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請實做以下兩種不同feature的模型，回答第(1) ~ (2) 題：

(1) 抽全部9小時內的污染源feature當作一次項(加bias)

(2) 抽全部9小時內pm2.5的一次項當作feature(加bias)

備註：

- a. NR請皆設為0，其他的非數值(特殊字元)可以自己判斷
- b. 所有 advanced 的 gradient descent 技術(如: adam, adagrad 等) 都是可以用的
- c. 第1-2題請都以題目給訂的兩種model來回答
- d. 同學可以先把model訓練好，kaggle死線之後便可以無限上傳。
- e. 根據助教時間的公式表示，(1) 代表 $p = 9 \times 18 + 1$ 而(2) 代表 $p = 9 \times 1 + 1$

1. (1%)記錄誤差值 (RMSE)(根據kaggle public+private分數)，討論兩種feature的影響

第一個model我train 500 個epoch後RMSE是5.4(kaggle 4.83487)，第二個則是5.67(kaggle:5.03893)。第一個model把所有資料都參考進去了，這樣子產生的function值域比較廣，但是因為training data的數量並不是趨近於無限大，所以取樣會有偏誤。因此第一個model訓練過後較容易有overfit的情形。然而第二個model因為只考慮一個feature，所以MSE會壓不下去。但是好處是他較不會overfitting。我認為第二個model考慮的feature太少了，所以她最後在kaggle的成績並不理想。

2. (1%)解釋什麼樣的data preprocessing 可以improve你的training/testing accuracy, ex. 你怎麼挑掉你覺得不適合的data points。請提供數據(RMSE)以佐證你的想法。

將有其中一個數字是超過65的都刪掉。原先的RMSE是18.02，應用後是7.1(大幅成長)

3.(3%) Refer to math problem

<https://hackmd.io/RFiulFsYR5uQTrrpdxUv1w?view>

1.

NO.

$$1. (a) \arg \min_{w, b} \sum_{i=1}^5 (y_i - (wx_i + b))^2, \quad \therefore \arg \min_b \sum_{i=1}^5 (z_i - b)^2 = \frac{1}{5} \sum_{i=1}^5 z_i \quad \therefore b = \frac{1}{5} \sum_{i=1}^5 (y_i - wx_i)$$

$$\hookrightarrow \text{let } \frac{1}{5} \sum_{i=1}^5 (z_i - b)^2 = \sum_{i=1}^5 (z_i - \bar{z})^2$$

$$\therefore \arg \min_w \left[\arg \min_b \sum_{i=1}^5 (y_i - (wx_i + b))^2 \right] = \arg \min_w \left[\sum_{i=1}^5 y_i^2 - 2 \sum_{i=1}^5 y_i x_i w + \sum_{i=1}^5 x_i^2 w^2 - \frac{1}{5} (\sum_{i=1}^5 y_i - \sum_{i=1}^5 x_i w)^2 \right]$$

$$= \arg \min_w \left[w^2 \left[\sum_{i=1}^5 x_i^2 - \frac{1}{5} (\sum_{i=1}^5 x_i)^2 \right] - 2w \left[\sum_{i=1}^5 x_i y_i - \frac{1}{5} (\sum_{i=1}^5 x_i \sum_{i=1}^5 y_i) \right] \right]$$

$$= \frac{\sum_{i=1}^5 x_i y_i - \frac{1}{5} (\sum_{i=1}^5 x_i \sum_{i=1}^5 y_i)}{\sum_{i=1}^5 x_i^2 - \frac{1}{5} (\sum_{i=1}^5 x_i)^2} = \frac{60.9 - 50.4}{55 - 45} = 1.05 \quad \therefore b = \frac{1}{5} (1.05) = 0.21.$$

$$(b) \text{ let } \tilde{x} = \begin{bmatrix} x \\ 1 \end{bmatrix}, \quad \tilde{w} = \begin{bmatrix} w \\ b \end{bmatrix}, \quad \text{Loss}(\tilde{w}) = \frac{1}{2N} \sum_{i=1}^N (y_i - \tilde{w}^T \tilde{x}_i)^2 = \frac{1}{2N} \|X^T \tilde{w} - y\|^2.$$

$$\text{Loss}(\tilde{w} + \delta \tilde{w}) = \|X^T (\tilde{w} + \delta \tilde{w}) - y\|^2 = \text{Loss}(\tilde{w}) + 2\delta \tilde{w}^T X (X^T \tilde{w} - y) + \delta \tilde{w}^T X X^T \delta \tilde{w}$$

$$\therefore \nabla_{\tilde{w}} \text{Loss}(\tilde{w}) = 2X(X^T \tilde{w} - y) \quad \Rightarrow \quad \nabla \text{Loss}(\tilde{w}) = 0 \Leftrightarrow \tilde{w} = (X X^T)^{-1} X^T y.$$

$$\text{Ans. } \tilde{w} = (X X^T)^{-1} X^T y, \text{ where } \tilde{w} = \begin{bmatrix} w \\ b \end{bmatrix}, \text{ and } X = [\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_N] \text{ and } \tilde{x}_i = \begin{bmatrix} x_i \\ 1 \end{bmatrix}$$

$$(c) \text{Lreg}(w, b) = \frac{1}{2N} \left(\sum_{i=1}^N (y_i - (w^T x_i + b))^2 + N\lambda \|w\|^2 \right) = \frac{1}{2N} (\|X^T \tilde{w} - y\|^2 + N\lambda \|\tilde{w}\|^2)$$

$$\therefore \text{Lreg}(w) = \frac{1}{2N} (\|X^T \tilde{w} - y\|^2 + N\lambda \|\tilde{w}\|^2), \quad \nabla_{\tilde{w}} \text{Lreg}(w) = 2X(X^T \tilde{w} - y) + 2N\lambda \tilde{w}$$

$$\text{let } \nabla_{\tilde{w}} \text{Lreg}(w) = 0 \Leftrightarrow [(X X^T + \lambda N I) \tilde{w} - X^T y] = 0 \Leftrightarrow \tilde{w} = (X X^T + \lambda N I)^{-1} X^T y$$

$$\therefore \tilde{w} = \begin{bmatrix} w \\ b \end{bmatrix}, \text{ and } \tilde{w} = (X X^T + \lambda N I)^{-1} X^T y$$

2.

NO.

$$\begin{aligned}
2. \quad E \left[\frac{1}{2N} \sum_{i=1}^N (f(x_i + \eta_i) - y_i)^2 \right] &= E \left[\frac{1}{2N} \| \omega^T (X + H) - y^T \|^2 \right], \text{ where } H = [\eta_1, \eta_2, \dots, \eta_N] \\
&= \frac{1}{2N} E \left[(\omega^T (X + H) - y^T) (X + H)^T \omega - y^T \right] = \frac{1}{2N} E \left[\omega^T (X + H) (X + H)^T \omega \right] + \frac{1}{2N} E \left[-2 \omega^T (X + H) y \right] + \frac{1}{2N} E \left[y^T y \right] \\
&= \frac{1}{2N} \left[E \left[\omega^T X X^T \omega \right] + E \left[\omega^T (H X^T + X H^T) \omega \right] + E \left[\omega^T H H^T \omega \right] + E \left[-2 \omega^T X y \right] + E \left[-2 \omega^T H y \right] + E \left[y^T y \right] \right] \\
&= \frac{1}{2N} \left[\omega^T X X^T \omega + 0 + N \sigma^2 \omega^T \omega - 2 (\omega^T X y) + y^T y \right] \\
&= \frac{1}{2N} \left(\| X^T \omega - y \|^2 + N \sigma^2 \| \omega \|^2 \right) = \frac{1}{2N} \sum_{i=1}^N (f(x_i) - y_i)^2 + \frac{\sigma^2}{2} \| \omega \|^2
\end{aligned}$$

3.

$$\begin{aligned}
3. (a) \quad e_k &= \frac{1}{N} \sum_{i=1}^N (g_k(x_i) - y_i)^2 = \frac{1}{N} \left(\sum_{i=1}^N g_k(x_i)^2 - 2 \sum_{i=1}^N g_k(x_i) y_i + \sum_{i=1}^N y_i^2 \right) = s_k - \frac{2}{N} \sum_{i=1}^N g_k(x_i) y_i + e_0 \\
&\therefore \sum_{i=1}^N g_k(x_i) y_i = \frac{N}{2} (s_k - e_k + e_0)
\end{aligned}$$

$$3. (b) \quad \frac{1}{N} \sum_{i=1}^N \left(\sum_{k=0}^K \alpha_k g_k(x_i) - y_i \right)^2 = \frac{1}{N} \sum_{i=1}^N \left[\sum_{k=0}^K \alpha_k (g_k(x_i) - y_i) \right]^2, \text{ where } g_0(x_i) = 0, \alpha_0 \equiv 1 - \sum_{k=1}^K \alpha_k$$

$$\frac{\partial L_{\text{test}}}{\partial \alpha_n} = \frac{1}{N} \sum_{i=1}^N \left[2 \alpha_n (g_n(x_i) - y_i) + \sum_{k=0}^K \alpha_k (g_k(x_i) - y_i) (g_n(x_i) - y_i) - \alpha_n (g_n(x_i) - y_i)^2 \right]$$

$$= \frac{1}{N} \sum_{i=1}^N [g_n(x_i) - y_i]^2 \cdot \alpha_n + \frac{1}{N} \sum_{k=0}^K \alpha_k \sum_{i=1}^N (g_k(x_i) - y_i) (g_n(x_i) - y_i)$$

$$= \alpha_n e_n + \frac{1}{N} \sum_{i=1}^N \left[g_n(x_i) \sum_{k=0}^K \alpha_k g_k(x_i) - g_n(x_i) y_i - \sum_{k=0}^K \alpha_k g_k(x_i) y_i + y_i^2 \right]$$

$$= \alpha_n e_n - \frac{1}{2} (s_n - e_n + e_0) + e_0 + \frac{1}{N} \sum_{i=1}^N \left[(g_n(x_i) - y_i) \sum_{k=0}^K \alpha_k g_k(x_i) \right]$$

$$\frac{\partial L_{\text{test}}}{\partial \alpha_n} = 0 \Leftrightarrow \alpha_n = \frac{1}{2 e_n} (s_n - e_n - e_0) - \frac{1}{2 e_n} \frac{1}{N} \sum_{i=1}^N [(g_n(x_i) - y_i) \sum_{k=0}^K \alpha_k g_k(x_i)]$$

$$= \frac{1}{2 e_n} (s_n - e_n - e_0) - \frac{1}{e_n} \frac{1}{N} \sum_{i=1}^N \sum_{k=0}^K \alpha_k g_k(x_i) g_n(x_i) + \frac{1}{e_n N} \sum_{k=0}^K \alpha_k \cdot \frac{N}{2} (s_k - e_k + e_0)$$

$$= \frac{1}{2 e_n} (s_n - e_n - e_0) + \frac{1}{2 e_n} \sum_{k=0}^K \alpha_k (s_k - e_k + e_0) - \frac{1}{e_n N} \sum_{i=1}^N \sum_{k=0}^K \alpha_k g_k(x_i) g_n(x_i)$$

$$\therefore \sum_{n=0}^K \alpha_n = 1 = \text{[I messed up]}$$