Finite Element Modelling for Geosciences: Numerical Integration and Changes of Coordinates

Patrick Sanan

ETH Zurich

The Problem

- For very simple cases, we can evaluate integrals exactly, when building our Finite Element system.

$$\int_0^L N_1(x)N_2(x)dx = \int_0^L \left(1 - \frac{x}{L}\right)\left(\frac{x}{L}\right) dx = \frac{L}{6}$$

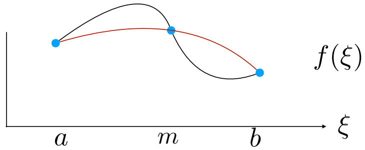
- But in general this is not possible, once arbitrary coefficient functions are involved

$$\int_0^L \kappa(x)\frac{\partial N_1}{\partial x}\frac{\partial N_2}{\partial x} dx = ?$$

- What can we do?

The Solution: Numerical Integration (aka Quadrature)

- How does one define integrals (areas under curves?)
- For well-behaved functions, recall the Trapezoidal rule or Simpson's rule:



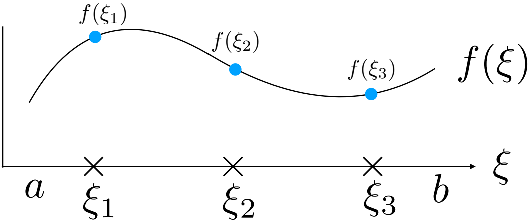
- The idea is to estimate the area by computing the area under a low-order polynomial which interpolates the function.
- These are both *Newton-Cotes formulae*. They all use equally-spaced "samples" of a function f
- If we have freedom to choose different sampling points, we can do better!

Numerical Integration (aka Quadrature)

- *Gaussian Quadrature*: Approximate an integral on a fixed domain as a weighted sum of point values, at specially chosen points.

$$\int_{\mathcal{I}} f(\xi) d\xi \approx \sum_{i=1}^{n} w_i f(\xi_i)$$

- The choice of w_i and x_i determines the specific quadrature rule.



- Easy to compute, as we only need to know f at a few points!

Numerical Integration (aka Quadrature)

- Gaussian Quadrature can *exactly* integrate polynomials of low order.
- Approximate an integral as a weighted sum of point values:

$$\int_a^b p(x)dx = \sum_{i=1}^{n} w_i p(x_i)$$

where p is a polynomial of degree $k \doteq 2n - 1$ or less.

Gauss-Legendre Quadrature

- Gaussian Quadrature rule over $[-1, 1]$.

$$\int_{-1}^{1} f(\xi) d\xi = \sum_{i=1}^{n} w_i f(\xi_i)$$

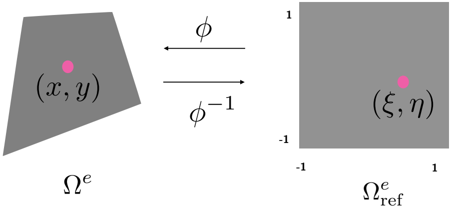
n	ξ_i	w_i	k
1	0.0	2.0	1
2	$\pm\sqrt{\frac{1}{3}}$	1.0	3
3	0.0	0.888888888888889	
	$\pm$0.774596669241483	0.555555555555556	5
4	$\pm$0.339981043584859	0.652145154862546	
	$\pm$0.861136311594053	0.347854845137454	7

(Table 4.1 in the notes)

- But... we don't just want to integrate over $[-1, 1]$!

Changes of Coordinates

- Looking ahead, we consider changes of coordinates in *several* dimensions.
- Consider a single-element reference domain Ω^e_{ref} and a physical domain Ω^e.
- Let $\vec{x} \doteq (x, y, \ldots)$ denote points in the physical domain.
- Let $\vec{\xi} \doteq (\xi, \eta, \ldots)$ denote points in the reference domain, with each coordinate in $[-1, 1]$.
- Let ϕ be an invertible function mapping the reference domain to the physical domain [1]. $\vec{x} = \phi(\vec{\xi})$



[1] A bijection $\phi : \Omega^e_{\text{ref}} \mapsto \Omega^e$

The Jacobian

- The Jacobian (matrix) captures information about the derivative(s) of ϕ.
- It describes how much local deformation occurs in mapping from the reference element to the physical one.
- To condense the notation, let's use the common shorthand that $\vec{x}$ is a function of ξ

$$\vec{x} \doteq (x, y, \ldots), \quad \vec{\xi} \doteq (\xi, \eta, \ldots), \quad \vec{x} = \phi(\xi)$$

- We'll write the Jacobian as

$$J(\vec{\xi}) \doteq \left(D\phi(\vec{\xi})\right)^T = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \cdots \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

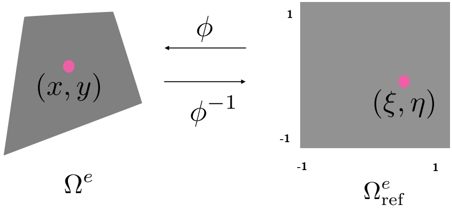
- Terminology warning! You will see the term "Jacobian" used to refer to the matrix above, its transpose, and its determinant.

The Jacobian in the Chain Rule

$$\frac{\partial f}{\partial \xi} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial \xi} + \cdots$$

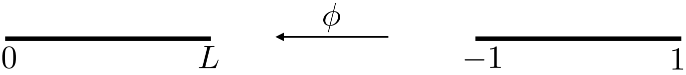
$$\begin{bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \vdots \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \cdots \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \vdots \end{bmatrix}$$

Change of Variables Formula



$$\int_{\Omega^e} f(\vec{x}) d\vec{x} = \int_{\Omega^e_{\mathrm{ref}}} f(\phi(\vec{\xi})) \det(J(\vec{\xi})) d\vec{\xi}$$

Change of Variables (1D)



$$x = \phi(\xi) = \frac{L}{2}(\xi + 1)$$

$$J(\xi) = \frac{\partial x}{\partial \xi} = \frac{L}{2}, \quad \det(J(\xi)) = \frac{L}{2}$$

Example: integrate a simple function.

$$\int_0^L x^2 dx = \int_{-1}^{1} (\phi(\xi))^2 \frac{L}{2} d\xi$$

$$= \int_{-1}^{1} \left(\frac{L}{2}(\xi + 1) \right)^2 \frac{L}{2} d\xi = \left(\frac{L}{2} \right)^3 \int_{-1}^{1} (\xi + 1)^2 d\xi$$

$$= \left(\frac{L}{2} \right)^3 \int_0^2 \xi'^2 d\xi' = \left(\frac{L}{2} \right)^3 \left(\frac{\xi'^3}{3} \Big|_0^2 \right) = \frac{L^3}{3}$$

Putting it Together

- Now, we can numerically approximate any 1D integral using Gauss-Legendre quadrature (See exercise 4.2).

$$\int_a^b f(x)dx = \int_{-1}^1 f(\phi(\xi)) \det\left(\frac{dx}{d\xi}(\xi)\right) d\xi$$

$$\approx \sum_{i=1}^n f(\phi(\xi_i)) w_i \det\left(\frac{dx}{d\xi}(\xi_i)\right)$$

- Note how this is just a weighted sum of quantities in the reference domain (functions of ξ_i). This is crucial to the efficiency of the FEM.
- Warning! In simple examples, the Jacobian is constant over an element. In general, this is not true, and you need it at each qudrature point.

What about Derivatives?

- If we use the chain rule and keep track of "where things live", we can use the usual change of coordinates formula

$$\begin{aligned}\int_a^b \frac{df}{dx}(x)dx \\ = \int_a^b \frac{df}{d\xi}(x)\frac{d\xi}{dx}(x)dx \\ = \int_{-1}^1 \frac{\partial f}{\partial \xi}(\phi(\xi))\frac{d\xi}{dx}(\phi(\xi))\det\left(\frac{dx}{d\xi}(\xi)\right)d\xi\end{aligned}$$

- This involves *inverse* Jacobian terms (e.g. $\frac{\partial \xi}{\partial dx}$) as well as the usual Jacobian determinant term.
- Again, note that everything can be evaluated in the reference domain, hence efficiently approximated using quadrature.
- See (4.13) in the notes.