Lecture 5: Regression Models

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In this lecture, we discuss regression problems. First, we review the training methods of linear regression models from different perspectives. Then, a basic nonlinear extension idea is introduced, feature mapping, and use it to introduce the first nonlinear regression model, polynomial regression. Afterward, we understand polynomial regression from the perspective of basis functions, and then introduce another commonly used nonlinear model, spline regression. At the end of this lecture, we introduce a new concept, the overfitting problem. It is a core challenge in machine learning from the training perspective, and we focus on it in the next lecture.

1 Linear Regression Model

Unlike classification problems, the target variable in regression is continuous, but it inherits the basic idea of classification problems, which is to predict the target variable using a weighted combination of feature variables, i.e.

$$y = w_0 + w_1 x_1 + \dots w_p x_p + \epsilon$$

where ϵ is a error term. The error term contains many things. It could be measurement errors, or random noise, or all the variations that can not be explained by all the feature variables. For the latest case, it also means we need more feature variables for a better prediction of the target variable.

Obviously, we have to apply some methods (algorithm) to learn the model, i.e. estimate the coefficients $w_0, w_1, \dots, w_p$ from a data set. Here, we mainly discuss two methods, least square methods and maximum likelihood method. Eventually, the two methods are equivalent for a regression problem, however, it is still necessary to explain maximum likelihood method for understanding logistic regression in lecture 7.

1.1 Least Square Method

Least Square method was proposed by the famous mathematician Gauss. He applied this method for data analysis to accurately predict the time of the second appearance of the asteroid, Ceres. His idea is quite simple: to use data to find the optimal line, represented by two coefficients, in order to minimize prediction errors, see the plot below.

Suppose that we have a set of paired observations, $(y_1, x_1), \dots, (y_n, x_n)$, then the mathematical formulation is

$$\hat{w}_0, \hat{w}_1 = \arg\min_{w_0, w_1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

where $\hat{y}_i = w_0 + w_1 x_i$.

The solution of this optimization problem is $\widehat{w}_1 = \frac{\sum_{i=1}^{N}(x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^{N}(x_i - \overline{x})^2}$, and $\widehat{w}_0 = \overline{y} - \widehat{w}_1 \overline{x}$

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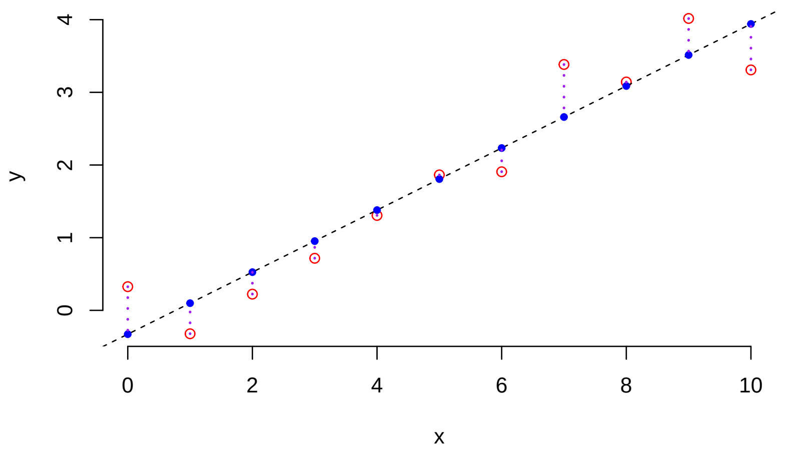


Figure 1: Simple Linear Regression Model: Red circles are observations, Black dashline is the regression model, Blue Dots on the dash line are prediction, the lenght of segment in purple is the prediction error.

1.2 Matrix Form (NE)

When we consider multiple feature variables in a linear regression model, the above calculation formula becomes somewhat cumbersome and inefficient. To compute all the regression coefficients more effectively, we typically need to consider the matrix form of the model. By expressing the linear regression model in matrix form, we can simplify the computation and make it more efficient. The model can be written as:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \epsilon$$

where: - $\mathbf{y}$ is the vector of observed values (target variable), $\mathbf{y} = (y_1, \dots, y_n)^\top$, - $\mathbf{X}$ is the design matrix, which contains the feature variables (including a column of ones for the intercept), i.e.

$$\mathbf{X} = \begin{pmatrix} 1 & x_{1,1} & \cdots & x_{1,p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & \cdots & x_{n,p} \end{pmatrix}$$

- $\mathbf{w}$ is the vector of regression coefficients, $\mathbf{w} = (w_0, w_1, \dots, w_p)^\top$ - $\boldsymbol{\epsilon}$ is the vector of errors, $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_n)^\top$.

To estimate the regression coefficients , we use the least squares method, which minimizes the sum of squared errors. The solution to this optimization problem is:

$$\widehat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$$

This formula provides an efficient way to calculate the coefficients for a linear regression model with multiple features. Using matrix operations not only simplifies the calculations but also allows for faster computation, especially when dealing with large data sets or numerous features. Thus, the matrix form of the model allows for a more streamlined approach to regression analysis, making it easier to implement and compute the necessary coefficients, particularly when working with multiple variables.

1.3 Maximum Likelihood Method

Different from least square method, next, we are going to reexamine the regression model from the perspective of probability models. To do so, we assume the error term ϵ is normally distributed, $\epsilon \sim \mathcal{N}(0, \sigma^2)$. Based on this assumption, the target variable is normally distributed conditional on feature variables. Therefore, we essentially predict the expected value of the target variable conditional on $X_1, \dots, X_p$ as a linear model, i.e.

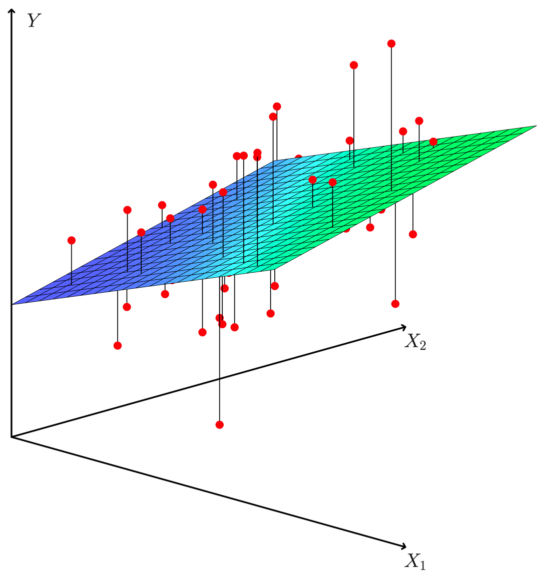


Figure 2: Regression Model: the expected value of target variable is a linear function of X1 and X2

$$\mathrm{E}(Y|X_1, \dots, X_p) = w_0 + w_1 X_1 + w_2 X_2 + \cdots + w_p X_p$$

Based on the normality assumption, another estimation method, MLE, for coefficients can be discussed.

MLE of regression model: Under the normality assumption, we have $y_i \sim \mathcal{N}(w_0 + w_1 x_1, \sigma^2)$. If you remember the secrete message behind the normal distribution, the likelihood of each observation, y_i, is inversely proportionally to the distance to the expected value, i.e.

$$f(y_i|w_0, w_1, \sigma^2) \propto -(y_i - (w_0 + w_1 x_1))^2$$

Therefore the likelihood function of the sample $\{y_i, x_i\}_{i=1}^n$ is

$$\log\left(L(w_0, w_1, \sigma^2|(y_i, x_i))\right) \propto -\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_1))^2$$

Notice that, on the LHS, it is sum square of residual. Therefore, minimize sum square of residuals is equivalent to maximize the log likelihood function. In other words, the two methods are equivalent.

1.4 Model Evaluation

Unlike classification problems, model evaluation for regression problems is quite straightforward. From the purpose of regression, our ultimate goal is to use feature variables to estimate a continuous target variable. A good regression model naturally minimizes prediction error. Therefore, we typically use the mean squared error (MSE) of the model predictions for evaluation. That is

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

where $\hat{y}_i$ is the prediction of the ith case, i.e. $\hat{w}_0 + \hat{w}_1 x_{i,1} + \cdots + \hat{w}_p x_{i,p}$, and therefore $y_i - \hat{y}_i$ is the prediction error of the ith case. To gain a more intuitive understanding, people often use RMSE (Root Mean

Squared Error), i.e. RMSE $= \sqrt{\text{MSE}}$. Sometimes, people also use Mean Absolute Error (MAE) to evaluate a regression model.

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

For all metrics, lower value indicates better model performance.

Quiz: Do you know why we don't use the average errors, i.e. $\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)$ to evaluate a regression model?

Tips: The simplest regression model is $y = w_0 + \epsilon$ and the estimation is $\hat{w}_0 = \bar{y}$, i.e. $\hat{y} = \bar{y}$.

1.5 Loss function

The attentive among you may have noticed that the objective function of the least squares method in regression problems is the same as the model evaluation metric, MSE. From another perspective, we can understand the estimation of regression models as finding a set of regression coefficients that minimize the MSE. In machine learning, estimating regression coefficients is framed as an optimization problem, where MSE is interpreted as the objective function of this optimization problem, also referred to as the model's loss function. For a regression problem, it is called MSE loss:

$$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

For different problem, we could have different loss functions, for example, Huber loss, cross entropy loss, hinge loss. We will explore this further in the lab exercises. This concept, connecting to Maximum Likelihood Estimation, will reappear and be discussed again in the context of logistic regression models.

2 5.2 Nonlinear Regression Models

So far, we have studied two linear models, however, it is by no means enough to solve the problems in reality. For example, the plot below displays a classification problem, and clearly, we cannot find a suitable linear classifier. In other words, we cannot identify a straight line that can divide this 2D feature space in such a way that the two classes of sample points are located on opposite sides of the line. At the same time, through data visualization, we can roughly observe that the boundary between the two classes is an ellipse. Therefore, to address this problem, we must extend our linear model to find a solution.

2.1 5.2.1 Basic ideas of Non-linear Extension

Nonlinear models are not the focus of our course, however, here we can explore the basic approach to finding nonlinear models, that is feature mapping. Feature mapping involves the basic idea of introducing new variables by transforming the original feature variables with functions. This expands the original feature space, allowing the exploration of potential linear solutions within the augmented feature space. Let's start with the toy example of classification problem above.

In the classification problem, we can consider three new variables $\left(h_1 = x_1^2, h_2 = \sqrt{2}x_1x_2, h_3 = x_2^2\right)$ instead of the two original variables x_1, x_2. The new data set is visualized in the following 3D plot.

If you rotate the 3D scatter plot above, you may notice that the same set of observed cases becomes linearly separable in the new feature space, see the LHS of plot below. For example, we can train an LDA classifier using three new feature variables, (h_1, h_2, h_3). The decision boundary of this classifier would correspond to the gray plane in the 3D space. By building the new feature space, the previously non-linearly separable data points may now become linearly separable, allowing the LDA classifier to effectively separate the two

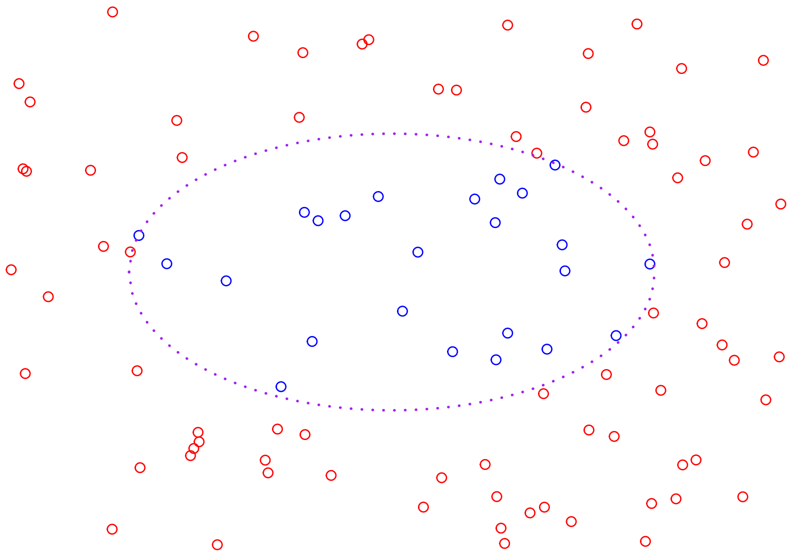


Figure 3: Classification Toy Example

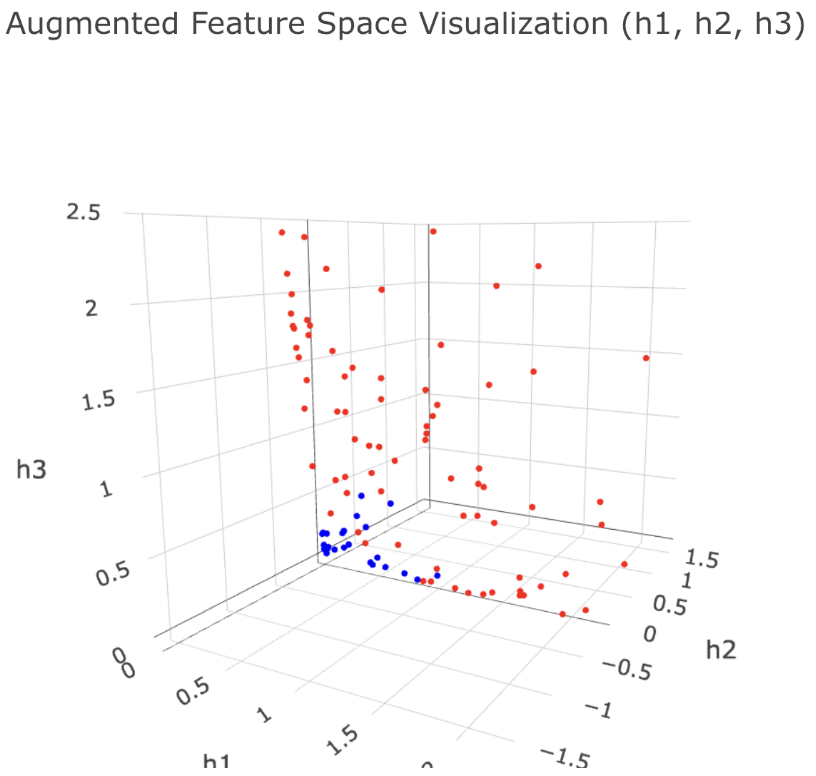


Figure 4: Augmented Feature Space

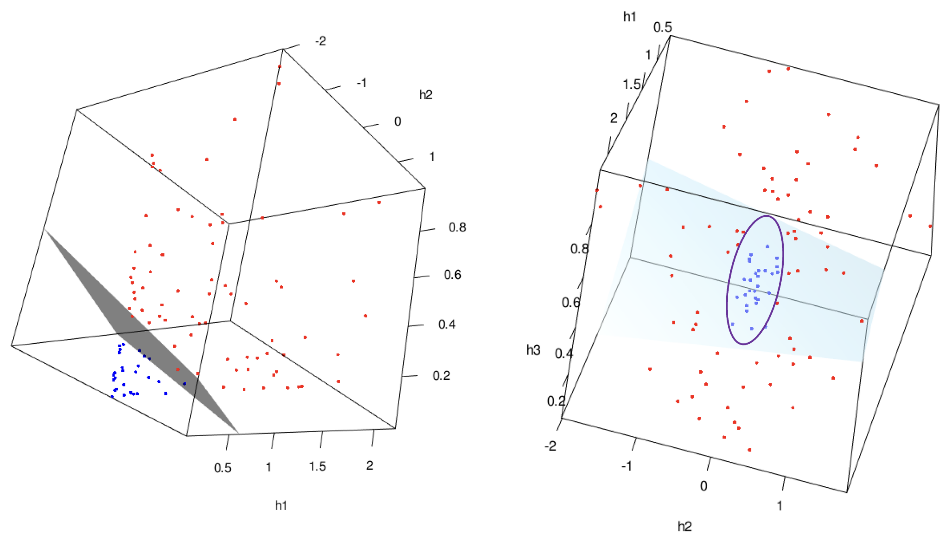


Figure 5: Augmented Feature Space

classes. Also, if we change the direction of our view, the linear model in the augmented feature space is eventually a nonlinear model in the original space, see the LHS of the plots below.

We can refer to this idea as the **feature mapping idea**. In simple terms, we need to find an appropriate new space, which we call the **augmented feature space**, and train our linear model within it. This augmented feature space is entirely determined by a transformation function, $\phi(\mathbf{x})$: p-D space $\rightarrow$ q-D space which we refer to as **feature mappings**.

This concept plays a significant role in machine learning, and almost all advanced nonlinear models are based on this idea. For example:

- Before **deep learning** dominated AI, the **Support Vector Machine (SVM)** applied this idea indirectly through the **kernel function**. The kernel allows the SVM to operate in a higher-dimensional space without explicitly computing the coordinates in that space.
- In the world of **ensemble methods**, which dominate structured data tasks, each **single model** can be seen as a form of feature mapping.
- In the foundation deep learning model, the **neural network**, the chain of transformations through neurons can also be seen as a feature transformation.

This idea of transforming data into a higher-dimensional space (whether directly or indirectly) enables models to handle complex, nonlinear relationships that would otherwise be difficult to capture in the original space.

2.2 5.2.2 Polynomial Regression Model

In this section, we will introduce a nonlinear regression model using the feature mapping idea, specifically focusing on polynomial regression. Let's begin by looking at a simple example.

In this example, we are dealing with a nonlinear regression problem, where the relationship between the feature variable and the target variable is clearly nonlinear. A linear model would not provide satisfactory results because it assumes a straight-line relationship between the features and the target. As you can see, the blue line in the plot, i.e. the simple linear model has totally unacceptable performance on the whole domain. However, by using the feature mapping idea, we can transform the feature space into a higher-dimensional space, where the relationship becomes linear, making it possible to apply linear regression successfully. To

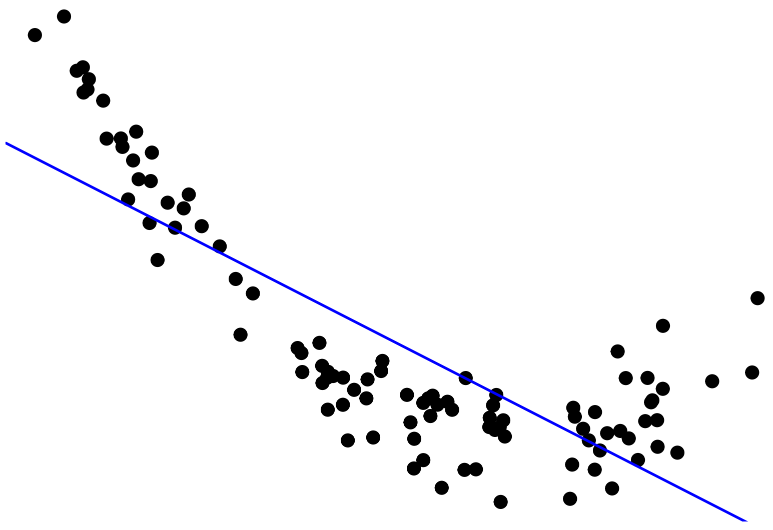


Figure 6: Regression Toy Example

do so, we introduce the augmented feature space by the feature mapping $\phi(x) = (x, x^2)$, i.e. a mapping from 1D to 2D, see the 3D scatter plot below.

You can see that all the points stand on a plane in the augmented space which means that we can find a linear model, i.e.

$$y = w_0 + w_1 x + w_2 x^2,$$

to solve the problem.

Remark: I believe you can see that the choice of feature mapping, $\phi()$, or basis functions, is extremely important. If we choose an inappropriate set of feature mappings, we may end up with very poor results. As shown in the figure below, we apply $\phi(x) = (x, x^5)$ to obtain the augmented feature space, then we eventually switch to another nonlinear problem. In other words, we can't find a plane in the new space such that all the sample points roughly all stand on it. So, we naturally have the following question and we will answer it in the next lecture.

Question: How to choose an appropriate feature mapping?

From another perspective, essentially, our idea in solving the above problem is to use polynomial functions to represent a nonlinear curve and then fit the data with this function. We refer to this regression model as **polynomial regression model**. The generic form of p-th order polynomial regression is

$$y = w_0 + w_1 x + w_2 x^2 + \cdots + w_p x^p + \epsilon$$

2.3 5.2.3 More Options for Basis functions

Basis functions are an essential concept in regression modeling, helping us to represent more complex relationships between the features and the target variable. In addition to polynomial basis functions, which we discussed earlier, there are other types of basis functions, such as **spline basis functions**. They are a set of piecewise polynomial functions used to model non-linear relationships. They are often preferred because they can offer a good balance between flexibility and smoothness. **Cubic splines**, for example, divide the data range into intervals and fit a cubic polynomial to each interval. The key advantage of splines is that they ensure continuity and smooth derivatives at the boundaries between these intervals, preventing abrupt changes in the model's behavior. For spline basis, you are recommended to read the textbook 7.2 to 7.4, and we will also study it through exercises in the Lab.

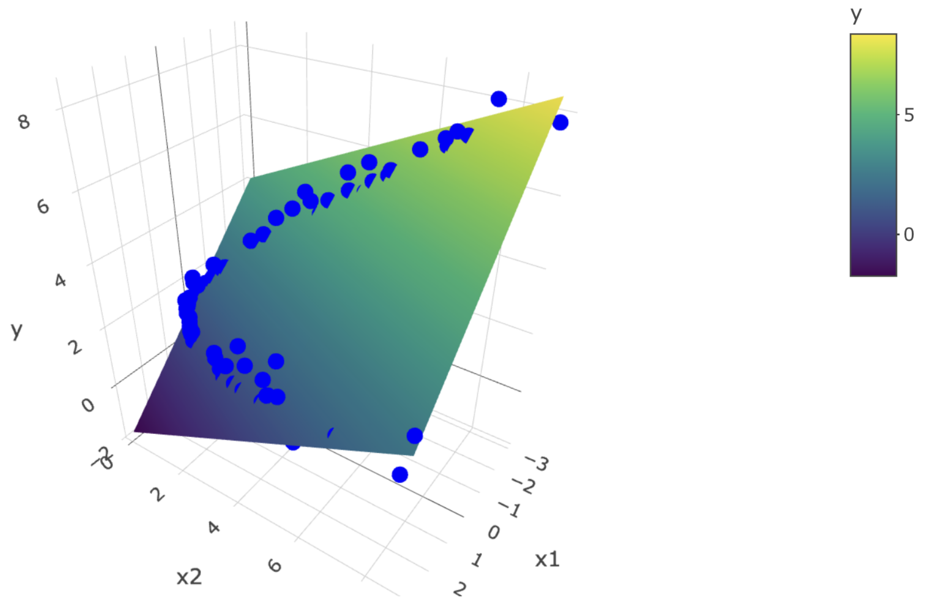


Figure 7: Augmented Feature Space

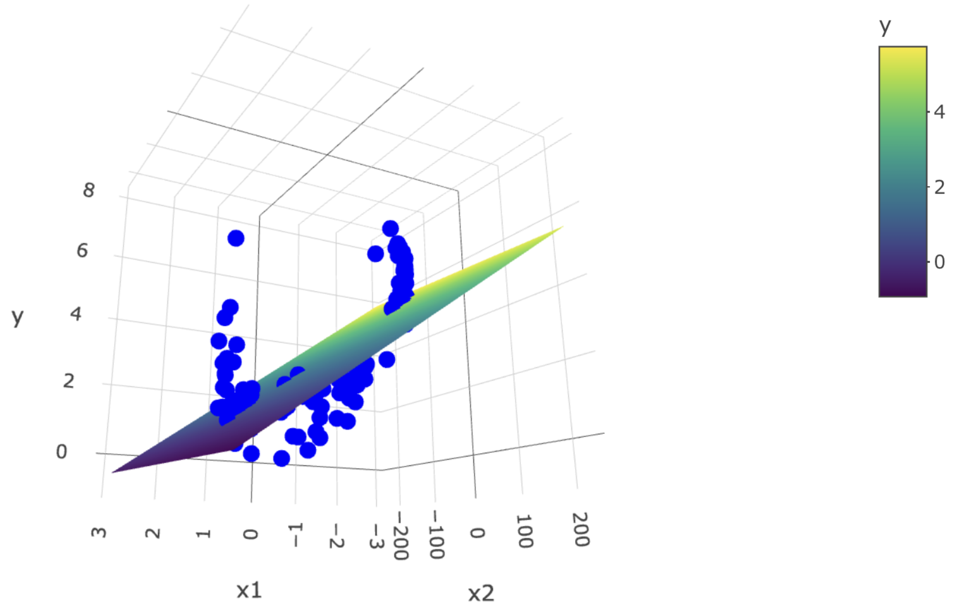
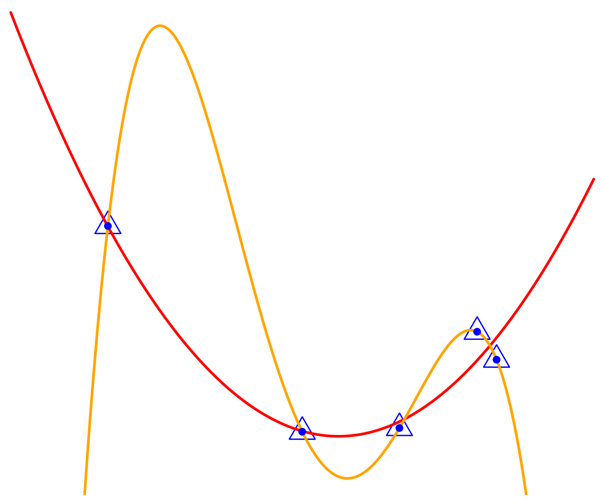


Figure 8: Augmented Feature Space

3 5.3 Over Fitting Problems

With the help of feature mapping or basis functions, it seems like we can achieve anything. It appears that as long as we continuously expand our feature space through feature mapping, we can always find a perfect linear model in a vast augmented feature space to solve the problem. But is it really that simple? Let's take a look at the following example.

3.1 5.3.1 Motivating Examples

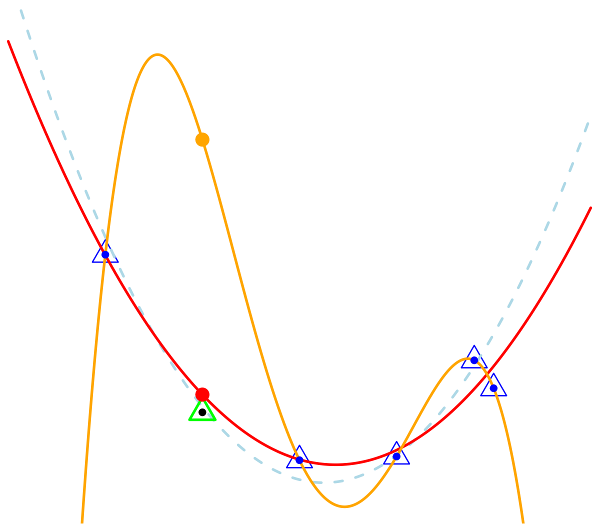


Here we have a set of data (blue triangles), and we want to use the values of the horizontal coordinate X to predict the vertical coordinate Y. There are two candidate models.

- Red model: 2nd-degree polynomial regression, which performs well enough, but makes some errors on the three points on the right side.
- Orange model: 4th-degree polynomial regression, which performs perfectly because it passes exactly through every observation point, meaning it makes no errors at all.

So, the question is, which model do you think is better?

You might like the orange model because it is "perfect." Indeed, people often pursue perfection, but behind perfection often lies a trap. Let me tell you the truth. As shown in the figure below, all the observation points are generated by the light blue dashed line plus a normal noise term. Now, let's generate another observation point, the green triangle. At this point, the red model still performs well, but the prediction of the perfect orange model seems rather absurd.



3.2 5.3.2 Over Fitting

Let's analyze this phenomenon. First, we need to weigh the pros and cons from two aspects, i.e. considering both the performance on the training samples and the testing samples. Therefore, I summarize the analysis of this phenomenon in the table below.

	Orange (4th order)	Red (2nd order)
Training set	Perfect	Good enough
Testing set	Poor	Good
Number of coefficients	5	3
Complexity	Complex	Simple

Training Set Performance

- The **orange model** perfectly fits the training data, capturing every fluctuation in the observations. This is often seen as an indicator of a model that is too complex, as it adjusts to every detail in the data, including noise or outliers.
- On the other hand, the **red model** provides a "good enough" fit. It captures the overall trend of the data without fitting every minor variation, resulting in a simpler and more generalizable model.

Performance on testing set

- When we introduce new observations (those not included in the training set), the **orange model**'s performance drops significantly. Despite its "perfect" fit on the training data, it fails to generalize well to unseen data, indicating that it has overfitted the training set. Overfitting occurs when a model learns not only the true underlying pattern but also random fluctuations or noise in the training data. As a result, the model performs poorly on new, real-world data.
- Conversely, the **red model**, with its simpler structure, generalizes better to new data points. It performs adequately on the training data and maintains reasonable performance on new observations, as it avoids overfitting by not capturing unnecessary complexity.

This phenomenon is called the **overfitting problem**. Simply put, if a model performs "perfectly" on the training samples but fails to generalize to new observations, it means we cannot apply the model for prediction, or in other words, we cannot extend the model to other observations.

Consequences of Overfitting:

- The model becomes overly sensitive to small variations in the training data, which doesn't reflect the true distribution of data in the population.
- It fails to make accurate predictions when new data points are introduced, making it less useful for real-world applications.

So, what causes the overfitting problem? Let me introduce a new concept, model complexity. It refers to how intricate or detailed a model is in terms of its structure and the number of parameters it uses. A more complex model has more parameters or can capture more intricate patterns in the data.

Model Complexity and Overfitting

- The **orange model** has 5 coefficients, making it more complex and prone to overfitting. The extra flexibility allowed by the 4th-order polynomial gives the model the ability to fit noise, leading to poor generalization.
- The **red model**, with only 3 coefficients, is simpler and less likely to overfit. While it may not fit the training data perfectly, its simpler structure helps it to better handle new observations.

Summary: This example demonstrates the classic **overfitting problem**: while complex models (like the orange model) may perform well on the training data, they fail to generalize to new data. Simpler models (like the red model) strike a better balance between fitting the data and maintaining the ability to generalize. This highlights the importance of selecting the appropriate model complexity to ensure that the model performs well not just on the training data, but also in real-world scenarios where new, unseen data is encountered.

3.3 5.3.3 An Analogy for Overfitting

I have had many frustrating experiences assembling IKEA furniture, and one of them is strikingly similar to the overfitting problem in machine learning. Imagine I'm putting together a chair, trying to screw the wooden slats into the metal frame. After tightening the first three screws, I feel like I'm almost done, but when I try to insert the fourth screw, it doesn't fit. I've tightened the first three screws so much that there's no room left to insert the last one.

This situation mirrors the concept of overfitting. By focusing too much on perfectly fitting the training data (the first three screws), I leave no flexibility for new, unseen data (the last screw). The model becomes too rigid, capturing every detail of the training data—just like I over-tightened the first screws—but fails to adapt when it encounters new observations.

3.4 5.3.4 Variance and Bias View

A 2nd-order polynomial regression model exhibits some prediction error for the y values in the training sample, whereas a 4th-order polynomial regression model always predicts the y values perfectly. As a result, the 4th-order model provides highly accurate predictions, while the 2nd-order model performs slightly worse. In statistical terms, the predictions of the 4th-order model have zero bias, whereas the 2nd-order model exhibits some bias.

However, if we repeatedly generate five observations from the light blue model and estimate the regression model each time, we will observe that the 2nd-order model produces very stable predictions. As shown in the figure, all its curves remain approximately within a certain range. In contrast, the 4th-order model

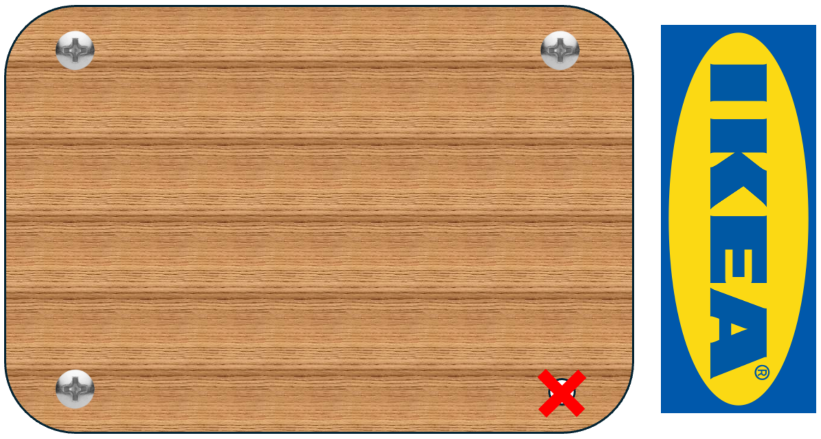


Figure 9: The Pain of Assembling IKEA Furniture: An Analogy for Overfitting

is highly unstable. In statistical terms, the 4th-order model has very high variance, while the variance of the 2nd-order model is much smaller. Therefore, overfitting occurs when the model has low bias and high variance. It fits the training data too closely, including noise, leading to excellent training performance but poor generalization on unseen data. So how can we avoid the overfitting problem? We will discuss this in the next section.

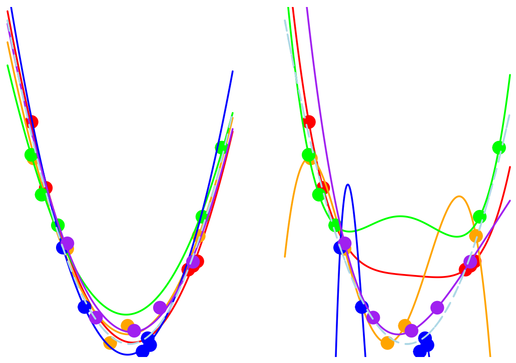


Figure 10: Variance-Bias Tradeoff: We have five sets of data generated by the true model, represented by the light blue dashed line, each shown in a different color. On the left-hand side (LHS), we fit a 2nd-order polynomial regression model to each dataset, while on the right-hand side (RHS), we fit a 4th-order polynomial regression model. As you can see, the fitted models on the LHS are very stable. However, on the RHS, although the models perfectly pass through the observation points, they are extremely unstable.