

Lecture Notes 2/4 - Hands-on Coding

In the coming weeks we'll consider two problem flavours

$$\textcircled{\text{IVP}} \quad \frac{u_j^{n+1} - u_j^n}{K} = D_+ D_- u|_j + N[u]|_j$$

$$\textcircled{\text{BVP}} \quad D_+ D_- u|_j + N[u]|_j = 0$$

- Depending on RHS for $\textcircled{\text{IVP}}$ being implicit/explicit will req. nonlinear solve
- So far we've only studied linear problems

Today's Exercise

- ① Learn to reliably solve non-linear systems of eqns
- ② Learn to solve for a linear stencil

In ~ 1 week we'll put it all together

Newton's Method -

- Find $f(x^*) = 0$

- Taylor expand around guess x^n

$$f(x^n) + f'(x^n)(x - x^n) = 0$$

- solve for $x \rightarrow x^{n+1}$

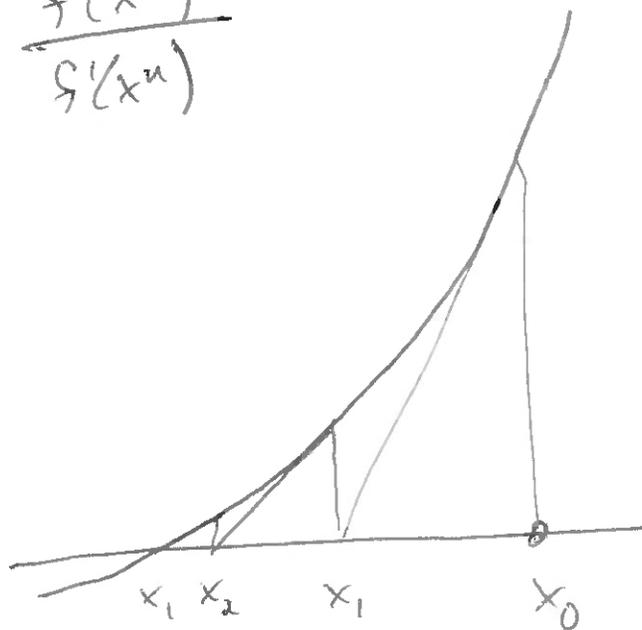
$$x^{n+1} = x^n - \frac{f(x^n)}{f'(x^n)}$$

(quadratic conv.)

Thm Let x^* solve f .

There exists $\delta > 0$ such that for $|x_0 - x^*| < \delta$

$$|x_{k+1} - x^*| \leq C |x_k - x^*|^2$$



Pf Let $e_k = x_k - x^*$

For $\xi_k \in [x_k, x^*]$

Expand at x^* →

$$f(x_k) = \underbrace{f(x^*)}_{=0} + f'(x^*)e_k + \frac{1}{2} f''(\xi_k) e_k^2$$

similarly $f'(x_k) = f'(x^*) + \frac{1}{2} f''(\xi_k) e_k$ for $\forall_k \in [x_k, x^*]$

Write Newton step minus x^*

$$\underbrace{x_{k+1} - x^*}_{e_{k+1}} = \underbrace{x_k - x^*}_{e_k} - \frac{f(x_k)}{f'(x_k)}$$

Substitute in Taylor series & simplify (that we did)

$$e_{k+1} = e_k \left(1 - \frac{1 + \frac{1}{2} \frac{f''(\xi_k)}{f'(x^*)} e_k^2}{1 + \frac{f''(\xi_k)}{f'(x^*)} e_k} \right)$$

For small $|e_k|$ $(1+x)^{-1} \approx 1-x + o(x^2)$

$$e_{k+1} = e_k \left(\frac{1}{2} \frac{f''(\xi_k)}{f'(x^*)} e_k + o(e_k^2) \right)$$

$|e_0| < \delta$ justifies

$$e_{k+1} = \underbrace{\frac{1}{2} \frac{f''(\xi_k)}{f'(x^*)}}_{\leq C} e_k^2 + \text{HOT}$$

Multivariate Case

$$\Delta_n = -J^{-1}(x^n) F(x^n)$$

$$x^{n+1} = x^n + \Delta_n$$

Back tracking

Newton requires $e_0 < \xi$ (good init guess)

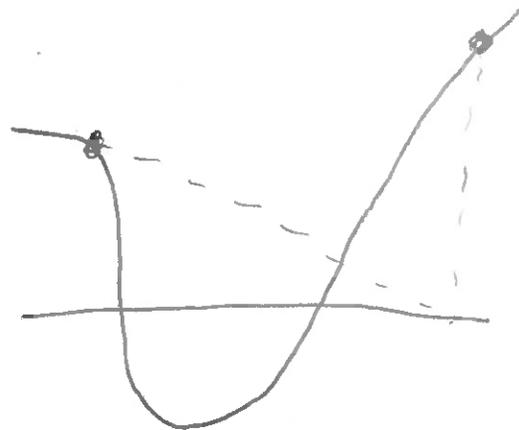
Error can get worse!

$$x^{n+1} = x^n + \alpha^n \Delta^n$$

\uparrow relaxation

$$\alpha \in [0, 1]$$

$\alpha \downarrow 0 \rightarrow$ gradient descent



How to pick α ? Armijo's Rule

Define $\phi(x)$ s.t. $\phi(x) = 0 \Rightarrow F(x) = 0$

(e.g. $\phi(x) = \frac{1}{2} \|F(x)\|^2$)

Armijo Pick maximum $\alpha_k \in [0, 1]$ s.t.

$$\phi(x_k + \alpha_k \Delta_k) \leq \phi(x_k) + c_1 \alpha_k \nabla \phi(x_k)^T \Delta_k$$

\uparrow typically 10^{-4}

Thm For cont. F , + differentiable $\phi(x_{k+1}) < \phi(x_k)$ if $\Delta \neq 0$

Pf Consider WLOG $\phi = \frac{1}{2} \|F\|^2$

$$\nabla \phi = J(x_k)^T F(x_k)$$

$$\begin{aligned} \nabla \phi(x_k)^T \Delta_k &= - (J(x_k)^T F(x_k))^T (J(x_k)^{-1} F(x_k)) \\ &= - \|F(x_k)\|^2 \end{aligned}$$

If J invertible

Taylor expansion

$$\phi(x_k + \alpha_k \Delta_k) = \phi(x_k) + \underbrace{\alpha_k \nabla \phi(x_k)^T \Delta_k}_{\text{showed this is negative}} + o(\alpha_k^2)$$

showed this is negative

$$\leq \phi(x_k) + c_1 \alpha_k \nabla \phi(x_k)^T \Delta_k$$

↑ for any $c_1 < 1$ □

Punchline

For small enough α , relaxation guaranteed to improve error

$\alpha_{k=0}^0 = 1$, $\alpha_k^{i+1} = \epsilon \alpha_k^i$ until ϕ decreases