

# Chapter 4 Classification

we cannot compare the normal logistic regression

Linear regression --> Least square

Logistic regression --> maximum likelihood

Logistic Regression is a specific type of Generalized Linear Model (Often Abbreviated GLM). Generalized Linear Models are a generalization of the concepts and abilities of regular Linear Models.

## 4. Classification

### Main goal

Predict a **qualitative** (categorical) response variable  $Y$  instead of a quantitative one.

Three classic examples used throughout the chapter:

1. Emergency room diagnosis: stroke, drug overdose, epileptic seizure?
2. Online banking: is this transaction fraudulent?
3. DNA sequence: is this mutation disease-causing or not?

### 4.1 An Overview of Classification

#### Key idea

Classification assigns an observation to one of a set of discrete categories (classes).

We still have training data  $(x_i, y_i)$  pairs, but now  $y_i$  is a label (e.g., Yes/No, stroke/overdose/seizure, default/no default).

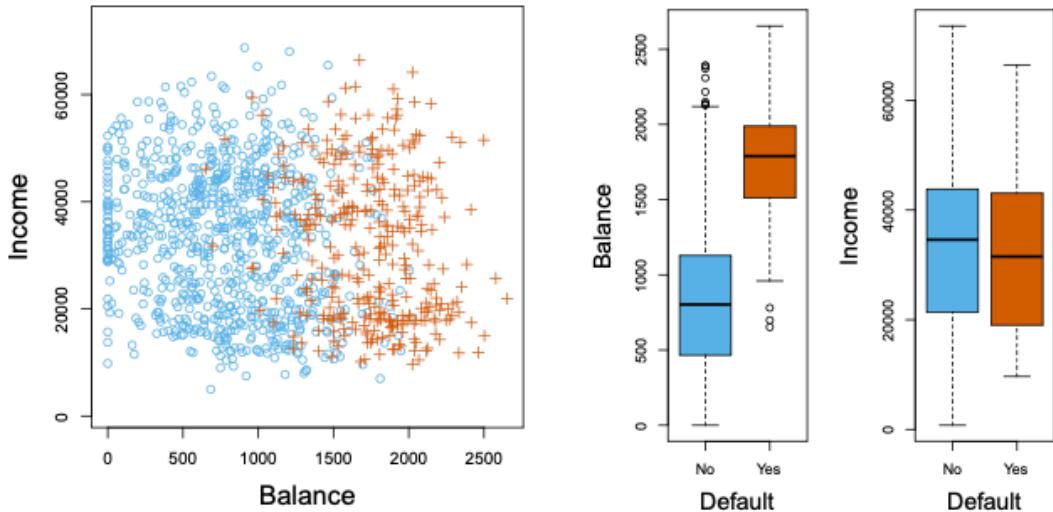
Most widely used methods covered in this chapter:

- Logistic regression
- Linear Discriminant Analysis (LDA)
- Quadratic Discriminant Analysis (QDA)
- Naïve Bayes
- K-nearest neighbors (mentioned briefly)

### 4.2 Why Not Linear Regression?

#### Core problem

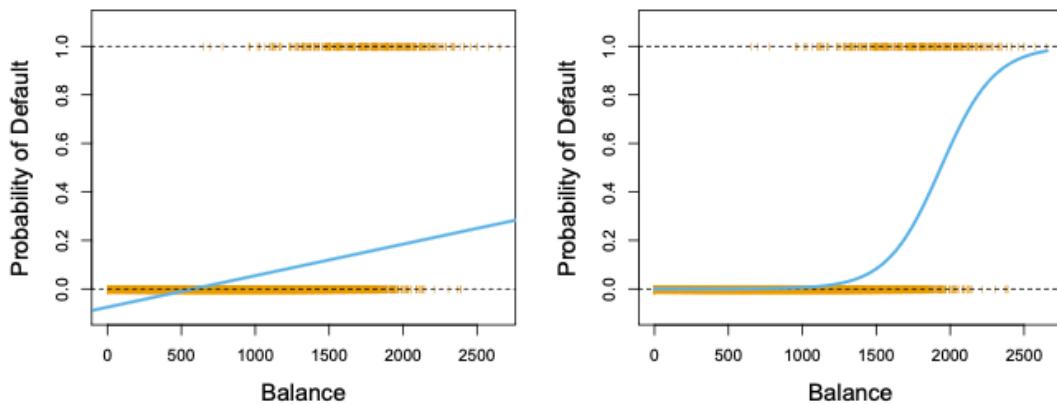
Linear regression assumes  $Y$  is continuous and unbounded. When  $Y$  is binary (0/1) or multi-class, it produces nonsense predictions (probabilities  $< 0$  or  $> 1$ ).



**Figure 4.1**

- Left: annual income vs monthly credit card balance, colored by default status
- Center & right: boxplots showing defaulters tend to have much higher balances

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**Figure 4.2** (most important figure in 4.2)

- Left panel: linear regression fit → line goes below 0 and above 1
- Right panel: logistic regression fit → nice S-shaped curve, stays in  $[0,1]$

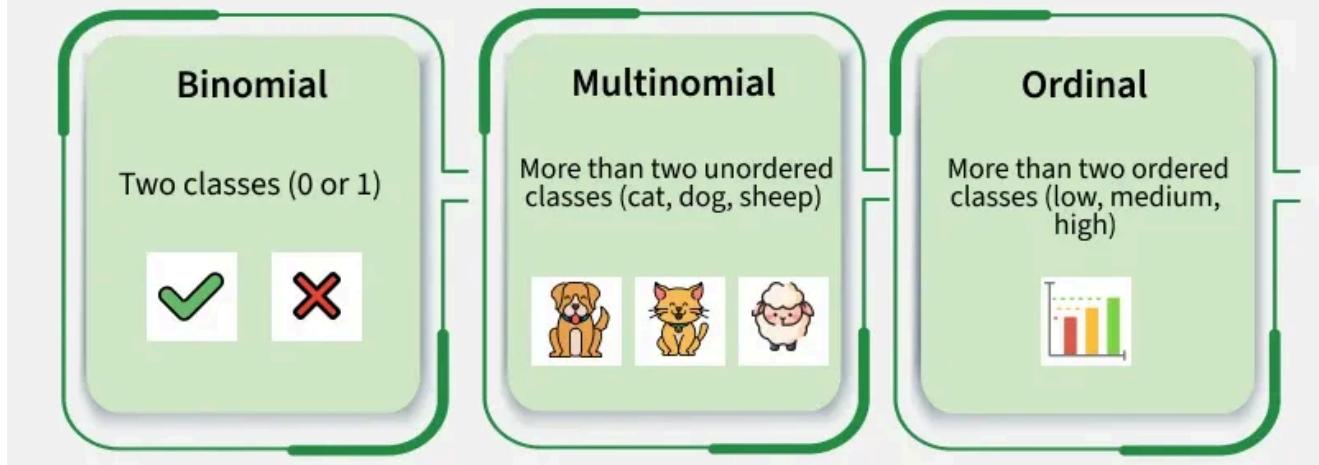
### Takeaway

Linear regression is inappropriate for classification because:

- Predicted values can fall outside  $[0,1]$
- The relationship between predictors and probability is usually not linear

## 4.3 Logistic Regression

# Types of Logistic Regression



## 4.3.1 The Logistic Model

### Core equation

Instead of modeling  $\Pr(Y=1|X)$  directly, model the **log-odds** linearly:

$$\log( p(X) / (1 - p(X)) ) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

Solving for probability gives the **logistic (sigmoid) function**:

$$\begin{aligned} p(X) &= e^{(\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p)} / (1 + e^{(\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p)}) \\ &= 1 / (1 + e^{-(\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p)}) \end{aligned}$$

Figure 4.2 (right panel) shows this S-shape perfectly on the Default data using balance.

## 4.3.2 Estimating the Regression Coefficients

We use **maximum likelihood** (not least squares) to find  $\beta$ .

	Coefficient	Std. error	z-statistic	p-value
Intercept	-10.6513	0.3612	-29.5	<0.0001
balance	0.0055	0.0002	24.9	<0.0001

**Table 4.1** (logistic regression with only balance)

- Intercept very negative → low baseline default risk
- $\beta$  balance  $\approx 0.00555$  → very strong positive effect

	Coefficient	Std. error	z-statistic	p-value
Intercept	-3.5041	0.0707	-49.55	<0.0001
student [Yes]	0.4049	0.1150	3.52	0.0004

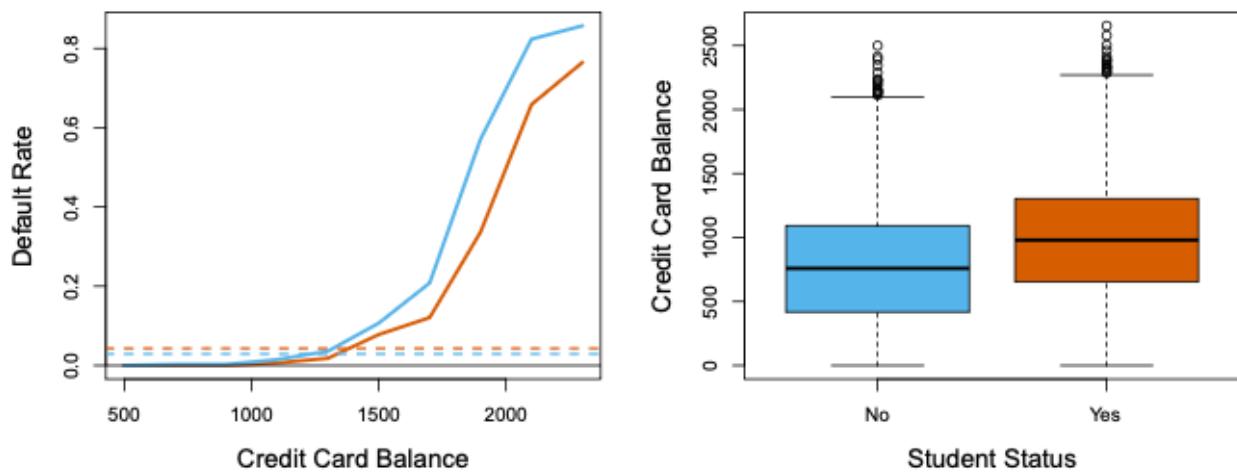
**Table 4.2** (logistic regression with only student status)

- Students appear to have slightly higher default probability

	Coefficient	Std. error	z-statistic	p-value
<b>Intercept</b>	-10.8690	0.4923	-22.08	<0.0001
<b>balance</b>	0.0057	0.0002	24.74	<0.0001
<b>income</b>	0.0030	0.0082	0.37	0.7115
<b>student [Yes]</b>	-0.6468	0.2362	-2.74	0.0062

**Table 4.3** (multiple logistic regression: balance + income + student)

- Now student coefficient is **negative** → students are actually less likely to default when balance and income are controlled for



**Figure 4.3** (classic confounding illustration)

- Left: default rate vs balance → separate lines for students (orange) and non-students (blue)
- Right: **box plot** → students have much higher balances on average  
→ **Confounding**: students borrow more, so look riskier overall, but are safer at the same balance level.

## +R-Square and P-Value

There is no consensus way to calculate the r-square and p-value for logistic regression.

### McFadden's Pseudo R-square

LL(fit) log likelihood fitted line

LL(Overall Probability)

And do it like the R-square in the Simple linear model

$$R^2 = \frac{\text{LL(overall probability)} - \text{LL(fit)}}{\text{LL(overall probability)}}$$

Chi-Squared value =  $2(\text{LL(Fit)} - \text{LL(Overall Probability)})$

### 4.3.3 Making Predictions

Once  $\beta$  are estimated, plug new X into the logistic formula to get predicted probability.

Example from Table 4.1:

balance = \$1,000 → predicted  $\Pr(\text{default}) \approx 0.00576$  (very low)

balance = \$2,000 → predicted  $\Pr(\text{default}) \approx 0.0586$  (much higher)

### 4.3.4 Multiple Logistic Regression

General form:

$$\log(p(X)/(1-p(X))) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

Same interpretation: each  $\beta_j$  is the change in log-odds per 1-unit change in  $X_j$  (holding others fixed).

### 4.3.5 Multinomial Logistic Regression

Extension to  $K > 2$  classes (e.g., stroke / overdose / seizure).

One class is chosen as baseline; we model log-odds relative to that baseline for each of the other classes.

## 4.4 Generative Models for Classification

### Big idea

Instead of directly modeling  $\Pr(Y=k|X)$ , model how X is generated in each class → then use Bayes rule.

$$\Pr(Y=k|X=x) = \Pr(X=x|Y=k) \times \Pr(Y=k) / \Pr(X=x)$$

$Y=k$  given X

Three main methods:

### Why discriminant Analysis?

-When classes are well-separated, the parameter estimate for the logistic regression model are

surprisingly unstable, so the linear discriminant analysis does not suffer from this problem.  
 -If n is small and the distribution of the predictors X is approximately normal in each of the classes, the linear discriminant model is again more stable than the logistic regression model.  
 -Linear discriminant analysis is popular when we have more than two response classes, because it also provides low-dimensional views of the data.

#### 4.4.1 Linear Discriminant Analysis for p = 1

The Gaussian density

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma_k}\right)^2}$$

Where

$\mu_k$  is the mean, and variance (in class k). we assume that variance K = normal variance

Assume each class is normal with same variance  $\sigma^2$ .

So plugging it into the Bayes Formula, we get the following

$$p_k(x) = \Pr(Y = k | X = x):$$

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma}\right)^2}}{\sum_{l=1}^K \pi_l \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu_l}{\sigma}\right)^2}}$$

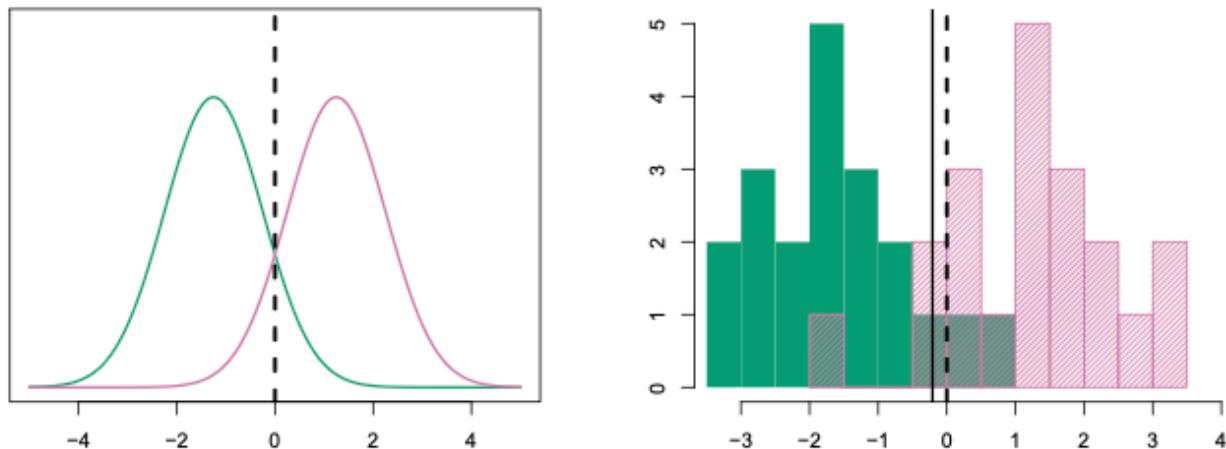
To classify at the value  $X = x$ , we need to see which of the  $p_k(x)$  is largest. Taking logs, and discarding terms that do not depend on  $k$ , we see that this is equivalent to assigning  $x$  to the class with the largest *discriminant score*:

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k) \quad \leftarrow$$

Note that  $\delta_k(x)$  is a *linear* function of  $x$ .

If there are  $K = 2$  classes and  $\pi_1 = \pi_2 = 0.5$ , then one can see that the *decision boundary* is at  $\text{---}$

$$x = \frac{\mu_1 + \mu_2}{2}.$$

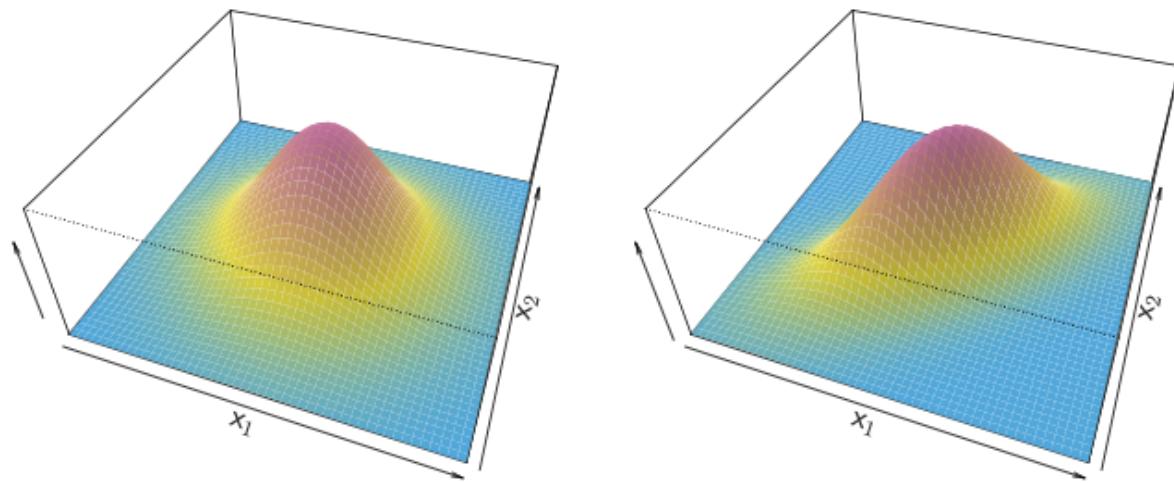


**Figure 4.4**

- Left: two overlapping normal densities + Bayes decision boundary (dashed vertical line)
- Right: 20 sampled points per class + histogram + LDA boundary (solid)

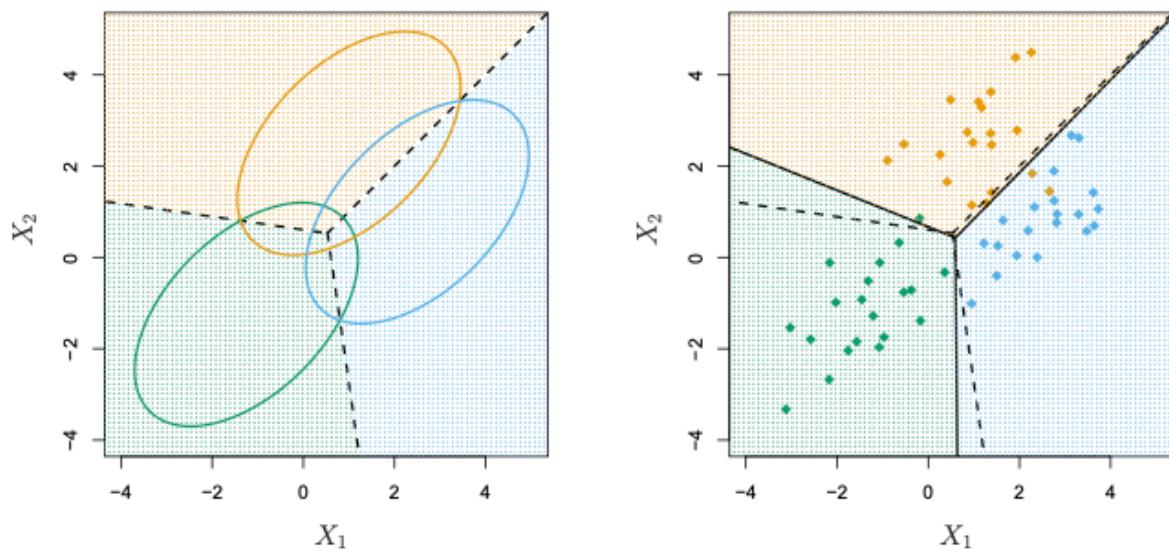
#### 4.4.2 Linear Discriminant Analysis for $p > 1$

Assume multivariate normal with class-specific means  $\mu_k$  but **common covariance matrix**  $\Sigma$  for all classes.



**Figure 4.5**

- Two multivariate Gaussians ( $p=2$ ) with correlation 0.7 → elliptical contours



**Figure 4.6** (very important)

- Left: three classes, 95% probability ellipses, Bayes boundaries (dashed), LDA boundaries (solid)
- Right: actual 20 points per class sampled → LDA boundaries very close to Bayes

**Confusion matrix examples (Default data, 10,000 observations)**

		<i>True default status</i>		Total
		No	Yes	
<i>Predicted default status</i>	No	9644	252	9896
	Yes	23	81	104
	Total	9667	333	10000

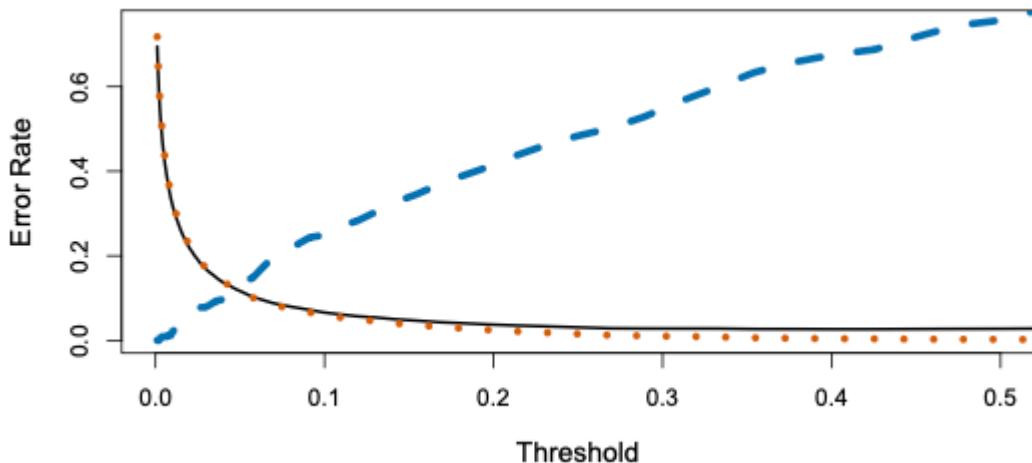
**Table 4.4** (LDA with default threshold 0.5)

- Overall error  $\approx 2.75\%$
- But misses  $252 / 333 = 75.7\%$  of actual defaulters  $\rightarrow$  very low sensitivity

		<i>True default status</i>		Total
		No	Yes	
<i>Predicted default status</i>	No	9432	138	9570
	Yes	235	195	430
Total		9667	333	10000

**Table 4.5** (LDA with lower threshold  $\sim 20\%$ )

- Predicts many more defaults (430 instead of 104)
- Catches more true defaulters but increases false positives



**Figure 4.7**

Error rates vs threshold:

- Black = overall error
  - Blue dashed = error among true defaulters
  - Orange dotted = error among true non-defaulters
- $\rightarrow$  Clear trade-off

#### 4.4.3 Quadratic Discriminant Analysis

Same as LDA but **allows different covariance matrices  $\Sigma_k$**  for each class  $\rightarrow$  decision boundaries become **quadratic**.

#### ROC Curve (Figure 4.8)

- x-axis = False Positive Rate ( $1 - \text{specificity}$ )
- y-axis = True Positive Rate (sensitivity / recall)
- AUC  $\approx 0.95$  for LDA on Default data  $\rightarrow$  very good performance

**Summary table – when to prefer which method**

METHOD	ASSUMPTION	BOUNDARY SHAPE	BEST WHEN ...
Logistic Regression	linear in log-odds	linear	many predictors, no strong normality needed
LDA	multivariate normal + equal $\Sigma$	linear	classes roughly normal, similar spread
QDA	multivariate normal + different $\Sigma_k$	quadratic	clear difference in variance between classes
Naïve Bayes	features independent given class	usually linear	high-dimensional data (text, genomics), sparse

#### 4.4.4 Naive bayes

Naive bayes is a ML classification algorithm that predicts the category of a data point using probability.

It assume that all features are independent of each other.

**Ex:** best use in spam filtering, document categorisation, sentiment analysis

Naive bayes use **Bayes's Theorem** to classify data based on the probabilities of different classes given the features of the data. It is used mostly in high-dimensional text classification.

**Naive bayes's Characteristic:**

- Very few number of parameters --> faster than other classification algorithm
- It assumes that each feature contributes to the predictions with no relation between each other

**Why is it called Naive Bayes?**

Because it assumes the presence of one feature does not affect other features.

**Assumption of the Naive Bayes**

- Feature independence:** when we are trying to classify sth, each feature or piece of information in the data does not affect any other feature.
- Continuos features are normally distributed:** If a feature is continuous, then it is assumed to be normally distributed within each class.
- Discrete features have multinomial distributions:** If a feature is discrete, then it is assumed to have a multinomial distribution within each class.
- Features are equally important:** all feature are assumed to contribute equally to the prediction of the class label.
- No missing data:** the data should not contain any missing values.

**Bayes's Theorem**

$$P(y|X) = \frac{P(X|y) \cdot P(y)}{P(X)}$$

Where:

- $P(y|X)$ : Posterior probability, probability of class  $y$  given features  $X$
- $P(X|y)$ : Likelihood, probability of features  $X$  given class  $y$
- $P(y)$ : Prior probability of class  $y$
- $P(X)$ : Marginal likelihood or evidence

The "naive" in Naive Bayes comes from the assumption that all features are independent given the class. That is:

$$P(x_1, x_2, \dots, x_n | y) = P(x_1 | y) \cdot P(x_2 | y) \cdots P(x_n | y)$$

Thus, Bayes' theorem becomes:

$$P(y|x_1, \dots, x_n) = \frac{P(y) \cdot \prod_{i=1}^n P(x_i | y)}{P(X)}$$

Since the denominator is constant for a given input, we can write:

$$P(y|x_1, \dots, x_n) \propto P(y) \cdot \prod_{i=1}^n P(x_i | y)$$

We compute the posterior for each class  $y$  and choose the class with the highest probability:

$$\hat{y} = \arg \max_y P(y) \cdot \prod_{i=1}^n P(x_i | y)$$

This becomes our Naive Bayes classifier.

### Naive Bayes for Continuous Features

For continuous features, we assume a Gaussian Distribution

$$P(x_i|y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left(-\frac{(x_i - \mu_y)^2}{2\sigma_y^2}\right)$$

## Type of Naive Bayes Model

1. **Gaussian Naive Bayes:** Continuous values associated with each feature are assumed to be distributed according to a gaussian distribution.
2. **Multinomial naive Bayes:** when features represent the frequency of terms (word count) in a doc. Commonly applied in text classification
3. **Bernoulli Naive Bayes:** binary feature, where each feature indicates whether a word appears or not in a document. It is suited for scenarios where the presence or absence of terms is more relevant than their frequency. Both models are widely used in document classification tasks