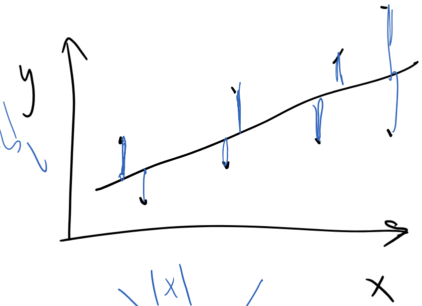
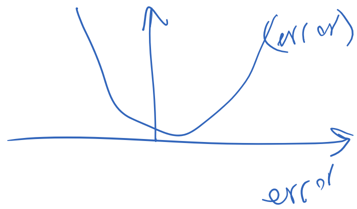
2022/10/04

Tuesday, October 4, 2022 11:21 AM

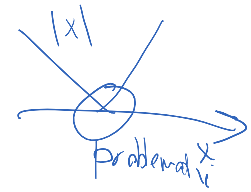
Least Square (LS) method

Least square concept is used in many different settings, for example in (linear) regression.





$(\text{error})^2 \geq 0$ & differentiable



$R_i(x) = u_h'' + q(x)$

$R_f = \bar{F} - F = 1 - u'(2)$

$$R^2 = \int_0^2 (R_i(x))^2 dx + (R_f)^2 \quad ①$$

(a) $x=2$

R2 is zero for the exact solution, but in discrete form, we want to find the solution that minimizes R2 (R2 may be > 0)

Let's find R2 for the problem with 2 unknowns:

$$u^h = \phi_p(x) + a_1\phi_1(x) + a_2\phi_2(x) = 1 + a_1 x + a_2 x^2 \qquad \phi_p = 1 \quad \phi = \{x, x^2\}$$

$$R_i = u'' + q(x) = 2a_2 + q(x) \quad ②$$

$$R_f = 1 - u'|_{x=2} = 1 - a_1 - 2a_2 x|_{x=2} = 1 - (a_1 + 4a_2) \quad ③$$

Plug ② & ③ in ①

$$R^2 = \int_0^2 R_i^2(x)\,dx + R_f^2 = \int_0^1 (2a_2 + \underbrace{(2-2x)}_{q(x)\text{ for }0<x<1})^2 dx + \int_1^2 (2a_2)^2 dx + (1 - (a_1 + 4a_2))^2$$

here $q(x)=0$

$$\boxed{R^2(a_1, a_2) = 1 + a_1^2 + 20a_2 - 2a_1 - 8a_2 + 8a_1 a_2}$$

want to minimize R^2

$$\nabla R^2 = 0$$

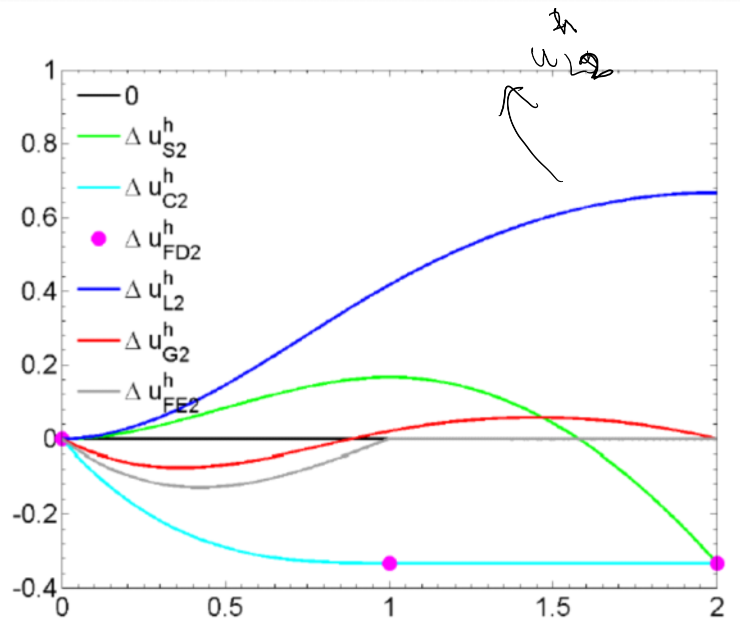
$$\begin{bmatrix} 2a_1 + 8a_2 - 2 \\ 8a_1 + 4a_2 - 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} 2 & 8 \\ \cdot & \cdot \end{bmatrix} \begin{bmatrix} a_1 \\ \cdot \end{bmatrix} = \begin{bmatrix} 2 \\ \cdot \end{bmatrix}$$

$$\begin{bmatrix} 2a_1 + 8a_2 - 2 \\ 8a_1 + 4a_2 - 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \rightarrow \underbrace{\begin{bmatrix} 2 & 8 \\ 8 & 4 \end{bmatrix}}_{K} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \underbrace{\begin{bmatrix} 2 \\ 4 \end{bmatrix}}_{F}$$

$$\rightarrow a = \begin{bmatrix} 2 \\ -\frac{1}{4} \end{bmatrix} \qquad \boxed{u^h_{L2} = 1 + 2x - \frac{1}{4}x^2}$$

We first discretized (-> a1, a2) then minimized (grad R2 = 0)

Bar example, $n = 2$, Comparison of solutions



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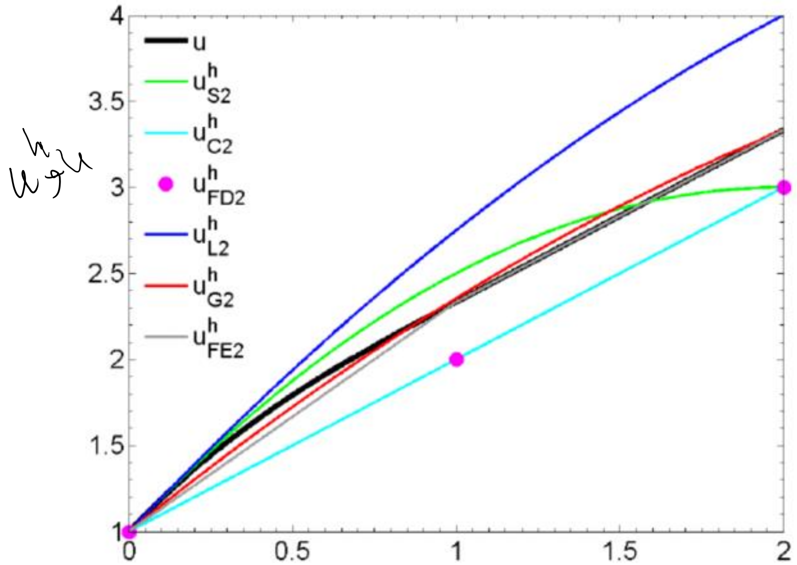

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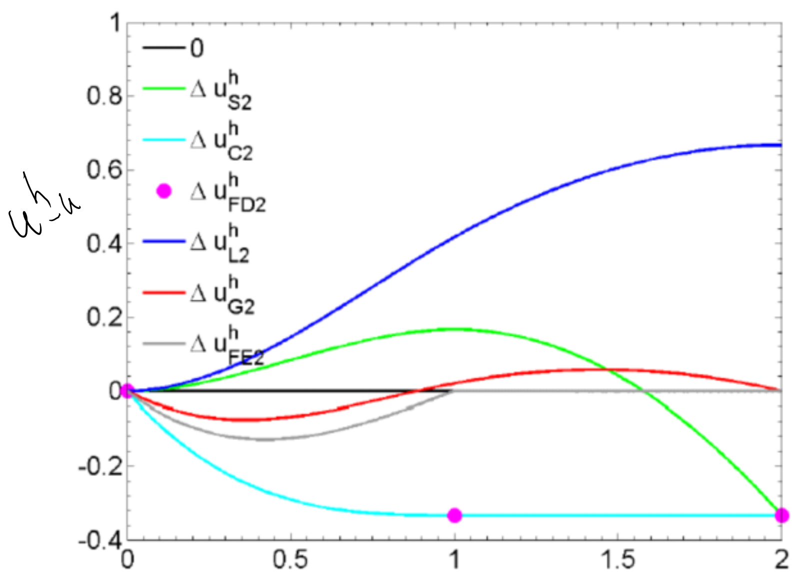


More modular & faster way to have K & F for LS method

inside DE: $R_i = L_M(u) - r$

source term

natural B: $R_f = \bar{F} - L_f(u)$

$$R^2 = \int R_i^2\, dV + \int R_f^2\, ds + \cancel{\int R_u^2\, ds}$$

$$R^2 = \int_{\Omega} R_i^2\, dV + \int_{\partial\Omega_f} R_f^2\, ds + \cancel{\int_{\partial\Omega_u} R_u^2\, ds}$$

$R_u = \bar{u} - u$

we strongly satisfy this

$$u^h = \phi_p + \sum_{i=1}^{n} a_i \phi_i$$

n unknowns $a_1, \dots, a_n$

$$R^2(a_1, \dots, a_n) = \int_{\Omega} R_i^2(a_1, \dots, a_n)\, dV + \int_{\partial\Omega_f} R_f^2(a_1, \dots, a_n)\, ds$$

inside (not an index)

minimize R^2

$$\nabla_a R^2 = 0$$

$$\frac{\partial R^2}{\partial a_j} = 0 \quad \forall j = 1, \dots, n$$

$$\int_{\Omega} \frac{\partial R_i^2}{\partial a_j}\, dV + \int_{\partial\Omega_f} \frac{\partial R_f^2}{\partial a_j}\, ds = 0 \quad (\star)$$

$$\frac{\partial R_i^2}{\partial a_j} = 2 R_i \frac{\partial R_i}{\partial a_j} \qquad \frac{\partial R_f^2}{\partial a_j} = 2 R_f \frac{\partial R_f}{\partial a_j}$$

we'll calculate these

$$R_i(a) = L_M(u^h) - r$$

linear Differential eqn

$$u^h = \phi_p + \sum_{k=1}^{n} a_k \phi_k(x)$$

$$R_i = L_M\left(\phi_p + \sum_{k=1}^{n} a_k \phi_k\right) - r = L_M(\phi_p) + \sum_{k=1}^{n} a_k L_M(\phi_k) - r$$

Dealing with a linear problem

$$R_i(a_1, \dots, a_n) = L_M(\phi_p) - r + a_1 L_M(\phi_1) + a_2 L_M(\phi_2) + \dots + a_n L_M(\phi_n)$$

side note

$L_M = (\,)''$ $\quad (f+g)'' = f'' + g''$

$L_M(u) = u u'$ I cannot open it as above as it's not linear

$$\frac{\partial R_i}{\partial a_j} = L_M(\phi_j)$$

$$R_f = \bar{F} - L_f(u^h) = \bar{F} - L_f\left(\phi_p + \sum_{k=1}^{n} a_k \phi_k(x)\right) \quad (L_f \text{ is linear})$$

$$R_f = \bar{F} - L_f(u^h) = \bar{F} - L_f\left(\phi_p + \sum_{k=1}^{n} a_k \phi_k(x)\right) = \bar{F} - L_f(\phi_p) - \sum_{k=1}^{n} a_k L_f(\phi_k) \quad (L_f \text{ is linear})$$

$$u^h = \phi_p + \sum_{k=1}^{n} a_k \phi_k(x)$$

$$\text{so } R_f = \bar{F} - L_f(\phi_p) - a_1 L_f(\phi_1) - a_2 L_f(\phi_2) - \dots - a_n L_f(\phi_n)$$

$$\frac{\partial R_f}{\partial a_j} = -L_f(\phi_j)$$

Summary

$$\frac{\partial \tilde{R}}{\partial a_j} = 2\left(\int_{\Omega} R_i \left(\frac{\partial R_i}{\partial a_j}\right) dV + \int_{\partial\Omega_f} R_f \left(\frac{\partial R_f}{\partial a_j}\right) ds \right) = 0$$

$$\frac{\partial R_i}{\partial a_j} \to L_M(\phi_j), \qquad \frac{\partial R_f}{\partial a_j} \to -L_f(\phi_j)$$

$\frac{\partial \tilde{R}}{\partial a_j} = 0$: Least square final result

$$\int_{\Omega} L_M(\phi_j) R_i \, dv + \int_{\partial\Omega_f} \left(-L_f(\phi_j)\right) R_f \, ds = 0$$

WRS

$$\int_{\Omega} W_j R_i \, dv + \int_{\partial\Omega_f} (W_f)_j R_f \, ds = 0$$

Least Square method is a WRS where we have different weights for inside and on natural boundary

$$W_j = L_M(\phi_j) \quad \text{on } \Omega$$
$$(W_f)_j = -L_f(\phi_j) \quad \text{on } \partial\Omega_f$$

Going back to our bar problem:

$$R_i = (EAw)' + q(x) = u'' + q(x) = L_M(u) - r_1(x)$$

$$R_i = (\underbrace{EA}_{EA=1}w)' + q(x) = u'' + q(x) = \underbrace{L_M(u)}_{=u''} - \underbrace{r(x)}_{-q(x)}$$

$$\boxed{L_M = (\ )''}$$

$$L_f = \bar F - F = \bar F - EAu' = \underbrace{1}_{f} - \underbrace{u'}_{L_f(u)}$$

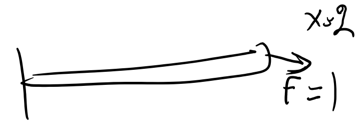
$$\boxed{L_f = (\ )'}$$

$$w = L_M(\phi) = \begin{pmatrix} x \\ x^2 \end{pmatrix}'' = \begin{pmatrix} 0 \\ 2 \end{pmatrix}$$

$$w_f = L_f(\phi) = -\begin{pmatrix} x \\ x^2 \end{pmatrix}' = -\begin{pmatrix} 1 \\ 2x \end{pmatrix}$$

WRS $$\int_0^2 \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \Big(\underbrace{\big(\phi_p + [\phi_1\ \phi_2]\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}\big)'' + q(x)}_{R_i} \Big) + \begin{bmatrix} w_{f_1} \\ w_{f_2} \end{bmatrix} \Big(1 - \big([\phi_1\ \phi_2]\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} + \phi_p\big)' \Big)$$

we had $\phi_p = 1$



$$K = \int_0^2 \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}'' [\phi_1\ \phi_2]'' dx + \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}' [\phi_1\ \phi_2]' \Big|_{x=2}$$

$$= \int_0^2 \begin{bmatrix} 0 \\ 2 \end{bmatrix} [0\ \ 2]\, dx + \begin{bmatrix} 1 \\ 2x \end{bmatrix} [1\ \ 2x] \Big|_{x=2}$$

$$= \begin{bmatrix} 0 & 0 \\ 0 & 4 \end{bmatrix} + \begin{bmatrix} 1 & 4 \\ 4 & 16 \end{bmatrix}$$

$$F = -\int_0^{\cancel{1}} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} q(x)\, dx - \begin{bmatrix} w_{f_1} \\ w_{f_2} \end{bmatrix}\Big|_{x=2} 1 = -\int_0^1 \begin{bmatrix} 0 \\ 2 \end{bmatrix} (2-2x)\, dx - \begin{bmatrix} -1 \\ -2x \end{bmatrix}\Big|_{x=2} 1$$

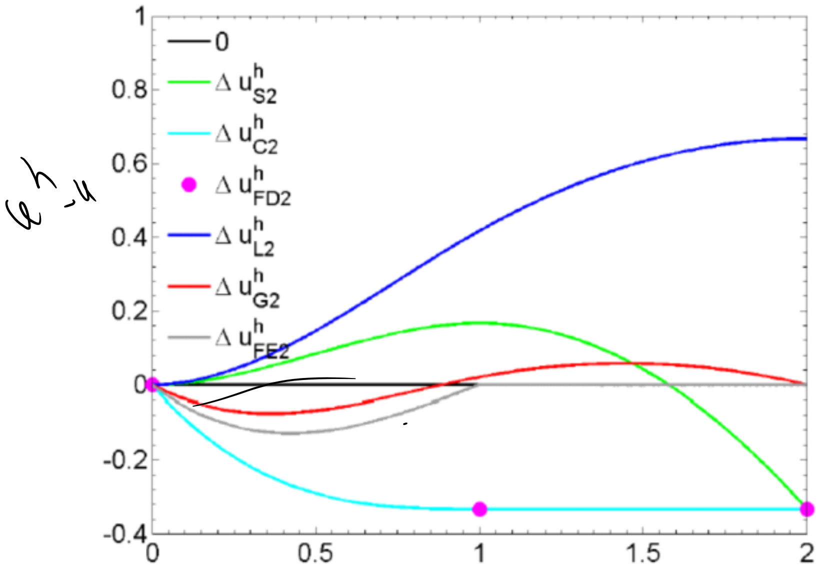
$$= \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$K = \begin{bmatrix} 1 & 4 \end{bmatrix} \quad \begin{bmatrix} 1 & 1 \end{bmatrix} \rightarrow a = K^{-1}F = \begin{bmatrix} 2 \end{bmatrix}$$

$$K = \begin{bmatrix} 1 & 4 \\ 4 & 20 \end{bmatrix}, \quad F = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \rightarrow \quad a = K^{-1}F = \begin{bmatrix} 2 \\ -1/4 \end{bmatrix}$$

this matches our earlier solution, but this approach is much faster & clearer

Bar example, $n = 2$, Comparison of solutions



Didn't we minimize R^2?

why compared to $\underbrace{G2, S2, C2}$

$u^h = \phi_p + \phi_1 a_1 + \phi_2 a_2$

$\phi_p \to 1$, $\phi_1 \to x$, $\phi_2 \to x^2$

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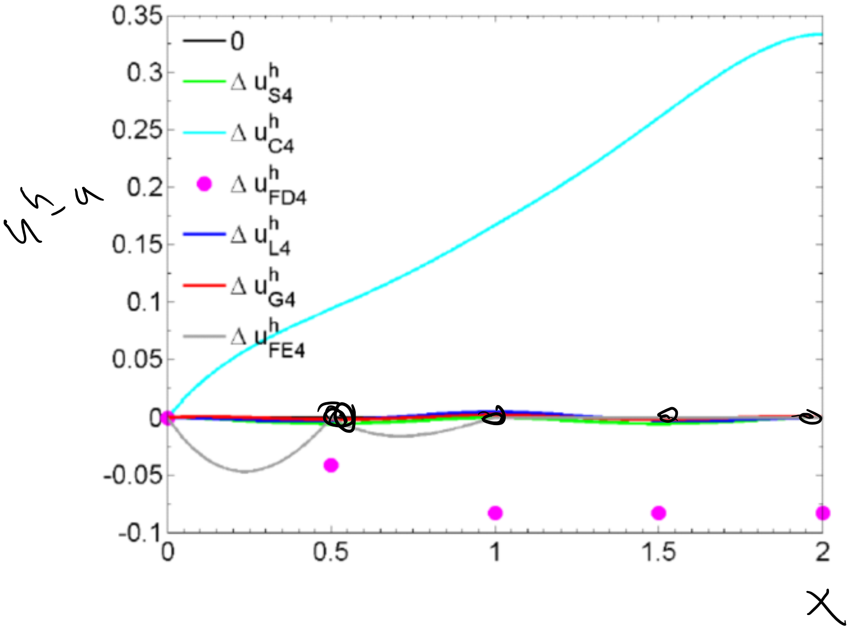
Least square minimizes the error in Differential Equation (Ri) and Natural BC (Rf) in an R2 fashion. This does not result in minimum solution error Norm(uh - u)

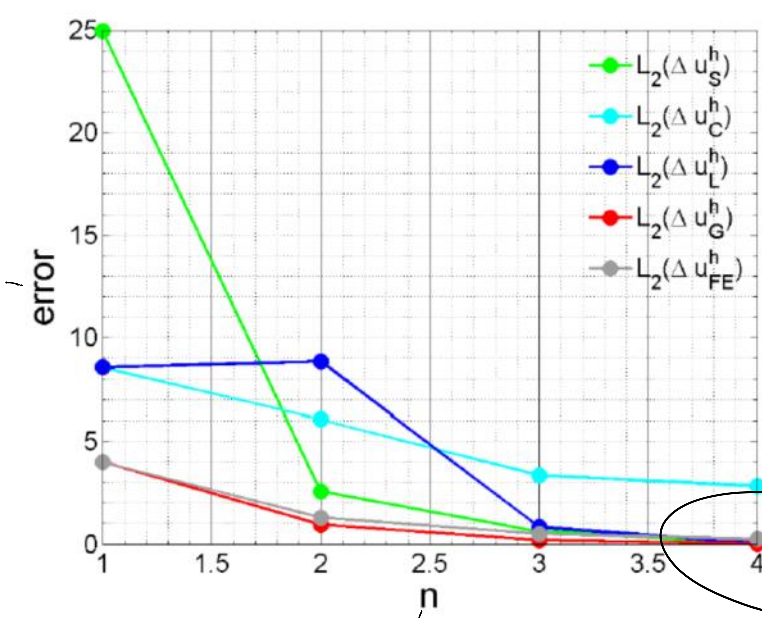
We already mentioned that in 1D FEM often we match the exact solution at nodes



Let's compare the errors of different methods

$$\text{error} = \sqrt{\int_0^2 (u^h - u)^2(x)\, dx} = \| u_h - u \|_2$$

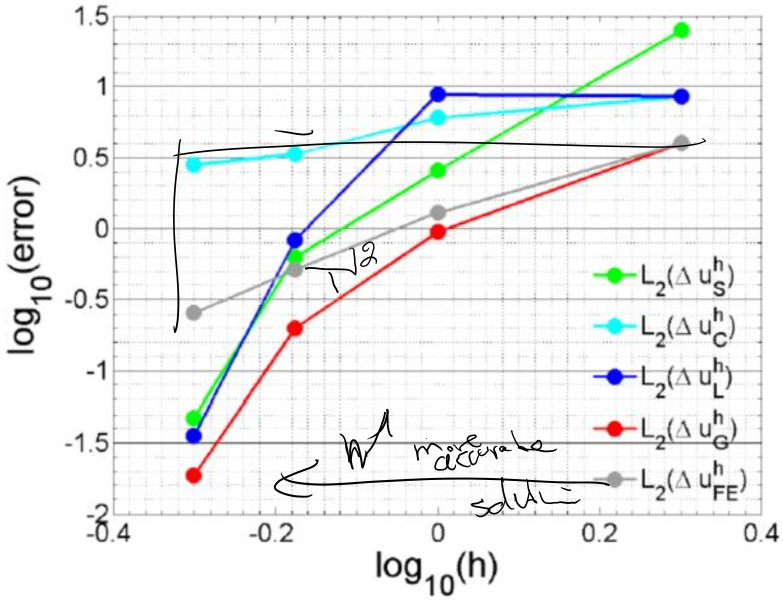
Bar example, Error Convergence



\# unknowns

not clear
we'll use log(error)

Bar example, Error Convergence



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$h = \frac{L}{n}$

$h \searrow (n \nearrow)$

FEM we have a linear relation between log(error) & log(h)

$$e^{\left(\log(\text{error}) = A + \underbrace{\text{slope}}_{\text{here}: 2} \log(h)\right)}$$

$$\text{error} = \underbrace{(e^A)}_{C} h^2$$

FEM $\boxed{\text{error} = C h^2}$

For linear FE formulation of a bar problem

General for FE & Discontinuous Galerkin

a priori error estimate

$$\boxed{\text{error} = C h^{a \min(p, s) + b}}$$

p: order of element

s: regularity of solution

error estimate

s: regularity of solution

a & b are factors that depend on DE and the type of error considered

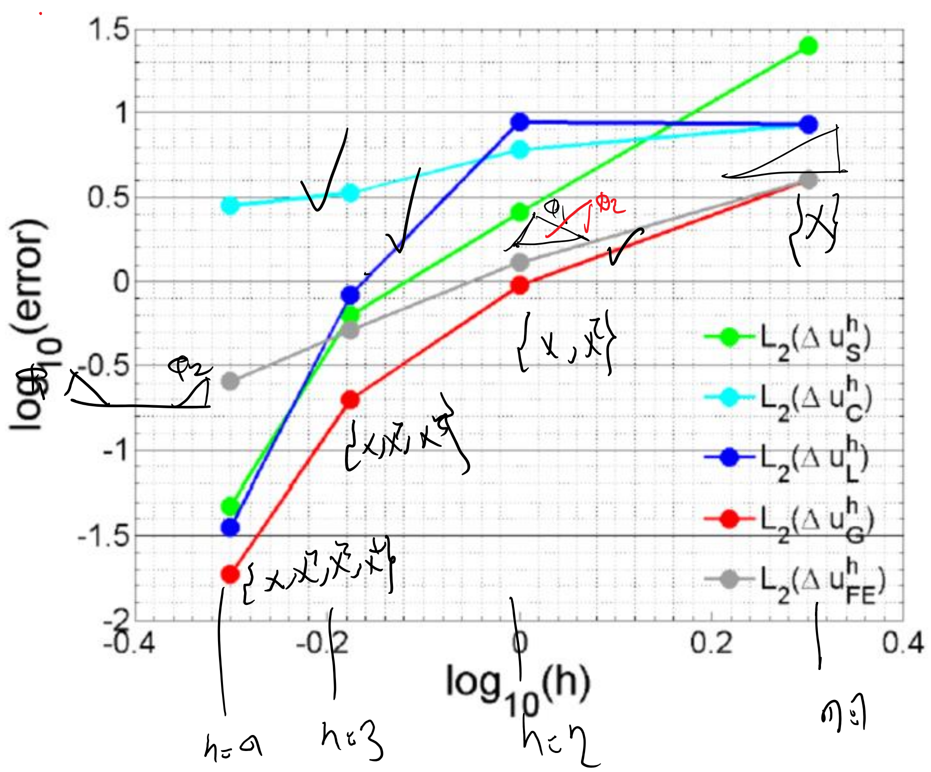
for sufficiently smooth problem

error = $C h^{ap+b}$

example here: $a=1$, $b=1$, $p=1$ (bar problem, L2 error)

error = Ch^2

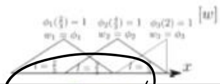
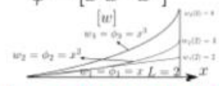
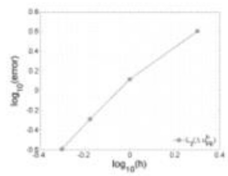
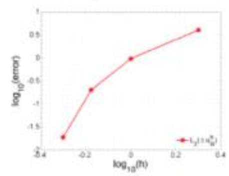
Bar example, Error Convergence



{x} → {x²}, ... convergence rate

they have a much faster

Observations: FE versus spectral methods

Feature	Finite Element	Spectral Methods
Trial Functions Example	Local / Finite Regularity hat functions 	Globally Smooth $\phi = [x\ x^2\ x^3]$ 
Matrix $\mathbf{K}$ Example	Sparse $\begin{bmatrix} 4 & -2 & 0 & 0 \\ -2 & 4 & -2 & 0 \\ 0 & -2 & 4 & -2 \\ 0 & 0 & -2 & 2 \end{bmatrix}$	Full (diagonal for orthogonal ϕ) $\begin{bmatrix} 2 & 4 & 8 & 16 \\ 4 & \frac{32}{3} & 24 & \frac{256}{5} \\ 8 & 24 & \frac{288}{5} & 128 \\ 16 & \frac{256}{5} & 128 & \frac{2048}{7} \end{bmatrix}$
order of accuracy of u^h (p)	fixed $(e.g., p = 1)$	$\nearrow$ vs. n $(e.g., p = n)$
Convergence Example	Linear: $e = Ch^{\alpha}$ $\alpha = 2$  	higher than linear exponential 
Geometry	Very general geometries	simple (*e.g.*, rectangular) in practice to get diagonal $\mathbf{K}$

spectral

Diagonal matrix for spectral methods

- The global nature of trial functions ϕ in spectral method results in full $\mathbf{K}$ matrices that are expensive to solve.
- To circumvent this problem we employ trial functions that make $\mathbf{K}$ diagonal.
- In weak statement $K_{ij} := \mathcal{A}(\phi_i, \phi_j) = \int_{\mathcal{D}} L_m^w(\phi_i) L_m(\phi_j)\, \mathrm{dv}$.
- If the problem is self-adjoint $\mathcal{A}(.,.)$ is an inner product and we can construct an orthogonal trial function basis ϕ_i for example using Gram Schmidt method.
- Given the particular form of $\mathcal{A}$ (from L_m^w and L_m) and domain of integration $\mathcal{D}$ ($[0\ 1]$, $[-1\ 1]$, semi-infinite, infinite, *etc.*) we employ various trigonometric and orthogonal polynomial spaces. Some examples are:
  - $\phi_k(x) = e^{ikx}$ Fourier spectral method.
  - $\phi_k(x) = T_k(x)$ Chebyshev spectral method.
  - $\phi_k(x) = L_k(x)$ or $P_k(x)$ Legendre spectral method.
  - $\phi_k(x) = \mathcal{L}_k(x)$ Laguerre spectral method.
  - $\phi_k(x) = H_k(x)$ Hermite spectral method.

  where $T_k(x)$, $L_k(x)(P_k(x))$, $\mathcal{L}_k(x)$, and $H_k(x)$ are the Chebyshev, Legendre, Laguerre, and Hermite polynomials of degree k, respectively.
- The orthogonal property of these functions is for simple geometries. That is why spectral methods are more popular for simple geometries where we can take advantage of their exponential convergence property while keeping computational costs low by using orthogonal trial functions.

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