Today: End of FDM
Onward to FEM

1/12

Before switching to FEM + Graphs in remainder of class, lets pause to discuss what we can and can't do w/ FDs for ML

1. Prove stability, energy cons, mom cons
2. Use Lax equiv theorem + polynomial reproduction to guarantee convergence
3. Integrate Hamiltonian systems w/ discrete energy cons. or use RK3+ to get stable, convergent solns
4. Pose physics learning as a nonlinear perturbation of "nice" problem

In engineering "V+V" is bedrock of trust in sim.

verification - is code correctly implemented, using unit test to verify reproduction of the claims theory provides (math ⇔ good code)

validation - is code predictive of experimental data (good code ⇔ good model)

> Note
> Sci. eng. term w/ specific meaning in scientific computing

We are not able to

1. Handle complex geometries, non-periodic BC, refine our approx, etc. $\Longrightarrow$ FEM

Some FEM history (Get some perspective away from ML hype!)

1915 - Boris Galerkin developed FEM to make subs

1909 - Walter Ritz establishes Rayleigh-Ritz for variational mechanics

No adoption in industry

30's - Courant solves PDEs ~~to solve~~ using piecewise polynomial functions, early theory in 40s

60's - Mathematical formalism

Called FEM by Clough in 1960

Shift from "spring-mass elements" to what we will learn today

80's - computers catch up, early Abacus

ML History

1957 First MLP (Rumelhart, Hinton, Williams)

00's Deep networks

10's ML Libraries

20's Transformers + Scaling

First "PINN" paper (Lagaris 1998)

1D FEM

Consider the poisson problem w/ Dirichlet BC

$$(P) \begin{cases} -u'' = f \\ u(0) = u(1) = 0 \end{cases}$$

ex sol $f = 1$

$$u(x) = \frac{x(x-1)}{2}$$

- Finite differences assume too much regularity in solution $\rightarrow u \in C^2([0,1])$

- Weak form poses the problem w/out requiring regularity

Note weak $\neq$ bad or not strong
actually a more general class of solutions

"Galerkin cookbook"

"error measurement"

① Take an arbitrary function v w/ $v(0) = v(1) = 0$

② Multiply (P) and integrate

$$-\int_0^1 u'' v \, dx = \int_0^1 f v \, dx$$

③ Integrate by parts until we get the least restrictive derivatives on u and v possible

$$\int_0^1 u'v' dx - \cancel{\left(u'(1)v(1) - u'(0)v(0)\right)} = \int_0^1 f v \, dx$$

By Dirichlet BC

This defines the Galerkin - form of (P)

Choose a function space V

(G) Find $u \in V$ such that for any $v \in V$

$$\int_0^1 u'v'\,dx = \int_0^1 f v\,dx$$

<u>Remarks</u> - there is a <u>symmetry</u> similar to what we've seen w/ D_h, D_h^* in the FDM

- how do we choose the space of functions V?

If (G) holds for <u>any</u> v, pick $v = u$

(E-G) $\int_0^1 u'^2 = \int_0^1 f u$ Needs to be <u>well-defined</u>

Define some useful common function spaces

$$L^2([0,1]) = \left\{ f,\ \int_0^1 f^2\,dx < \infty \right\}$$

$$H^1([0,1]) = \left\{ f \in L^2,\ f' \in L^2 \right\}$$

$$H_0^1([0,1]) = \left\{ f \in H^1,\ f(0) = f(1) = 0 \right\}$$

LHS of (EG) finite if $u \in H^1$

RHS $\left|\int f u\right|^2 \leq \int |fu|^2 \leq |f|^2 |u|^2 < \infty$ if $f \in L^2$, $u \in L^2$

$H_0^1 \Rightarrow$ Don't worry about the boundary terms during IBP

$\Rightarrow \boxed{V = H_0^1}$ But different for other PDEs

What makes FEM "finite"?

Choose $V_h \subseteq V$, $\dim(V_h) = N$

(aka pick a basis w/ N shape functions)

$$u \in V_h \Rightarrow u(x) = \sum_i \hat{u}_i \, \phi_i(x)$$

basis coeffs — basis

Many choices

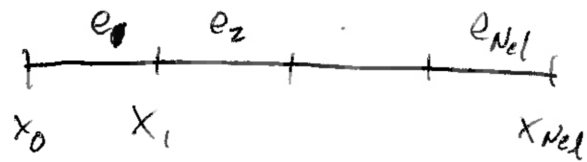
ϕ_i	
discontinuous piecewise constant	Finite Volume
piecewise polynomial	Discontinuous Galerkin
Continuous polynomial	(Bubnov) Galerkin
Trig/orthogonal polynomial	Spectral Element
Gaussians	Meshfree

⋮

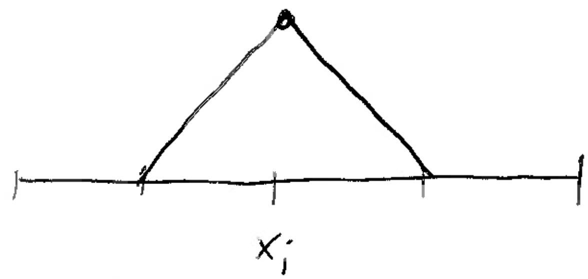
Take $V_h = \{\text{piecewise linear functions}\}$

$$X_h = \{ih, \ i = 0, 1, \dots N_{el}\}$$

$$e_{i+1} = [ih, (i+1)h]$$



Let
$$\phi_i = \begin{cases} \dfrac{x - x_{i-1}}{x_i - x_{i-1}} & x \in e_i \\ 1 - \dfrac{x - x_i}{x_{i+1} - x_i} & x \in e_{i+1} \\ 0 & \text{else} \end{cases}$$



Rewrite (G) Find $u \in V_h$ such that ~~for~~ any $v \in V_h$

$$\Rightarrow \quad \int_0^1 u'v'\,dx = \int_0^1 fv\,dx$$

As $\Rightarrow$ Find $\hat{u} \in \mathbb{R}^{N_{el}}$ s.t. $\forall$ $\hat{v} \in \mathbb{R}^{N_{el}}$

$$\sum_{i,j} \hat{v}_i \int_0^1 \phi_i' \phi_j'\,dx\ \hat{u}_j = \sum_i \hat{v}_i \int_0^1 \phi_i f\,dx$$

Group
$$\sum_i \hat{v}_i \left[\underbrace{\int_0^1 \phi_i' \phi_j'\,dx}_{S_{ij}}\ \hat{u}_j - \int_0^1 \phi_i f\,dx \right] = 0$$

True if $\rightarrow$ $S\hat{u} = b, \quad b_i = \int_0^1 \phi_i f\,dx$

<u>Thm</u> FEM discretization of $\textcircled{G}$ is unique

<u>Pf</u> - Let u_1, u_2 solve G

- $$\int_0^1 u_1' v' dx = \int_0^1 f v \, dx$$ for any $v \in V_h$
$$\int_0^1 u_2' v' dx = \int_0^1 f v \, dx$$

$$\int_0^1 (u_1 - u_2)' v' dx = 0$$

Pick $v = u_1 - u_2$

$$\int_0^1 \left[(u_1 - u_2)'\right]^2 = 0$$

$\Rightarrow$ $(u_1 - u_2)' = 0$ pointwise

$u_1 - u_2 = \text{constant}$

if $V_h \subseteq H_0^1$, $u_1 - u_2 = 0$ on boundary

$\Rightarrow$ $u_1 - u_2 = 0$ everywhere

<u>Thm</u> S is sym. pos. def.

<u>Pf</u> $$\hat{y}^T S \hat{y} = \sum_{i,j} \hat{y}_i \int \phi_i' \phi_j' \, dx \, \hat{y}_j$$
$$= \int y'^2 dx \geq 0$$, w/ equality only if $y = 0$

So we can solve the matrix problem, but how to construct it?

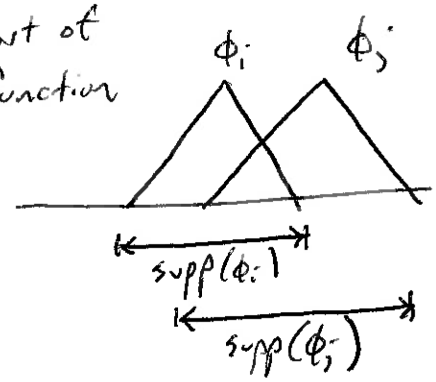
$$S_{ij} = \int_0^1 \phi_i' \phi_j' \, dx$$

- only non-zero if $\text{supp}(\phi_i) \cap \text{supp}(\phi_j) \neq \emptyset$

  ↑ support of function

- most of S_{ij} are 0

  "sparse"



Quadrature (aka how to integrate)

def A quad. rule is a set of N_q

w_i – quad weights

x_i – quad points

such that

$$\int_{-1}^{1} f(x)\,dx = \sum_{i=1}^{N_q} f(x_i)\, w_i$$

That is exact for some class of functions

Catch details on wikipedia

Gauss – Legendre QR

Exact for polynomial f of degree $2(N_q - 1)$

- x_i are zeros of Legendre polynomials
- $w_i = \dfrac{2}{(1-x_i^2)\,[P_n'(x_i)]^2}$

N_q	x_i	w_i
1	0	2
2	$\pm\sqrt{3}$	1
3	$0, \pm\sqrt{3/5}$	$8/9, 5/9, 5/9$

Change of variables

To map domain of integration from $[-1, 1]$ to $[a, b]$

u-substitution $\quad u = 2\left(\dfrac{x-a}{b-a}\right) - 1$

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{a+b}{2}\right)\frac{b-a}{2}\,dx$$

$$= \frac{b-a}{2}\sum_{i=1}^{n} w_i\, f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

Connection between energy minimization & Galerkin

(From Klaes Johnston)

Consider the functional

$$F(v) = \frac{1}{2}(v', v') - (f, v)$$

Define Ritz method (R)

$$\min_{v \in V_h} F(v)$$

To solve, use our old friend the functional derivative

$$(\delta_v F(v), \delta v) = \lim \frac{1}{\varepsilon}\Big(F(v + \varepsilon \delta v) - F(v)\Big)$$

$$= \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon}\Big[\frac{1}{2}(v' + \varepsilon \delta v', v' + \varepsilon \delta v') - \frac{1}{2}(v', v') - (f, v + \varepsilon \delta v) + (f, v)\Big]$$

$$= \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon}\Big[\varepsilon(v', \delta v') + \frac{\varepsilon^2}{2}(\delta v', \delta v') - \varepsilon(f, \delta v)\Big]$$

$$= (v', \delta v') - (f, \delta v)$$

For any $\delta v \in V$ which is Galerkin!

Remark Not all PDEs can be written as an energy min.

What's special about Galerkin – optimal error

If the exact soln is $u \in V$, FEM $u_h \in V_h$

$$(u', v') = (f, v)$$
$$(u_h', v') = (f, v)$$
$$(u' - u_h', v') = 0$$

← Galerkin Orthogonality

Thm For any $v \in V_h$

$$\|(u - u_h)'\| \leq \|(u - v)'\|$$

← soln is best possible in your space of functions

Pf Let $v \in V_h$ and $w = u_h - v \in V_h$

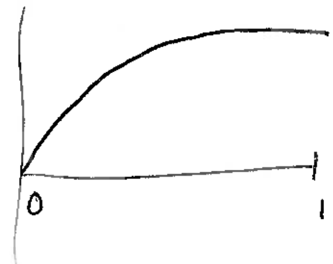
$$\|(u - u_h)'\|^2 = ((u - u_h)', (u - u_h)')$$
$$= ((u - u_h)', (u - u_h)') + ((u - u_h)', w')$$

← galerkin orthogonality

$$= ((u - u_h)', (u - u_h + w)')$$
$$= ((u - u_h)', (u - v)')$$
$$\leq \|(u - u_h)'\| \, \|(u - v)'\|$$

Handling Neumann BCs

$$u'' = 1$$
$$u(0) = 0$$
$$u'(1) = 0$$



Soln $u(x) = x\left(1 - \frac{x}{2}\right)$

Returning to original form of PDE

$$-\int u'' v \, dx = \int f v \, dx$$

$$\int u' v' \, dx - \big(u'(1) v(1) - u'(0) v(0) \big) = \int f v \, dx$$

If $u'(1) = g$, substitute it in