# ETC3250/5250: Introduction to Machine Learning

## Categorical response regression

Lecturer: *Professor Di Cook*

Department of Econometrics and Business Statistics

ETC3250.Clayton-x@monash.edu

Week 3a

# Categorical responses

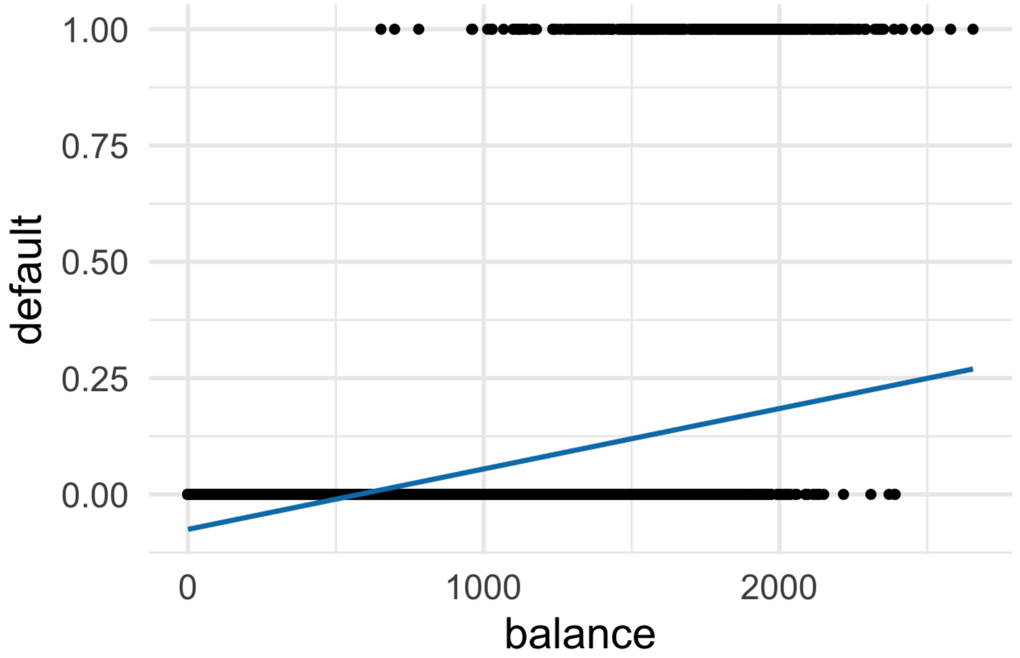
In **classification**, the output $Y$ is a categorical variable. For example,

- Loan approval: $Y \in \{\text{successful}, \text{unsuccessful}\}$
- Type of business culture: $Y \in \{\text{clan}, \text{adhocracy}, \text{market}, \text{hierarchical}\}$
- Historical document author: $Y \in \{\text{Austen}, \text{Dickens}, \text{Imitator}\}$
- Email: $Y \in \{\text{spam}, \text{ham}\}$

Map the categories to a numeric variable, or possibly a binary matrix.

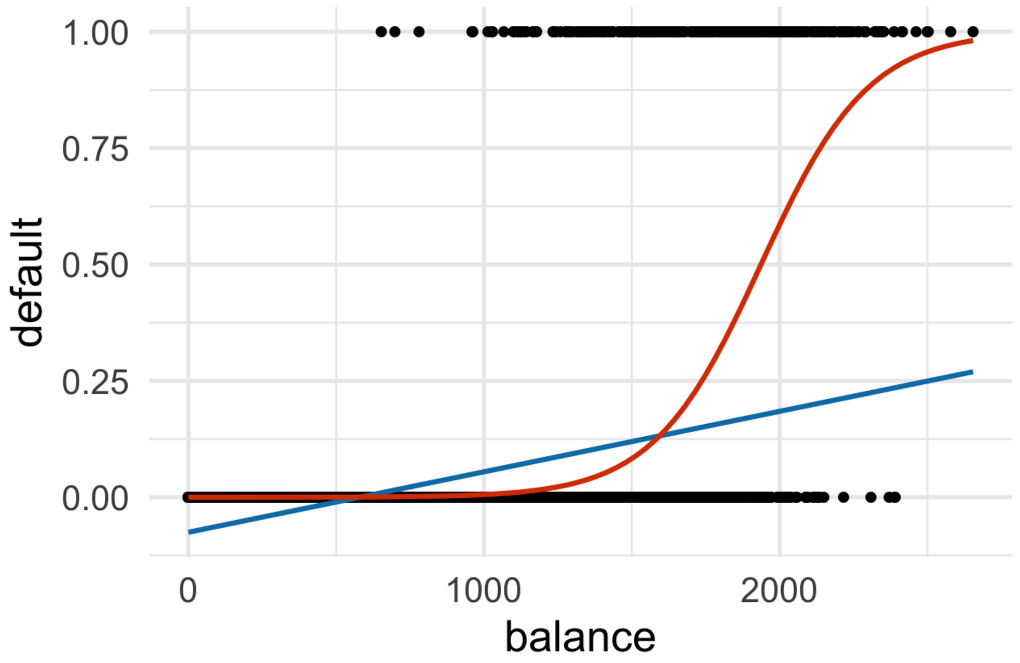
# When linear regression is not appropriate

Consider the following data `simcredit` in the ISLR R package (textbook) which looks at the default status based on credit balance.




> **?** Why is a linear model less than ideal for this data?

# Modelling binary responses




Orange line is a loess smooth of the data. It's much better than the linear fit.

- To model **binary data**, we need to link our **predictors** to our response using a *link function*. Another way to think about it is that we will transform $Y$ to convert it to a proportion, and then build the linear model on the transformed response.
- There are many different types of link functions we could use, but for a binary response we typically use the logistic link function.

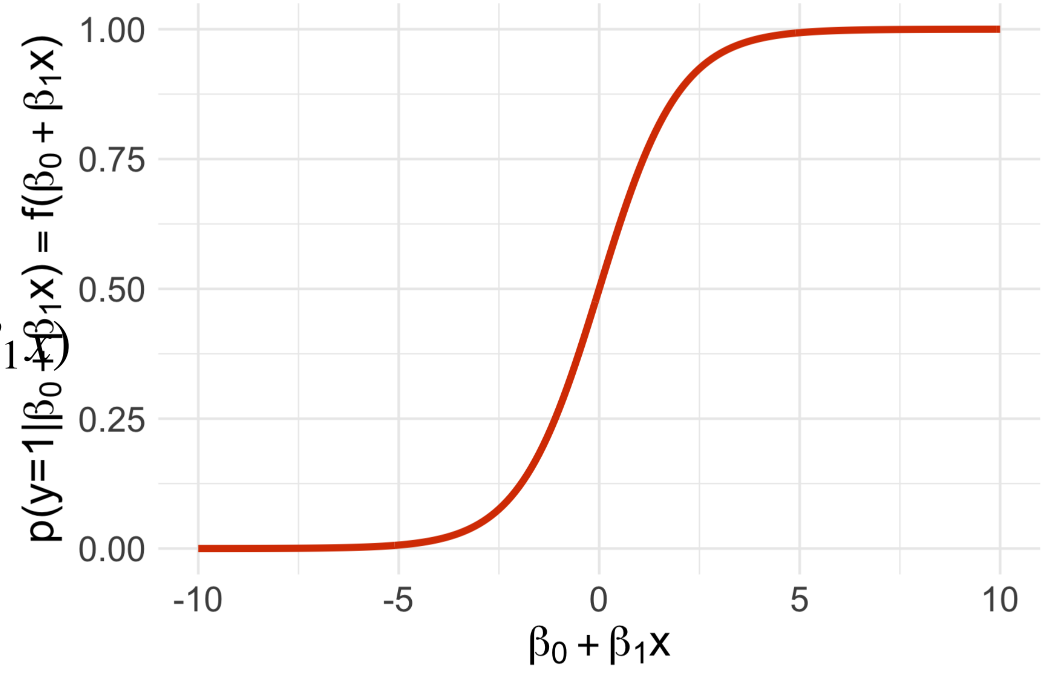
# The logistic function

Instead of predicting the outcome directly, we instead predict the probability of being class 1, given the (linear combination of) predictors, using the logistic link function.

$$p(y = 1|\beta_0 + \beta_1 x) = f(\beta_0 + \beta_1 x)$$

where

$$f(\beta_0 + \beta_1 x) = \frac{e^{\beta_0+\beta_1 x}}{1 + e^{\beta_0+\beta_1 x}}$$



# Logistic function

Transform the function:

$$y = \frac{e^{\beta_0+\beta_1 x}}{1 + e^{\beta_0+\beta_1 x}}$$

$\longrightarrow y = \frac{1}{1/e^{\beta_0+\beta_1 x}+1}$

$\longrightarrow 1/y = 1/e^{\beta_0+\beta_1 x} + 1$

$\longrightarrow 1/y - 1 = 1/e^{\beta_0+\beta_1 x}$

$\longrightarrow \frac{1}{1/y-1} = e^{\beta_0+\beta_1 x}$

$\longrightarrow \frac{y}{1-y} = e^{\beta_0+\beta_1 x}$

$\longrightarrow \log_e \frac{y}{1-y} = \beta_0 + \beta_1 x$

Transforming the response $\log_e \frac{y}{1-y}$ makes it possible to use a linear model fit.

The left-hand side, $\log_e \frac{y}{1-y}$, is known as the log-odds ratio or logit.

# The logistic regression model

The fitted model, where $P(Y = 0|X) = 1 - P(Y = 1|X)$ is then written as:

$$\log_e \frac{P(Y=1|X)}{1-P(Y=1|X)} = \beta_0 + \beta_1 X$$

When there are more than two categories:

- the formula can be extended, using dummy variables.
- follows from the above, extended to provide probabilities for each level/category, and the last category is 1-sum of the probabilities of other categories.
- the sum of all probabilities has to be 1.

# Interpretation

- **Linear regression**
  - $\beta_1$ gives the average change in $Y$ associated with a one-unit increase in $X$
- **Logistic regression**
  - Because the model is not linear in $X$, $\beta_1$ does not correspond to the change in response associated with a one-unit increase in $X$
  - However, increasing $X$ by one unit changes the log odds by $\beta_1$ or equivalently it multiplies the odds by $e^{\beta_1}$

# Maximum Likelihood Estimation

Given the logistic $p(x_i) = \frac{1}{e^{-(\beta_0+\beta_1 x_i)}+1}$ choose parameters $\beta_0, \beta_1$ to maximize the likelihood:

$$l_n(\beta_0, \beta_1) = \prod_{i=1}^{n} p(x_i)^{y_i}(1 - p(x_i))^{1-y_i}.$$

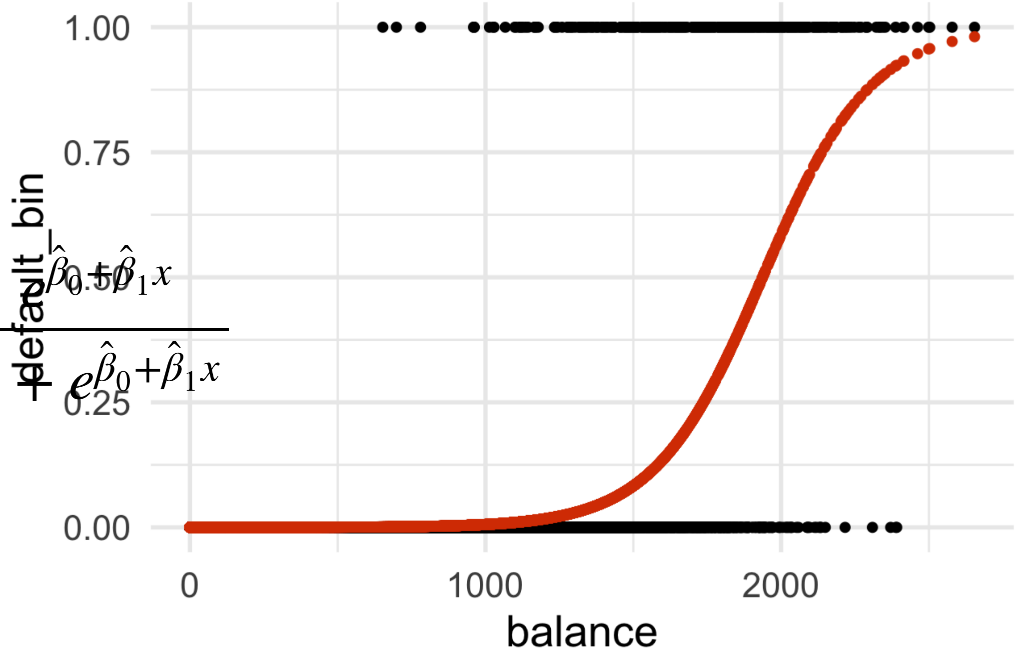
It is more convenient to maximize the *log-likelihood*:

$$\begin{aligned} \log l_n(\beta_0, \beta_1) &= \sum_{i=1}^{n} \Big( y_i \log p(x_i) + (1 - y_i) \log(1 - p \\ &= \sum_{i=1}^{n} \Big( y_i(\beta_0 + \beta_1 x_i) - \log\left(1 + e^{\beta_0+\beta_1 x}\right. \end{aligned}$$

# Making predictions

With estimates from the model fit, $\hat{\beta}_0, \hat{\beta}_1$ we can predict the **probability of belonging to class 1** using:

$$p(y = 1|\hat{\beta}_0 + \hat{\beta}_1 x) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 x}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 x}}$$




Orange points are fitted values, $\hat{y}_i$. Black points are observed response, $y_i$ (either 0 or 1).

- Round to 0 or 1 for class prediction.
- Residual could be calculated as the difference between observed and predicted. Mostly, the misclassification (correct or incorrect) is used to assess the model fit.

# Fitting credit data in R

We use the `glm` function in R to fit a logistic regression model. The `glm` function can support many response types, so we specify `family="binomial"` to let R know that our response is *binary*.

```
logistic_mod <- logistic_reg() %>%
  set_engine("glm") %>%
  set_mode("classification") %>%
  translate()

logistic_fit <-
  logistic_mod %>%
  fit(default ~ balance,
      data = simcredit)
```

# Examine the fit

```
tidy(logistic_fit)
```

```
## # A tibble: 2 × 5
##   term        estimate std.error statistic   p.value
##   <chr>          <dbl>     <dbl>     <dbl>     <dbl>
## 1 (Intercept) -10.7     0.361        -29.5 3.62e-191
## 2 balance       0.00550 0.000220      25.0 1.98e-137
```

```
glance(logistic_fit)
```

```
## # A tibble: 1 × 8
##   null.deviance df.null logLik   AIC   BIC deviance df.residual  nobs
##           <dbl>   <int>  <dbl> <dbl> <dbl>    <dbl>       <int> <int>
## 1         2921.    9999  -798. 1600. 1615.    1596.        9998 10000
```

# Write out the model

$\hat{\beta}_0 = -10.6513306$

$\hat{\beta}_1 = 0.0054989$

# Model fit summary

Null model deviance 2920.6 (think of this as TSS)

Model deviance 1596.5 (think of this as RSS)

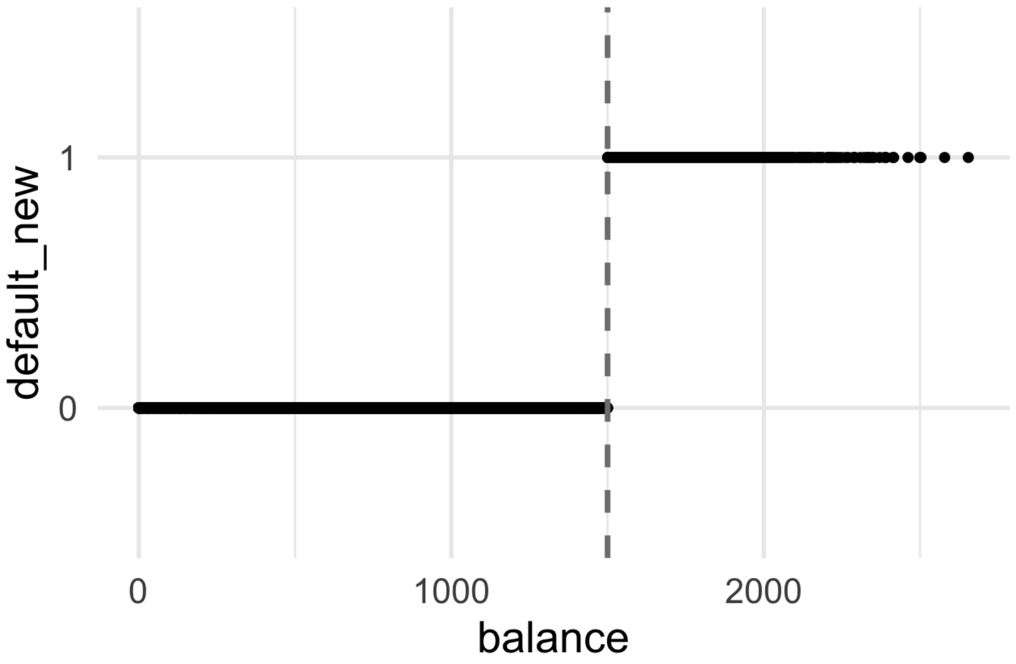
# Check model fit

```
simcredit_fit <- augment(logistic_fit, simcredit)
simcredit_fit %>%
  count(default, .pred_class) %>%
  pivot_wider(names_from = "default", values_from = n)

## # A tibble: 2 × 3
##   .pred_class    No   Yes
##   <fct>       <int> <int>
## 1 No           9625   233
## 2 Yes            42   100
```

Note: Residuals not typically used.

# A warning for using GLMs!




Logistic regression model fitting fails when the data is *perfectly* separated.

MLE fit will try and fit a step-wise function to this graph, pushing coefficients sizes towards infinity and produce large standard errors.

Pay attention to warnings!

```
logistic_fit <-
  logistic_mod %>%
  fit(default_new ~ balance,
      data = simcredit)

## Warning: glm.fit: algorithm did not converge

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

# More on supervised classification to come

Logistic regression is a technique for supervised classification. We'll see a lot more techniques: linear discriminant analysis, trees, forests, support vector machines, neural networks.

Lecturer: *Professor Di Cook*

Department of Econometrics and Business Statistics

ETC3250.Clayton-x@monash.edu

Week 3a