

Lecture Notes 2/4 - Hands-on Coding

In the coming weeks we'll consider two problem flavors

(I) IVP

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D_+ D_- u_j + N[u] \Big|_j$$

(II) BVP

$$D_+ D_- u_j + N[u] \Big|_j = 0$$

- Depending on RHS for 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 $x \rightarrow x^{n+1}$

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

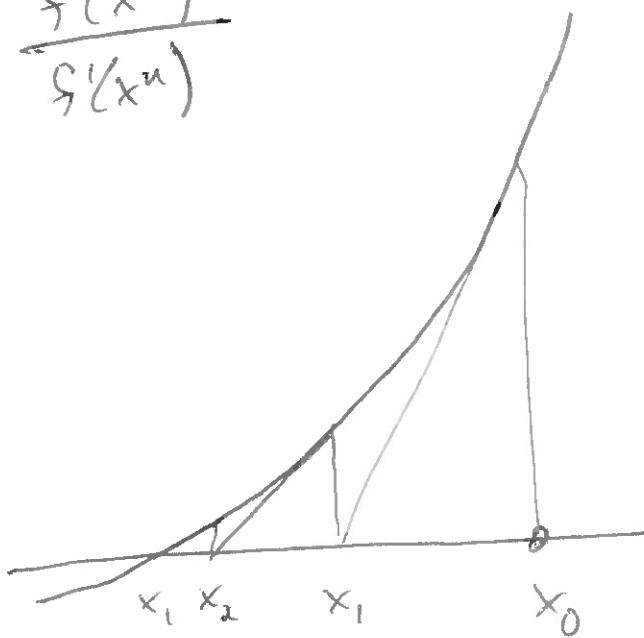
(quadratic conv.)

Then 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^* \rightarrow

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

similarly $f'(x_k) = f'(x^*) + f''(\xi_k) e_k$ for $\xi_k \in [x_k, x^*]$

Write Newton step move x^*

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

Substitute in Taylor series + simplify (that we do)

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

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

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

$|e_0| < \delta$ justifies

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

Multivariate Case

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

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

Backtracking

Newton requires $\epsilon_0 < \gamma$ (good init guess)

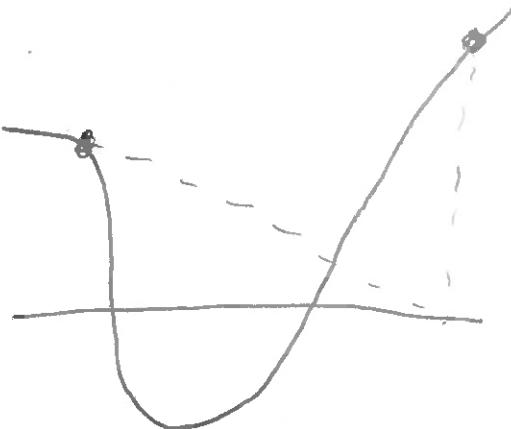
Error can get worse!

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

\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 $\alpha \in [0,1]$ 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
if $\Delta \neq 0$

$$\phi(x_{k+1}) < \phi(x_k)$$

Pf Consider wlog $\phi = \frac{1}{2} \|F\|_2^2$

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

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

Taylor expansion

If J invertible

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

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

↑ for any $c_1 < 1$

◻

Conclusion

For small enough α , relaxation guaranteed to
improve error

$\alpha_k^0 = 1$, $\alpha_k^{i+1} = \varepsilon \alpha_k^i$ until ϕ decreases