

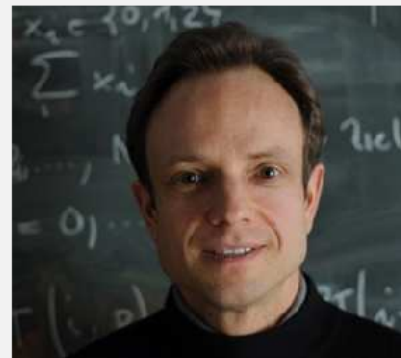
Course Video

Section 8.7: Non-linear Least Squares

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Dependencies. Section 3.1.1

Duration: || minutes

VIII Iterative Methods for Non-Linear Systems of Equations

8.7 Non-Linear Least Squares

$$\text{LSE : } \underline{A}\underline{x} = \underline{b} \quad , \quad A \in \mathbb{R}^{m,n}$$

overdetermined $\leftarrow m > n$

$$\text{NLSE} \quad F(\underline{x}) = 0 \quad , \quad F: D \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$$

overdetermined $\leftarrow m > n$

▷ LSE : generalized concept of solutions

Definition 3.1.1.1. Least squares solution

For given $\underline{A} \in \mathbb{R}^{m,n}$, $\underline{b} \in \mathbb{R}^m$ the vector $\underline{x} \in \mathbb{R}^n$ is a **least squares solution** of the linear system of equations $\underline{Ax} = \underline{b}$, if

$$\underline{x} \in \underset{\underline{y} \in \mathbb{R}^n}{\operatorname{argmin}} \|\underline{Ay} - \underline{b}\|_2^2 ,$$

$$\Updownarrow$$

$$\|\underline{Ax} - \underline{b}\|_2^2 = \min_{\underline{y} \in \mathbb{R}^n} \|\underline{Ay} - \underline{b}\|_2^2 = \min_{y_1, \dots, y_n \in \mathbb{R}} \sum_{i=1}^m \left(\sum_{j=1}^n (A)_{i,j} y_j - (b)_i \right)^2 .$$

Definition 8.7.0.6. Non-linear least-squares solution

Given $F : D \subset \mathbb{R}^n \mapsto \mathbb{R}^m$, $m, n \in \mathbb{N}$, $m > n$, we call $\mathbf{x}^*$ a **non-linear least squares solution** of $F(\mathbf{x}) = \mathbf{0}$, if

$$\mathbf{x}^* = \operatorname{argmin}_{\mathbf{x} \in D} \|F(\mathbf{x})\|_2^2.$$

Non-linear least squares problem

Given: $F : D \subset \mathbb{R}^n \mapsto \mathbb{R}^m$, $m, n \in \mathbb{N}$, $m > n$.

Find: $\mathbf{x}^* \in D$: $\mathbf{x}^* = \operatorname{argmin}_{\mathbf{x} \in D} \Phi(\mathbf{x})$, $\Phi(\mathbf{x}) := \frac{1}{2} \|F(\mathbf{x})\|_2^2$. (8.7.0.7)

Ex. 8.7.0.1 (Least squares data fitting)

Recall: Linear least-squares fitting ($\rightarrow$ 5.7)

General Linear least squares fitting problem:

Given: $\blacklozenge$ data points $(\mathbf{t}_i, \mathbf{y}_i) \in \mathbb{R}^k \times \mathbb{R}^d$, $i = 1, \dots, m$

$\blacklozenge$ basis functions $\mathbf{b}_j : D \subset \mathbb{R}^k \mapsto \mathbb{R}$, $j = 1, \dots, n$, $n < m$

Sought: coefficients $x_j \in \mathbb{R}$, $j = 1, \dots, n$, such that

$$\mathbf{x} := [x_1, \dots, x_n]^\top := \operatorname{argmin}_{\mathbf{z} \in \mathbb{R}^d} \sum_{i=1}^m \left\| \sum_{j=1}^n z_j \mathbf{b}_j(\mathbf{t}_i) - \mathbf{y}_i \right\|_2^2. \quad (5.7.0.9)$$

linear combination

Non-linear least squares fitting problem in $\mathcal{D}$

Given: $\blacklozenge$ data points (t_i, y_i) , $i = 1, \dots, m$

$\blacklozenge$ (symbolic formula) for parameterized function

$$f(x_1, \dots, x_n; \cdot) : D \subset \mathbb{R} \mapsto \mathbb{R}, \quad n < m$$

Sought: parameter values $x_1^*, \dots, x_n^* \in \mathbb{R}$ such that

$$(x_1^*, \dots, x_n^*) = \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^n} \sum_{i=1}^m |f(x_1, \dots, x_n; t_i) - y_i|^2. \quad (8.7.0.3)$$

Linear case: $f(x_1, \dots, x_n, t) = \sum_{j=1}^n x_j b_j(t)$

$\Leftrightarrow$ overdet. NLS $\exists \mathbf{x} \in \mathbb{R}^n$ s.t. $F(\mathbf{x}) = \mathbf{0}$

$$F(\mathbf{x}) := \begin{bmatrix} f(x_1, \dots, x_n, t_1) - y_1 \\ \vdots \\ f(x_1, \dots, x_n, t_m) - y_m \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}. \quad (8.7.0.4)$$

Fitting Gaussians: ($n = 3$)

$$f(x_1, x_2, x_3, t) := x_1 e^{-x_2(t-x_3)}$$

③

▷ Review questions 8.7.0.10

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