Optimização pelo Método dos Mínimos Quadrados

Pretende-se encontrar os coeficientes da função paramétrica, pela optimização dos mínimos quadrados, dada pela função;

$$f(a_i) = \sum_{k=0}^{n} \left(a_1 + a_2 V_k + a_3 \alpha_k + a_4 V_k^2 + a_5 V_k \alpha_k + a_6 \alpha_k^2 + a_7 V_k \alpha_k^2 + a_8 V_k^2 \alpha_k^2 + a_9 V_k^3 + a_{10} \alpha_k^3 - MatrizDisc\right)^2$$

Sabe-se que esses coeficientes que minimizam a função $f(a_i)$ têm de satisfazer:

$$\frac{\partial f(a_i)}{\partial a_i} = 0$$

Isso leva-nos a um sistema de equações lineares; $C.a = q$, sendo:

$$C = \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} & c_{1,6} & c_{1,7} & c_{1,8} & c_{1,9} & c_{1,10} \\ c_{2,1} & c_{2,2} & c_{2,3} & c_{2,4} & c_{2,5} & c_{2,6} & c_{2,7} & c_{2,8} & c_{2,9} & c_{2,10} \\ c_{3,1} & c_{3,2} & c_{3,3} & c_{3,4} & c_{3,5} & c_{3,6} & c_{3,7} & c_{3,8} & c_{3,9} & c_{3,10} \\ c_{4,1} & c_{4,2} & c_{4,3} & c_{4,4} & c_{4,5} & c_{4,6} & c_{4,7} & c_{4,8} & c_{4,9} & c_{4,10} \\ c_{5,1} & c_{5,2} & c_{5,3} & c_{5,4} & c_{5,5} & c_{5,6} & c_{5,7} & c_{5,8} & c_{5,9} & c_{5,10} \\ c_{6,1} & c_{6,2} & c_{6,3} & c_{6,4} & c_{6,5} & c_{6,6} & c_{6,7} & c_{6,8} & c_{6,9} & c_{6,10} \\ c_{7,1} & c_{7,2} & c_{7,3} & c_{7,4} & c_{7,5} & c_{7,6} & c_{7,7} & c_{7,8} & c_{7,9} & c_{7,10} \\ c_{8,1} & c_{8,2} & c_{8,3} & c_{8,4} & c_{8,5} & c_{8,6} & c_{8,7} & c_{8,8} & c_{8,9} & c_{8,10} \\ c_{9,1} & c_{9,2} & c_{9,3} & c_{9,4} & c_{9,5} & c_{9,6} & c_{9,7} & c_{9,8} & c_{9,9} & c_{9,10} \\ c_{10,1} & c_{10,2} & c_{10,3} & c_{10,4} & c_{10,5} & c_{10,6} & c_{10,7} & c_{10,8} & c_{10,9} & c_{10,10} \end{bmatrix}$$

Onde;

$$a = [a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \quad a_8 \quad a_9 \quad a_{10}]$$

$$q = [q_1 \quad q_2 \quad q_3 \quad q_4 \quad q_5 \quad q_6 \quad q_7 \quad q_8 \quad q_9 \quad q_{10}]^T$$

Onde:

$$q_1 = \sum_{k=1}^{n} MatrizDisc_k \ , \quad q_2 = \sum_{k=1}^{n} V_k MatrizDisc_k \ , \quad q_3 = \sum_{k=1}^{n} \alpha_k MatrizDisc_k \ , \quad q_4 = \sum_{k=1}^{n} V^2 MatrizDisc_k \ ,$$

$$q_5 = \sum_{k=1}^{n} V\alpha MatrizDisc_k \ , \quad q_6 = \sum_{k=1}^{n} \alpha^2 MatrizDisc_k \ , \quad q_7 = \sum_{k=1}^{n} V_k \alpha_k^2 MatrizDisc_k \ ,$$

$$q_8 = \sum_{k=1}^{n} V_k^2 \alpha_k^2 MatrizDisc_k \ , \quad q_9 = \sum_{k=1}^{n} V_k^3 MatrizDisc_k \ , \quad q_{10} = \sum_{k=1}^{n} \alpha_k^3 MatrizDisc_k \ ,$$

$$c_{1,1} = n, \quad c_{1,2} = \sum_{k=1}^{n} V_k \ , \quad c_{1.3} = \sum_{k=1}^{n} \alpha_k \ , \quad c_{1,4} = \sum_{k=1}^{n} V_k^2 \ , \quad c_{1,5} = \sum_{k=1}^{n} V_k \alpha_k \ ,$$

$$c_{1,6} = \sum_{k=1}^{n} \alpha_k^2 \ , \quad c_{1,7} = \sum_{k=1}^{n} V_k \alpha_k^2 \ , \quad c_{1,8} = \sum_{k=1}^{n} V_k^2 \alpha_k^2 \ , \quad c_{1,9} = \sum_{k=1}^{n} V_k^3 \ , \quad c_{1,10} = \sum_{k=1}^{n} \alpha_k^3 \ ,$$

$$c_{2,2} = \sum_{k=1}^{n} V_k^2 \ , \quad c_{2,3} = \sum_{k=1}^{n} V_k \alpha_k \ , \quad c_{2,4} = \sum_{k=1}^{n} V_k^3 \ , \quad c_{2,5} = \sum_{k=1}^{n} V_k^2 \alpha_k \ , \quad c_{2,6} = \sum_{k=1}^{n} V_k \alpha_k^2 \ ,$$

$$c_{2,7} = \sum_{k=1}^{n} V_k^2 \alpha_k^2 \ , \quad c_{2,8} = \sum_{k=1}^{n} V_k^3 \alpha_k^2 \ , \quad c_{2,9} = \sum_{k=1}^{n} V_k^4 \ , \quad c_{2,10} = \sum_{k=1}^{n} V_k \alpha_k^3 \ , \quad c_{3,3} = \sum_{k=1}^{n} \alpha_k^2 \ ,$$

$$c_{3,4} = \sum_{k=1}^{n} V_k^2 \alpha_k \ , \quad c_{3,5} = \sum_{k=1}^{n} V_k \alpha_k^2 \ , \quad c_{3,6} = \sum_{k=1}^{n} \alpha_k^3 \ , \quad c_{3,7} = \sum_{k=1}^{n} V_k \alpha_k^3 \ , \quad c_{3,8} = \sum_{k=1}^{n} V_k^2 \alpha_k^3 \ ,$$

$$c_{3,9} = \sum_{k=1}^{n} V_k^3 \alpha_k \ , \quad c_{3,10} = \sum_{k=1}^{n} \alpha_k^4 \ , \quad c_{4,4} = \sum_{k=1}^{n} V_k^4 \ , \quad c_{4,5} = \sum_{k=1}^{n} V_k^3 \alpha_k \ , \quad c_{4,6} = \sum_{k=1}^{n} V_k^2 \alpha_k^2 \ ,$$

$$c_{4,7} = \sum_{k=1}^{n} V_k^3 \alpha_k^2 \ , \quad c_{4,8} = \sum_{k=1}^{n} V_k^4 \alpha_k^2 \ , \quad c_{4,9} = \sum_{k=1}^{n} V_k^5 \ , \quad c_{4,10} = \sum_{k=1}^{n} V_k^2 \alpha_k^3 \ , \quad c_{5,5} = \sum_{k=1}^{n} V_k^2 \alpha_k^2 \ ,$$

$$c_{5,6} = \sum_{k=1}^{n} V_k \alpha_k^3 \ , \quad c_{5,7} = \sum_{k=1}^{n} V_k^2 \alpha_k^3 \ , \quad c_{5,8} = \sum_{k=1}^{n} V_k^3 \alpha_k^3 \ , \quad c_{5,9} = \sum_{k=1}^{n} V_k^4 \alpha_k \ , \quad c_{5,10} = \sum_{k=1}^{n} V_k \alpha_k^4 \ ,$$

$$c_{6,6} = \sum_{k=1}^{n} \alpha_k^4 \ , \quad c_{6,7} = \sum_{k=1}^{n} V_k \alpha_k^4 \ , \quad c_{6,8} = \sum_{k=1}^{n} V_k^2 \alpha_k^4 \ , \quad c_{6,9} = \sum_{k=1}^{n} V_k^3 \alpha_k^2 \ , \quad c_{6,10} = \sum_{k=1}^{n} \alpha_k^5 \ ,$$

$$c_{7,7} = \sum_{k=1}^{n} V_k^2 \alpha_k^4 \ , \quad c_{7,8} = \sum_{k=1}^{n} V_k^3 \alpha_k^4 \ , \quad c_{7,9} = \sum_{k=1}^{n} V_k^4 \alpha_k^2 \ , \quad c_{7,10} = \sum_{k=1}^{n} V_k \alpha_k^5 \ , \quad c_{8,8} = \sum_{k=1}^{n} V_k^4 \ \alpha_k^4 \ ,$$

$$c_{8,9} = \sum_{k=1}^{n} V_k^5 \alpha_k^2 \ , \quad c_{8,10} = \sum_{k=1}^{n} V_k^2 \alpha_k^5 \ , \quad c_{9,9} = \sum_{k=1}^{n} V_k^6 \ , \quad c_{9,10} = \sum_{k=1}^{n} V_k^3 \alpha_k^3 \ , \quad c_{10,10} = \sum_{k=1}^{n} \alpha_k^6 \ ,$$

De realçar que a matriz C é simétrica. Caso se queira considerar uma superfície quadrática, a matriz C deverá ter dimensão 6×6 (com os primeiros elementos) e os vectores $\boldsymbol{a}$ e $\boldsymbol{q}$ deverão conter os 6 primeiros elementos dos apresentados acima.

O critério que define a figura de mérito é a raiz da média do erro quadrático, em inglês; RMS_{ERROR}:

$$RMS_{ERROR} = \sqrt{\frac{1}{n}\sum_{k=1}^{n}[MatrizDisc_k - MatrizParam(V_k, \alpha_k)]^2}$$

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