

# Logistic Regression and Classification

## Introduction to Statistical Modelling

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# Overview

- ① Introduction: what are classification problems?
- ② K-nearest neighbors classification
- ③ Logistic regression
- ④ Classification

# Introduction

# Classification

In many problems, the outcome is a **categorical** variable:

- Figure out whether mutation is deleterious (yes/no), based on DNA sequencing data.
- Predict a person's eye color (blue/brown/green)
- Predict the outcome of surgery (success/failure) for patients with ovarian cancer, based on patient characteristics
- Classify iris (flower) variety given dimensions of leaves

These problems are examples of **classification** problems.

# Techniques for classification

- **Logistic regression**
- **K-nearest neighbors**
- Linear discriminant analysis
- Support vector classification (SVC)
- Decision trees
- ...

The techniques in **bold** are discussed in this lecture.

Each technique has its advantages and disadvantages.

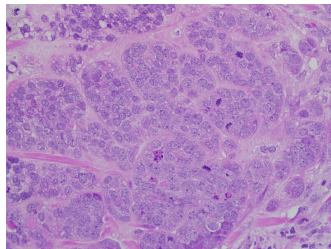
# References

- *An Introduction to Statistical Learning*. Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. Available for free online at <https://www.statlearning.com/>.
  - Logistic regression: sections 4.1 - 4.3

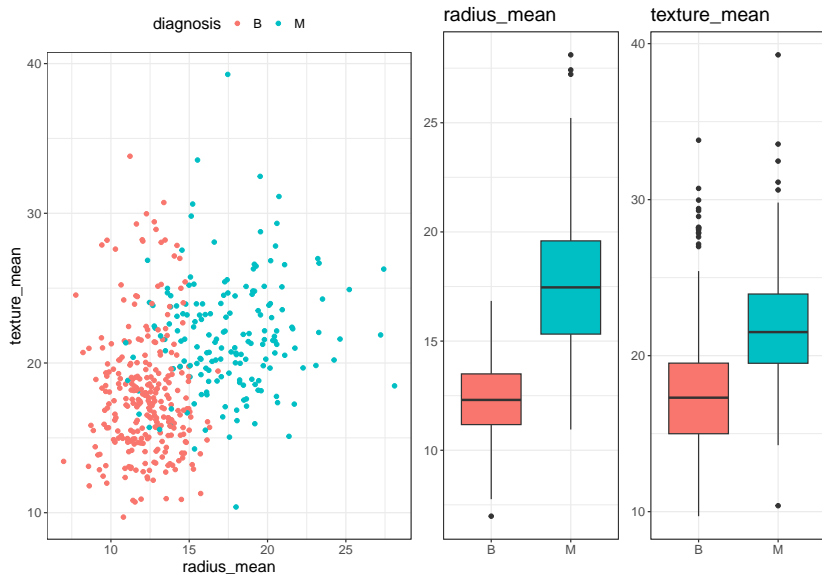
# Dataset

bdiag – Wisconsin breast cancer diagnostic dataset (*Nuclear feature extraction for breast tumor diagnosis*. W. Street, W. Wolberg, O. Mangasarian. Electronic imaging 29 (1993))

- Cell nuclei from 569 tumor samples
- Classified as malignant or benign
- Features:
  - radius of the cell nucleus
  - texture (variance of gray-scale values)



# A first look at the data

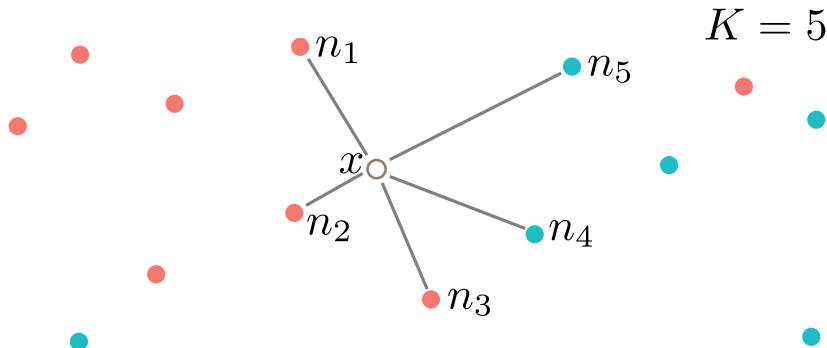




## K-nearest neighbors classification

# Principle

- Find  $K$  nearest neighbors to  $x$
- Probability of belonging to class  $i$  is proportional to number of neighbors in that class



- $P(\text{red}|X = x) = \frac{3}{5} = 60\%$
- $P(\text{green}|X = x) = \frac{2}{5} = 40\%$

# Properties

K-nearest neighbor (KNN) classification estimates probabilities

$$P(Y = j|X = x) = \frac{1}{|\mathcal{N}_K(x)|} \sum_{i=1}^{|\mathcal{N}_K(x)|} I(y_i = j)$$

Here:

- $\mathcal{N}_K(x)$  is the set of  $K$  nearest datapoints to  $x$
- $I(y_i = j)$  is equal to 1 if  $y_i = j$  and to 0 otherwise

# Advantages and disadvantages

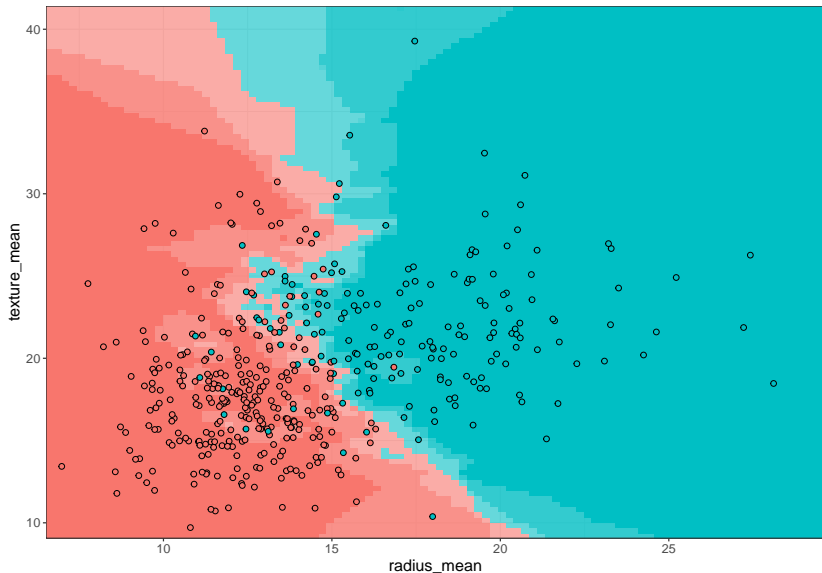
## Advantages:

- No “training” necessary
- Robust to outliers
- Can easily deal with more than 2 labels

## Disadvantages:

- Not very interpretable – why was class decided?
- Memory-intensive

## Decision boundary ( $K = 5$ )



## Logistic regression

## Reminder: odds

- If  $\pi$  is the probability of having a malignant tumor, then the **odds** are defined as

$$\text{Odds} = \frac{\pi}{1 - \pi}.$$

For example: if  $\pi = 0.8$  then  $\text{Odds} = 4$ , meaning that for every benign tumor there are 4 malignant ones (on average).

- Odds range from 0 (impossible event) to  $+\infty$  (almost certain).

## Reminder: odds ratio

- **Odds ratio** (OR): indicates by how much the odds change between two treatments. For example: suppose in the treatment group the probability of a malignant tumor drops to  $\pi_T = 0.75$  (compared to  $\pi_C = 0.8$  in the untreated group). Then

$$\text{OR} = \frac{\text{Odds}(T)}{\text{Odds}(C)} = \frac{3}{4} = 0.75$$

- If  $\text{OR} < 1$ , then the odds for treatment 1 decrease compared to treatment 2. If  $\text{OR} > 1$ , the odds increase.



## Log-odds (logits)

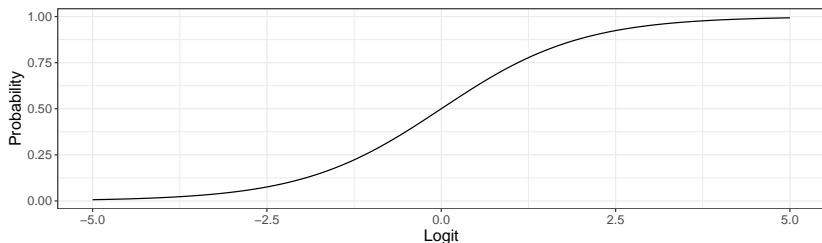
Often it makes sense to work with the logarithm of the odds (**logits**):

$$\text{logit}(\pi) = \ln \text{Odds} = \ln \left( \frac{\pi}{1 - \pi} \right).$$

To convert back to probabilities, use the **logistic** function:

$$\pi = \frac{1}{1 + e^{-\text{logit}}}.$$

Logits are unbounded:  $\text{logit} \rightarrow \pm\infty$  for  $p \rightarrow 0, 1$



# Regression for classification

- Given data  $(X_1, Y_1), \dots, (X_n, Y_n)$  where:
  - Outcomes  $Y_i$  are categorical (0 or 1)
  - Predictors  $X_i$  can be continuous or discrete
- We will model  $Y_i$  as a Bernoulli random variable (0 or 1) with probability  $\pi(X_i)$ :

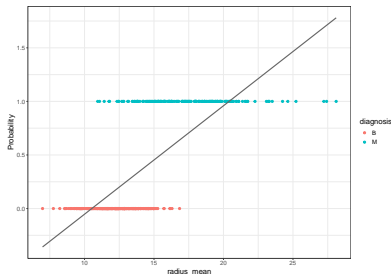
$$Y_i = 0 \quad \text{with probability } \pi(X_i)$$

$$Y_i = 1 \quad \text{with probability } 1 - \pi(X_i)$$

- Now we need to determine how  $\pi(X)$  depends on  $X$ .

## Idea 1: linear regression (bad)

- One predictor  $X = \text{radius\_mean}$ , outcome  $Y = 0$  (benign) or  $Y = 1$  (malignant).
- Assume  $\pi(X) = \alpha + \beta X$  and determine  $\alpha, \beta$  through linear regression.



Problems:

- Fitted probabilities can take on values outside  $[0, 1]$ .
- Does not easily generalize to more than two classes.

## Idea 2: logistic regression (better)

- Let  $\pi(X)$  depend on  $X$  through the logistic function

$$\pi(X) = \frac{1}{1 + \exp(-(\alpha + \beta X))}.$$

- **Nonlinear** model in parameters  $\alpha, \beta$
- Alternatively, apply the logit transformation

$$\text{logit}(\pi) = \alpha + \beta X.$$

- Linear in the logits.

## Determining the regression parameters: MLE

- **Likelihood function**  $\mathcal{L}$ : probability of observing the data given the parameters  $\alpha, \beta$ :

$$\mathcal{L}(\alpha, \beta) = \prod_{i=1}^n P(Y = Y_i | X = X_i),$$

where

$$P(Y = Y_i | X = X_i) = \pi(X_i)^{Y_i} (1 - \pi(X_i))^{1-Y_i}.$$

is the probability of observing one data point  $(X_i, Y_i)$ .

- In practice, often better to use the log of the likelihood:

$$\ell(\alpha, \beta) = \ln \mathcal{L}(\alpha, \beta).$$

## Determining the regression parameters: MLE

- **Maximum likelihood estimation** (MLE): find parameters that maximize  $\mathcal{L}(\alpha, \beta)$  or  $\ell(\alpha, \beta)$
- Finding maximum: set partial derivatives (score functions) equal to zero:

$$\frac{\partial \ell}{\partial \alpha} = 0, \quad \frac{\partial \ell}{\partial \beta} = 0.$$

- Complicated equations, usually maximum cannot be found analytically (unlike least squares)
- Use numerical methods to find maximum (R does this automatically with the `glm` command)

## Simplified example: MLE for binomial variable

- Suppose there are *no* predictors. We just have a bunch of categorical outcomes  $Y_i = 0, 1$ , e.g.

$$Y = (0, 0, 1, 0, 1, 0, \dots, 1, 1, 0, 0, 1)$$

- In semester 1 we saw that a good estimate for the probability  $\pi = P(Y = 1)$  is given by the proportion of 1s in the data:

$$\hat{\pi} = \frac{1}{N} \sum_{i=1}^N Y_i = \bar{Y}.$$

- We'll use MLE to re-derive this result.

## Simplified example: MLE for binomial variable

- Likelihood

$$\begin{aligned}\mathcal{L}(\pi) &= \prod_{i=1}^n P(Y = Y_i) \\ &= \pi^{n\bar{Y}} (1 - \pi)^{n(1-\bar{Y})}\end{aligned}$$

- Log likelihood:  $\ell(\pi) = n\bar{Y} \ln \pi + n(1 - \bar{Y}) \ln(1 - \pi)$ .
- Maximum occurs when first derivative vanishes:

$$\frac{d\ell}{d\pi} = \frac{n\bar{Y}}{\pi} - \frac{n(1 - \bar{Y})}{1 - \pi} = 0.$$

- Simplifies to  $\hat{\pi} = \bar{Y}$ .



# MLE for logistic regression in R

```
m_simple <- glm(diagnosis ~ radius_mean, data = train, family = "binomial")
summary(m_simple)
```

Call:

```
glm(formula = diagnosis ~ radius_mean, family = "binomial", data = train)
```

Coefficients:

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	-15.8086	1.5310	-10.326	<2e-16 ***
radius_mean	1.0662	0.1066	9.998	<2e-16 ***

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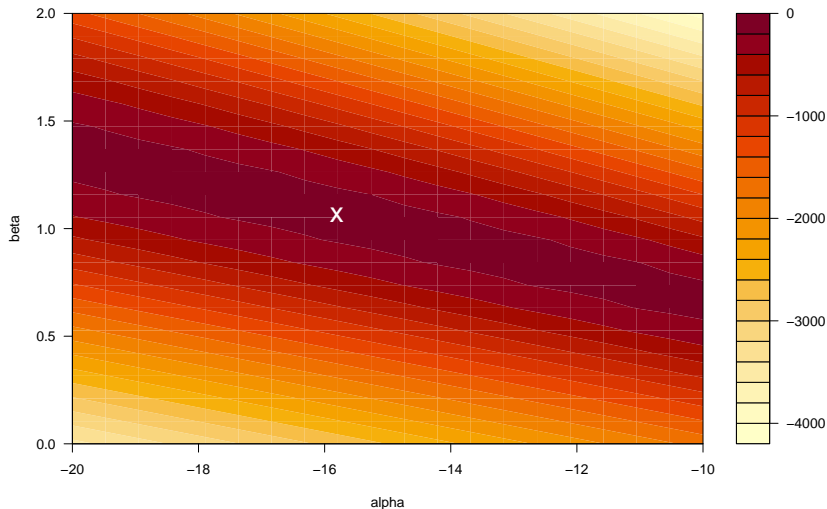
Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 604.40 on 454 degrees of freedom  
Residual deviance: 256.54 on 453 degrees of freedom  
AIC: 260.54

Number of Fisher Scoring iterations: 6

## The log likelihood



- Value of log likelihood at MLE:  $\ell = -128.2701$ .
- R reports (residual) deviance:  $D = -2 \times \ell = 256.54$

## Multiple logistic regression

- Like in linear regression, often the outcome  $Y$  is influenced by several predictors  $X_1, X_2, \dots, X_p$ .
- For example: `diagnosis` depends on `radius_mean` and `texture_mean`:

$$\text{logit}(\pi) = \alpha + \beta_1 \cdot \text{radius\_mean} + \beta_2 \cdot \text{texture\_mean}.$$

- Parameters  $\alpha, \beta_1, \dots, \beta_p$  determined through MLE.

# In R

```
m_multi <- glm(diagnosis ~ radius_mean + texture_mean,  
               data = train, family = "binomial")  
summary(m_multi)
```

Call:

```
glm(formula = diagnosis ~ radius_mean + texture_mean, family = "binomial",  
    data = train)
```

Coefficients:

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	-20.51694	2.04729	-10.021	< 2e-16 ***
radius_mean	1.09536	0.11727	9.341	< 2e-16 ***
texture_mean	0.21749	0.04034	5.391	7.01e-08 ***

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 604.40 on 454 degrees of freedom  
Residual deviance: 223.68 on 452 degrees of freedom  
AIC: 229.68

Number of Fisher Scoring iterations: 7

## Interactions between variables

```
m_inter <- glm(diagnosis ~ radius_mean * texture_mean,  
               data = train, family = "binomial")
```

Coefficient	Estimate	SE	z value	p value
(Intercept)	-8.3046	7.4554	-1.114	0.2653
radius	0.2182	0.5288	0.413	0.6798
texture	-0.4133	0.3855	-1.072	0.2836
radius:texture	0.0455	0.0276	1.647	0.0995

Interaction between radius and texture is not significant

## Making predictions (by hand)

What is the probability of a tumor being malignant if the radius is 13 mm?

$$\begin{aligned}\pi(\text{radius\_mean} = 13) &= \frac{1}{1 + \exp(15.8086 - 1.0662 \times 13)} \\ &= 0.1247716\end{aligned}$$

No easy formula for confidence interval on the prediction.

## Making predictions (using R)

```
predict(m_simple,  
        newdata = data.frame(radius_mean = 13),  
        type = "response")
```

1

0.1247961

# Computing a confidence interval for the prediction

Proceeds in three steps:

- 1 Make a prediction on the **logit** scale (`type = "link"`)
- 2 Compute CI on logit scale from SE (`se.fit = TRUE`)
- 3 Map CI back to probabilities

For step 3, use `plogis` to undo the logit transformation:

$$\text{plogis}(x) = \frac{1}{1 + \exp(-x)}.$$



# Computing an CI: example

**Step 1:** Prediction on the logit scale.

```
pred <- predict(m_simple,  
               newdata = data.frame(radius_mean = 13),  
               type = "link", se.fit = TRUE)
```

**Step 2:** CI on the logit scale.

```
ci_logits <- c(pred$fit - 1.96 * pred$se.fit,  
               pred$fit + 1.96 * pred$se.fit)  
ci_logits
```

	1	1
	-2.358216	-1.537335

### Step 3: CI on the original scale (probabilities)

```
ci_probs <- c(plogis(ci_logits[1]), plogis(ci_logits[2]))  
ci_probs
```

```
          1          1  
0.08641491 0.17692307
```

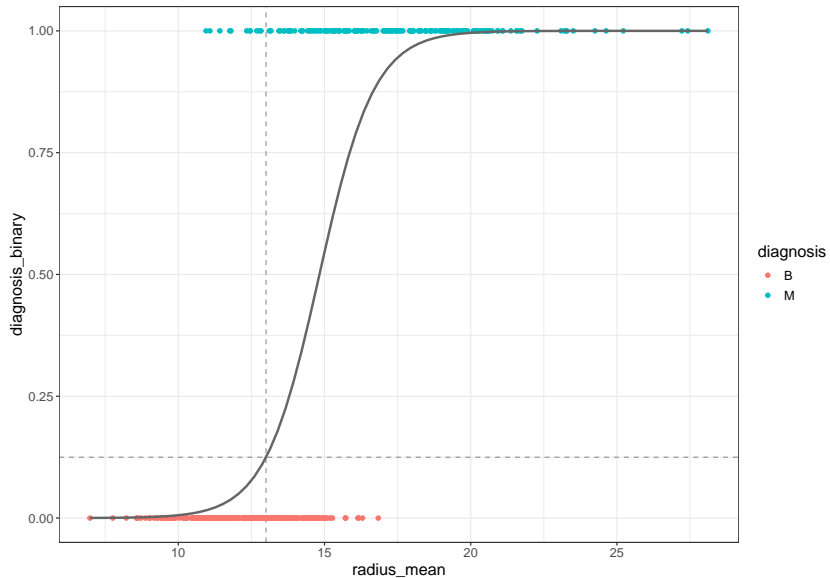
Original prediction:

```
pred_probs <- plogis(pred$fit)  
pred_probs
```

```
          1  
0.1247961
```

**Conclusion:** The predicted probability that a tumor of radius 13mm is malignant is 12.5% (95% CI: [8.6%, 17.7%])

# Making predictions



## Quantifying the strength of an association

Write the logistic regression model in terms of odds as

$$\text{logit}(\pi) = \ln \text{Odds} = \alpha + \beta X.$$

After some algebra:

$$e^{\beta} = \frac{\text{Odds}(X + 1)}{\text{Odds}(X)}.$$

In other words:  $e^{\beta}$  is the odds ratio (OR) associated to a 1-unit increase in  $X$ .

### **i** Breast cancer dataset

Here  $\beta = 1.0662$ , so  $\text{OR} = \exp(1.0662) = 2.90$ . An increase in 1 mm in tumor radius is associated with odds that are 2.90 times higher (risk increase).

# Testing an association

- Often, we want to test whether a model coefficient  $\beta$  is significant.
- Related: check if complex and simple nested models are equivalent (recall  $F$ -test from linear regression).

Several ways of testing:

- Wald test (reported in `summary`): can be conservative
- Likelihood ratio test (via `anova` command): more power, preferred
- Score test (not covered)

## Testing an association: Wald test

- Null hypothesis  $H_0 : \beta = 0$ , alternative hypothesis  $H_A : \beta \neq 0$
- Test statistic follows  $N(0, 1)$  under  $H_0$

$$z = \frac{\hat{\beta}}{SE(\beta)} \sim N(0, 1) \quad \text{under } H_0.$$

- Reported in the R regression output (summary):

Coefficient	Estimate	SE	z value	p value
(Intercept)	-20.5169	2.0473	-10.021	< 2e-16
radius_mean	1.0954	0.1173	9.341	< 2e-16
texture_mean	0.2175	0.0403	5.391	7.01e-08

# Testing an association: Likelihood ratio test

Useful for:

- Comparing nested models (simple/complex)
- Testing single coefficient

Hypothesis:

- $H_0$ : simple and complex model are equivalent
- $H_A$ : complex model is better

Test statistic: **deviance**

$$\begin{aligned} D &= -2 \ln \frac{\mathcal{L}(\text{simple})}{\mathcal{L}(\text{complex})} \\ &= -2\ell(\text{simple}) + 2\ell(\text{complex}). \end{aligned}$$

Under  $H_0$ ,  $D$  follows a  $\chi_k^2$  distribution, where  $k$  is the number of extra parameters in the complex model.

## Worked out example

Nested models:

- Simple: includes `radius_mean` only
- Complex: includes both `radius_mean` and `texture_mean`.

From R summary (listed as residual deviance) or direct calculation:

- $-2\ell(\text{simple}) = 256.54$
- $-2\ell(\text{complex}) = 223.68$

Hence  $D = 256.54 - 223.68 = 32.86 > 3.841459 = \chi^2_{1;0.95}$ .

Conclusion: reject  $H_0$ , significant evidence to decide (at 5% significance level) that complex model is better.



## Likelihood ratio test in R (single variable)

```
anova(m_simple, m_multi)
```

Analysis of Deviance Table

Model 1: diagnosis ~ radius\_mean

Model 2: diagnosis ~ radius\_mean + texture\_mean

	Resid. Df	Resid. Dev	Df	Deviance
1	453	256.54		
2	452	223.68	1	32.864

Compare with critical values for  $\chi^2_1$  to draw conclusion

## Likelihood ratio test in R (groups of variables)

Nested models:

- Simple: includes radius\_mean and texture\_mean.
- Complex: adds concavity\_mean and symmetry\_mean.

R output:

```
anova(m_multi, m_multi_4)
```

Analysis of Deviance Table

Model 1: diagnosis ~ radius\_mean + texture\_mean

Model 2: diagnosis ~ radius\_mean + texture\_mean + concavity

	Resid. Df	Resid. Dev	Df	Deviance
1	452	223.68		
2	450	129.99	2	93.686

Compare with critical value  $\chi^2_{2;0.95} = 5.991465$  to conclude that complex model is better.

# Confidence interval for regression parameters

Wald-type **approximate**  $(1 - \alpha) \times 100\%$  confidence interval for  $\beta$ :

$$\hat{\beta} \pm z_{1-\alpha/2} \cdot SE(\beta)$$

**i** Breast cancer dataset

95% confidence interval for  $\beta_{\text{radius\_mean}}$ :

$$1.095 \pm 1.96 \times 0.117 = [0.866, 1.324].$$

## Confidence interval for regression parameters in R

```
confint(m_multi)
```

	2.5 %	97.5 %
(Intercept)	-24.8846042	-16.8233485
radius_mean	0.8840034	1.3456187
texture_mean	0.1405734	0.2993915

R uses the so-called profile method to compute CI:

- Different from Wald method (narrower CIs, but close)
- Preferred to use this method through R

## Confidence interval for odds ratio

- Recall that  $\exp(\beta) = \text{OR}$  for a 1-unit change in  $X$
- $(1 - \alpha) \times 100\%$  confidence interval for the OR:

$$\exp\left(\hat{\beta} \pm z_{1-\alpha/2} \cdot SE(\beta)\right).$$

### **i** Breast cancer dataset

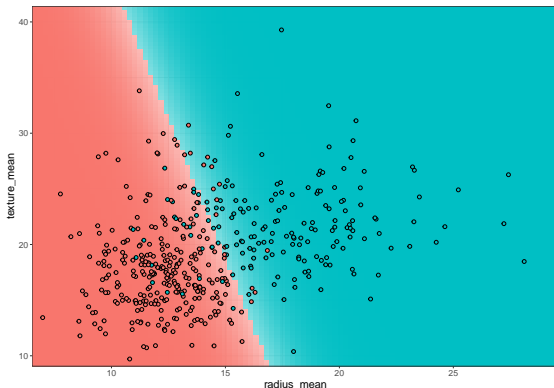
95% confidence interval for  $\text{OR}_{\text{radius\_mean}}$ :

$$\begin{aligned}\exp(1.095 \pm 1.96 \times 0.117) &= [\exp(0.866), \exp(1.324)] \\ &= [2.377, 3.759]\end{aligned}$$

# Classification

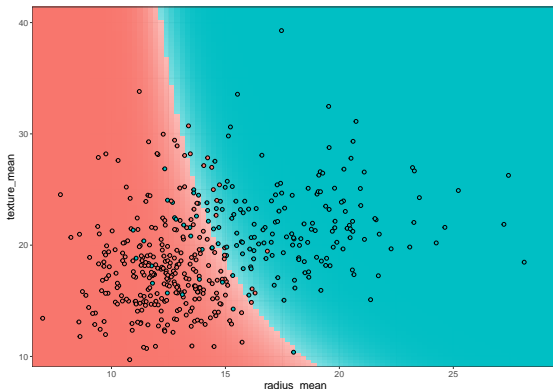
## Decision boundary (no interaction terms)

- Model:  $\text{logit}(\text{diagnosis}) \sim \text{radius} + \text{texture}$
- Decision boundary is **straight** line



# Decision boundary (with interaction terms)

- Model:  
 $\text{logit}(\text{diagnosis}) \sim \text{radius} + \text{texture} + \text{radius} : \text{texture}$
- Decision boundary is **curved** line





# Classification

- Once we have a (logistic) model for  $\pi(X)$ , we can use it to classify new data  $X$  as negative ( $Y = 0$ ) or positive ( $Y = 1$ ), by comparing  $\pi(X)$  with a fixed threshold  $C$ :

$$Y = 1 \quad \text{if } \pi(X) > C, \text{ otherwise } Y = 0.$$

- Performance **depends on choice of  $C$**

## **i** Breast cancer dataset

We computed earlier that  $\pi(\text{radius\_mean} = 13) = 0.12$ . Assuming that the threshold for malignant samples is  $C = 0.5$ , this sample would be classified as **benign**.

# Confusion matrix

By comparing labels given by our model with “actual” labels, we can get an idea of the performance of our classifier.

		Predicted condition	
Total population = P + N		Positive (PP)	Negative (PN)
Actual condition	Positive (P)	True positive (TP)	False negative (FN)
	Negative (N)	False positive (FP)	True negative (TN)

Figure source: [https://en.wikipedia.org/wiki/Confusion\\_matrix](https://en.wikipedia.org/wiki/Confusion_matrix)

## Performance metrics

Name	Definition	Value for example
Accuracy	$(TP + TN)/(P + N)$	0.84
Sensitivity (recall)	$TP / P$	0.93
Specificity	$TN / N$	0.67
PPV (precision)	$TP / PP$	0.84
NPV	$TN / NN$	0.84

- Many other metrics exist
- Which one is important depends on the problem
- Metrics can give surprising results in case of unbalanced data

# In R (via caret package)

## Confusion Matrix and Statistics

	Reference	
Prediction	B	M
B	64	6
M	11	33

Accuracy : 0.8509

95% CI : (0.772, 0.9107)

No Information Rate : 0.6579

P-Value [Acc > NIR] : 3.039e-06

Kappa : 0.6786

Mcnemar's Test P-Value : 0.332

Sensitivity : 0.8462

Specificity : 0.8533

Pos Pred Value : 0.7500

Neg Pred Value : 0.9143

Prevalence : 0.3421

Detection Rate : 0.2895

Detection Prevalence : 0.3860

Balanced Accuracy : 0.8497

'Positive' Class : M

# Trading sensitivity and specificity

What is important?

- Diagnostic test: **sensitivity** (don't tell people with tumor that they are healthy). Choose low threshold.
- Classifying email as spam: **specificity** (don't put regular email in the spam folder). Choose high threshold.

By changing the threshold, sensitivity and specificity can be traded against one another.

- Lowering threshold: Sensitivity  $\uparrow$ , Specificity  $\downarrow$ .
- Increasing threshold: Sensitivity  $\downarrow$ , Specificity  $\uparrow$ .

**i** Breast cancer dataset

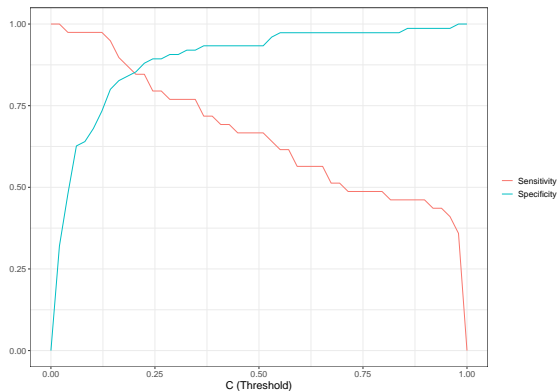
- For  $C = 0.5$ : sensitivity 0.84

Prediction	Reference	B	M
B		70	<b>13</b>
M		5	26

- For  $C = 0.2$ : sensitivity **0.85**

Prediction	Reference	B	M
B		64	<b>6</b>
M		11	33

# Sensitivity and specificity as a function of threshold

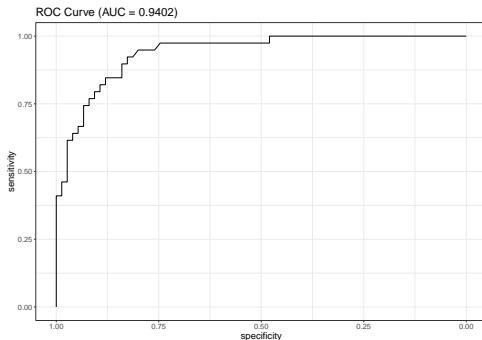


As threshold increases:

- Sensitivity **decreases** (less true positives)
- Specificity **increases** (less false positives)

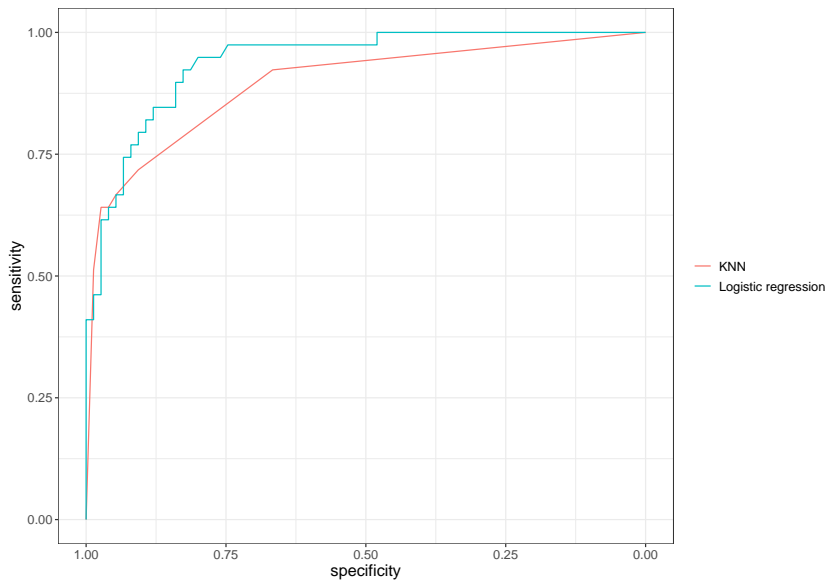
# ROC curve

- By varying  $C$  from 0 to 1, sensitivity and specificity change continuously and trace out the **Receiver Operator Curve (ROC)**.
- The closer the curve sticks to the upper left corner, the better
- Can be used to compare classifiers





## ROC: KNN versus logistic regression



# AUC: Area under the ROC

Single number to quantify performance of classifier:

- $AUC = 1.0$ : distinguishes perfectly between two classes
- $AUC = 0.5$ : classifier no better than guessing randomly
- $0.5 < AUC < 1.0$ : varying degrees of performance.

# AUC: Link with concordance probability

**Concordance probability:** probability that classifier will give a negative sample a lower probability than a positive sample.

The AUC is equal to the concordance probability

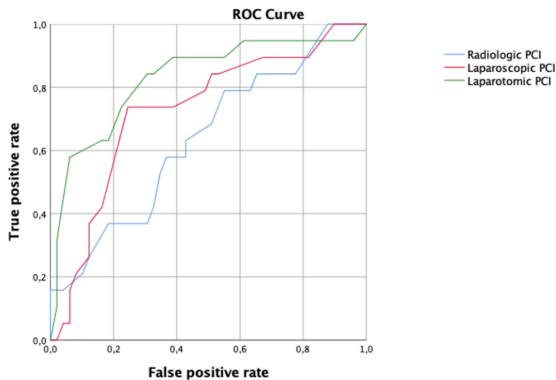
$$\text{AUC} = P(\pi(x_{\text{neg}}) \leq \pi(x_{\text{pos}}))$$

Important for model calibration:

- Often, we don't care much about probability  $\pi$  to belong to the positive class
- But, want negative samples to have lower probability than positive samples

# In clinical research

The ROC and AUC are often reported in clinical research.



**Figure 4.** Receiver operating characteristic (ROC) curve comparing radiologic (blue line), laparoscopic (red line) and laparotomic (green line) peritoneal cancer index (PCI) in women who underwent primary debulking surgery.

Regarding the PCI score (Figure 4), the best performance to predict residual disease, with an AUC 0.83, CI 95% 0.71–0.95 was observed applying the laparotomic PCI, while the accuracy of the radiological PCI and laparoscopic PCI was AUC 0.64, CI 95% 0.49–0.78 and AUC 0.73, CI 95% 0.59–0.86, respectively. The cut-off value associated with the best performance of the laparotomic PCI score was 18.

Figure and text from Di Donna *et al.*, Concordance of Radiological, Laparoscopic and Laparotomic Scoring to Predict Complete Cytoreduction in Women with Advanced Ovarian Cancer. *Cancers* (2023)