Homework 1 Report - PM2.5 Prediction

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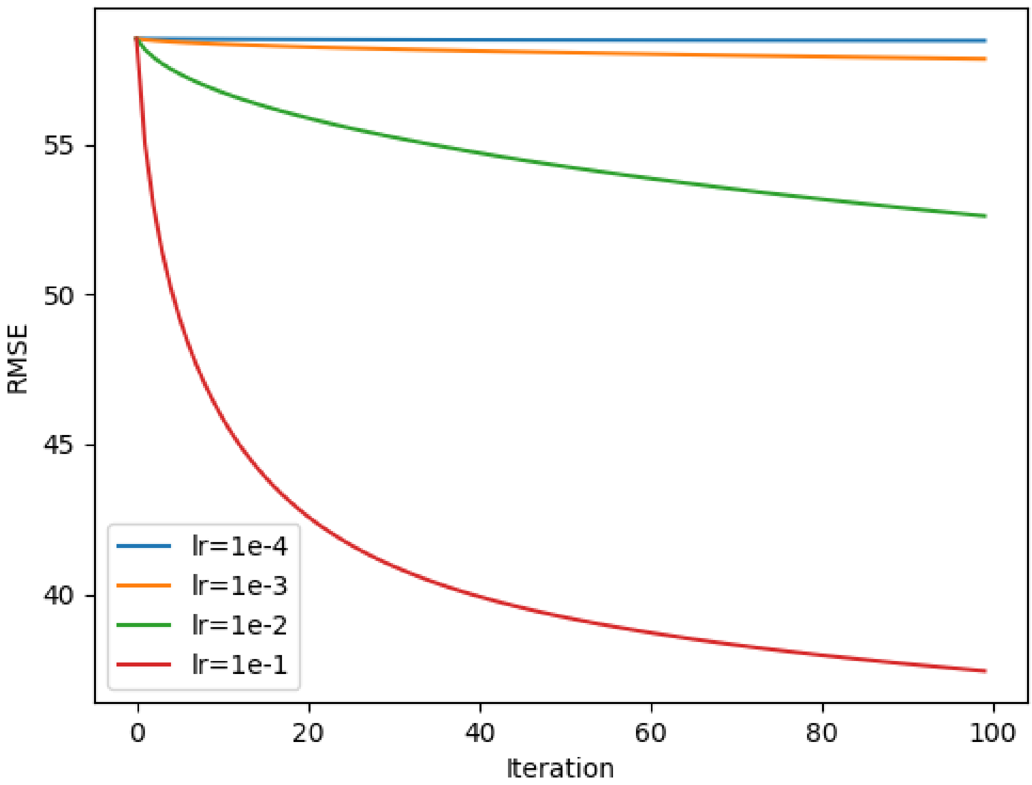
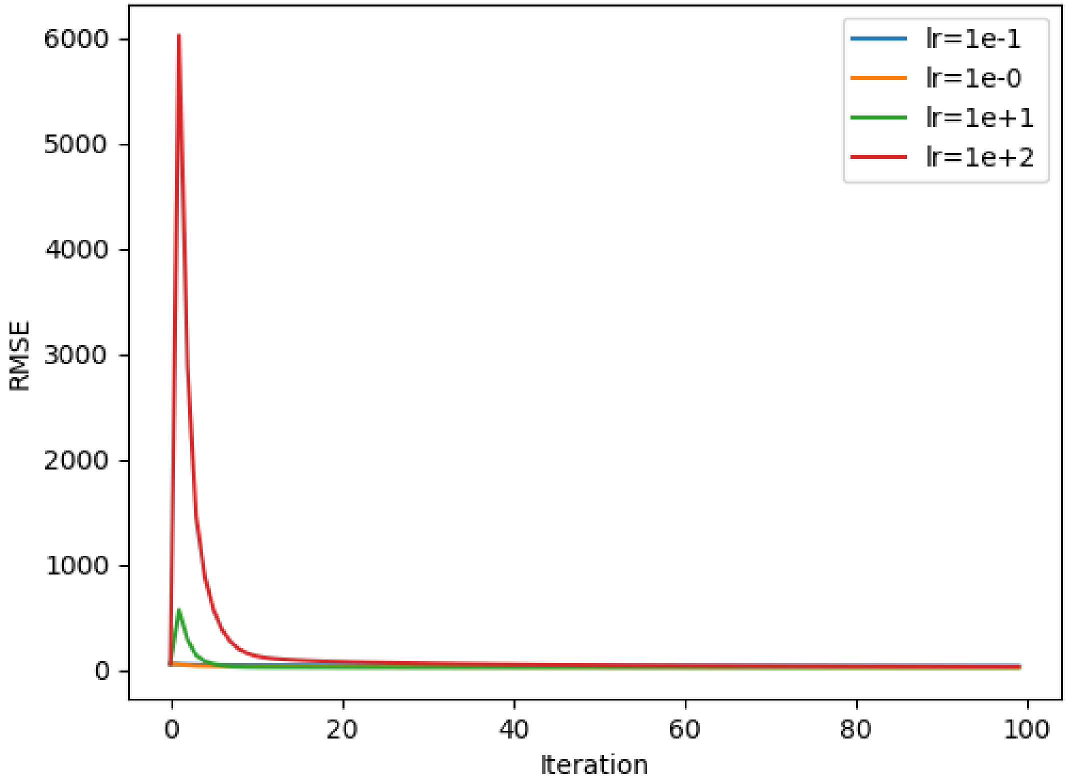
1. **(1%) 請分別使用至少 4 種不同數值的 learning rate 進行 training（其他參數需一致），對其作圖，並且討論其收斂過程差異。**





本題採用七種 learning rate 0.0001/0.001/0.01/0.1/1/10/100，從圖中可以看出 learning rate 為 0.1 時收斂的最快，如果 learning rate 再繼續提高到 1.0 或 10.0 時 RMSE 會呈現一個暴增的山峰然後才慢慢收斂，原因是因為本題採用 gradient descent，雖然過程中會修正每一步的位移量，但太極端的 learning rate 則需要經過多個回合的修正才能開始收斂。

不過本圖也可看出在 gradient descent 的方法裡，learning rate 過高會比過低的收斂速度來的快。

2. (1%) 請分別使用每筆 data9 小時內所有 feature 的一次項（含 bias 項）以及每筆 data9 小時內 PM2.5 的一次項（含 bias 項）進行 training，比較並討論這兩種模型的 root mean-square error（根據 kaggle 上的 public/private score）。

Score	Private	Public
All Feature	8.73094	8.35278
PM2.5	9.71723	9.61511

根據結果可以發現 feature 全取比只取 PM2.5 不管在 private 還是 public 的結果都還要好，因此可以判斷出除了 PM2.5 以外至少還有一個 feature 會影響未來 PM2.5 的數值。

3. (1%)請分別使用至少四種不同數值的 regulization parameter λ 進行 training（其他參數需一至），討論及討論其 RMSE(traning, testing)（testing 根據 kaggle 上的 public/private score）以及參數 weight 的 L2 norm。

λ	Train RMSE	L2 norm	Private Score	Public Score
10.0	25.008061	353.875457	9.42694	8.79099
0.1	23.115629	692.218842	8.66211	8.29411
0.01	23.113938	702.882058	8.66601	8.30637
0.00001	23.113909	704.103165	8.66655	8.30788

根據結果可以發現 λ 越大則 L2 norm 越小，原因是因為 minimize error 的過程中若λ越大則 weight 必須越小才能最小化，但 training RMSE 則會上升，原因是因為阻礙了 weight 的更新(變化較平滑)，而比較 Private 與 Public 的結果可以發現λ從大至小的 score 表現先降後升，原因與老師所講的結論一樣，function 不夠平滑與太平滑都不好。

4 (1%)

(4-a)

Given t_n is the data point of the data set $\mathcal{D} = \{t_1, \ldots, t_N\}$. Each data point t_n is associated with a weighting factor $r_n > 0$.
The sum-of-squares error function becomes:

$$E_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N} r_n(t_n - \mathbf{w}^{\mathbf{T}}\mathbf{x}_n)^2$$

Find the solution $\mathbf{w}^*$ that minimizes the error function.

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$\mathrm{w}^* = \arg\min_{w} E_D(w)$ ➔ compute $\frac{dE_D}{dw}|_{w=w^0}$ ➔find $\frac{\partial E_D}{\partial w} = 0$

對其微分展開得$\frac{\partial \boldsymbol{E_D}}{\partial \boldsymbol{w}} = \sum_{n=1}^{N} \boldsymbol{r_n}(\boldsymbol{t_n} - \boldsymbol{w}^T\boldsymbol{x_n})(-\boldsymbol{x_n}) = \mathbf{0}$ **，故只需找到w* 使其滿足左式即可最小化 error function**

$$\frac{\partial E_D}{\partial w_j} = \sum_{n=1}^{N} \frac{\partial}{\partial w_j}\left(\frac{1}{2} r_n (t_n - w^T x_n)^2\right) = \sum_{n=1}^{N} r_n x_{n,j}(t_n - w^T x_n) = 0$$

➔ $\sum_{n=1}^{N} r_n x_{n,j}\, t_n = \left(\sum_{n=1}^{N} r_n x_{n,j}\, x_n\right) w$

令 A=$\left(\sum_{n=1}^{N} r_n x_{n,j}\, x_n\right)$，b=$\sum_{n=1}^{N} r_n x_{n,j}\, t_n$，則 Aw=b 解出 w=$A^{-1}$b 即可，若 A 不可逆則採用$\sum_{n=1}^{N} r_n (t_n - w^T x_n)(-x_n) = 0$ 解聯立方程式一樣可求出$\mathbf{w}^*$，底下 4-b 即是採用解聯立方法求出

(4-b)

Following the previous problem(2-a), if

$$\mathbf{t} = [t_1 t_2 t_3] = [0 \quad 10 \quad 5], \mathbf{X} = [\mathbf{x_1 x_2 x_3}] = \begin{bmatrix} 2 & 5 & 5 \\ 3 & 1 & 6 \end{bmatrix}$$

$$r_1 = 2, r_2 = 1, r_3 = 3$$

Find the solution $\mathbf{w}^*$.

令$\mathrm{w}^* = [w_1\ w_2]^T$，代入 4-a 所得公式展開可得兩個聯立方程式，展開解聯立方程式得

$\mathbf{w}^* = \begin{bmatrix} \mathbf{2.282752536391707} \\ \mathbf{-1.135862373180415} \end{bmatrix}$

5 (1%)

Given a linear model:

$$y(x, \mathbf{w}) = w_0 + \sum_{i=1}^{D} w_i x_i$$

with a sum-of-squares error function:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \left(y(x_n, \mathbf{w}) - t_n\right)^2$$

where t_n is the data point of the data set $\mathcal{D} = \{t_1, \ldots, t_N\}$

Suppose that Gaussian noise ϵ_i with zero mean and variance σ^2 is added independently to each of the input variables x_i.
By making use of $\mathbb{E}[\epsilon_i \epsilon_j] = \delta_{ij}\sigma^2$ and $\mathbb{E}[\epsilon_i] = 0$, show that minimizing E averaged over the noise distribution is equivalent to minimizing the sum-of-squares error for noise-free input variables with the addition of a weight -decay regularization term, in which the bias parameter w_0 is omitted from the regularizer.
Hint

- $$\delta_{ij} = \begin{cases} 1(i = j), \\ 0(i \neq j). \end{cases}$$

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將x_n加上 noise: $\widetilde{\mathrm{x}_n} = \mathrm{x}_n + \epsilon_n$，則 minimizing E averaged over the noise distribution 為

$$\min\{\frac{1}{2}\sum_{n=1}^{N}(w_0 + \sum_{i=1}^{D} w_i(x_i + \epsilon_i) - t_n)^2\} = \min\{\frac{1}{2}\sum_{n=1}^{N}(w_0 + \sum_{i=1}^{D} w_i x_i + \sum_{i=1}^{D} w_i \epsilon_i - t_n)^2\}$$

令$\mathrm{A}_n = w_0 + \sum_{i=1}^{D} w_i x_i - t_n$，並將常數項$\frac{1}{2}$省略不影響 min，繼續展開

原式$= \min\left\{\sum_{n=1}^{N}\left(\mathrm{A}_n + \sum_{i=1}^{D} w_i \epsilon_i\right)^2\right\} = \min\{\sum_{n=1}^{N}({\mathrm{A}_n}^2 + 2 * \mathrm{A}_n * \sum_{i=1}^{D} w_i \epsilon_i + (\sum_{i=1}^{D} w_i \epsilon_i)^2)\}$

其中期望值$\mathbb{E}[{\mathrm{A}_n}^2] = {\mathrm{A}_n}^2$，$\mathbb{E}[2 * \mathrm{A}_n * \sum_{i=1}^{D} w_i \epsilon_i] = 2\mathrm{A}_n \sum_{i=1}^{D} w_i \mathbb{E}[\epsilon_i] = 2\mathrm{A}_n \sum_{i=1}^{D} w_i * 0 = 0$，$\mathbb{E}\left[\left(\sum_{i=1}^{D} w_i \epsilon_i\right)^2\right] = \mathbb{E}[({w_1}^2{\epsilon_1}^2 + {w_2}^2{\epsilon_2}^2 + \cdots + {w_D}^2{\epsilon_D}^2)] + 2\mathbb{E}[(w_1\epsilon_1 w_2\epsilon_2 + w_1\epsilon_1 w_3\epsilon_3 + \cdots + w_{D-1}\epsilon_{D-1} w_D \epsilon_D)] = ({w_1}^2\delta_{11}\sigma^2 + {w_2}^2\delta_{22}\sigma^2 + \cdots + {w_D}^2\delta_{DD}\sigma^2) + 2(w_1 w_2 \delta_{12}\sigma^2 + w_1 w_3 \delta_{13}\sigma^2 + \cdots + w_{D-1} w_D \delta_{D-1D}\sigma^2) = \sum_{i=1}^{D} {w_i}^2\sigma^2 + 0 = \sigma^2 \sum_{i=1}^{D} {w_i}^2$ 帶回原式

原式$= \min\{\sum_{n=1}^{N}({\mathrm{A}_n}^2 + \sigma^2 \sum_{i=1}^{D} {w_i}^2\} = \min\{\sum_{n=1}^{N}((w_0 + \sum_{i=1}^{D} w_i x_i - t_n)^2 + \sigma^2 \sum_{i=1}^{D} {w_i}^2\}$

前面項$(\boldsymbol{w_0} + \sum_{i=1}^{D} \boldsymbol{w_i x_i} - \boldsymbol{t_n})^2$是 minimizing the sum-of-squares error for noise-free input variables，而後面項 $\boldsymbol{\sigma^2} \sum_{i=1}^{D} \boldsymbol{{w_i}^2}$是 addition of a weight–decay regulation term，故兩者結果相等得證#

6 (1%)

$\mathbf{A} \in \mathbb{R}^{n \times n}$, α is one of the elements of $\mathbf{A}$, prove that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} ln|\mathbf{A}| = Tr\left(\mathbf{A}^{-1} \frac{\mathrm{d}}{\mathrm{d}\alpha} \mathbf{A}\right)$$

where the matrix $\mathbf{A}$ is a real, symmetric, non-sigular matrix.

Hint:

- The determinant and trace of $\mathbf{A}$ could be expressed in terms of its eigenvalues.

Derivation of Jacobi's formula by Laplace:

$\mathrm{d}|\mathrm{A}| = \sum_j A_{ij} adj^T(A)_{ij}$ 又 $|\mathrm{A}| = \mathrm{F}(\mathrm{A}_{11}, \mathrm{A}_{12}, \dots, \mathrm{A}_{21}, \mathrm{A}_{22}, \dots, \mathrm{A}_{nn})$

➔ $\mathrm{d}|\mathrm{A}| = \sum_i \sum_j \frac{\partial F}{\partial A_{ij}} dA_{ij}$ ➔ $\frac{\partial |\mathrm{A}|}{\partial A_{ij}} = \frac{\partial \sum_k A_{ik} adj^T(A)_{ik}}{\partial A_{ij}} = \sum_k \frac{\partial A_{ik} adj^T(A)_{ik}}{\partial A_{ij}} = \sum_k \frac{\partial A_{ik}}{\partial A_{ij}} adj^T(A)_{ik} + \sum_k \frac{\partial adj^T(A)_{ik}}{\partial A_{ij}} A_{ik} = \sum_k \frac{\partial A_{ik}}{\partial A_{ij}} adj^T(A)_{ik} + 0 = \sum_k \frac{\partial A_{ik}}{\partial A_{ij}} adj^T(A)_{ik} = adj^T(A)_{ij}$ ➔ $\mathbf{d|A|} = \boldsymbol{Tr(adj(A)dA)}$

因為 A 可逆➔ $\frac{\mathbf{d|A|}}{\boldsymbol{d\alpha}} = \boldsymbol{|A| Tr(A^{-1} \frac{dA}{d\alpha})}$

$\frac{d}{d\alpha} \ln|A| = Tr\left(adj(\ln A) \frac{d \ln A}{d\alpha}\right) = Tr\left(\ln|A| * \frac{1}{\ln A} * \frac{d \ln A}{d\alpha}\right) = \ln|A| \operatorname{Tr}\left(\ln A^{-1} \frac{d \ln A}{d\alpha}\right)$

$= \ln|A| \operatorname{Tr}\left(\ln A^{-1} \frac{d \ln A}{dA} * \frac{dA}{d\alpha}\right) = \ln|A| \operatorname{Tr}\left(\frac{1}{\ln A} * A^{-1} * \frac{dA}{d\alpha}\right)$

設 A 的 eigenvalues 為$\lambda_1, \lambda_2, \lambda_3 \dots, \lambda_n$，則$|A| = \lambda_1 \lambda_2 \lambda_3 \dots \lambda_n$，$\mathrm{Tr}(A) = \lambda_1 + \lambda_2 + \lambda_3 + \cdots + \lambda_n$繼續展開

$$\frac{d}{d\alpha} \ln|A| = \ln(\lambda_1 \lambda_2 \lambda_3 \dots \lambda_n) * \frac{1}{\ln(\lambda_1) + \ln(\lambda_2) + \ln(\lambda_3) + \cdots + \ln(\lambda_n)} * \operatorname{Tr}\left(A^{-1} * \frac{dA}{d\alpha}\right)$$

又$\ln(\lambda_1 \lambda_2 \lambda_3 \dots \lambda_n) = \ln(\lambda_1) + \ln(\lambda_2) + \ln(\lambda_3) + \cdots + \ln(\lambda_n)$

故$\frac{d}{d\alpha} \ln|A| = \frac{1}{1} \operatorname{Tr}\left(A^{-1} * \frac{d}{d\alpha} A\right) = \operatorname{Tr}\left(A^{-1} * \frac{d}{d\alpha} A\right)$ 得證#