

Logistic Regression

Mehdi ATTAOUI

Master: Machine Learning and Artificial Intelligence

Faculty of Science, Tetouan

19 December 2024

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1 Introduction to Logistic Regression

1.1 Definition

Logistic regression is a statistical model used to predict the probability that a binary target variable (or a categorical variable with two classes) takes a particular value based on independent variables. Unlike linear regression, which is suited for predicting continuous values, logistic regression is specifically used for classification problems where the target variable is discrete, typically binary.

The fundamental principle of logistic regression is to model the probability that an event belongs to one of the two classes (for example, 0 or 1, or "yes" or "no") based on multiple explanatory variables. The logistic function, also known as the sigmoid function, is used to perform this modeling. It transforms a linear combination of the explanatory variables into a probability between 0 and 1, which allows for classification.

The logistic regression model can be expressed as follows:

$$P(y = 1 | X) = \frac{1}{1 + e^{-Z}}$$

where:

$P(y = 1 | X)$ represents the probability that the event y takes the value 1, given the explanatory variables X .

θ is the vector of coefficients of the model, which are adjusted during training.

\mathbf{X} is the vector of explanatory variables (features).

$\exp(-z)$ is the base of the natural logarithm.

Z represents the dot product of the coefficient vector and the feature vector X plus the Bias

$$Z = \theta^T X + b$$

with:

$$\theta = (\theta_1, \theta_2, \dots, \theta_n), \quad X = (X_1, X_2, \dots, X_n)$$

This sigmoid function,

$$\frac{1}{1 + e^{-z}}$$

where $z = \theta^T X$, ensures that the model output is always between 0 and 1, which is essential for interpretation as a probability.

The goal of the logistic regression algorithm is to determine the coefficients θ that minimize the error between the model's predictions and the observed values in the training data. This is generally achieved through an optimization method, such as gradient descent, which seeks to adjust the parameters to maximize the likelihood of the observed data.

Another important aspect of logistic regression is that the coefficients θ can be interpreted as the effect of each explanatory variable on the probability of belonging to class 1. In particular, the exponent of coefficient θ_j of an explanatory variable X_j represents the factor by which the probability of the event increases when X_j increases by one unit, holding all other factors constant.

Logistic regression is widely used in many fields, including biostatistics (for example, predicting the presence of a disease), marketing (predicting the likelihood that a customer will purchase a product), and finance (predicting credit risk). Its simplicity, efficiency, and the interpretability of its results make it a model of choice for binary classification tasks.

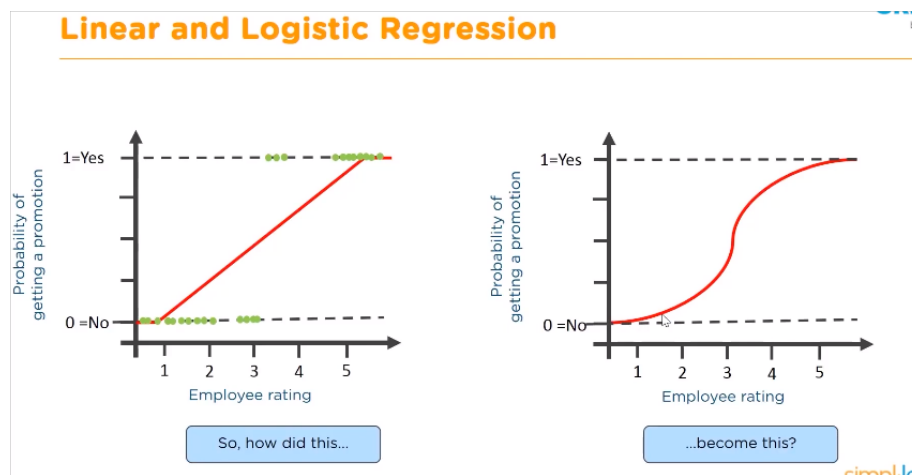
1.2 Linear regression vs logistic regression

Linear regression and logistic regression are fundamental techniques in machine learning and statistics, each serving distinct purposes. Linear regression is primarily used for predicting continuous outcomes, such as house prices, sales revenue, or temperature. It assumes a linear relationship between the input variables and the output and can be expressed as $y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n + \epsilon$, where β_0 is the intercept, β_i are the coefficients, and ϵ is the error term. In contrast, logistic regression is designed for binary classification tasks, where the target variable has two categories (e.g., spam/not spam or diseased/healthy). Logistic regression uses the logistic function to model the probability of a binary outcome. The sigmoid function maps the linear relationship to the range $[0, 1]$, and is defined as $P(y = 1 | X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n)}}$.

Linear regression produces a continuous numerical output, while logistic regression provides probabilities that are typically converted into binary outcomes using a threshold, often set at 0.5. Linear regression minimizes the mean squared error (MSE) as its loss function, which calculates the average squared difference between predicted and actual values. Logistic regression, on the other hand, uses log loss (or binary cross-entropy) as its loss function, which measures the

error in terms of predicted probabilities. Linear regression assumes a linear relationship between variables, normality of residuals, and homoscedasticity, while logistic regression assumes no multicollinearity and a linear relationship between the input variables and the log-odds of the target variable.

Applications of linear regression include predicting stock prices, energy consumption, and other numerical outcomes. Logistic regression is commonly used in classification problems such as fraud detection, disease diagnosis, and spam email detection. Despite their differences, both models are simple, interpretable, and foundational in machine learning, forming the basis for more complex algorithms.



Linear Regression Vs Logistic Regression

1.3 Objectives of Logistic Regression

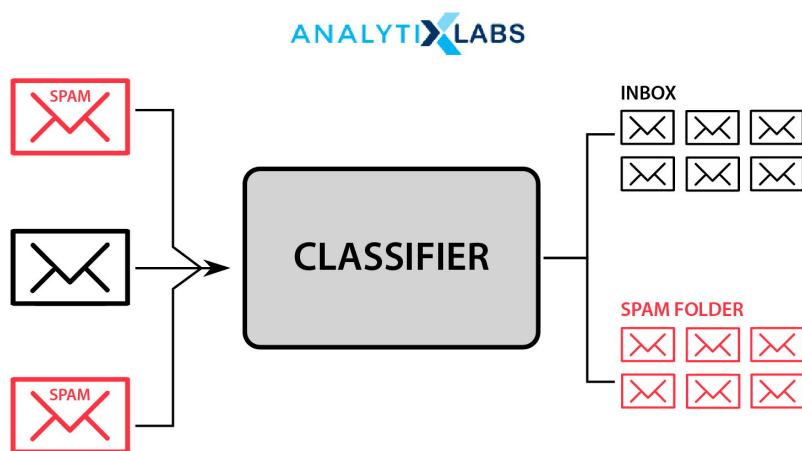
The primary objective of logistic regression is to model the relationship between a set of input features and a binary outcome variable, where the output represents the probability of the occurrence of a specific event. Logistic regression aims to estimate the parameters of a logistic function that maps the input features to probabilities within the range $[0, 1]$. By applying a sigmoid function to the linear combination of the features, the model converts raw predictions into probabilities. These probabilities can then be used for classification by setting a decision threshold, often 0.5, to distinguish between the two classes. Logistic regression also provides insights into the influence of each feature on the outcome through its coefficients, making it both a predictive and interpretable tool. Additionally, it ensures that predictions are probabilistic and interpretable, allowing for applications in areas such as medical diagnosis, risk assessment, and binary decision-making.

2 Mathematical Foundation of Logistic Regression

2.1 Binary Classification and Logistic Regression

2.1.1 What is Classification?

Classification is a supervised learning task in machine learning where the goal is to predict the categorical label of a given input based on its features. In this context, the model learns a mapping from input variables (features) to a discrete output variable (class labels). The primary objective is to assign each data point to one of the predefined classes based on the patterns learned from the training data. Classification problems can be binary, where there are only two possible outcomes, or multiclass, where more than two classes are possible.



Spam Detection Using Classification Algorithm

2.1.2 Linear Discriminant Analysis

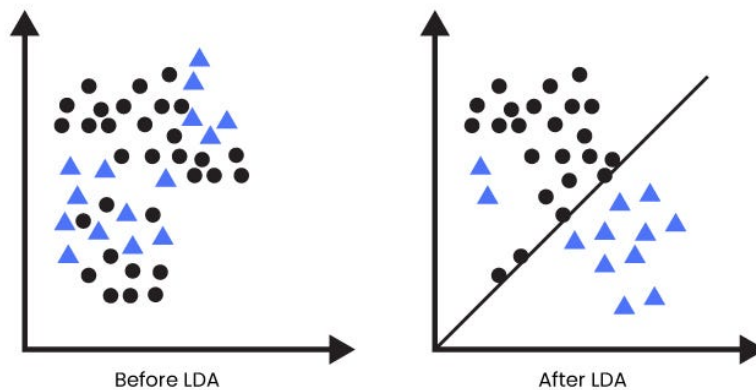
Linear Discriminant Analysis (LDA) is a method used for classification that aims to find a linear combination of features that best separates the classes. It assumes that the data from different classes follow a Gaussian distribution and tries to maximize the distance between class means while minimizing the variance within each class. LDA is effective when the classes are linearly separable.

and the assumptions about the data distribution hold, but it struggles when those assumptions are violated or when the classes are not well separated.

However, LDA has several limitations:

- **Linear Separability:** LDA assumes that the classes are linearly separable. When the data is not linearly separable, LDA's performance can degrade, and it may fail to find an optimal solution.
- **Convergence Issues:** LDA relies on maximizing the likelihood of the data under the assumption of normality and equal covariance matrices. However, if the assumptions are violated, the algorithm may struggle to converge to a meaningful solution, especially in cases with overlapping class distributions.
- **Lack of Probabilistic Interpretation:** LDA does not provide a probabilistic output; it only gives a hard classification decision. This limits the ability to assess the model's confidence in its predictions, which is essential for many applications that require uncertainty quantification.

These limitations highlight the need for more flexible models that can handle non-linearity, provide meaningful probability outputs, and work effectively in situations where the assumptions of LDA do not hold.



Linear Discriminant Analysis (LDA)

2.1.3 The Perceptron

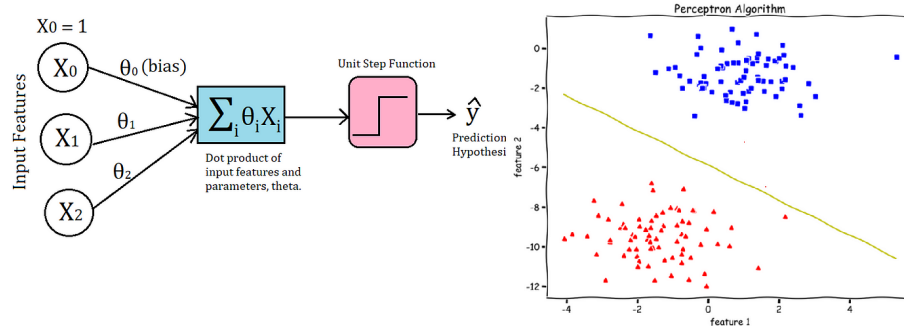
The perceptron is one of the earliest neural network models introduced in the 1950s for binary classification. It uses a linear decision boundary to separate the classes, where the model's parameters (weights) are updated based on the

classification error. While simple and intuitive, the perceptron is limited by its inability to handle non-linear relationships between features and classes. It only works well when the classes are linearly separable, and struggles with more complex decision boundaries.

However, the perceptron has several limitations:

- **Linear Separability:** The perceptron assumes that the classes are linearly separable. If the classes cannot be separated by a straight line (or hyperplane in higher dimensions), the perceptron will fail to find a suitable solution and may never converge.
- **Convergence Issues:** The perceptron algorithm updates the weights based on misclassified examples. If the data is not linearly separable, the algorithm may keep adjusting the weights indefinitely without finding an optimal solution, causing convergence problems.
- **Lack of Probabilistic Interpretation:** The perceptron uses a hard threshold function to classify data points, outputting only binary labels (0 or 1). It does not provide any probabilistic interpretation or measure of certainty, which limits its usefulness when probabilities or confidence levels are required.

These limitations highlight the need for more sophisticated algorithms that can handle non-linearities, ensure convergence, and offer probabilistic outputs for classification tasks.



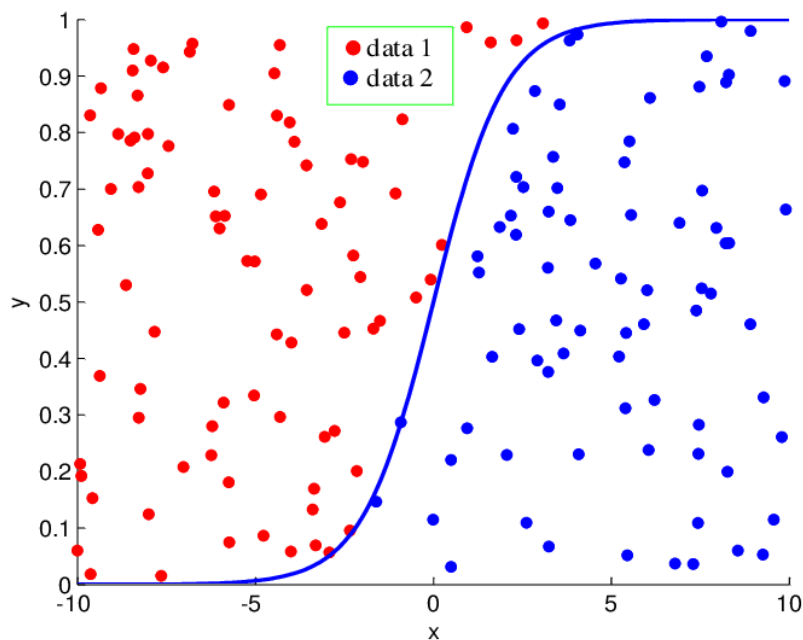
the Perceptron Algorithm for Classification

2.1.4 Why Logistic Regression for Classification ?

Logistic Regression addresses these limitations by providing a more flexible and interpretable framework for binary classification. Unlike the perceptron, logistic regression does not rely on a hard threshold function but instead uses the

sigmoid function, which outputs probabilities between 0 and 1. This allows logistic regression to handle non-linear relationships through the introduction of additional features or transformations.

- **Linear Separability:** Logistic regression still assumes linear separability, but it can work better with non-linearly separable data by employing regularization techniques and mapping data into higher-dimensional spaces (e.g., polynomial features).
- **Convergence Issues:** Logistic regression is optimized using a **likelihood function**, which guarantees convergence to a global optimum when using methods like **gradient descent**. Unlike the perceptron, which may fail to converge with non-linearly separable data, logistic regression will always find the optimal solution that maximizes the likelihood.
- **Probabilistic Interpretation:** One of the key advantages of logistic regression is its ability to provide a probabilistic interpretation of the output. Instead of making a hard decision, it estimates the probability of a data point belonging to a certain class, allowing for more nuanced predictions and uncertainty quantification.



Binary Logistic Regression

2.2 The Sigmoid Function

2.2.1 Definition

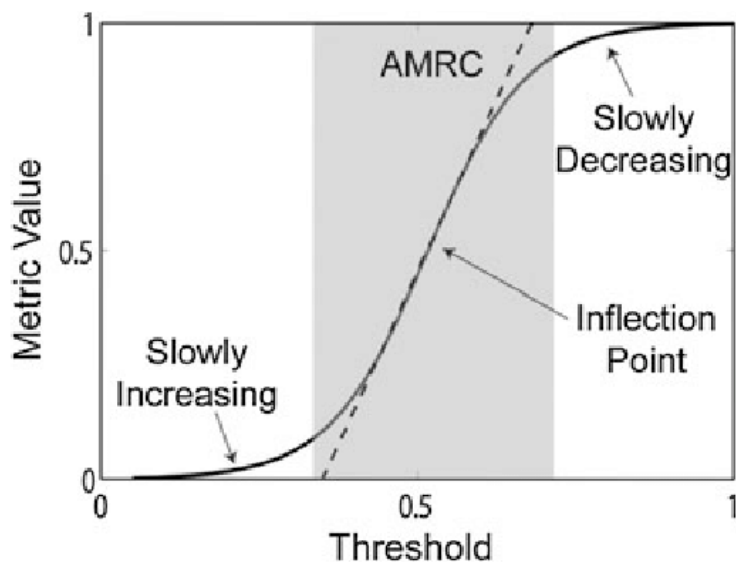
The sigmoid function, also known as the logistic function, is a mathematical function commonly used in machine learning and statistics, particularly for binary classification tasks. It maps any real-valued input into a value between 0 and 1, making it suitable for modeling probabilities.

Mathematically, the sigmoid function is defined as:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

where:

- $\sigma(x)$ is the output of the sigmoid function, a value between 0 and 1.
- x is the input to the function, typically a linear combination of features (i.e., $x = \beta_0 + \beta_1x_1 + \beta_2x_2 + \dots + \beta_nx_n$ in logistic regression).
- e is the base of the natural logarithm (approximately 2.718).



Sigmoid Function

2.2.2 Mathematical Properties

- **Symmetry:** The sigmoid function is *symmetric* about the point $x = 0$. Specifically, the function satisfies the relationship $\sigma(-x) = 1 - \sigma(x)$. This symmetry means that if the input to the function is negative, the output is complementary to the output for the positive input, making the sigmoid well-suited for modeling binary outcomes (e.g., class 0 or class 1).
- **Derivative:** The derivative of the sigmoid function is crucial for optimization algorithms, particularly gradient descent. It is given by:

$$\sigma'(x) = \sigma(x)(1 - \sigma(x))$$

This property shows that the rate of change of the sigmoid function at any point is directly related to the output of the function. The derivative is largest when $\sigma(x) = 0.5$, and it decreases as the output approaches 0 or 1.

- **Monotonicity:** The sigmoid function is *monotonically increasing*, meaning it consistently rises as x increases. As x becomes more negative, the output approaches 0, and as x becomes more positive, the output approaches 1. This behavior ensures that the sigmoid function always moves in the same direction, making it suitable for classification tasks.
- **Concavity and Convexity:**

The **concavity and convexity** of the sigmoid function are important properties that help understand its behavior and how it changes as the input x varies.

- **Concave Down for Positive x :** For values of $x > 0$, the sigmoid function is concave down, meaning that its second derivative is negative. This indicates that the function's rate of change is slowing down as x increases. The function is not increasing as rapidly when x is large and positive. To understand why, consider the behavior of the sigmoid function when x is large. As x grows, $\sigma(x)$ approaches 1, but the rate at which this happens diminishes, making the curve flatten out. This is a result of the decreasing slope, indicating diminishing returns from increasing x .
- **Convex Up for Negative x :** For values of $x < 0$, the sigmoid function is convex up, meaning that its second derivative is positive. In this region, as x becomes more negative, the function increases more rapidly. The curve steepens, reflecting a faster rate of change of the function as x approaches zero. This convexity happens because the sigmoid function moves toward 0 at an increasing rate as x becomes more negative.
- **Inflection Point:** The transition from concave to convex occurs at the inflection point, which happens at $x = 0$. At this point,

the sigmoid function changes from increasing at a diminishing rate (concave down) to increasing at an accelerating rate (convex up). The inflection point corresponds to the value where the function's rate of change is the greatest, and the slope is $\frac{1}{4}$ (this is derived from the derivative formula).

- **Local and Global Minima:** The sigmoid function is globally smooth, continuous, and differentiable, and its behavior shows no local minima or maxima within its domain. The function has no **local minima** or **local maxima** because it is monotonic. It steadily increases from 0 to 1 as x moves from negative to positive infinity. There is only one **global minimum** at $x \rightarrow -\infty$, where $\sigma(x)$ approaches 0, and one **global maximum** at $x \rightarrow +\infty$, where $\sigma(x)$ approaches 1. The absence of local minima or maxima means that the sigmoid function does not have turning points that can be confused with local optima. This is important when using the sigmoid function in optimization algorithms like gradient descent, as it ensures the optimization process converges in a predictable manner without the risk of getting stuck in local optima.

The **concavity and convexity** of the sigmoid function are important properties that help understand its behavior and how it changes as the input x varies.

To prove concavity and convexity, we first calculate the first and second derivatives of the sigmoid function.

First Derivative

The sigmoid function is defined as:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

To compute the first derivative, we apply the chain rule. Let $u = e^{-x}$, so $\sigma(x) = \frac{1}{1+u}$.

Now, differentiate $\sigma(x)$ with respect to x :

$$\begin{aligned} \frac{d\sigma(x)}{dx} &= -\frac{1}{(1+u)^2} \cdot \frac{d}{dx}(1+u) \\ &= -\frac{1}{(1+e^{-x})^2} \cdot (-e^{-x}) \\ &= \frac{e^{-x}}{(1+e^{-x})^2} \end{aligned}$$

This can be rewritten as:

$$\sigma'(x) = \sigma(x)(1 - \sigma(x))$$

Second Derivative

Next, we calculate the second derivative to analyze the convexity and concavity. Differentiate $\sigma'(x) = \sigma(x)(1 - \sigma(x))$ using the product rule:

$$\begin{aligned}\sigma''(x) &= \frac{d}{dx} [\sigma(x)(1 - \sigma(x))] \\ &= \sigma'(x)(1 - \sigma(x)) + \sigma(x)(-\sigma'(x))\end{aligned}$$

Substitute $\sigma'(x) = \sigma(x)(1 - \sigma(x))$ into this:

$$\begin{aligned}\sigma''(x) &= \sigma(x)(1 - \sigma(x))(1 - \sigma(x)) - \sigma(x)\sigma(x)(1 - \sigma(x)) \\ &= \sigma(x)(1 - \sigma(x)) [(1 - \sigma(x)) - \sigma(x)] \\ &= \sigma(x)(1 - \sigma(x))(1 - 2\sigma(x))\end{aligned}$$

Proof of Concavity and Convexity

- ****Concave Down for Positive x ****: For values of $x > 0$, the second derivative $\sigma''(x) = \sigma(x)(1 - \sigma(x))(1 - 2\sigma(x))$ is negative. This means the sigmoid function is concave down for positive x . Specifically, for $\sigma(x)$ to be less than 0.5, $1 - 2\sigma(x)$ is negative, leading to a negative second derivative.

- ****Convex Up for Negative x ****: For values of $x < 0$, the second derivative $\sigma''(x)$ is positive. In this region, $\sigma(x)$ is greater than 0.5, and $1 - 2\sigma(x)$ is positive, making the second derivative positive, so the function is convex up.

- ****Inflection Point****: The transition from concave to convex occurs at the inflection point, which happens at $x = 0$. At this point, the second derivative $\sigma''(x) = 0$, and the rate of change of the sigmoid function switches from slowing down to accelerating. The inflection point corresponds to $\sigma(x) = 0.5$, where the function's rate of change is maximal.

In summary, the concavity and convexity of the sigmoid function reflect the way the output changes as x increases or decreases. These properties are important when analyzing the behavior of models that use the sigmoid, particularly in logistic regression where the goal is to predict probabilities. The lack of local minima or maxima ensures that optimization algorithms can efficiently find the global solution.

2.2.3 Why the Sigmoid Function is Important in Logistic Regression

The sigmoid function plays a crucial role in logistic regression, which is one of the most commonly used methods in machine learning for binary classification tasks. Logistic regression aims to model the probability that a given input belongs to one of two classes, and the sigmoid function is central to achieving this objective. Let's explore in detail why the sigmoid

function is important in logistic regression.

1. Mapping Linear Predictions to Probabilities

One of the core challenges in classification tasks is to transform a linear model (which produces real-valued outputs) into a probabilistic interpretation (values between 0 and 1). In logistic regression, we use the sigmoid function to map the output of a linear equation to a probability that is easy to interpret.

Consider a typical logistic regression model where the input features x_1, x_2, \dots, x_n are linearly combined with weights $\beta_1, \beta_2, \dots, \beta_n$, and an intercept β_0 . The model computes a linear prediction:

$$z = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$

This linear combination, z , can take any real value, ranging from $-\infty$ to $+\infty$. However, we need to convert this into a value between 0 and 1, representing the probability that the instance belongs to a certain class (say, class 1). The sigmoid function provides a smooth transformation from real-valued inputs to outputs in the desired range:

$$P(y = 1 \mid x) = \sigma(z) = \frac{1}{1 + e^{-z}}$$

Here, $P(y = 1 \mid x)$ is the probability that the instance belongs to class 1, given the input features x , and $\sigma(z)$ is the sigmoid function applied to the linear model's output z . The sigmoid function ensures that this probability is always between 0 and 1.

2. Probabilistic Interpretation of Classification

The output of the sigmoid function is interpreted as the probability that a given input belongs to class 1. Specifically:

- If $\sigma(z)$ is close to 1, the model predicts that the input is more likely to belong to class 1.
- If $\sigma(z)$ is close to 0, the model predicts that the input is more likely to belong to class 0.
- If $\sigma(z) = 0.5$, the model is uncertain and assigns equal probability to both classes.

This probabilistic output allows logistic regression to quantify uncertainty in its predictions, which is important for decision-making in real-world applications where confidence in a prediction matters. For example, in medical diagnosis, a model might predict the probability of a patient having a disease, and decisions can be made based on that probability.

3. Decision Boundary and Thresholding

Logistic regression often involves making a hard classification decision based on the probability predicted by the sigmoid function. By

setting a threshold (typically 0.5), we can decide whether to classify a given input as belonging to class 1 or class 0.

For example:

- If $P(y = 1 | x) \geq 0.5$, predict class 1.
- If $P(y = 1 | x) < 0.5$, predict class 0.

The threshold at 0.5 corresponds to the point where the model is equally likely to assign the instance to either class. The sigmoid function allows us to interpret the raw output of the linear model z in a way that is meaningful for classification, with the threshold representing the point where we are most uncertain.

4. Smooth and Differentiable Nature

The sigmoid function is smooth and differentiable, which makes it ideal for optimization algorithms such as gradient descent. Gradient descent is commonly used in logistic regression to find the optimal values for the model parameters $\beta_0, \beta_1, \dots, \beta_n$ by minimizing a loss function (typically the log-likelihood or cross-entropy loss).

The smoothness and differentiability of the sigmoid function allow for efficient computation of the gradient (derivative) at each step of the optimization process. This ensures that the algorithm can make incremental updates to the model parameters to gradually improve the model's performance. The logistic regression model's ability to smoothly transition between 0 and 1 makes the optimization process more stable and efficient.

2.3 Likelihood Function and Model Fitting

2.3.1 Introduction to Likelihood Functions

- **Definition of Likelihood Function:** The likelihood function represents the probability of observing the given data under different values of the model parameters. For a logistic regression model, it describes the probability of the observed binary outcomes as a function of the model's parameters.
- **Connection Between Likelihood and Probability:** In classical statistics, likelihood is similar to probability but is viewed in reverse: given the data, we seek to find the most likely model parameters. While probability asks about the chance of observing an event given a model, likelihood asks about the probability of the model parameters given the data.
- **Importance in Parameter Estimation:** Likelihood is crucial because it forms the basis of Maximum Likelihood Estimation (MLE), the standard approach for fitting logistic regression models. MLE seeks to maximize the likelihood function to find parameter estimates that best explain the observed data.

2.3.2 Maximum Likelihood Estimation (MLE)

- **Concept of MLE in Logistic Regression:** MLE is a method used to estimate the parameters of the logistic regression model. It selects the values for the model parameters that maximize the likelihood of observing the data. In logistic regression, the parameters are the weights (or coefficients) of the features.
- **Deriving the Likelihood Function for Logistic Regression:** In logistic regression, the likelihood function is based on the Bernoulli distribution. If we denote y_i as the binary response for the i -th observation, and \hat{p}_i as the predicted probability for the i -th observation, the likelihood function $L(\theta)$ is:

$$L(\theta) = \prod_{i=1}^n \hat{p}_i^{y_i} (1 - \hat{p}_i)^{1-y_i}$$

Where $\hat{p}_i = \frac{1}{1+e^{-(X_i\theta)}}$, and X_i represents the feature vector for the i -th observation.

- **Log-Likelihood Function:** Taking the natural logarithm of the likelihood function simplifies the calculations, and the log-likelihood function for logistic regression is:

$$\log L(\theta) = \sum_{i=1}^n [y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i)]$$

- **Simplification Using the Log-Likelihood:** The log-likelihood simplifies the product of probabilities into a sum, making optimization more computationally feasible. Log-likelihood is also easier to handle analytically, especially when applying gradient-based optimization methods.
- **Properties of MLE (Consistency, Efficiency, etc.):** MLE estimators are consistent (they converge to the true parameter values as the sample size increases) and asymptotically efficient (they achieve the lowest possible variance among all unbiased estimators in large samples).

In logistic regression, the log-likelihood function measures how well the model explains the observed data, with values typically ranging from $-\infty$ to positive values. A higher log-likelihood (closer to 0) indicates that the model assigns high probabilities to the observed outcomes, reflecting a better fit. Conversely, a log-likelihood approaching $-\infty$ suggests poor model performance, as it corresponds to low probabilities assigned to the observed data. During training, the objective of logistic regression is to maximize the log-likelihood, ensuring the model parameters are adjusted to achieve the best possible fit to the data.

2.4 The Cost Function

The cost function in logistic regression is a measure of how well the model's predictions align with the actual data. It is designed to quantify the difference between the predicted outcomes (based on the model's parameters) and the actual outcomes. The most commonly used cost function in logistic regression is the *log-loss* (or cross-entropy) function, which is derived from the log-likelihood. The log-loss function penalizes incorrect predictions more heavily, especially when the model is confident but wrong. It is expressed as:

$$J(\theta) = -\frac{1}{n} \sum_{i=1}^n [y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i)]$$

where \hat{p}_i is the predicted probability for the i -th observation, and y_i is the actual binary outcome. The cost function is minimized using optimization algorithms such as gradient descent, where the goal is to find the parameters θ that reduce the cost function, thus improving the model's accuracy. A smaller value of the cost function corresponds to better model performance, as it indicates that the model's predictions are closer to the true values. In summary, the cost function in logistic regression helps guide the optimization process by quantifying the error between predicted and actual outcomes, and minimizing it results in a more accurate model.

2.5 Optimization Through Stochastic Gradient Descent

Stochastic Gradient Descent (SGD) is one of the most widely used optimization algorithms in machine learning, particularly for minimizing a cost function in models such as linear regression, logistic regression, and neural networks. The core idea of stochastic gradient descent is to adjust the parameters (weights) of a model iteratively in order to minimize a given objective function, typically the cost function or loss function. Unlike traditional gradient descent, which uses the entire dataset to compute the gradient, SGD updates the parameters using a **single training example** (or a small mini-batch) at each iteration. This makes the optimization process faster but more stochastic and noisy.

In machine learning, we aim to find the model parameters θ that minimize a cost function $J(\theta)$. The cost function quantifies how well the model's predictions match the actual data, and minimizing it means improving the model's performance. In SGD, the gradient of the cost function is calculated for each randomly selected data point (or mini-batch) and used to update the parameters iteratively.

At each step of the optimization, we compute the gradient of the cost function with respect to the parameters and update the parameters in the

direction that reduces the function's value most quickly. This direction is determined by the gradient at the specific data point used in the current iteration. While SGD introduces more variability in the parameter updates due to its use of a single example, this noisy update can help escape local minima and speed up convergence, especially in large datasets or complex models like neural networks.

Stochastic Gradient and Direction of Descent (SGD)

In Stochastic Gradient Descent, the gradient of the cost function is computed using a **single training example** (or a small batch of examples) at each iteration, rather than the entire dataset. The gradient is a vector of partial derivatives that indicates the rate of change of the function with respect to each parameter. In stochastic gradient descent, we calculate the gradient of the cost function $J(\theta)$ with respect to the model's parameters using just one data point:

$$\nabla_{\theta} J(\theta) = \left[\frac{\partial J(\theta)}{\partial \theta_1}, \frac{\partial J(\theta)}{\partial \theta_2}, \dots, \frac{\partial J(\theta)}{\partial \theta_n} \right] \quad \text{for a randomly selected data point.}$$

This approximation of the gradient, using only a single data point, leads to more frequent updates and can cause the algorithm to fluctuate more compared to batch gradient descent. However, this stochastic nature can also help escape local minima and lead to faster convergence in some cases.

Parameter Update Rule (SGD)

In each iteration, Stochastic Gradient Descent updates the parameters θ using the following formula:

$$\theta_j := \theta_j - \alpha \frac{\partial J(\theta)}{\partial \theta_j} \quad \text{for a randomly chosen training example.}$$

Where:

- θ_j is the j -th model parameter (e.g., weight in logistic regression).
- α is the learning rate, a hyperparameter that controls the step size in the direction of the gradient.
- $\frac{\partial J(\theta)}{\partial \theta_j}$ is the partial derivative of the cost function with respect to the parameter θ_j , computed using a single data point (or mini-batch).

Since updates are made after evaluating just one (or a few) data point(s), SGD tends to have noisy updates compared to batch gradient descent, but it can lead to faster learning.

Iterative Process (SGD)

Stochastic Gradient Descent is an iterative algorithm, meaning the parameter updates happen over multiple steps (iterations). In each iteration, the model parameters are adjusted based on the gradient calculated from a single data point (or mini-batch), and this process continues until the parameters converge to the optimal values or the change in the cost function becomes sufficiently small.

Unlike in batch gradient descent, where the parameters are updated after processing the entire dataset, SGD updates the parameters much more frequently (after each training example), which can lead to faster convergence but also more fluctuation in the path toward convergence.

Key Differences Between Gradient Descent and Stochastic Gradient Descent:

- **Data used for updates:**
 - * **Gradient Descent:** Uses the entire dataset to compute the gradient.
 - * **Stochastic Gradient Descent:** Uses one data point (or mini-batch) at a time.
- **Convergence:**
 - * **Gradient Descent:** Provides smoother convergence, as it uses the full dataset to compute the gradient.
 - * **Stochastic Gradient Descent:** Leads to noisier updates and more fluctuations, but it can escape local minima and converge faster in practice.
- **Computation Time:**
 - * **Gradient Descent:** Requires more computation per iteration as it computes the gradient over the entire dataset.
 - * **Stochastic Gradient Descent:** Requires less computation per iteration since it only processes a single or few examples.

3 Real-World Applications of Logistic Regression

3.1 Medical Diagnosis

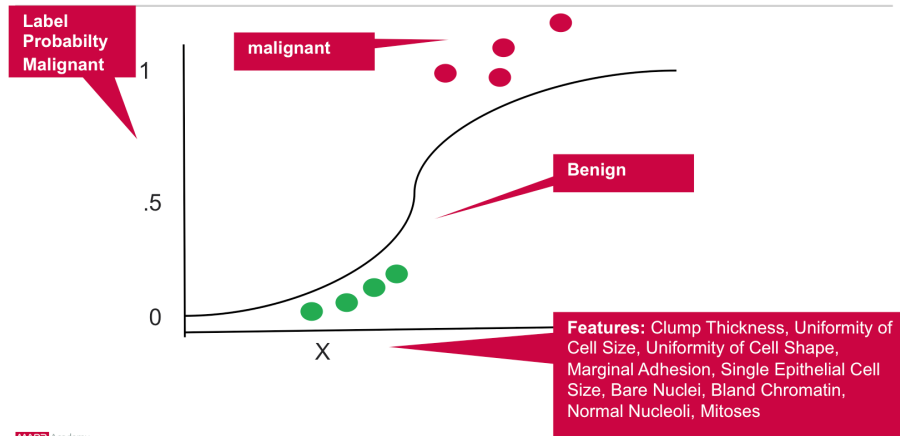
Logistic regression plays a critical role in medical diagnostics, particularly in predicting the likelihood of diseases based on various factors. It is widely used in fields like oncology, cardiology, and epidemiology to predict binary outcomes such as whether a patient has a disease (e.g., cancer, diabetes) or not.

Real-Life Example: Breast Cancer Prediction

In medical research, logistic regression can be used to predict whether a patient has breast cancer based on factors like age, tumor size, and results from diagnostic tests. One widely used dataset for this purpose is the *Wisconsin Breast Cancer Dataset*, which includes patient information such as:

- **Features:**
 - * Radius of the tumor
 - * Texture of the tumor
 - * Perimeter of the tumor
 - * Area of the tumor
 - * Smoothness of the tumor surface
 - * Compactness of the tumor
 - * Concavity
 - * Symmetry
 - * Fractal dimension of the tumor
- **Target Variable:**
 - * 0: Benign (No cancer)
 - * 1: Malignant (Cancer present)

Breast Cancer Logistic Regression Example



Binary Logistic Regression

By using logistic regression, researchers can predict the likelihood of a tumor being benign or malignant based on these features. For example, if a patient has a tumor with a high perimeter, large area, and high compactness, logistic regression could predict a high probability that the tumor is malignant.

3.2 Credit Scoring and Risk Assessment

In finance, logistic regression is often used to assess the creditworthiness of loan applicants and predict the likelihood of default. This application is critical for banks and lending institutions to make informed decisions about issuing loans.

Real-Life Example: Credit Scoring Model

Consider a *Credit Scoring Dataset*, where the goal is to predict whether a person will default on a loan. The dataset might include the following features:

- **Features:**
 - Age
 - Income
 - Loan amount
 - Employment status (Employed/Unemployed)
 - Credit score (e.g., FICO score)
 - Debt-to-income ratio
 - Previous default history (Yes/No)
 - Marital status

- **Target Variable:**

- 0: No default
- 1: Default

Using logistic regression, a bank can calculate the probability that a person will default on a loan based on these factors. For instance, a logistic regression model might find that the probability of default increases significantly if a person has a high debt-to-income ratio or a low credit score. A potential application of the model would be to determine whether to approve a loan application, where the model's output could be used as a threshold for approval (e.g., if the probability of default is less than 0.4, the loan is approved).

3.3 Marketing and Customer Segmentation

Logistic regression is used extensively in marketing to understand customer behavior and improve marketing strategies. It helps companies predict customer actions, such as purchasing a product, clicking on an advertisement, or subscribing to a service.

Real-Life Example: Predicting Customer Purchase Behavior

Consider a *Customer Purchase Behavior Dataset*, where the goal is to predict whether a customer will purchase a product based on certain demographic and behavioral characteristics. The dataset might include:

- **Features:**

- Age
- Gender
- Income level
- Past purchase history (e.g., frequency of purchases)
- Engagement with marketing campaigns (e.g., email opens, ad clicks)
- Product category preferences (e.g., electronics, clothing)

- **Target Variable:**

- 0: No purchase
- 1: Purchase

Customer Segmentation Example:

Companies can also use logistic regression for customer segmentation by creating multiple models to identify distinct customer groups. For example, a retailer

could use logistic regression to classify customers into high-value and low-value segments based on their likelihood to make purchases. These models can be trained on features like average order value, frequency of purchases, and product preferences. With this data, the company can tailor marketing efforts, discounts, and product recommendations based on the characteristics of each segment.

Logistic regression can be used to predict the probability of a customer making a purchase based on these features. For instance, if a customer is young, has a high income, and frequently clicks on marketing emails, logistic regression may predict a high probability that the customer will make a purchase. This information can help companies target their marketing efforts more effectively by focusing on high-probability customers and personalizing campaigns.

4 Disadvantages of Logistic Regression

4.1 Limited to Linear Boundaries

- **Explanation:** Logistic regression assumes a linear relationship between the independent variables and the log-odds of the dependent variable. This can limit its applicability in cases where the true decision boundary is nonlinear.
- **Example:** If the data has a circular or complex decision boundary, logistic regression will struggle to classify it accurately.
- **Mitigation:** Use techniques like feature engineering, kernel methods, or switch to more advanced models like support vector machines (SVMs) or neural networks.

4.2 Sensitive to Outliers

- **Explanation:** Logistic regression is sensitive to extreme values or outliers in the independent variables, as they can disproportionately affect the coefficients.
- **Example:** A single extreme data point can skew the logistic function and lead to incorrect predictions.
- **Mitigation:** Use robust scaling techniques (like MinMaxScaler or RobustScaler) to identify and remove outliers using methods like the IQR rule.

4.3 Requires Large Sample Size

- **Explanation:** Logistic regression requires a large number of samples to estimate coefficients accurately, especially when there are many independent variables.
- **Example:** If there are too few observations relative to the number of predictors, logistic regression can overfit or fail to converge.
- **Mitigation:** Collect more data, reduce the dimensionality of the data (using PCA, for example), or consider regularization methods like L1 (Lasso) or L2 (Ridge) penalties.

4.4 Feature Independence Assumption

- **Explanation:** Logistic regression assumes that independent variables are not highly correlated with each other (no multicollinearity).
- **Example:** If two predictors are strongly correlated, it can distort the estimated coefficients, leading to unreliable results.
- **Mitigation:** Check for multicollinearity using Variance Inflation Factor (VIF) and remove or combine correlated features.

4.5 Limited to Binary Classification (in Base Form)

- **Explanation:** Standard logistic regression is inherently a binary classifier, making it less effective for multi-class problems.
- **Example:** For a problem with three classes (A, B, and C), logistic regression must be extended to support multi-class classification.
- **Mitigation:** Use one-vs-all (OvA) or one-vs-one (OvO) schemes, or use models like multinomial logistic regression, decision trees, or neural networks.

4.6 Lack of Interpretability with High-Dimensional Data

- **Explanation:** As the number of features grows, it becomes difficult to interpret the relationship between individual predictors and the outcome.
- **Example:** In natural language processing (NLP) with thousands of features (words), interpreting each feature's contribution is nearly impossible.
- **Mitigation:** Use dimensionality reduction techniques (like PCA) or choose models with better interpretability (like decision trees or rule-based classifiers).

4.7 Overfitting on Noisy Data

- **Explanation:** Logistic regression can overfit if there are too many predictors relative to the number of observations or if the data contains noise.
- **Example:** If many irrelevant features are included, logistic regression can "memorize" the training data.
- **Mitigation:** Use regularization (L1 or L2), reduce dimensionality, or apply feature selection techniques.

5 Extensions of Logistic Regression

5.1 Multinomial Logistic Regression

Multinomial Logistic Regression is a generalization of binary logistic regression used when the dependent variable has more than two categorical outcomes. Unlike binary logistic regression, which predicts the probability of one of two possible outcomes, multinomial logistic regression predicts the probabilities of each of the multiple possible outcomes of a categorical dependent variable. This method is commonly used in fields like machine learning, healthcare, and social sciences to classify observations into one of several classes.

To understand the mathematical formulation, let's denote the dependent variable Y as a categorical variable that takes values from the set $\{1, 2, \dots, K\}$, where K is the total number of possible categories. For each observation i , we have a feature vector $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T$, where p is the number of predictors. The goal is to estimate the probability that $Y = k$ for each category k given the feature vector \mathbf{x}_i .

The core of multinomial logistic regression is to model the log-odds (logits) of each category relative to a reference category (usually the last category, K). The probability that $Y = k$ given \mathbf{x}_i is modeled using the following softmax function:

$$P(Y = k | \mathbf{x}_i) = \frac{e^{\mathbf{x}_i^T \beta_k}}{\sum_{j=1}^K e^{\mathbf{x}_i^T \beta_j}}$$

where β_k is the coefficient vector associated with the k -th category, and it determines how the predictors influence the log-odds of category k relative to the reference category. Note that one of the categories is chosen as the reference category, typically K , and for that category, we set $\beta_K = 0$ to identify the model.

To better understand this, consider a simple case where $K = 3$ (i.e., the dependent variable has 3 categories) and there are two predictors x_1 and x_2 . For this case, the probability that an observation i belongs to category 1, 2, or 3 is given by:

$$P(Y = 1|\mathbf{x}_i) = \frac{e^{\mathbf{x}_i^T \beta_1}}{e^{\mathbf{x}_i^T \beta_1} + e^{\mathbf{x}_i^T \beta_2} + e^{\mathbf{x}_i^T \beta_3}}$$

$$P(Y = 2|\mathbf{x}_i) = \frac{e^{\mathbf{x}_i^T \beta_2}}{e^{\mathbf{x}_i^T \beta_1} + e^{\mathbf{x}_i^T \beta_2} + e^{\mathbf{x}_i^T \beta_3}}$$

$$P(Y = 3|\mathbf{x}_i) = \frac{e^{\mathbf{x}_i^T \beta_3}}{e^{\mathbf{x}_i^T \beta_1} + e^{\mathbf{x}_i^T \beta_2} + e^{\mathbf{x}_i^T \beta_3}}$$

The last probability is simplified because the coefficients for the reference category (category 3) are set to zero, i.e., $\beta_3 = 0$.

The parameters β_{kj} (where $k = 1, 2, \dots, K-1$ and $j = 0, 1, \dots, p$) are estimated using maximum likelihood estimation (MLE). The likelihood function for the multinomial logistic regression model is:

$$L(\beta_1, \beta_2, \dots, \beta_{K-1}) = \prod_{i=1}^n \prod_{k=1}^K P(y_{ik}|\mathbf{x}_i)^{y_{ik}}$$

The log-likelihood function is:

$$\ell(\beta_1, \beta_2, \dots, \beta_{K-1}) = \sum_{i=1}^n \sum_{k=1}^K y_{ik} \log(P(y_{ik}|\mathbf{x}_i))$$

The goal is to maximize this likelihood function with respect to the coefficients β_k for $k = 1, 2, \dots, K-1$. This is usually done using iterative optimization algorithms like gradient descent or Newton-Raphson.

Maximum Likelihood Estimation (MLE) can be written as:

$$\hat{\beta}_k = \arg \max_{\beta_k} \ell(\beta_1, \dots, \beta_{K-1})$$

Once the coefficients are estimated, we can predict the category for a new observation \mathbf{x} by selecting the category with the highest predicted probability. Specifically, we compute $P(Y = k|\mathbf{x})$ for each k and assign the observation to the class with the largest probability:

$$P(Y = k|\mathbf{x}) = \frac{e^{\mathbf{x}^T \beta_k}}{\sum_{j=1}^K e^{\mathbf{x}^T \beta_j}}$$

Multinomial logistic regression can be seen as a generalization of binary logistic regression. When $K = 2$, the model reduces to the standard logistic regression model. For larger K , the model simultaneously models $K - 1$ log-odds equations relative to the reference category. Unlike the binary case, the decision boundaries between categories in the predictor space are no longer linear, which makes the multinomial logistic model more flexible in handling complex classification problems.

In summary, multinomial logistic regression predicts probabilities for multiple outcome categories using the softmax function. It models the log-odds of each class relative to a reference category, and the coefficients are estimated using maximum likelihood estimation. The model can be used for classification, where each observation is assigned to the category with the highest predicted probability.

The cost function, which is the negative log-likelihood, is given by:

$$J(\beta_1, \beta_2, \dots, \beta_{K-1}) = - \sum_{i=1}^n \sum_{k=1}^K y_{ik} \log(P(y_{ik}|\mathbf{x}_i))$$

5.2 Ordinal Logistic Regression

Ordinal Logistic Regression is a type of regression used when the dependent variable is ordinal, meaning it has more than two categories with a clear order, but the distances between categories are not necessarily equal. This model is often used when the goal is to predict the probability of an observation falling into one of the ordered categories.

Let Y be an ordinal dependent variable that takes values from the set $\{1, 2, \dots, K\}$, where K is the total number of ordered categories. For each observation i , we have a feature vector $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T$, where p is the number of predictors. The goal is to estimate the probability that $Y \leq k$ for each category k given the feature vector \mathbf{x}_i .

The cumulative probability that $Y \leq k$ given \mathbf{x}_i is modeled using a cumulative logit function, which can be written as:

$$P(Y \leq k | \mathbf{x}_i) = \frac{1}{1 + e^{-(\mathbf{x}_i^T \beta_k + \theta_k)}}$$

where β_k is the coefficient vector associated with the k -th category and θ_k is the threshold parameter for category k . The thresholds $\theta_1, \theta_2, \dots, \theta_{K-1}$ help define the cut-off points between adjacent categories.

For the probability that $Y = k$ (i.e., the probability that Y belongs to category k), we can compute the difference between the cumulative probabilities for adjacent categories:

$$P(Y = k | \mathbf{x}_i) = P(Y \leq k | \mathbf{x}_i) - P(Y \leq k - 1 | \mathbf{x}_i)$$

The likelihood function for ordinal logistic regression is based on the cumulative probabilities for each observation. It is written as:

$$L(\beta_1, \beta_2, \dots, \beta_{K-1}) = \prod_{i=1}^n \prod_{k=1}^K P(y_{ik} | \mathbf{x}_i)^{y_{ik}}$$

The log-likelihood function is:

$$\ell(\beta_1, \beta_2, \dots, \beta_{K-1}) = \sum_{i=1}^n \sum_{k=1}^K y_{ik} \log(P(y_{ik} | \mathbf{x}_i))$$

The goal is to maximize this likelihood function with respect to the coefficients β_k for $k = 1, 2, \dots, K - 1$. This is typically done using iterative optimization methods such as gradient descent or Newton-Raphson.

Maximum Likelihood Estimation (MLE) for the ordinal logistic regression model is:

$$\hat{\beta}_k = \arg \max_{\beta_k} \ell(\beta_1, \dots, \beta_{K-1})$$

Once the coefficients are estimated, we can predict the cumulative probability for a new observation \mathbf{x} by computing the cumulative probabilities for each category.

Specifically, we compute $P(Y \leq k|\mathbf{x})$ for each k and assign the observation to the category with the highest probability.

Ordinal logistic regression can be seen as a generalization of binary logistic regression. When $K = 2$, the model reduces to the standard logistic regression model. For larger K , the model simultaneously models the cumulative log-odds for each category. Unlike multinomial logistic regression, the ordinal model assumes that the categories have a natural order, making it more appropriate for ordinal data.

In summary, ordinal logistic regression predicts the cumulative probability for an ordered categorical outcome using the cumulative logit function. The coefficients are estimated using maximum likelihood estimation, and the model can be used for classification where each observation is assigned to the category with the highest predicted probability.

The cost function, which is the negative log-likelihood, is given by:

$$J(\beta_1, \beta_2, \dots, \beta_{K-1}) = - \sum_{i=1}^n \sum_{k=1}^K y_{ik} \log(P(y_{ik}|\mathbf{x}_i))$$

5.3 Regularized Logistic Regression (L1, L2, ElasticNet)

Regularized Logistic Regression is a type of logistic regression that adds a penalty term to the cost function to prevent overfitting by discouraging excessively large coefficients. Regularization helps improve the generalization ability of the model.

Let Y be the binary dependent variable, which takes values from the set $\{0, 1\}$. For each observation i , we have a feature vector $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T$, where p is the number of predictors. The logistic regression model estimates the probability that $Y = 1$ given the feature vector \mathbf{x}_i using the sigmoid function:

$$P(Y = 1|\mathbf{x}_i) = \frac{1}{1 + e^{-\mathbf{x}_i^T \beta}}$$

where β is the coefficient vector associated with the predictors.

The likelihood function for logistic regression is:

$$L(\beta) = \prod_{i=1}^n P(y_i|\mathbf{x}_i)^{y_i} (1 - P(y_i|\mathbf{x}_i))^{1-y_i}$$

The log-likelihood function is:

$$\ell(\beta) = \sum_{i=1}^n [y_i \log(P(y_i|\mathbf{x}_i)) + (1 - y_i) \log(1 - P(y_i|\mathbf{x}_i))]$$

In regularized logistic regression, a regularization term is added to the log-likelihood function to penalize large coefficients. The most common forms of regularization are **L2 regularization** (Ridge) and **L1 regularization** (Lasso).

1. **L2 Regularization** (Ridge):

The cost function with L2 regularization is:

$$J(\beta) = -\ell(\beta) + \lambda \sum_{j=1}^p \beta_j^2$$

where λ is the regularization parameter that controls the strength of the penalty. The higher the value of λ , the stronger the penalty on large coefficients.

2. **L1 Regularization** (Lasso):

The cost function with L1 regularization is:

$$J(\beta) = -\ell(\beta) + \lambda \sum_{j=1}^p |\beta_j|$$

where λ is the regularization parameter, similar to L2 regularization.

The goal in regularized logistic regression is to maximize the log-likelihood function with the regularization term added:

$$\hat{\beta} = \arg \max_{\beta} \left(\ell(\beta) - \lambda \sum_{j=1}^p \text{Penalty}(\beta_j) \right)$$

The regularization term can either be $\sum_{j=1}^p \beta_j^2$ for L2 regularization or $\sum_{j=1}^p |\beta_j|$ for L1 regularization.

The gradient of the cost function with respect to β for L2 regularization is:

$$\nabla_{\beta} J(\beta) = - \sum_{i=1}^n [y_i - P(y_i|\mathbf{x}_i)] \mathbf{x}_i + 2\lambda\beta$$

The gradient for L1 regularization is:

$$\nabla_{\beta} J(\beta) = - \sum_{i=1}^n [y_i - P(y_i|\mathbf{x}_i)] \mathbf{x}_i + \lambda \text{sign}(\beta)$$

where $\text{sign}(\beta)$ is the element-wise sign function of β .

Once the coefficients are estimated using regularized logistic regression, we can predict the probability for a new observation \mathbf{x} using the logistic function:

$$P(Y = 1|\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{x}^T \hat{\beta}}}$$

The regularization in logistic regression helps prevent overfitting by ensuring that the model does not rely too heavily on any individual predictor.

In summary, regularized logistic regression adds a penalty term to the logistic regression cost function to control the complexity of the model. The regularization term can either be L1 (Lasso) or L2 (Ridge) regularization. The coefficients are estimated by maximizing the regularized log-likelihood function, and the model can then be used for prediction.

The cost function with L2 regularization is:

$$J(\beta) = - \sum_{i=1}^n [y_i \log(P(y_i|\mathbf{x}_i)) + (1 - y_i) \log(1 - P(y_i|\mathbf{x}_i))] + \lambda \sum_{j=1}^p \beta_j^2$$

The cost function with L1 regularization is:

$$J(\beta) = - \sum_{i=1}^n [y_i \log(P(y_i|\mathbf{x}_i)) + (1 - y_i) \log(1 - P(y_i|\mathbf{x}_i))] + \lambda \sum_{j=1}^p |\beta_j|$$

6 Code Implementation

6.1 Sigmoid Function

This section defines the sigmoid activation function used for binary classification. The sigmoid function maps any real-valued number to a value between 0 and 1, making it suitable for probability estimation in logistic regression.

6.2 Logistic Regression Model with L2 Regularization

This section introduces the custom `LogisticRegression` class, which includes methods for training the model (`fit`) and making predictions (`predict`). The model incorporates L2 regularization to prevent overfitting by adding a penalty to the cost function, which discourages large weights.

6.3 Loading the Dataset

Here, the Breast Cancer dataset from `sklearn.datasets` is loaded and the data is split into features (\mathbf{X}) and target labels (\mathbf{y}). This dataset is used to demonstrate the logistic regression model.

6.4 Data Preprocessing

This step involves selecting a subset of features (in this case, only the first two) for visualization and standardizing the feature values using `StandardScaler`. Feature scaling is essential for gradient-based optimization to ensure faster convergence.

6.5 Model Training

The logistic regression model is trained using the preprocessed training data. Parameters such as learning rate (`lr`), number of iterations (`n_iters`), and regularization strength (`reg_strength`) are set to optimize model performance during training.

6.6 Model Prediction

After training, the model is used to predict the target labels on the test dataset. The `predict` method applies the learned weights and bias to the input features and outputs the predicted class labels.

6.7 Accuracy Calculation

A function to compute the accuracy of the model's predictions is implemented. The accuracy is calculated as the proportion of correct predictions on the test set, providing a measure of the model's performance.

6.8 Visualization: Loss Function

A plot is generated showing the loss function over the course of the model's training iterations. The loss decreases as the model learns, indicating successful training.

6.9 Visualization: Decision Boundary

A decision boundary is visualized on a 2D plot, with the decision boundary separating the classes based on the trained logistic regression model. This helps to understand how the model classifies different regions of the feature space.

7 Conclusion

Logistic regression stands as one of the most fundamental and widely used techniques in machine learning and statistical modeling. Its simplicity, interpretability, and mathematical elegance make it a preferred choice for binary classification problems across a diverse range of fields, from medical diagnostics to financial risk assessment. By leveraging the sigmoid function and optimizing through maximum likelihood estimation, logistic regression provides a probabilistic framework for classification, offering insight into the likelihood of class membership.

However, like any model, logistic regression has its limitations. It is constrained by its reliance on linear decision boundaries and its sensitivity to outliers, multicollinearity, and small sample sizes. Despite these challenges, its extensions — such as multinomial and ordinal logistic regression — expand its applicability to more complex, multi-class problems. Regularization techniques like L1, L2, and ElasticNet further enhance its robustness, mitigating overfitting in high-dimensional datasets.

Ultimately, logistic regression serves as a vital entry point into the world of classification algorithms. Its principles lay the groundwork for more advanced models while remaining a powerful, interpretable, and efficient option for solving practical, real-world classification tasks. By understanding its strengths, limitations, and extensions, practitioners can make informed choices about when and how to apply this indispensable tool in machine learning and data analysis.