Approximation Functions and Numerical Integration for 1D Problems

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Outline

- Strong form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(E(x)A(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}\right)+b(x)=0,$$

- Weighted residual method: multiplying the strong solution by an arbitrary (weight) function δu and integrating over the domain on which it holds:

$$\int_\Omega \delta u(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\left(E(x)A(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}\right)+b(x)\right)=0,$$

- Integration by parts:

$$\int_\Gamma \delta u(x)E(x)A(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}n(x)\mathrm{d}x-\int_\Omega \frac{\mathrm{d}\delta u(x)}{\mathrm{d}x}E(x)A(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}\mathrm{d}x+\int_\Omega \delta u(x)b(x)\mathrm{d}x=0$$

- Integral on the boundary:

$$\int_{\Gamma^u}\underbrace{\delta u(x)}_{=0}E(x)A(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}n(x)\mathrm{d}x+\int_{\Gamma^t}\delta u(x)\underbrace{E(x)A(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}n(x)}_{=\bar{t}}\mathrm{d}x$$

- Weak form:

$$\int_\Omega \frac{\mathrm{d}\delta u(x)}{\mathrm{d}x}E(x)A(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}\mathrm{d}x=\int_\Omega \delta u(x)b(x)\mathrm{d}x+\int_{\Gamma^t}\delta u(x)\bar{t}\mathrm{d}x$$

- Convergence of the FEM - The accuracy of FEM improves with mesh refinement, i.e. as element size h, decreases, the solution tends to be the correct solution.
- The two necessary conditions for convergence of the FEM are:
  - Continuity
  - Completeness
- *Continuity* - The trial solutions and weight functions must be sufficiently smooth. The required degree of smoothness depends on the order of the derivatives that appear in the weak form. For the second-order differential equations, derivatives in the weak form are the first derivatives, and the weight functions and trial solutions must be C^0 continuous.
- *Completeness* is the capability of a series of functions to approximate a given smooth function with arbitrary accuracy. For convergence of the FEM, it is sufficient that as the element sizes approach zero, the trial solutions and weight functions, and their derivatives up to and including the highest order derivative appearing in the weak form, be capable of assuming constant values.

- The trial function is denoted $\phi(x)$, the global FEM approximation $\phi^h(x)$; this function is for a particular element $\phi^e(x)$.
- Nodal values for the trial function are denoted by subscript; for element-related nodal value, the local node number is used x_1^e.

The solution is supposed to be approximated in each element by a polynomial function for $\phi^e(x)$:

$$\phi^e(x) = \alpha_0^e + \alpha_1^e x + \alpha_2^e x^2 + \alpha_3^e x^3 + \ldots, \tag{1}$$

where α_i are coefficients selected so that continuity is satisfied. The continuity $\phi^h(x)$ has to be satisfied within each element and between elements, too.

Consider an approximation $\phi^e(x) = \alpha_0^e + \alpha_1^e x$
This approximation satisfies completeness:

- The term α_0^e can represent any constant function
- The term α_1^e can represent any function with a constant derivative

For the complete and C^0 continuous function, we express the approximation in the element in terms of the nodal values. We can write the approximation $\phi^e(x)$:

$$\phi^e(x) = \underbrace{\begin{bmatrix} 1 & x \end{bmatrix}}_{\boldsymbol{p}(x)} \underbrace{\begin{bmatrix} \alpha_0^e \\ \alpha_1^e \end{bmatrix}}_{\boldsymbol{\alpha}^e} = \boldsymbol{p}(x)\boldsymbol{\alpha}^e \tag{2}$$

Coefficients are expressed in term of nodal values:

$$\begin{array}{rrrl} \phi^e(x_1^e) \equiv & \phi_1^e = & \alpha_0^e + \alpha_1^e x_1^e & \\ \phi^e(x_2^e) \equiv & \phi_2^e = & \alpha_0^e + \alpha_2^e x_2^e & \end{array} \rightarrow \underbrace{\begin{bmatrix} \phi_1^e \\ \phi_2^e \end{bmatrix}}_{\boldsymbol{d}^e} = \underbrace{\begin{bmatrix} 1 & x_1^e \\ 1 & x_2^e \end{bmatrix}}_{\boldsymbol{M}^e} \underbrace{\begin{bmatrix} \alpha_0^e \\ \alpha_1^e \end{bmatrix}}_{\boldsymbol{\alpha}^e}, \tag{3}$$

where $\boldsymbol{d}^e$ is the vector of approximated nodal values of the function ϕ in element e.
The coefficients α are obtained by the inverse form of the previous equation:

$$\boldsymbol{\alpha}^e = (\boldsymbol{M}^e)^{-1}\boldsymbol{d}^e. \tag{4}$$

The approximation can be expressed now:

$$\phi^e = \boldsymbol{N}^e\boldsymbol{d}^e, \qquad \boldsymbol{N}^e = \boldsymbol{p}^e(\boldsymbol{M}^e)^{-1}. \tag{5}$$

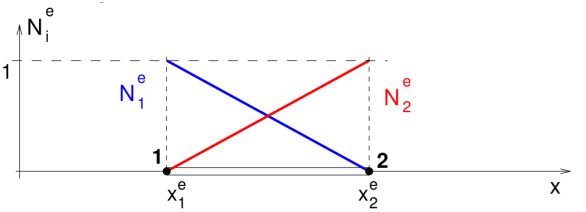
From the inverse matrix

$$(\boldsymbol{M}^e)^{-1} = \frac{1}{x_2^e - x_1^e}\begin{bmatrix} x_2^e & -x_1^e \\ -1 & 1 \end{bmatrix}, \tag{6}$$

we obtain the element shape function matrix:

$$\boldsymbol{N}^e = \begin{bmatrix} \frac{x_2^e - x}{l^e}, & \frac{x - x_1^e}{l^e} \end{bmatrix} = [N_1^e, N_2^e]\,. \tag{7}$$

The approximation ϕ^e is written as $\phi^e = \boldsymbol{N}^e(x)\boldsymbol{d}^e$, where $\boldsymbol{N}^e(x)$ is the element shape function matrix.



The previous approximation can be interpreted as a linear combination of shape functions N_i^e:

$$\phi^e = \boldsymbol{N}^e(x)\boldsymbol{d}^e = \sum_i N_i^e \phi_i^e. \tag{8}$$

Properties of approximation functions:

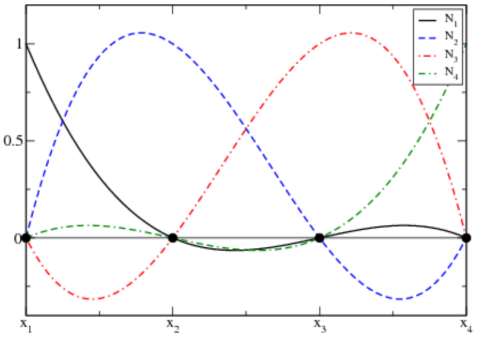
- Kronecker delta property $N_i^e(x_j^e) = \delta_{ij}$:

$$\phi^e(x_j) = \sum_{i=1}^{2} N_i^e(x_j^e)\phi_i^e = \sum_{i=1}^{2} \delta_{ij}\phi_i^e. \tag{9}$$

- $\sum_{i=1}^{2} N_i^e(x_j^e) = 1$, shape functions have to approximate a constant function $\phi(x) = c$, $\phi_i^e = c$. For $\forall i$, we have:

$$c = \sum_{i=1}^{2} N_i^e \phi_i^e = \sum_{i=1}^{2} N_i^e c = c\left(\sum_{i=1}^{2} N_i^e\right). \tag{10}$$

Lagrange interpolation functions exploit the Kronecker delta property. The i-th shape function is equal to zero at all nodes except the j-th.



$$N_i^e = \frac{(x - x_1)\dots(x - x_{i-1})(x - x_{x+1})\dots(x - x_n)}{(x_i - x_1)\dots(x_i - x_{i-1})(x_i - x_{x+1})\dots(x_i - x_n)}, \tag{11}$$

where the numerator expresses Kronecker delta property and the denominator norms the numerator so that the value of shape functions are equal to one at i-th node

- Linear approximation functions for 1D problems:

$$N_1^e = \frac{(x - x_2)}{(x_1 - x_2)},$$
$$N_2^e = \frac{(x - x_1)}{(x_2 - x_1)}.$$

- The vector of linear approximation functions for 1D problems reads:

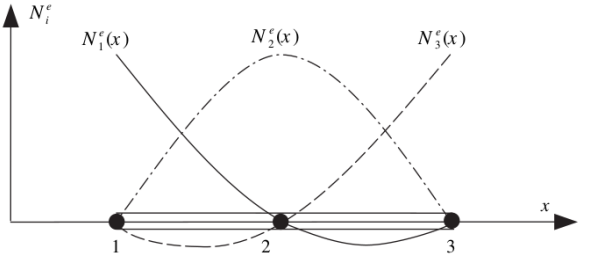
$$\boldsymbol{N}^e = \frac{1}{l^e}\left[(x_2 - x), (x - x_1)\right]. \tag{12}$$

- Quadratic approximation functions for 1D problems:

$$N_1^e = \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)},$$
$$N_2^e = \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)},$$
$$N_3^e = \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)}.$$

- The vector of quadratic approximation functions for 1D problems reads:

$$\boldsymbol{N}^e = \frac{2}{l^{e2}} \left[(x - x_2)(x - x_3), -2(x - x_1)(x - x_3), (x - x_1)(x - x_2) \right]. \tag{13}$$



In general, the weak form cannot be integrated in closed form. For the evaluation of integrals in the weak form, it is better to map the physical domain $[a, b]$ to the parent domain $[-1, 1]$ with the natural coordinate ξ. And then the numerical integration is performed from $x_1^e = -1$ to $x_2^e = 1$. The shape functions are transferred into the following forms:

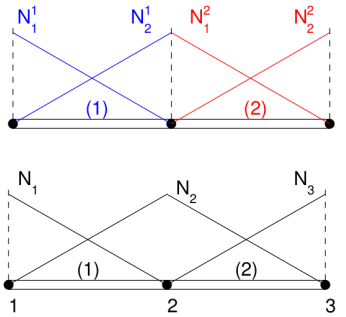
- Linear:

$$N_1^e = \frac{1}{2}(1 - \xi),$$
$$N_2^e = \frac{1}{2}(1 + \xi).$$

- Quadratic:

$$\begin{aligned} N_1^e &= \frac{1}{2}(1 - \xi) - \frac{1}{2}(1 - \xi^2), \\ N_2^e &= (1 - \xi^2), \\ N_3^e &= \frac{1}{2}(1 + \xi) - \frac{1}{2}(1 - \xi^2), \end{aligned}$$

The global approximation of the trial function (and the weight function) is a sum of contribution from individual elements:



$$\phi^h = \sum_{e=1}^{n_{el}} \boldsymbol{N}^e \boldsymbol{d}^e = \boldsymbol{N}^1 \boldsymbol{d}^1 + \boldsymbol{N}^2 \boldsymbol{d}^2$$

$$\phi^h = \left[\; N_1^1, \quad N_2^1 + N_1^2, \quad N_2^2 \; \right] \left\{ \begin{array}{c} \xi_1 \\ \xi_2 \\ \xi_3 \end{array} \right\}$$

$$\phi^h = \boldsymbol{N}\boldsymbol{d}$$

- In the Ritz method, approximation functions are selected for the whole domain respecting the shape of the domain, boundary conditions, etc. - the selection is difficult.
- The FEM selects shape functions very easily - they are nonzero in the vicinity of the given node (only in adjacent elements).
- Refinement in the Ritz method is obtained by adding other linear independent basis functions. In the FEM, we perform the refinement of the FE mesh - the domain is discretized by a greater number of elements (more basis (approximation) functions).

- The weak form requires the calculation of integrals which is difficult for arbitrary domains. Therefore, numerical integration is needed. There are many numerical integration techniques. Gauss quadrature is one of the most efficient techniques for polynomials.
- Consider the following integral over a parent domain:

$$I = \int_{-1}^{1} f(\xi) \mathrm{d}\xi. \tag{14}$$

- The integral value, we approximate by

$$\hat{I} = \sum_{i=1}^{n} w_i f(\xi_i), \tag{15}$$

where w_i are the weights and ξ_i are the points at which the integrand is to be evaluated.

- The basic idea of the Gauss quadrature is to choose the weights and the integration points so that the highest possible polynomial is integrated precisely. We have $2n$ unknown parameters to select.
- The consequence is that we have n integration points (Gauss points), then we can integrate the polynomial of order $p \leq 2n - 1$.
- The number of integration points needed to integrate a polynomial of order p exactly is given by

$$n \geq \frac{p+1}{2}. \tag{16}$$

- Consider $n = 1$:

$$w_1 f(\xi_1) \approx \int_{-1}^{1} f(\xi)\mathrm{d}\xi. \tag{17}$$

We try to find such a weight w_1 and the point ξ_1 so that the integral will be precise for polynomials of the highest order (the first order). Let's consider $f(\xi) = a\xi + b$, where $a, b \in R$ are constants. We have:

$$w_1 f(\xi_1) = \int_{-1}^{1} f(\xi)\mathrm{d}\xi \implies w_1(a\xi_1 + b) = \int_{-1}^{1} (a\xi_1 + b)\mathrm{d}\xi \implies$$

$$w_1(a\xi_1 + b) = \left[(a\frac{\xi^2}{2} + b\xi)\right]_{-1}^{1} \implies a\xi_1 w_1 + bw_1 = 0 \cdot a + 2 \cdot b. \tag{18}$$

- For the arbitrary polynomial of the first order ($a, b \neq 0$):

$$\begin{aligned} \xi_1 w_1 &= 0, \\ w_1 &= 2. \end{aligned}$$

- The required solution is:

$$\xi_1 = 0, \quad w_1 = 2, \quad \int_{-1}^{1} f(\xi)\mathrm{d}\xi \approx 2f(0).$$

- Consider $n = 2$:

$$w_1 f(\xi_1) + w_2 f(\xi_2) \approx \int_{-1}^{1} f(\xi)\mathrm{d}\xi. \tag{19}$$

We try to find such weights w_1, w_2 and the points ξ_1, ξ_2 so that the integral will be precise for polynomials of the highest order. Let's consider $f(\xi) = a\xi^3 + b\xi^2 + c\xi + d$. Introduction into Eq. (19), we get:

$$\begin{aligned}
w_1 f(\xi_1) + w_2 f(\xi_2) &= \int_{-1}^{1} f(\xi)\mathrm{d}\xi \implies \\
w_1[a\xi_1^3 + b\xi_1^2 + c\xi_1 + d] + w_2[a\xi_2^3 + b\xi_2^2 + c\xi_2 + d] &= \int_{-1}^{1} [a\xi^3 + b\xi^2 + c\xi + d]\mathrm{d}\xi \implies \\
w_1[a\xi_1^3 + b\xi_1^2 + c\xi_1 + d] + w_2[a\xi_2^3 + b\xi_2^2 + c\xi_2 + d] &= \left[\frac{a\xi^4}{4} + \frac{b\xi^3}{3} + \frac{c\xi^2}{2} + d\xi\right]_{-1}^{1} \implies \\
a[w_1\xi_1^3 + w_2\xi_2^3] + b[w_1\xi_1^2 + w_2\xi_2^2 - 2/3] &+ c[w_1\xi_1 + w_2\xi_2] - d[w_1 + w_2 - 2] = 0.
\end{aligned}$$

- For the arbitrary polynomial of the third order ($a, b, c, d \neq 0$):

$$\begin{aligned} w_1\xi_1^3 + w_2\xi_2^3 &= 0, \\ w_1\xi_1^2 + w_2\xi_2^2 - 2/3 &= 0, \\ w_1\xi_1 + w_2\xi_2 &= 0, \\ w_1 + w_2 - 2 &= 0. \end{aligned}$$

- The required solution is:

$$\xi_1 = \frac{-1}{\sqrt{3}}, \quad \xi_2 = \frac{1}{\sqrt{3}}, \qquad w_1 = w_2 = 1.$$

The previous algorithm is not really used for determining of weights and positions of Gauss points. For the optimal precision of polynomial integration (order $2n-1$, interval $[-1,1]$), the coordinates of Gauss points are determined as roots of Legendre polynomials. Legendre polynomials are defined by a "recursive formula":

$$P_{k+1}(x) = \frac{2k+1}{k+1} x P_k(x) - \frac{k}{k+1} P_{k-1}(x), \quad \text{where} \quad P_0(x) = 1, \quad P_1(x) = x.$$

The weights are defined by:

$$w_i = \int_{-1}^{1} \prod_{k=1, k\neq i}^{n} \frac{x - x_i}{x_k - x_i} \mathrm{d}x.$$

Table of position of Gauss points and corresponding weights:

n	ξ_i	w_i
1	0.0	2.0
2	$\pm 1/\sqrt{3}$	1.0
3	$\pm$ 0.7745966692	0.555 555 5556
	0.0	0.888 888 8889
4	$\pm$ 0.8611363116	0.347 854 8451
	$\pm$ 0.3399810436	0.652 145 1549
5	$\pm$ 0.9061798459	0.236 926 8851
	$\pm$ 0.5384693101	0.478 628 6705
	0.0	0.568 888 8889
6	$\pm$ 0.9324695142	0.171 324 4924
	$\pm$ 0.6612093865	0.360 761 5730
	$\pm$ 0.2386191861	0.467 913 9346

Numerical example:

- Determine the value of the integral:

$$I = \int_{-1}^{1} \left(x^4 + 4 \cdot x^3 - 2 \cdot x^2 - 2 \cdot x + 1\right) \mathrm{d}x \tag{20}$$

- Analytical solution:

- Gauss quadrature:

Numerical example:

- Elements with the same approximation of trial function and the geometry (coordinates x, y, z), For 1D bar element with linear approximation functions:

$$x^e(\xi) = N_1^e(\xi)x_1^e + N_2^e(\xi)x_2^e = \frac{1}{2}(1-\xi)x_1^e + \frac{1}{2}(1+\xi)x_2^e. \tag{21}$$

- Integration is in natural coordinate system (parent domain):

$$\int_{x_1}^{x_2} f(x)\mathrm{d}x = \int_{-1}^{1} f\left(x(\xi)\right) J\mathrm{d}\xi = \sum_i f\left(x(\xi)\right) J w_i, \tag{22}$$

where $J = \frac{\mathrm{d}x}{\mathrm{d}\xi} = \frac{l^e}{2}$ is the Jacobian of transformation.

References

- English course of "Numerical analysis of structures" by J. Zeman (jan.zeman@fsv.cvut.cz)
- Czech course of "Numerická analýza konstrukcí" (Numerical analysis of structures) by B. Patzák (borek.patzak@fsv.cvut.cz)
- J. Fish and T. Belytschko: A First Course in Finite Elements, John Wiley & Sons, 2007