Linear Regression
(Problems & Solutions)

Dr. JASMEET SINGH
ASSISTANT PROFESSOR, CSED
TIET, PATIALA

Problem 1: Multicollinearity

- In regression, "multicollinearity" refers to predictors that are correlated with other predictors.
- Multicollinearity occurs when our model includes multiple factors that are correlated not just to your response variable, but also to each other.
- In other words, it results when we have factors that are a bit redundant.
- Multicollinearity increases the standard errors of the coefficients.
- Increased standard errors in turn means that coefficients for some independent variables may be found not to be significantly different from 0.
- In other words, by overinflating the standard errors, multicollinearity makes some variables statistically insignificant when they should be significant.

Problem 2 & 3: Underfitting & Overfitting

- In order to understand the concept of overfitting and underfitting, consider following example (shown in Figure 1(a)) where we have to fit a regression function (hypothesis) that can predict the value of output variable (y) given input variable (x).
- Let us fit three regression hypothesis on the data as shown in Figure 1(b), 1(c), and 1 (d)

Figure 1(a)

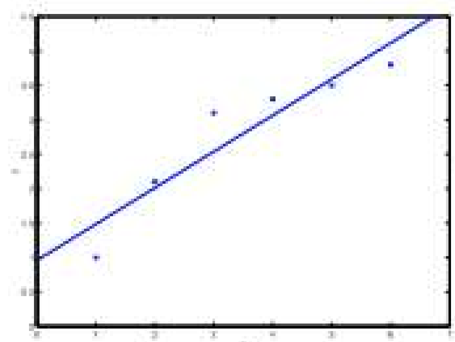


Figure 1(b)
$y^\wedge = \beta_0 + \beta_1 x$
(Underfit)

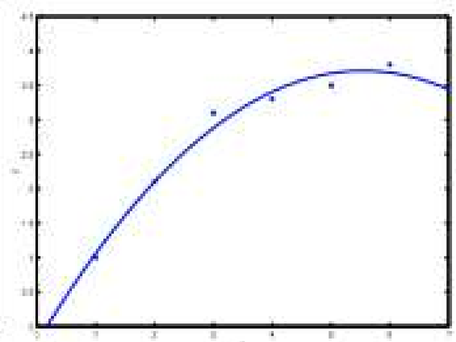


Figure 1(c)
$y^\wedge = \beta_0 + \beta_1 x + \beta_2 x^2$
(Good Fit)

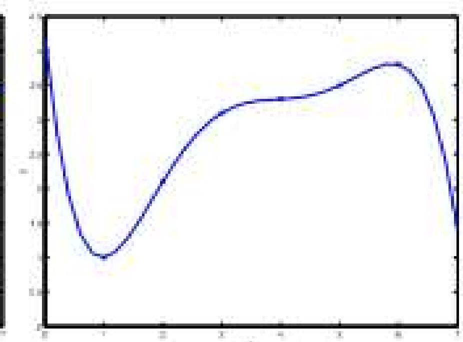


Figure 1(d)
$y^\wedge = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4\, x^4$
(Overfit)

Underfitting

- The figure 1(a) shows the result of fitting a linear hypothesis $y^{\wedge} = \beta_0 + \beta_1 x$.
- We can see that the data doesn't really lie on straight line, and so the fit is not very good.
- The figure shows an instance of **underfitting**—in which the data clearly shows structure not captured by the model.
- **Underfitting, or high bias**, is when the form of our hypothesis function h maps poorly to the trend of the data.
- It is usually caused by a function that is too simple or uses too few features.
- Underfitting can be solved by increasing the number of features in our training data.

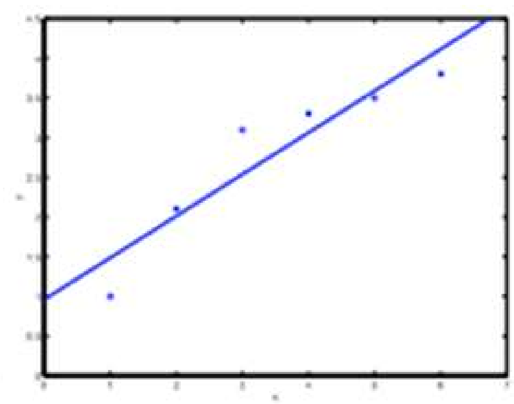


Figure 1(b)
$y^{\wedge} = \beta_0 + \beta_1 x$
(Underfit)

Overfitting

- The figure 1(d) shows the result of fitting a high order polynomial hypothesis $y^\wedge = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4$.
- The figure is an example of **overfitting.**
- **O**verfitting, or high variance, is caused by a hypothesis function that fits the available data but does not generalize well to predict new data.
- It is usually caused by a complicated function that creates a lot of unnecessary curves and angles unrelated to the data.
- For example, a quadratic fit shown in Figure 1(c) (slide number 3) is a good fit as it fits well to data and generalizes well.

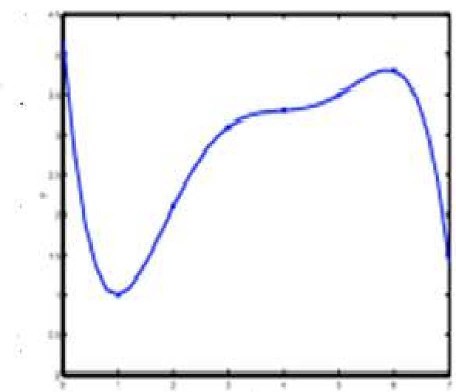
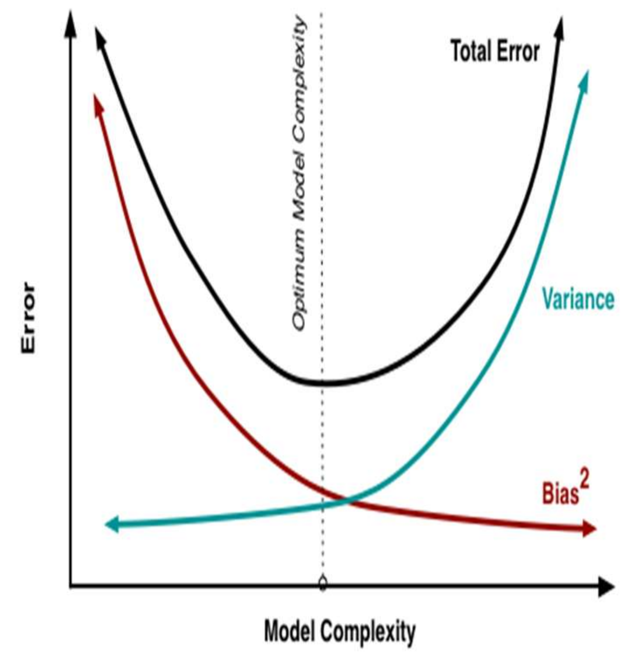


Figure 1(d)
$y^\wedge = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4$
(Overfit)

Bias and Variance Tradeoff

- If we have less number of features i.e., low model complexity, the fit is underfit with high bias error.
- the bias is an error from a faulty assumption in the learning algorithm.
- when the bias is too large, the algorithm would be able to correctly model the relationship between the features and the target outputs.
- As we keep on increasing the model complexity (number of features) bias decreases but variance increases (overfit).
- Variance is an error resulting from fluctuations int he training dataset.
- A high value for variance would cause the algorithm may capture the most data points put would not be generalized enough to capture new data points.
- The tradeoff between bias and variance can be controlled using controlling the complexity of model.



Solutions to Regression Problems

- The problems of multicollinearity, and overfitting can be controlled by handling the complexity of the model.
- The model complexity can be controlled using any of these features:

1. **Remove highly correlated predictors from the model**
   - Manually select which features to keep.
   - Use feature selection methods to choose features that maximizes relevancy or minimizes redundancy.
   - Use feature extraction techniques models such as PCA, SVD, and LDA.
2. **Regularization**

- Keep all the features, but reduce the magnitude of parameters
- Regularization works well when we have a lot of slightly useful features.

Regularization/ Shrinkage

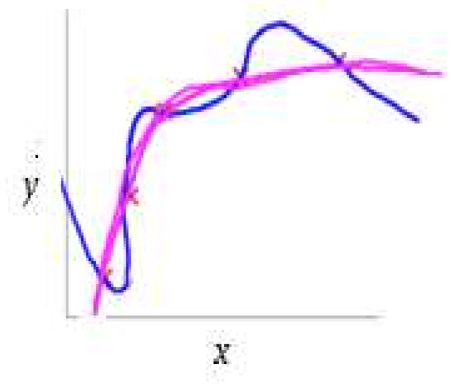
- Regularization is a technique used for tuning the function by adding an additional penalty term in the error function that reduces the magnitude of parameters .
- The additional term controls the excessively fluctuating function such that the coefficients don’t take extreme values.
- This technique of keeping a check or reducing the value of error coefficients are called **shrinkage methods**.
- If we have overfitting from our hypothesis function (as shown in Figure 1(d)), we can reduce the weight of some of the terms in our function carry by increasing their cost.

Regularization/ Shrinkage Contd…

- Without actually getting rid of these features or changing the form of our hypothesis, we can instead modify our **cost function**:

$$Cost\ Function = J(\beta_0, \beta_1, \beta_2, \beta_3, \beta_4) + 5000\ \beta_3^2 + 5000\beta_4^2$$

- We've added two extra terms at the end to inflate the cost of β_3 *and* β_4.
- Now, in order for the cost function to get close to zero, we will have to reduce the values of β_3 *and* β_4 to near zero.
- This will in turn greatly reduce the values of β_3 *and* β_4 in our hypothesis function.
- As a result, we see that the new hypothesis (depicted by the pink curve) looks like a quadratic function but fits the data better due to the extra small terms $\beta_3 x^3 + \beta_4\ x^4$



Regularization in Linear Regression

- In regression models, we do not know which regression coefficients we should shrink by adding their penalty in the cost function.
- So, the general tendency of applying regularization in regression is to shrink the weight (regression coefficients) of all the input variables.
- Two most commonly used regularization in linear regression are:

1. Ridge Regression (L2 Normalization)
2. Least Absolute Selection and Shrinkage Operator (LASSO) Regression (L1 Normalization)

Ridge Regression

- Ridge regression performs '**L2 regularization**', i.e. it adds a factor of sum of squares of coefficients in the optimization objective.

- Thus, ridge regression optimizes the following:

$\boldsymbol{Cost\ (Objective) Function = Mean\ Square\ Error +}$ **λ(sum of square of coefficients)**

i.e., $\boldsymbol{J = \frac{1}{2n}\sum_{i=1}^{n}((y_i - \beta_0 - \beta_1 x_{i1} - \beta_2 x_{i2} - \beta_3 x_{i3} - \cdots \ldots \ldots \ldots .. - \beta_k x_{ik})^2 + \lambda \sum_{j=0}^{k} \beta_j^2)}$

where n are the total number of training examples; k are the number of features; β_j represents regression coefficients of jth input variable and λ is the regularization parameter.

Ridge Regression Contd…

λ can take various values:

1. **$\lambda = 0$:**

- The objective becomes same as simple linear regression.
- We'll get the same coefficients as simple linear regression.

2. $\lambda = \infty$:

- The coefficients will be zero.
- Because of infinite weightage on square of coefficients, anything less than zero will make the objective infinite.

3. $0 < \lambda < \infty$:

- The magnitude of α will decide the weightage given to different parts of objective.
- The coefficients will be somewhere between 0 and ones for simple linear regression.

Ridge Regression using Gradient Descent

- We know in gradient descent optimization, we update the regression coefficients as follows:

$$\beta_j = \beta_j - \alpha \frac{\partial(J(\beta))}{\partial \beta_j} \; for \; j = 0,1,2, \dots \dots .. k$$

- For Ridge Regression, cost function is given by:

$$J = \frac{1}{2n} \sum_{i=1}^{n} ((y_i - \beta_0 - \beta_1 x_{i1} - \beta_2 x_{i2} - \beta_3 x_{i3} - \cdots \dots \dots \dots .. -\beta_k x_{ik})^2 + \lambda \sum_{j=0}^{k} \beta_j^2)$$

- The gradient of cost function w.r.t β's is given by:

$$\frac{\partial J}{\partial \beta_0} = \frac{1}{n} \sum_{i=1}^{n} ((\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \cdots \dots \dots \dots .. + \beta_k x_{ik} - y_i) + \lambda \, \beta_0)$$

Ridge Regression using Gradient Descent Contd…

Similarly, $\frac{\partial J}{\partial \beta_1} = \frac{1}{n}\sum_{i=1}^{n}((\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \cdots \ldots \ldots \ldots .. + \beta_k x_{ik} - y_i) \times x_{i1} + \lambda\ \beta_1)$

$$\frac{\partial J}{\partial \beta_2} = \frac{1}{n}\sum_{i=1}^{n}((\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \cdots \ldots \ldots \ldots .. + \beta_k x_{ik} - y_i) \times x_{i1} + + \lambda\ \beta_2)$$

$$\frac{\partial J}{\partial \beta_3} = \frac{1}{n}\sum_{i=1}^{n}((\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \cdots \ldots \ldots \ldots .. + \beta_k x_{ik} - y_i) \times x_{i3} + + \lambda\ \beta_3)$$

$$\vdots$$

In general, $\boldsymbol{\frac{\partial J}{\partial \beta_j} = \frac{1}{n}\sum_{i=1}^{n}((\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \cdots \ldots \ldots \ldots .. + \beta_k x_{ik} - y_i) \times x_{ij} + \lambda\ \beta_j)}$

Ridge Regression using Gradient Descent Contd…

- Therefore, the regression coefficients are updated as:

$$\beta_j = \beta_j - \frac{\alpha}{n}\sum_{i=1}^{n}((\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \cdots \ldots \ldots \ldots .. + \beta_k x_{ik} - y_i) \times x_{ij} + \lambda \beta_j)$$

or $$\boldsymbol{\beta_j} = \boldsymbol{\beta_j}\left(\mathbf{1} - \frac{\boldsymbol{\alpha\lambda}}{\boldsymbol{n}}\right) - \frac{\boldsymbol{\alpha}}{\boldsymbol{n}}\sum_{i=1}^{n}(\boldsymbol{\beta_0} + \boldsymbol{\beta_1 x_{i1}} + \boldsymbol{\beta_2 x_{i2}} + \boldsymbol{\beta_3 x_{i3}} + \cdots \ldots \ldots \ldots .. + \boldsymbol{\beta_k x_{ik}} - \boldsymbol{y_i}) \times \boldsymbol{x_{ij}}$$

Since the factor $\left(\mathbf{1} - \frac{\boldsymbol{\alpha\lambda}}{\boldsymbol{n}}\right)$ is less than 1, therefore, the algorithm, will keep on shrinking the values of the regression coefficients, and will handle the problem of overfitting.

Ridge Regression using Least Square Error Fit

- In least Square error fit, we represent error in matrix form as:

$$\epsilon = y - X\beta$$

- Where $\epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \vdots \\ \epsilon_n \end{bmatrix}$; y= $\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_n \end{bmatrix}$; β $= \begin{bmatrix} \beta_0 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}$

and $X = \begin{bmatrix} 1 & x_{11} & x_{12} \cdots & x_{1k} \\ 1 & x_{21} & x_{22} \cdots & x_{2k} \\ \vdots & \vdots & \vdots \quad \vdots & \vdots \\ 1 & x_{n1} & x_{n2} \cdots & x_{nk} \end{bmatrix}$

$$\boldsymbol{Cost\ (Objective) Function = Mean\ Square\ Error +\ \lambda}\textbf{(sum of square of coefficients)}$$

Ridge Regression using Least Square Error Fit Contd….

$\boldsymbol{Cost\ (Objective) Function = Mean\ Square\ Error +\ \lambda}$**(sum of square of coefficients)**

$$J(\beta) = \frac{1}{2n}\sum_{i=1}^{n}\left(\epsilon_i^2 + \lambda\sum_{j=1}^{k}\beta_j^2\right) = \frac{1}{2n}(\epsilon^T\epsilon + \lambda\beta^T\beta)$$

$$= \frac{1}{2n}((y - X\beta)^T(y - X\beta) + \lambda\beta^T\beta)$$

$$= \frac{1}{2n}((y^T - \beta^T X^T)(y - X\beta) + \lambda\beta^T\beta)$$

$$J(\beta) = \frac{1}{2n}(y^T y - \beta^T X^T y - y^T X\beta + \beta^T X^T X\beta + \lambda\beta^T\ \beta)$$

$$\boldsymbol{J(\beta)} = \frac{1}{2n}\ (\boldsymbol{y^T y} - \boldsymbol{2y^T X\beta} + \boldsymbol{\beta^T X^T} X\beta + \lambda\beta^T\ \beta)$$

[Because $y^T X\beta$ and $\beta^T X^T y$ is always equal with only one entry. The square error function is minimized using **second derivative test**]

Ridge Regression using Least Square Error Fit Contd….

- **Step 1: Compute the partial derivate of J($\boldsymbol{\beta}$) w.r.t $\boldsymbol{\beta}$**

$$\frac{\partial \mathrm{J}(\beta)}{\partial \beta} = \frac{1}{2n}\frac{\partial (y^T y - 2y^T X\beta + \beta^T X^T\, X\beta + \lambda\beta^T\, \beta)}{\partial \beta}$$

$$= \frac{1}{2n} \times \frac{\partial y^T y}{\partial \beta} - \frac{\partial 2y^T X\beta}{\partial \beta} + \frac{\partial \beta^T X^T\, X\beta}{\partial \beta} + \frac{\partial \lambda\beta^T \beta}{\partial \beta}$$

$$= \frac{1}{2n} \times \left(0 - 2X^T y\frac{\partial \beta}{\partial \beta} + \frac{\partial \beta^T X^T\, X\beta}{\partial \beta} + \frac{\partial \lambda\beta^T \beta}{\partial \beta}\right) [Because\ \frac{\partial AX}{\partial X} = A^T]$$

$$= \frac{1}{2n} \times (-2X^T y + 2X^T\, X\beta + 2\lambda I\beta) = -X^T y + X^T\, X\beta + \lambda I\beta$$

$$[Because\ \frac{\partial X^T AX}{\partial X} = 2AX]$$

Ridge Regression using Least Square Error Fit Contd….

- **Step 2: Compute $\boldsymbol{\beta}$ˆ for $\boldsymbol{\beta}$ for which $\frac{\partial \mathbf{J}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \mathbf{0}$**

$$-X^T y + X^T X\beta\hat{} + \lambda I\beta\hat{} = 0$$

$$(X^T X + \lambda I)\beta\hat{} = X^T y$$

$$\boldsymbol{\beta\hat{} = (X^T X + \lambda I)^{-1} X^T y}$$

- **Step 3: Compute $\frac{\partial^2 \mathbf{J}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}^2}$ and prove it to be minimum for $\boldsymbol{\beta}$ˆ**

$$\frac{\partial^2 \mathrm{J}(\beta)}{\partial \beta^2} = \frac{\partial(-X^T y + X^T X\beta + \lambda I\beta)}{\partial \beta} = 0 + 2\, X^T X + \lambda I = +ve\ semi - definite\ matrix$$

- Thus, β is updated as $\beta\hat{} = (X^T X + \lambda I)^{-1} X^T y$. It will solve the problem of overfitting and multicollinearity as $|X^T X + \lambda I|$ will not be zero for correlated features.