FIT2086 Lecture 7
Classification and logistic regression

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Outline

Revision from last week (1)

- Linear regression

$$\mathbb{E}[Y_i] = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \cdots + \beta_p x_{i,p}$$

  - β_0 is the intercept (value of $\mathbb{E}[Y_i]$ when all predictors are zero)
  - β_j is a coefficient (change in $\mathbb{E}[Y_i]$ per unit change in $x_{j,i}$)
- Residuals (errors)

$$e_i = y_i - \beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \cdots - \beta_p x_{i,p}$$

- Residual sum-of-squares

$$\text{RSS}(\beta_0, \beta_1, \ldots, \beta_p) = \sum_{i=1}^{n} e_i^2$$

- Least-squares estimates linear model by finding $\beta_0, \beta_1, \ldots, \beta_p$ that minimise the RSS

Revision from last week (2)

- R^2 goodness-of-fit

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}$$

  where TSS is the sum of squared errors for the mean model
- Model fitting:
  - Overfitting = including unimportant predictors
  - Underfitting = excluding important predictors
- Hypothesis testing to determine if variable is important
  - Test $H_0 : \beta_j = 0$ vs $H_A : \beta_j \neq 0$
  - The smaller the p-value the stronger predictor j is associated with the target
- Model selection methods:
  - Add complexity penalty to the negative log-likelihood
- Finding good models – all subsets selection, stepwise selection

Outline

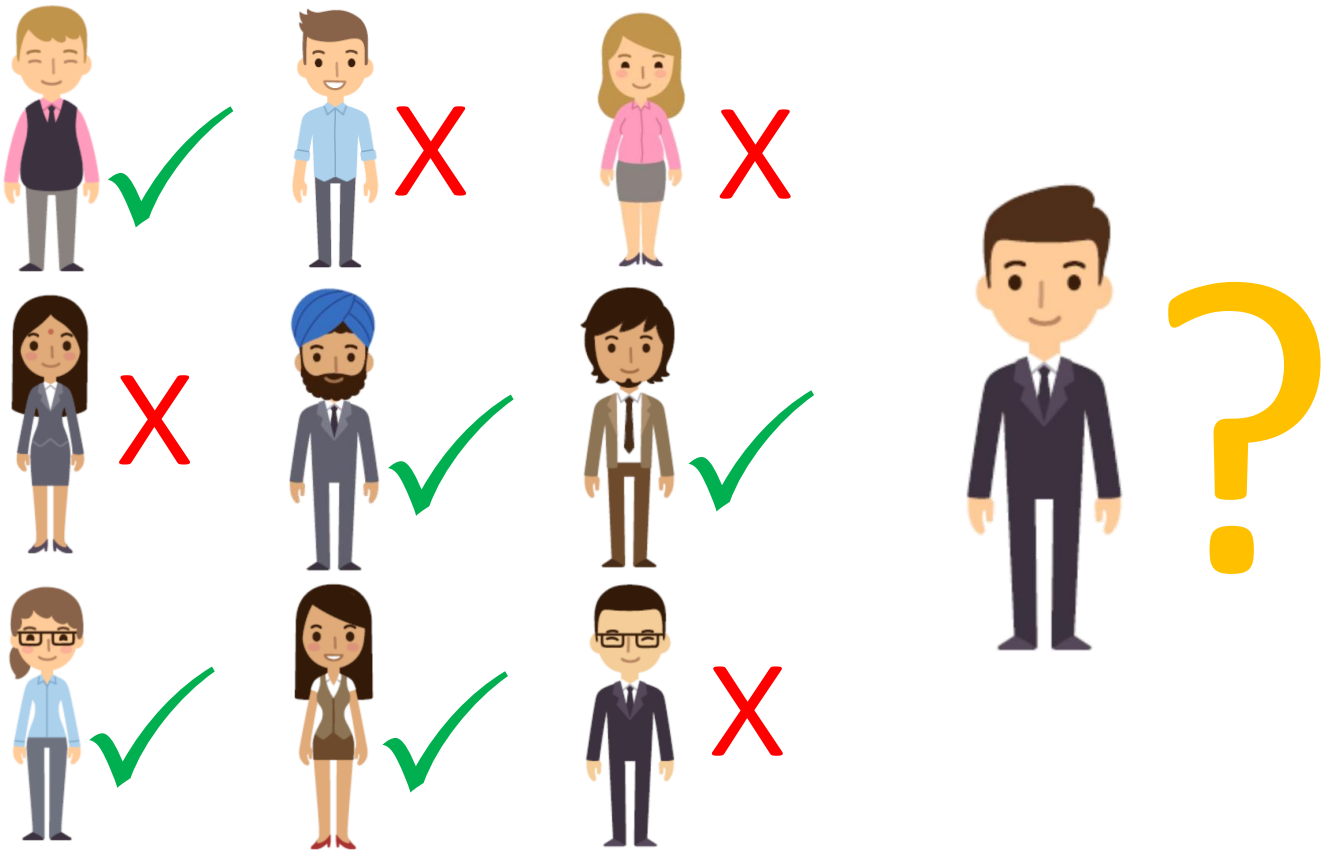
Supervised Learning – recap (1)

- Imagine we have measured $p+1$ variables on n individuals (people, objects, things)
- We would like to predict one of the variables using the remaining p variables
- If the variable we are predicting is categorical, we are performing classification
  - Example: predicting if someone has diabetes from medical measurements.
- If the variable we are predicting is numerical, we are performing regression
  - Example: Predicting the quality of a wine from chemical and seasonal information.

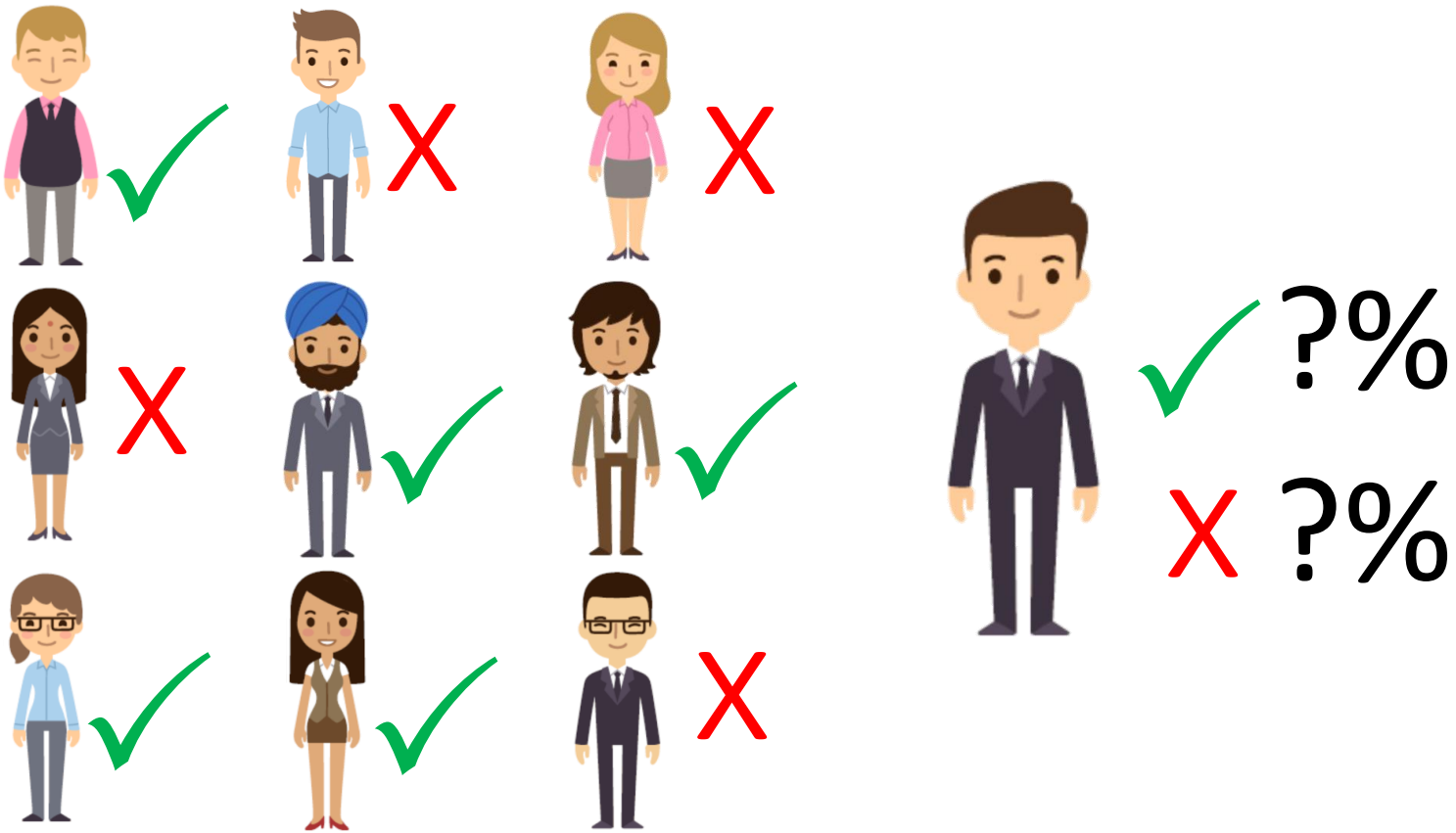
Supervised Learning – recap (2)

- The variable we are predicting is designated the "y" variable
  - We have $(y_1, \ldots, y_n)$
- This variable is often called the:
  - target;
  - response;
  - outcome.
- The other variables are usually designated "X" variables
  - We have $(x_{i,1}, \ldots, x_{i,p})$ for $i = 1, \ldots, n$
- These variables are often called the
  - explanatory variables;
  - predictors;
  - covariates;
  - features;
  - exposures.
- Usually we assume the targets are random variables and the predictors are known without error

Classifiers



Probabilistic classifiers



Classification – Key Slide

- We begin by defining a classifier in terms of probability
- Imagine we have a categorical outcome variable Y
- We also have p predictor variables $X_1, \ldots, X_p$
  $\Rightarrow$ often called features in classification literature
- We can build a classifier for Y using our predictors, i.e., we want to find

$$\mathbb{P}(Y = y \,|\, X_1 = x_1, X_2 = x_2, \ldots, X_p = x_p)$$

- This is the conditional probability of Y given $X_1, \ldots, X_p$.
- Gives us the probability of an individual being in class $Y = y$, given the values of their predictors $x_1, \ldots, x_p$

Classifiers (1)

- Let us now specialise our problem
- Assume that all the predictors are also categorical
- The formula for conditional probability is:

$$\mathbb{P}(Y = y \,|\, X_1 = x_1, \ldots, X_p = x_p) = \frac{\mathbb{P}(Y = y, X_1 = x_1, \ldots, X_p = x_p)}{\mathbb{P}(X_1 = x_1, \ldots, X_p = x_p)}$$

where

- the numerator is the joint probability of $(Y = y, X_1 = x_1, \ldots, X_p = x_p)$;
- the denominator is the marginal probability of $(X_1 = x_1, \ldots, X_p = x_p)$.

Classifiers (2)

- So if we have the joint probability we can build a classifier
- Consider the following example:

	No Heart Disease ($H = 0$)	Heart Disease ($H = 1$)
No Mutation ($M = 0$)	0.35	0.30
Mutation ($M = 1$)	0.10	0.25

Population joint probabilities of heart disease/LDLR mutation.

- Then we have

$$P(H = 1 \,|\, M = 0) = \frac{P(H = 1, M = 0)}{P(M = 0)} = 0.4615$$

$$P(H = 1 \,|\, M = 1) = \frac{P(H = 1, M = 1)}{P(M = 1)} = 0.7143$$

Classifiers (3)

- In our example we got told the population joint probabilities
- But in reality we don't know these – we just have data
- We can try and estimate them from the data
- For our example:
  - our target is heart disease, $H \in \{0, 1\}$,
  - predictor is LDLR mutation, $M \in \{0, 1\}$

Classifiers (4)

- Imagine we had n realisations of this random variables, $\mathbf{m} = (m_1, \ldots, m_n)$ and $\mathbf{h} = (h_1, \ldots, h_n)$
- We could estimate joint probability by proportions

$$F(H = h, M = m) = \frac{1}{n} \sum_{i=1}^{n} I(h_i = h \text{ and } m_i = m)$$

- Weak law of large numbers guarantees this will converge on population proportions for large enough n

Classifiers (5)

- Example, imagine we had
  - $\mathbf{m} = (1, 1, 0, 1, 1, 1, 0, 0)$ and
  - $\mathbf{h} = (1, 0, 1, 1, 0, 0, 1, 0)$
- Then estimated joint probabilities are

	No Heart Disease ($H = 0$)	Heart Disease ($H = 1$)
No Mutation ($M = 0$)	$1/8$	$2/8$
Mutation ($M = 1$)	$3/8$	$2/8$

Estimated joint probabilities of heart disease/LDLR mutation

- Now we can estimate $\mathbb{P}(H = h \,|\, M = m)$ using

$$\frac{F(H = h, M = m)}{F(H = 0, M = m) + F(H = 1, M = m)}$$

- For large n the proportions will be close to population probabilities

Classifiers (6)

- Simple enough – but there is a problem
- For our simple problem H and M were binary
  $\Rightarrow$ only need to estimate $2 \times 2 = 4$ joint probabilities
- What if we had two binary genetic mutations, M_1 and M_2?
- Now have $2 \times 2 \times 2 = 8$ probabilities to estimate
- For p predictors, there are 2^{p+1} probabilities to estimate
  $\Rightarrow$ exponential growth in p
- This rapidly outstrips our sample size n no matter how big n is

Classifiers (7)

- We need to constrain the problem
- Two simple approaches popular in literature

- Naïve Bayes classifiers
  - Make simplifying assumptions about joint probabilities
  - Easily handle categorical predictors
  - Easily handles multi-class targets
  - Popular in text mining and classification
  - We don't examine – but simple enough for you to learn yourself if interested

- Logistic regression
  - Adaptation of the linear model, widely used
  - Directly estimates conditional probabilities
  - Handles categorical and continuous predictors
  - More difficult to handle multi-class targets

Logistic Regression (1)

- The direct approach we examined used the joint probabilities to find the conditional probability of the targets using Bayes rule.
- This is (potentially) a round-about way of solving problem
- Logistic regression directly models the conditional probabilities
  $\Longrightarrow$ extends the linear regression model to binary data
- This approach also extends to other classification methods
  - Decision trees and forests (in two weeks time)
  - Support vector machines
  - Neural networks
  - And many more ...

Logistic Regression (2)

- Given predictors $x_{i,1}, \ldots, x_{i,p}$ multiple linear regression predicts the target as

$$\mathbb{E}\left[Y_i\right] = \eta_i = \beta_0 + \sum_{j=1}^{p} \beta_j x_{i,j}$$

  where η_i is shorthand for our linear predictor for individual i
- We find $\beta_0, \beta_1, \ldots, \beta_j$ by least-squares
- If our target is binary, we *could* fit a linear model using least-squares and approximate

$$\mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p}) \approx \eta_i$$

- Serious problem: our predicted value η_i could be less than zero, or greater than one, for certain values of the features!

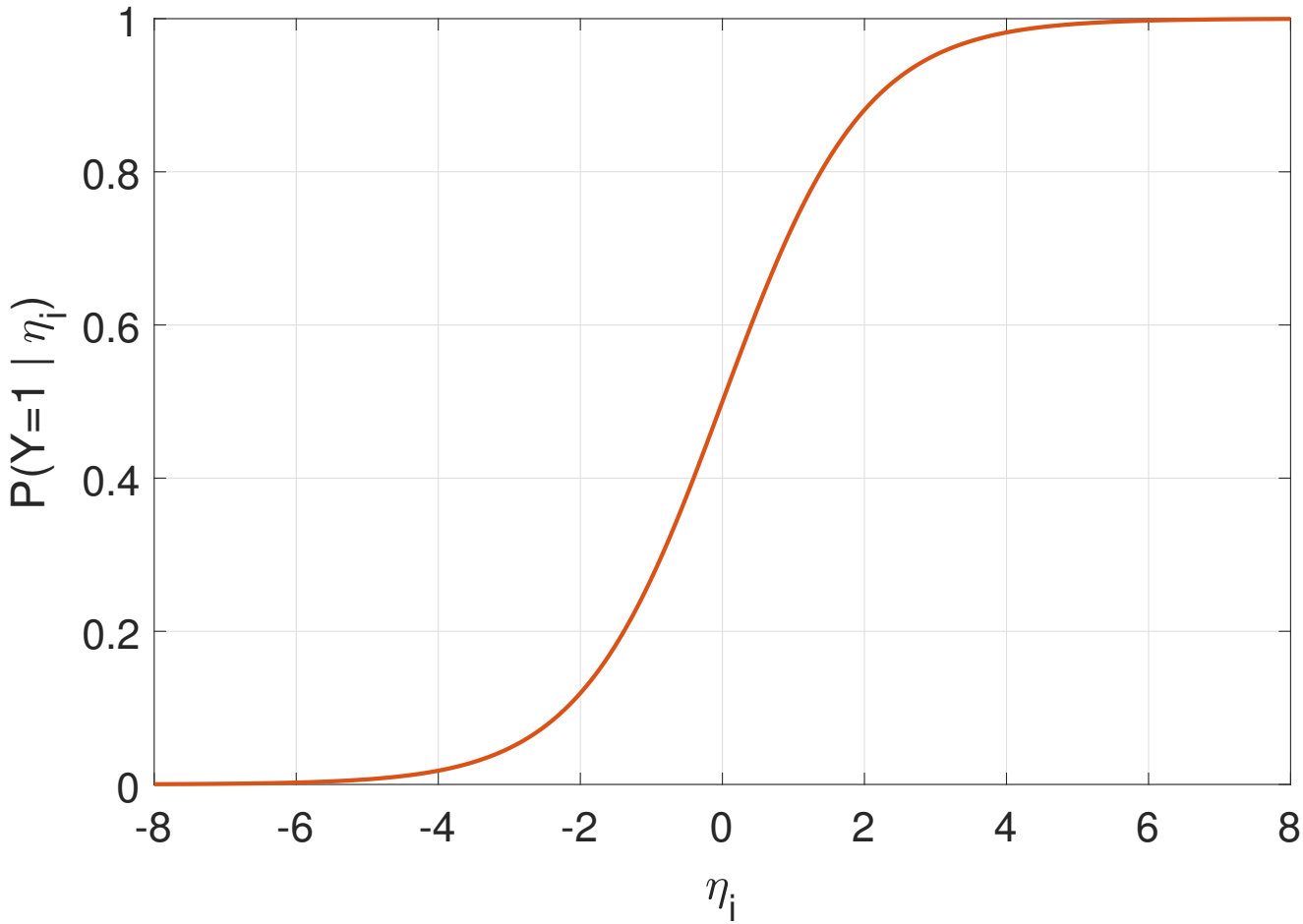
Logistic Regression (3)

- One solution is to bound η_i to (0,1)
- There exist a lot of ways of bounding η_i
- Logistic regression chooses to use the logistic function

$$\mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p}) = \frac{1}{1 + \exp(-\eta_i)}$$

- This function smoothly
  - tends to 0 as $\eta_i \equiv \beta_0 + \sum_{j=1}^{p} \beta_j x_{i,j} \to -\infty$;
  - tends to 1 as $\eta_i \equiv \beta_0 + \sum_{j=1}^{p} \beta_j x_{i,j} \to \infty$.

Logistic Regression (4)



The logistic function. As $\eta_i \to -\infty$, then $\mathbb{P}(Y_i = 1 \,|\, \eta_i) \to 0$, and as $\eta_i \to \infty$, then $\mathbb{P}(Y_i = 1 \,|\, \eta_i) \to 1$.

Logistic Regression (5)

- We can interpret the logistic model in terms of log-odds
- Given $\mathbb{P}(Y = 1)$ and $\mathbb{P}(Y = 0)$, the odds for $Y = 1$ are

$$\mathbb{P}(Y = 1)/\mathbb{P}(Y = 0)$$

- They reflect how *many more times likely* the event $Y = 1$ is to occur than the event $Y = 0$
- Example: probability of a heads from coin toss is 0.75; then
  - the odds for seeing a head are $0.75/0.25 = 3$;
  - the odds for seeing a tail are $0.25/0.75 = 1/3$.
- The log-odds make this symmetric:
  - the log-odds for seeing a head are $\log(0.75/0.25) = \log 3$;
  - the log-odds for seeing a tail are $\log(0.25/0.75) = -\log 3$.

Logistic Regression (6) – Key Slide

- A logistic regression models the conditional log-odds as

$$\log\left(\frac{\mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p})}{\mathbb{P}(Y_i = 0 \,|\, x_{i,1}, \ldots, x_{i,p})}\right) = \beta_0 + \sum_{j=1}^{p} \beta_j x_{i,j} \equiv \eta_i$$

- So the log-odds of a success, given the values of the predictors, is equal to the linear predictor η_i
  - the intercept β_0 is the log-odds when all the predictors are zero, i.e., $x_{i,1} = x_{i,2} = \ldots = x_{i,p} = 0$;
  - the coefficient β_j is the increase in log-odds per unit change of predictor x_j

- The odds for $Y = 1$ are $\exp(\eta_i)$
  - when $\eta_j > 0$, $Y = 1$ is more likely than $Y = 0$, and $e^{\eta_i} > 1$
  - when $\eta_j < 0$, $Y = 0$ is more likely than $Y = 1$, and $e^{\eta_i} < 1$

Logistic Regression (7)

- To see that setting log-odds equal to η_i leads to logistic regression, write:

$$\log\left(\frac{\mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p})}{1 - \mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p})}\right) = \eta_i$$

- Now exponentiate both sides

$$\frac{\mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p})}{1 - \mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p})} = \exp(\eta_i)$$

- Solving for $\mathbb{P}(Y_i = 1 \,|\, \cdots)$ yields

$$\mathbb{P}(Y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,p}) = \frac{\exp(\eta_i)}{1 + \exp(\eta_i)} = \frac{1}{1 + \exp(-\eta_j)}$$

(noting $1/e^a = e^{-a}$) which is the logistic function.

Fitting Logistic Regression Models (1)

- How to estimate the regression coefficients?
- Many packages use maximum likelihood
- Let $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)$ be our regression coefficients
- Assume our targets are independent RVs;
- Each Y_i is then distributed as per a Bernoulli distribution

$$Y_i \sim \mathrm{Be}\left(\theta_i(\beta_0, \boldsymbol{\beta})\right)$$

where

$$\theta_i(\beta_0, \boldsymbol{\beta}) = \frac{1}{1 + \exp\left(-\beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j}\right)}$$

is the probability of success for individual i, given the predictors $x_{i,1}, \ldots, x_{i,p}$ and the parameters $\beta_0, \beta_1, \ldots, \beta_p$.

Fitting Logistic Regression Models (2)

- If $\mathbf{y} = (y_1, \ldots, y_n)$ are binary targets, the likelihood for a logistic regression is then

$$\begin{aligned} p(\mathbf{y} \,|\, \beta_0, \boldsymbol{\beta}) &= \prod_{i=1}^{n} p(y_i | \beta_0, \boldsymbol{\beta}) \\ &= \prod_{i=1}^{n} \theta_i(\beta_0, \boldsymbol{\beta})^{y_i} \left(1 - \theta_i(\beta_0, \boldsymbol{\beta})\right)^{1-y_i} \end{aligned}$$

  from the pdf of the Bernoulli distribution.

- The negative log-likelihood is then

$$L(\mathbf{y} \,|\, \beta_0, \boldsymbol{\beta}) = -\sum_{i=1}^{n} \left[y_i \log \theta_i(\beta_0, \boldsymbol{\beta}) + (1 - y_i) \log \left(1 - \theta_i(\beta_0, \boldsymbol{\beta})\right) \right]$$

Fitting Logistic Regression Models (3)

- The negative log-likelihood is then

$$\begin{aligned} L(\mathbf{y} \mid \beta_0, \boldsymbol{\beta}) &= -\sum_{i=1}^{n} \left[y_i \log \theta_i(\beta_0, \boldsymbol{\beta}) + (1 - y_i) \log \left(1 - \theta_i(\beta_0, \boldsymbol{\beta})\right) \right] \\ &= -y_i \eta_i + \log \left(1 + e^{\eta_i}\right) \end{aligned}$$

  where $\eta_i = \beta_0 + \sum_{j=1}^{p} \beta_j x_{i,j}$ is the log-odds (linear predictor)

- The values $\hat{\beta}_0$, $\hat{\boldsymbol{\beta}}$ of β_0 and $\boldsymbol{\beta}$ that minimise this quantity are the maximum likelihood estimates

- No closed form solution exists, must be found numerically
  $\Longrightarrow$ But luckily always only a single, global minimum

- Time complexity roughly cubic in number of predictors p

Goodness-of-fit

- The minimised negative log-likelihood

$$L(\mathbf{y} \mid \hat{\beta}_0, \hat{\boldsymbol{\beta}})$$

  is a measure of goodness-of-fit of a model.
- The difference in minimised negative log-likelihoods

$$L(\mathbf{y} \mid \hat{\beta}_0) - L(\mathbf{y} \mid \hat{\beta}_0, \hat{\boldsymbol{\beta}})$$

  is a measure similar to R^2; (bigger differences $\Rightarrow$ better fit)
- Relative to model with an intercept only (no predictors); equivalent to assuming $P(Y = 1)$ is same for all individuals
- Sometimes maximised log-likelihood is reported instead, or two times (negative) log-likelihoods; depends on package

Predicting with a Logistic Regression

- Once we have found estimates $\hat{\beta}_0$, $\hat{\boldsymbol{\beta}}$ it is easy to predict with a logistic regression
- For some new values of features $x'_1, \ldots, x'_p$, we calculate

$$\hat{\eta} = \hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x'_j$$

- Then we can estimate the probability that $Y' = 1$ for these features:

$$\mathbb{P}(Y' = 1 \,|\, x'_1, \ldots, x'_p) = \frac{1}{1 + \exp(-\hat{\eta})}$$

- If we need to guess at most likely class, choose value of Y' that maximises this probability

Extensions

- A strength of logistic regression is that it builds on the tools used in linear regression
- Handle categorical predictors same as linear regression
  $\Rightarrow$ form new indicator variables for each category
- They can also handle non-linearities the same way as linear regressions, e.g.,
  - logarithmic transformations of predictors;
  - polynomial transformations of predictors.

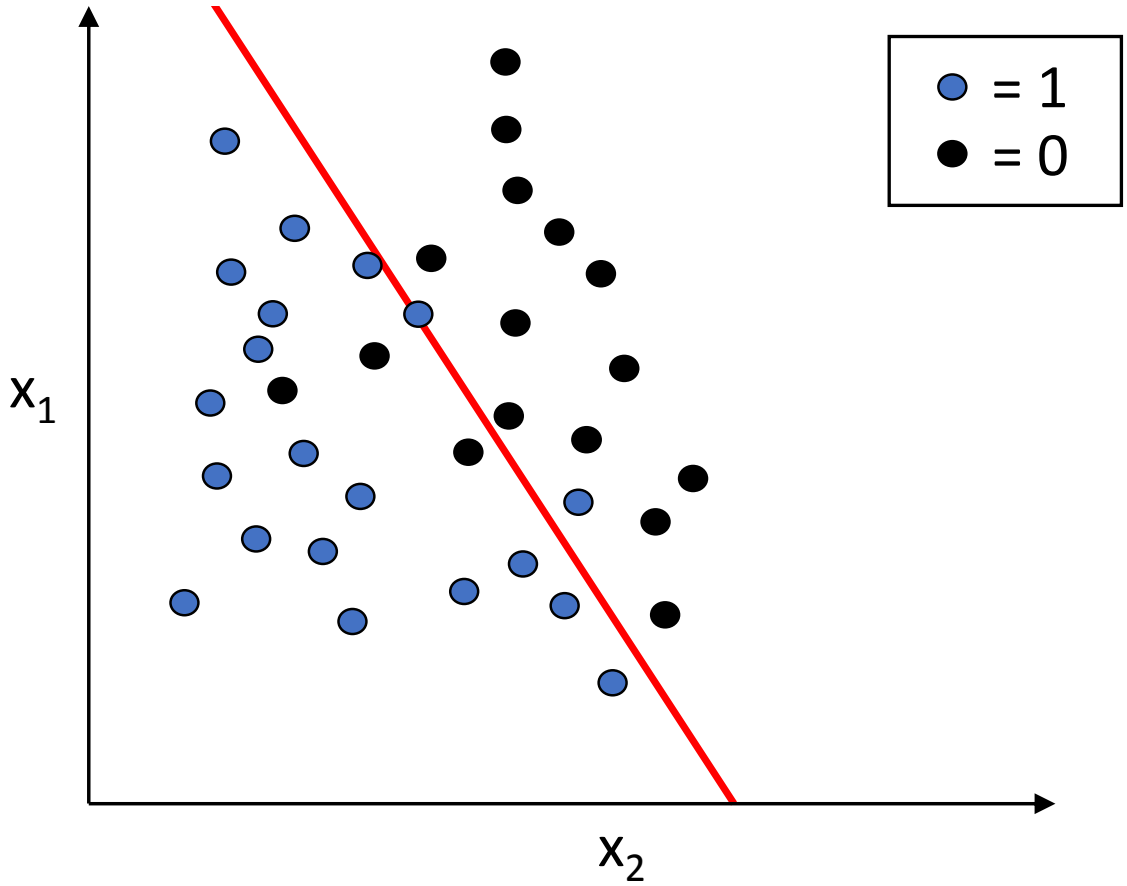
Finding logistic regression models

- Same approaches as for linear models
  $\Rightarrow$ try to avoid under/over-fitting
- Hypothesis testing $H_0 : \beta_j = 0$ vs $H_A : \beta_j \neq 0$
  - Smaller p-value $\Rightarrow$ more likely predictor j is important
- Model selection
  - Use penalized likelihood:

$$L(\mathbf{y} \,|\, \hat{\beta}_0, \hat{\boldsymbol{\beta}}) + k\alpha_n$$

    where:
    - k is number of predictors in model;
    - $\alpha_n = 1$ for Akaike information criterion (AIC);
    - $\alpha_n = 3/2$ for Kullback information criterion (KIC);
    - $\alpha_n = (1/2)\log n$ for Bayesian information criterion (BIC).
  - Sometimes two times these quantities are used (e.g., in R)
- Forward/backwards selection of predictors

Logistic regressions are linear



A logistic regression seperates successes from failures by using a linear seperation surface. The line is defined by the values of the two features x_1 and x_2 that satisfy $\mathbb{P}(Y = 1 \,|\, x_1, x_2) = 1/2$. For models with p features, this becomes a p-dimensional plane.

Outline

Performance Measures for Classifiers (1)

- Imagine we have trained a classifier on some data (logistic regression or something else)
- We now get a new body of data and want to test how well our classifier performs
- What measures of performance exist for classification problems?
  - Classification error
  - Sensitivity and specificity
  - Area-under-the-curve (AUC)
  - Logarithmic loss

Performance Measures for Classifiers (2)

- Let $\mathbf{y}' = (y'_1, \ldots, y'_{n'})$ be a vector of new data to test on
  - For simplicity, let us assume y'_i is binary
- Let $\mathbf{x}'_j = (x'_{1,j}, \ldots, x'_{n',j})$ be the vector for feature j
- For each of the new individuals, we can calculate our best guess at which class it belongs to using:

$$\hat{y}'_i = \underset{y \in \{0,1\}}{\arg\max} \left\{ \mathbb{P}(Y'_i = y \,|\, x'_{i,1}, \ldots, x'_{i,p}) \right\}$$

where the probabilities are estimated using the model we have learned from our training data

Classification Accuracy (1) – Key Slide

- The most straightforward measure of performance is classification accuracy
- This is given by:

$$\text{CA} = \frac{1}{n'} \sum_{i=1}^{n'} I\left(y_i' = \hat{y}_i'\right)$$

  where $I(\cdot)$ is one if the condition inside the parenthesis is met, and a zero otherwise
- The proportion of times our classifier correctly guesses the class of a new individual
- This ranges from 0 (perfectly incorrect), through to $1/2$ (only as good as random guessing) to 1 (perfectly correct)
- Realistically $1/2$ is worst accuracy – if $< 1/2$ we can swap our classification output

Classification Accuracy (2)

- More generally, we can form a confusion matrix

	$y_i = 0$	$y_i = 1$
$\hat{y}_i = 0$	True Negative (TN)	False Negative (FN)
$\hat{y}_i = 1$	False Positive (FP)	True Positive (TP)

- Classification accuracy is then

$$\text{CA} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

Specificity and Sensitivity (1) – Key Slide

- Can form other useful information
- Sensitivity is the true positive rate:

$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

- Specificity is the true negative rate:

$$\text{TNR} = \frac{\text{TN}}{\text{TN} + \text{FP}}$$

  - Sensitivity of 1 means we correctly classify all individuals for which $y_i' = 1$
  - Specificity of 1 means we correctly classify all individuals for which $y_i' = 0$
- High sensitivity can be achieved at expense of decreased sensitivity, and vice versa

Specificity and Sensitivity (2)

- Set a detection threshold $T \in (0, 1)$ for our classifier.
- For each of the new individuals, we say that $\hat{y}'_i = 1$ if

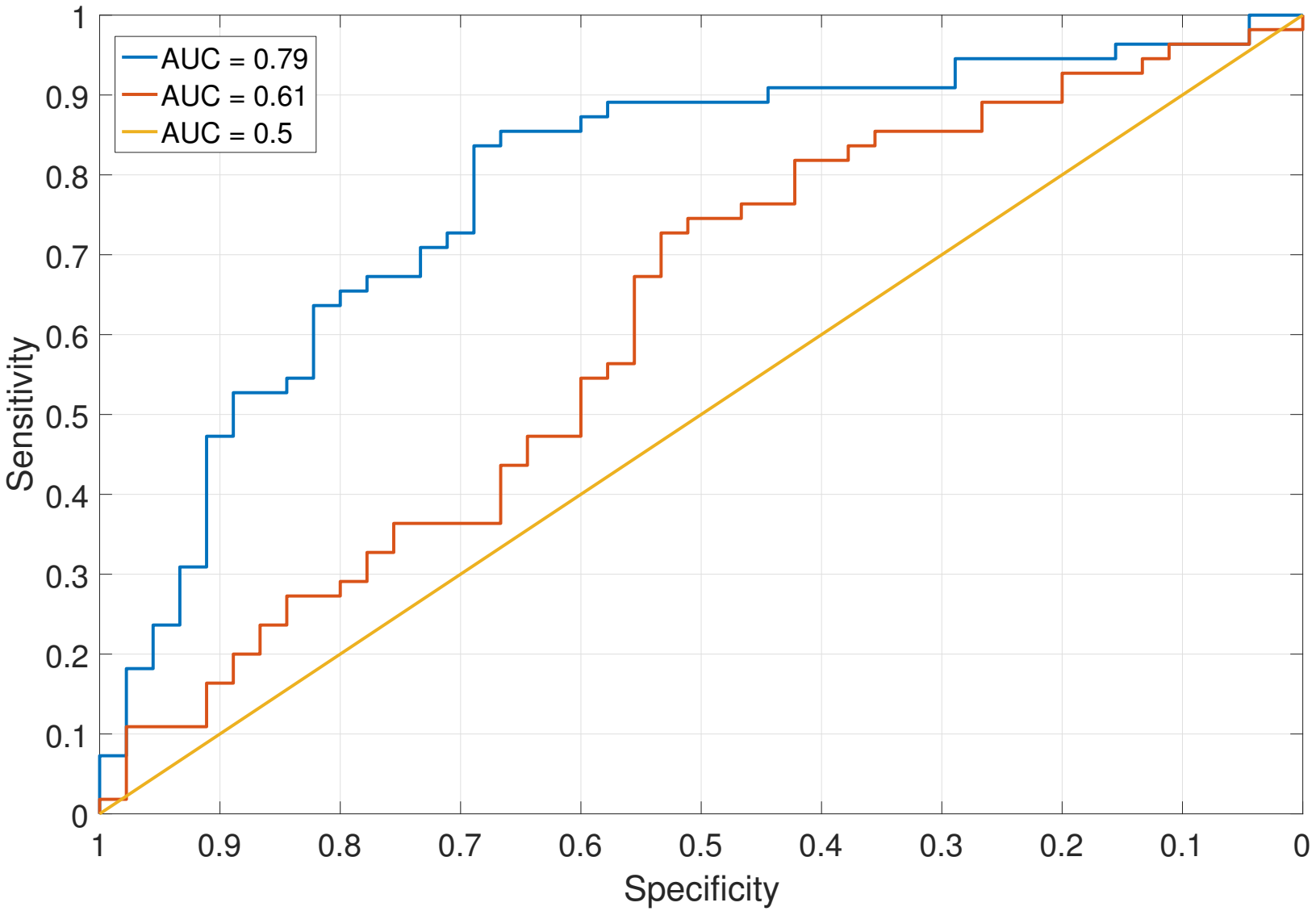
$$\mathbb{P}(Y'_i = 1 \,|\, x'_{i,1}, \ldots, x'_{i,p}) \geq T,$$

  otherwise they are in class $\hat{y}'_i = 0$.
- Classifying an individual based on which class is more likely is equivalent to using $T = 1/2$
- Varying T produces different values of sensitivity, specificity
- Let $\mathrm{TPR}(T)$, $\mathrm{TNR}(T)$ be the sensitivity, specificity for threshold T
  - Small $T \Rightarrow$ increased sensitivity;
  - Large $T \Rightarrow$ increased specificity

Area-under-the-curve (AUC) (1)

- If we vary T from 0 to 1 we get a range of different classification rules $\Longrightarrow$ each will yield a different TPR and TPN
- We can plot these different values to get a "reciever operating curve"
- The area under this curve is called the AUC
- The bigger the area, the better the classifier

Area-under-the-curve (AUC) (2)



Area-under-the-curve (AUC) (2) – Key Slide

- AUC is always between 0 and 1
  - AUC of 1 means we can achieve perfect classification;
  - AUC of 0 means we can achieve perfect misclassification;
  - AUC of $1/2$ means we do no better than a random guess.
- How to interpret AUC?
- An AUC of p means that if we randomly sampled an individual i from our test group for whom $y'_i = 1$, and randomly sampled an individual k from our test group for whom $y'_k = 0$ then

$$\mathbb{P}\left[\mathbb{P}(Y'_i = 1 \,|\, x'_{i,1}, \ldots, x'_{i,p}) > \mathbb{P}(Y'_k = 1 \,|\, x'_{k,1}, \ldots, x'_{k,p})\right] = p$$

  that is, it is the probability that a random individual i sampled from class 1 will be rated more likely to be in class 1 than random individual k sampled from class 0.

Logarithmic Loss (1) – Key Slide

- The final performance measure we consider is logarithmic loss
- For each sample i in our test group, we score

$$L(y_i') = \begin{cases} -\log \mathbb{P}(Y_i' = 1 \,|\, x_{i,1}', \ldots, x_{i,p}') & \text{for } y_i' = 1 \\ -\log \mathbb{P}(Y_i' = 0 \,|\, x_{i,1}', \ldots, x_{i,p}') & \text{for } y_i' = 0 \end{cases}.$$

  This is the negative-log-probability of the test data point y_i' under our classification model
- The total logarithmic loss is then

$$L(\mathbf{y}') = \sum_{i=1}^{n} L(y_i')$$

  $\Longrightarrow$ the negative-log-likelihood of this new, future data
- Smaller the score, the better our classifier predicts this data
- Log-loss measures how well the model predicts the probabilities of an individual being in a class (calibration)

Logarithmic Loss (2)

- Classification accuracy measures how good our guesses at the most likely class are
- Log-loss measures how well the model predicts the probabilities of an individual being in a class
- Why is this important?
- It tells you how confident you should be in your predicted class
- Example: Both $P(Y = 1 \,|\, x_1, \ldots, x_p) = 0.501$ and $P(Y = 1 \,|\, x_1, \ldots, x_p) = 0.99$ would predict the most likely class for Y to be $Y = 1$.
  $\Longrightarrow$ we are much more confident about latter than the former
- Estimating conditional probabilities well lets us get better idea of how confident we should we in our predicted classes

Reading/Terms to Revise

- Terms you should know:
  - Conditional independence
  - Odds, log-odds
  - Logistic regression
  - Classification accuracy
  - Specificity, sensitivity
  - Area-under-the-curve (AUC)
  - Logarithmic loss
- Next week we will be examined some more recent developments in fitting and estimating linear and logistic regression models.