EE2211 Lecture 6: Linear Classification, Ridge Regression, Polynomial Regression

Vincent Y. F. Tan

Department of Electrical and Computer Engineering, NUS

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Outline

Review of Linear Regression

- (Learning/Training) Given a dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$ where $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$, the least squares solution (with offset) is

$$\overline{\mathbf{w}}^* = \begin{bmatrix} b^* \\ \mathbf{w}^* \end{bmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \in \mathbb{R}^{d+1}$$

where the design matrix and target vector are

$$\mathbf{X} = \begin{bmatrix} - \overline{\mathbf{x}}_1^\top - \\ - \overline{\mathbf{x}}_2^\top - \\ \vdots \\ - \overline{\mathbf{x}}_m^\top - \end{bmatrix} = \begin{bmatrix} 1 & - \mathbf{x}_1^\top - \\ 1 & - \mathbf{x}_2^\top - \\ \vdots & \vdots \\ 1 & - \mathbf{x}_m^\top - \end{bmatrix} \in \mathbb{R}^{m \times (d+1)} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^m.$$

- (Prediction/Testing) Given a new feature vector (sample, example) $\mathbf{x}_{\text{new}}$, the prediction based on the least squares solution is

$$\hat{y}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{w}}^* = b^* + \mathbf{x}_{\text{new}}^\top \mathbf{w}^*.$$

Review of Linear Regression With Multiple Outputs

- Suppose there are h outputs we want to predict (above $h = 3$).
- Given a dataset $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m$ where $\mathbf{x}_i \in \mathbb{R}^d$ (column vector) and $\mathbf{y}_i \in \mathbb{R}^{1\times h}$ (row vector), the model to be used is

$$\underbrace{\begin{bmatrix} y_{1,1} & y_{1,2} & \dots & y_{1,h} \\ y_{2,1} & y_{2,2} & \dots & y_{2,h} \\ \vdots & \vdots & \ddots & \vdots \\ y_{m,1} & y_{m,2} & \dots & y_{m,h} \end{bmatrix}}_{\mathbf{Y}\in\mathbb{R}^{m\times h}} = \underbrace{\begin{bmatrix} 1 & x_{1,1} & \dots & x_{1,d} \\ 1 & x_{2,1} & \dots & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m,1} & \dots & x_{m,d} \end{bmatrix}}_{\mathbf{X}\in\mathbb{R}^{m\times(d+1)}} \underbrace{\begin{bmatrix} b_1 & b_2 & \dots & b_h \\ w_{1,1} & w_{1,2} & \dots & w_{1,h} \\ \vdots & \vdots & \ddots & \vdots \\ w_{d,1} & w_{d,2} & \dots & w_{d,h} \end{bmatrix}}_{\overline{\mathbf{W}}\in\mathbb{R}^{(d+1)\times h}}$$

- When $h = 1$, this particularizes to standard linear regression.
- This is exactly h separate linear regression problems.

Review of Linear Regression With Multiple Outputs

- (Training/Learning) Least Squares Solution

$$\overline{\mathbf{W}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} \in \mathbb{R}^{(d+1)\times h}.$$

- (Testing/Prediction) Given a new feature vector $\mathbf{x}_{\text{new}} \in \mathbb{R}^d$, we can predict its h outputs as

$$\hat{\mathbf{y}}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^* \in \mathbb{R}^{1\times h}$$

- The k-th ($1 \le k \le h$) component of $\hat{\mathbf{y}}_{\text{new}}$ is the prediction of the k-th output based the dataset $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m$.

Outline

- We have a collection of m labelled samples $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$ where
  1. $\mathbf{x}_i = [x_{i,1}, x_{i,2}, \ldots, x_{i,d}]^\top \in \mathbb{R}^d$ is the i-th feature vector;
  2. y_i is a discrete label.
- In binary classification, we can encode y_i as $y_i = +1$ (positive class) and $y_i = -1$ (negative class).
- m is the number of data samples (feature vectors) in the dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$.
- d is the dimension of each data sample, i.e., length of each $\mathbf{x}_i$.
- We assume the affine model

$$f_{\mathbf{w},b}(\mathbf{x}) = \mathbf{x}^\top \mathbf{w} + b = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}^\top \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} = \overline{\mathbf{x}}^\top \overline{\mathbf{w}},$$

where

$$\overline{\mathbf{x}} = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix} \in \mathbb{R}^{d+1} \qquad \overline{\mathbf{w}} = \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} \in \mathbb{R}^{d+1}$$

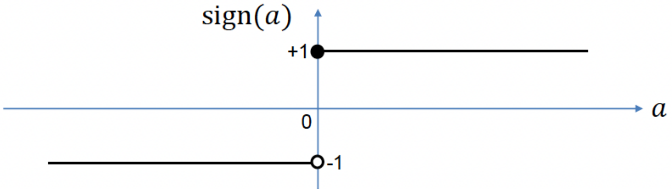
Linear Models for Classification

- The main idea is to treat binary classification as regression where each label y_i can only take on -1 or $+1$.
- If in testing/prediction, $\bar{\mathbf{x}}_{\text{new}}^\top \bar{\mathbf{w}}^*$ is positive (resp. negative), predict that $\hat{y}_{\text{new}} = +1$ (resp. $\hat{y}_{\text{new}} = -1$). For example, distinguishing between cats and dogs.
- (Learning/Training) Given a dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$ (where each $y_i \in \{+1, -1\}$), learn the weights using least squares

$$\bar{\mathbf{w}}^* = \begin{bmatrix} b^* \\ \mathbf{w}^* \end{bmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \in \mathbb{R}^{d+1}.$$

- (Prediction/Testing) Given a new data sample $\mathbf{x}_{\text{new}} \in \mathbb{R}^d$, its predicted label is

$$\hat{y}_{\text{new}} = \mathrm{sign}\left(\bar{\mathbf{x}}_{\text{new}}^\top \bar{\mathbf{w}}^*\right) = \mathrm{sign}\left(\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \bar{\mathbf{w}}^*\right) \in \{+1, -1\}.$$



For example,

- If the raw prediction $\overline{\mathbf{x}}_{\text{new}}^{\top}\overline{\mathbf{w}}^{*} = 0.2$, the predicted class is $+1$;
- If the raw prediction $\overline{\mathbf{x}}_{\text{new}}^{\top}\overline{\mathbf{w}}^{*} = -0.8$, the predicted class is -1;
- If the raw prediction $\overline{\mathbf{x}}_{\text{new}}^{\top}\overline{\mathbf{w}}^{*} = 0.0$, we declare error.

Numerical Example for Binary Classification

- Dataset $(\mathbf{x}_i, y_i), i = 1, 2, 3, 4$ includes the samples

$$\mathbf{x}_1 = -7, \quad \mathbf{x}_2 = -5, \quad \mathbf{x}_3 = 1, \quad \mathbf{x}_4 = 5$$
$$y_1 = -1, \quad y_2 = -1, \quad y_3 = +1, \quad y_4 = +1$$

- Here, $m = 4$ and $d = 1$ (scalar features).
- Design matrix and target vector are

$$\mathbf{X} = \begin{bmatrix} 1 & -7 \\ 1 & -5 \\ 1 & 1 \\ 1 & 5 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} -1 \\ -1 \\ +1 \\ +1 \end{bmatrix}$$

- The linear system $\mathbf{X}\overline{\mathbf{w}} = \mathbf{y}$ is overdetermined and there is no solution for $\overline{\mathbf{w}}$ because

$$\text{rank}(\mathbf{X}) < \text{rank}(\tilde{\mathbf{X}}).$$

Numerical Example for Binary Classification

- Using some numerical software, we can find the least square approximation

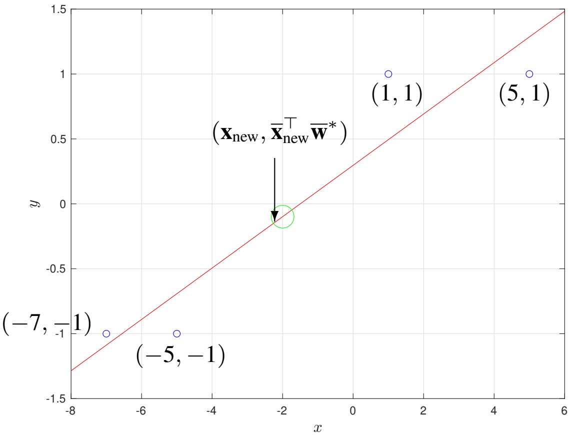
$$\overline{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} = \begin{bmatrix} 0.2967 \\ 0.1978 \end{bmatrix}$$

- If we want to predict what's the label for $\mathbf{x}_{\text{new}} = -2$, we plug $\mathbf{x}_{\text{new}} = -2$ into the learned affine model to get

$$\begin{aligned} \hat{y}_{\text{new}} &= \text{sign}\left(\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{w}}^* \right) \\ &= \text{sign}\left(1 \times (0.2967) + (-2) \times (0.1978)\right) \\ &= \text{sign}(-0.0989) = -1. \end{aligned}$$

- So we predict that the label of the new test point $\mathbf{x}_{\text{new}} = -2$ is $\hat{y}_{\text{new}} = -1$ (negative class). [Python demo]

Numerical Example for Binary Classification



The predicted label of new point $\mathbf{x}_{\mathrm{new}}$ is $\mathrm{sign}(\overline{\mathbf{x}}_{\mathrm{new}}^\top \overline{\mathbf{w}}^*) = -1$ as $\overline{\mathbf{x}}_{\mathrm{new}}^\top \overline{\mathbf{w}}^*$ is negative.

Python Demo 1

```python
# EE2211 Lecture 6 Demo 1 Binary classification
import numpy as np
from numpy.linalg import inv

X = np.array([[1,-7], [1,-5], [1,1], [1,5]])
y = np.array([[-1], [-1], [1], [1]])
## Linear regression for classification
w = inv(X.T @ X) @ X.T @ y
print("Estimated w")
print(w)
print("\n")

Xt = np.array([[1,-2]])
y_predict = Xt @ w
print("Predicted y")
print(y_predict)
y_class_predict = np.sign(y_predict)
print("Predicted y class")
print(y_class_predict)
```

Linear Models for Multi-Class Classification

- Suppose we want to distinguish between cats, dogs and birds. These are labelled as 1, 2, 3 respectively.
- Idea is to do one-hot encoding of the labels, say $\{1, 2, \ldots, C\}$, where $C > 2$ is the number of classes.
- If sample i has class 1, its label vector is

$$\mathbf{y}_i = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \end{bmatrix}$$

- If sample i has class 2, its label vector is

$$\mathbf{y}_i = \begin{bmatrix} 0 & 1 & 0 & \ldots & 0 \end{bmatrix}$$

- If sample i has class C, its label vector is

$$\mathbf{y}_i = \begin{bmatrix} 0 & 0 & 0 & \ldots & 1 \end{bmatrix}$$

Linear Models for Multi-Class Classification

- Stack all these label vectors into the $m \times C$ label matrix

$$\mathbf{Y} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_m \end{bmatrix} = \begin{bmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,C} \\ y_{2,1} & y_{2,2} & \cdots & y_{2,C} \\ \vdots & \vdots & \ddots & \vdots \\ y_{m,1} & y_{m,2} & \cdots & y_{m,C} \end{bmatrix}$$

- This is a $\{0, 1\}$-valued matrix with m (number of samples) rows and C (number of classes) columns.
- Essentially, we are doing C separate linear classification problems.
- Each determining the "likelihood" of whether we are in class $k \in \{1, 2, \ldots, C\}$.

Linear Models for Multi-Class Classification

- (Training/Learning) The design matrix $\mathbf{X}$ is the same. If it has full column rank, find the least squares solution

$$\overline{\mathbf{W}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} \in \mathbb{R}^{(d+1)\times C}.$$

- (Testing/Prediction) Given a new feature vector $\mathbf{x}_{\text{new}} \in \mathbb{R}^d$, we can predict its class as

$$\hat{y}_{\text{new}} = \underset{k\in\{1,2,\ldots,C\}}{\arg\max} \left(\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^*[:,k] \right) \in \{1,2,\ldots,C\}$$

where $\overline{\mathbf{W}}^*[:,k] \in \mathbb{R}^{d+1}$ is the k-column of $\overline{\mathbf{W}}^*$.

Numerical Example for Multi-Class Classification

- Our $m = 4$ feature vectors are

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \mathbf{x}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \quad \mathbf{x}_2 = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \quad \mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

  Each is of dimension $d = 2$.
- The raw classes (there are $C = 3$ of them) are

$$y_1 = \text{cat}, \quad y_2 = \text{dog}, \quad y_3 = \text{cat}, \quad y_4 = \text{bird}.$$

- First encode the raw classes into numerical classes, e.g.,

$$y_1 = 1, \quad y_2 = 2, \quad y_3 = 1, \quad y_4 = 3.$$

  Thus $\text{cat} \equiv 1$, $\text{dog} \equiv 2$, $\text{bird} \equiv 3$.
- One-hot encoding in operation!

$$\mathbf{y}_1 = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}, \ \mathbf{y}_2 = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}, \ \mathbf{y}_3 = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}, \ \mathbf{y}_4 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix},$$

Numerical Example for Multi-Class Classification

- Design matrix (with bias all-ones column) and target matrix are

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 3 \\ 1 & 1 & 0 \end{bmatrix} \in \mathbb{R}^{m \times (d+1)} \qquad \mathbf{Y} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{m \times C}.$$

  Please check that you know where these numbers came from.

- (Training/Learning) Least squares approximation

$$\overline{\mathbf{W}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} = \begin{bmatrix} 0 & 0.5 & 0.5 \\ 0.2857 & -0.5 & 0.2143 \\ 0.2857 & 0 & -0.2857 \end{bmatrix} \in \mathbb{R}^{(d+1) \times C}$$

Numerical Example for Multi-Class Classification

- (Prediction/Testing) Given a new sample $\mathbf{x}_{\text{new}} = \begin{bmatrix} 0 & -1 \end{bmatrix}^\top$.
- For each $k = 1, 2, 3$, calculate $\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^*[:, k]$.
- We obtain

$$\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^*[:, 1] = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}^\top \begin{bmatrix} 0 \\ 0.2857 \\ 0.2857 \end{bmatrix} = -0.2857$$

$$\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^*[:, 2] = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}^\top \begin{bmatrix} 0.5 \\ -0.5 \\ 0 \end{bmatrix} = 0.5,$$

$$\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^*[:, 3] = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}^\top \begin{bmatrix} 0.5 \\ 0.2143 \\ -0.2857 \end{bmatrix} = 0.7857$$

- (Prediction/Testing) Its predicted class is

$$\hat{y}_{\text{new}} = \underset{k \in \{1,2,3\}}{\arg\max} \left(\begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^*[:, k] \right) = 3 \in \{1, 2, 3\}$$

The column position $k \in \{1, 2, 3\}$ of the largest number determines the predicted class label. [Python Demo]

Python Demo 2: Setting Up and One-Hot Encoding

```python
# EE2211 Lecture 6 Demo 2 Multi-class classification
import numpy as np
from numpy.linalg import inv
from sklearn.preprocessing import OneHotEncoder
X = np.array([[1, 1, 1], [1, -1, 1], [1, 1, 3], [1, 1, 0]])
y_class = np.array([[1], [2], [1], [3]])
y_onehot = np.array([[1, 0, 0], [0, 1, 0], [1, 0, 0], [0, 0, 1]])
print("One-hot encoding manual")
print(y_class)
print(y_onehot)
print("\n")

print("One-hot encoding function")
onehot_encoder=OneHotEncoder(sparse=False)
print(onehot_encoder)
Ytr_onehot = onehot_encoder.fit_transform(y_class)
print(Ytr_onehot)
```

Python Demo 2: Training and Testing

```
## Linear Classification
print("Estimated W")
W = inv(X.T @ X) @ X.T @ Ytr_onehot
print(W)
X_test = np.array([[1, 0, -1]])
yt_est = X_test@W;
print("\n")
print("Test")
print(yt_est)
yt_class = [[1 if y == max(x) else 0 for y in x] for x in yt_est ]
print("\n")
print("class label test")
print(yt_class)

print("\n")
print("class label test using argmax")
print(np.argmax(yt_est)+1)
```

Outline

Motivation for Ridge Regression

- I was involved in the Manchester Asthma & Allergy Study (MAAS)
- About $m \approx 1000$ children (subjects are expensive to recruit)
- Number of variables $d \approx 10^6$ (modern equipment can acquire huge amounts of data)
- Environmental, Physiological and Genetic variables (e.g., Single Nucleotide Polymorphisms or SNPs)






Motivation for Ridge Regression

- This is the case of modern datasets which have many variables/attributes (d is large) and few samples (m is small).
- What happens to the least squares estimate?

$$\bar{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \in \mathbb{R}^{d+1}?$$

Recall that this was obtained from minimizing

$$J(\bar{\mathbf{w}}) = \sum_{i=1}^{m} \left(f_{\mathbf{w},b}(\mathbf{x}_i) - y_i \right)^2 = (\mathbf{X}\bar{\mathbf{w}} - \mathbf{y})^\top (\mathbf{X}\bar{\mathbf{w}} - \mathbf{y})$$

over $\bar{\mathbf{w}} = \left[b, \mathbf{w}^\top \right]^\top \in \mathbb{R}^{d+1}$.

- The design matrix $\mathbf{X} \in \mathbb{R}^{m \times (d+1)}$ is very "wide".
- $\mathbf{X}$ is highly unlikely to have full column rank.
- $(\mathbf{X}^\top \mathbf{X})^{-1}$ does not exist.
- We need to mitigate this problem.

Motivation for Ridge Regression

New Objective Function for Ridge Regression

- For a fixed $\lambda \geq 0$, consider

$$J(\overline{\mathbf{w}}) = \sum_{i=1}^{m} \left(f_{\mathbf{w},b}(\mathbf{x}_i) - y_i\right)^2 + \lambda \sum_{i=0}^{d} w_j^2$$
$$= (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y})^\top (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y}) + \lambda \overline{\mathbf{w}}^\top \overline{\mathbf{w}}$$

  Note that $w_0 = b$, the offset or bias.
- The term $\lambda \overline{\mathbf{w}}^\top \overline{\mathbf{w}}$ encourages the weight vector to have small components (also known as shrinkage.
- The new objective results in ridge regression or Tikhonov regularization.
- When $\lambda = 0$, we recover usual linear regression.

Solution for Ridge Regression

Solution for Ridge Regression

- Recall that we wish to solve

$$\overline{\mathbf{w}}^* = \underset{\overline{\mathbf{w}}=[b,\mathbf{w}]^\top}{\arg\min} \ (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y})^\top (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y}) + \lambda \overline{\mathbf{w}}^\top \overline{\mathbf{w}}.$$

- Expanding the objective, we obtain

$$\begin{aligned}
&(\mathbf{X}\overline{\mathbf{w}} - \mathbf{y})^\top (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y}) + \lambda \overline{\mathbf{w}}^\top \overline{\mathbf{w}} \\
&= \overline{\mathbf{w}}^\top \mathbf{X}^\top \mathbf{X}\overline{\mathbf{w}} - \overline{\mathbf{w}}^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\overline{\mathbf{w}} + \mathbf{y}^\top \mathbf{y} + \lambda \overline{\mathbf{w}}^\top \overline{\mathbf{w}} \\
&= \overline{\mathbf{w}}^\top \mathbf{X}^\top \mathbf{X}\overline{\mathbf{w}} + \overline{\mathbf{w}}^\top (\lambda \mathbf{I}) \overline{\mathbf{w}} - 2\overline{\mathbf{w}}^\top (\mathbf{X}^\top \mathbf{y}) + \mathbf{y}^\top \mathbf{y} \\
&= \overline{\mathbf{w}}^\top (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}) \overline{\mathbf{w}} - 2\overline{\mathbf{w}}^\top (\mathbf{X}^\top \mathbf{y}) + \mathbf{y}^\top \mathbf{y}
\end{aligned}$$

- Differentiating w.r.t. $\overline{\mathbf{w}}$ and setting the result to zero yields

$$2(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})\overline{\mathbf{w}}^* = 2(\mathbf{X}^\top \mathbf{y}) \quad \Longleftrightarrow \quad \overline{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}.$$

- Voila! For any $\lambda > 0$, $\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}$ is always invertible (why?) so the calculation above is legitimate.

Ridge Regression in Primal Form

- Training/Learning: Minimizing the ridge regression objective $J(\overline{\mathbf{w}}) = (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y})^\top (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y}) + \lambda \overline{\mathbf{w}}^\top \overline{\mathbf{w}}$ yields

$$\overline{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}.$$

- Testing/Prediction: Given a new test sample $\mathbf{x}_{\text{new}}$, its prediction is

$$\hat{y}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{w}}^*.$$

Ridge Regression in Primal Form

- The solution is known as the

$$\text{[Primal Form]} \qquad \overline{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_{d+1})^{-1} \mathbf{X}^\top \mathbf{y}.$$

  Use $\mathbf{I}_{d+1}$ to emphasize that the identity matrix is of size $(d+1) \times (d+1)$.
- What's the problem with inverting the $(d+1) \times (d+1)$ matrix $\mathbf{X}^\top \mathbf{X} + \lambda_{d+1} \mathbf{I}$?
- $d > m$ is very large. Inverting the $(d+1) \times (d+1)$ matrix is not advisable!
- This takes $\approx d^3$ operations (multiplications and additions). **[You don't need to know why.]**
- If $m > d$, we can still use

$$\overline{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_{d+1})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Ridge Regression in Dual Form

- Fact: For every $\lambda > 0$,

$$(\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_{d+1})^{-1} \mathbf{X}^\top \mathbf{y} = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda \mathbf{I}_m)^{-1} \mathbf{y}. \qquad \text{(P-D)}$$

- Training/Learning: So when $d > m$ (modern datasets), we use the

$$\text{[Dual Form]} \qquad \overline{\mathbf{w}}^* = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda \mathbf{I}_m)^{-1} \mathbf{y}.$$

- Testing/Prediction: Given a new test sample $\mathbf{x}_{\text{new}}$, its prediction is

$$\hat{y}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{w}}^*.$$

- To show (P-D), we use the Woodbury formula

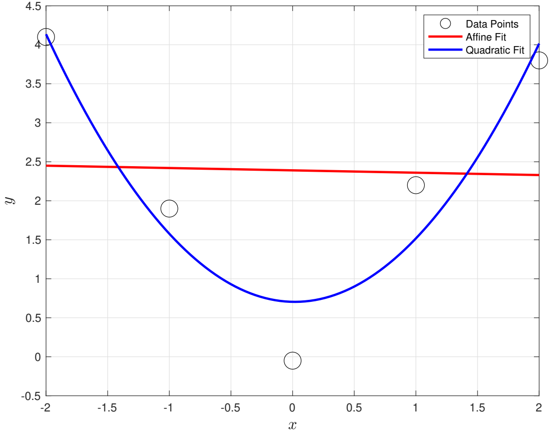
$$(\mathbf{I} + \mathbf{U}\mathbf{V})^{-1} = \mathbf{I} - \mathbf{U}(\mathbf{I} + \mathbf{V}\mathbf{U})^{-1}\mathbf{V}.$$

This will be an exercise in Tutorial 6.

Outline

Motivation for Polynomial Regression

Sometimes affine functions do not do a good job!

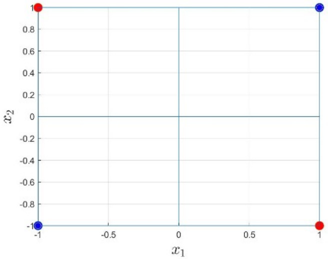


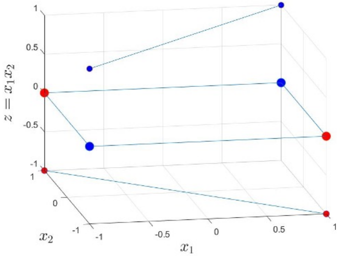
Data points come from a quadratic. Class of affine functions is not sufficiently rich.

Motivation for Polynomial Regression

XOR dataset in $d = 2$ dimensions.

$$\mathbf{x}_1 = \begin{bmatrix} +1 & +1 \end{bmatrix}^\top \quad \mathbf{x}_2 = \begin{bmatrix} -1 & +1 \end{bmatrix}^\top \quad \mathbf{x}_3 = \begin{bmatrix} +1 & -1 \end{bmatrix}^\top \quad \mathbf{x}_4 = \begin{bmatrix} -1 & -1 \end{bmatrix}^\top$$





- No linear/affine classifier can separate the training samples without error.
- The quadratic function $f(x_1, x_2) = x_1x_2$ (product of first and second components) can separate the training samples without error.

Polynomials

- We would like to model nonlinear decision boundaries or surfaces.
- A polynomial function of order 2 with $d = 1$ variables

$$f_{\mathbf{w}}(x) = w_0 + w_1 x + w_2 x^2 \qquad \mathbf{w} = (w_0, w_1, w_2)$$

- A polynomial function of order p with $d = 1$ variables

$$f_{\mathbf{w}}(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_p x^p \qquad \mathbf{w} = (w_0, w_1, \ldots, w_p)$$

- A polynomial function of order 1 with $d = 2$ variables

$$f_{\mathbf{w}}(x_1, x_2) = w_0 + w_1 x_1 + w_2 x_2 \qquad \mathbf{w} = (w_0, w_1, w_2)$$

- A polynomial function of order 2 with $d = 2$ variables

$$f_{\mathbf{w}}(x_1, x_2) = w_0 + w_1 x_1 + w_2 x_2 + w_{1,2} x_1 x_2 + w_{1,1} x_1^2 + w_{2,2} x_2^2$$
$$\mathbf{w} = (w_0, w_1, w_2, w_{1,2}, w_{1,1}, w_{2,2})$$

- For example, a polynomial function of order 2 in dimension $d = 2$

$$f_{\mathbf{w}}(x_1, x_2) = w_0 + w_1 x_1^{1} + w_2 x_2^{1} + w_{1,2} x_1^{1} x_2^{1} + w_{1,1} x_1^{2} + w_{2,2} x_2^{2}$$
$$\mathbf{w} = (w_0, w_1, w_2, w_{1,2}, w_{1,1}, w_{2,2})$$

Each term in $f_{\mathbf{w}}(x_1, x_2)$ is called a monomial. The maximum sum of powers (degree) of the x_1, x_2 terms is 2, e.g.,

$$\deg(w_2 x_2^{1}) = 0 + 1 = 1$$
$$\deg(w_{1,2} x_1^{1} x_2^{1}) = 1 + 1 = 2$$
$$\deg(w_{2,2} x_2^{2}) = 0 + 2 = 2$$

- In general, for d-variable quadratic (order-2) model,

$$f_{\mathbf{w}}(x_1, x_2, \ldots, x_d) = w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{1 \le i \le j \le d} w_{i,j} x_i x_j.$$

[Optional to know] How many terms are there here?

Polynomials

- For d-variable, cubic model,

$$f_{\mathbf{w}}(x_1, x_2, \ldots, x_d) = w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{1 \le i \le j \le d} w_{i,j} x_i x_j + \sum_{1 \le i \le j \le k \le d} w_{i,j,k} x_i x_j x_k$$

[Optional to know] How many terms are there here?

$$\binom{d-1}{0} + \binom{d}{1} + \binom{d+1}{2} + \binom{d+2}{3} = \binom{d+3}{3}.$$

- For a d-variable, order-p polynomial, there are

$$\binom{d+p}{p} \quad \text{terms.}$$

- The point is that if d and/or p is large, this is a very large number.

Polynomial Regression

- Generalized Linear Discriminant Function

$$f_{\mathbf{w}}(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{1 \le i \le j \le d} w_{i,j} x_i x_j + \sum_{1 \le i \le j \le k \le d} w_{i,j,k} x_i x_j x_k$$

- Noting that $x_{l,i}$ is the i-th ($1 \le i \le d$) component of the l-th ($1 \le l \le m$) sample, we can stack this into

$$f_{\mathbf{w}}(\mathbf{x}) = \mathbf{P}\mathbf{w} = \begin{bmatrix} \mathbf{p}_1^\top \mathbf{w} \\ \vdots \\ \mathbf{p}_m^\top \mathbf{w} \end{bmatrix}$$

and

$$\mathbf{p}_l^\top \mathbf{w} = \begin{bmatrix} 1 & x_{l,1} & \ldots & x_{l,d} & \ldots & x_{l,i}x_{l,j} & \ldots & x_{l,i}x_{l,j}x_{l,k} & \ldots \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \\ \vdots \\ w_{i,j} \\ \vdots \\ w_{i,j,k} \\ \vdots \end{bmatrix}$$

Polynomial Regression

- Note that the polynomial matrix

$$\mathbf{P} = \mathbf{P}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m) = \begin{bmatrix} - \mathbf{p}_1^\top - \\ - \mathbf{p}_2^\top - \\ \vdots \\ - \mathbf{p}_m^\top - \end{bmatrix} \in \mathbb{R}^{m \times \binom{d+p}{p}}$$

  is a function of the data samples $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m\}$.
- For an d-variable, order-p polynomial, the matrix $\mathbf{P}$ is of size $m \times \binom{d+p}{p}$.
- When we do not use a polynomial, then for a d-variable, order-1 polynomial (affine model), $\mathbf{P}$ is of size $m \times \binom{d+1}{1} = m \times (d+1)$.
- Offset term $w_0 = b$ is automatically taken into account in an order-1 polynomial.

- Data are

$$\mathbf{x}_1 = \begin{bmatrix}+1 & +1\end{bmatrix}^\top \quad \mathbf{x}_2 = \begin{bmatrix}-1 & +1\end{bmatrix}^\top \quad \mathbf{x}_3 = \begin{bmatrix}+1 & -1\end{bmatrix}^\top \quad \mathbf{x}_4 = \begin{bmatrix}-1 & -1\end{bmatrix}^\top$$

  and $y_1 = y_4 = +1$, $y_2 = y_3 = -1$.

- Second-order polynomial in $d = 2$ variables

$$f_{\mathbf{w}}(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + w_{1,2} x_1 x_2 + w_{1,1} x_1^2 + w_{2,2} x_2^2 = \mathbf{p}^\top \mathbf{w}$$

  where

$$\mathbf{w} = \begin{bmatrix} w_0 & w_1 & w_2 & w_{1,2} & w_{1,1} & w_{2,2} \end{bmatrix}$$
$$\mathbf{p} = \begin{bmatrix} 1 & x_1 & x_2 & x_1 x_2 & x_1^2 & x_2^2 \end{bmatrix}$$

- Can stack the 4 training samples into the polynomial matrix

$$\mathbf{P} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & x_{1,1}x_{1,2} & x_{1,1}^2 & x_{1,2}^2 \\ 1 & x_{2,1} & x_{2,2} & x_{2,1}x_{2,2} & x_{2,1}^2 & x_{2,2}^2 \\ 1 & x_{3,1} & x_{3,2} & x_{3,1}x_{3,2} & x_{3,1}^2 & x_{3,2}^2 \\ 1 & x_{4,1} & x_{4,2} & x_{4,1}x_{4,2} & x_{4,1}^2 & x_{4,2}^2 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \end{bmatrix}$$

- Notice that the magenta column perfectly distinguishes the training points. [Python Demo]

Summary of Polynomial Regression

- Ridge regression in primal form (when $m > d' = \binom{p+d}{p}$)
  - Learning/Training:

$$\mathbf{w}^* = (\mathbf{P}^\top \mathbf{P} + \lambda \mathbf{I})^{-1} \mathbf{P}^\top \mathbf{y}$$

  - Prediction/Testing: Given a new sample $\mathbf{x}_{\text{new}}$

$$\hat{y}_{\text{new}} = \mathbf{p}_{\text{new}}^\top \mathbf{w}^*$$

  where $\mathbf{p}_{\text{new}}$ is the polynomial vector associated to $\mathbf{x}_{\text{new}}$.

- Ridge regression in dual form (when $m < d' = \binom{p+d}{p}$)
  - Learning/Training:

$$\mathbf{w}^* = \mathbf{P}^\top (\mathbf{P}\mathbf{P}^\top + \lambda \mathbf{I})^{-1} \mathbf{y}$$

  - Prediction/Testing: Given a new sample $\mathbf{x}_{\text{new}}$

$$\hat{y}_{\text{new}} = \mathbf{p}_{\text{new}}^\top \mathbf{w}^*.$$

Summary of Polynomial Regression

- For regression applications:
  - Learn continuous-valued y by using either primal or dual forms
  - Prediction:

$$\hat{y}_{\text{new}} = \mathbf{p}_{\text{new}}^{\top} \mathbf{w}^{*}.$$

- For classification applications:
  - Learn discrete-valued $y \in \{-1, +1\}$ (for binary classification) or one-hot encoded $\mathbf{Y}$ (for $y \in \{1, 2, \ldots, C\}$ for multi-class classification) using either primal or dual forms
  - Binary prediction

$$\hat{y}_{\text{new}} = \operatorname{sign}\left(\mathbf{p}_{\text{new}}^{\top} \mathbf{w}^{*}\right)$$

  - Multi-class prediction

$$\hat{y}_{\text{new}} = \underset{k \in \{1,2,\ldots,C\}}{\arg\max} \left(\mathbf{p}_{\text{new}}^{\top} \mathbf{W}^{*}[:, k]\right)$$

The XOR Example Revisited

- We can compute the weight vector (with $\lambda = 0$)

$$\mathbf{w}^* = \mathbf{P}^\top(\mathbf{P}\mathbf{P}^\top)^{-1}\mathbf{y} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

Recall that

$$\mathbf{P} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}.$$

- Note that $\mathbf{w}^*$ picks out the coefficient $w_{1,2}$ corresponding x_1x_2.

The XOR Example Revisited

- Given a new test sample $\mathbf{x}_{\text{new}} = \begin{bmatrix} 0.2 & 0.5 \end{bmatrix}^\top$, the polynomial vector associated to $\mathbf{x}_{\text{new}}$ is

$$\begin{aligned}\mathbf{p}_{\text{new}} &= \begin{bmatrix} 1 & x_{\text{new},1} & x_{\text{new},2} & x_{\text{new},1}x_{\text{new},2} & x_{\text{new},1}^2 & x_{\text{new},2}^2 \end{bmatrix}^\top \\ &= \begin{bmatrix} 1 & 0.2 & 0.5 & 0.1 & 0.04 & 0.25 \end{bmatrix}^\top\end{aligned}$$

- Its predicted label is

$$\begin{aligned}\hat{y}_{\text{new}} &= \text{sign}\left(\mathbf{p}_{\text{new}}^\top \mathbf{w}^*\right) \\ &= \text{sign}(0 \times 1 + 0 \times 0.2 + 0 \times 0.5 + 1 \times 0.1 + 0 \times 0.04 + 0 \times 0.25) \\ &= 1.\end{aligned}$$

- Intuitively this is because the product of $\mathbf{x}_{\text{new}}$'s coordinates is positive. [Python Demo]

Python Demo 3: Training/Learning

```
#EE2211 Lecture 6 Demo 3 Training/Learning
import numpy as np
from numpy.linalg import inv
from numpy.linalg import matrix_rank
from sklearn.preprocessing import PolynomialFeatures
X = np.array([ [1, 1], [-1, 1], [1, -1], [-1, -1]])
y = np.array([[1], [-1], [-1], [1]])
## Generate polynomial features
order = 2
poly = PolynomialFeatures(order)
print(poly)
P = poly.fit_transform(X)
print("matrix P")
print(P)
print("Under-determined system")
#print(matrix_rank(P))
#PY = np.vstack((P.T, y.T))
#print(matrix_rank(PY.T))

## dual solution m < d (without ridge)
w_dual = P.T @ inv(P @ P.T) @ y
print("Unique constrained solution, no ridge")
print(w_dual)
```

Python Demo 3: Prediction/Testing

```
#testing
print("Prediction")
#Xnew= np.array([ [0.2, 0.5]])
# Two test points
Xnew= np.array([ [0.2, 0.5], [-0.9, 0.7]])
Pnew = poly.fit_transform(Xnew)
Ynew=Pnew@w_dual
print(Ynew)
print(np.sign(Ynew))
```

Summary

- Primal Form
  - Learning/Training

$$\mathbf{w}^* = (\mathbf{P}^\top \mathbf{P} + \lambda \mathbf{I})^{-1} \mathbf{P} \mathbf{y}$$

  - Prediction/Testing

$$\hat{y}_{\text{new}} = \mathbf{p}_{\text{new}}^\top \mathbf{w}^*$$

- Dual Form
  - Learning/Training

$$\mathbf{w}^* = \mathbf{P}^\top (\mathbf{P} \mathbf{P}^\top + \lambda \mathbf{I})^{-1} \mathbf{y}$$

  - Prediction/Testing

$$\hat{y}_{\text{new}} = \mathbf{p}_{\text{new}}^\top \mathbf{w}^*$$

- Useful Python packages and functions

`sklearn.preprocessing PolynomialFeatures`, `np.sign`,
`sklearn.model_selection train_test_split`,
`sklearn.preprocessing OneHotEncoder`