Introduction to Numerical Integration

Theoretical Acoustics

Motivation

- BEM matrix elements (in the collocational formalism) are

$$G_{ij} = \int_{\Gamma_j} G(\mathbf{x}_i, \mathbf{x}) \, \mathrm{d}\mathbf{x}$$

$$H_{ij} = \int_{\Gamma_j} \frac{\partial G(\mathbf{x}_i, \mathbf{x})}{\partial n(\mathbf{x})} \, \mathrm{d}\mathbf{x}$$

- In case of a 3D problem the fundamental solution G is

$$G = \frac{\mathrm{e}^{-\mathrm{j}kr}}{4\pi r}$$

$$\frac{\partial G}{\partial n} = -\frac{\mathrm{e}^{-\mathrm{j}kr}}{4\pi r^2} (1 + \mathrm{j}kr) \frac{\mathbf{r} \cdot \mathbf{n}}{r}$$

where $\mathbf{r} = \mathbf{x} - \mathbf{x}_0$ and $r = |\mathbf{r}|$

- We need numerical integration of complex functions over simple domains (plane triangular domains in our case)
- First, the quadrature principle is introduced over standardized domains, then, domain mapping is discussed

Problem definition

- Quadrature rule: the integral is approximated as a weighted sum of the function values at predefined base points

$$\int_{-1}^{1} f(\xi)\,\mathrm{d}\xi \approx \sum_{j=1}^{n} f(\xi_j) w_j$$

- Different strategies for choosing base points ξ_j and weights w_j define different quadrature families
- Classification:
  - Newton – Cotes quadrature (equidistant interpolation)
  - Gaussian quadrature
- Main properties
  - Size: n number of function samples
  - Order: Highest polynomial order integrated accurately
- Note that the standard domain is $-1 \leq \xi \leq +1$ hereafter

Newton – Cotes quadrature

- Lagrange interpolation with equidistant samples

$$f(\xi) \approx \sum_{j=1}^{n} f(\xi_j) L_j(\xi), \quad L_j(\xi) = \prod_{k=1, k\neq j}^{n} \frac{\xi - \xi_k}{\xi_j - \xi_k}$$

- $L_j(\xi)$ are the Lagrange polynomials, as defined above
- The weights w_j are the integral of the polynomials

$$\int_{-1}^{1} f(\xi)\mathrm{d}\xi \approx \sum_{j=1}^{n} f(\xi_j) \underbrace{\int_{-1}^{1} L_j(\xi)\mathrm{d}\xi}_{w_j}$$

- Examples
  - Brick rule: $n = 1$, $\xi_j = 0$, $w_j = 2$ (0-th order)
  - Trapezoid rule: $n = 2$, $\xi_j = [-1, 1]$, $w_j = [1, 1]$ (first order)
  - Simpson's $\frac{1}{3}$ rule: $n = 3$, $\xi_j = [-1, 0, 1]$, $w_j = \left[\frac{1}{3}, \frac{4}{3}, \frac{1}{3}\right]$ (second order)

The Gaussian quadrature I.

- Newton – Cotes rules are inefficient, i.e., higher polynomial order is achievable using the same number of base points.
- A better idea is based on polynomial division.
- Let $f(\xi)$ be a polynomial of order $2n-1$

$$f(\xi) = p_{2n-1}(\xi) \qquad -1 \leq \xi \leq +1$$

- Divide p by the n-th order polynomial q as

$$p_{2n-1}(\xi) = q_n(\xi) d_{n-1}(\xi) + r_{n-1}(\xi)$$

- Then, the integral of p is written as

$$\int_{-1}^{1} p_{2n-1}(\xi)\mathrm{d}\xi = \int_{-1}^{1} q_n(\xi) d_{n-1}(\xi)\mathrm{d}\xi + \int_{-1}^{1} r_{n-1}(\xi)\mathrm{d}\xi$$

- The next idea is to use *orthogonal polynomials* as q_n.
  Note that two functions f and g are orthogonal if, and only if

$$\int_{-1}^{1} f(\xi) g(\xi)\mathrm{d}\xi = 0$$

The Gaussian quadrature II.

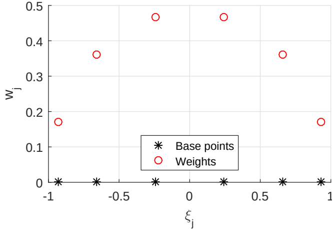
- If q is orthogonal to every polynomial up to order $n-1$ then the integral of p simplifies to the integral of the remainder r

$$\int_{-1}^{1} p_{2n-1}(\xi)\mathrm{d}\xi = \int_{-1}^{1} r_{n-1}(\xi)\mathrm{d}\xi$$

- Legendre polynomials $P_n(\xi)$ are orthogonal in $-1 \le \xi \le +1$
- Let ξ_j be the n roots of $q_n(\xi) = P_n(\xi)$. In this case

$$p_{2n-1}(\xi_j) = r_{n-1}(\xi_j)$$

- Thus, we have n samples of the $n-1$-th order remainder. The remainder is then reconstructed and integrated.



n	q	x_j	w_j
1	x	0	2
2	$3x^2-1$	$\pm 1/\sqrt{3}$	1
3	$5x^3-3x$	$0, \pm\sqrt{3/5}$	$8/9,\ 5/9$

Domain mapping

- The standard domain $-1 \le \xi \le +1$ is *mapped* to $x_1 \le x \le x_2$

$$x(\xi) = \frac{1-\xi}{2} x_1 + \frac{1+\xi}{2} x_2$$

- The integration is rewritten from x to ξ as

$$\int_{x_1}^{x_2} f(x)\,\mathrm{d}x = \int_{-1}^{1} f(x(\xi))\, \underbrace{\frac{\mathrm{d}x}{\mathrm{d}\xi}}_{J(\xi)}\, \mathrm{d}\xi$$

  where $J(\xi)$ is the Jacbian of the coordinate transform. Note that $J(\xi) = (x_2 - x_1)/2$ in this case.

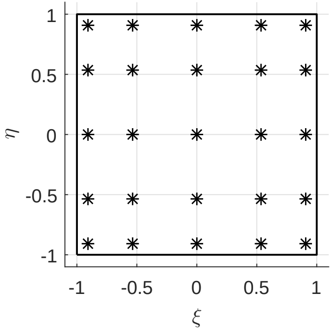
- Using the mapping quadrature rules can be transformed to arbitrary intervals in x.
- Similar coordinate transformations are used in multiple dimensions as well.

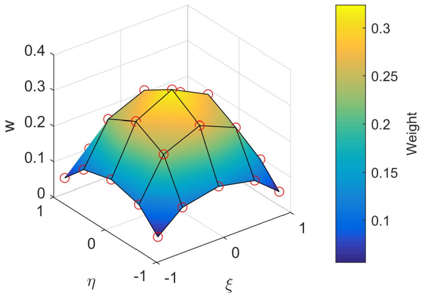
Integration over rectangles

- Tensor product quadrature

$$\int_{-1}^{1}\int_{-1}^{1} f(\xi,\eta)\mathrm{d}\xi\mathrm{d}\eta = \sum_i \left(\sum_j f(\xi_i,\eta_j) w_j \right) w_i \qquad (1)$$

- Quadrature points: (ξ_i, η_j), weights: $w_i \cdot w_j$



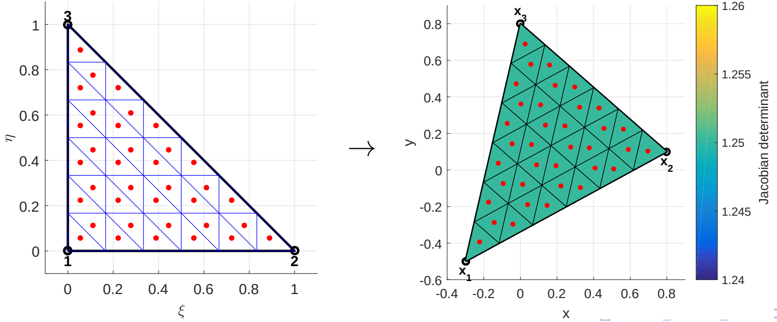


Standard triangular domain

- The mapping of a standard triangular domain: $0 \leq \xi \leq 1$, $0 \leq \eta \leq 1 - \xi$ is performed using the following linear map

$$\mathbf{x}(\xi, \eta) = \xi \mathbf{x}_1 + \eta \mathbf{x}_2 + (1 - \xi - \eta)\mathbf{x}_3$$

- The mapping functions $N_1(\xi, \eta) = \xi$, $N_2(\xi, \eta) = \eta$ and $N_3(\xi, \eta) = 1 - \xi - \eta$ are also referred to as *shape functions*
- The Jacobian of the transfom is constant, $J(\xi, \eta) = 2A$, where A is the area of the element in the (x, y, z) space



Duffy's transform

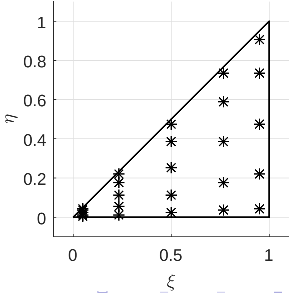
- An alternative standardized triangular domain can also be defined as $0 \leq \xi \leq 1$, $0 \leq \eta \leq \xi$
- In this case, we define the integral as:

$$\int_0^1 \int_0^\xi f(\xi, \eta) \mathrm{d}\xi \mathrm{d}\eta$$

- Duffy's transform: $\eta = \xi\mu$, $\mathrm{d}\eta = \xi \mathrm{d}\mu$

$$\int_0^1 \int_0^1 f(\xi, \mu) \xi \mathrm{d}\mu \mathrm{d}\xi \approx \sum_i \sum_j f(\xi_i, \xi_i \mu_j) \xi_i w_i w_j$$

- Equivalent to integration over a distorted rectangle with corners $(0,0), (1,0), (1,1), (0,0)$
- The transformed base points of the quadrature are shown in the figure to the right



Singular integrals using Duffy's transform I

- Remember that we need to calculate

$$G_{ij} = \int_{\Gamma_j} G(\mathbf{x}_i, \mathbf{x}) \mathrm{d}\mathbf{x} = \int_{\Gamma_j} \frac{\mathrm{e}^{-\mathrm{j}k|\mathbf{x}_i - \mathbf{x}|}}{4\pi\,|\mathbf{x}_i - \mathbf{x}|} \mathrm{d}\mathbf{x} = \int_{\Gamma_j} \frac{\mathrm{e}^{-\mathrm{j}kr}}{4\pi r} \mathrm{d}\mathbf{x}$$

  which is singular in the case $i = j$ (i.e., the receiver point is the middle of the source element)
- The problem is that the function is $\sim \frac{1}{r}$
- This singularity of type $\sim \frac{1}{r}$ can be cancelled by using polar transformation

$$\int\int f(x,y)\mathrm{d}x\mathrm{d}y = \int\int f(r,\theta) \underbrace{r}_{J(\rho,\theta)} \mathrm{d}r\mathrm{d}\theta$$

  as r is the Jacobian of the transform that cancels $1/r$. Here $x = r\cos\theta$ and $y = r\sin\theta$.

Singular integrals using Duffy's transform II

- Write the integral over the triangle in polar form

$$\int_0^1 \int_0^{\xi} f(\xi, \eta) \mathrm{d}\eta \mathrm{d}\xi = \int_0^{\pi/4} \int_0^{\rho_e(\theta)} f(\rho, \theta) \underbrace{\rho}_{J(\rho,\theta)} \mathrm{d}\rho \mathrm{d}\theta$$

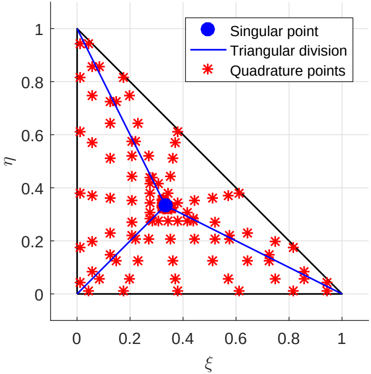
  where $\xi = \rho \cos\theta$ and $\eta = \rho \sin\theta$ and $\rho_e(\theta)$ denotes that the upper limit in ρ depends on θ.
- We can utilize Duffy's transformation

$$\int_0^1 \int_0^1 f(\xi, \mu) \xi \mathrm{d}\mu \mathrm{d}\xi \approx \sum_i \sum_j f(\xi_i, \xi_i \mu_j) \xi_i w_i w_j$$

  here $\xi_i = \rho_i \cos\theta_i$, which means that the summation weight $\xi_i w_i w_j$ automatically cancels the singularity of $1/r$
- Thus, it is also referred to as Duffy's *polar transformation*

Singular integrals using Duffy's transform III

- The singular quadrature is created by subdividing the original elements into smaller elements and using Duffy's transform to create the base points
- Notice that the base points are very dense near the singular point



- The other singular integral in the 3D Helmholtz BEM

$$H_{ij} = \int_{\Gamma_j} \frac{\partial G(\mathbf{x}_i, \mathbf{x})}{\partial n(\mathbf{x})} \, \mathrm{d}\mathbf{x} = 0 \qquad \text{if} \quad i = j$$

is zero over all planar elements.

Summary

- Numerical integration is performed using quadrature rules
- One very efficient strategy is the Gaussian quadrature
- The standardized domain of integration $-1 \leq \xi \leq 1$ is *mapped* to the actual integration domain
- When integrating in the standard domain, the Jacobian of the coordinate transform needs to be accounted for
- The same strategy is pursued in multiple dimensions
- Duffy's polar transform can be used to evaluate both regular and weakly singular[1] integrals over triangular domains
- Using planar triangular elements is efficient because we have a simple Jacobian and do not need to integrate $\partial G / \partial n$
- Using these strategies the matrix elements needed in the acoustical Helmholtz BEM can efficiently be evaluated

[1] functions containing $1/r$ singularity