\ }$

- Goal: approximately find the root using only $+, -, \times, \div$

- Naive method: Bisection method

$f(a)f(b) < 0 \Rightarrow \exists$ root $x^* \in [a, b]$



$$x_n = \frac{a_n + b_n}{2}$$

if $\text{sign}(f(x_n)) = \text{sign}(f(a_n))$

$a_{n+1} = x_n$, $b_{n+1} = b_n$

otherwise $a_{n+1} = a_n$, $b_{n+1} = x_n$

Error analysis :

$$e_n := |x_n - x^*| \le \frac{1}{2}(b_n - a_n) = \frac{b-a}{2^n} \longrightarrow 0 \quad \text{as} \quad n \to +\infty$$

$$e_{n+1} \approx \frac{1}{2} e_n \qquad \text{Linear convergence}$$

Can we do it faster ? (Have only access to $f(x)$)

Yes. One possible method:

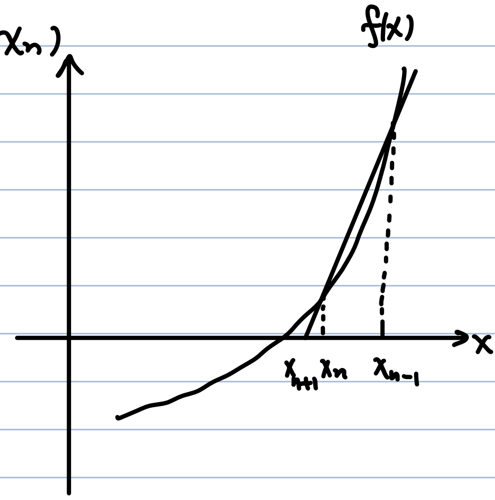
- Secant method

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

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

$$= 0$$

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



Error analysis:

$e_{n+1} := x_{n+1} - x^*$

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

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

$$= \underbrace{\frac{f(x_n) e_n^{-1} - f(x_{n-1}) e_{n-1}^{-1}}{f(x_n) - f(x_{n-1})}}_{\text{claim : } C_n \approx C} e_n e_{n-1}$$

check : $f(x_n) \approx f'(x^*) e_n + \frac{1}{2} f''(x^*) e_n^2$

$f(x_{n-1}) \approx f'(x^*) e_{n-1} + \frac{1}{2} f''(x^*) e_{n-1}^2$

$$C_n = \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \cdot \boxed{\frac{f(x_n) e_n^{-1} - f(x_{n-1}) e_{n-1}^{-1}}{x_n - x_{n-1}}}$$

$$\approx \frac{1}{2} f''(x^*) \underbrace{\frac{e_n - e_{n-1}}{x_n - x_{n-1}}}_{= 1}$$

(Since $x_n - x_{n-1}$
$= (x_n - x^*) - (x_{n-1} - x^*)$)

$$\approx \frac{1}{f'(x^*)} \cdot \frac{1}{2} f''(x^*) =: C$$

We arrive at

$$e_{n+1} = C e_n e_{n-1}$$

Let $e_{n+1} \approx A e_n^p \quad (p > 1)$

$$A e_n^p \approx c\, e_n \left(\frac{e_n}{A}\right)^{1/p} = \frac{c}{A^{1/p}} e_n^{1+\frac{1}{p}}$$

$$\Rightarrow A^{1+1/p} = c\, e_n^{1+1/p-p}$$

Since $e_n \to 0$ as $n \to +\infty$,

we should have $1 + \frac{1}{p} - p = 0 \Rightarrow p = \frac{1+\sqrt{5}}{2} \approx 1.618$

That is $e_{n+1} \approx c^{0.618} e_n^{1.618}$ faster than bisection

super linear convergence $\square$

most fundamental part

<u>numerical analysis</u>
- nonlinear equations
- data interpolation/approximation
- numerical integration/differentiation
- solution of ODE's/PDE's
- etc. (18.S190 + 18.S191/18.S097/18.S192)

<u>numerical linear algebra</u> (NLA)

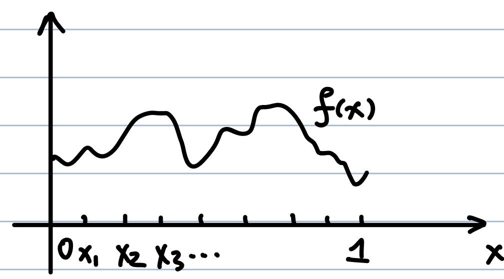
Example: Numerical methods for PDEs

a) Poisson equations

$$\begin{cases} \Delta u := \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = f \\ u|_{\partial\Omega} = 0 \end{cases}$$

In 1D, $\dfrac{d^2 u}{dx^2} = f$

$u(0) = u(-1) = 0$



Discretization:

$u(x_i) \approx u_i$

$f(x_i) \approx f_i$

$h = x_{i+1} - x_i$

$$\frac{d^2 u}{dx^2}(x_i) \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

$$\Longrightarrow \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & & \ddots & & \\ & & & & 1 \\ & & & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}$$

Solve large linear system

$$Au = f$$

b) Schrödinger Equation

$$-\Delta u + Vu = Eu$$

u: wave function

V: potential

E: Quantized energy (eigenvalues)

• Discretization :

$$\frac{1}{h^2}\begin{bmatrix} 2+V_1h^2 & -1 & & \\ -1 & 2+V_2h^2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2+V_nh^2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} = E\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}$$

$$Au = Eu$$

Solve large eigenvalue problems

Outline

$\boxed{\text{fundamentals of numerical analysis}}$

NLA

Given $A \in \mathbb{R}^{n\times m}$, $b \in \mathbb{R}^n$	Given $A \in \mathbb{R}^{n\times n}$
Solve $Ax = b$	Find all (λ, x) s.t. $Ax = \lambda x$

$\boxed{\text{Krylov subspace methods}}$

Other topics :
- Nonlinear optimization
- Numerical integration
- FFT etc