有限元素法：

1. Weighted Residue Methods.（最小余量 子空间）

类似于最小二乘法：

$\{(x_i, y_i) \mid i=1, \cdots, N\}$

$y=f(x)=ax+b$.

的最合适的 a 与 b 是什么？

$$L = \sum_i (ax_i+b-y_i)^2$$

$\frac{\partial L}{\partial a}=0$, $\frac{\partial L}{\partial b}=0$.

$\sum_i x_i(ax_i+b-y_i)=0$. $\sum_i ax_i+b-y_i=0$

变分法：

$H\psi_0=E_0\psi_0$

假设 $\psi_0 = f(\vec{x};\beta_1,\cdots\beta_n)$, $|f|^2=1$.

$$E_0=\langle\psi_0|H|\psi_0\rangle=\int d\vec{x}\ f^*\hat{H}f$$

确定参量.

共性：①限定解集在某受限子空间：
- 例1. 最小二乘：线性函数集合.
- 例2. 变分求基态：试探函数.

②找出真实解应满足的方程.
- 例1：最小二乘：平方和为零（最小）.
- 例2：变分法：能量为极值.

③假定此方程性质对限定解集也成立，求出解.

微分方程：

$$L\phi=\nabla\cdot(p(\vec{r})\nabla\phi(\vec{r}))+q(\vec{r})\cdot\phi(\vec{r})=f(\vec{r})$$

则 $L\phi(\vec{r})-f(\vec{r})=0$. 恒成立.

考虑完整函数空间的一个子空间，其基为：$|w_i\rangle$, $i=1,\cdots,N$.

则 $\langle w_i|L\phi(\vec{r})-f(\vec{r})\rangle=0$ 恒成立.

（注：若 $|w_i\rangle$ 组成完整空间，则为严格解）

$\phi(\vec{r}) = \sum C_i \phi_i(\vec{r})$

$\uparrow$

一些试探解.

则目的为求 C_i.

$\Rightarrow \sum_i C_i \langle w_j | L\phi_i \rangle = \langle w_j | f(\vec{r}) \rangle$

$\Downarrow$

构成 C_i 的线性方程组.

Galerkin 法: $|w_j\rangle = |\phi_j\rangle$. (同空间).

(设: $\phi \in Real$)

$\Updownarrow$

$\mathcal{L} = \langle \phi | L\phi - 2f \rangle$

$= -2\sum_i C_i \langle \phi_i | f \rangle + \sum_{ij} C_i C_j \langle \phi_i | L \phi_j \rangle$

$\frac{\partial \mathcal{L}}{\partial C_i} = 0 \Rightarrow -2\langle \phi_i | f \rangle + \sum_j C_j \langle \phi_i | L\phi_j \rangle + \sum_j C_j \langle \phi_j | L \phi_i \rangle = 0$

若: $\phi_i|_{\partial D} = 0$ 或 $\nabla \phi_i|_{\partial D} = 0$ (边界处不需分).

则: $\langle \phi_j | L \phi_i \rangle = \langle \phi_i | L \phi_j \rangle$

$\Rightarrow \sum_j C_j \langle \phi_i | L \phi_j \rangle = \langle \phi_i | f \rangle$

(退回原方程)

变分方程与边条件.

1D:

$$L\phi = \frac{d}{dx}\left(p(x)\frac{d\phi}{dx}\right) + q(x)\phi(x) = f(x), \quad \phi|_{\partial D} = 0$$

$$\langle \phi_i | L\phi_j \rangle = \int \phi_i \left(\frac{d}{dx} p(x) \frac{d\phi_j}{dx} + q(x)\phi_j(x)\right) dx$$

$$= \phi_i\, p(x) \frac{d\phi_j}{dx}\Big|_a^b - \int_a^b p(x)\phi_i'\phi_j' \, dx + \int_a^b q(x)\phi_i\phi_j \, dx$$

若 $\phi_i|_{\partial D} = 0$

$$\Rightarrow \langle \phi_i | L\phi_j \rangle = -\int_a^b p(x)\phi_i'\phi_j' \, dx + \int_a^b q(x)\phi_i\phi_j \, dx$$

= 阶导数消失了.

2D: $\nabla^2\phi = -\rho$ (Poisson Equation)

$$\phi|_{\partial D} = f(s)$$

变分 $\delta\phi$: $\delta\phi|_{\partial D} = 0$

$$\Rightarrow L = \langle \phi | \nabla^2\phi + 2\rho \rangle$$

$$= \int \phi \nabla^2\phi \, d\vec{r} + 2\int \rho\phi \, dr$$

$$= -\int \nabla\phi\cdot\nabla\phi \, d\vec{r} + 2\int \rho\phi \, d\vec{r}$$

$$\frac{\partial L}{\partial \delta\phi} = \nabla^2\phi + \rho = 0$$

$$L\phi = -\nabla\cdot(p\nabla\phi) + q\phi = \rho$$

$$\phi|_{\Gamma_1} = F(s), \quad \frac{\partial\phi}{\partial n} + q(s)\phi = b(s), \ s\in\Gamma_2, \quad \Gamma_1 \oplus \Gamma_2 = \partial D.$$

$$\mathcal{L}\phi = \int (p|\nabla\phi|^2 + g\phi^2 - 2\rho\phi)\,d\vec{r} + \int_{\Gamma_2} (p q\,\phi^2 - 2 p\cdot b\,\phi)\,ds$$

变分：$\delta\phi$，$\delta\phi|_{\Gamma_1} = 0$.

$$\frac{\partial \mathcal{L}}{\partial \delta\phi} = 2\int_{\Gamma_2} p\frac{\partial\phi}{\partial n}\cdot\delta\phi\,ds - 2\int \delta\phi\,\overset{\nabla\cdot(p\nabla\phi)}{}\,d\vec{r} + 2\int(g\phi\,\delta\phi - \rho\,\delta\phi)\,d\vec{r}$$

$$+\ 2\int_{\Gamma_2}(p\cdot q\phi\,\delta\phi - p\cdot b\,\delta\phi)\,ds$$

$$\Rightarrow\ -\nabla\cdot(p\nabla\phi) + g\phi = \rho$$

$$\Gamma_2:\ p\cdot\frac{\partial\phi}{\partial n} + p\cdot q\,\phi = p\cdot b$$

$$\Rightarrow\ \frac{\partial\phi}{\partial n} + q\phi = b,\quad s\in\Gamma_2.$$

1D 案例：

$$-p(x)\,\phi''(x) + q(x)\,\phi(x) = f(x),\quad x\in[0,1]$$

$$\phi(0) = \phi(1) = 0$$

(假设：$p(x) = p > 0$，$q(x) = q \geq 0$)

$$L = \int_0^1 p(x)\,\phi'(x)\,\phi'(x)\,dx + \int_0^1 (2q\phi^2 - 2f\phi)\,dx$$

(1) 分割：$[0,1]$ 分成 N 份（不需均匀）

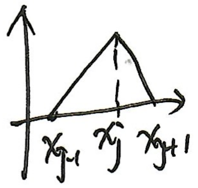
$0 = x_0 < x_1 < \cdots < x_{N-1} < x_N = 1.$

$[x_{j-1}, x_j]$ 长为 $h_j = x_j - x_{j-1}$（有限元素）.

② 选基：

ϕ_j： $[x_{j-1}, x_j] \cup [x_j, x_{j+1}]$，节点：$x_{j-1}, x_{j+1}$ 以x_j

图：



$$\phi_j = \begin{cases} \dfrac{x - x_{j-1}}{x_j - x_{j-1}}, & x_{j-1} \le x \le x_j \\ \dfrac{x_{j+1} - x}{x_{j+1} - x_j}, & x_j \le x \le x_{j+1} \\ 0, & \text{otherwise.} \end{cases}$$

$\phi_j(x_k) = \delta_{jk}.$

③ 近似解：$\phi(x) = \sum_{j=1}^{N-1} c_j \phi_j(x)$

（注：已用到边条件 $\phi(0) = \phi(1) = 0$）

否则：

$\phi(x) = \sum_{j=0}^{N} c_j \phi_j(x)$，

$\phi_0 = \dfrac{x - x_0}{x_1 - x_0}$，

$\phi_N = \dfrac{x_N - x}{x_N - x_{N-1}}$，

$c_0 = \phi(0)$, $c(1) = \phi(1)$）

④ 方程组：

$\langle \phi_i | L\phi - f \rangle = 0, \quad \forall\, i \in [1, N-1]$

注：i 的范围不含 0 与 N，则变分自动包含 $\delta\phi(0) = \delta\phi(1) = 0$.