

Generalization of least square method (廣義最小平方法)

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1 機器學習情境回顧

給定已知 $N + 1$ 筆, $M + K$ 維”連續變數”資料集, $\mathcal{D} := \left\{ \left(\underbrace{x_1^{(n)}, x_2^{(n)}, \dots, x_M^{(n)}}_{\vec{x}^{(n)}}, \underbrace{y_1^{(n)}, y_2^{(n)}, \dots, y_K^{(n)}}_{\vec{y}^{(n)}} \right) \right\}_{n=1}^{N+1}$

- 切割資料集

$$\forall \sigma \in \mathcal{S}_{N+1}, \mathcal{D} = \mathcal{D}_\sigma^{\text{train}} \cup \mathcal{D}_\sigma^{\text{valid}},$$

- 本文只考慮 **Leave-One-Out**: $|\mathcal{D}_\sigma^{\text{train}}| = N, |\mathcal{D}_\sigma^{\text{valid}}| = 1$ 即 $\sigma \in \mathcal{S}_{N+1}^{\text{LoO}}, |\mathcal{S}_{N+1}^{\text{LoO}}| = C_N^{N+1} = N + 1$

- 只根據 $\mathcal{D}_\sigma^{\text{train}}$, 可建構迴歸模型 $F_\sigma: \mathbb{R}^M \rightarrow \mathbb{R}^K$, 並同時使用 $\mathcal{D}_\sigma^{\text{train}}, \mathcal{D}_\sigma^{\text{valid}}$ 來評估建模成效

$$\text{終極目標: } \forall \sigma \in \mathcal{S}_{N+1}, \forall n = 1, 2, \dots, N + 1 \quad \underbrace{F_\sigma(\vec{x}^{(n)})}_{\text{predicted}} \approx \underbrace{\vec{y}^{(n)}}_{\text{target}}$$

- 根據多維向量定義, 可以把單一模型 $F: \mathbb{R}^M \rightarrow \mathbb{R}^K$ 問題, 想成獨立 K 個模型 $f: \mathbb{R}^M \rightarrow \mathbb{R}$

$$F_\sigma(\vec{x}^{(n)}) = \begin{bmatrix} f_1(\vec{x}^{(n)}) \\ f_2(\vec{x}^{(n)}) \\ \dots \\ f_K(\vec{x}^{(n)}) \end{bmatrix} \approx \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_K \end{bmatrix} = \vec{y}^{(n)}$$

- 於是只需研究 $f(\vec{x}^{(n)}) \approx y^{(n)} \in \mathbb{R}$ 迴歸問題如何建模 !!
- 損失函數(Loss function)越小越好概念:

$$f(\vec{x}^{(n)}) \approx y^{(n)} \implies \left(f(\vec{x}^{(n)}) - y^{(n)} \right)^2 \approx 0$$

$$\xRightarrow{\text{overall data}} \underbrace{\frac{1}{N} \sum_{n=1}^N \left(f(\vec{x}^{(n)}) - y^{(n)} \right)^2}_{\text{training_loss}(\mathcal{D}_\sigma^{\text{train}})} \approx 0, \underbrace{\left(f(\vec{x}^{(N+1)}) - y^{(N+1)} \right)^2}_{\text{validation_loss}(\mathcal{D}_\sigma^{\text{valid}})} \approx 0$$

- 交叉驗證(cross validation)最大誤差越小概念:

$$\xRightarrow{\text{overall } \sigma} \max_{\sigma} \text{training_loss}(\mathcal{D}_\sigma^{\text{train}}) \approx 0, \max_{\sigma} \text{validation_loss}(\mathcal{D}_\sigma^{\text{valid}}) \approx 0$$

2 模型假設 = 參數化 + 線性組合假設

- $f(\vec{x}^{(n)}) \xrightarrow{\text{引入模型假設}} f(\vec{w}, \vec{x}^{(n)}) := \sum_{b \in \mathcal{B}} w_b \cdot g_b(\vec{x}^{(n)}) \in \text{Span} \left\{ g_b \right\}_{b \in \mathcal{B}} =: \text{Span } g_{\mathcal{B}}$ (linear combinations of given basis $g_{\mathcal{B}}$)

- 常見 basis $g_{\mathcal{B}}, (M = 1)$

– Simple Intepolation:

$$g_{\mathcal{B}} := \left\{ 1, x_1, x_1^2, \dots, x_1^{N-1} \right\}$$

– Special Functions:

$$g_{\mathcal{B}} := \text{Hermite's, Chebyshev's, Legendre's, Laguerre's, Bessel's ...}$$

– Fourier Series:

$$g_{\mathcal{B}} := \left\{ e^{ikx_1} \right\}_{k \in \mathbb{Z}}$$

– ODE(微分方程)

$$g_{\mathcal{B}} := \left\{ e^{\lambda x_1} \right\}_{\lambda \in \text{eigenvalues}}$$

- 常見 basis $g_{\mathcal{B}}, (M \geq 1)$:

– Linear Regression:

$$g_{\mathcal{B}} := \left\{ 1, x_1, x_2, \dots, x_M \right\}$$

– Response Surface Methodology:

$$g_{\mathcal{B}} := \left\{ 1, \underbrace{x_1, x_2, \dots, x_M}_{\text{first-order } M \text{ terms}}, \underbrace{x_1^2, \dots, x_M^2, x_1 x_2, x_1 x_3, \dots, x_{M-1} x_M}_{\text{second-order } \frac{M(M-1)}{2} \text{ terms (features interaction)}} \right\}$$

– DIY or data transform by domain knowledge ...

3 核心推導

- 計算 \vec{w}^* 使得 $\text{training_loss}(\vec{w}^*, \mathcal{D}_\sigma^{\text{train}})$ 最小，則必須滿足 first-order optimality condition

$$\begin{aligned}
& \frac{\partial}{\partial w_b} \left[\frac{1}{2} \sum_{n=1}^N \left(f(\overbrace{w_b, w_{-b}}^{\vec{w}}, \vec{x}^{(n)}) - y^{(n)} \right)^2 \right] = \sum_{n=1}^N \left[\frac{1}{2} \cdot \frac{\partial}{\partial w_b} \left(f(\overbrace{w_b, w_{-b}}^{\vec{w}}, \vec{x}^{(n)}) - y^{(n)} \right)^2 \right] = 0 \\
& \Rightarrow \sum_{n=1}^N \frac{1}{2} \times 2 \left(f(\vec{w}, \vec{x}^{(n)}) - y^{(n)} \right) \cdot g_b(\vec{x}^{(n)}) = \sum_{n=1}^N \left(\sum_{b' \in \mathcal{B}} w_{b'} g_{b'}(\vec{x}^{(n)}) - y^{(n)} \right) \cdot g_b(\vec{x}^{(n)}) = 0 \\
& \Rightarrow \bigwedge_{b \in \mathcal{B}} \left\{ \sum_{b' \in \mathcal{B}} \sum_{n=1}^N g_{b'}(\vec{x}^{(n)}) g_b(\vec{x}^{(n)}) w_{b'} = \sum_{n=1}^N y^{(n)} \cdot g_b(\vec{x}^{(n)}) \right\} \\
& \equiv \underbrace{\left[\sum_{n=1}^N \phi^{(n)} \phi^{(n)T} \right] \vec{w}}_{\text{Matrix}(|\mathcal{B}| \times |\mathcal{B}|) \cdot \text{Vector}(|\mathcal{B}| \times 1) \text{ Multiplication}} = \underbrace{\left[\sum_{n=1}^N y^{(n)} \phi^{(n)} \right]}_{\text{Vector}(|\mathcal{B}| \times 1)} \quad \text{where } \phi^{(n)} := [g_b(\vec{x}^{(n)})]_{b \in \mathcal{B}} \text{ is column vector (also called kernel !!)}
\end{aligned}$$

- analytic optimal solution :

$$\vec{w}^* = \left[\sum_{n=1}^N \phi^{(n)} \phi^{(n)T} \right]^{-1} \left[\sum_{n=1}^N y^{(n)} \phi^{(n)} \right]$$

- 使用 Sherman-Morrison formula 高效率計算反矩陣

$$\begin{cases} A_1^{-1} = \left(\phi^{(1)} \phi^{(1)T} \right)^{-1} \\ A_{n+1}^{-1} = \left[A_n + \phi^{(n+1)} \phi^{(n+1)T} \right]^{-1} = A_n^{-1} - \frac{A_n^{-1} \phi^{(n+1)} \phi^{(n+1)T} A_n^{-1}}{1 + \phi^{(n+1)T} A_n^{-1} \phi^{(n+1)}} \quad n \geq 1 \end{cases}$$