Probability Modeling

DS 6030 | Fall 2024

prob-modeling.pdf

Contents

1 Probability Modeling Intro

1.1 Credit Card Default data (`Default`)

The textbook *An Introduction to Statistical Learning (ISL)* has a description of a simulated credit card default dataset. The interest is on predicting whether an individual will default on their credit card payment.

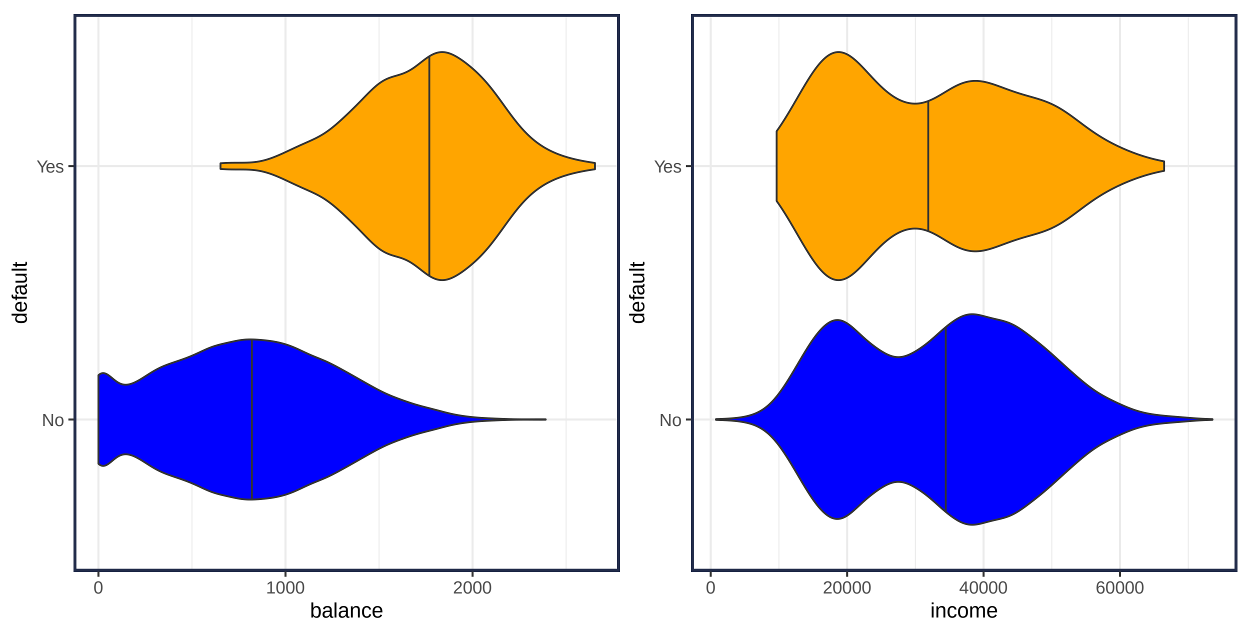
```r
data(Default, package="ISLR")
```

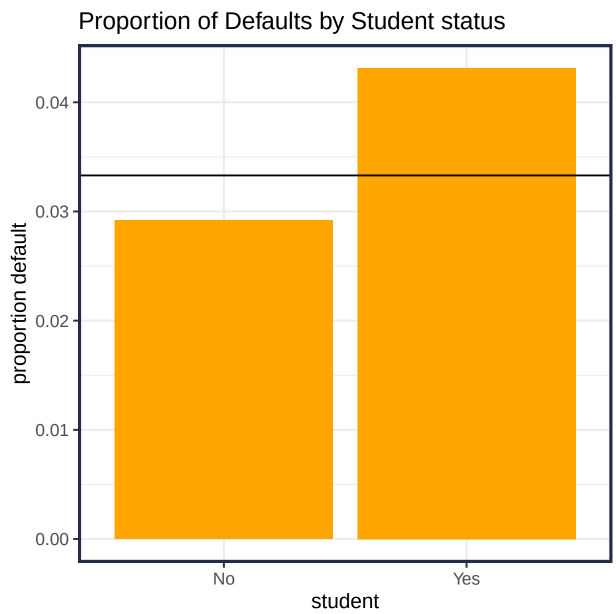
The variables are:

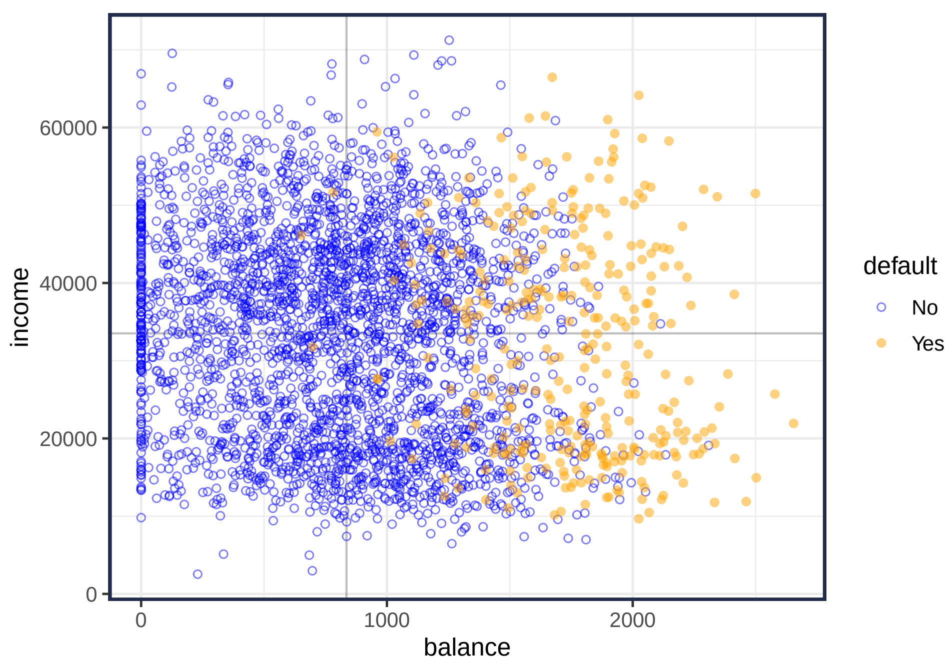
- *outcome variable* is categorical (factor) `Yes` and `No`, (`default`)
- the categorical (factor) variable (`student`) is either `Yes` or `No`
- the average balance a customer has after making their monthly payment (`balance`)
- the customer's income (`income`)

default	student	balance	income
No	No	396.5	41970
No	No	913.6	46907
No	Yes	561.4	21747
Yes	Yes	1889.3	22652
No	No	491.0	37836
No	Yes	282.2	19809

```r
Default %>% summary
#>  default    student       balance          income     
#>  No :9667   No :7056   Min.   :   0   Min.   :  772  
#>  Yes: 333   Yes:2944   1st Qu.: 482   1st Qu.:21340  
#>                        Median : 824   Median :34553  
#>                        Mean   : 835   Mean   :33517  
#>                        3rd Qu.:1166   3rd Qu.:43808  
#>                        Max.   :2654   Max.   :73554  
```




Proportion of Defaults by Student status
proportion default
0.04
0.03
0.02
0.01
0.00
No
Yes
student


income
60000
40000
20000
0
0
1000
2000
balance
default
No
Yes

Your Turn #1 : Credit Card Default Modeling

How would you construct a model to predict the risk of default?

Linear Regression
Expected Value E[Y|X] = Pr(Y = 1|X)*1 + Pr(Y=0|X)*0
E[Y|X] = Pr(Y=1|X)

For linear regression, our loss is MSE (Means Squared Error). We are trying to minimizing our MSE value.

1.2 Set-up

- The outcome variable is *categorical* and denoted $G \in \mathcal{G}$
  - Default Credit Card Example: $\mathcal{G} = \{$"Yes", "No"$\}$
  - Medical Diagnosis Example: $\mathcal{G} = \{$"stroke", "heart attack", "drug overdose", "vertigo"$\}$
- The training data is $D = \{(X_1, G_1), (X_2, G_2), \ldots, (X_n, G_n)\}$
- The optimal decision/classification is often based on the posterior probability $\Pr(G = g \mid \mathbf{X} = \mathbf{x})$

1.3 Binary Probability/Risk Modeling

- Modeling is simplified when there are only 2 classes.
  - Many multi-class problems can be addressed by solving a set of binary classification problems (e.g., one-vs-rest).
- It is often convenient to transform the outcome variable to a binary $\{0, 1\}$ variable:

$$Y_i = \begin{cases} 1 & G_i = \mathcal{G}_1 \quad \text{(outcome of interest)} \\ 0 & G_i = \mathcal{G}_2 \end{cases}$$

- In the `Default` data, it would be natural to set `default=Yes` to 1 and `default=No` to 0.

1.3.1 Linear Regression

- In this set-up we can run linear regression

$$\hat{y}(\mathbf{x}) = \hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x_j$$

```
#: Create binary column (y)
Default = Default %>% mutate(y = if_else(default == "Yes", 1L, 0L))

#: Fit Linear Regression Model
fit_lm = lm(y~student + balance + income, data = Default)
```

term	estimate	std.error	statistic	p.value
(Intercept)	-0.08118	0.00838	-9.685	0.00000
studentYes	-0.01033	0.00566	-1.824	0.06817
balance	0.00013	0.00000	37.412	0.00000
income	0.00000	0.00000	1.039	0.29896

Your Turn #2 : OLS for Binary Responses

1. For the binary Y, what is linear regression estimating?

2. What is the *loss function* that linear regression is using?

3. How could you create a *hard classification* from the linear model?

threshold

$\hat{y} \geq$ threshold $\to \hat{y} =$ yes default

4. Does is make sense to use linear regression for binary risk modeling and classification?

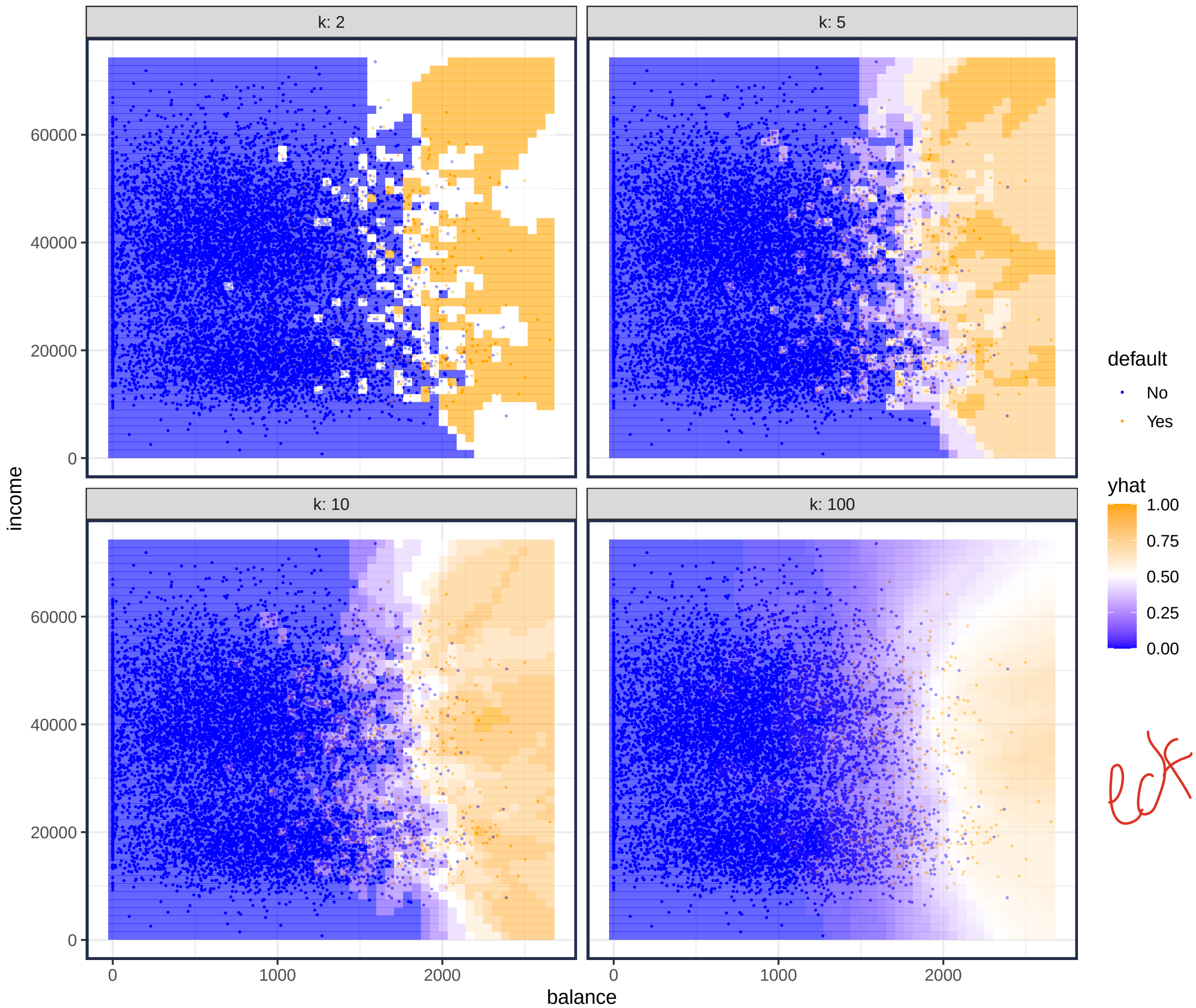
1.3.2 k-nearest neighbor (kNN)

- The k-NN method is a non-parametric *local* method, meaning that to make a prediction $\hat{y}|x$, it only uses the training data in the *vicinity* of x.
  - contrast with OLS linear regression, which uses all X's to get prediction.
- The model (for regression and binary classification) is simple to describe

$$
\begin{aligned}
f_{\text{knn}}(x;k) &= \frac{1}{k} \sum_{i:x_i \in N_k(x)} y_i \\
&= \text{Avg}(y_i \mid x_i \in N_k(x))
\end{aligned}
$$

  - $N_k(x)$ are the set of k nearest neighbors
  - only the k closest y's are used to generate a prediction
  - it is a *simple mean* of the k nearest observations
- When y is binary (i.e., $y \in \{0, 1\}$), the kNN model estimates

$$f_{\text{knn}}(x;k) \approx p(x) = \Pr(Y = 1|X = x)$$



edf = n/k

Your Turn #3 : Thoughts about kNN

The above plots show a kNN model using the *continuous* predictors of `balance` and `income`.

- How could you use kNN with the categorical `student` predictor?

model 1 : student

model 2 : non-student

- The k-NN model also has a more general description when the outcome variable is categorical $G_i \in \mathcal{G}$

$$f_g^{\text{knn}}(x;k) = \frac{1}{k}\sum_{i:x_i \in N_k(x)} \mathbb{1}(g_i = g)$$
$$= \widehat{\Pr}(G_i = g \mid x_i \in N_k(x))$$

  - $N_k(x)$ are the set of k nearest neighbors

- only the k closest y's are used to generate a prediction
- it is a *simple proportion* of the k nearest observations that are of class g

Your Turn #4 : kNN for multi-class outcomes

If using a categorical outcome, kNN models will output a *vector* of probabilities that sum to 1. For small k or if many categories, this vector may be *sparse* meaning that most entries are 0.

- How could we use concepts like Laplace smoothing to produce better predictions in these scenarios?

2 Logistic Regression

2.1 Basics

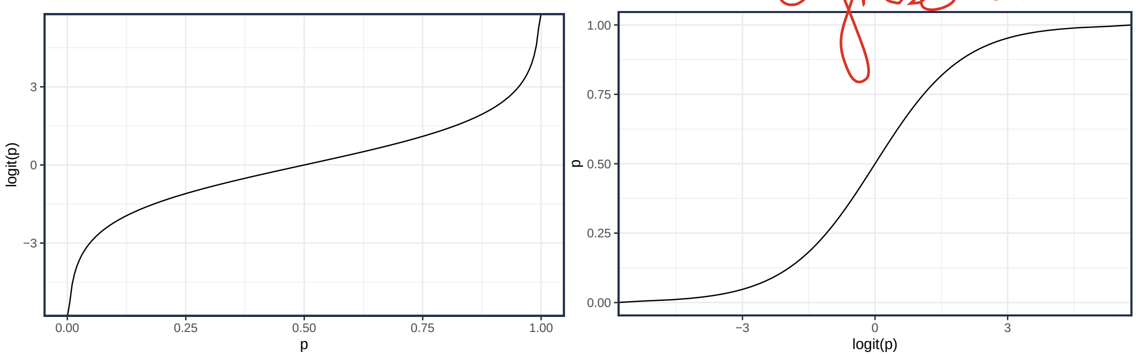
- Let $0 \le p \le 1$ be a probability.
- The log-odds of p is called the *logit*

$$f = \text{logit}(p) = \log\left(\frac{p}{1-p}\right)$$

- The inverse logit is the *logistic function* (or *sigmoid function*). Let $f = \text{logit(p)}$, then

$$\begin{aligned} p &= \frac{e^f}{1+e^f} \\ &= \frac{1}{1+e^{-f}} \end{aligned}$$

Logistic $f = \sum_{j=0}^{p} x_j \beta_j$
regression



Logistic Regression models have the form:

$$\text{logit}\,\Pr(Y=1 \mid X=x) = \log\left(\frac{\Pr(Y=1 \mid X=x)}{1-\Pr(Y=1 \mid X=x)}\right) = \beta^{\mathsf{T}}x$$

and thus,

$$\begin{aligned} \Pr(Y=1 \mid X=x) &= \frac{e^{\beta^{\mathsf{T}}x}}{1+e^{\beta^{\mathsf{T}}x}} \\ &= \left(1+e^{-\beta^{\mathsf{T}}x}\right)^{-1} \end{aligned}$$

Note

For binary outcome variables $Y \in \{0,1\}$, Linear Regression models

$$\mathrm{E}[Y \mid X=x] = \Pr(Y=1 \mid X=x) = \beta^{\mathsf{T}}x$$

2.2 Estimation

- The input data for logistic regression are: $(\mathbf{x}_i, y_i)_{i=1}^n$ where $y_i \in \{0,1\}$, $\mathbf{x}_i = (x_{i0}, x_{i1}, \ldots, x_{ip})^{\mathsf{T}}$.
- $y_i \mid \mathbf{x}_i \sim \text{Bern}(p_i(\beta))$

  - $p_i(\beta) = \Pr(Y = 1 \mid \mathbf{X} = \mathbf{x}_i; \beta) = \left(1 + e^{-\beta^\mathsf{T}\mathbf{x}_i}\right)^{-1}$
  - where $\beta^\mathsf{T}\mathbf{x}_i = \mathbf{x}_i^\mathsf{T}\beta = \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j$

- Bernoulli Likelihood Function

likelihood

$$
\begin{aligned}
L(\beta) &= \prod_{i=1}^{n} p_i(\beta)^{y_i}(1 - p_i(\beta))^{1-y_i} \\
&= \sum_{i=1}^{n} \begin{cases} p_i(\beta) & y_i = 1 \\ 1 - p_i(\beta) & y_i = 0 \end{cases}
\end{aligned}
$$

loglikelihood

$$
\begin{aligned}
\log L(\beta) &= \sum_{i=1}^{n} \{y_i \ln p_i(\beta) + (1 - y_i)\ln(1 - p_i(\beta))\} \\
&= \sum_{i=1}^{n} \begin{cases} \ln p_i(\beta) & y_i = 1 \\ \ln(1 - p_i(\beta)) & y_i = 0 \end{cases} \\
&= \sum_{i:y_i=1} \ln p_i(\beta) + \sum_{i:y_i=0} \ln(1 - p_i(\beta)
\end{aligned}
$$

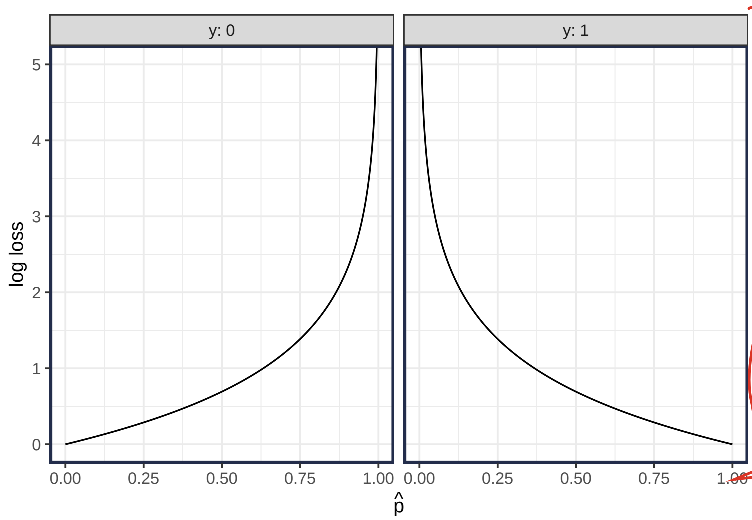
- The usual approach to estimating the Logistic Regression coefficients is *maximum likelihood*

$$
\begin{aligned}
\hat{\beta} &= \arg\max_{\beta}\ L(\beta) \\
&= \arg\max_{\beta}\ \log L(\beta)
\end{aligned}
$$

- We can also view this as the coefficients that minimize the *loss function* $\ell(\beta)$, where the loss function is the negative log-likelihood

$$
\hat{\beta} = \arg\min_{\beta}\ \ell(\beta)
$$

using loss $\ell(\beta) = -C \log L(\beta)$ where $C > 0$ is some positive constant, e.g., $C = 1/n$



Log Loss

- The *log-loss* is the negative Bernoulli log-likelihood.
- The *cross-entropy* loss is also the negative Bernoulli log-likelihood.
- $-\log(p) = \log(1/p)$

- This view facilitates *penalized logistic regression*

$$\hat{\beta} = \arg\min_{\beta} \; \ell(\beta) + \underline{\lambda P(\beta)}$$

Penalty term

Ridge Penalty	$P(\beta) = \|\beta\|_2^2 = \sum_{j=1}^{p} \|\beta_j\|^2 = \beta^\mathsf{T}\beta$
Lasso Penalty	$P(\beta) = \|\beta\|_1 = \sum_{j=1}^{p} \|\beta_j\|$
Best Subsets	$P(\beta) = \|\beta\|_0 = \sum_{j=1}^{p} \|\beta_j\|^0 = \sum_{j=1}^{p} 1_{(\beta_j \neq 0)}$
Elastic Net	$P(\beta, \alpha) = (1-\alpha)\|\beta\|_2^2/2 + \alpha\|\beta\|_1 = \sum_{j=1}^{p}(1-\alpha)\|\beta_j\|^2/2 + \alpha\|\beta_j\|$

2.3 Logistic Regression in Action

- In **R**, logistic regression can be implemented with the `glm()` function since it is a type of *Generalized Linear Model*.
- Because logistic regression is a special case of *Binomial* regression, use the `family=binomial()` argument

```
#: Fit logistic regression model
fit_lr = glm(y~student + balance + income,
             family = "binomial",  <-- logistic regression call
             data = Default)
```

term	estimate	std.error	statistic	p.value
(Intercept)	-10.869	0.492	-22.080	0.000
studentYes	-0.647	0.236	-2.738	0.006
balance	0.006	0.000	24.738	0.000
income	0.000	0.000	0.370	0.712

Your Turn #5 : Interpreting Logistic Regression

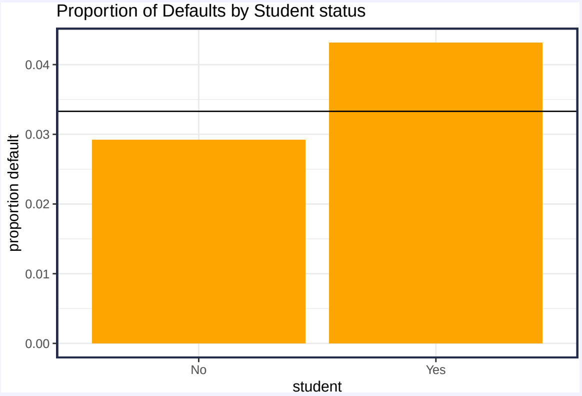
1. What is the estimated probability of default for a Student with a balance of $1000?

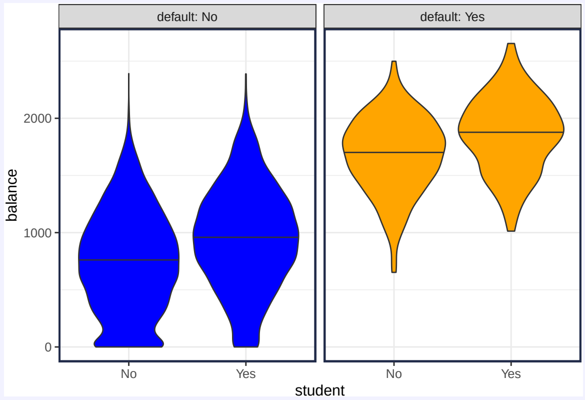
$\text{logit}(\hat{p}) = -10.869 - 0.647 + 10{,}000(0.006) =$

$\hat{p} = e^{\text{logit}(\hat{p})} / 1 + e^{\text{logit}(\hat{p})}$

2. What is the estimated probability of default for a *Non-Student* with a balance of $1000?

3. Why does `student=Yes` appear to lower risk of default, when the plot of student status vs. default appears to increase risk?





2.3.1 Logistic vs. Linear Regression predictions

```
fit_logistic = glm(y~student + balance + income, family="binomial", data = Default)
```

term	estimate	std.error	statistic	p.value
(Intercept)	-10.869	0.492	-22.080	0.000
studentYes	-0.647	0.236	-2.738	0.006
balance	0.006	0.000	24.738	0.000
income	0.000	0.000	0.370	0.712

```
fit_linear = lm(y~student + balance + income, data = Default)
```

term	estimate	std.error	statistic	p.value
(Intercept)	-0.08118	0.00838	-9.685	0.00000
studentYes	-0.01033	0.00566	-1.824	0.06817
balance	0.00013	0.00000	37.412	0.00000
income	0.00000	0.00000	1.039	0.29896

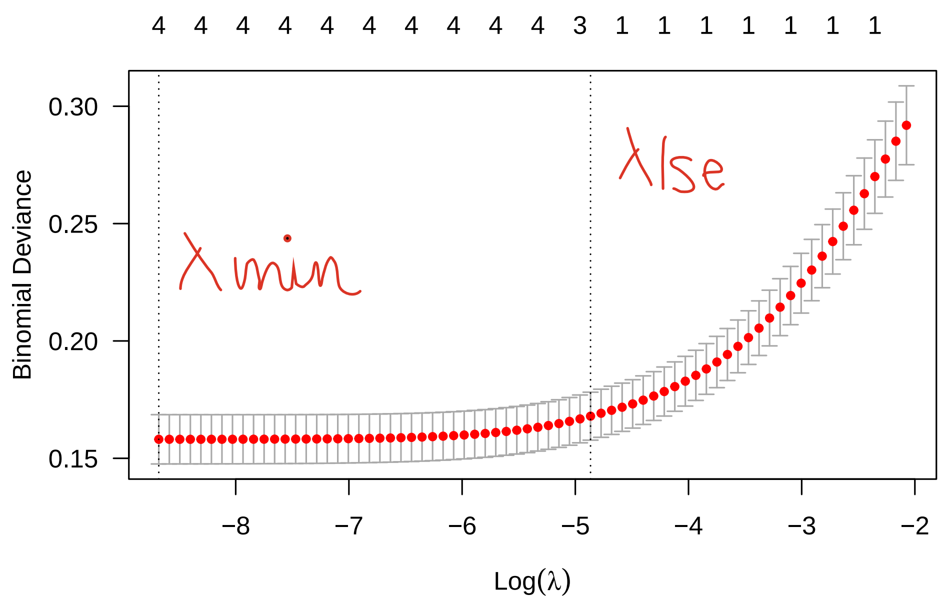
Compare predictions:

student	balance	income	logistic_p	linear_p
Yes	1000	40000	0.003	0.049
No	1000	40000	0.007	0.059

2.3.2 Penalized Logistic Regression

- The `glmnet()` package can estimate logistic regression using an elastic net penalty (e.g., ridge, lasso).

```
#: Fit *penalized* logistic regression model
library(glmnet)
set.seed(2020)
X = makeX(Default %>% select(student, balance, income))
Y = Default$y
fit.enet = cv.glmnet(X, Y,
                     alpha=.5,
                     family="binomial")

#: CV performance plot
plot(fit.enet, las=1)
```



term	unpenalized	lambda.min	lambda.1se
(Intercept)	-10.869	-11.056	-7.937
studentYes	-0.647	-0.299	-0.041
balance	0.006	0.006	0.004
income	0.000	0.000	0.000
studentNo	NA	0.325	0.044

2.4 Logistic Regression Summary

- Logistic Regression (both penalized and unpenalized) estimates a *posterior probability*, $\hat{p}(x) = \widehat{\Pr}(Y = 1 \mid X = x)$

- This estimate is a function of the estimated coefficients

$$
\begin{aligned}
\hat{p}(x) &= \frac{e^{\hat{\beta}^\mathsf{T} x}}{1 + e^{\hat{\beta}^\mathsf{T} x}} \\
&= \left(1 + e^{-\hat{\beta}^\mathsf{T} x}\right)^{-1}
\end{aligned}
$$

Your Turn #6

1. Given a person's `student` status, `balance`, and `income`, how could you use Logistic Regression to decide if they will `default`? (i.e., make a hard classification)

Probability

3 Evaluating Binary Risk Models

3.1 Common Binary Loss Functions

- Suppose we are going to predict a binary outcome $Y \in \{0, 1\}$ with $0 \le \hat{p}(x) \le 1$.
  - Call $\hat{p}(x)$ the *risk score*
- **Brier Score / Squared Error**

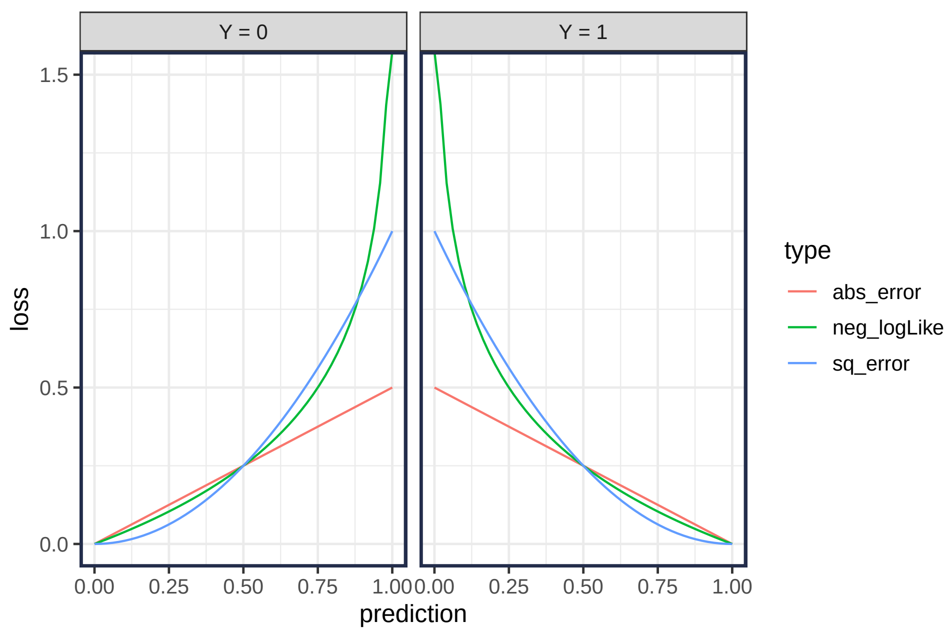
$$
\begin{aligned}
L(y, \hat{p}) &= (y - \hat{p})^2 \\
&= \begin{cases} (1-\hat{p})^2 & y = 1 \\ \hat{p}^2 & y = 0 \end{cases}
\end{aligned}
$$

- **Absolute Error**

$$
\begin{aligned}
L(y, \hat{p}) &= |y - \hat{p}| \\
&= \begin{cases} 1-\hat{p} & y = 1 \\ \hat{p} & y = 0 \end{cases}
\end{aligned}
$$

- **Bernoulli negative log-likelihood (Log-Loss / Cross-entropy)**
  - This is the loss function used in Logistic Regression

$$
\begin{aligned}
L(y, \hat{p}) &= -\left\{ y \log \hat{p} + (1-y)\log(1-\hat{p}) \right\} \\
&= \begin{cases} -\log \hat{p} & y = 1 \\ -\log(1-\hat{p}) & y = 0 \end{cases}
\end{aligned}
$$



Loss functions scaled to be equal at .50

3.2 Model Comparison

```
#: Evaluation Function
evaluate <- function(p_hat, y){
  tibble(
    mn_log_loss = -mean(dbinom(y, prob = p_hat, size=1, log=TRUE)),
    mse = mean((y-p_hat)^2),
    mae = mean(abs(y-p_hat))
  )
}
```

```
#: train/test split
set.seed(2019)
test = sample(nrow(Default), size=2000)
train = -test
```

```
#: fit logistic regression on training data
fit_lm = glm(y~student + balance + income, family='binomial',
             data=Default[train, ])
p_hat.lm = predict(fit_lm, Default[test,], type="response")
evaluate(p_hat.lm, y = Default$y[test])
#> # A tibble: 1 x 3
#>   mn_log_loss    mse    mae
#>         <dbl>  <dbl>  <dbl>
#> 1      0.0815 0.0228 0.0457


#: Fit lasso logistic regression (choose lambda with 10-fold cv)
X = glmnet::makeX(Default |> select(student, balance, income))
Y = Default$y
set.seed(2022)
fit_lasso = cv.glmnet(X[train,], Y[train], alpha = 1, family = "binomial")
p_hat.lasso = predict(fit_lasso, X[test,], type="response", s = "lambda.min")
evaluate(p_hat.lasso, y=Y[test])
#> # A tibble: 1 x 3
#>   mn_log_loss    mse    mae
#>         <dbl>  <dbl>  <dbl>
#> 1      0.0815 0.0228 0.0459

#: Fit ridge penalized linear regression (choose lambda with 10-fold cv)
set.seed(2022)
fit_linear_ridge = cv.glmnet(X[train,], Y[train],
                             alpha = 0, family = "gaussian")
p_hat.linear_ridge = predict(fit_linear_ridge, X[test,], s = "lambda.min") %>%
  pmin(1) |> pmax(0)   # force to [0,1]
evaluate(p_hat.linear_ridge, y=Y[test])
#> # A tibble: 1 x 3
#>   mn_log_loss    mse    mae
#>         <dbl>  <dbl>  <dbl>
#> 1       0.108 0.0280 0.0698
```

3.3 Area under the ROC curve (AUC or AUROC or C-Statistic)

$Y=1$

The AUROC of a risk model is: the probability that the model will score a randomly chosen positive example $(Y = 1)$ higher than a randomly chosen negative example $(Y = 0)$, i.e.

$$\text{AUROC} = \Pr(\hat{p}(\tilde{X}_1) > \hat{p}(\tilde{X}_0))$$

where $\tilde{X}_k$ is a randomly chosen example from class $Y = k$ and $\hat{p}(x) = \widehat{\Pr}(Y = 1 \mid X = x)$ is the estimated probability from a fitted model.

3.3.1 Naive AUC estimator

To *estimate* the AUROC you will fit a model to training data and make predictions on hold-out (test) data with known labels. Hopefully the model will assign large probabilities to the outcome of interest ($Y = 1$) and low probabilities to the other class.

The *naive AUC estimator* compares the probabilities between all pairs of observations where one comes from the $Y = 1$ set and the other from the $Y = 0$ set. The estimated AUROC is the proportion of the pairs where the estimated probability for the outcome of interest is larger then the probability for the other outcome.

$$\widehat{\text{AUROC}} = \frac{1}{n_1 n_0} \sum_{i:y_i=1} \sum_{j:y_j=0} \mathbb{1}(\hat{p}_i > \hat{p}_j) + \overbrace{\frac{1}{2}\,\mathbb{1}(\hat{p}_i = \hat{p}_j)}^{\text{handles ties}}$$

- The extra term ($\frac{1}{2}\,\mathbb{1}(\hat{p}_i = \hat{p}_j)$) is to handle ties in predicted probability.

- Note: see below for a more efficient way to estimate AUC using the ranked order of test predictions

3.3.2 AUC properties

- The AUROC assesses the *discrimination ability* of the model. It gives a different assessment on model performance from *calibration*.
- Notice that the AUROC is the same for any monotonic transformation of the estimated probabilities. E.g., we can use $\hat{p}$ or $\log(\hat{p})$ or logit$(\hat{p})$ or $\hat{p}/10$ and still get the same AUROC.
- We will discuss the Receiver Operating Curves (ROC) during Classification: Decision Theory lesson.
- Note: calibration assesses how closely the estimated probabilities match the actual probabilities as well as helping to identify the regions in feature space where the predictions are poor.

Calculating AUC from Ranked Sums

The AUC is related to the test statistic form a Wilcoxon rank-sum test (also known as the Mann-Whitney U test). Steps:

1. Rank all predictions $\{\hat{p}(x_i)\}$ from *smallest to largest*.
2. Calculate R_1, the sum of the ranks for the observations correspond to the outcome of interest ($Y = 1$). Hopefully, the sum of the ranks is large.
3. Estimate the AUC as
$$\widehat{\text{AUC}} = \frac{R_1 - n_1(n_1 + 1)/2}{n_1 n_0}$$
This calculation makes it clear that AUC may be better viewed as a ranking metric rather than a probability assessment.

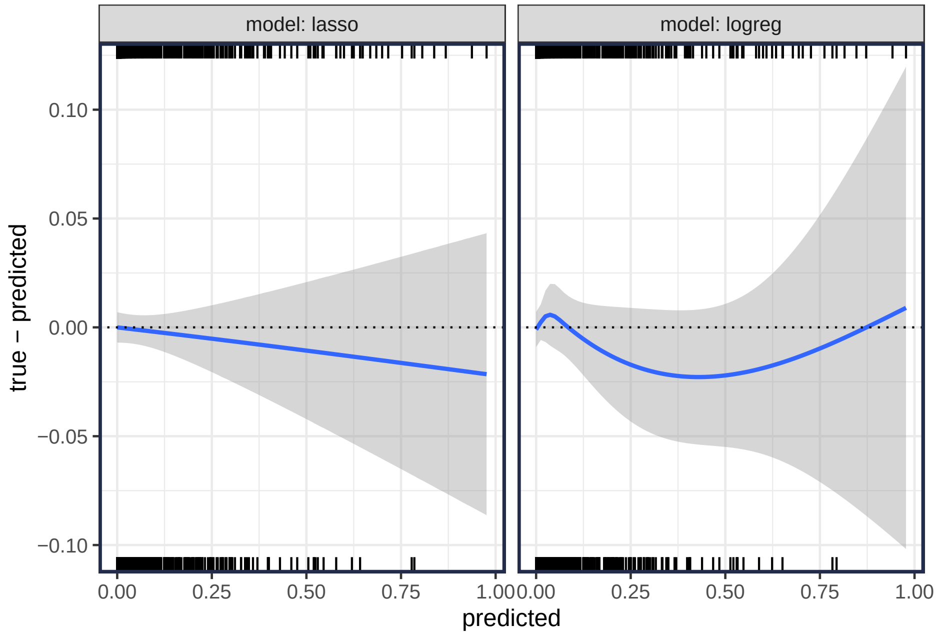
- If your problem is not fundamentally based on *ranking a set of unlabeled observations*, then AUC may not be the best metric for the problem.

A helpful discussion on AUROC (including calculation): https://stats.stackexchange.com/questions/145566/how-to-calculate-area-under-the-curve-auc-or-the-c-statistic-by-hand

3.4 Calibration

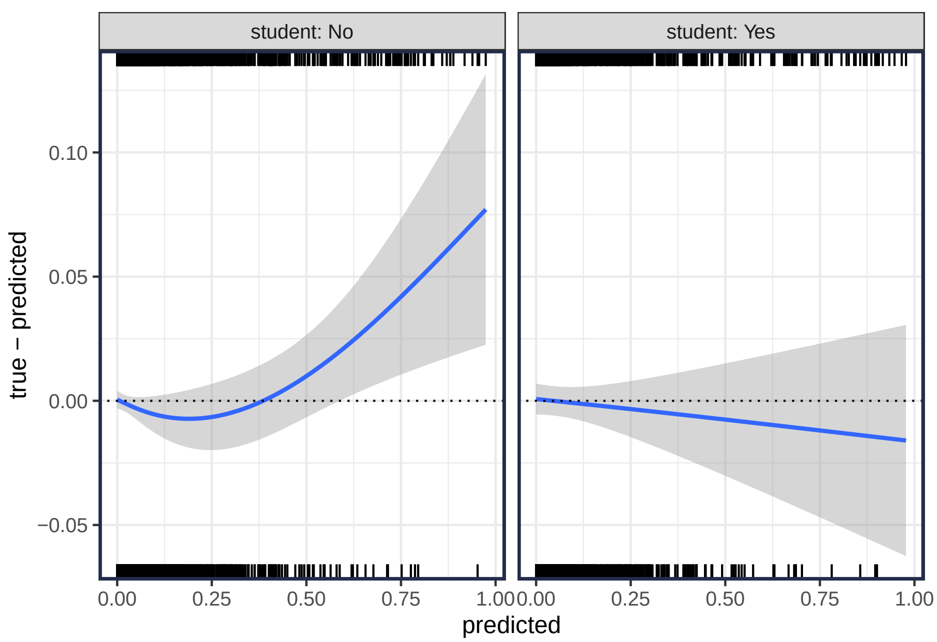
A risk model is said to be calibrated if the *predicted* probabilities are equal to the *true* probabilities.

$$\Pr(Y = 1 \mid \hat{p} = p) = p \qquad \text{for all } p$$



Calibration plots can be used to measure drift, fairness, and model/algorithmic bias. Consider comparing the predictive performance of our models for Students and Non-Students.

$$\Pr(Y = 1 \mid \hat{p} = p, X = x) = p \qquad \text{for all } p \text{ and } x$$



3.4.1 Estimating Calibration

To measure mis-calibration, we can treat the predictions as features and use the predictions as an offset. E.g., to check for linear deviation

$$\text{logit}\, p(x) = \beta_0 + \beta_1 \hat{p}(x) + \text{logit}\, \hat{p}(x)$$

fit on a hold-out set, and check how far β_0 and β_1 are from 0.

We will dive into calibration later in the course.

4 Appendix: R Code

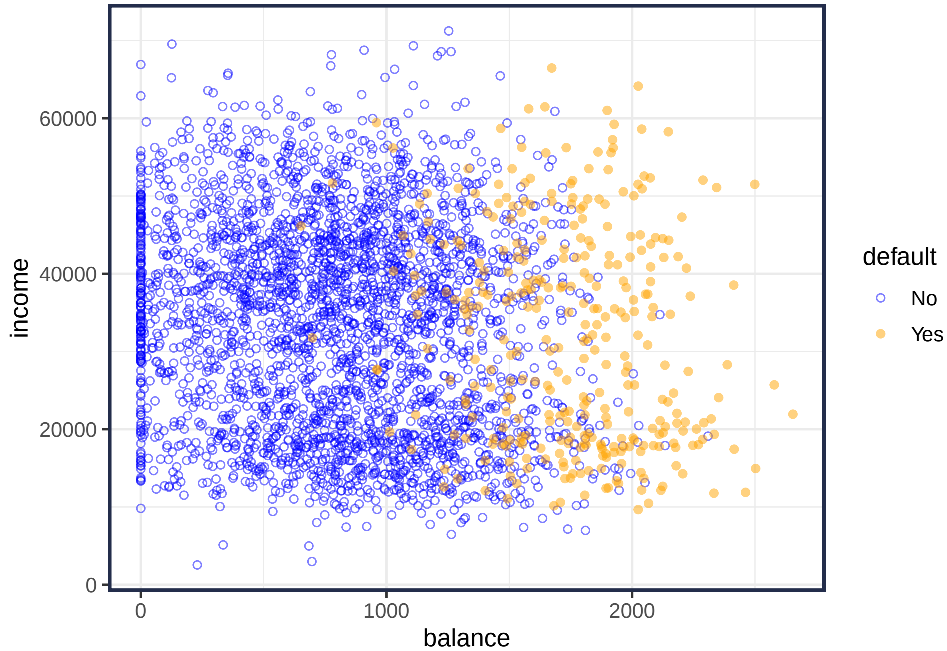
Set-up

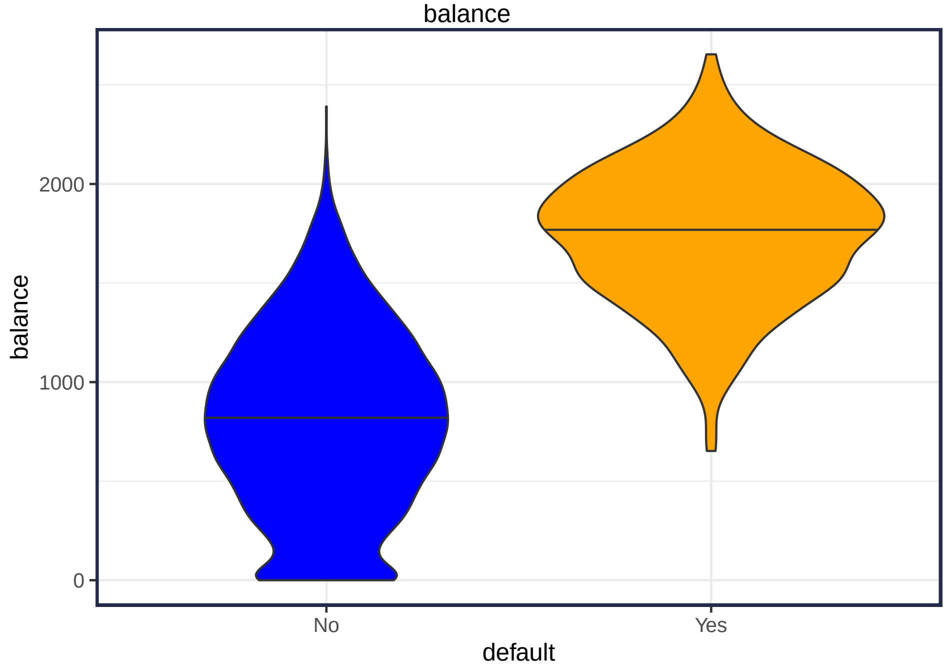
```
#: Load Required Packages
library(ISLR)
library(FNN)
library(broom)
library(yardstick)
library(tidyverse)
```

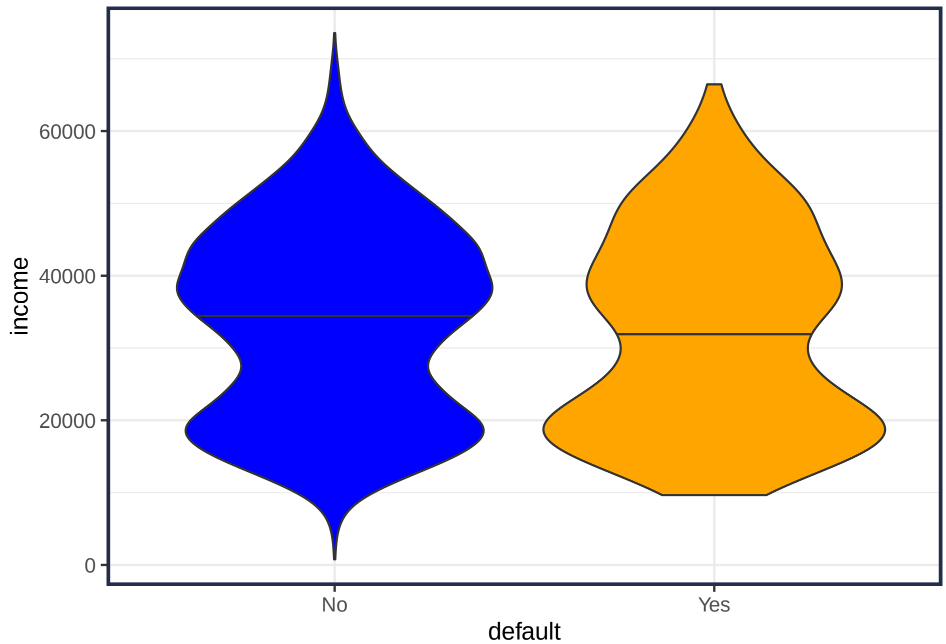
```
#--------------------------------------------------------------------------#
#: Default Data
#  From the ISLR package
#  The outcome variable is `default`
#--------------------------------------------------------------------------#
library(ISLR)
data(Default, package="ISLR")    # load the Default Data

#: Create binary column (y)
Default = Default %>% mutate(y = ifelse(default == "Yes", 1L, 0L))

#: Summary Stats (Notice only 333 (3.3%) have defaulted)
summary(Default)
#>  default    student       balance         income            y
#>  No :9667   No :7056   Min.   :   0   Min.   :  772   Min.   :0.0000
#>  Yes: 333   Yes:2944   1st Qu.: 482   1st Qu.:21340   1st Qu.:0.0000
#>                        Median : 824   Median :34553   Median :0.0000
#>                        Mean   : 835   Mean   :33517   Mean   :0.0333
#>                        3rd Qu.:1166   3rd Qu.:43808   3rd Qu.:0.0000
#>                        Max.   :2654   Max.   :73554   Max.   :1.0000
```

```
#: Plots
plot_cols = c(Yes="orange", No="blue")  # set colors

Default %>%
  group_by(default) %>%
    slice(1:3000) %>%  # choose max of 3000 from each group
  ggplot( aes(balance, income, color=default, shape=default)) +
  geom_point(alpha=.5) +
  scale_color_manual(values=plot_cols) +
  scale_shape_manual(values=c(Yes=19, No=1))

ggplot(Default, aes(default, balance, fill=default)) +
  geom_violin(draw_quantiles=.5) +  #alternative: geom_boxplot() +
  scale_fill_manual(values=plot_cols, guide="none")

ggplot(Default, aes(default, income, fill=default)) +
  geom_violin(draw_quantiles=.5) +
  scale_fill_manual(values=plot_cols, guide="none")

count(Default, default, student) %>%
  group_by(student) %>% mutate(p=n/sum(n)) %>%
  filter(default == "Yes") %>%
  ggplot(aes(student, p, fill=default)) +
  geom_col() +
  geom_hline(yintercept=mean(Default$default == "Yes")) +
  scale_fill_manual(values=plot_cols, guide="none") +
  labs(title="Proportion of Defaults by Student status",
```

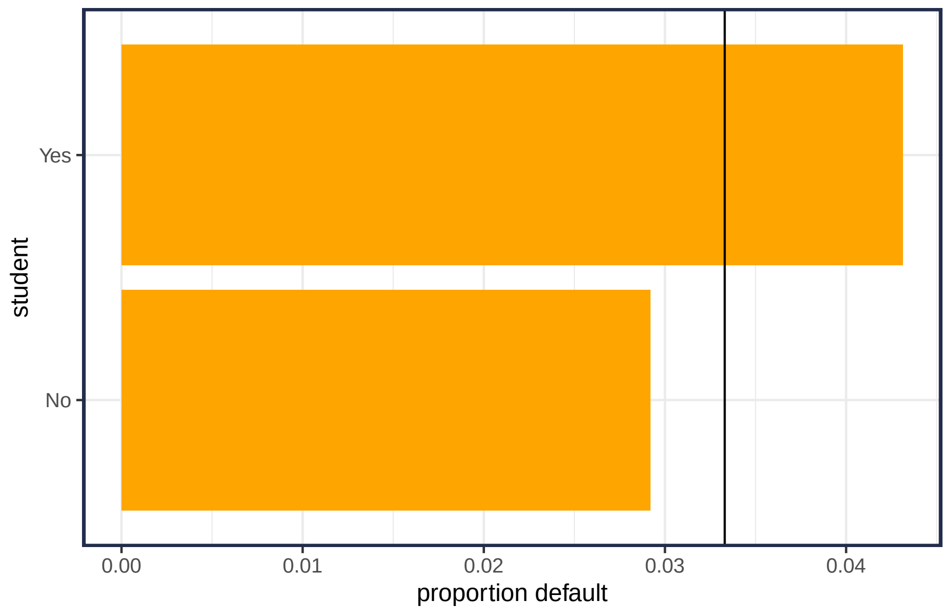
```
      y="proportion default") +
  coord_flip()
```







Proportion of Defaults by Student status



Linear Regression (for binary response)

```
library(broom) # to extract good stuff from models

#: Fit Linear Regression Model
fit_lm = lm(y~student + balance + income, data=Default)

#: Extract coefficients
coef(fit_lm)          # generic coef function to get coefficients
#> (Intercept)  studentYes     balance      income
#>  -8.118e-02  -1.033e-02   1.327e-04   1.992e-07
broom::tidy(fit_lm)     # tidy way to get coefficients
#> # A tibble: 4 x 5
```

```
#>   term            estimate   std.error statistic   p.value
#>   <chr>              <dbl>       <dbl>     <dbl>     <dbl>
#> 1 (Intercept) -0.0812      0.00838         -9.68 4.37e- 22
#> 2 studentYes  -0.0103      0.00566         -1.82 6.82e-  2
#> 3 balance      0.000133    0.00000355      37.4  8.04e-287
#> 4 income       0.000000199 0.000000192      1.04 2.99e-  1
```

k nearest neighbor

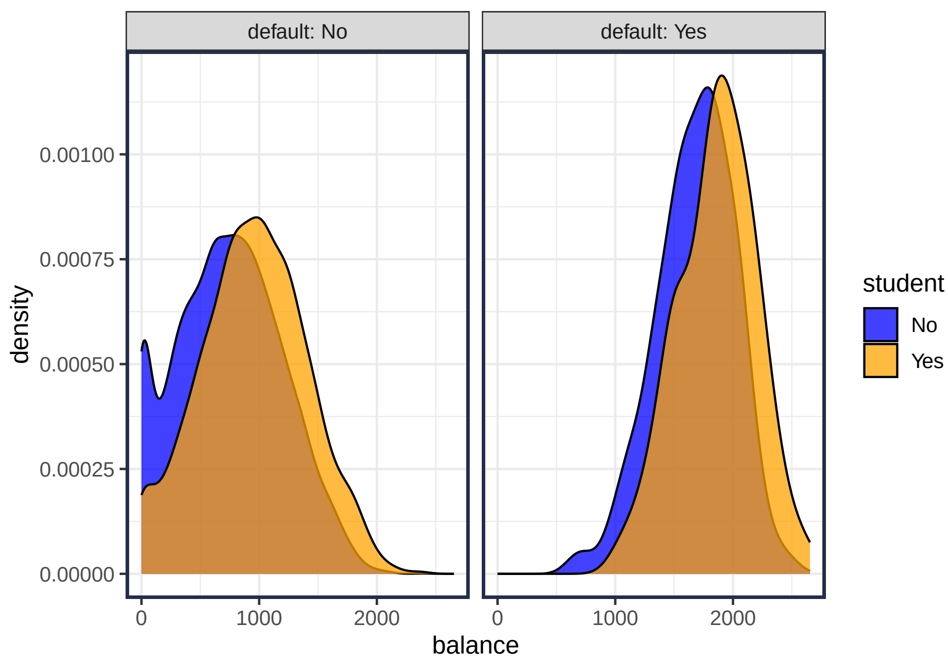
```
library(FNN)          # for knn.reg() function
library(tidymodels)   # for recipe functions

#: center and scale predictors so Euclidean distance makes more sense
library(tidymodels)
pre_process =
  recipe(y ~ balance + income, data = Default) %>% # specify formula
  step_normalize(all_predictors()) %>%         # center and scale
  prep()                                       # estimate means and sds

#: apply the transformation to the predictors
X.scale = bake(pre_process, Default, all_predictors())
Y = bake(pre_process, Default, all_outcomes())$y
# Y = Default$y


#: Evaluation Points
eval.pts = expand_grid(
  balance = seq(min(Default$balance), max(Default$balance), length=50),
  income = seq(min(Default$income), max(Default$income), length=50)
  )

X.eval = bake(pre_process, eval.pts)  # scale eval pts too
#  Note: this uses the same center and scale from the *training data*.
#        This is important!
#        Don't rescale the hold-out data separately!

#: fit knn model
knn5 = FNN::knn.reg(X.scale, y=Y, test=X.eval, k=5)
#  Note: I'm using knn.reg() using the binary coded Y.
#        we could use the knn() function (suitable for categorical outcomes),
#        but to get at the probabilities isn't straightforward. They give the
#        same solutions for two-class problems, so it doesn't matter.
```

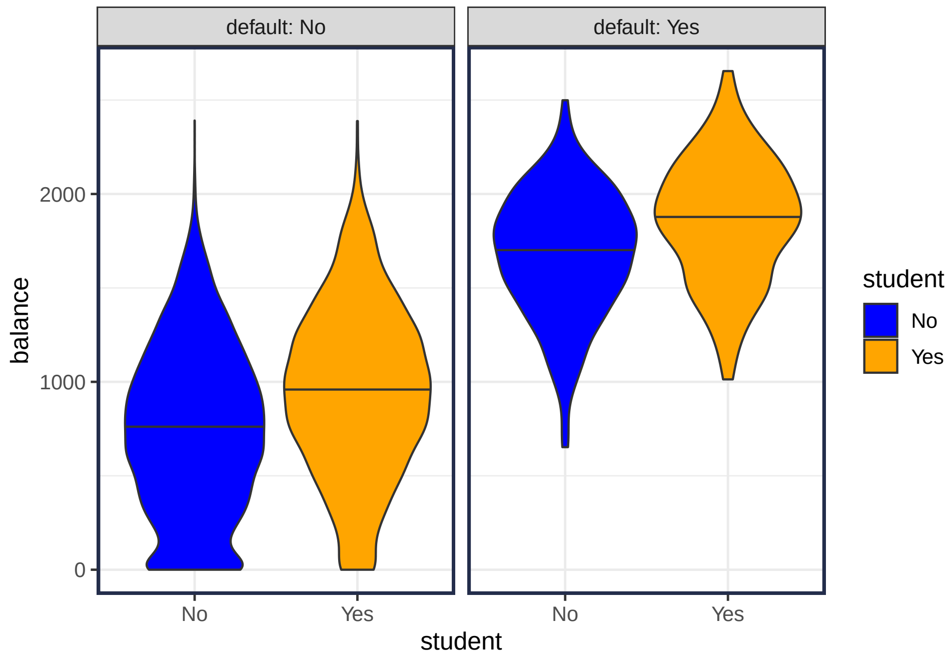
Logistic Regression

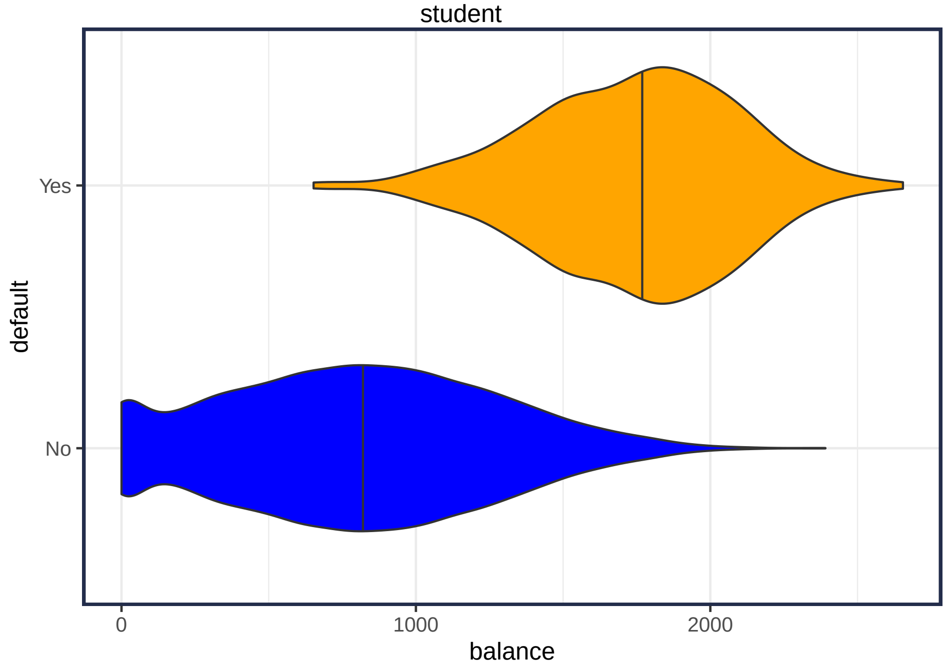
```
#  More details in ISL_v2 4.7.2

#: Fit logistic regression model
fit_lr = glm(y ~ student + balance + income,
             family = "binomial",   # this make it logistic regression
             data = Default)

## Alternatively, you can replace the binary y with a factor/character column
# fit_lr = glm(default~student + balance + income, data=Default,
#                family="binomial")
```

```
#: Get coefficients
tidy(fit_lr)
#> # A tibble: 4 x 5
#>   term            estimate  std.error statistic   p.value
#>   <chr>              <dbl>      <dbl>     <dbl>     <dbl>
#> 1 (Intercept) -10.9        0.492        -22.1   4.91e-108
#> 2 studentYes   -0.647      0.236         -2.74  6.19e-  3
#> 3 balance       0.00574    0.000232      24.7   4.22e-135
#> 4 income        0.00000303 0.00000820     0.370 7.12e-  1

#: Get predictions (for training data)
prob.lr = predict(fit_lr, type="response") # probabilities
link.lr = predict(fit_lr, type="link")     # logit (linear part)


#: Interpret
# Notice that Student=Yes has a negative coefficient, but the plot of
#  defaults by student status suggests otherwise.
# Reason is because students have more balance on average than non-students,
#  and they get over-estimated once balance is in the model

plot_cols = c(Yes="orange", No="blue")  # set colors

ggplot(Default, aes(balance, fill=student)) +
  geom_density(alpha=.75) +
  facet_wrap(~default, labeller=label_both) +
  scale_fill_manual(values=plot_cols)

ggplot(Default, aes(student, balance, fill=student)) +
  geom_violin(draw_quantiles = .5) +
  facet_wrap(~default, labeller=label_both) +
  scale_fill_manual(values=plot_cols)


#: probability at certain values
eval.pts = tibble(
  student = c("Yes", "No"),
  balance = c(1000, 1000),     # balance = 1000
  income  = c(40000, 40000)    # income set to 40K
  )

predict(fit_lr, eval.pts, type="link")
#>      1      2
#> -5.658 -5.011
predict(fit_lr, eval.pts, type="response")
#>        1        2
#> 0.003477 0.006619

#: Simpson's Paradox

# Students have higher default rate
Default %>%
  group_by(student) %>% summarize(n=n(), p_default = mean(default == 'Yes'))
#> # A tibble: 2 x 3
#>   student     n p_default
#>   <fct>   <int>     <dbl>
#> 1 No       7056    0.0292
#> 2 Yes      2944    0.0431
```

```
# People with higher balances have higher default rate
ggplot(Default, aes(balance, default, fill=default)) +
  geom_violin(draw_quantiles=.5) +  #alternative: geom_boxplot() +
  scale_fill_manual(values=plot_cols, guide = "none")

Default %>%
  group_by(default) %>% summarize(avg_balance = mean(balance))
#> # A tibble: 2 x 2
#>   default avg_balance
#>   <fct>         <dbl>
#> 1 No             804.
#> 2 Yes           1748.

# Students have higher balances on average, so they appear to be more likely
#  to default if the balance is not taken into account
Default %>%
  group_by(student) %>% summarize(avg_balance = mean(balance))
#> # A tibble: 2 x 2
#>   student avg_balance
#>   <fct>         <dbl>
#> 1 No             772.
#> 2 Yes            988.


# This is why the logistic regression model correctly adjusts the student status
#  negative.
Default %>%
  mutate(p_hat = prob.lr) %>%
  group_by(student) %>%
  summarize(n=n(), default_rate = mean(default == 'Yes'), avg_p = mean(p_hat))
#> # A tibble: 2 x 4
#>   student     n default_rate  avg_p
#>   <fct>   <int>        <dbl>  <dbl>
#> 1 No       7056       0.0292 0.0292
#> 2 Yes      2944       0.0431 0.0431
```







Convert data frame to model matrix

The `glmnet` package only handles model matrix and not data frames, so we have to convert the data into model matrix. When all predictors are numeric, this is easy (e.g., data.matrix() or model.matrix() if formula), but categorical/factor data needs to be handled separately and consistently if there are multiple data sets (e.g., train and test).

Here are a few options:

```
#: Create model formula (or vector of column names)
fmla = as.formula(y ~ student + balance + income)
vars = fmla %>% terms() %>% labels()
```

tidymodels recipe package

`tidymodels` are a collection of useful modeling packages (like `tidyverse`). The main package to pre-process, transform, and prepare a data frame for passing into a modeling function is `recipe`.

- `recipe()` sets the variables: predictor, outcome, case_weight, or ID. And optionally provides the training data.
- `prep()` performs (i.e., fits) the pre-processing/transformations using the training data.
- `bake()` applies the pre-processing to new data

```
#-----------------------------------------#
#: Option 1: using tidymodels()
#-----------------------------------------#
library(tidymodels)

rec = recipe(fmla, data = Default) %>%  # sets the variable roles
  step_dummy(all_nominal(), one_hot = TRUE) %>% # one-hot encoding
  prep()                                # "fits" using Default data.

# to get the "matrix", set `composition = "matrix"`
X.train = bake(rec, new_data = Default, all_predictors(), composition="matrix")

# Convert the outcome variable to a vector with `pull()`
Y.train = bake(rec, new_data = Default, all_outcomes()) %>% pull()
# Now any new data, like test data, can be obtained by changing the new_data argument
# X.test = bake(rec, new_data = test, all_predictors(), composition="matrix")
```

glmnet::makeX()

The `glmnet` package provides a basic function `makeX()` to properly create training and testing model matrices.

```
#-----------------------------------------#
#: Option 2: using glmnet::makeX()
#-----------------------------------------#
X.train = glmnet::makeX(Default |> select(any_of(vars)))

# if test data is available, pass it in at same time
# X = glmnet::makeX(
#   train = Default |> select(-y),
#   test = train |> select(-y)
#   )
# X.train = X$x
# X.test = X$xtest
```

Other approaches

```
#-----------------------------------------#
#: Option 3: Manually using dplyr::select() + as.matrix()
#-----------------------------------------#
# Note: must manually transform, dummy, interactions, etc.
X.train = select(Default, !!vars) %>%
  mutate(dummy = 1) %>%
  pivot_wider(
    names_from = student,
    values_from = dummy,
```

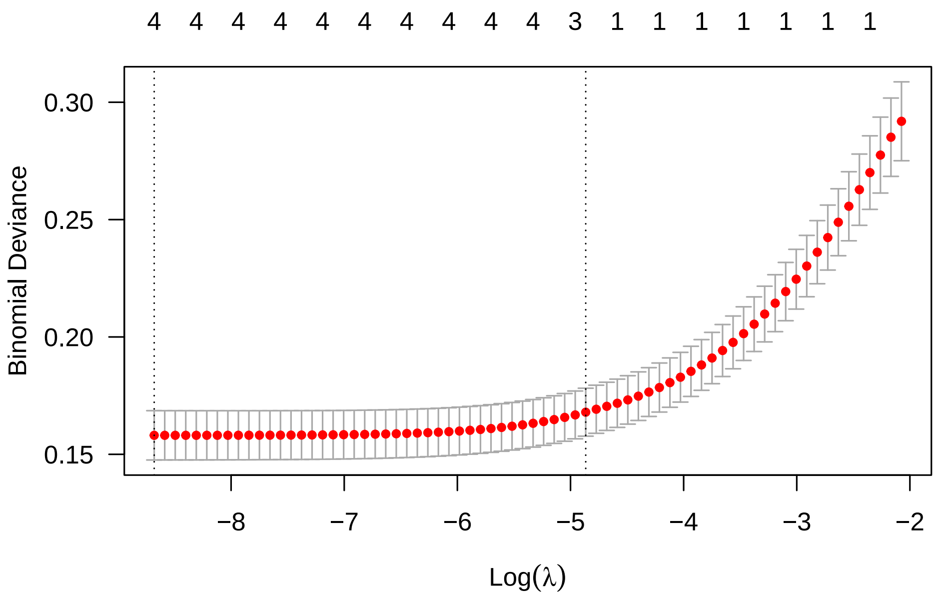
```
    values_fill = 0L
  ) %>%
  as.matrix()                                         # make X matrix
Y.train = Default$y              # make Y vector
# X.test = select(test, !!vars) %>%
#   mutate(dummy=1) %>% pivot_wider(names_from = student, values_from = dummy, values_fill = 0L) %>%
#   as.matrix()


#-----------------------------------------#
#: Option 4: using model.matrix()
#-----------------------------------------#
X.train = model.matrix(fmla, data = Default)[,-1] # remove intercept term
Y.train = Default$y
# X.test = model.matrix(fmla, data = test)[,-1] # remove intercept term
```

Penalized Logistic Regression

```
library(tidymodels)
rec = recipe(y~student + balance + income, data = Default) %>%
  step_dummy(all_nominal(), one_hot = TRUE) %>%
  prep()
X.train = bake(rec, new_data = Default, all_predictors(), composition="matrix")
Y.train = bake(rec, new_data = Default, all_outcomes()) %>% pull()
X.eval = bake(rec, new_data = eval.pts, all_predictors(), composition="matrix")
#> Warning: ! There was 1 column that was a factor when the recipe was prepped:
#> * `student`
#> i This may cause errors when processing new data.

# library(glmnet)
# vars = c("student", "balance", "income")
# X = glmnet::makeX(select(Default, !!vars), select(eval.pts, !!vars))
# X.train = X$x
# Y.train = Default$y
# X.eval = X$xtest
```

```
#: Elastic net with alpha = .5. Use CV to select lambda.
library(glmnet)
set.seed(2020)
fit_enet = cv.glmnet(X.train, Y.train,
                     alpha=.5,
                     family="binomial")

#: CV performance plot
plot(fit_enet, las=1)

#: probability at certain values
predict(fit_enet, X.eval, s="lambda.min", type="response")
#>      lambda.min
#> [1,]   0.003722
#> [2,]   0.006929
predict(fit_enet, X.eval, s="lambda.1se", type="response")
#>      lambda.1se
#> [1,]    0.01444
#> [2,]    0.01569

#: Compare with intercept only model. Set large penalty (s large)
```

```
predict(fit_enet, X.eval, s=1000, type="response") # intercept only (effectively)
#>          s1
#> [1,] 0.0333
#> [2,] 0.0333
mean(Default$y)                                       # actual intercept only
#> [1] 0.0333

#: Compare with unpenalized logistic regression. Set penalty s=0.
predict(fit_enet, X.eval, s=0, type="response") # unpenalized (effectively)
#>            s1
#> [1,] 0.003722
#> [2,] 0.006929
```



Performance Metrics

```
#: train/test split
set.seed(2019)
test = sample(nrow(Default), size=1000)
train = -test
```

```
#: Elastic net with alpha = .5. Use CV to select lambda.
library(glmnet)
set.seed(2020)
fit_enet = cv.glmnet(X.train, Y.train,
                     alpha=.5,
                     family="binomial")
X.test = bake(rec, all_predictors(),
              new_data = Default[test,],  composition="matrix")


#: Fit logistic regression model
fit_logr = glm(y ~ student + balance + income, data=Default,
             family="binomial")
```

The `yardstick` package is part of `tidymodels` and deals with predictive evaluation metrics.

```
library(yardstick)

# create evaluation dataframe
data_eval =
  tibble(
    default = Default %>% slice(test) %>% pull(default),
    p_enet = predict(fit_enet, X.test , s="lambda.min", type = "response")[,1],
    p_logr = predict(fit_logr, Default[test,], type = "response"),
  ) %>%
    pivot_longer(-default, names_to = "model", values_to = "p_hat")

# set threshold at p_hat = 0.50 and calculate metrics
data_eval |>
  mutate(G_hat = ifelse(p_hat > .50, "Yes", "No") %>% factor) %>%
  group_by(model) %>%
  metrics(default, G_hat, p_hat)
#> # A tibble: 8 x 4
#>   model  .metric     .estimator .estimate
#>   <chr>  <chr>       <chr>          <dbl>
#> 1 p_enet accuracy    binary         0.97
#> 2 p_logr accuracy    binary         0.97
#> 3 p_enet kap         binary         0.431
#> 4 p_logr kap         binary         0.431
#> 5 p_enet mn_log_loss binary         6.08
#> 6 p_logr mn_log_loss binary         6.15
#> # i 2 more rows
```