New homework assignment posted to canvas
Due 2/8

Plan for today
- Mixture models
  ↳ over fitting
- Regression theory
  - finite elements
  - local polynomial reproduction
  - curse of dimensionality
  - intro to DNNs ← no black boxes!

Some final comments on building probability distributions

Multivariate Gaussian

$y \in \mathbb{R}^N$

$y \sim N(\mu, \Sigma)$ (det)

$$p(y) = 2\pi^{-N/2} |\Sigma| \exp\left[-\frac{1}{2}(y-\mu)^T \Sigma^{-1}(y-\mu)\right]$$

ex If $\Sigma = \text{diag}(\sigma_i^2)$ show that y may be viewed as joint distribution of indep univariate gaussians

Mixture of experts

Let $C \sim \text{categorical}(\pi)$
$\text{cat}(\pi)$

$0 \le \pi \le 1$

$\sum_i \pi_i = 1$

Define MOE

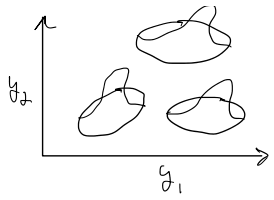
$$p(y|x) = \sum_c \underbrace{p(y|c,x)}_{\text{expert model}} \underbrace{p(c|x)}_{\text{gating function}}$$

IDEA: Tool For Blending Multiple Models Potentially Allowing Specialization

Example Gaussian Mixture model

$$p(y) = \sum_{c=1}^{N_c} p(c)\, p(y|c)$$

$$\approx \sum_{c=1}^{N_c} \pi_c\, N(y; \mu_c, \Sigma_c)$$



Some exercises

- Compute $p(c|y)$

$$p(c|y) = \frac{p(y|c)\,p(c)}{p(y)} \qquad \text{Bayes Thm}$$

$$= \frac{p(y|c)\,p(c)}{\sum_{c'} p(y|c')\,p(c')} \qquad \text{Total Probability}$$

$$= \frac{\pi_c\, N(y; \mu_c, \Sigma_c)}{\sum_{c'} \pi_{c'}\, N(y; \mu_{c'}, \Sigma_{c'})}$$

Remark $\Rightarrow$ Mixture models allow Bayesian inference of cluster ownership

Exercises Compute $\mathbb{E}_{c \sim p(c|y)}[c]$

$\mathrm{Var}_{c \sim p(c|y)}[c]$

Overfitting in MLE

Consider fitting two clusters to scattered data w/ max. likelihood

$$NLL(\pi, \mu, \Sigma) = \log p(y_1 \cdots y_d) = \sum_{i=1}^{d} \log p(y_d)$$

$$= \sum_{i=1}^{d} \log \sum_{c} \pi_c\, p(y_d|c)$$

Remark: First time we've gotten log of sum $\rightarrow$ not nice for optimization

Take $\pi_{c_1} = 1$

$$\mu_{c_1} = y_{d_1}$$
$$\Sigma_{c_1} = \varepsilon^2 I << 1$$

Then $NLL = -\sum_{i=1}^{d} \log N(y_d; y_{d_{11}}, \varepsilon^2 I)$

$$= -\log N(y_{d_1}; y_{d_1}, \varepsilon^2 I) - \sum_{i \neq 1}^{d} \log N(y_d; y_{d_1}, \varepsilon^2 I)$$

$$= C + \frac{d}{2} \log \varepsilon + \frac{1}{2} \frac{0}{\varepsilon^2} + \text{STUFF}$$

Note that $\lim_{\varepsilon \to 0} NLL = -\infty$

So that we can make the NLL arbitrarily small by attaching a cluster to a single point

Overfitting is a danger of MLE

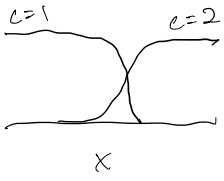
Soln. Stabilization for GMM

$$N(y \mid \mu_c, \Sigma_c + \varepsilon^2 I)$$

$\varepsilon^2 > 0$ Fixed Background Noise

Another MoE example — Piecewise Polynomial Regression

$$p(y|x) = \sum_c p(y|c,x)\, p(c|x)$$



$$p(c|x) = \text{cat}(\sigma(wx+\beta))$$
$$p(y|c,x) = N(y; A_c x + B_c, \sigma_c^2)$$

Classical Regression — Introductory Functional Analysis

Let $L_2(\Omega) = \{ f \mid \int_\Omega f^2 dx < \infty \}$

$C_1(\Omega) = \{ f \mid$

Finite Elements Let $0 = x_0 < \cdots < x_N = 1$

Let $\mathcal{S}$ be a linear space of functions $\mathcal{S} = \text{span}(\{v_1, \ldots, v_N\})$ satisfying

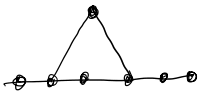
1) $v \in C^0([0,1])$ continuous on unit interval

2) $v|_{[x_i, x_{i+1}]}$ is a linear polynomial

3) $v(0) = 0$

Define $\phi_i(x)$ by requiring "Kronecker delta" property

$$\phi_i(x_j) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & \text{else} \end{cases}$$



ML def of PL functions

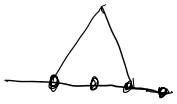
Recall $\mathrm{ReLU}(x) = \begin{cases} x & x > 0 \\ 0 & \text{else} \end{cases}$

ex Express $\phi_i(x)$ in terms of ReLU

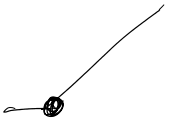
$$\phi_i(x) = A\,\mathrm{ReLU}(x - x_{i-1}) + B\,\mathrm{ReLU}(x - x_i) + C\,\mathrm{ReLU}(x - x_{i+1})$$

$\phi_i(x_j) = \delta_{ij}$ implies

$$1 = \phi_i(x_i) = A(x_i - x_{i-1}) + 0 + 0$$
$$0 = \phi_i(x_{i+1}) = A(x_{i+1} - x_{i-1}) + B(x_{i+1} - x_i) + 0$$
$$0 = \phi_i(x_{i+2}) = A(x_{i+2} - x_{i-1}) + B(x_{i+2} - x_i) + C(x_{i+2} - x_{i+1})$$

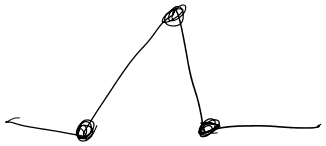


$$A = \frac{1}{x_i - x_{i-1}} \qquad B = \frac{-A(x_{i+1} - x_{i-1})}{x_{i+1} - x_i} \qquad C = \frac{-A(x_{i+2} - x_{i-1}) - B(x_{i+2} - x_i)}{x_{i+2} - x_{i+1}}$$



Activation 1

Activation 2



Activation 3

Lemma ϕ_i form a basis for S

Pf - ϕ_i is a basis if $\sum c_i \phi_i(x_j) = 0$ implies $c_i = 0$ for all i

- From Kronecker-δ property

$$\sum_i c_i \phi_i(x_j) = \sum_i c_i \delta_{ij}$$

$= c_j = 0$

Thm $\mathcal{S} \subset L^2([0,1])$ if

$f \in$

Define The interpolant $v_I \in \mathcal{S}$ satisfying

$v_I(x_j) = v(x_j)$ for all j

is $v_I(x) = \sum_i v(x_i)\,\phi_i(x_i)$

Pf $v_I(x_j) = \sum_i c_i\,\phi_i(x_j)$

$= \sum_i c_i\,\delta_{ij}$

$= c_j$

Thm Let $h = \max_i |x_{i+1} - x_i|$. If u'' defined

Then $|u(x) - u_I(x)| \le \frac{1}{2} h^2 \max_{x \in [0,1]} |u''(x)|$

Pf for $x \in [x_i, x_{i+1}]$

- $u(x) - u_I(x) = \int_{x_i}^{x} (u - u_I)'(t)\,dt$ Fundamen Thm Calc

- Mean value thm $\Rightarrow$ can find $x^* \in [x_i, x_{i+1}]$ s.t.

$u'(x^*) = \dfrac{u(x_{i+1}) - u(x_i)}{x_{i+1} - x_i} = u_I'$

so $(u - u_I)'(x^*) = 0$

F.T.C. $(u-u_I)'(t) = \int_{x^*}^{t} (u-u_I)''(s)$

$$= \int_{x_i}^{x} \int_{x^*}^{t} (u-u_I)''(s)\, ds\, dt$$

$$= \int_{x_i}^{x} \int_{x^*}^{t} u''(s)\, ds\, dt$$

$$|u-u_I|(x) \le \max_{s\in[x_i, x_{i+1}]} u''(s) \int_{x_i}^{x} \int_{x^*}^{t} ds\, dt$$

$$|u-u_I| \le \frac{1}{2} h^2 \left(\max_{[0,1]} u''\right)$$

We can understand this informally

→ the interpolant can match the constant + linear term of the Taylor series on each element. Integrating the remainder on the element gives h^2 scaling

Exercise Develop higher-order polynomial spaces using ReLU networks (HW problem)

First glimpse at DNN

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$= 0$

Def A shallow neural network of width N

$$NN: \mathbb{R}^{N_{in}} \to \mathbb{R}^{N_{out}}$$

with ReLU activation consists of a "hidden layer"

$$L_H(x) = \text{ReLU}(Wx + b)$$

$$W \in \mathbb{R}^{N \times N_{in}}, \quad b \in \mathbb{R}^N$$

composed w/ a "linear layer"

$$L_L(x) = Cx$$

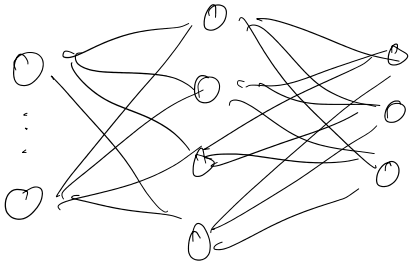
$$C \in \mathbb{R}^{N_{out} \times N}$$

$$NN_\theta(x) = L_L \circ L_H(x)$$

and we denote trainable params

$$\theta = \{W, B, C\}$$

We draw this as a network w/ weights + biases represented as edges



crude model of brain

Some history This is an example of a

Some history

This is an example of a "Multilayer Perceptron" (MLP)

More generally a deep NN / dense / feed forward can consist of many layers and other nonlinear activation functions

$$y(x) = L_L \circ L_{H_M} \circ \cdots \circ L_{H_1}(x)$$

$$L_{H_i}(x) = \sigma(W_i x + b_i)$$

(σ: activation, W_i: weight, b_i: bias)

1958 - single hidden, trainable linear only

1970 - first backprop

2003 - renewed interest due to architectures

$$NN(x) = \sum c_i \bar{\Phi}_i(x;\theta)$$

(c_i: LL, θ: W, b)

$$\bar{\Phi}_i(x;\theta) = \sigma(Wx + b)$$

Thm Consider $N_{in} = N_{out} = 1$ (1D scalar data)

$$\mathcal{D} = (x_i, y_i)_{i=1}^{N_D} \qquad N_D = N - 1$$

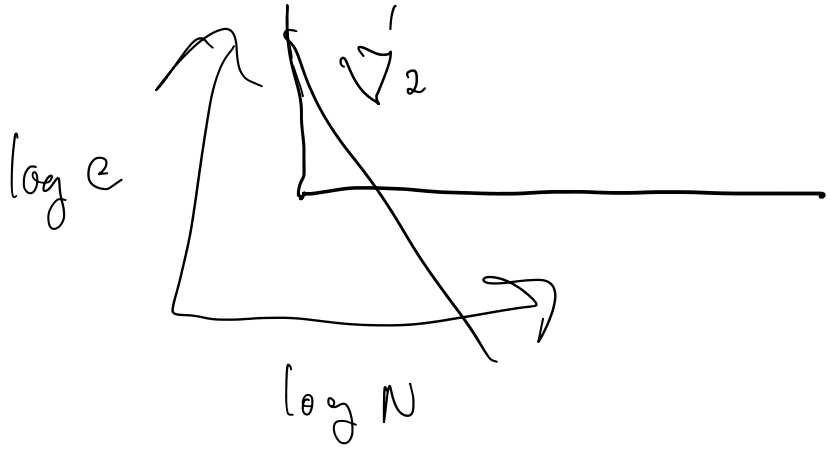
satisfying $x_i \neq x_j$ $\forall i, j$

satisfying $x_i \neq x_j \quad \forall i,j$

then

$$\min_{\theta} \sqrt{\frac{1}{N_D} \sum_{i=1}^{N_D} | NN_\theta(x_i) - y_i |^2} \leq C h^2$$

Pf Set: biases to match nodes
weights to 1
linear layer to interpolant of data



— This is drastically over simplistic

- Does an interpolant exist for arbitrary scattered data?
- How does that depend on dimension

- A NN can emulate PW linears in 1D — what about higher dimensions?
- When can a NN beat a traditional finite element space?
- How do we initialize a DNN when training w/ gradient descent?

Understanding the curse of dimensionality

(See "Scattered data approximation" By Holger Wendland)

- Consider a scattered dataset

$$\mathcal{D} = \{x_i, y_i\}_{i=1}^{N} \qquad x \in \mathbb{R}^d, \; y \in \mathbb{R}$$

- Aim to build a "quasi-interpolant" of $\mathcal{D}$

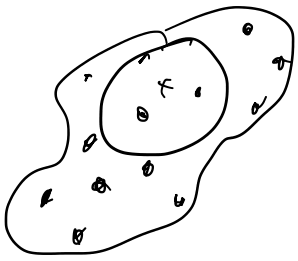
$$s(x) = \sum_{j=1}^{N} y_j \, u_j(x)$$

(u_j: TBD)

where $s \approx y$ at x

- Def fill-distance

$$h_{x,\Omega} = \sup_{x \in \Omega} \min_{1 \le j \le N} \|x - x_j\|_2$$



the largest distance one needs to go to find a data pt.

- def A local polynomial reproduction of degree ℓ assigns u_j s.t.

polynomial reproducing

(1) $\sum_j p_j u_j(x) = p(x) \quad \forall p \in \Pi_\ell(\mathbb{R}^d)$

"not too big"

(2) $\sum_j |u_j(x)| < C_1 \quad \forall x \in \Omega$

compact support

(3) $u_j(x) = 0$ if $\|x - x_j\|_2 \ge C_2 h_{x,\Omega}, \forall x \in \Omega$

For a polynomial reproduction of order m on a compact Ω

$$|f(x) - s(x)| \le C h_{x,\Omega}^{m+1} |f|_{C^{m+1}}$$

where $|f|_{C^{m+1}} = \max_{|\alpha| = m+1} \|D^\alpha f\|_{L^\infty}$

sketch proof

Pf Let $p \in \Pi_m$ be a polynomial of order m. Then

$$|f(x) - s(x)| \le |f(x) - p(x)| + |p(x) - \sum_j f_j u_j(x)|$$

$$= \quad " \quad + \left| \sum p_j u_j(x) - f_j u_j(x) \right|$$

$$\leq |f(x) - p(x)| + \sum |p_j - f_j| \, |u_j(x)|$$

$$\leq \|f - p\|_{L^\infty(B(x, c_2 h_{x,\Omega}))} \left(1 + \sum_j |u_j(x)|\right)$$

$$\leq (1 + c_1) \|f - p\|_{L^\infty(B(x, c_2 h_{x,\Omega}))}$$

Taking p as the Taylor polynomial

$$\|f - p\|_{L^\infty(B(x, c_2 h_{x,\Omega}))} \leq C h_{x,\Omega}^{m+1} |f|_{C^{m+1}}$$

@ So error depends on scaling of $h_{x,\Omega}$

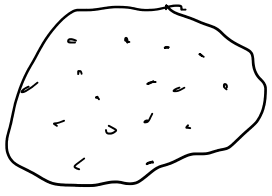
→ how does that depend on dimension?

def separation distance $q_X = \frac{1}{2} \min_{i \neq j} \|x_j - x_i\|$

def data sites X are quasi-uniform if

$$q_X < h_{x,\Omega} < c_{qu} q_X \,, \quad c_{qu} > 0$$

informally → $q_X \sim h_{x,\Omega}$



thm Given N quasi-uniform data sites

$$C N^{-1/d} \leq h_{X,\Omega} \leq C N^{-1/d}$$

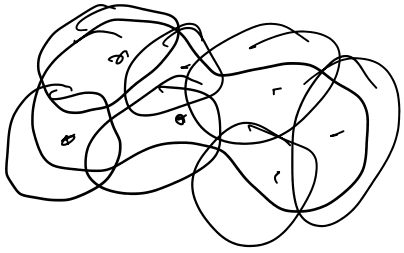
$$C N^{-1/d} \le h_{X,\Omega} \le C N^{-1/d}$$

Pf ($\Rightarrow$) $\Omega \subseteq \bigcup_{i=1}^{N} B(x_i, h_{X,\Omega})$

$$\mathrm{vol}(\Omega) \le \sum \mathrm{vol}\left(B(x_i, h_{X,\Omega})\right)$$

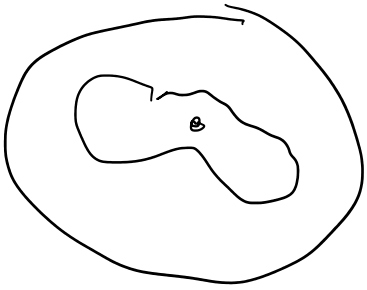
$$\le C N h^d$$

$$N^{-1/d} \le C h$$



($\Leftarrow$) Since Ω bounded, there is a x_0, R s.t.

$$\Omega \subseteq B(x_0, R)$$



$$\bigcup_{i=1}^{N} B(x_i, q_X) \subseteq \Omega$$

disjoint balls

$$N q_X^d \le \mathrm{vol}(\Omega)$$

$$q_X \le C N^{-1/d}$$

quasi-uniformity $\quad h_{X,\Omega} \le C N^{-1/d}$

Punchline To hit a given error

$$N \sim \varepsilon^{-\frac{m+1}{d}}$$

$$\|u - s\|_{\infty} \sim C h^{m+1} \sim C N^{-\frac{m+1}{d}}$$

Today – Introduction to the finite element method and solving diff. eq. models

Control Volume Analysis

Recall the generalized Stokes theorem:

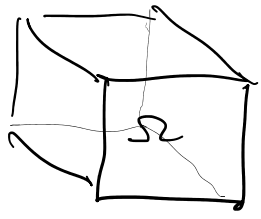
Gauss Div thm $$\int_C \nabla \cdot F \, dV = \int_{f \in \partial C} F \cdot dA$$

Stokes / Greens thm $$\iint_f \nabla \times F \, dA = \oint_{e \in \partial f} F \cdot dl$$

Fund. Thm of calculus $$\oint_e \nabla \phi \cdot dl = \phi(e_+) - \phi(e_-)$$

Conservation laws

- Consider an arbitrary subdomain Ω



- Express change of system as balance of flux in/out

$$\frac{d}{dt}\int_\Omega \text{stuff}\, dx = \oint_{\partial\Omega} \text{Flux(stuff)} \cdot dA$$

ex Cons of Mass

$$\frac{d}{dt}\,\text{MASS} = \frac{d}{dt}\int_\Omega \rho\, dx = \int_{\partial\Omega} \rho\vec{u}\cdot dA = \text{MASS FLUX}$$

Applying GDT

$$\int_\Omega \left(\partial_t \rho + \nabla\cdot \rho u\right) dx = 0$$

Must hold independent of choice for Ω

$\Rightarrow$ integrand $=0$

$$\partial_t \rho + \nabla\cdot \rho u = 0 \qquad \text{PDE Model}$$

Examples

① Conservation of Momentum

- $\rho \partial_{tt} u = \nabla\cdot \vec{\vec{\sigma}}(u)$ (solids, u = displacements)
- $\rho \partial_t u = \nabla\cdot \vec{\vec{\sigma}}(u)$ (fluids, u = velocity)

② Conservation of thermal energy

- $\rho\, c_p\, \partial_t T = \nabla\cdot \vec{q}(T)$ $\quad q \to$ heat flux

③ Conservation of magnetic flux

- $\partial_t B = \nabla\times(v\times B)$ $\quad v\times B \to$ magnetic flux

We will consider the abstract problem

(CL)
$$\begin{cases} \partial_t u + \nabla \cdot F = f(x,t) & (A) \\ F = N(u;\theta) + g(x,t) & (B) \end{cases}$$

Notes
- (CLA) is known physics
- (CLB) is unknown closure
- (CLA) encodes conservation structure independent of θ

$$\int_\Omega \partial_t u + \nabla \cdot F \, dx = \int_\Omega f \, dx$$

$$= \frac{d}{dt}\int_\Omega u \, dx + \oint_{\partial\Omega} F \cdot dA = \int_\Omega f \, dx$$

$$\Rightarrow \frac{d}{dt}\int_\Omega u \, dx = 0 \quad \text{if} \quad F \cdot \hat{n}\big|_{\partial\Omega} = 0, \; f = 0$$

Classical Modelling: Develop $N(u;\theta)$ either empirically or analytically

So that
1. Easily calibrate θ from experiments
   e.g. rheometry
2. Guarantee (CL) is:
   - well-posed

- easily solved
  - computer vs analytically
- physically - realizable
- amenable to UQ

Data-driven modeling

Instead use data to select F_θ via an equality constrained opt. problem.

$$\underset{\theta}{\text{argmin}} \; \|u - u_{data}\|^2 + \varepsilon^2 \|F - F_{data}\|^2$$

s.t. (CL) holds

We have the pieces:
- probability
- regression
- how to numerically solve PDEs

last piece →

Next week - Finite Elements vs DNNs for PDEs

How to solve heat eqn w/ FEM

Let $\Omega = [0, 1]$

Eqn 1 Solve $\partial_t u + c^2 \partial_{xx} u = f$

for now ↙

$$u(x=0, t) = u_L = 0$$

$$u(x=1, t) = u_R = 0$$

Variational Formulation

Choose trial space $u(x) \in H_0^1(\Omega)$

$$H_0^1 = \left\{ \int u^2 < \infty,\ \int u'^2 < \infty,\ u|_{\partial\Omega} = 0 \right\}$$

IDEA → u are candidate solutions

Pick a test space V ← more on how to choose this later

IDEA $v \in V$ will be how we measure the error

In continuous Galerkin method $V = H_0^1(\Omega)$

Variational procedure. Let $v(x) \in V$

$$\partial_t u + c^2 \partial_{xx} u = f$$

$$\int_\Omega v\left(\partial_t u + c^2 \partial_{xx} u\right) dx = \int_\Omega v f \, dx$$

$$\frac{d}{dt} \int v u \, dx + c^2 \int v \partial_{xx} u \, dx = \int_\Omega v f \, dx$$

Integrate 2nd term by parts

$$\frac{d}{dt} \int v u \, dx - c^2 \int \partial_x v \, \partial_x u + v \partial_x u \Big|_0^1 = \int_\Omega v f \, dx$$

$v \partial_x u = 0$ because $v(0) = v(1) = 0$

With the notation $(f, g) = \int f g \, dx$

$$\frac{d}{dt}(v, u) - c^2 (\partial_x v, \partial_x u) = (v, f)$$

Why rewrite in this way?

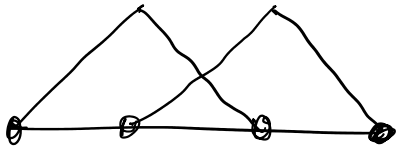
- Any soln of "strong form" (Eqn 1) will satisfy this equation
- Eqn 1 needs u'' to be defined, while this one only needs to be able to integrate products of first derivatives (hence "weak form")
- exposes symmetry that we'll use to prove stuff

How to solve

Define $V_h = \{$ piecewise linears & sat. BCs $\}$

$$u = \sum_{i=1}^{N-1} \hat{u}_i \, \phi_i(x)$$

$$= \phi(x)^T \hat{u}$$



And substitute in

$$\frac{d}{dt}(v,u) - c^2 (\partial_x v, \partial_x u) = (v, f)$$

$$\frac{d}{dt} \sum \hat{v}_i (\phi_i, \phi_j) \hat{u}_j - c^2 \hat{v}_i (\partial_x \phi_i, \partial_x \phi_j) \hat{u}_j = \sum \hat{v}_i (\phi_i, f)$$

$$\frac{d}{dt}\sum_{ij}\hat{v}_i(\phi_i,\phi_j)\hat{u}_j - c^2\hat{v}_i(\partial_x\phi_i,\partial_x\phi_j)\hat{u}_j = \sum_i \hat{v}_i(\phi_i,f)$$

Regrouping

$$\sum_i\left[\hat{v}_i\left(\sum_j \underbrace{(\phi_i,\phi_j)}_{M_{ij}}\hat{u}_j - c^2\underbrace{(\partial_x\phi_i,\partial_x\phi_j)}_{S_{ij}}\hat{u}_j - \underbrace{(\phi_i,f)}_{b_i=0}\right)\right]$$

M_{ij}: mass matrix

S_{ij}: stiffness matrix

$$\hat{v}^T\left(\frac{d}{dt}M + c^2 S\right)\hat{u} = \hat{v}^T b$$

Require to hold for any $v \in V_h$

$$\Rightarrow \boxed{M\frac{d}{dt}\hat{u} + c^2 S\hat{u} = b}$$

linear system of ODEs

To solve, discretize in time

ex: if $\hat{u}^n = \hat{u}(t^n)$

$$\frac{d}{dt}\hat{u}(t^n) \approx \frac{\hat{u}^{n+1} - \hat{u}^n}{\Delta t}$$

explicit Euler

$$M \hat{u}^{n+1} = \left(M - c^2 \Delta t\, S\right) \hat{u}^n + \Delta t\, b^n$$

Required calculation: Build M, S, b

Gauss quadrature $\int_{-1}^{1} f(x)\,dx = \sum_q w_q f(x_q)$

2pt $\quad x_1 = \frac{-1}{\sqrt{3}}, \; x_2 = \frac{1}{\sqrt{3}}$

or w/ change of var $\quad w_1 = w_2 = 1$

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