PM2.5 Final Report

Three method to linear regression:

Gradient descent ...know how and why

Maximum likelihood estimation ...know how only

Maximum a posterior ...know how only

PM2.5 dataset

Features:17D

8	U		2 .	3	4 ,	5 (6 ,	/ {	8	1	IU	188	12	13	14	15	16	l /
Г		AMB_TE	CH4	CO	NMHC	ИО	NO2	NOx	03	PM10	RAINFAI	RH	SO2	THC	WD_HR	WIND_D	WIND_SI	WS_HR
н		19.5	1.9	0.4175	0.089167	1.054167	10.78333	11.97917	42.95833	54.04167	0	71.29167	2.383333	1.9875	62.04167	62.16667	2.770833	2.320833
н		18.70833	1.9625	0.60375	0.173333	5.420833	20.225	25.64583	26.17083	89.375	0.016667	83.66667	2.495833	2.120833	76.25	87.70833	1.529167	1.1125
		19.16667	2.079167	0.721667	0.27375	14.7375	29.58333	44.41667	4.904167	55.29167	0.816667	90.41667	2.408333	2.354167	94.91667	84.375	1.15	0.758333
н		20.20833	2.154167	0.996667	0.360417	23.4	22.975	46.41667	9.4375	42.75	0.008333	88.54167	2.9125	2.504167	188.5417	186.7083	0.883333	0.491667
н		20.375	2.033333	0.654583	0.324583	15.87391	24.69565	40.52174	7.291667	55.08696	0.008333	87.33333	3.433333	2.345833	119.9167	133.5417	1.3375	0.895833
н		18.25	1.9	0.375417	0.16125	1.779167	17.14167	19.02083	24.61667	26.20833	1.825	86.45833	2.258333	2.075	62.04167	60.66667	2.633333	1.8375
н		18	1.881818	0.41875	0.135455	2.426087	12.31304	14.68696	38.75	47.5	0	75.04167	2.583333	1.990909	61.33333	62.08333	3.675	2.920833
н		16.875	1.891667	0.44875	0.12375	1.3125	14.025	15.44583	36.70833	51.20833	0.083333	77.375	2.420833	1.9875	65.04167	67.5	2.85	2.325
н		17.33333	1.9125	0.557917	0.144583	3.441667	17.87083	21.26667	32.91667	49.16667	0	71.54167	3.554167	2.045833	63.66667	61.91667	2.8375	2.204167
н		18.375	1.954167	0.542917	0.189583	5.879167	17.65	23.67083	21.25417	45.625	0	81.45833	2.654167	2.145833	94.125	85.79167	1.425	1.029167
П		16.875	1.845833	0.415833	0.1325	3.841667	19.50417	23.35833	27.7375	19.625	2.3	89.41667	1.666667	1.991667	68	75.375	1.904167	1.329167
н	1	16.29167	1.854545	0.382174	0.099545	2.104348	10.78261	12.90435	34	32.82609	0.066667	80.125	1.326087	1.945455	64.08333	64.875	3.629167	2.766667
н		14.25	1.9	0.477917	0.117917		11.39167	12.31667	33.79167	27.125	0	82.33333	1.1625	1.983333	64.54167	64.45833	3.525	2.641667
н		14.66667	1.941667	0.64375	0.17375	3.016667	17.6125	20.625	31	61.33333	0	75.58333	3.420833	2.116667	66.875	66.79167	2.895833	
ш		15.625		0.653333	0.213333	4.929167	26.125	31.08333		70.29167		83.75		2.183333		69.25	1.725	1.408333
н		18.66667	1.929167	0.515	0.146667	3.020833	17.99167		26.72083		0.016667	77	2.466667	2.075	74.91667	80.58333	2.116667	1.683333
н		16.875	1.945833	0.51375	0.148333	7.004167	16.49167	23.54167	22.95417			89.83333		2.095833	114.8083	126.5833	1.5625	0.925
П		14.833333	1.913043	0.542917	0.100.10	2.816667			36.58333				2.083333	2.03913	71.375	71.625		2.741667
н		14.58333	1.895833		0.149167		15.51667				0.033333	74.58333			71.20833		3.7	3.0625
н		15.5	1.883333	0.011001		4.416667	19.25		26.81667	26.75	0	78	3.0625		82.58333			2.266667
П		15.54167		0.374583		5.254167		21.29583		18.45833				2.033333				1.495833
н		15.25			0.135417		15.8375		26.81667			86			61.70833	61.625		2.254167
н		10.0375			0.082917		10.62083		32.29167		0.9	84.5	2.1375		64.79167			3.716667
ı		4.970833	1.804167	0.3225		1.604167				40.16667								
		7.833333	1.841667		0.098333						_		2.270833				3.795833	
			1.047006															

Target:

2	#Date	PM2.5
Ś	2016/1/1	27.70833
Ş	2016/1/2	46.08333
ζ	2016/1/3	38.47826
5	2016/1/4	23.52174
2	2016/1/5	31.47826
	2016/1/6	6.916667
	2016/1/7	21.625
	2016/1/8	25.5
	2016/1/9	22.29167
	2016/1/10	21.16667
	2016/1/11	6.375
	2016/1/12	11.13043
	2016/1/13	11.75
	2016/1/14	34.95833
	2016/1/15	43.29167
	2016/1/16	14.91667
	2016/1/17	10.16667
	2016/1/18	24.65217
	2016/1/19	44
	2016/1/20	10.58333
	2016/1/21	5.666667
	2016/1/22	2.958333
	2016/1/23	17.625
	2016/1/24	12.75

Four basic function: Polynomial (M=1): $h(x,\theta) = \sum_{i=0}^{\infty} \theta_i x_i$

Polynomial (M=2):
$$h(x,\theta) = \sum_{i=0}^{17} \theta_i x_i + \sum_{i=1}^{27} \sum_{j=1}^{i} \theta_n x_i x_j$$
, $n \text{ in range } (18,171)$

Sigmoidal:
$$S(x) = \frac{e^x}{1 + e^x}$$

Gaussian:
$$f(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)}$$

Error estimation: RMSE

Polynomial (M=1)

Dataset: $\begin{cases} training: 80\% \\ testing: 20\% \end{cases}$

data

Normalization

Shuffle

Train test split

Linear regression (G.D and MLE)

PM2.5(M=1)—gradient descent

Hypothesis:
$$h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \dots + \theta_{17} x_{17}$$

Cost function:
$$J(\theta_0, \theta_1, ..., \theta_{16}, \theta_{17}) = \frac{1}{2N} \sum_{i=1}^{N} (h_{\theta}(x^i) - T^i)^2$$

Gradient descent: repeat before convergence{

$$\theta_n = \theta_n - \alpha \frac{\partial J(\theta_0, \theta_1, \dots, \theta_{17})}{\partial \theta_n}$$

PM2.5(M=1)—gradient descent

Pseudocode:

Read the data Split into training set and testing set



Initialize theta Update theta by gradient descent



Get the hypothesis function





Use the training target to test the model

Use the testing target to test the model

PM2.5(M=1)hypothesis function

 x_i^j :the ith feature in the jth data

$$h_{\theta}(x) = [\theta_{0} \quad \theta_{1} \quad \dots \quad \theta_{16} \quad \theta_{17}]_{1X18} \cdot \begin{bmatrix} x_{0}^{1} & x_{0}^{2} & \dots & x_{0}^{N-1} & x_{0}^{N} \\ x_{1}^{1} & x_{1}^{2} & \dots & x_{1}^{N-1} & x_{1}^{N} \\ \dots & \dots & \dots & \dots \\ x_{16}^{1} & x_{16}^{2} & \dots & x_{17}^{N-1} & x_{17}^{N} \end{bmatrix}_{18XN}$$
Just to put the constant of the hypothesis function into the matrix
$$= [y^{1} \quad y^{2} \quad \dots \quad y^{N-1} \quad y^{N}]_{1XN}$$

 $x_0^i = 1$ Just to put the constant of the

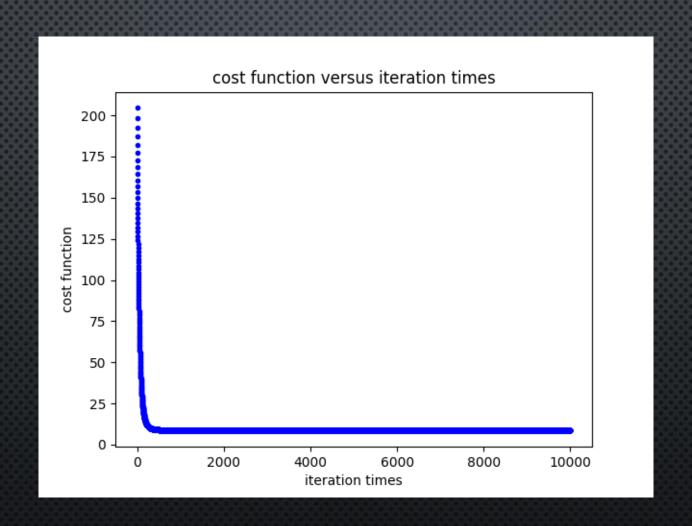
Transpose from the original data

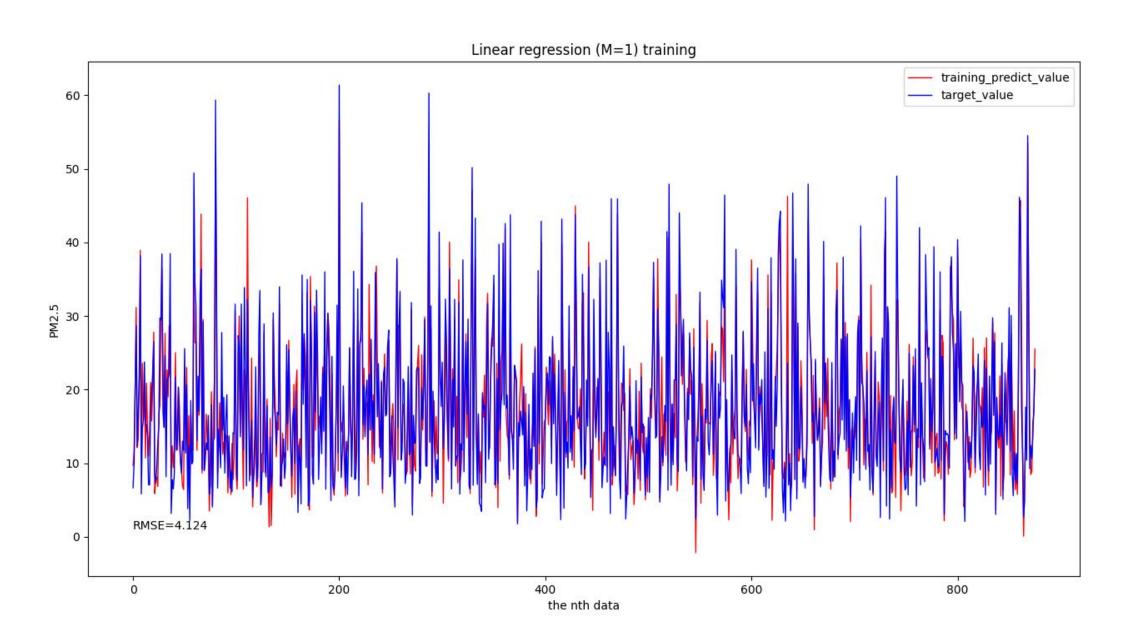
$$\begin{aligned} \text{Theta_grad:} &= \left[\frac{\partial J}{\partial \theta_0} \ \frac{\partial J}{\partial \theta_1} \ \dots \ \frac{\partial J}{\partial \theta_{16}} \ \frac{\partial J}{\partial \theta_{17}} \right]_{1X18} \\ &= \frac{1}{N} \Bigg[\sum_{i=1}^N \left(h_\theta(x^i) - T^i \right) \cdot x_0^i \ \sum_{i=1}^N \left(h_\theta(x^i) - T^i \right) \cdot x_1^i \ \dots \ \sum_{i=1}^N \left(h_\theta(x^i) - T^i \right) \cdot x_{16}^i \ \sum_{i=1}^N \left(h_\theta(x^i) - T^i \right) \cdot x_{17}^i \Bigg]_{1X18} \\ &= \frac{1}{N} \left([y^1 \ y^2 \ \dots \ y^{N-1} \ y^N]_{1XN} - [T^1 \ T^2 \ \dots \ T^{N-1} \ T^N]_{1XN} \right) \cdot \begin{bmatrix} x_0^1 \ x_0^2 \ \dots \ x_0^{N-1} \ x_0^N \\ x_1^1 \ x_1^2 \ \dots \ x_1^{N-1} \ x_1^N \\ \dots \ \dots \ \dots \ \dots \ \dots \\ x_{16}^1 \ x_{16}^2 \ \dots \ x_{17}^{N-1} \ x_{17}^N \end{bmatrix}_{18XN} \end{aligned}$$
 Hypothesis: $h_\theta(x) = \theta_0 x_0 + \theta_1 x_1 + \dots + \theta_{17} x_{17}$

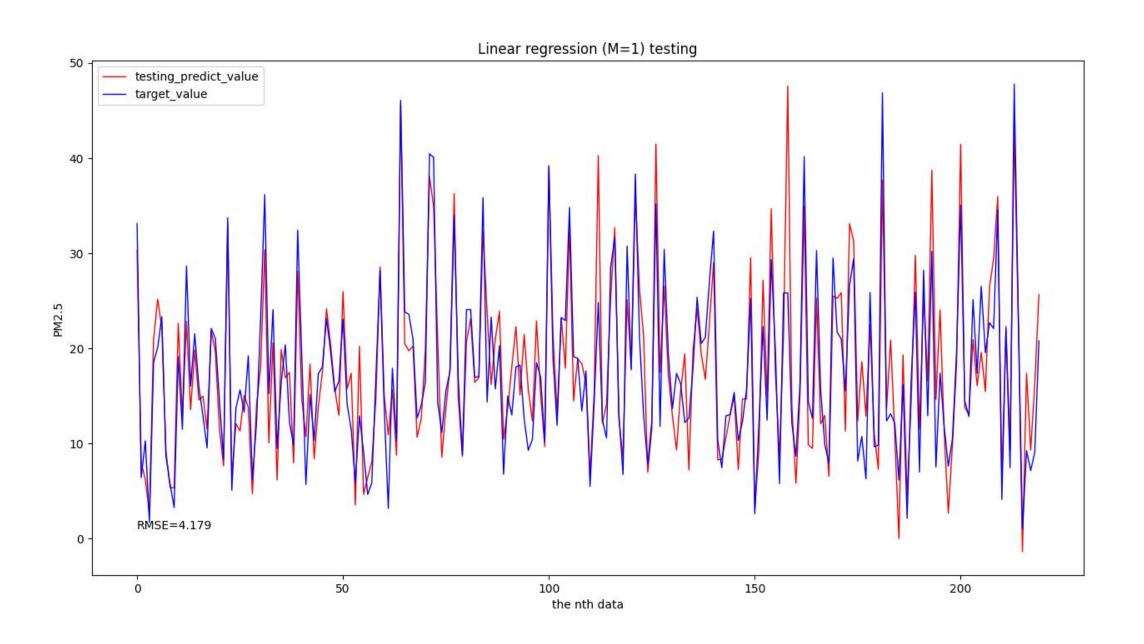
Hypothesis: $h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \dots + \theta_{17} x_{17}$

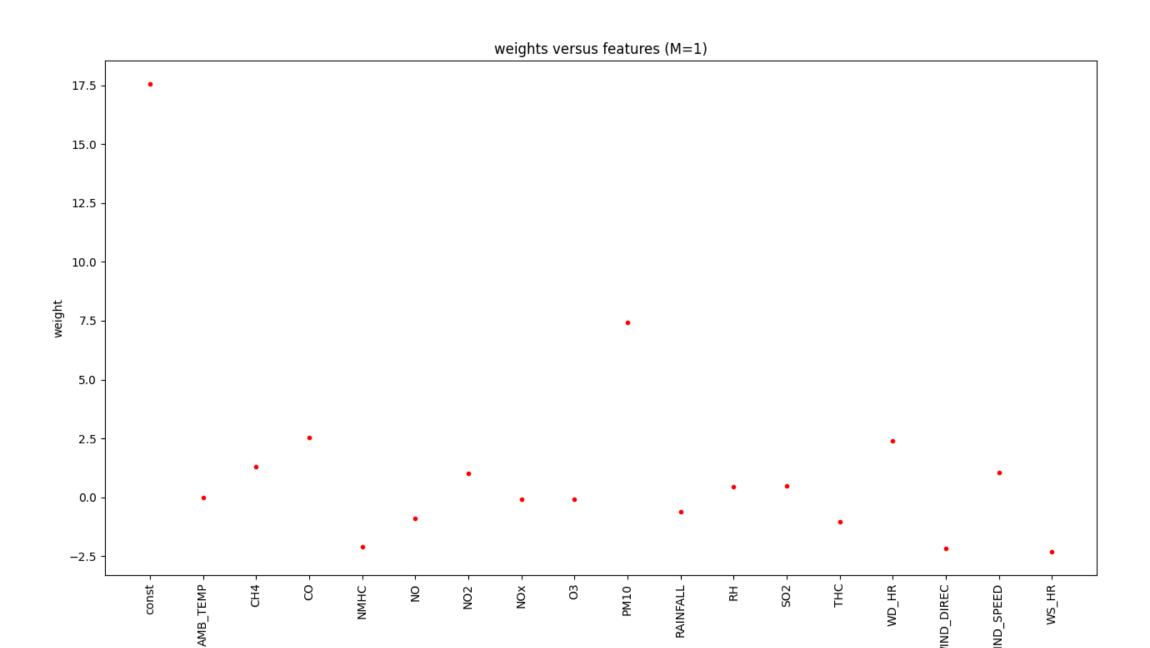
Cost function:
$$J(\theta_0, \theta_1, ..., \theta_{16}, \theta_{17}) = \frac{1}{2N} \sum_{i=1}^{N} (h_{\theta}(x^i) - T^i)^2$$

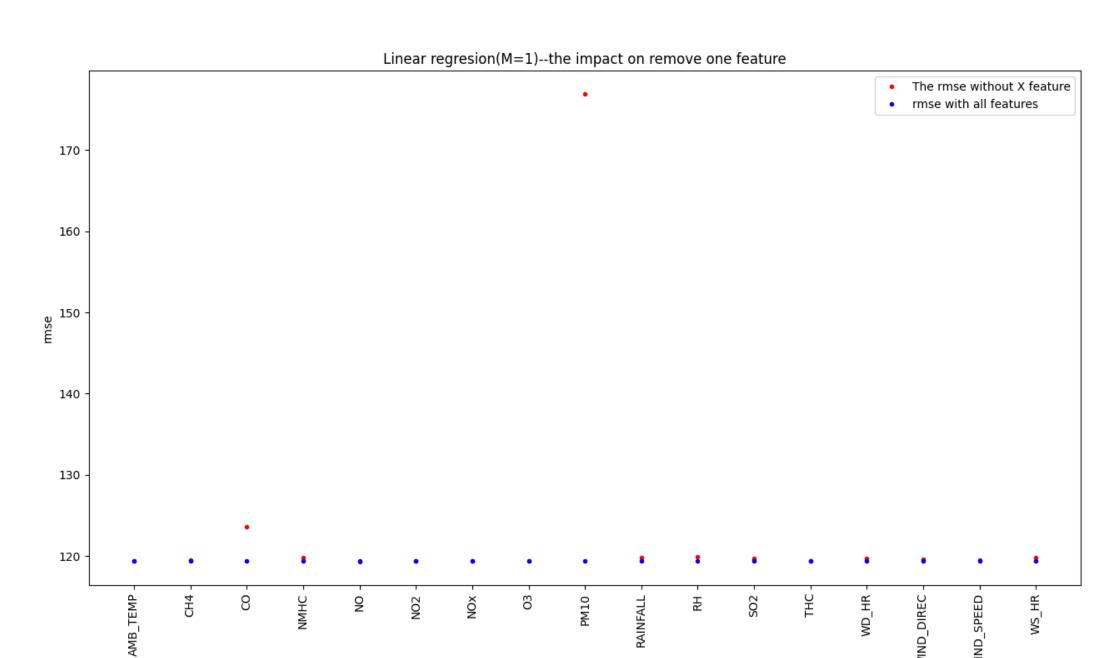
Gradient descent:
$$\theta_n = \theta_n - \alpha \frac{\partial J(\theta_0, \theta_1, \dots, \theta_{17})}{\partial \theta_n}$$











PM2.5(M=2)—gradient descent

Hypothesis:
$$h_{\theta}(x) = \theta_{0}x_{0} + \theta_{1}x_{1} + \ldots + \theta_{17}x_{17} + \theta_{18}x_{1}x_{1} + \theta_{19}x_{2}x_{1} + \theta_{20}x_{2}x_{2} + \theta_{21}x_{3}x_{1} + \theta_{22}x_{3}x_{2} + \theta_{23}x_{3}x_{3} + \ldots + \theta_{169}x_{17}x_{16} + \theta_{170}x_{17}x_{17}$$

$$\Rightarrow h_{\theta}(x) = \sum_{i=0}^{17} \theta_{i}x_{i} + \sum_{j=1}^{i} \theta_{n}x_{i}x_{j}, n \ in \ range(18,171)$$

Cost function:
$$J(\theta_0, \theta_1, \dots, \theta_{169}, \theta_{170}) = \frac{1}{2N} \sum_{i=1}^{N} (h_{\theta}(x^i) - T^i)^2$$

Gradient descent: repeat before convergence{

$$\theta_n = \theta_n - \alpha \frac{\partial J(\theta_0, \theta_1, \dots, \theta_{170})}{\partial \theta_n}$$

PM2.5(M=2)—gradient descent

Data preprocess

Append the data (or features) by multiplied two features:

<u>0 1 2 3 4 5 6 7</u> 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22.......169 170

	AMB_TE	CH4	CO	NMHC	NO	NO2	NOx	03	PM10	RAINFAI	RH	SO2	THC	WD_HR	WIND_D	WIND_SI	WS_HR					
e e	19.5	1.9	0.4175	0.089167	1.054167	10.78333	11.97917	42.95833	54.04167	0	71.29167	2.383333	1.9875	62.04167	62.16667	2.770833	2.320833					
5	18.70833	1.9625	0.60375	0.173333	5.420833	20.225	25.64583	26.17083	89.375	0.016667	83.66667	2.495833	2.120833	76.25	87.70833	1.529167	1.1125					
9	19.16667	2.079167	0.721667	0.27375	14.7375	29.58333	44.41667	4.904167	55.29167	0.816667	90.41667	2.408333	2.354167	94.91667	84.375	1.15	0.758333					
	20.20833	2.154167	0.996667	0.360417	23.4	22.975	46.41667	9.4375	42.75	0.008333	88.54167	2.9125	2.504167	188.5417	186.7083	0.883333	0.491667					
9	20.375	2.033333	0.654583	0.324583	15.87391	24.69565	40.52174	7.291667	55.08696	0.008333	87.33333	3.433333	2.345833	119.9167	133.5417	1.3375	0.895833					1 1
9	18.25	1.9	0.375417	0.16125	1.779167	17.14167	19.02083	24.61667	26.20833	1.825	86.45833	2.258333	2.075	62.04167	60.66667	2.633333	1.8375					
8	18	1.881818	0.41875	0.135455	2.426087	12.31304	14.68696	38.75	47.5	0	75.04167	2.583333	1.990909	61.333333	62.08333	3.675	2.920833					1 6
9	16.875	1.891667	0.44875	0.12375	1.3125	14.025	15.44583	36.70833	51.20833	0.083333	77.375	2.420833	1.9875	65.04167	67.5	2.85	2.325					
9	17.33333	1.9125	0.557917	0.144583	3.441667	17.87083	21.26667	32.91667	49.16667	0	71.54167	3.554167	2.045833	63.66667	61.91667	2.8375	2.204167					
8	18.375	1.954167	0.542917	0.189583	5.879167	17.65	23.67083	21.25417	45.625	0	81.45833	2.654167	2.145833	94.125	85.79167	1.425	1.029167				17	17
	16.875	1.845833	0.415833	0.1325	3.841667	19.50417	23.35833	27.7375	19.625	2.3	89.41667	1.666667	1.991667	68	75.375	1.904167	1.329167		121	2	17	17
	16.29167	1.854545	0.382174	0.099545	2.104348	10.78261	12.90435	34	32.82609	0.066667	80.125	1.326087	1.945455	64.08333	64.875	3.629167	2.766667	-JL	4	*	*	
	14.25	1.9	0.477917	0.117917	1.129167	11.39167	12.31667				82.33333	1.1625	1.983333	64.54167	64.45833	3.525	2.641667	*	_ ^	^	 *	^
	14.66667	1.941667	0.64375	0.17375	3.016667	17.6125	20.625	31	61.33333	0	75.58333	3.420833	2.116667	66.875	66.79167	2.895833	2.266667					
5	15.625	1.958333	0.653333	0.213333	4.929167	26.125	31.08333		70.29167		83.75	3.1625		68.83333	69.25		1.408333			2	16	17
9	18.66667	1.929167	0.515	0.146667	3.020833	17.99167	20.85	26.72083	33.25	0.016667	77	2.466667	2.075	74.91667	80.58333	2.116667	1.683333					
		1.945833			7.004167	16.49167	23.54167	22.95417	26.45833	2.025	89.83333	1.795833	2.095833	114.8083		1.5625	0.925					
8			0.542917					36.58333		0.008696							2.741667					
	14.58333	1.895833	0.5875	0.149167		15.51667	18.74583	36.58333		0.033333	74.58333	3.708333		71.20833			3.0625					
	15.5	1.883333	0.511667		4.416667			26.81667	26.75	0	78		2.075	82.58333	83.91667		2.266667					
9			0.374583		5.254167				18.45833					77.79167			1.495833					
9			0.329167			15.8375			14.20833			2.083333		61.70833	61.625		2.254167					
		1.866667			2.216667				34.95833	0.9		2.1375		64.79167								
		1.804167	0.3225		1.604167				40.16667							3.458333						
		1.841667			2.991667								1.945833			3.795833						
	13.87917	1.947826	0.59	0.266957	12.38696	23.82609	36.13043	22.23913	35.73913	0	64.25	3.117391	2.217391	111.9167	108.4583	1.445833	0.991667					

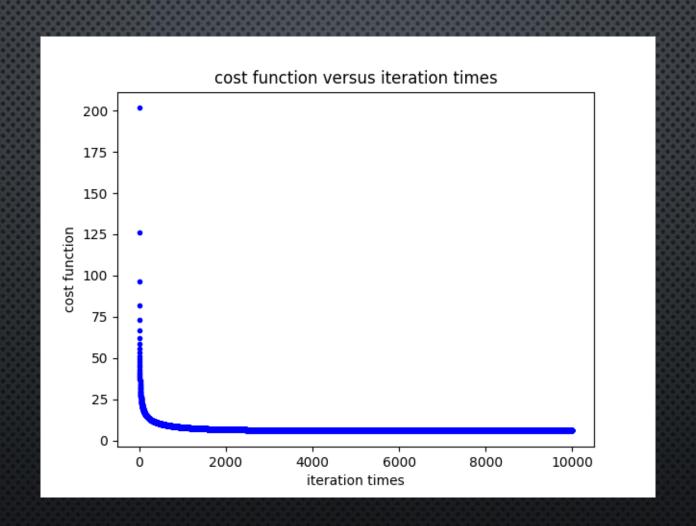
PM2.5(M=2)—gradient descent

$$h_{\theta}(x) = \sum_{i=0}^{17} \theta_i x_i + \sum_{i=1}^{17} \sum_{j=1}^{i} \theta_n x_i x_j, n \text{ in } range(18,171)$$

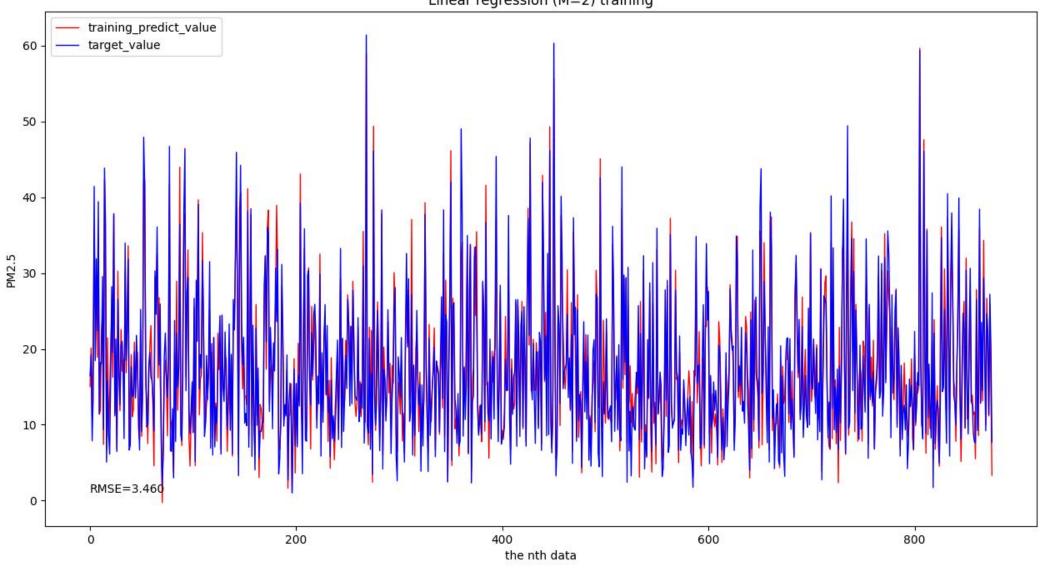
$$\Rightarrow h_{\theta}(x) = \sum_{i=0}^{17} \theta_{i} x_{i} + \sum_{i=18}^{170} \theta_{i} x_{i} = \sum_{i=0}^{170} \theta_{i} x_{i} = [\theta_{0} \quad \theta_{1} \quad \dots \quad \theta_{169} \quad \theta_{170}]_{1X171} \cdot \begin{bmatrix} x_{0}^{1} & x_{0}^{2} & \dots & x_{0}^{N-1} & x_{0}^{N} \\ x_{1}^{1} & x_{1}^{2} & \dots & x_{1}^{N-1} & x_{1}^{N} \\ \dots & \dots & \dots & \dots & \dots \\ x_{169}^{1} & x_{170}^{2} & \dots & x_{17}^{N-1} & x_{17}^{N} \end{bmatrix}_{171XN}$$

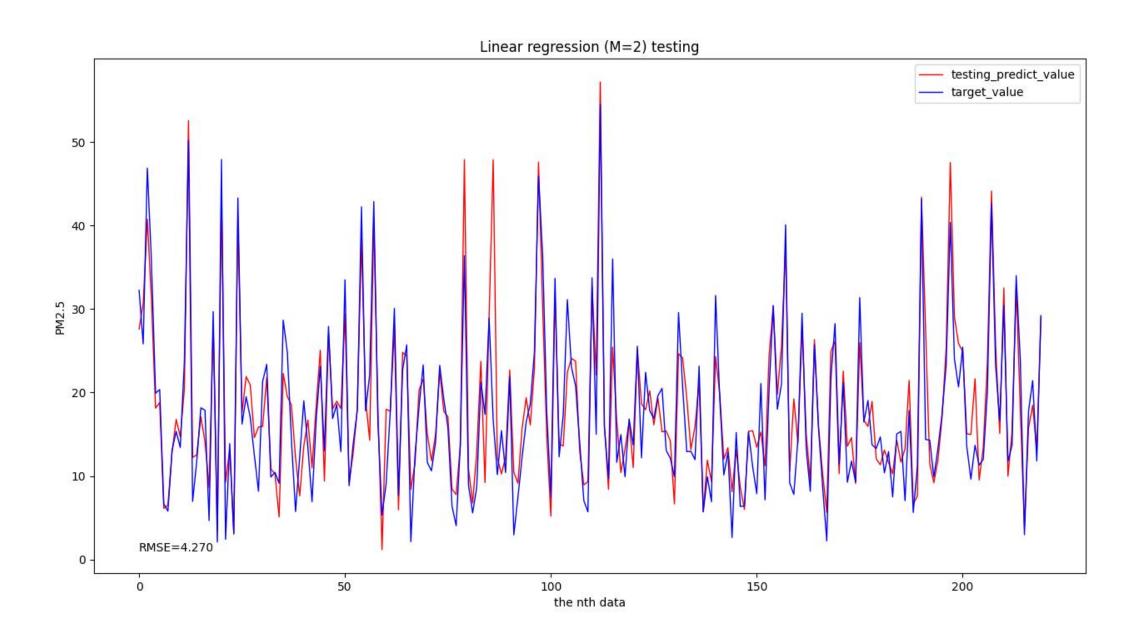
$$= [y^{1} \quad y^{2} \quad \dots \quad y^{N-1} \quad y^{N}]_{1XN}$$

Transpose from the original data









Model evaluation

RMSE	training	testing
	1. 4.116	1. 4.160
	2. 4.093	2. 4.258
M=1 (gradient	3. 4.190	3. 3.879
descent)	4. 4.066	4. 4.345
	5. 4.093	5. 4.245
	Avg: 4.111	Avg: 4.177
	1. 3.361	1. 4.128
	2. 3.365	2. 4.242
M=2 (gradient	3. 3.414	3. 5.051
descent)	4. 3.351	4. 4.183
	5. 3.408	5. 4.864
	Avg: 3.379	Avg: 4.493

由以上梯度下降實作中可以看到當m=1的時候,training的rmse與testing的rmse差距其實蠻小的,但是當m=2的時候,可以觀察到training的rmse降到很小,表示比起m=1找到更適合的參數去貼合模型,但是當到了testing的時候,可以發現rmse比起training的時候增加了許多,甚至超過了m=1的testing的rmse,因此可以推斷出這邊發生了過擬合的現象,因此面對陌生的資料時會較敏感。

PM2.5--MLE

data

Normalization

Data Transform

Shuffle

Sigmoidal:
$$S(x) = \frac{e^x}{1 + e^x}$$

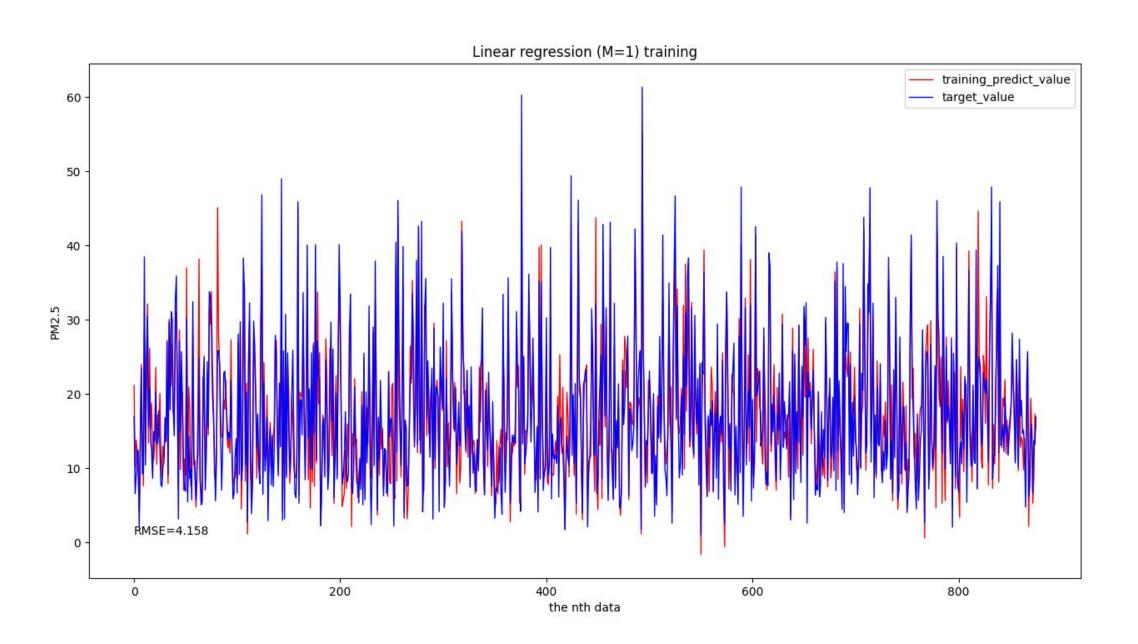
Gaussian: $f(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)}$

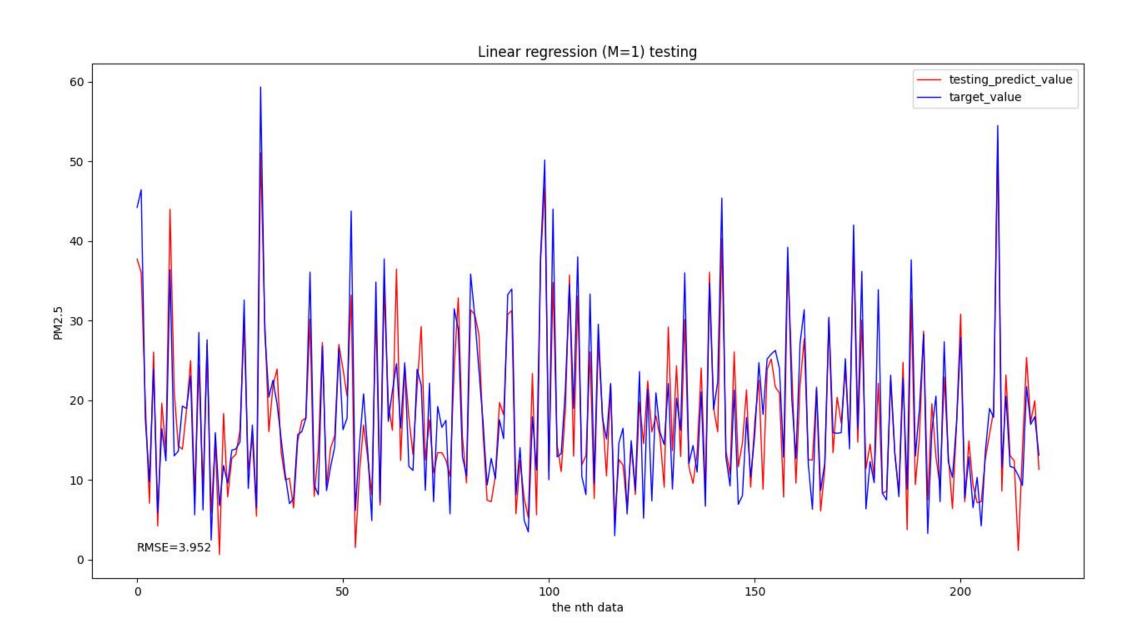
Train test split

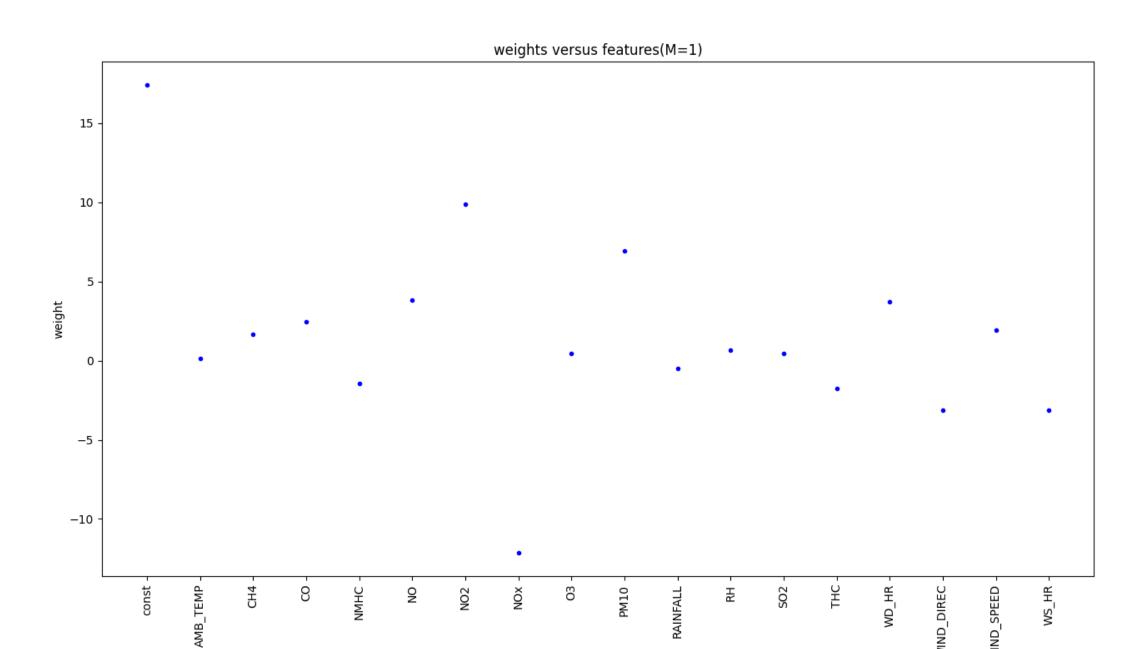
Linear regression

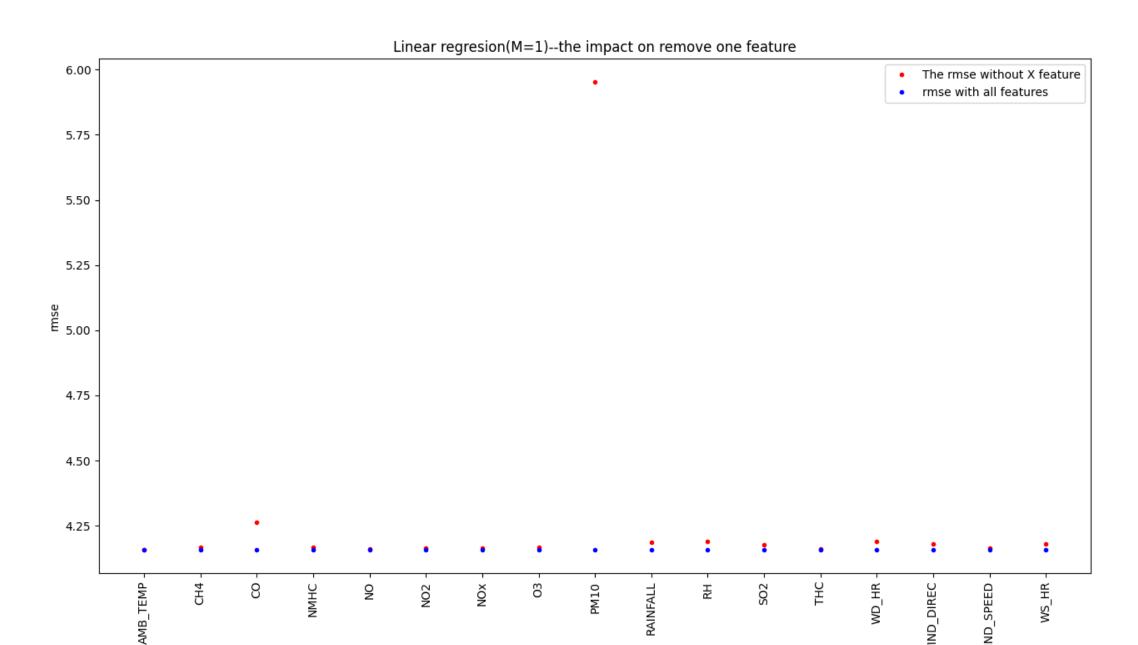
Linear regression: $w = (X^T X)^{-1} X^T Y$

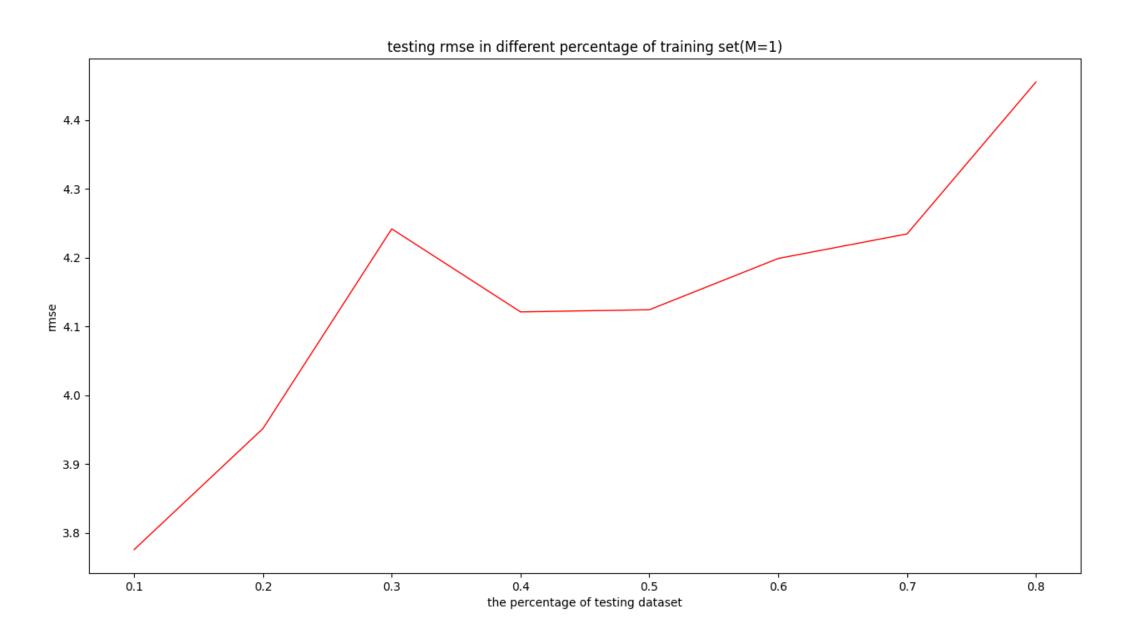
Polynomial (M=1)-MLE

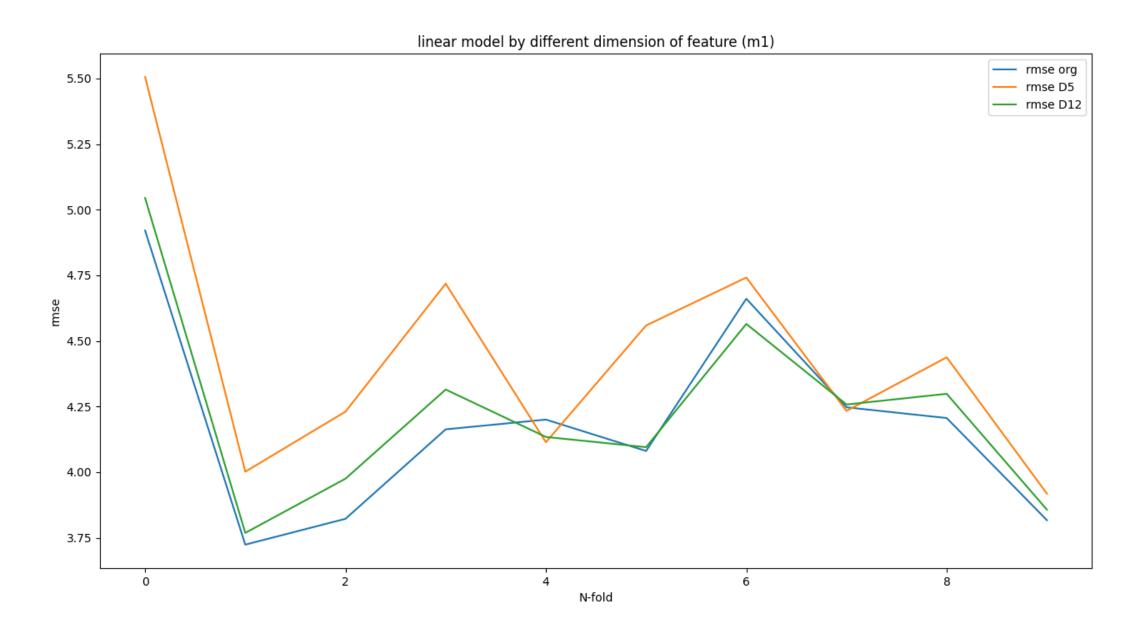




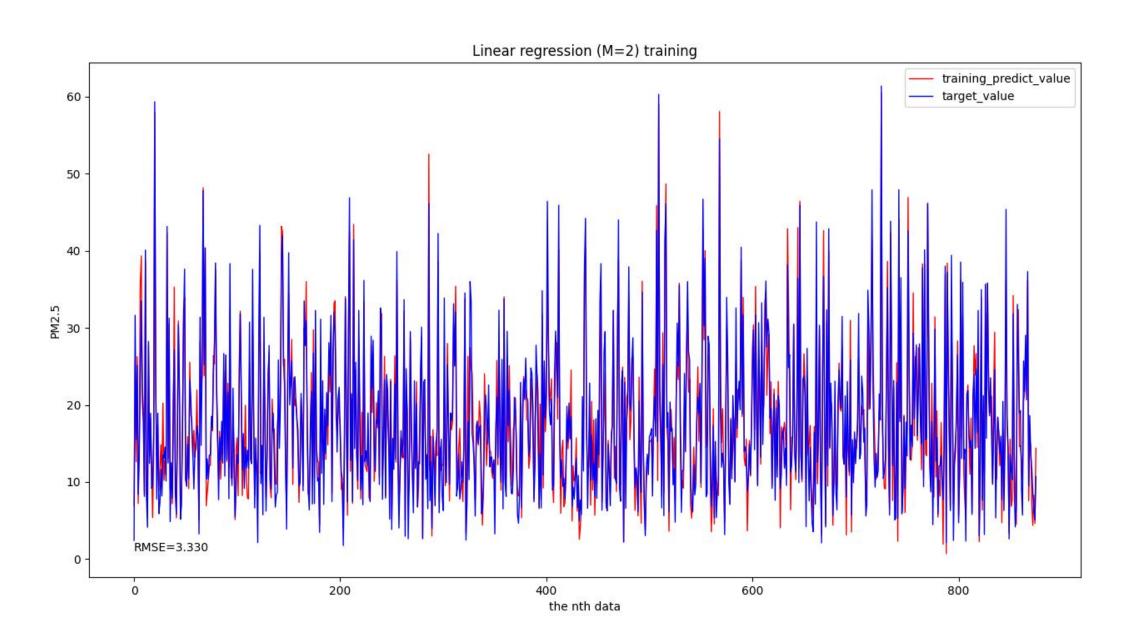


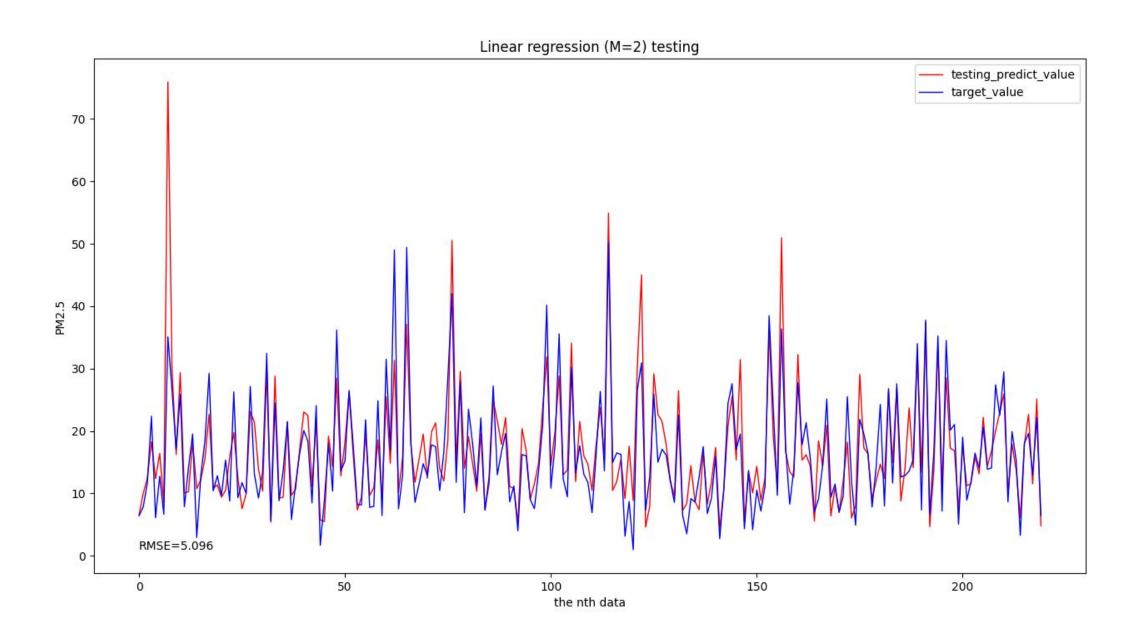


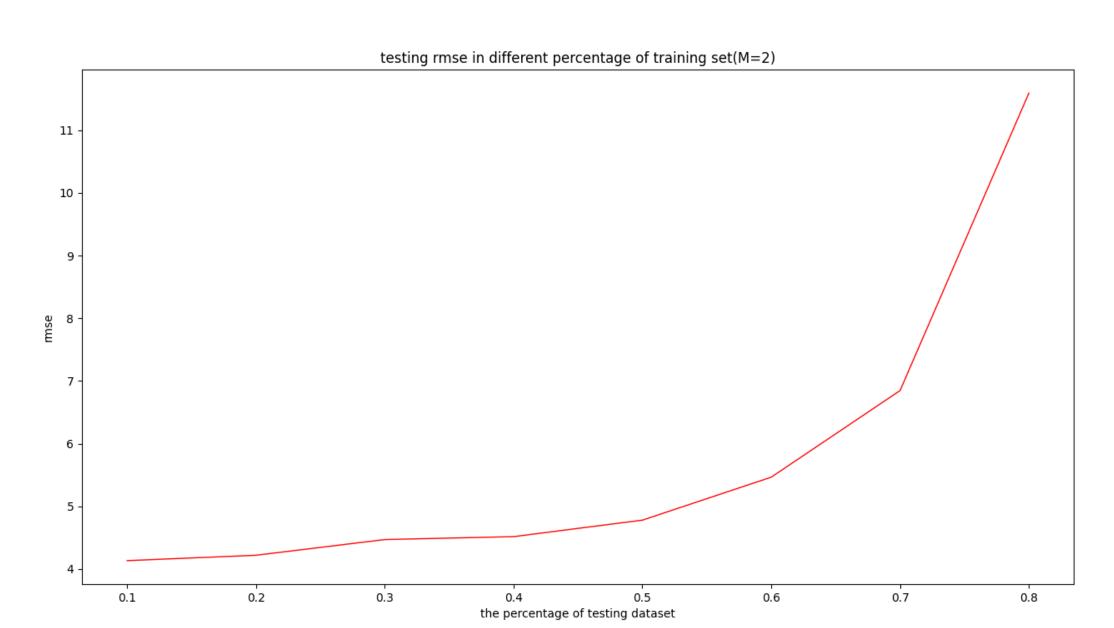


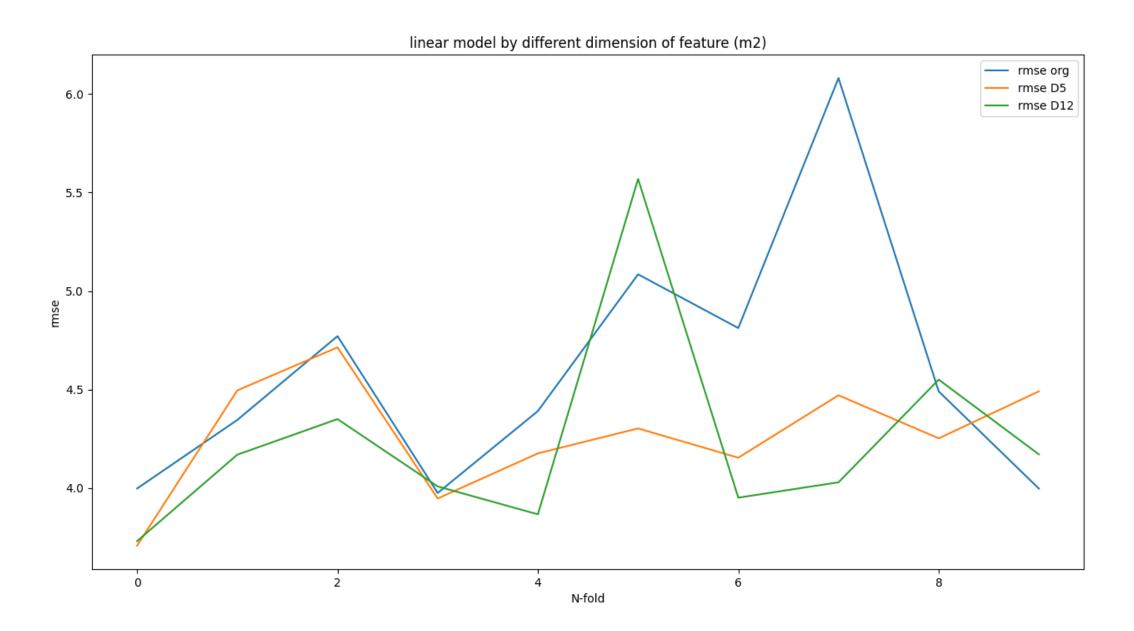


Polynomial (M=2)-MLE

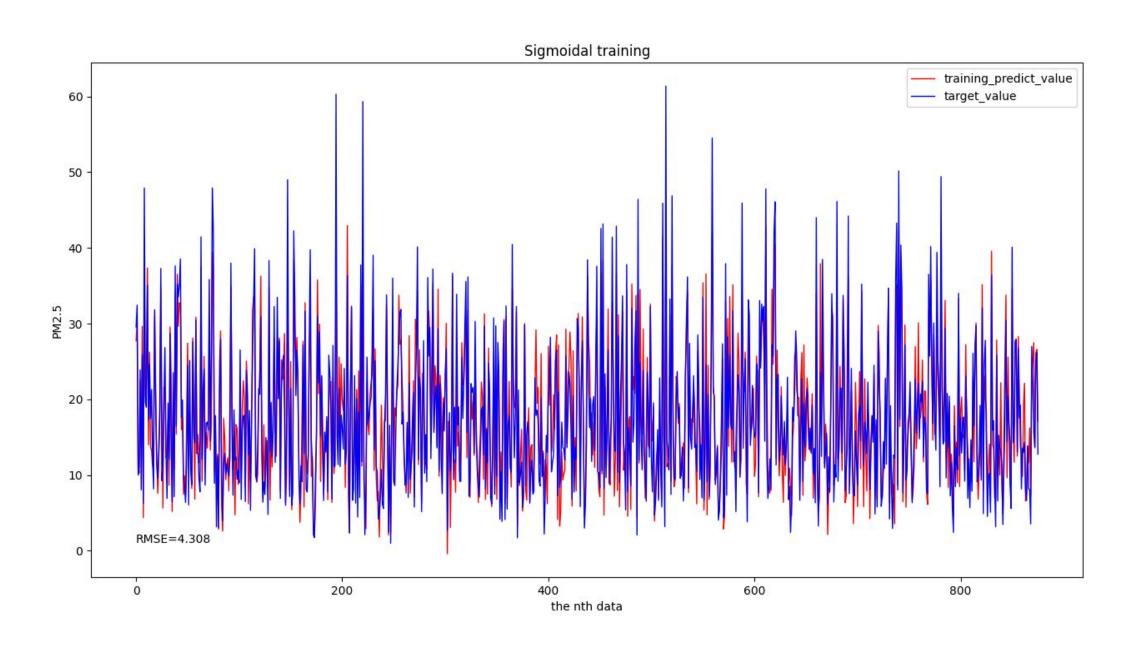


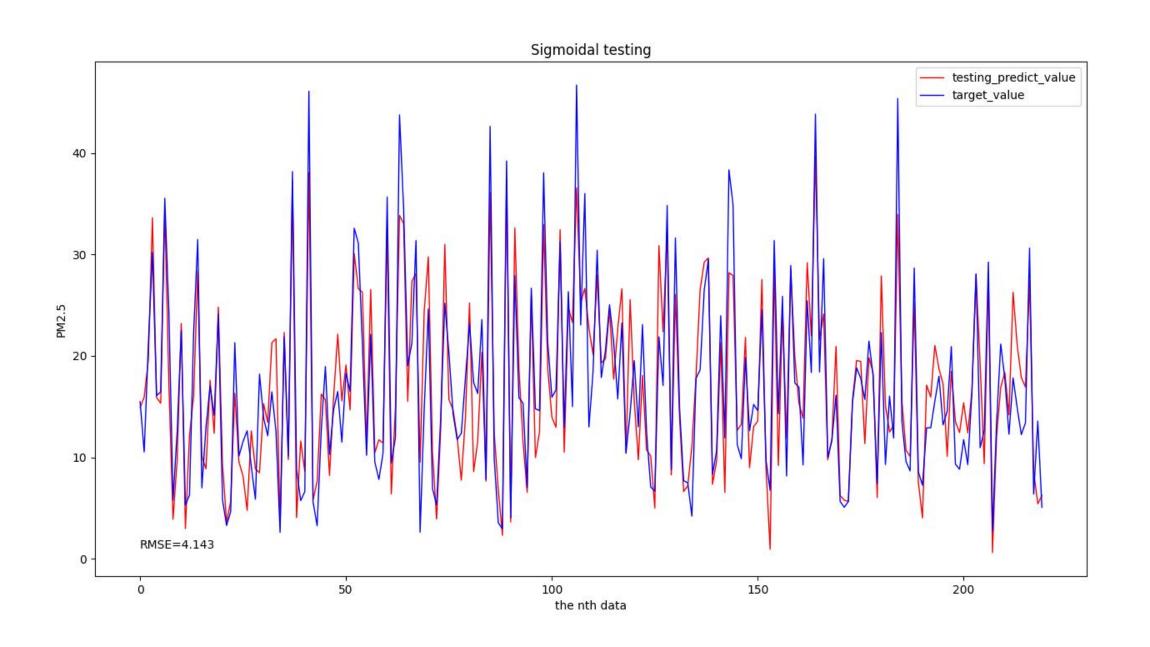


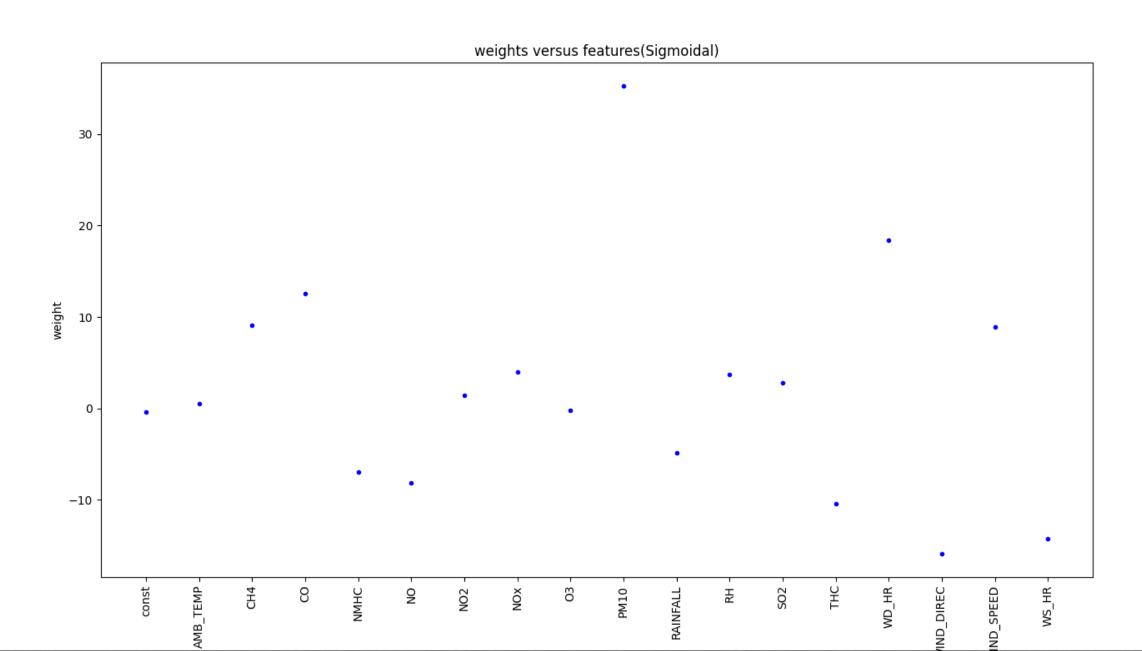


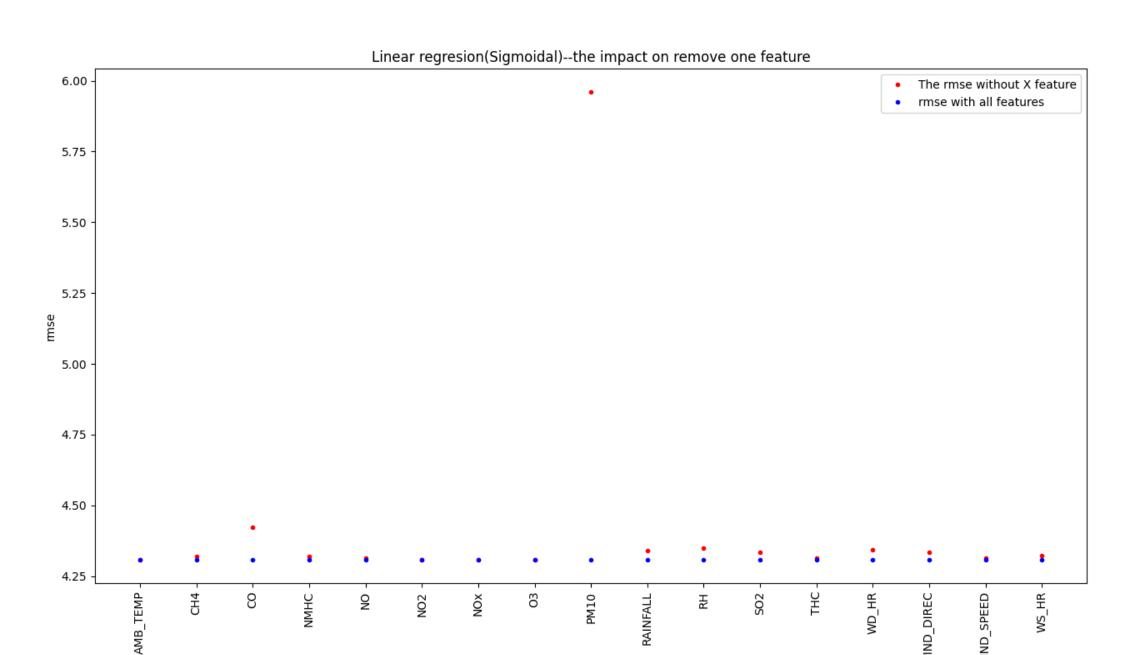


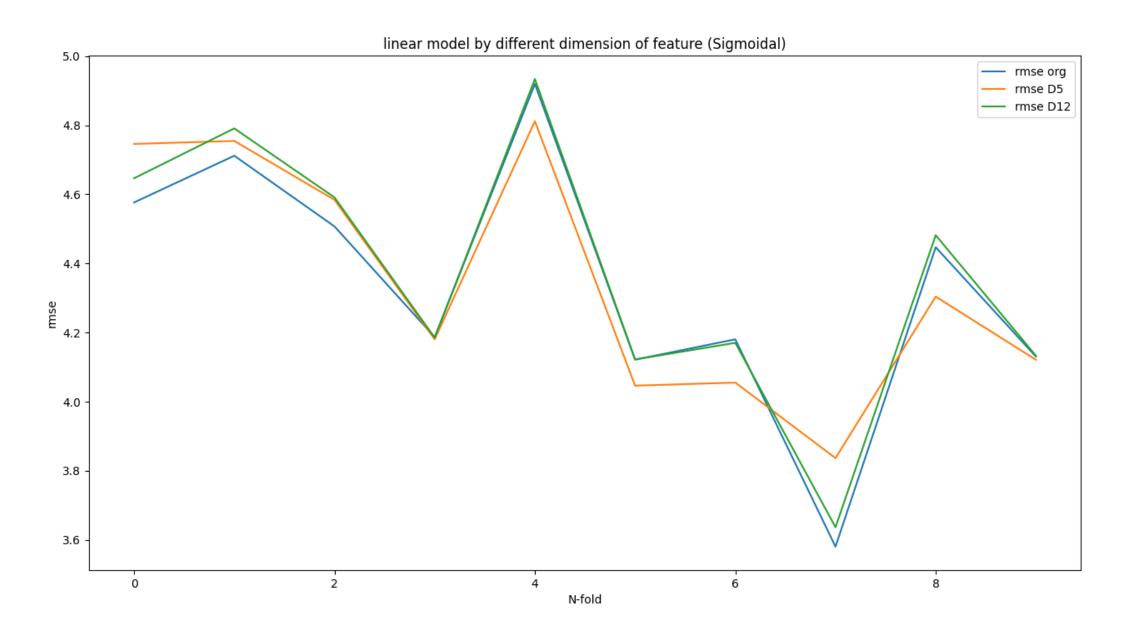
Sigmoidal $S(x) = \frac{e^x}{1 + e^x}$



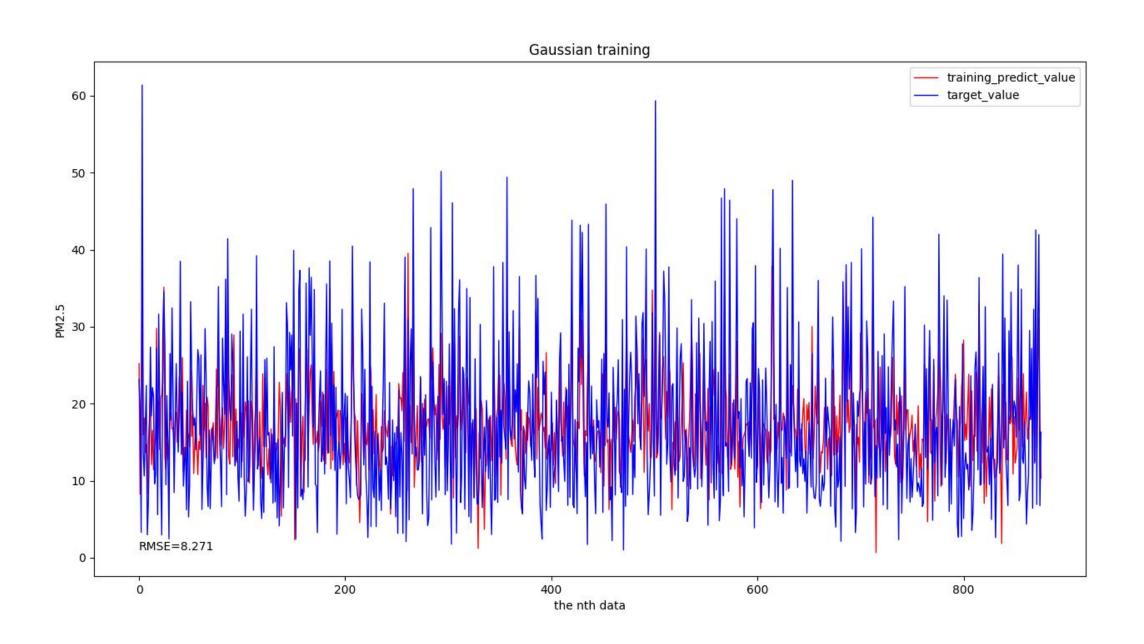


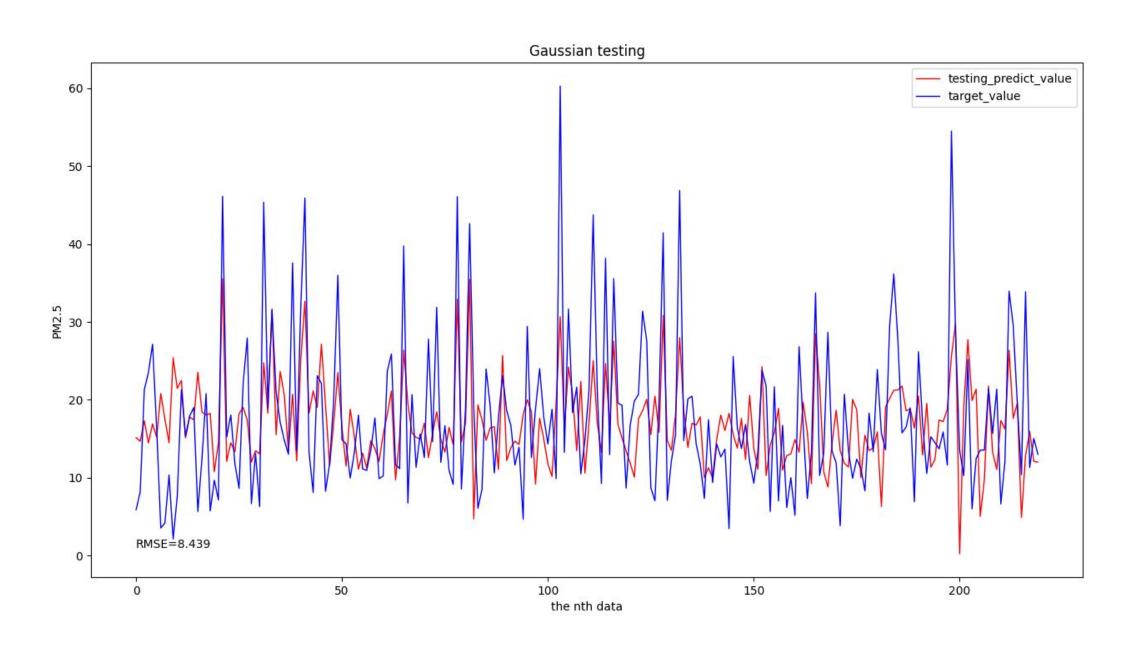


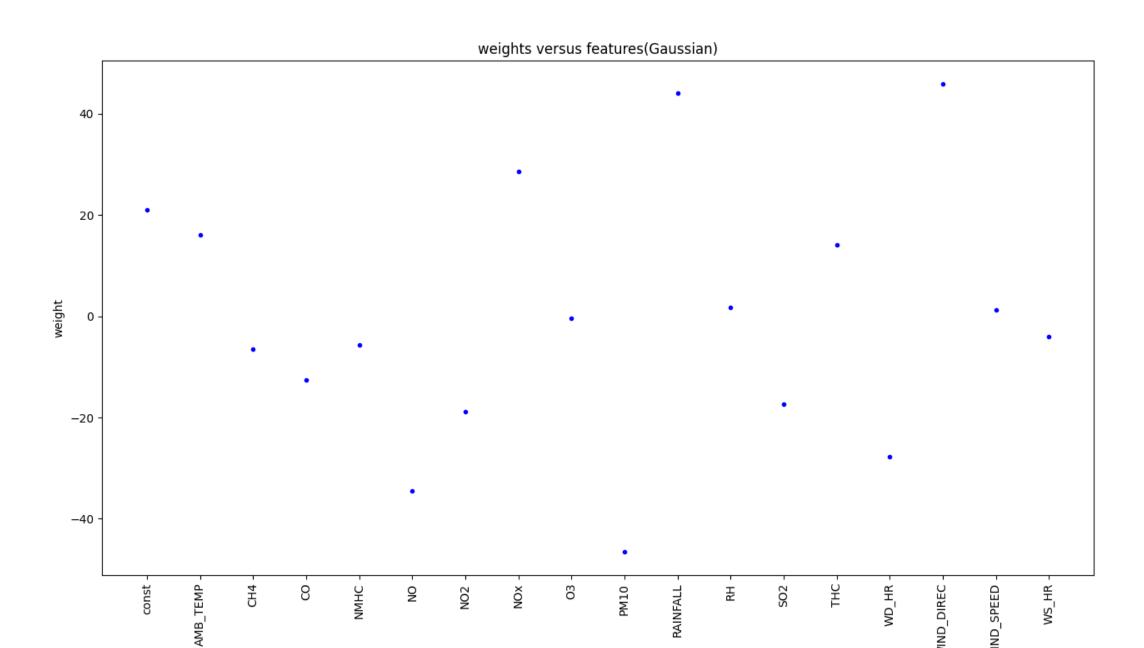


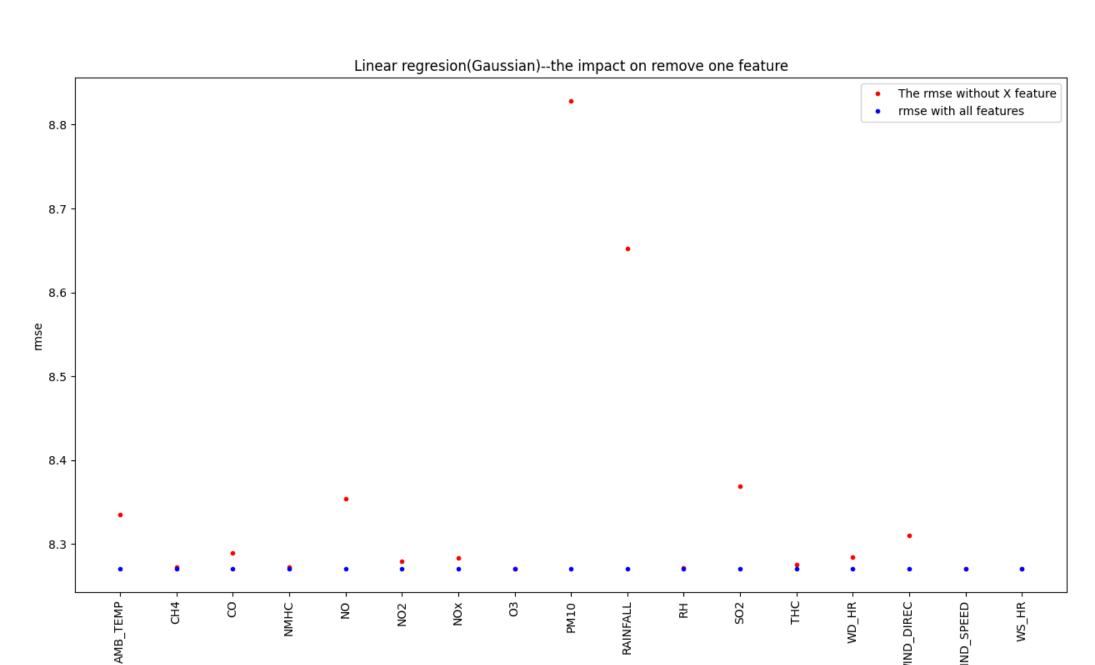


Gaussian
$$f(x,\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)}$$

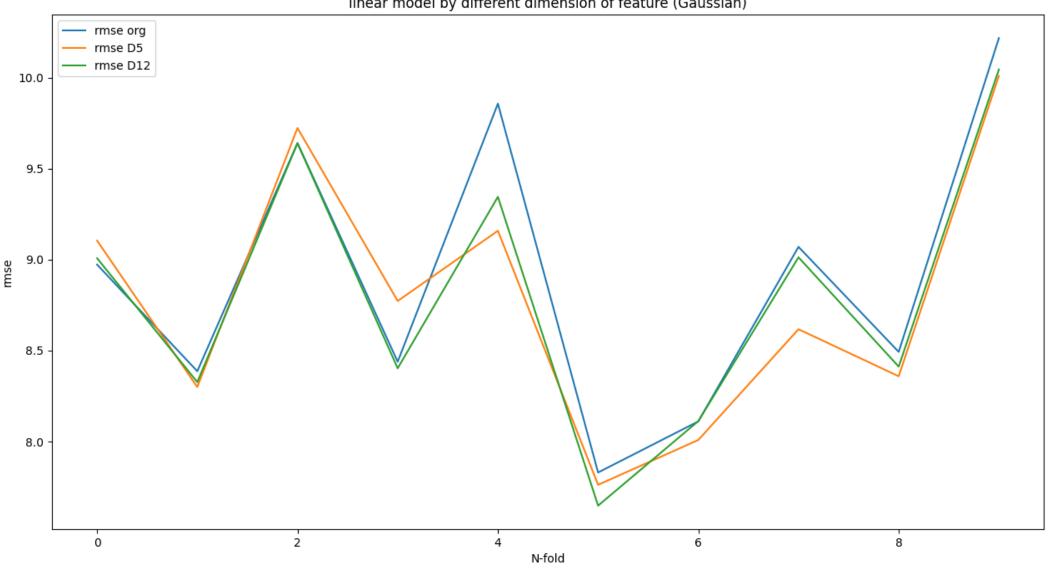












MLE rmse testing comparison:

	Rmse
M=1	5.543
M=2	5.971
Sigmoidal	5.658
Gaussian	8.806

我們可以從這邊testing的rmse中發現Gaussian的模型是四個裡面表現最差的,可能的推論原因是因為Gaussian的basic function較為複雜,因此使其沒有很好的表現。

另外,在這邊我們也透過減少模型的特徵數來觀察是否可以解決過擬合的現象發生,因此我們選了三種模型,分別是不進行任何處理的original(D=17)與考慮影響最大的五個特徵(D=5)及去除影響最小的五個特徵(D=12),來做比較,從上面的結果圖中可以發現:D=5的fold幾乎都在最下面,而D=12的fold則是與D=17沒有進行特徵篩選的模型很貼合,因此我們可以推斷,對於取D=5的這幾種特徵可以很好的去減少testing的rmse,透過做這個測試,我也了解到可以,不一定是要去使用所有的特徵才能去train出一個很好的model,如何去篩選所需要的特徵,對於model的效率及精準度都是一個很重要的事情。

Maximum a posterior (MAP)

data

Normalization

Shuffle

Function Transform

Sigmoidal:
$$S(x) = \frac{e^x}{1 + e^x}$$

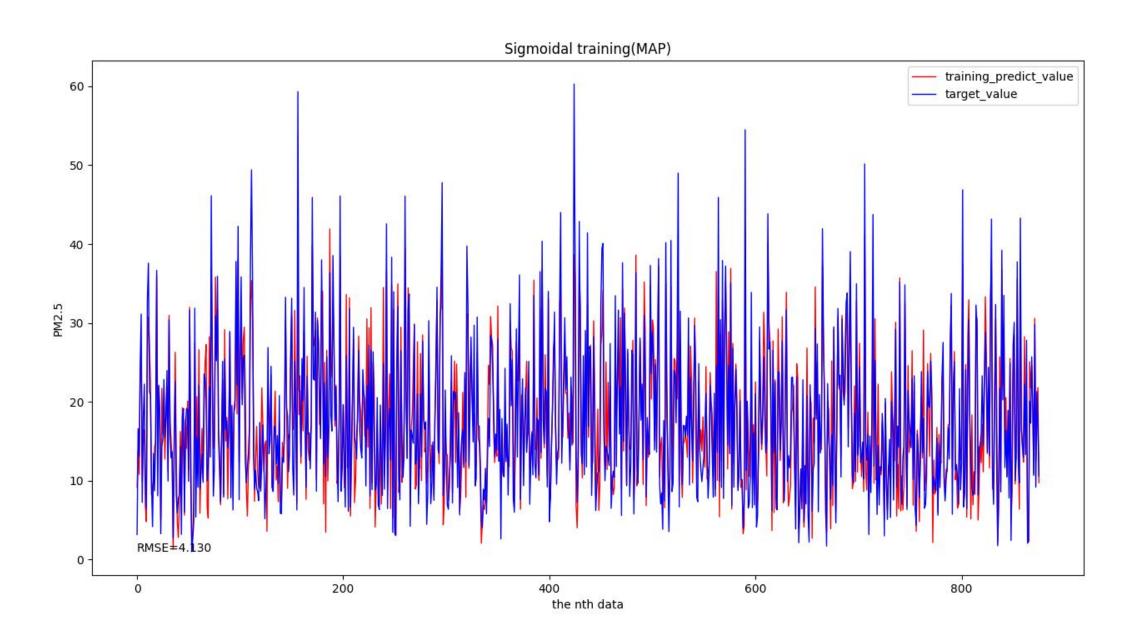
Gaussian: $f(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)}$

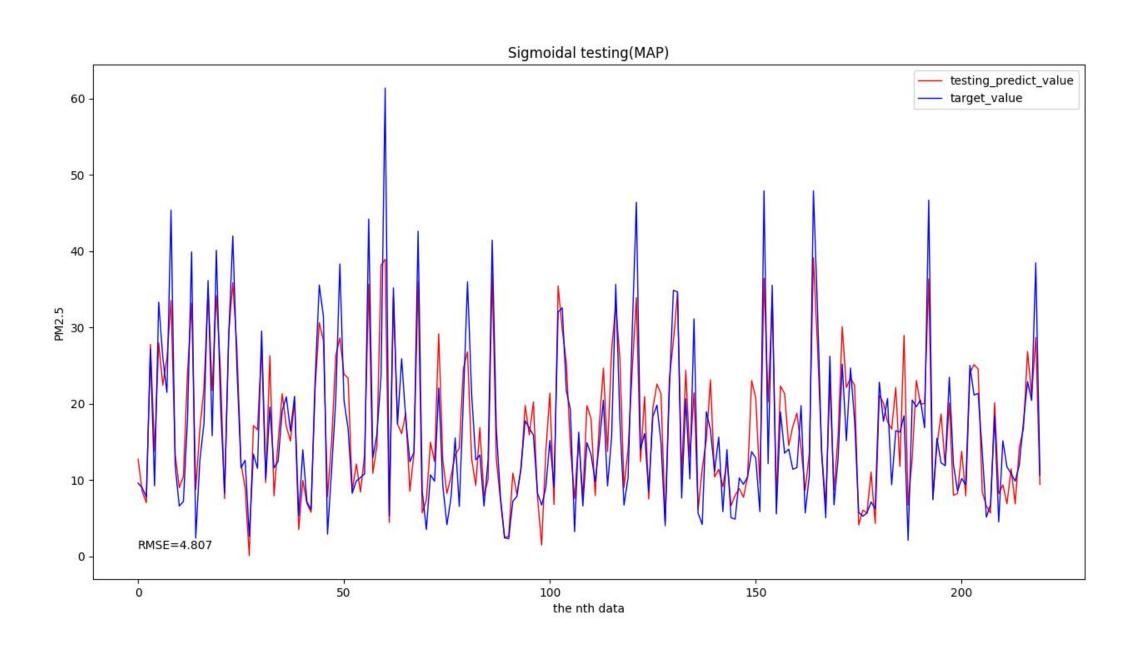
Train test split

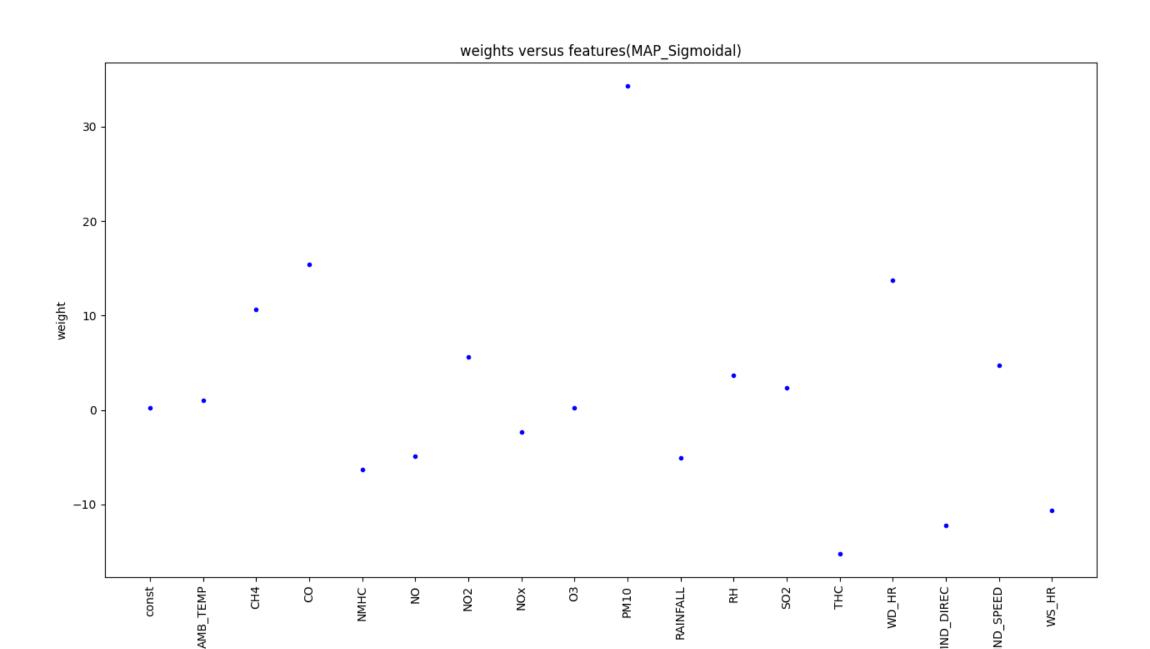
Linear regression(MAP)

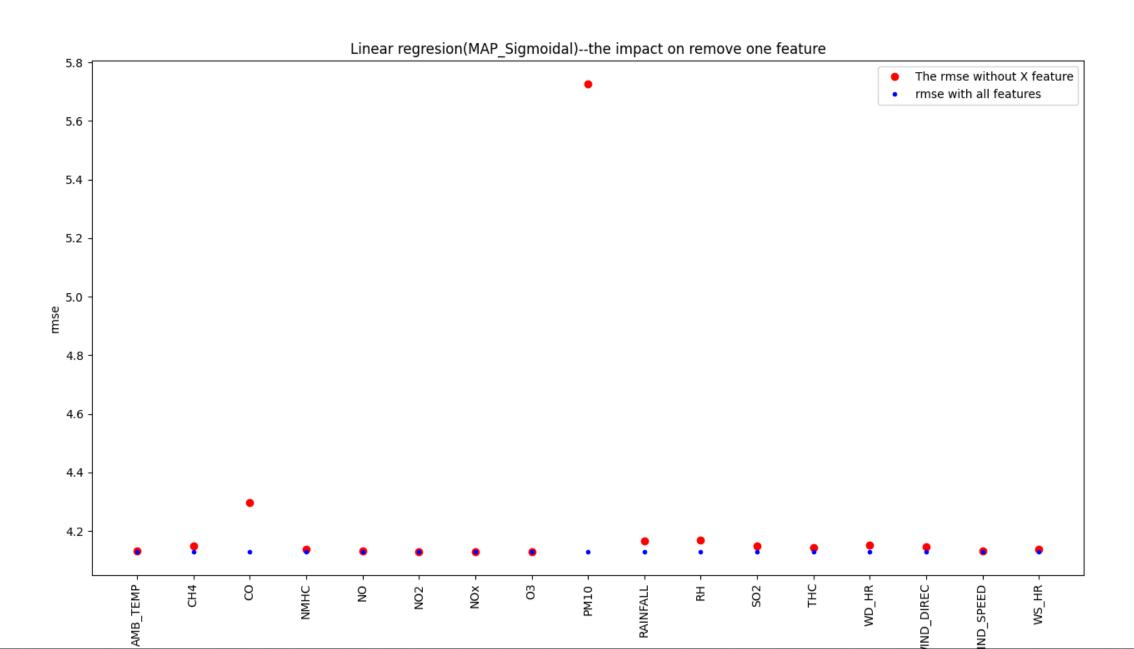
How to update the weight: $\theta_{map} = (X^TX + \lambda I)^{-1}X^Ty$ With $\lambda = 0.0001$

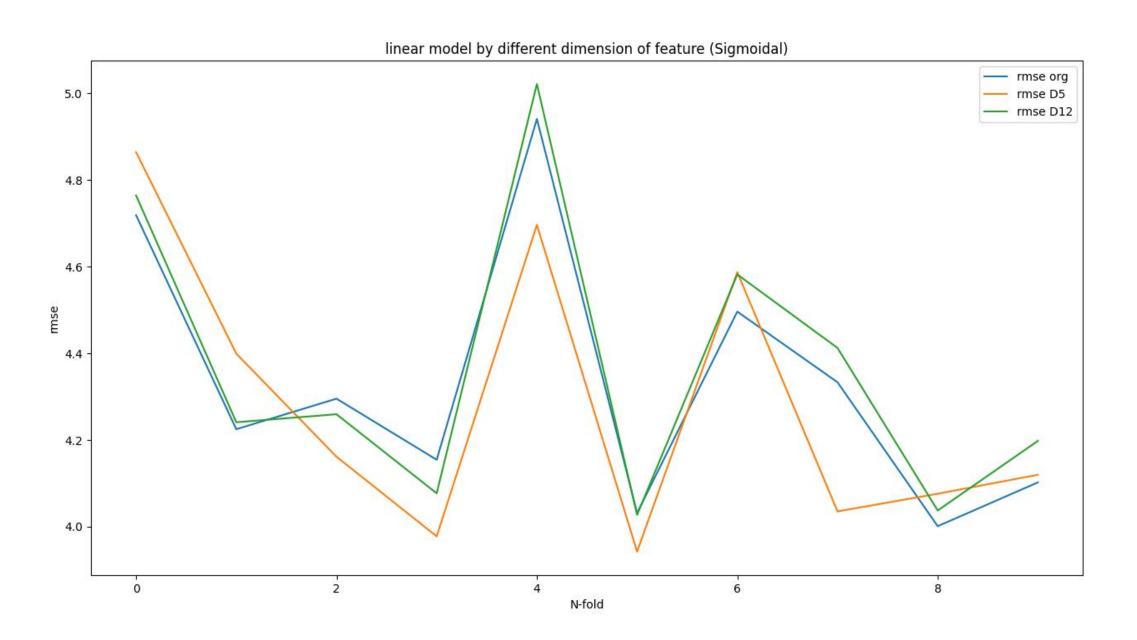
Sigmoidal $S(x) = \frac{e^x}{1 + e^x}$



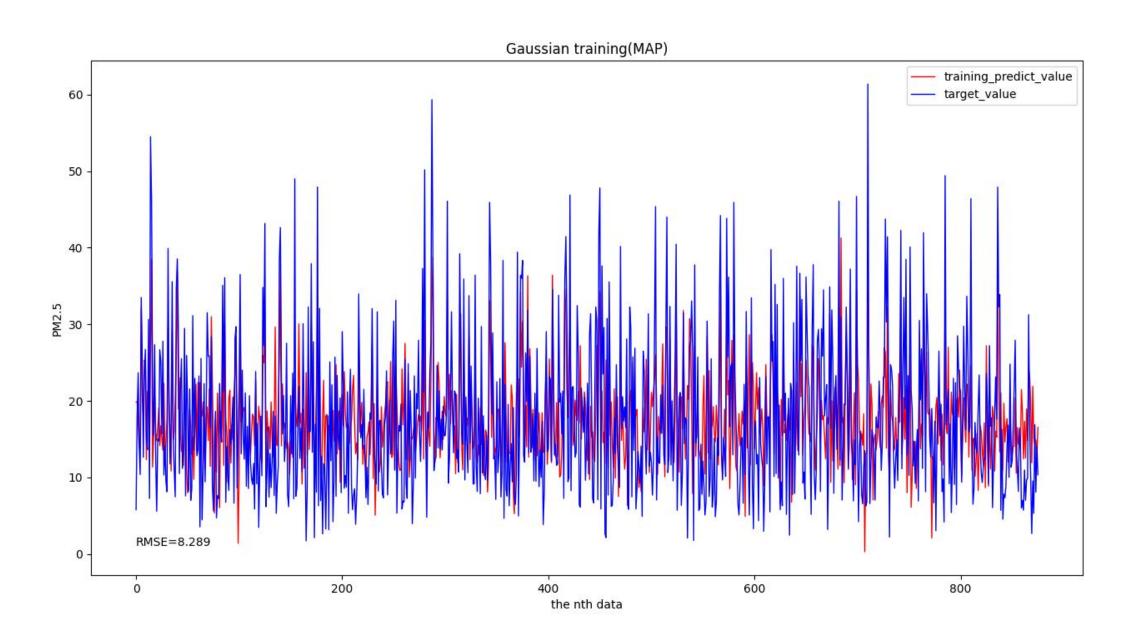


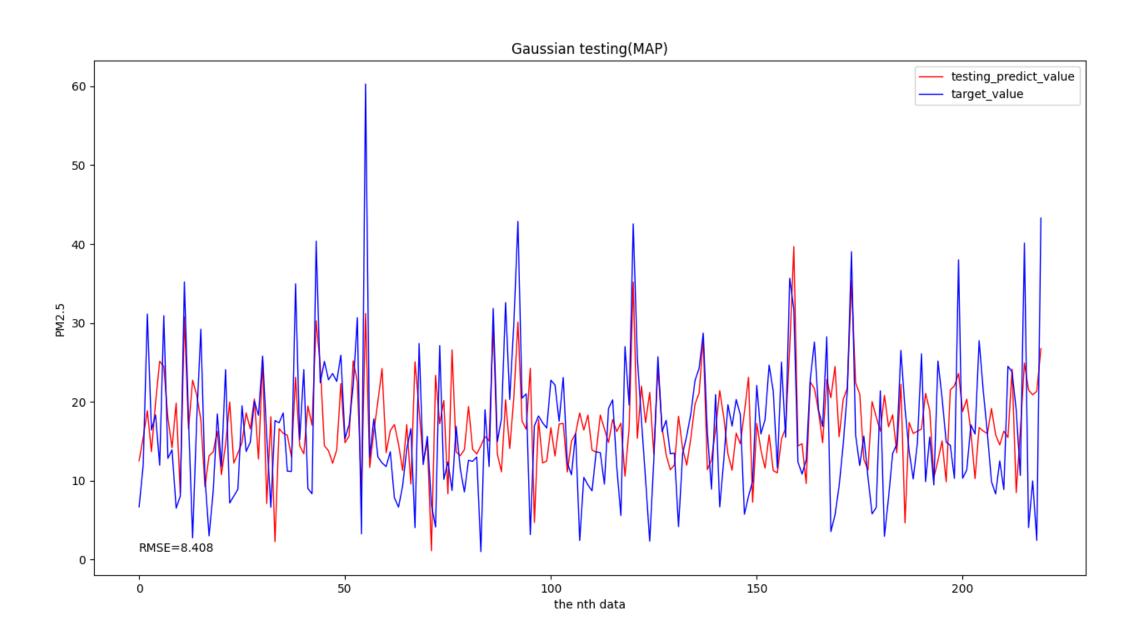


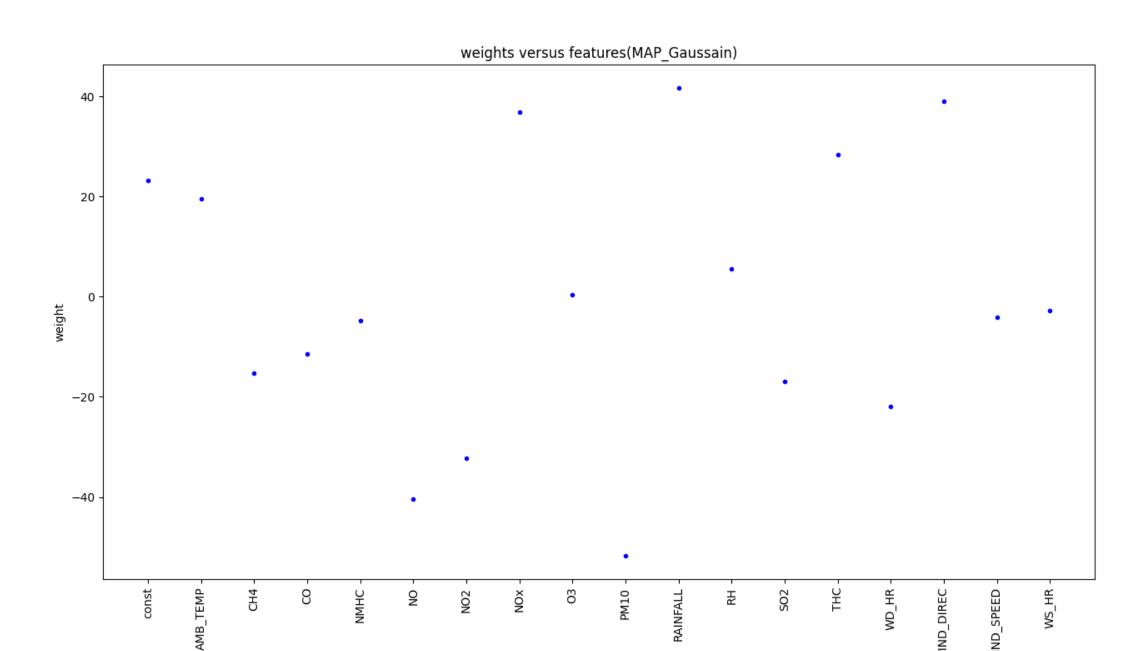


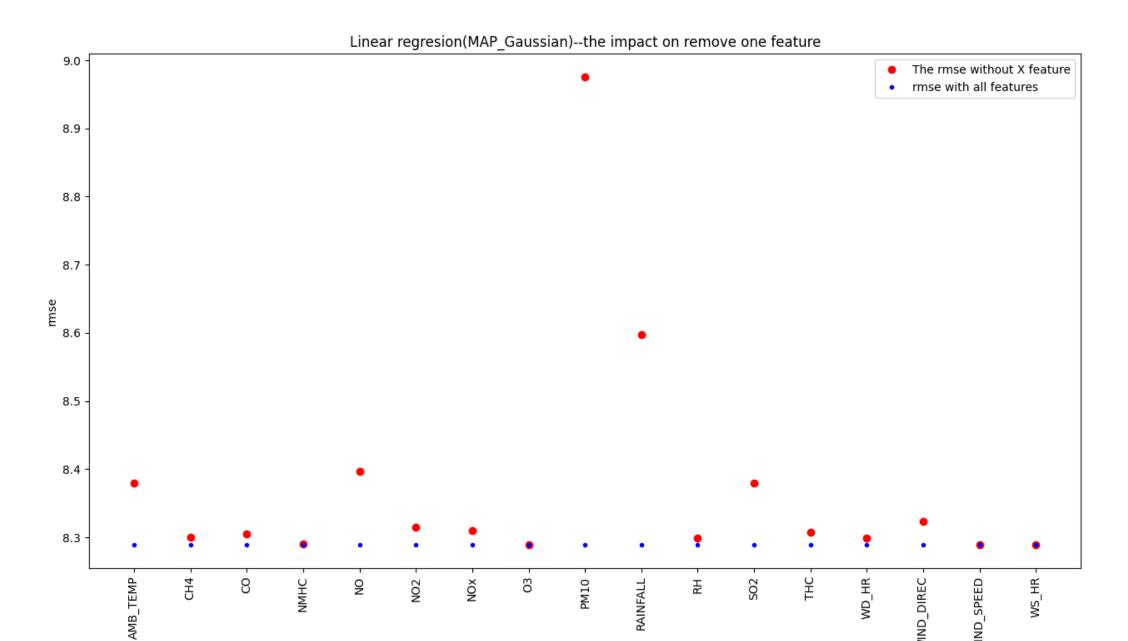


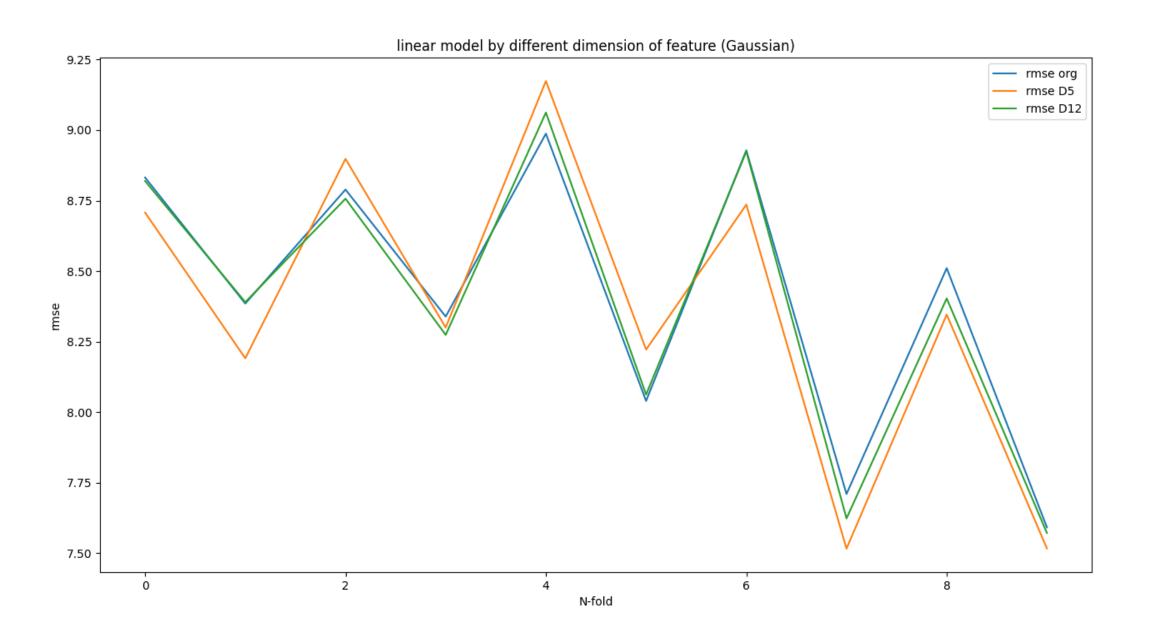
Gaussian
$$f(x,\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)}$$











Compare testing between MLE and MAP:

Linear regression(rmse)	MLE	MAP
Sigmoidal(Train)	4.125	4.222
Sigmoidal(Test)	5.658	4.453
Gaussian(Train)	8.234	8.275
Gaussian(Test)	8.806	8.678

由上表可以看到MAP的表現結果比MLE小一點點,因此推斷 MAP是能夠比MLE在更精準一點的線性回歸方法。