

## 2.2. 目标轮廓曲线的表示. (傅立叶展开)

$$L: (x(\sigma), y(\sigma)).$$

①  $x(\sigma), y(\sigma)$  满足 Dirichlet 条件  $x(0)=x(\pi)=0$   $y(0)=y(\pi)=0$

$$x(\sigma) = \sum_{n=1}^{+\infty} X_n \sin(n\sigma) \quad y(\sigma) = \sum_{n=1}^{+\infty} Y_n \sin(n\sigma) \quad \sigma \in [0, \pi]$$

$$X_n = \frac{2}{\pi} \int_0^{\pi} x(\sigma) \sin(n\sigma) d\sigma \quad Y_n = \frac{2}{\pi} \int_0^{\pi} y(\sigma) \sin(n\sigma) d\sigma$$

②  $x(\sigma), y(\sigma)$  满足 Neuman 条件  $\left. \frac{dx}{d\sigma} \right|_{\sigma=0} = \left. \frac{dx}{d\sigma} \right|_{\sigma=\pi} = \left. \frac{dy}{d\sigma} \right|_{\sigma=0} = \left. \frac{dy}{d\sigma} \right|_{\sigma=\pi} = 0$

$$x(\sigma) = \sum_{n=1}^{+\infty} X_n \cos(n\sigma) \quad y(\sigma) = \sum_{n=1}^{+\infty} Y_n \cos(n\sigma)$$

$$X_n = \frac{2}{\pi} \int_0^{\pi} x(\sigma) \cos(n\sigma) d\sigma \quad Y_n = \frac{2}{\pi} \int_0^{\pi} y(\sigma) \cos(n\sigma) d\sigma$$

③  $x(0)=x_s$   $x(\pi)=x_e$   $y(0)=y_s$   $y(\pi)=y_e$

$$\begin{aligned} \text{变换 } \bar{x}(\sigma) &= x(\sigma) - x_s - \frac{x_e - x_s}{\pi} \sigma \\ \bar{y}(\sigma) &= y(\sigma) - y_e - \frac{y_e - y_s}{\pi} \sigma \end{aligned} \quad \sigma \in [0, \pi]$$

条件化为 ①.

$$\bar{x}(\sigma) = \sum_{n=1}^{+\infty} X_n \sin(n\sigma) \quad \bar{y}(\sigma) = \sum_{n=1}^{+\infty} Y_n \sin(n\sigma) \quad \sigma \in [0, \pi]$$

$$\therefore x(\sigma) = x_s + \frac{x_e - x_s}{\pi} \sigma + \sum_{n=1}^{+\infty} X_n \sin(n\sigma)$$

$$y(\sigma) = y_s + \frac{y_e - y_s}{\pi} \sigma + \sum_{n=1}^{+\infty} Y_n \sin(n\sigma)$$

$$x'(\sigma) = \frac{x_e - x_s}{\pi} + \sum_{n=1}^{+\infty} n X_n \cos(n\sigma) \quad y'(\sigma) = \frac{y_e - y_s}{\pi} + \sum_{n=1}^{+\infty} n Y_n \cos(n\sigma)$$

$$x''(\sigma) = - \sum_{n=1}^{+\infty} n^2 X_n \sin(n\sigma) \quad y''(\sigma) = - \sum_{n=1}^{+\infty} n^2 Y_n \sin(n\sigma)$$

### 3.1 目标轮廓模型的建立.

$$E_{tol} = E_{int} + E_{ext}$$

$$\text{动能 } E_{int-1} = \frac{1}{2} \int_0^{\pi} ((x'(\sigma))^2 + (y'(\sigma))^2) d\sigma$$

$$\text{势能 } E_{int-2} = \frac{1}{2} \int_0^{\pi} ((x''(\sigma))^2 + (y''(\sigma))^2) d\sigma$$

$$E_{int} = \alpha E_{int-1} + \beta E_{int-2} \quad \alpha, \beta \text{ 权重系数}$$

$$E_{ext} = \int_0^{\pi} f(x, y) d\sigma \quad f(x, y) = 1 - |\nabla(x(\sigma), y(\sigma))|^2$$

$$E_{tol} = \frac{1}{2} \int_0^{\pi} \alpha ((x'(\sigma))^2 + (y'(\sigma))^2) + \beta ((x''(\sigma))^2 + (y''(\sigma))^2) d\sigma + \int_0^{\pi} f(x, y) d\sigma$$

$$\int_0^{\pi} (x'(\sigma))^2 d\sigma = \int_0^{\pi} \left( \frac{x_e - x_s}{\pi} + \sum_{n=1}^{+\infty} n X_n \cos(n\sigma) \right)^2 d\sigma = \frac{(x_e - x_s)^2}{\pi} + \frac{\pi}{2} \sum_{n=1}^{+\infty} n^2 X_n^2$$

$$\int_0^{\pi} (x''(\sigma))^2 d\sigma = \int_0^{\pi} \left( - \sum_{n=1}^{+\infty} n^2 X_n \sin(n\sigma) \right)^2 d\sigma = \frac{\pi}{2} \sum_{n=1}^{+\infty} n^4 X_n^2$$

$$\int_0^{\pi} (y'(\sigma))^2 d\sigma = \frac{(y_e - y_s)^2}{\pi} + \sum_{n=1}^{+\infty} n^2 Y_n^2 \quad \int_0^{\pi} (y''(\sigma))^2 d\sigma = \frac{\pi}{2} \sum_{n=1}^{+\infty} n^4 Y_n^2$$

$$E_{tol} = \frac{\pi}{4} \sum_{n=1}^{+\infty} (\alpha n^2 + \beta n^4) (X_n^2 + Y_n^2) + \frac{\alpha[(x_e - x_s)^2 + (y_e - y_s)^2]}{2\pi} + \int_0^{\pi} f(x(\sigma), y(\sigma)) d\sigma$$

$$\text{离散化} \quad E_{tol} \approx \frac{\pi}{4} \sum_{n=1}^{+\infty} (\alpha n^2 + \beta n^4) (X_n^2 + Y_n^2) + \frac{\alpha[(x_e - x_s)^2 + (y_e - y_s)^2]}{2\pi} + \frac{\pi}{m} \sum_{m=1}^M f(x(\frac{m\pi}{m}), y(\frac{m\pi}{m}))$$

$$\text{极小值条件} \quad \frac{\partial E_{tol}}{\partial X_n} = \frac{\partial E_{tol}}{\partial Y_n} = 0 \quad n=1, 2, \dots, N$$

$$\left\{ \begin{aligned} (\alpha + \beta) X_1 + \frac{\pi}{m} \sum_{m=1}^M f_x(x(\frac{m\pi}{m}), y(\frac{m\pi}{m})) \sin \frac{m\pi}{m} &= 0 \\ (\alpha n^2 + \beta n^4) X_n + \frac{\pi}{m} \sum_{m=1}^M f_x(x(\frac{m\pi}{m}), y(\frac{m\pi}{m})) \sin \frac{mn\pi}{m} &= 0 \\ (\alpha + \beta) Y_1 + \frac{\pi}{m} \sum_{m=1}^M f_y(x(\frac{m\pi}{m}), y(\frac{m\pi}{m})) \sin \frac{m\pi}{m} &= 0 \\ (\alpha n^2 + \beta n^4) Y_n + \frac{\pi}{m} \sum_{m=1}^M f_y(x(\frac{m\pi}{m}), y(\frac{m\pi}{m})) \sin \frac{mn\pi}{m} &= 0 \end{aligned} \right.$$

$$(\alpha n^2 + \beta n^4) X_n + \frac{\pi}{m} \sum_{m=1}^M f_x(x(\frac{m\pi}{m}), y(\frac{m\pi}{m})) \sin \frac{mn\pi}{m} = 0$$

$$(\alpha + \beta) Y_1 + \frac{\pi}{m} \sum_{m=1}^M f_y(x(\frac{m\pi}{m}), y(\frac{m\pi}{m})) \sin \frac{m\pi}{m} = 0$$

$$(\alpha n^2 + \beta n^4) Y_n + \frac{\pi}{m} \sum_{m=1}^M f_y(x(\frac{m\pi}{m}), y(\frac{m\pi}{m})) \sin \frac{mn\pi}{m} = 0$$

### 3.2 模型求解

$$\begin{cases} g_1(x_1, \dots, x_n, y_1, \dots, y_n) = 0 \\ g_2(x_1, \dots, x_n, y_1, \dots, y_n) = 0 \\ \vdots \\ g_{2n}(x_1, \dots, y_n) = 0 \end{cases} \quad \text{记 } G(z) = [g_1(z), \dots, g_n(z)]^T$$

$$z = (x_1, \dots, y_n)^T$$

$$\Rightarrow G(z) = 0$$

迭代法  $z' = \varphi(z)$   $\varphi: D \subset \mathbb{R}^n \rightarrow \mathbb{R}^n$   $\varphi(z) = [\varphi_1(z), \dots, \varphi_n(z)]^T$

$z_{k+1} = \varphi(z_k)$  需要  $\|\varphi(x) - \varphi(y)\| \leq L \|x - y\| \quad \forall x, y \in \mathbb{R}^n \quad L \in (0, 1)$

Taylor  $G(z) \approx G(z_k) + G'(z_k)(z - z_k)$  取  $z_{k+1} = G(z_k) + G'(z_k)(z_{k+1} - z_k)$

取  $G(z_{k+1}) \approx 0$   $z_{k+1} = z_k - (G'(z_k))^{-1} G(z_k)$  需要  $G'(z_k)$  可逆.

#### 3.2.1 逆 Broyden 秩 1 法

$$A_k = G'(z_k) \quad z_{k+1} = z_k - A_k^{-1} G(z_k)$$

用差商代替求解导数  $A_{k+1}(z_{k+1} - z_k) = G(z_{k+1}) - G(z_k)$  ①

设  $A_{k+1} = A_k + \Delta A_k$   $\text{rank}(\Delta A_k) = 1$  设  $\Delta A_k = u_k v_k^T$  代入 ①

$$u_k = \frac{1}{v_k^T s_k} (y_k - A_k s_k) \quad s_k = z_{k+1} - z_k \quad y_k = G(z_{k+1}) - G(z_k)$$

令  $v_k = s_k$   $u_k = \frac{1}{\|s_k\|^2} (y_k - A_k s_k)$  记  $B_k = A_k^{-1}$

由 Sherman-Morrison 公式 对非奇异阵  $A_k$  当  $1 + v_k^T A_k u_k \neq 0$

$$(A_k + u_k v_k^T)^{-1} = A_k^{-1} - \frac{A_k^{-1} u_k v_k^T A_k^{-1}}{1 + v_k^T A_k^{-1} u_k}$$

$$\therefore B_{k+1} = (A_k + u_k v_k^T)^{-1} = B_k - \frac{1}{s_k^T B_k^T y_k} (B_k y_k - s_k) B_k^T$$

至此  $z_{k+1} = z_k - B_k G(z_k)$

$B_0$  可取  $G'(z_0)^{-1}$

#### 4.1 建立目标轮廓能量泛出模型.

$$E_{tot} = E_{int} + E_{ext}. \quad E_{ext} = \int_L f(x, y) ds. \quad f(x, y) \text{ 为势函数}$$

$$\text{取 } f(x, y) = e^{-\frac{1}{2} \| (x(\sigma), y(\sigma)) \|^2}$$

$$E_{tot} = \frac{\pi}{4} \sum_{n=1}^{\infty} (\alpha n^2 + \beta n^4) (X_n^2 + Y_n^2) + \frac{\int_L [(Xe - Xs)^2 + (Ye - Ys)^2]}{2\pi} + \int_L f(x, y) ds$$

离散化.

$$E_{tot} = \frac{\pi}{4} \sum_{n=1}^{\infty} (\alpha n^2 + \beta n^4) (X_n^2 + Y_n^2) + \frac{\int_L [(Xe - Xs)^2 + (Ye - Ys)^2]}{2\pi} + \sum_{m=0}^{M-1} f(x(\frac{m\pi}{M}), y(\frac{m\pi}{M})) \beta S_m$$

$$\Delta S_m = \sqrt{(x(\frac{(m+1)\pi}{M}) - x(\frac{m\pi}{M}))^2 + (y(\frac{(m+1)\pi}{M}) - y(\frac{m\pi}{M}))^2}$$

#### 4.2 简模型求解.

##### 4.2.1 响应函数.

$$h_{\sigma_0}(\sigma) : (1) h_{\sigma_0}(\sigma) \geq 0. (2) h_{\sigma_0}(0) = h_{\sigma_0}(\pi) = 0. h_{\sigma_0}(\sigma_0) = 1.$$

$$(3) h_{\sigma_0}(\sigma) \text{ 在 } [0, \sigma_0] \text{ 上单增 } [\sigma_0, \pi] \text{ 递减 } (4) h_{\sigma_0}''(\sigma) \text{ 连续}$$

$$\text{取 } h_{\sigma_0}(\sigma) = e^{-r(\sigma-\sigma_0)^2} - a(\sigma-\sigma_0)^{2n} \quad n \geq 2.$$

$$\text{由 (2)} \Rightarrow a = \begin{cases} \frac{e^{-r\sigma_0^2}}{\sigma_0^{2n}} & 0 < \sigma < \sigma_0 \\ \frac{e^{-r(\pi-\sigma_0)^2}}{(\sigma_0 - \pi)^{2n}} & \sigma_0 < \sigma < \pi. \end{cases}$$

$$\therefore h_{\sigma_0}(\sigma) \text{ 满足 Dirichlet 条件} \quad h_{\sigma_0}(\sigma) = \sum_{n=1}^{\infty} H(\sigma_0, n) \sin n\sigma.$$

$$H_n = \frac{2}{\pi} \int_0^{\pi} h_{\sigma_0}(\sigma) \sin n\sigma d\sigma \approx \frac{2}{m} \sum_{m=0}^{M-1} h_{\sigma_0}(\frac{m\pi}{M}) \sin(\frac{m\pi}{M}).$$

$$\begin{cases} x_1(\sigma) = x_0(\sigma) + d h_{\sigma_0}(\sigma) \\ y_1(\sigma) = y_0(\sigma) + d h_{\sigma_0}(\sigma) \end{cases} \quad \begin{cases} x_1(\sigma) = X_s + \frac{X_e - X_s}{\pi} \sigma + \sum_{n=1}^{\infty} (X_n + d H(\sigma_0, n)) \sin n\sigma \\ y_1(\sigma) = Y_s + \frac{Y_e - Y_s}{\pi} \sigma + \sum_{n=1}^{\infty} (Y_n + d H(\sigma_0, n)) \sin n\sigma \end{cases}$$

迭代前系数  $X_{01}, \dots, X_{0m}, Y_{01}, \dots, Y_{0m}$ .

$$\begin{cases} X_{1i} = X_{0i} + d H_{\sigma_0}(i) \\ Y_{1i} = Y_{0i} + d H_{\sigma_0}(i) \end{cases}$$

初始值  $X_i = Y_i = 0$

$$\begin{cases} x(\sigma) = X_s + \frac{X_e - X_s}{\pi} \sigma + \sum_{m=1}^m x_i h_{\sigma_i}(\sigma) \\ y(\sigma) = Y_s + \frac{Y_e - Y_s}{\pi} \sigma + \sum_{m=1}^m y_i h_{\sigma_i}(\sigma) \end{cases} \quad \begin{cases} X_n = \sum_{m=1}^m x_i H_{\sigma_i}(n) \\ Y_n = \sum_{m=1}^m y_i H_{\sigma_i}(n) \end{cases}$$

## 4.2.2 模型求解

(1) 选取初始状态

$$\begin{cases} x(0) = x_s + \frac{x_e - x_s}{\pi} \delta & x_m = y_m = 0 \\ y(0) = y_s + \frac{y_e - y_s}{\pi} \delta & x_n = y_n = 0 \end{cases}$$

$$E_{int} = \frac{\sqrt{[(x_e - x_s)^2 + (y_e - y_s)^2]}}{2\pi} \quad E_{ext} = \sum_{m=0}^{M-1} f\left(x\left(\frac{m\pi}{M}\right), y\left(\frac{m\pi}{M}\right)\right) \delta s_m$$

$$E_{tol} = E_{int} + E_{ext}$$

(2) 设置可变范围

$$0x, 0y \in [-d, d]$$

$$\text{找 } E_{min} = \min_{\substack{1 \leq m_0 \leq M \\ -d \leq 0x \leq d \\ -d \leq 0y \leq d}} E(x(0) + 0x h_{\delta m_0}, y(0) + 0y h_{\delta m_0}(\delta))$$

(3) 若  $E_{min} < E(x(0), y(0))$  取  $E_{tol} = E_{min}$

更新  $x_n, y_n$ , 转回(2) 否则 终止