

Machine Learning Homework 2

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Exercise 1: Projection

1.

Assume that there are two $\mathbf{P}_A(\mathbf{x})$, which we can denote them as $\mathbf{P}_A(\mathbf{x})$ and $\mathbf{P}_A(\mathbf{x})'$.

First, we are going to prove that $\mathcal{C}(A)$ is a convex set:

we can choose any two points in $\mathcal{C}(A)$, which we can call $\mathbf{x}_1, \mathbf{x}_2$, because $\mathcal{C}(A)$ is a linear space, so we can get,

$$\forall \lambda_1, \lambda_2 \in \mathbb{R}, \lambda_1 \mathbf{x}_1 + \lambda_2 \mathbf{x}_2 \in \mathcal{C}(A)$$

So, it is easy to assert that

$$\forall \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{C}(A) \text{ and } \forall \theta \in [0, 1], \text{ we have: } \theta \mathbf{x}_1 + (1 - \theta) \mathbf{x}_2 \in \mathcal{C}(A).$$

Therefore, $\mathcal{C}(A)$ is convex.

Next, we are going to prove that two $\mathbf{P}_A(\mathbf{x})$ is ridiculous:

Because $\mathcal{C}(A)$ is a convex set, so there is a line in $\mathcal{C}(A)$ which is between $\mathbf{P}_A(\mathbf{x})$ and $\mathbf{P}_A(\mathbf{x})'$. We denote the midpoint of this line as \mathbf{m} . So, we have:

$$\mathbf{m} = \frac{\mathbf{P}_A(\mathbf{x}) + \mathbf{P}_A(\mathbf{x})'}{2}$$

Then, we can get:

$$\begin{aligned} \|\mathbf{m} - \mathbf{z}\|_2 &= \left\| \frac{\mathbf{P}_A(\mathbf{x}) + \mathbf{P}_A(\mathbf{x})'}{2} - \mathbf{z} \right\|_2 = \left\| \frac{\mathbf{P}_A(\mathbf{x})' - \mathbf{z}}{2} + \frac{\mathbf{P}_A(\mathbf{x}) - \mathbf{z}}{2} \right\|_2 \\ &\leq \left\| \frac{\mathbf{P}_A(\mathbf{x}) - \mathbf{z}}{2} \right\|_2 + \left\| \frac{\mathbf{P}_A(\mathbf{x})' - \mathbf{z}}{2} \right\|_2 = \|\mathbf{P}_A(\mathbf{x}) - \mathbf{z}\|_2 \end{aligned}$$

That is ridiculous, which is against the definition of projection.

So, we can conclude that $\mathbf{P}_A(\mathbf{x})$ is unique.

2.

(a)

We have: $\mathbf{P}_{\mathbf{v}_1}(\mathbf{w}) = \underset{\mathbf{z} \in \mathbb{R}^n}{\operatorname{argmin}} \{\|\mathbf{w} - \mathbf{z}\|_2 : \mathbf{z} \in \mathcal{C}(\mathbf{v}_1)\}$

Because $\mathbf{v}_i \in \mathbb{R}^n$, so we can get:

$$\mathbf{P}_{\mathbf{v}_1}(\mathbf{w}) = \underset{\mathbf{z} \in \mathbb{R}^n}{\operatorname{argmin}} \{\|\mathbf{w} - \mathbf{z}\|_2 : \mathbf{z} \in \mathcal{C}(\mathbf{v}_1)\} = \underset{\mathbf{w} \in \mathbb{R}^n}{\operatorname{argmin}} \{\|\mathbf{w} - \lambda \mathbf{v}_1\|_2, \lambda \in \mathbb{R}\}$$

Let $f(\lambda) = (\mathbf{w} - \lambda \mathbf{v}_1)^T (\mathbf{w} - \lambda \mathbf{v}_1) = \mathbf{w}^T \mathbf{w} + \lambda^2 \mathbf{v}_1^T \mathbf{v}_1 - 2\lambda \mathbf{v}_1^T \mathbf{w}$,

then we let:

$$\frac{\partial f}{\partial \lambda} = 2\lambda \mathbf{v}_1^T \mathbf{v}_1 - 2\mathbf{v}_1^T \mathbf{w} = 0$$

So, we have:

$$\lambda = \frac{\mathbf{v}_1^T \mathbf{w}}{\mathbf{v}_1^T \mathbf{v}_1}$$

Therefore, we have:

So, we have:

$$\mathbf{P}_{\mathbf{v}_1}(\mathbf{w}) = \frac{\mathbf{v}_1^T \mathbf{w}}{\mathbf{v}_1^T \mathbf{v}_1} \mathbf{v}_1$$

(b)

$$\begin{aligned} \mathbf{P}_{\mathbf{v}_1}(\alpha \mathbf{u} + \beta \mathbf{w}) &= \underset{\mathbf{w}, \mathbf{u} \in \mathbb{R}^n}{\operatorname{argmin}} \{ \|\alpha \mathbf{u} + \beta \mathbf{w} - \lambda \mathbf{v}_1\|_2, \lambda \in \mathbb{R} \} = (\alpha \mathbf{u} + \beta \mathbf{w}) \cdot \mathbf{v}_1 (\mathbf{v}_1^T \mathbf{v}_1)^{-1} \\ &= \alpha (\mathbf{u} \mathbf{v}_1) \cdot \mathbf{v}_1 (\mathbf{v}_1^T \mathbf{v}_1)^{-1} + \beta (\mathbf{w} \mathbf{v}_1) \cdot \mathbf{v}_1 (\mathbf{v}_1^T \mathbf{v}_1)^{-1} = \alpha \mathbf{P}_{\mathbf{v}_1}(\mathbf{u}) + \beta \mathbf{P}_{\mathbf{v}_1}(\mathbf{w}) \end{aligned}$$

(c)

$$\text{Let } \mathbf{P}_{\mathbf{v}_1}(\mathbf{w}) = \mathbf{H}_1 \mathbf{w} = \frac{\mathbf{v}_1^T \mathbf{w}}{\mathbf{v}_1^T \mathbf{v}_1} \mathbf{v}_1$$

$$\text{So we have : } \mathbf{H}_1 = \mathbf{v}_1 \mathbf{v}_1^T (\mathbf{v}_1^T \mathbf{v}_1)^{-1}$$

(d)

$$\text{Let } f(\lambda) = (\mathbf{w} - \sum_{i=1}^d \lambda_i \mathbf{v}_i)^T (\mathbf{w} - \sum_{i=1}^d \lambda_i \mathbf{v}_i) = \mathbf{w}^T \mathbf{w} - \sum_{i=1}^d \lambda_i \mathbf{v}_i^T \mathbf{w} - \sum_{i=1}^d \lambda_i \mathbf{w}^T \mathbf{v}_i + (\sum_{i=1}^d \lambda_i \mathbf{v}_i^T) (\sum_{i=1}^d \lambda_i \mathbf{v}_i)$$

Then we let:

$$\frac{\partial f}{\partial \lambda_i} = -\mathbf{v}_i^T \mathbf{w} - \mathbf{w}^T \mathbf{v}_i + \mathbf{v}_i^T (\sum_{i=1}^d \lambda_i \mathbf{v}_i) + (\sum_{i=1}^d \lambda_i \mathbf{v}_i^T) \mathbf{v}_i = 2[\mathbf{v}_i^T (\sum_{i=1}^d \lambda_i \mathbf{v}_i) - \mathbf{v}_i^T \mathbf{w}] = 0$$

So, we have:

$$\mathbf{v}_i^T (\sum_{i=1}^d \lambda_i \mathbf{v}_i) = \mathbf{v}_i^T \mathbf{w}$$

不会写，但是d个方程确实有d对应d个未知数，但是写不出来解的表达式。

If we have $\mathbf{v}_i^T \mathbf{v}_j = 0, \forall i \neq j$, then we have:

$$\mathbf{v}_i^T (\sum_{i=1}^d \lambda_i \mathbf{v}_i) = \lambda_i \mathbf{v}_i^T \mathbf{v}_i = \mathbf{v}_i^T \mathbf{w}$$

So, we have:

$$\lambda_i = \frac{\mathbf{v}_i^T \mathbf{w}}{\mathbf{v}_i^T \mathbf{v}_i}$$

Therefore, we have:

$$\mathbf{P}_{\mathbf{v}}(\mathbf{w}) = \sum_{i=1}^d \frac{\mathbf{v}_i^T \mathbf{w}}{\mathbf{v}_i^T \mathbf{v}_i} \mathbf{v}_i$$

3.

(a)

The coordinates unique, and they are $[\mathbf{x} \cdot (1, 0), \mathbf{x} \cdot (0, 1)]$.

(b)

The column vectors in A are not linearly independent, so we cannot get a unique coordinate.

Exercise 2: Projection to a Matrix Space

1.

The first question is easy to prove, because we can get:

$\forall A, B \in \mathbb{R}^{n \times n}$, which are two diagonal matrices, we have $\alpha A + \beta B$ is a diagonal matrix. And, the other conditions are obviously satisfied.

So, we assert that Show that the set of diagonal matrices in $\mathbb{R}^{n \times n}$ forms a linear space.

Let $\Sigma = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$, where $\lambda_i \in \mathbb{R}$.

Then we have:

$$\mathbf{P}_{\Sigma}(\mathbf{A}) = \underset{\mathbf{z} \in \Sigma}{\operatorname{argmin}} \{ \|\mathbf{A} - \mathbf{z}\|_2 : \mathbf{z} \in \Sigma \}$$

Here, A is a matrix in $\mathbb{R}^{n \times n}$, then we can get:

$$\begin{aligned} \|\mathbf{A} - \mathbf{z}\|_2 &= \|\mathbf{A} - \Sigma\|_2 = \operatorname{tr}[(\mathbf{A} - \Sigma)^T(\mathbf{A} - \Sigma)] \\ &= \operatorname{tr}(\mathbf{A}^T \mathbf{A} - \mathbf{A}^T \Sigma - \Sigma^T \mathbf{A} + \Sigma^T \Sigma) \\ &= \operatorname{tr}(\mathbf{A}^T \mathbf{A}) - 2\operatorname{tr}(\mathbf{A}^T \Sigma) + \operatorname{tr}(\Sigma^T \Sigma) \text{ denoted as } f(\lambda) \end{aligned}$$

Then, we let:

$$\frac{\partial f}{\partial \lambda_i} = 2\lambda_i - 2a_{ii} = 0$$

So, we have: $\lambda_i = a_{ii}$

Therefore, we have:

$$\mathbf{P}_{\Sigma}(\mathbf{A}) = \text{diag}(a_{11}, a_{22}, \dots, a_{nn})$$

2.

The second question is also easy to prove, because we can get:

The set of symmetric matrices, which is denoted as \mathcal{S} , we have any two symmetric matrices, their linear combination is absolutely symmetric.

So, we assert that Show that the set of symmetric matrices in $\mathbb{R}^{n \times n}$ is a linear space.

We can easily compute the dimension of this linear space:

the diagonal dimension is n , the off-diagonal dimension is the total number of the matrix elements n^2 minus the diagonal elements n , because the matrix is symmetric, so we have:

$$\dim(\mathcal{S}) = n + \frac{n^2 - n}{2} = \frac{n^2 + n}{2}$$

3.

First ,we are going to prove $\text{tr}(\mathbf{AB}) = \text{tr}(\mathbf{BA})$:

$$\begin{aligned}\text{tr}(\mathbf{AB}) &= \sum_{i=1}^n [\mathbf{AB}]_{ii} = \sum_{i=1}^n \sum_{j=1}^n a_{ij} b_{ji} = \sum_{j=1}^n \sum_{i=1}^n b_{ji} a_{ij} = \\ &= \sum_{j=1}^n [\mathbf{BA}]_{jj} = \text{tr}(\mathbf{BA})\end{aligned}$$

Then,we consider a symmetric matrix \mathbf{A} and a skew-symmetric matrix \mathbf{B} , we have:

$$\langle \mathbf{A}, \mathbf{B} \rangle = \text{tr}(\mathbf{A}^T \mathbf{B}) = \text{tr}(\mathbf{AB})$$

Because \mathbf{B} is skew-symmetric, so we have:

$$\text{tr}(\mathbf{AB}) = \text{tr}((\mathbf{AB})^T) = \text{tr}(\mathbf{B}^T \mathbf{A}^T) = \text{tr}(-\mathbf{BA}) = -\text{tr}(\mathbf{BA}) = -\text{tr}(\mathbf{AB})$$

So, we have:

$$\langle \mathbf{A}, \mathbf{B} \rangle = 0$$

Next, we are going to prove any matrix can be decomposed as the sum of a symmetric matrix and a skew-symmetric matrix.

Let \mathbf{A} be a matrix, then we let:

$$\mathbf{A}_1 = (\mathbf{A} + \mathbf{A}^T)/2, \mathbf{A}_2 = (\mathbf{A} - \mathbf{A}^T)/2$$

It is easy to see that \mathbf{A}_1 is a symmetric matrix and \mathbf{A}_2 is a skew-symmetric matrix.

4.

Let \mathbf{A} be a matrix, then we have:

$$\mathbf{A} = \mathbf{Q} + \mathbf{P}$$

In this case, \mathbf{Q} is a symmetric matrix and \mathbf{P} is a skew-symmetric matrix.

Let us denote symmetric matrices space as \mathcal{S} , then we have:

$$\mathbf{P}_{\mathcal{S}}(\mathbf{A}) = \underset{\mathbf{z} \in \mathcal{S}}{\text{argmin}} \{ \|\mathbf{A} - \mathbf{z}\|_2 : \mathbf{z} \in \mathcal{S} \}$$

So, we have:

$$\begin{aligned}\|\mathbf{A} - \mathbf{z}\|_2 &= \|\mathbf{A} - \mathbf{z}\|_2 = \|\mathbf{P} + \mathbf{Q} - \mathbf{z}\|_2 \\ &= \text{tr}((\mathbf{Q} + \mathbf{P} - \mathbf{z})^T (\mathbf{Q} + \mathbf{P} - \mathbf{z})) \\ &= \text{tr}(\mathbf{QQ} + \mathbf{QP} - \mathbf{Qz} - \mathbf{PQ} - \mathbf{PP} + \mathbf{Pz} - \mathbf{zQ} - \mathbf{zP} + \mathbf{zz}) \\ &= \text{tr}(\mathbf{QQ}) - \text{tr}(\mathbf{Qz}) - \text{tr}(\mathbf{zQ}) - \text{tr}(\mathbf{PP}) + \text{tr}(\mathbf{zz}) \\ &= \text{tr}(\mathbf{QQ}) - 2\text{tr}(\mathbf{zQ}) + \text{tr}(\mathbf{PP}) + \text{tr}(\mathbf{zz}) \\ &\quad \text{denoted as } f(\mathbf{z})\end{aligned}$$

In this $f(\mathbf{z})$, the part which can be influenced by \mathbf{z} is:

$$-2\text{tr}(\mathbf{zQ}) + \text{tr}(\mathbf{zz}) = \text{tr}[\mathbf{z}(\mathbf{z} - 2\mathbf{Q})] = \sum_{i=1}^n \sum_{j=1}^n z_{ij} (z_{ij} - 2q_{ij})$$

So, we let:

$$\frac{\partial f}{\partial z_{ij}} = 2z_{ij} - 2q_{ij} = 0$$

So, we have:

$$z_{ij} = q_{ij}$$

Therefore, we have:

$$\mathbf{P}_S(\mathbf{A}) = \mathbf{Q} = (\mathbf{A} + \mathbf{A}^T)/2$$

Exercise 3: Projection to a Function Space

1.

(a)

$L^2(\Omega)$ is a linear space,;

▮ $\forall X, Y \in L^2(\Omega)$, we have: $\mathbb{E}[(\alpha X + \beta Y)^2] < \infty$

And the projection $\mathbf{P}_\Omega(Y)$ is defined as:

$$\mathbf{P}_\Omega(Y) = \underset{\mathbf{z} \in \Omega}{\operatorname{argmin}} \{ \|\mathbf{Y} - \mathbf{z}\|_2 : \mathbf{z} \in \Omega \}$$

We know that

$$\begin{aligned} \|\mathbf{Y} - \mathbf{z}\|_2^2 &= \mathbb{E}(\mathbf{Y} - \mathbf{z})^2 = \mathbb{E}(Y^2 - 2Y\mathbf{z} + \mathbf{z}^2) = \mathbb{E}(Y^2) - 2\mathbb{E}(Y\mathbf{z}) + \mathbb{E}(\mathbf{z}^2) \\ &= \mathbb{E}(Y^2) - 2\mathbf{z}\mathbb{E}(Y) + \mathbf{z}^2 \text{ denoted as } f(z) \end{aligned}$$

So, we let:

$$\frac{\partial f}{\partial z} = 2(\mathbb{E}(Y) - z) = 0$$

So, we have:

$$z = \mathbb{E}(Y)$$

Therefore, we have:

$$\mathbf{P}_\Omega(Y) = \mathbb{E}(Y)$$

(b)

$$\hat{c} = \underset{c \in \mathbb{R}}{\operatorname{argmin}} \mathbb{E}[(Y - c)^2].$$

We have:

$$\begin{aligned} \mathbb{E}[(Y - c)^2] &= \mathbb{E}[Y^2 - 2Y\mathbf{c} + \mathbf{c}^2] = \mathbb{E}(Y^2) - 2\mathbb{E}(Y\mathbf{c}) + \mathbb{E}(\mathbf{c}^2) \\ &= \mathbb{E}(Y^2) - 2\mathbf{c}\mathbb{E}(Y) + \mathbf{c}^2 \text{ denoted as } f(c) \end{aligned}$$

So, we let:

$$\frac{\partial f}{\partial c} = 2(\mathbb{E}(Y) - c) = 0$$

So, we have:

$$c = \mathbb{E}(Y)$$

Therefore, we have:

$$\hat{c} = \mathbb{E}(Y)$$

(c)

$$\begin{aligned}\mathbb{E}[(Y - c)^2] &= \mathbb{E}[Y^2 - 2Y\mathbf{c} + \mathbf{c}^2] = \mathbb{E}(Y^2) - 2\mathbb{E}(Y\mathbf{c}) + \mathbb{E}(\mathbf{c}^2) \\ &= \mathbb{E}(Y^2) - 2\mathbf{c}\mathbb{E}(Y) + \mathbf{c}^2 \text{ denoted as } f(c)\end{aligned}$$

Let $c = \mathbb{E}(Y)$, we have:

$$\frac{\partial f}{\partial c} = 2(\mathbb{E}(Y) - c) = 0$$

So, we have $\mathbb{E}[(Y - c)^2]$ get its minimum value at $\mathbb{E}(Y)$.

$$\mathbb{E}[(Y - c)^2]_{\min} = \mathbb{E}(Y^2)$$

The necessary and sufficient condition is $c = \mathbb{E}(Y)$.

Let we treat \mathbf{c} and \mathbf{Y} as vectors, we have $(Y - c)^2$ is the distance between them.

And the minimum distance between any two vectors is $\mathbb{E}[(Y - c)^2]_{\min} = \mathbb{E}(Y^2)$, if and only if $c = \mathbb{E}(Y)$, that is \mathbf{c} is the projection of \mathbf{Y} onto Ω .

2.

(a)

$$\mathbb{E}[(f(X) - Y)^2] = \iint (y - f(x))^2 p(x, y) dx dy$$

So, the solution of (a) is the same to:

$$\min_f \left\{ J[f] := \iint (y - f(x))^2 p(x, y) dx dy \right\}$$

Let:

$$\frac{\partial J[f]}{\partial f} = \lim_{\epsilon \rightarrow 0} \frac{J[f + \epsilon h] - J[f]}{\epsilon} = 0$$

We have:

$$\int -2(y - f^*(x))p(x, y) dy = 0$$

So, we have:

$$f^*(\mathbf{x}) = \frac{\int yp(\mathbf{x}, y)dy}{\int p(\mathbf{x}, y)dy} = \int y \frac{p(\mathbf{x}, y)}{p(\mathbf{x})} dy = \int yp(y|\mathbf{x})dy = \mathbb{E}[Y|\mathbf{X}]$$

So, the solution is $f(\mathbf{X}) = \mathbb{E}[Y|\mathbf{X}]$

(b)

And the projection $\mathbf{P}_{\mathcal{C}}(Y)$ is defined as:

$$\begin{aligned}\mathbf{P}_{\mathcal{C}}(Y) &= \underset{f(\mathbf{X}) \in \mathcal{C}}{\operatorname{argmin}} \{ \|\mathbf{Y} - f(\mathbf{X})\|_2 : f(\mathbf{X}) \in \mathcal{C} \} \\ &= \underset{f(\mathbf{X}) \in \mathcal{C}}{\operatorname{argmin}} \{ \mathbb{E}[(\mathbf{Y} - f(\mathbf{X}))^2] : f(\mathbf{X}) \in \mathcal{C} \}\end{aligned}$$

So, we can assert that the solution of (a) is $\mathbf{P}_{\mathcal{C}}(Y)$, their function is the same.

(c)

The question 1 is the special case of the question 2, where $\mathcal{C} = \Omega$, \mathbf{X} is not a random value but a constant value.

The conditional expectation is the projection of Y onto \mathcal{C} .

Exercise 4: Multicollinearity

1.

(a)

$$\begin{aligned}\mathbb{E}(\hat{\mathbf{w}}) &= \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}] = \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{X} \mathbf{w} + \mathbf{e})] \\ &= \mathbb{E}[\mathbf{w}] + \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{e}] = \mathbf{w} + \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T] \mathbb{E}[\mathbf{e}] = \mathbf{w}\end{aligned}$$

Here, we consider that \mathbf{X} is independent of \mathbf{e} .

So, we can get $\mathbb{E}(\hat{\mathbf{w}}) = \mathbf{w}$.

(b)

$$\begin{aligned}\operatorname{Cov}(\hat{\mathbf{w}}) &= \mathbb{E}[(\hat{\mathbf{w}} - \mathbb{E}(\hat{\mathbf{w}}))(\hat{\mathbf{w}} - \mathbb{E}(\hat{\mathbf{w}}))^T] \\ &= \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{X} \mathbf{w} + \mathbf{e}) - \mathbf{w}][(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{X} \mathbf{w} + \mathbf{e}) - \mathbf{w}]^T] \\ &= \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{e}][(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{e}]^T] \\ &= \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{e} \mathbf{e}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1}] \\ &= \mathbb{E}[\mathbf{e} \mathbf{e}^T] \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1}] \\ &= \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}\end{aligned}$$

2.

$$\begin{aligned}
\text{MSE}(\hat{\mathbf{w}}) &= \mathbb{E}[\|\hat{\mathbf{w}} - \mathbf{w}\|^2] \\
&= \mathbb{E}[(\hat{\mathbf{w}} - \mathbf{w})^T (\hat{\mathbf{w}} - \mathbf{w})] \\
&= \mathbb{E}[\hat{\mathbf{w}}^T \hat{\mathbf{w}} - \hat{\mathbf{w}}^T \mathbf{w} - \mathbf{w}^T \hat{\mathbf{w}} + \mathbf{w}^T \mathbf{w}] \\
&= \mathbb{E}\left\{\sum_{i=1}^p \hat{w}_i^2 - 2 \sum_{i=1}^p \hat{w}_i w_i + \sum_{i=1}^p w_i^2\right\} \\
&= \sum_{i=1}^p [\mathbb{E}\hat{w}_i^2 - (\mathbb{E}\hat{w}_i)^2 + (\mathbb{E}\hat{w}_i)^2 + \mathbb{E}w_i^2 - 2\mathbb{E}(\hat{w}_i w_i)] \\
&= \sum_{i=1}^p \text{Var}(\hat{w}_i) + \sum_{i=1}^p (\mathbb{E}\hat{w}_i - \mathbb{E}w_i)^2 \\
&= \sum_{i=1}^p \text{Var}(\hat{w}_i) + \sum_{i=1}^p (\mathbb{E}\hat{w}_i - w_i)^2
\end{aligned}$$

3.

$$\begin{aligned}
\text{MSE}(\hat{\mathbf{w}}) &= \mathbb{E}[\|\hat{\mathbf{w}} - \mathbf{w}\|^2] \\
&= \mathbb{E}[(\hat{\mathbf{w}} - \mathbf{w})^T (\hat{\mathbf{w}} - \mathbf{w})] \\
&= \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{X} \mathbf{w} + \mathbf{e}) - \mathbf{w}]^T [(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{X} \mathbf{w} + \mathbf{e}) - \mathbf{w}] \\
&= \mathbb{E}[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{e}]^T [(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{e}] \\
&= \mathbb{E}[\mathbf{e}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2} \mathbf{X}^T \mathbf{e}] \\
&= \mathbb{E}[\text{tr}(\mathbf{e}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2} \mathbf{X}^T \mathbf{e})] \\
&= \text{tr}(\mathbb{E}[\mathbf{e}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2} \mathbf{X}^T \mathbf{e}]) \\
&= \text{tr}(\mathbb{E}[\mathbf{e} \mathbf{e}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2} \mathbf{X}^T]) \\
&= \text{tr}(\mathbb{E}[\mathbf{e} \mathbf{e}^T] \mathbb{E}[\mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2} \mathbf{X}^T]) \\
&= \text{tr}(\sigma^2 \mathbf{I} \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2} \mathbf{X}^T) \\
&= \sigma^2 \text{tr}(\mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2} \mathbf{X}^T) \\
&= \sigma^2 \text{tr}(\mathbf{X}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-2}) \\
&= \sigma^2 \text{tr}((\mathbf{X}^T \mathbf{X})^{-1}) \\
&= \sigma^2 \sum_{i=1}^p \frac{1}{\lambda_i}, \text{ where } \lambda_1, \lambda_2, \dots, \lambda_p \text{ are the eigenvalues of } \mathbf{X}^T \mathbf{X}.
\end{aligned}$$

这里用到的公式或者性质有：二次型 $x^T A x = \text{tr}(A x x^T)$, 以及迹的循环性质

4.

It means that MSE will be infinity, which means that the model is not suitable for the given data.

Exercise 5: Regularized least squares

1.

Let v be any d -dimensional vector.

We have $v^T \mathbf{X}^T \mathbf{X} v = (\mathbf{X} v)^T (\mathbf{X} v)$ is a 2-norm of vector $\mathbf{X} v$, so it is absolutely ≥ 0 .

So is $\mathbf{X}^T \mathbf{X}$ always definite semi-definite.

If we have $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_d$ is linear independent, then $(\mathbf{X} v) = \mathbf{0}$ if and only if $v = \mathbf{0}$.

So, we can say that $\mathbf{X}^T \mathbf{X}$ is always positive definite.

2.

We have $\mathbf{X}^T \mathbf{X}$ is semi-definite, and $\lambda \mathbf{I}$ is positive.

So, Let v be any d-dimensional vector but not a zero vector, we can get :

$$v^T (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}) v = v^T \mathbf{X}^T \mathbf{X} v + \lambda v^T v > 0$$

So, $\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}$ is positive definite, so its eigenvalues are all positive, so it is always invertible.

Exercise 6: High-Dimensional Linear Regression for Image Warping (Programming Exercise)

1.

$$\hat{\phi}(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b} + \mathbf{W}\phi(\mathbf{x})$$

$$\min_{\mathbf{W}, \mathbf{A}, \mathbf{b}} l := \sum_{i=1}^N \|\mathbf{A}\mathbf{x}_i + \mathbf{b} + \mathbf{W}\phi(\mathbf{x}_i) - \mathbf{y}_i\|_2^2 + \lambda_1 \|\mathbf{A} - \mathbf{I}\|_f^2 + \lambda_2 \|\mathbf{b}\|_2^2 + \lambda_3 \|\mathbf{W}\|_f^2$$

Let $\mathbf{M} = [\mathbf{A}, \mathbf{b}, \mathbf{W}] \in \mathbb{R}^{n \times (n+1+N)}$, $\mathbf{Y} = [\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N] \in \mathbb{R}^{n \times N}$,

And

$$\mathbf{Z}_i = \begin{bmatrix} \mathbf{x}_i^T \\ 1 \\ \phi^T(\mathbf{x}_i) \end{bmatrix} \in \mathbb{R}^{n+1+N}, \mathbf{X} = [\mathbf{Z}_1, \mathbf{Z}_2, \dots, \mathbf{Z}_N] \in \mathbb{R}^{(n+1+N) \times N}$$

So we can write the problem as:

$$\min_{\mathbf{M}} l := \|\mathbf{MX} - \mathbf{Y}\|_f^2 + \left\| (\mathbf{M} - [\mathbf{I}_n, 0]_{n \times (n+1+N)}) \text{diag}(\sqrt{\lambda_1^{(n)}}, \sqrt{\lambda_2^{(1)}}, \sqrt{\lambda_3^{(N)}}) \right\|_f^2, \text{ Let's denote } \arg(\sqrt{\lambda_1^{(n)}}, \sqrt{\lambda_2^{(1)}}, \sqrt{\lambda_3^{(N)}}) \text{ as } \mathbf{E}$$

Then, we can write the problem as:

$$\min_{\mathbf{M}} l := \|\mathbf{MX} - \mathbf{Y}\|_f^2 + \|(\mathbf{M} - [\mathbf{I}_n, 0])\mathbf{E}\|_f^2$$

Let:

$$\frac{\partial l}{\partial \mathbf{M}} = 2(\mathbf{MX} - \mathbf{Y})\mathbf{X}^T + 2\mathbf{ME}^2 - [\mathbf{I}_n, 0]\mathbf{E}^2 = 0$$

We can get:

$$\hat{\mathbf{M}} = (\mathbf{YX}^T + [\mathbf{I}_n, 0]\mathbf{E}^2)(\mathbf{XX}^T + \mathbf{E}^2)^{-1}$$

2.



This is a sample image after warping.

Exercise 7: Bias-Variance Trade-off (Programming Exercise)

1.

The design matrix $\Phi(\mathbf{X})^{(l)}$ is an $N \times 25$ matrix, where N represents the number of data points and 25 denotes the dimension of $\phi(x) = (1, \phi_1(x), \dots, \phi_{24}(x))^T$.

And the column vector $\mathbf{Y}^{(l)}$ is an N -dimensional vector representing the $y_n^{(l)}$

So, the loss function can be written as:

$$L^{(l)}(w) = \frac{1}{2}(\mathbf{Y} - \Phi^{(l)}w)^T(\mathbf{Y} - \Phi^{(l)}w) + \frac{\lambda}{2}w^T w$$

Then, we let:

$$\frac{\partial L^{(l)}}{\partial w} = -(\Phi^{(l)})^T(\mathbf{Y} - \Phi^{(l)}w) + \lambda w = 0$$

We can get:

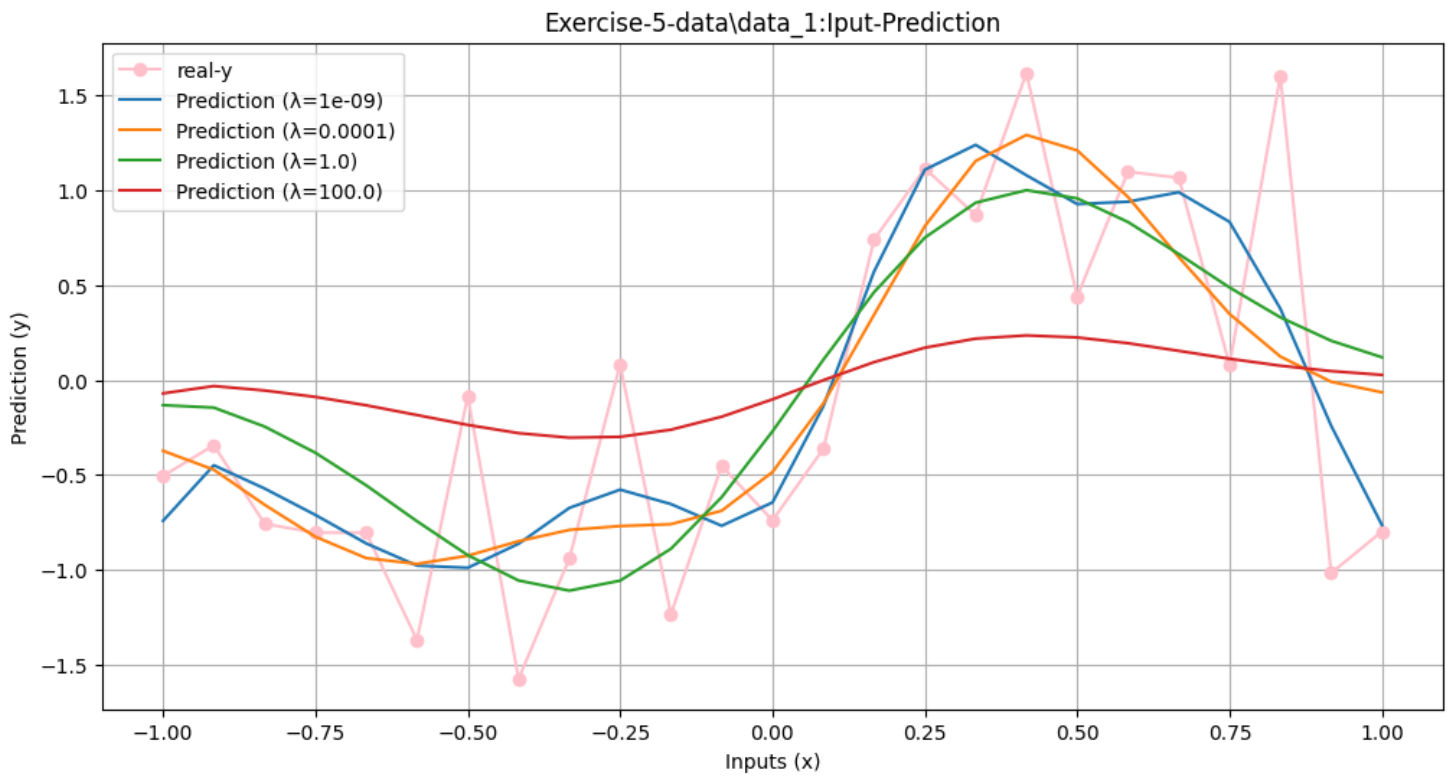
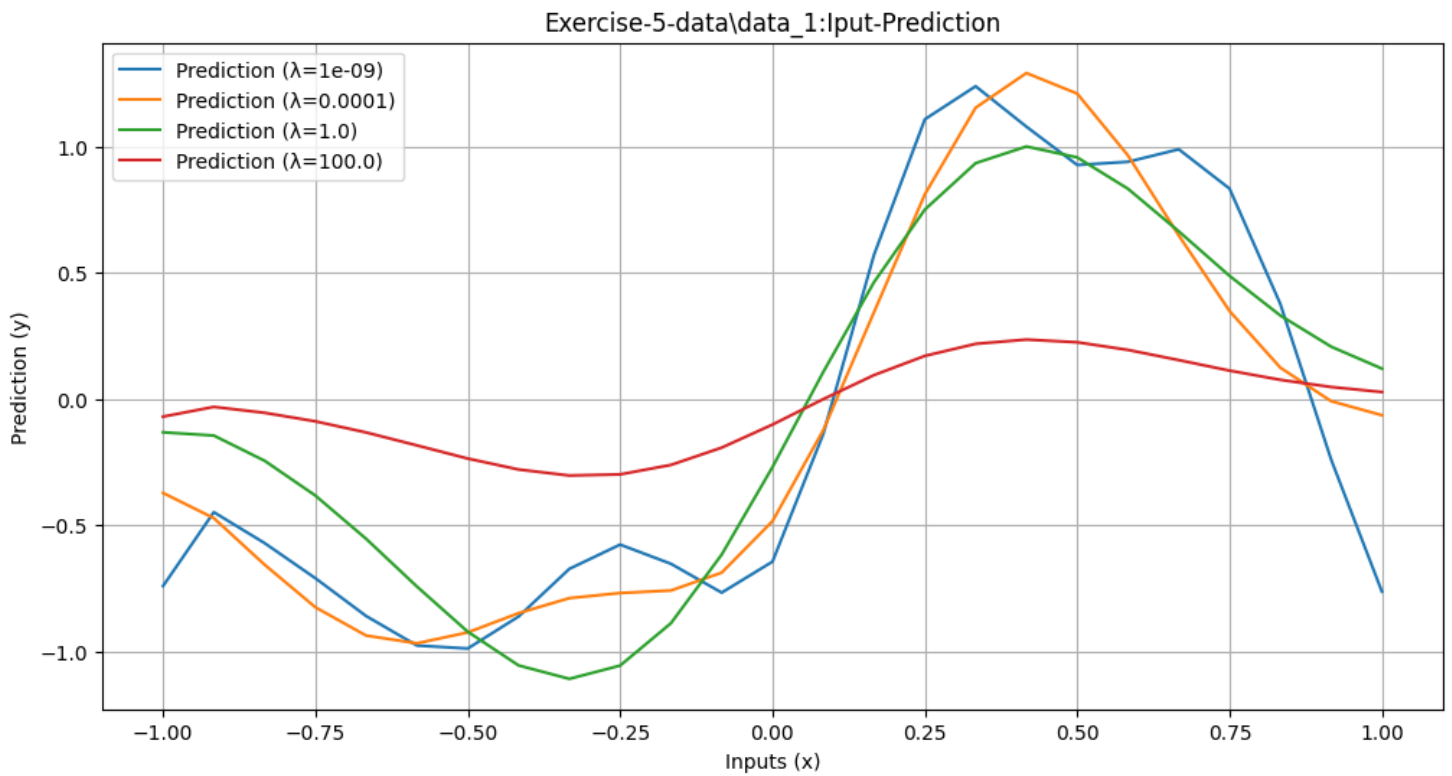
$$\hat{w}^{(l)} = ((\Phi^{(l)})^T \Phi^{(l)} + \lambda I)^{-1} (\Phi^{(l)})^T \mathbf{Y}$$

2.

We can write $f_{\mathcal{D}^{(l)}}(x)$ as $(w^{(l)})^T \phi(x)$

So, $y^{(l)}(x) = f_{\mathcal{D}^{(l)}}(x) = (w^{(l)})^T \phi(x)$

So, $\mathbf{Y}^{(l)}(\mathbf{x}^{(l)}) = f_{\mathcal{D}^{(l)}}(x) = \phi(\mathbf{x})^{(l)}(w^{(l)})$



3.

We have the column vector $\hat{\mathbf{y}}^{(l)}$ is an N-dimensional vector representing the $\hat{y}_n^{(l)}$, so we can let $\hat{\mathbf{Y}} = [\hat{\mathbf{y}}^{(1)}, \hat{\mathbf{y}}^{(1)}, \dots, \hat{\mathbf{y}}^{(L)}]$

Let $\bar{\mathbf{Y}} = \hat{\mathbf{Y}}$'s column mean, let $\mathbf{H} = [h(x_1), h(x_2), \dots, h(x_N)]^T$

Then, we can write:

$$(\text{bias})^2 = (\bar{\mathbf{Y}} - \mathbf{H})^T (\bar{\mathbf{Y}} - \mathbf{H}) / N$$

$$variance = \|\hat{\mathbf{Y}} - \overline{\mathbf{Y}}\|_f / NL$$

Here, $\overline{\mathbf{Y}}$ has been performed broadcasting along the columns.

