
CSIE 5432 — Machine Learning Foundations

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Homework 4

Due Date: December 4 2020, 13:00

Deterministic Noise

1. Answer: [c]

由題意可得 $L_{square} = \frac{1}{2} \int_0^2 (e^x - w \cdot x)^2 dx = \frac{1}{2} \int_0^2 (e^{2x} - 2w \cdot x e^x + w^2 x^2) dx = \frac{8}{2} w^2 - (2e^2 + 2)w + \frac{1}{2}(e^2 + 1)$,
令 $\frac{dL_{square}}{dw} = 0$, $\frac{8}{3}w - 1 - e^2 = 0$, 得 $w = \frac{3+3e^2}{8}$ 。

Learning Curve

2. Answer: [b]

令 $h^* = \operatorname{argmin}_{h \in \mathcal{H}} E_{out}(h)$, 因為 $\mathcal{A}(\mathcal{D})$ 為使 E_{in} 最小的 hypothesis, 在給定任意 \mathcal{D} 的條件下, $E_{in}(\mathcal{A}(\mathcal{D})) \leq E_{in}(h^*)$ 恆成立, 則 $\mathbb{E}_{\mathcal{D}}[E_{in}(\mathcal{A}(\mathcal{D}))] \leq \mathbb{E}_{\mathcal{D}}[E_{in}(h^*)]$ 亦恆成立。

令 \mathcal{D} 為由 N 筆 *i.i.d.* 資料 $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$ 構成的資料集, 則:

$$\begin{aligned} \mathbb{E}_{\mathcal{D}}[E_{in}(h^*)] &= \int_{\mathcal{D}} P(\mathcal{D}) E_{in}(h^*) d\mathcal{D} = \int_{\mathcal{D}} P(\mathcal{D}) \left[\frac{1}{N} \sum_{i=1}^N \operatorname{err}(h^*(\mathbf{x}_i), y_i) \right] d\mathcal{D}, \quad \because \{(\mathbf{x}_i, y_i)\}_{i=1}^N \text{ 為 } i.i.d. \\ &= \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} \dots \int_{\mathbf{x}_N} P(\mathbf{x}_1) P(\mathbf{x}_2) \dots P(\mathbf{x}_N) \left[\frac{1}{N} \sum_{i=1}^N \operatorname{err}(h^*(\mathbf{x}_i), y_i) \right] d\mathbf{x}_1 d\mathbf{x}_2 \dots d\mathbf{x}_N \\ &= \frac{1}{N} \sum_{i=1}^N \left[\left(\prod_{\substack{j=1 \\ j \neq i}}^N \int_{\mathbf{x}_j} P(\mathbf{x}_j) d\mathbf{x}_j \right) \int_{\mathbf{x}_i} P(\mathbf{x}_i) \operatorname{err}(h^*(\mathbf{x}_i), y_i) d\mathbf{x}_i \right], \quad \because \int_{\mathbf{x}_j} P(\mathbf{x}_j) d\mathbf{x}_j = 1, \\ &= \frac{1}{N} \sum_{i=1}^N \int_{\mathbf{x}_i} P(\mathbf{x}_i) \operatorname{err}(h^*(\mathbf{x}_i), y_i) d\mathbf{x}_i \\ &= \frac{1}{N} \sum_{i=1}^N \mathcal{E}_{\mathbf{x}_i \sim \mathcal{P}} \operatorname{err}(h^*(\mathbf{x}_i), y_i), \quad \because \mathcal{E}_{\mathbf{x}_i \sim \mathcal{P}} \operatorname{err}(h^*(\mathbf{x}_i), y_i) = E_{out}(h^*), \\ &= \frac{1}{N} \sum_{i=1}^N E_{out}(h^*) = \frac{1}{N} \cdot N \cdot E_{out}(h^*) = E_{out}(h^*) \end{aligned}$$

$E_{out}(h^*)$ 與 \mathcal{D} 無關, 對隨機變數 \mathcal{D} 可視為一常數, 因此 $E_{out}(h^*) = \mathbb{E}_{\mathcal{D}}[E_{out}(h^*)]$ 。此外, 給定任意 \mathcal{D} 的條件下, $E_{out}(h^*) \leq E_{out}(\mathcal{A}(\mathcal{D}))$ 恆成立, 則 $\mathbb{E}_{\mathcal{D}}[E_{out}(h^*)] \leq \mathbb{E}_{\mathcal{D}}[E_{out}(\mathcal{A}(\mathcal{D}))]$ 恆成立。

綜上所述, $\mathbb{E}_{\mathcal{D}}[E_{in}(\mathcal{A}(\mathcal{D}))] \leq \mathbb{E}_{\mathcal{D}}[E_{in}(h^*)] = E_{out}(h^*) = \mathbb{E}_{\mathcal{D}}[E_{out}(h^*)] \leq \mathbb{E}_{\mathcal{D}}[E_{out}(\mathcal{A}(\mathcal{D}))]$, 可推得 $\mathbb{E}_{\mathcal{D}}[E_{in}(\mathcal{A}(\mathcal{D}))] \leq \mathbb{E}_{\mathcal{D}}[E_{out}(\mathcal{A}(\mathcal{D}))]$ 恆成立, $\mathbb{E}_{\mathcal{D}}[E_{in}(\mathcal{A}(\mathcal{D}))] > \mathbb{E}_{\mathcal{D}}[E_{out}(\mathcal{A}(\mathcal{D}))]$ 的情況與結果矛盾, 必 always false。

Noisy Virtual Examples

3. Answer: [d]

$$\text{令 } \mathbf{X} = \begin{pmatrix} -\mathbf{x}_1^T - \\ -\mathbf{x}_2^T - \\ \vdots \\ -\mathbf{x}_N^T - \end{pmatrix}, \xi = \begin{pmatrix} -\epsilon^T - \\ -\epsilon^T - \\ \vdots \\ -\epsilon^T - \end{pmatrix}, \tilde{\mathbf{X}} = \begin{pmatrix} -\mathbf{x}_1^T + \epsilon^T - \\ -\mathbf{x}_2^T + \epsilon^T - \\ \vdots \\ -\mathbf{x}_N^T + \epsilon^T - \end{pmatrix} = \mathbf{X} + \xi$$

$$\mathbf{X}_h = \begin{pmatrix} \mathbf{X} \\ \tilde{\mathbf{X}} \end{pmatrix}, \mathbf{X}_h^T = (\mathbf{X}^T, \tilde{\mathbf{X}}^T), \text{ 其中 } \mathbf{X}^T \mathbf{X} \text{ 為常數, } \mathbb{E}(\mathbf{X}^T \mathbf{X}) = \mathbf{X}^T \mathbf{X}$$

$$\begin{aligned} \mathbb{E}(\mathbf{X}_h^T \mathbf{X}_h) &= \mathbb{E}(\mathbf{X}^T \mathbf{X} + \tilde{\mathbf{X}}^T \tilde{\mathbf{X}}) = \mathbb{E}(\mathbf{X}^T \mathbf{X} + (\mathbf{X} + \xi)^T (\mathbf{X} + \xi)) = \mathbb{E}(2\mathbf{X}^T \mathbf{X} + \xi^T \mathbf{X} + \mathbf{X}^T \xi + \xi^T \xi) \\ &= 2\mathbf{X}^T \mathbf{X} + \mathbb{E}(\xi)^T \mathbf{X} + \mathbf{X}^T \mathbb{E}(\xi) + \mathbb{E}(\xi^T \xi) \\ &= 2\mathbf{X}^T \mathbf{X} + \begin{pmatrix} \mathbb{E}(-\epsilon^T -) \\ \mathbb{E}(-\epsilon^T -) \\ \vdots \\ \mathbb{E}(-\epsilon^T -) \end{pmatrix}^T \mathbf{X} + \mathbf{X}^T \begin{pmatrix} \mathbb{E}(-\epsilon^T -) \\ \mathbb{E}(-\epsilon^T -) \\ \vdots \\ \mathbb{E}(-\epsilon^T -) \end{pmatrix} + \mathbb{E}(\sum_{n=1}^N \epsilon \epsilon^T), \quad \because \mathbb{E}(\epsilon) = 0, \\ &= 2\mathbf{X}^T \mathbf{X} + \begin{pmatrix} -\mathbf{0}^T - \\ -\mathbf{0}^T - \\ \vdots \\ -\mathbf{0}^T - \end{pmatrix}^T \mathbf{X} + \mathbf{X}^T \begin{pmatrix} -\mathbf{0}^T - \\ -\mathbf{0}^T - \\ \vdots \\ -\mathbf{0}^T - \end{pmatrix} + \mathbb{E}(\sum_{n=1}^N \epsilon \epsilon^T) \\ &= 2\mathbf{X}^T \mathbf{X} + \mathbb{E}(\sum_{n=1}^N \epsilon \epsilon^T) = 2\mathbf{X}^T \mathbf{X} + \sum_{n=1}^N \mathbb{E}(\epsilon \epsilon^T) = 2\mathbf{X}^T \mathbf{X} + \sum_{n=1}^N \sigma^2 \mathbf{I}_{d+1} = 2\mathbf{X}^T \mathbf{X} + N\sigma^2 \mathbf{I}_{d+1} \end{aligned}$$

4. Answer: [e]

$$\mathbb{E}(\mathbf{X}_h^T \mathbf{y}_h) = \mathbb{E}(\mathbf{X}^T \mathbf{y} + \tilde{\mathbf{X}}^T \mathbf{y}) = \mathbb{E}(\mathbf{X}^T \mathbf{y} + (\mathbf{X}^T + \xi^T) \mathbf{y}), \quad \because \mathbf{X}, \mathbf{y} \text{ 為常數, 可得下面結果,}$$

$$= 2\mathbf{X}^T \mathbf{y} + \mathbb{E}(\xi)^T \mathbf{y} = 2\mathbf{X}^T \mathbf{y} + \begin{pmatrix} \mathbb{E}(-\epsilon^T -) \\ \mathbb{E}(-\epsilon^T -) \\ \vdots \\ \mathbb{E}(-\epsilon^T -) \end{pmatrix}^T \mathbf{y} = 2\mathbf{X}^T \mathbf{y} + \begin{pmatrix} -\mathbf{0}^T - \\ -\mathbf{0}^T - \\ \vdots \\ -\mathbf{0}^T - \end{pmatrix}^T \mathbf{y} = 2\mathbf{X}^T \mathbf{y}$$

Regularization

5. Answer: [d]

$$\mathbf{Z} = \mathbf{X}\mathbf{Q}, \text{ 則 } \mathbf{Z}^T \mathbf{Z} = \mathbf{Q}^T \mathbf{X}^T \mathbf{X} \mathbf{Q} = \mathbf{Q}^T (\mathbf{Q} \Gamma \mathbf{Q}^T) \mathbf{Q} = \mathbf{I}_{d+1} \Gamma \mathbf{I}_{d+1} = \Gamma$$

根據 Lecture 14 slides 第 10 頁得最佳解公式並由題意代入 $\mathbf{Z}^T \mathbf{Z} = \Gamma$:

$$\mathbf{v} = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{y} = \Gamma^{-1} \mathbf{Z}^T \mathbf{y}, \quad \because \Gamma \text{ 為對角矩陣, 則 } \Gamma^{-1} \text{ 亦為對角矩陣, 得 } v_i = \frac{1}{\gamma_i} (\mathbf{Z}^T \mathbf{y})_i \quad \circ$$

$$\mathbf{u} = (\mathbf{Z}^T \mathbf{Z} + \lambda \mathbf{I}_{d+1})^{-1} \mathbf{Z}^T \mathbf{y} = (\Gamma + \lambda \mathbf{I}_{d+1})^{-1} \mathbf{Z}^T \mathbf{y}, \quad \because (\Gamma, \lambda \mathbf{I}_{d+1}) \text{ 為對角矩陣, 則 } (\Gamma + \lambda \mathbf{I}_{d+1})^{-1} \text{ 亦為對角矩陣, 得 } u_i = \frac{1}{\gamma_i + \lambda} (\mathbf{Z}^T \mathbf{y})_i \quad \circ$$

$$\text{綜上所述, 得 } \frac{u_i}{v_i} = \frac{\gamma_i}{\gamma_i + \lambda} \cdot \frac{(\mathbf{Z}^T \mathbf{y})_i}{(\mathbf{Z}^T \mathbf{y})_i} = \frac{\gamma_i}{\gamma_i + \lambda} \quad \circ$$

6. Answer: [a]

$$\text{令 } \mathbf{X} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix}_{N \times 1}, \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}_{N \times 1}$$

根據 Lecture 14 slides 第 10 頁得最佳解公式 $w^* = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{1 \times 1})^{-1} \mathbf{X}^T \mathbf{y} = \frac{\sum_{n=1}^N x_n y_n}{\sum_{n=1}^N x_n x_n + \lambda}$

由題意可知最佳解在 constraint 邊界, 得 $C = (w^*)^2 = \left(\frac{\sum_{n=1}^N x_n y_n}{\sum_{n=1}^N x_n x_n + \lambda} \right)^2$ 。

7. Answer: [d]

令 $\Omega(y) = (y + c)^2$, 當 $\frac{d}{dy} \left\{ \frac{1}{N} (\sum_{n=1}^N (y - y_n)^2 + 2K(y + c)^2) \right\} = 0$ 時, y 為最佳解,

$\frac{d}{dy} \left\{ \frac{1}{N} (\sum_{n=1}^N (y - y_n)^2 + 2K(y + c)^2) \right\} = 0$, 則 $\sum_{n=1}^N (y - y_n) + 2K(y + c) = 0$

移項整理得 $y = \frac{\sum_{n=1}^N y_n - 2K \cdot c}{N + 2K}$, 又由題意得 $\frac{\sum_{n=1}^N y_n - 2K \cdot c}{N + 2K} = \frac{\sum_{n=1}^N y_n + K}{N + 2K}$,

綜上所述, 因 $-2K \cdot c = K$, 可得 $c = -0.5$, 因此 $\Omega(y) = (y - 0.5)^2$ 。

8. Answer: [b]

$$\text{令 } \begin{cases} \tilde{L}(\tilde{\mathbf{w}}) = \frac{1}{N} \sum_{n=1}^N (\tilde{\mathbf{w}}^T \Phi(\mathbf{x}_n) - y_n)^2 + \frac{\lambda}{N} (\tilde{\mathbf{w}}^T \tilde{\mathbf{w}}) \\ L(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N (\mathbf{w}^T \mathbf{x}_n - y_n)^2 + \frac{\lambda}{N} \Omega(\mathbf{w}) \end{cases}$$

$$\tilde{\mathbf{w}}^T \Phi(\mathbf{x}_n) = \tilde{\mathbf{w}}^T \Gamma^{-1} \mathbf{x}_n = \tilde{\mathbf{w}}^T ((\Gamma^{-1})^T)^T \mathbf{x}_n = ((\Gamma^{-1})^T \tilde{\mathbf{w}})^T \mathbf{x}_n = ((\Gamma^T)^{-1} \tilde{\mathbf{w}})^T \mathbf{x}_n$$

因為對角矩陣 Γ 為對稱, $\Gamma = \Gamma^T$, 因此 $\tilde{\mathbf{w}}^T \Phi(\mathbf{x}_n) = (\Gamma^{-1} \tilde{\mathbf{w}})^T \mathbf{x}_n$ 。

令 $\mathbf{w} = \Gamma^{-1} \tilde{\mathbf{w}}$, 可得 $L = \frac{1}{N} \sum_{n=1}^N (\tilde{\mathbf{w}}^T \Phi(\mathbf{x}_n) - y_n)^2 + \frac{\lambda}{N} \Omega(\mathbf{w})$, 當 $L = \tilde{L}$, 由封閉性得 $\Omega(\mathbf{w}) = \tilde{\mathbf{w}}^T \tilde{\mathbf{w}}$, 轉換之對角矩陣 Γ^{-1} 可逆, 可代入 $\tilde{\mathbf{w}} = \Gamma \mathbf{w}$, $\Omega(\mathbf{w}) = (\Gamma \mathbf{w})^T (\Gamma \mathbf{w}) = \mathbf{w}^T \Gamma^T \Gamma \mathbf{w} = \mathbf{w}^T \Gamma \mathbf{w} = \mathbf{w}^T \Gamma^2 \mathbf{w}$ 。

因為 \mathbf{w} 和 $\tilde{\mathbf{w}}$ 轉換關係為 bijective, 當 $\mathbf{w} = \Gamma^{-1} \tilde{\mathbf{w}}$, $\Omega(\mathbf{w}) = \mathbf{w}^T \Gamma^2 \mathbf{w}$ 時,

$$\frac{1}{N} \sum_{n=1}^N (\tilde{\mathbf{w}}^T \Phi(\mathbf{x}_n) - y_n)^2 + \frac{\lambda}{N} \tilde{\mathbf{w}}^T \tilde{\mathbf{w}} = \frac{1}{N} \sum_{n=1}^N (\mathbf{w}^T \mathbf{x}_n - y_n)^2 + \frac{\lambda}{N} \Omega(\mathbf{w}) \text{ 恆成立,}$$

則 $\min_{\mathbf{w}} \left\{ \frac{1}{N} \sum_{n=1}^N (\tilde{\mathbf{w}}^T \Phi(\mathbf{x}_n) - y_n)^2 + \frac{\lambda}{N} \tilde{\mathbf{w}}^T \tilde{\mathbf{w}} \right\} = \min_{\mathbf{w}} \left\{ \frac{1}{N} \sum_{n=1}^N (\mathbf{w}^T \mathbf{x}_n - y_n)^2 + \frac{\lambda}{N} \Omega(\mathbf{w}) \right\}$ 必成立, 其中, 最佳解關係亦為 $\mathbf{w}^* = \Gamma^{-1} \tilde{\mathbf{w}}^*$ 。

9. Answer: [b]

$$\text{令 } L(\mathbf{w}) = \sum_{n=1}^N (\mathbf{w}^T \mathbf{x}_n - y_n)^2$$

Stage 1:

因為 \mathbf{B} 為對角矩陣, $\sum_{i=0}^d \beta_i w_i^2 = \mathbf{w}^T \mathbf{B} \mathbf{w}$, 其中 \mathbf{B} 具對稱性, 故 $\mathbf{B} = \mathbf{B}^T$,

$$\begin{aligned} \frac{d}{d\mathbf{w}} \left\{ \frac{1}{N} (L(\mathbf{w}) + \lambda \mathbf{w}^T \mathbf{B} \mathbf{w}) \right\} &= \frac{1}{N} (L'(\mathbf{w}) + \lambda \frac{d}{d\mathbf{w}} \{\mathbf{w}\} \mathbf{B} \mathbf{w} + \lambda \frac{d}{d\mathbf{w}} \{\mathbf{B} \mathbf{w}\} \mathbf{w}) \\ &= \frac{1}{N} (L'(\mathbf{w}) + \lambda (\mathbf{B} + \mathbf{B}^T) \mathbf{w}) = \frac{1}{N} (L'(\mathbf{w}) + 2\lambda \mathbf{B} \mathbf{w}) \end{aligned}$$

當 \mathbf{w} 為最佳解時, $L'(\mathbf{w}) = -2\lambda \mathbf{B} \mathbf{w}$

Stage 2:

$$\begin{aligned}
 \frac{d}{d\mathbf{w}} \left\{ \frac{1}{N+K} (L(\mathbf{w}) + \sum_{k=1}^K (\mathbf{w}^T \tilde{\mathbf{x}}_k - \tilde{y}_k)^2) \right\} &= \frac{1}{N+K} (L'(\mathbf{w}) + \frac{d}{d\mathbf{w}} \{\|\tilde{\mathbf{X}}\mathbf{w} - \tilde{\mathbf{y}}\|^2\}) \\
 &= \frac{1}{N+K} (L'(\mathbf{w}) + 2(\frac{d}{d\mathbf{w}} \{\tilde{\mathbf{X}}\mathbf{w}\}(\tilde{\mathbf{X}}\mathbf{w} - \tilde{\mathbf{y}}))) \\
 &= \frac{1}{N+K} (L'(\mathbf{w}) + 2(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}}\mathbf{w} - \tilde{\mathbf{X}}^T \tilde{\mathbf{y}}))
 \end{aligned}$$

當 \mathbf{w} 為最佳解時, $L'(\mathbf{w}) = -2(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}}\mathbf{w} - \tilde{\mathbf{X}}^T \tilde{\mathbf{y}})$

由 Stage 1 和 Stage 2 結果得:

$$\lambda \mathbf{B}\mathbf{w} - \mathbf{0} = \tilde{\mathbf{X}}^T \tilde{\mathbf{X}}\mathbf{w} - \tilde{\mathbf{X}}^T \tilde{\mathbf{y}}, \text{ 由封閉性得 } \begin{cases} \tilde{\mathbf{X}}^T \tilde{\mathbf{X}} = \lambda \mathbf{B} \\ \tilde{\mathbf{X}}^T \tilde{\mathbf{y}} = \mathbf{0} \end{cases}, \text{ 可推至 } \begin{cases} \tilde{\mathbf{X}} = \sqrt{\lambda} \cdot \sqrt{\mathbf{B}} \\ \tilde{\mathbf{y}} = \mathbf{0} \end{cases}.$$

Leave-one-out

10. Answer: [e]

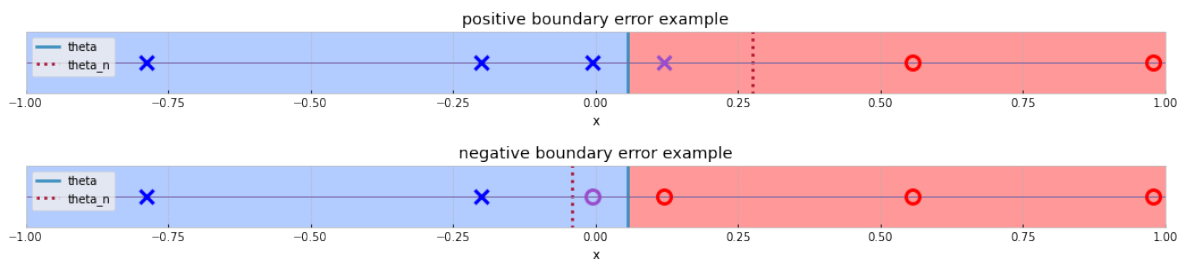
當 \mathbf{x}_n 為 positive, 則 negative examples 的數量會大於 positive examples, 預測結果必為 negative, $\mathbf{e}_n = 1$; 當 \mathbf{x}_n 為 negative, 則 negative examples 的數量會小於 positive examples, 預測結果必為 positive, $\mathbf{e}_n = 1$, 綜上所述, $\mathcal{A}_{majority}$ 在任何 leave-one-out 的情況皆必答錯, $\mathbf{e}_n = 1$ 恆成立, 得 $E_{loocv}(\mathcal{A}_{majority}) = \frac{1}{2N} \sum_{n=1}^{2N} 1 = 1$ 。

11. Answer: [c]

令所有 N 筆訓練資料得到的 hypothesis 為 θ ; 使用 \mathbf{x}_n 作為 valid sample, 剩下 $N-1$ 筆訓練資料求得的 hypothesis 為 θ_n , 將所有 \mathbf{e}_n 的可能分成兩種情況討論:

(1) 若 valid sample 為在 θ 的左/右的邊界 sample:

以下圖為例, 當 valid sample 在 θ 左或右邊的情況時, 有可能發生兩種 valid sample 同時都預測錯誤的狀況。



(2) 若 valid sample 不是 θ 的邊界 sample:

假使存在一非邊界 sample \mathbf{x}_n 在成為 valid sample 後會使 θ_n 將其誤判, 若 \mathbf{x}_n 為 positive, 代表 \mathbf{x}_n 在 θ_n 左邊, 但如果 \mathbf{x}_n 不是 θ 的邊界 sample, 表示必存在一 \mathbf{x}'_n 比 \mathbf{x}_n 更小, 但仍為 positive, 代表 θ_n 最大只能位在大於 \mathbf{x}'_n 且小於 \mathbf{x}_n 的區間內, 與假設矛盾; 若 \mathbf{x}_n 為 negative, 代表 \mathbf{x}_n 在 θ_n 右邊, 但如果 \mathbf{x}_n 不是 θ 的邊界 sample, 表示必存在一 \mathbf{x}'_n 比 \mathbf{x}_n 更大, 但仍為 negative, 代表 θ_n 最大只能位在小於 \mathbf{x}'_n 且大於 \mathbf{x}_n 的區間內, 與假設矛盾, 綜上所述, valid samples 不是在 θ 的時候, $\mathbf{e}_n = 0$ 恆成立。

由 (1)(2) 得, 有可能發生 $\mathbf{e}_n = 1$ 的情況只有在 \mathbf{x}_n 為決定 θ 的左右兩個點的時候, 因此 $\sum_{n=1}^N \mathbf{e}_n \leq 2$, 得 $E_{loocv} = \frac{1}{N} \sum_{n=1}^N \mathbf{e}_n \leq \frac{2}{N}$, 且根據題意 $N \geq 4$, 則 $\frac{2}{N} \leq \frac{1}{2}$, 得 $\frac{2}{N}$ 為 tightest upper bound。

12. Answer: [e]

(1) constant model:

令 i, j 為訓練參數資料的 index, $L_{constant}(w_0) = (w_0 - y_i)^2 + (w_0 - y_j)^2$, $L'_{constant}(w_0) = 2(2w_0 - y_i - y_j)$, 當 $w_0 = \frac{y_i + y_j}{2}$ 時為最佳解:

$$w_0|_{\mathbf{e}_1} = \frac{2+0}{2} = 1, \mathbf{e}_1 = (1-0)^2 = 1$$

$$w_0|_{\mathbf{e}_2} = \frac{0+0}{2} = 0, \mathbf{e}_2 = (0-2)^2 = 4$$

$$w_0|_{\mathbf{e}_3} = \frac{0+2}{2} = 1, \mathbf{e}_3 = (1-0)^2 = 1$$

$$E_{loocv-constant} = \frac{1}{3}(1+4+1) = 2$$

(2) linear model:

令 i, j 為訓練參數資料的 index, $L_{linear}(w_0, w_1) = (w_0 + w_1 x_i - y_i)^2 + (w_0 + w_1 x_j - y_j)^2$, 訓練資料兩點構成一線, 則 $w_0 = \frac{x_i y_j - x_j y_i}{x_i - x_j}$, $w_1 = \frac{y_i - y_j}{x_i - x_j}$:

$$w_0|_{\mathbf{e}_1} = \frac{\rho \cdot 0 - (-3) \cdot 2}{\rho - (-3)} = \frac{6}{\rho + 3}, w_1|_{\mathbf{e}_1} = \frac{2 - 0}{\rho - (-3)} = \frac{2}{\rho + 3}, \mathbf{e}_1 = (\frac{6}{\rho + 3} + \frac{2}{\rho + 3} \cdot 3 - 0)^2 = (\frac{12}{\rho + 3})^2$$

$$w_0|_{\mathbf{e}_2} = \frac{3 \cdot 0 - (-3) \cdot 0}{3 - (-3)} = 0, w_1|_{\mathbf{e}_2} = \frac{0 - 0}{3 - (-3)} = 0, \mathbf{e}_2 = (0 + 0 \cdot \rho - 2)^2 = 4$$

$$w_0|_{\mathbf{e}_3} = \frac{3 \cdot 2 - \rho \cdot 0}{3 - \rho} = \frac{6}{3 - \rho}, w_1|_{\mathbf{e}_3} = \frac{2 - 0}{\rho - 3} = \frac{2}{\rho - 3}, \mathbf{e}_3 = (\frac{6}{3 - \rho} + \frac{2}{\rho - 3} \cdot (-3) - 0)^2 = (\frac{12}{\rho - 3})^2$$

$$E_{loocv-linear} = \frac{1}{3}((\frac{12}{\rho + 3})^2 + 4 + (\frac{12}{\rho - 3})^2)$$

根據題意, $E_{loocv-constant} = E_{loocv-linear}$, 由 (1)(2) 得 $2 = \frac{1}{3}((\frac{12}{\rho + 3})^2 + 4 + (\frac{12}{\rho - 3})^2)$,

整理移項得多項式 $\rho^4 - 162\rho^2 - 1215 = 0$, 因式分解為 $(\rho^2 - (81 + 36\sqrt{6}))(\rho^2 - (81 - 36\sqrt{6})) = 0$,

其中, [e] 選項滿足其中一解 $\rho = \sqrt{81 + 36\sqrt{6}}$ 。

13. Answer: [d]

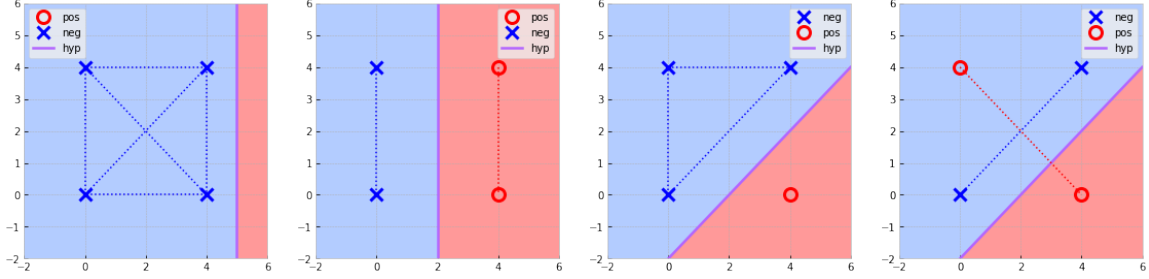
令 (\mathbf{x}_i, y_i) 為第 i 個從分佈 \mathcal{P} 抽到的 sample, 證明如下:

$$\begin{aligned} \text{Var}_{\mathcal{D}_{\text{val}} \sim \mathcal{P}^k}[E_{\text{val}}(h)] &= \text{Var}_{\mathcal{D}_{\text{val}} \sim \mathcal{P}^k}[\frac{1}{K} \sum_{i=1}^K \text{err}(h(\mathbf{x}_i), y_i)], \mathbf{x}_i \text{ 為 mutually independent, Var 可拆成線性疊加,} \\ &= \sum_{i=1}^K \text{Var}_{(\mathbf{x}_i, y_i) \sim \mathcal{P}}[\frac{1}{K} \text{err}(h(\mathbf{x}_i), y_i)], (\mathbf{x}_i, y_i) \text{ 來自同一分佈 } \mathcal{P} \text{ 可全部記作 } (\mathbf{x}, y), \\ &= K \cdot \text{Var}_{(\mathbf{x}, y) \sim \mathcal{P}}[\frac{1}{K} \text{err}(h(\mathbf{x}), y)] = K \cdot \frac{1}{K^2} \cdot \text{Var}_{(\mathbf{x}, y) \sim \mathcal{P}}[\text{err}(h(\mathbf{x}), y)] \\ &= \frac{1}{K} \cdot \text{Var}_{(\mathbf{x}, y) \sim \mathcal{P}}[\text{err}(h(\mathbf{x}), y)] \end{aligned}$$

14. Answer: [c]

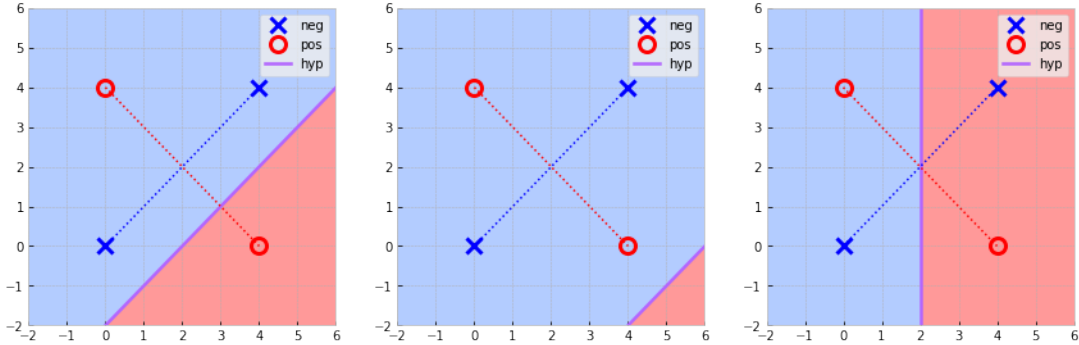
$$\mathbb{E}_{y_1, y_2, y_3, y_4} \left(\min_{\mathbf{w} \in \mathbb{R}^{2+1}} E_{in}(\mathbf{w}) \right) = \sum_{i=1}^{16} P(y_1, y_2, y_3, y_4) \min_{\mathbf{w} \in \mathbb{R}^{2+1}} E_{in}(\mathbf{w})|_{y_1, y_2, y_3, y_4}$$

每個同 label 的頂點和其他同 label 的頂點連線形成 connected component, 兩個 label 對應到兩個 connected component, 四個頂點所有 label 可能的組合可以簡化成四種 connected component 的情況討論:



若 hyper-line 與任一 connected component 的 edge 發生交點, 代表 edge 對應到的兩頂點介於 hyper-line 兩邊, 兩頂點必為異號, 表示本該同號的兩頂點被 hyper-line 分錯, 代表該 hyper-line 無法使 $E_{in}(\mathbf{w})|_{y_1, y_2, y_3, y_4} = 0$ 成立, 因此當 $E_{in}(\mathbf{w})|_{y_1, y_2, y_3, y_4} = 0$ 時, hyper-line 與任一 connected component 的 edge 必定不會發生交點。

第一種情況只有一個 connected component, 上述交點條件不發生一定能使 $E_{in} = 0$; 第二種情況兩 connected component 分別為兩線段, 只要兩線段不產生交點, 必能找到一條 hyper-line 劃分兩線段, 使 $E_{in} = 0$; 第三種情況為一三角形與一頂點, 只要一頂點不位在三角形內, 必能找到一條 hyper-line 劃分兩條線, 使 $E_{in} = 0$; 第四種為矩形同邊異號對角同號的狀況, $E_{in} \neq 0$ 恆成立, 證明如下:



如上圖所示, 若 hyper-line 沒有介於兩 connected component 之間, 則無法劃分不同的 connected component, 所有頂點將被歸類為同號, 無法將四點正確分類; 若 hyper-line 介於兩 connected component 之間, 會與至少一對角線產生交點, 而產生交點表示對角線兩端位在 hyper-line 的兩邊, hyper-line 兩邊的頂點必為異號, 在所有該情況的可能下, 不存在一 hypothesis 能夠使 $E_{in} = 0$, 但如第一張圖所示, 可以利用一三角形與一頂點對應的 hypothesis 分對其中三點, 使得 $E_{in} = \frac{1}{4}$ 。

綜上所述, 第四種 connected component 同邊異號對角同號的情況共有 2 個, 其他前三種 connected component 共有 14 個, 每一頂點 label 的組合發生的機率為 $\frac{1}{4}$ 可得:

$$\begin{aligned} \mathbb{E}_{y_1, y_2, y_3, y_4} \left(\min_{\mathbf{w} \in \mathbb{R}^{2+1}} E_{in}(\mathbf{w}) \right) &= 2 \cdot P[\text{同邊異號對角同號}] \cdot \min_{\mathbf{w} \in \mathbb{R}^{2+1}} E_{in}(\mathbf{w})|_{\text{同邊異號對角同號}} \\ &\quad + 14 \cdot P[\text{其他}] \cdot \min_{\mathbf{w} \in \mathbb{R}^{2+1}} E_{in}(\mathbf{w})|_{\text{其他}} \\ &= 2 \cdot \frac{1}{16} \cdot \frac{1}{4} + 14 \cdot \frac{1}{16} \cdot 0 = \frac{2}{64} \end{aligned}$$

15. Answer: [a]

$E_{out}(g) = p\epsilon_+ + (1-p)\epsilon_-$, 根據題意得 $E_{out}(g) = E_{out}(g_c) = 1-p$, 則 $p\epsilon_+ + (1-p)\epsilon_- = 1-p$, $p(\epsilon_+ - \epsilon_- + 1) = 1 - \epsilon_-$, 得 $p = \frac{1-\epsilon_-}{\epsilon_+ - \epsilon_- + 1}$ 。

Experiment

程式碼實作細節如下, 可以透過 parser 的 `--tra_path/--tst_path` 設置訓練資料和測試資料的路徑

```
python code.py --tra_path hw4_train.dat --tst_path hw4_test.dat
```

```
from liblinearutil import *
import numpy as np
import argparse

'''Define Function'''

def Q_transform(X):
    X_scnd = []
    for i in range(1, X.shape[1]):
        for j in range(i, X.shape[1]):
            X_scnd.append(X[:, i] * X[:, j])
    X_scnd = np.array(X_scnd).T
    return np.hstack((X, X_scnd))

def get_data(path, bias=1.0, transform=None):
    X = []
    for x in open(path, 'r'):
        x = x.strip().split(' ')
        x = [float(v) for v in x]
        X.append([bias] + x)

    X = np.array(X)
    X, Y = np.array(X[:, :-1]), np.array(X[:, -1])

    if transform is not None:
        X = transform(X)

    return X, Y

def main():
    '''Parsing'''
    parser = argparse.ArgumentParser(
        description='Argument Parser for MLF HW4.')

    parser.add_argument('--tra_path', default='hw4_train.dat')
```

```

parser.add_argument('--tst_path', default='hw4_test.dat')
args = parser.parse_args()

# load data
X_tra, Y_tra = get_data(path=args.tra_path, transform=Q_transform)
X_tst, Y_tst = get_data(path=args.tst_path, transform=Q_transform)

log10_lambda_choices = [-4, -2, 0, 2, 4]
lambda_choices = [10**lmd for lmd in log10_lambda_choices]

'''Answer questions'''
print('RUNNING Q16...')
best_log_lmd = 0
max_acc = 0
for i in range(len(lambda_choices)):
    lmd = lambda_choices[i]
    model = train(
        Y_tra, X_tra, '-s 0 -c {:f} -e 0.000001 -q'.format(1 / (2*lmd)))
    _, pre_acc, _ = predict(Y_tst, X_tst, model, '-q')
    if pre_acc[0] >= max_acc:
        best_log_lmd = log10_lambda_choices[i]
        max_acc = pre_acc[0]
print('Answer of Q16 : {:2d}\n'.format(best_log_lmd))

print('RUNNING Q17...')
best_log_lmd = 0
max_acc = 0
for i in range(len(lambda_choices)):
    lmd = lambda_choices[i]
    model = train(
        Y_tra, X_tra, '-s 0 -c {:f} -e 0.000001 -q'.format(1 / (2*lmd)))
    _, pre_acc, _ = predict(Y_tra, X_tra, model, '-q')
    if pre_acc[0] >= max_acc:
        best_log_lmd = log10_lambda_choices[i]
        max_acc = pre_acc[0]
print('Answer of Q17 : {:2d}\n'.format(best_log_lmd))

print('RUNNING Q18...')
best_lmd_idx = 0
max_acc = 0
for i in range(len(lambda_choices)):
    lmd = lambda_choices[i]
    model = train(Y_tra[:120], X_tra[:120],
        '-s 0 -c {:f} -e 0.000001 -q'.format(1 / (2*lmd)))
    _, pre_acc, _ = predict(
        Y_tra[120:], X_tra[120:], model, '-q')
    if pre_acc[0] >= max_acc:
        best_lmd_idx = i
        max_acc = pre_acc[0]
model = train(Y_tra[:120], X_tra[:120],
    '-s 0 -c {:f} -e 0.000001 -q'.format(1 / (2*lambda_choices[best_lmd_idx])))

```



```

_, pre_acc, _ = predict(Y_tst, X_tst, model, '-q')
print('Answer of Q18 : {:.4f}\n'.format((100 - pre_acc[0]) * 0.01))

print('RUNNING Q19...')
model = train(Y_tra, X_tra,
              '-s 0 -c {:.f} -e 0.000001 -q'.format(1 / (2*lambda_choices[best_lmd_idx])))
_, pre_acc, _ = predict(Y_tst, X_tst, model, '-q')
print('Answer of Q19 : {:.4f}\n'.format((100 - pre_acc[0]) * 0.01))

print('RUNNING Q20...')
folds_num = 5
X_folds = np.vsplit(X_tra, folds_num)
Y_folds = np.hsplit(Y_tra, folds_num)
best_lmd_idx = 0
max_acc = 0
for i in range(len(lambda_choices)):
    lmd = lambda_choices[i]
    acc_list = []
    for fold_idx in range(folds_num):
        X_tra_cv = np.vstack([X_folds[f_idx]
                               for f_idx in range(folds_num) if fold_idx != f_idx])
        Y_tra_cv = np.hstack([Y_folds[f_idx]
                               for f_idx in range(folds_num) if fold_idx != f_idx])
        X_val_cv = X_folds[fold_idx]
        Y_val_cv = Y_folds[fold_idx]
        model = train(Y_tra_cv, X_tra_cv,
                      '-s 0 -c {:.f} -e 0.000001 -q'.format(1 / (2*lmd)))
        _, pre_acc, _ = predict(Y_val_cv, X_val_cv, model, '-q')
        acc_list.append(pre_acc[0])
    acc = np.mean(acc_list)
    if acc >= max_acc:
        best_lmd_idx = i
        max_acc = acc
print('Answer of Q20 : {:.4f}\n'.format((100 - max_acc) * 0.01))

if __name__ == "__main__":
    main()

```

16. Answer: [b]	17. Answer: [a]	18. Answer: [e]	19. Answer: [d]	20. Answer: [c]
-2	-4	0.1433	0.13	0.12