

Probability Modeling

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prob-modeling.pdf

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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.

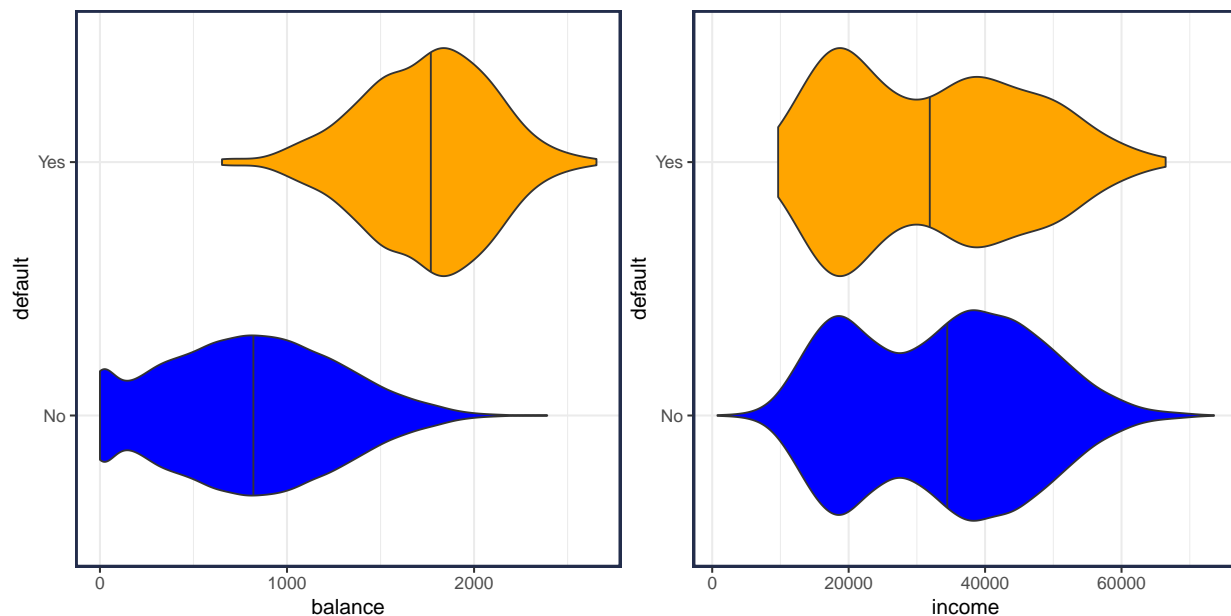
```
data(Default, package="ISLR")
```

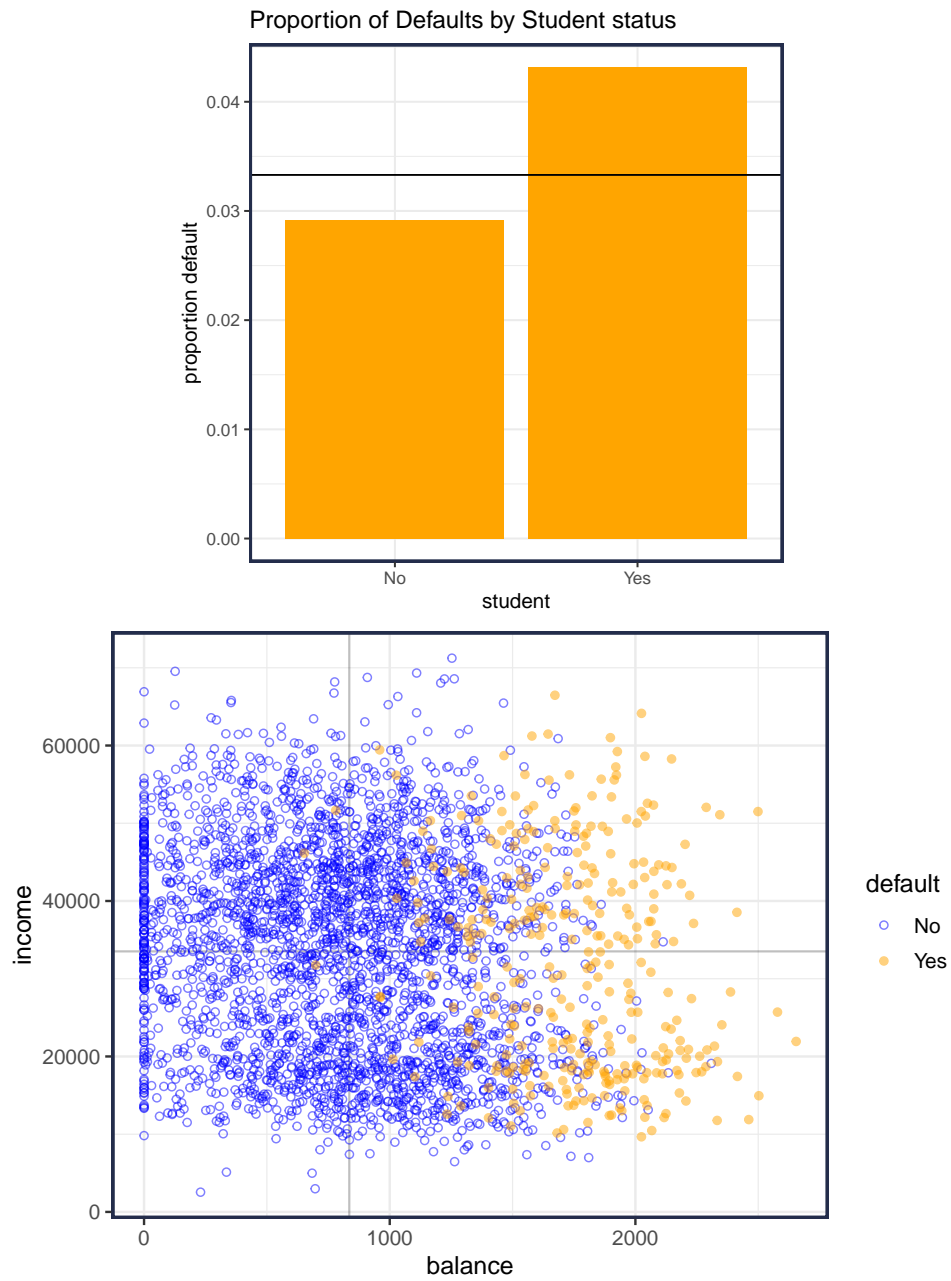
The variables are:

- *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

```
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
```





Your Turn #1 : Credit Card Default Modeling

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

1.2 Set-up

- The outcome variable is *categorical* and denoted $G \in \mathcal{G}$
 - Default Credit Card Example: $\mathcal{G} = \{\text{"Yes"}, \text{"No"}\}$
 - Medical Diagnosis Example: $\mathcal{G} = \{\text{"stroke"}, \text{"heart attack"}, \text{"drug overdose"}, \text{"vertigo"}\}$
- The training data is $D = \{(X_1, G_1), (X_2, G_2), \dots, (X_n, G_n)\}$
- 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

- Classification 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

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

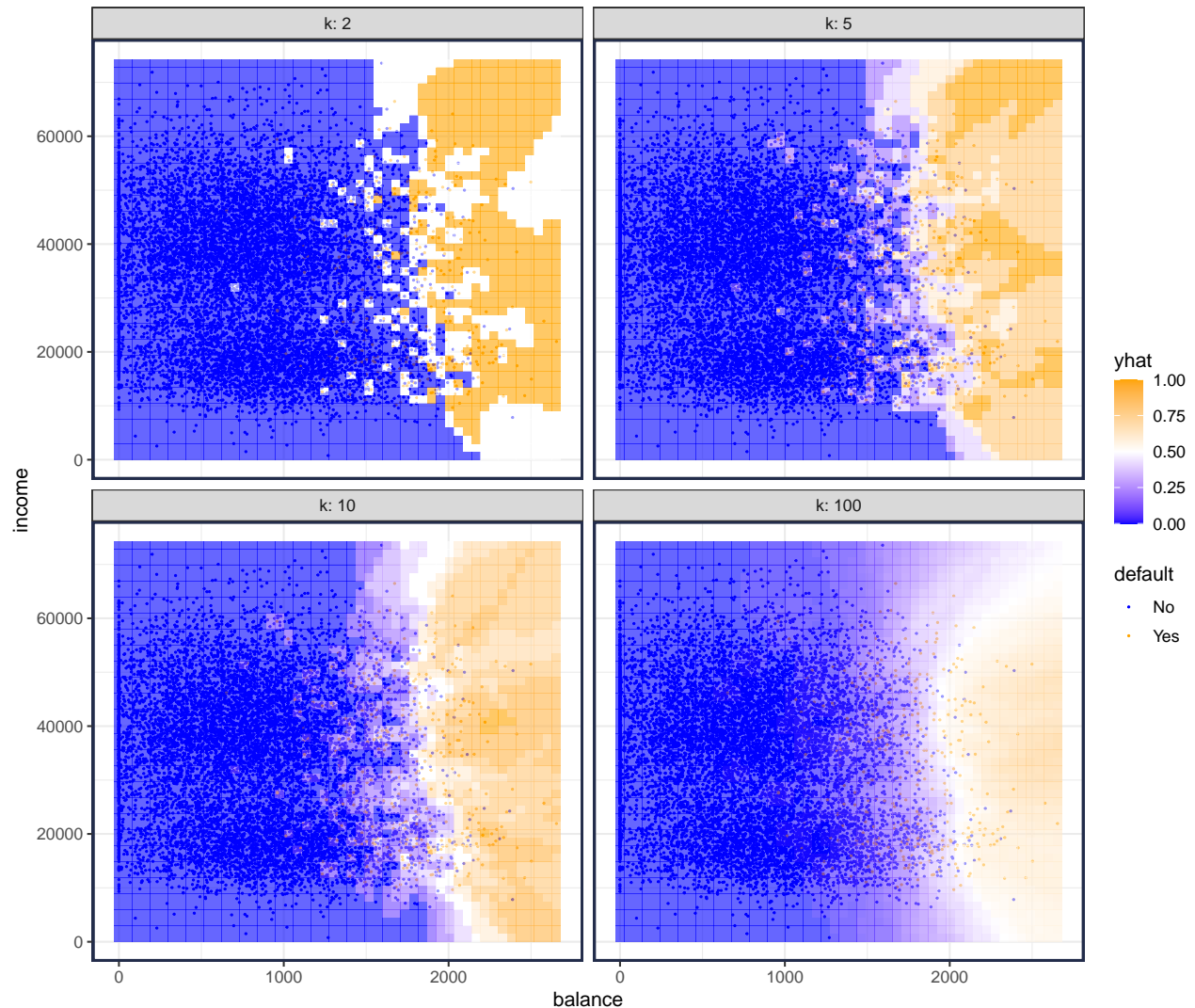
1.3.2 *k*-nearest neighbor (kNN)

- 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

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



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?

- The k -NN model also has a more general description when the outcome variables 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

2 Logistic Regression

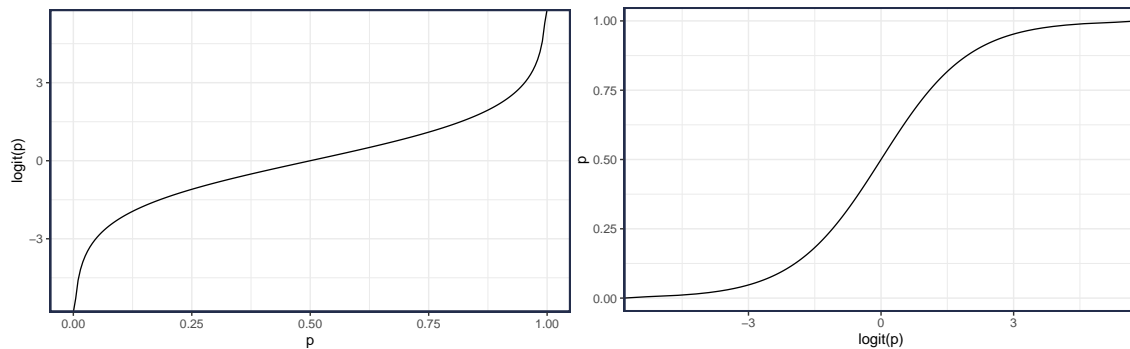
2.1 Basics

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

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

- 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 Regression models have the form:

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

and thus,

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

Note

For binary outcome variables $Y \in \{0, 1\}$, [Linear Regression](#) models

$$E[Y \mid X = x] = \Pr(Y = 1 \mid X = x) = \beta^\top x$$

2.2 Estimation

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

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

- Bernoulli Likelihood Function

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

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

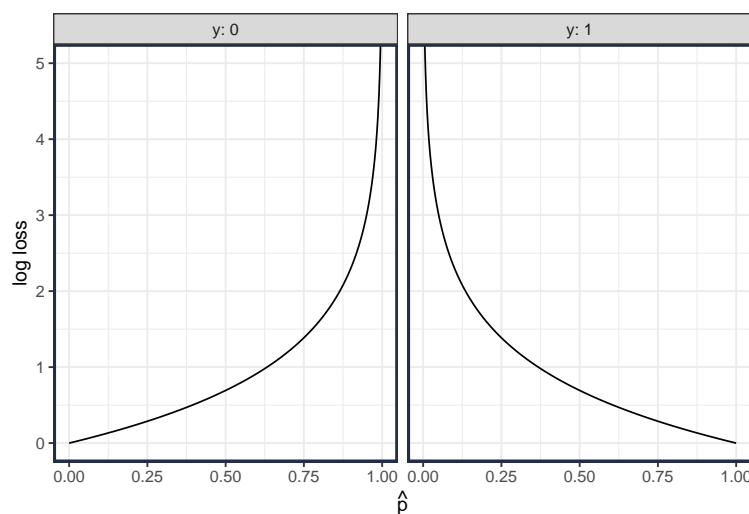
- The usual approach to estimating the Logistic Regression coefficients is *maximum likelihood*

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

- 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., $C = 1/n$



Note

The *log-loss* is the negative Bernoulli log-likelihood.

- This view facilitates *penalized logistic regression*

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

Ridge Penalty	$P(\beta) = \ \beta\ _2^2 = \sum_{j=1}^p \beta_j ^2 = \beta^T \beta$
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

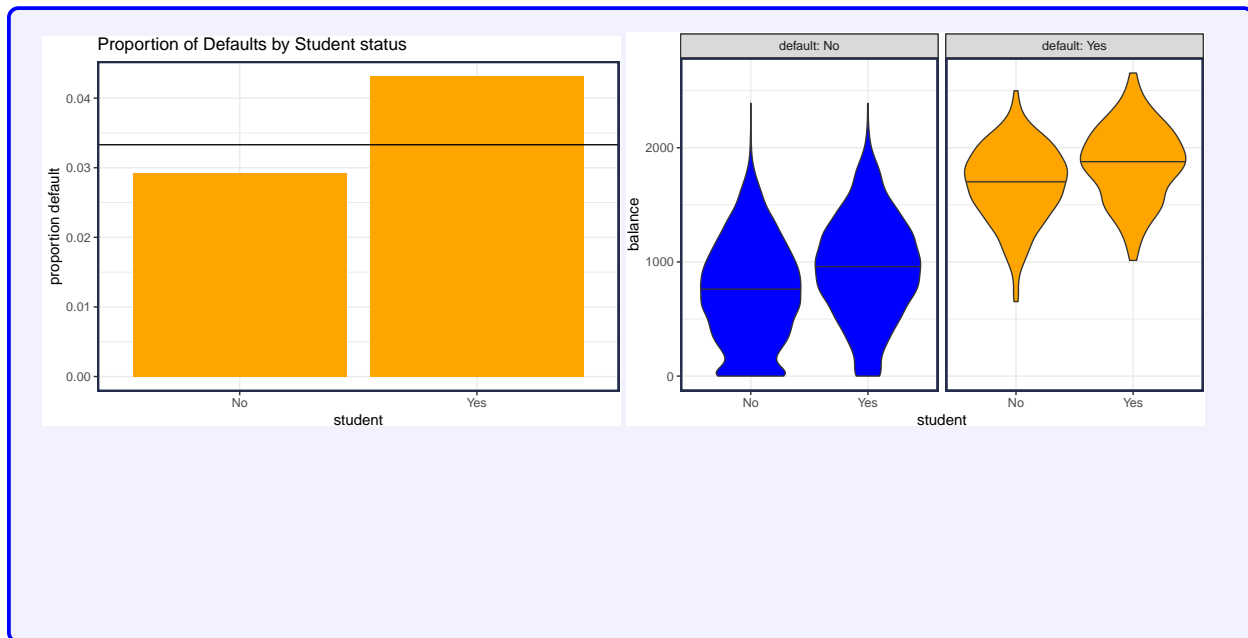
- In **R**, logistic regression can be implemented with the `glm()` function since it is a type of *Generalized Linear Model*.
- Because logistic regression is a special case of *Binomial* regression, use the `family=binomial()` argument

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

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 #4 : Interpreting Logistic Regression

1. What is the estimated probability of default for a Student with a balance of \$1000?
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, data = Default, family="binomial")
```

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

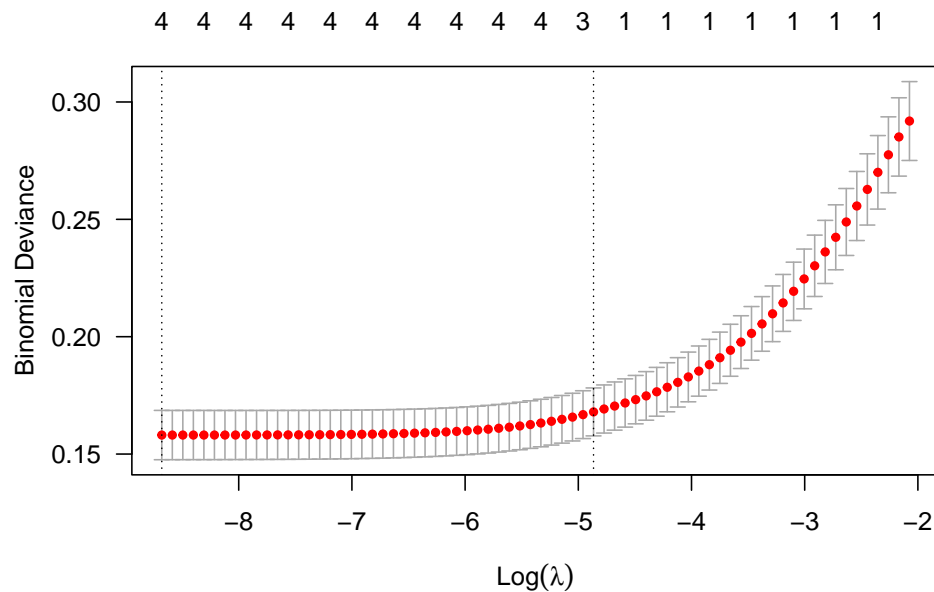
- The `glmnet()` package can estimate logistic regression using an elastic net penalty (e.g., ridge, lasso).

```

#: 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

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

Your Turn #5

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)

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 $0 \leq \hat{p}(x) \leq 1$.

- Call $\hat{p}(x)$ the *risk score*

- **Brier Score / Squared Error**

$$L(y, \hat{p}) = (y - \hat{p})^2$$

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

- **Absolute Error**

$$L(y, \hat{p}) = |y - \hat{p}|$$

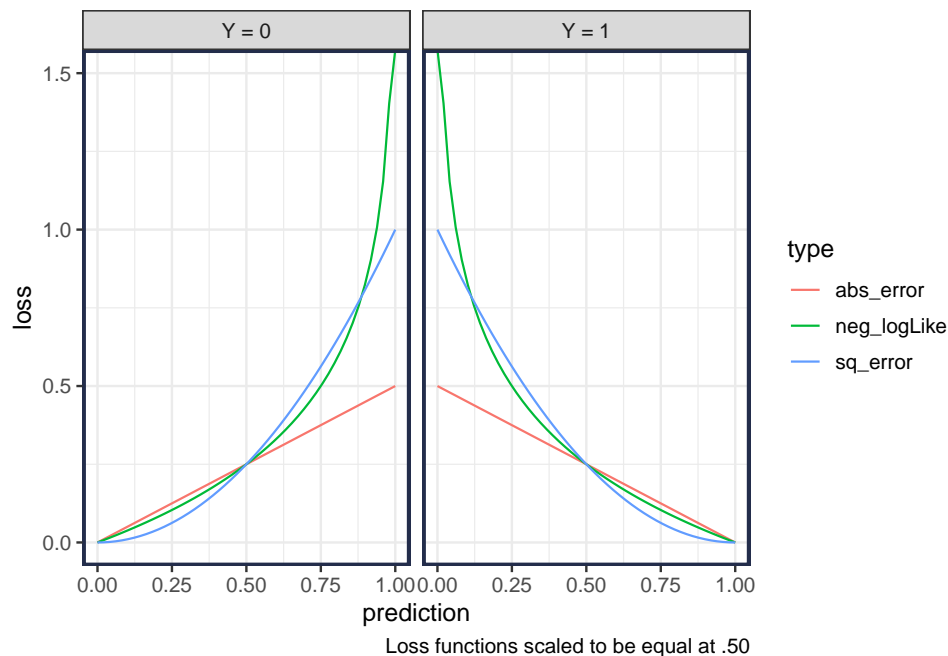
$$= \begin{cases} 1 - \hat{p} & y = 1 \\ \hat{p} & y = 0 \end{cases}$$

- **Bernoulli negative log-likelihood (Log-Loss)**

- This is the loss function for Logistic Regression

$$L(y, \hat{p}) = -\{y \log \hat{p} + (1 - y) \log(1 - \hat{p})\}$$

$$= \begin{cases} -\log \hat{p} & y = 1 \\ -\log(1 - \hat{p}) & y = 0 \end{cases}$$



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(select(Default, student, balance, income))
Y = Default$y
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 0.0458
```

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

The AUROC of a risk model is: the probability that the model will rank 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.

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. Then compare the probabilities between all pairs of observations where one comes from the $Y = 1$ set and the other from the $Y = 0$ set. The AUROC is the proportion of the pairs where the estimated probability for the outcome of interest is larger than the probability for the other outcome. The extra term is to handle ties in predicted probability.

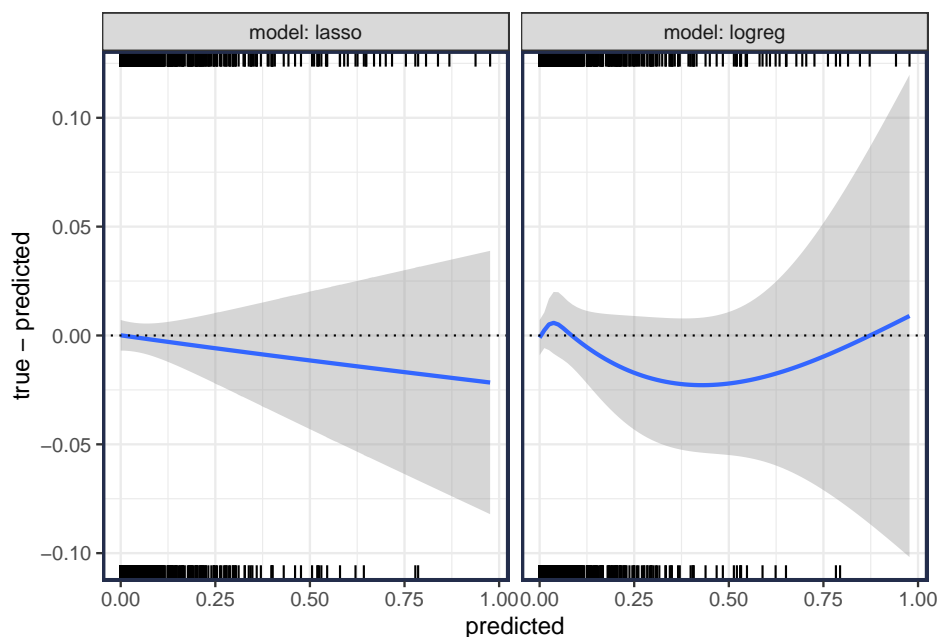
$$\widehat{\text{AUROC}} = \frac{1}{n_1 n_0} \sum_{i: y_i=1} \sum_{j: y_j=0} \mathbb{1}(\hat{p}_i > \hat{p}_j) + \frac{1}{2} \mathbb{1}(\hat{p}_i = \hat{p}_j)$$

- 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 $\text{logit}(\hat{p})$ or $\hat{p}/10$ and still get the same AUROC.
- A helpful discussion on AUROC: <https://stats.stackexchange.com/questions/145566/how-to-calculate-area-under-the-curve-auc-or-the-c-statistic-by-hand>
- 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.

3.4 Calibration

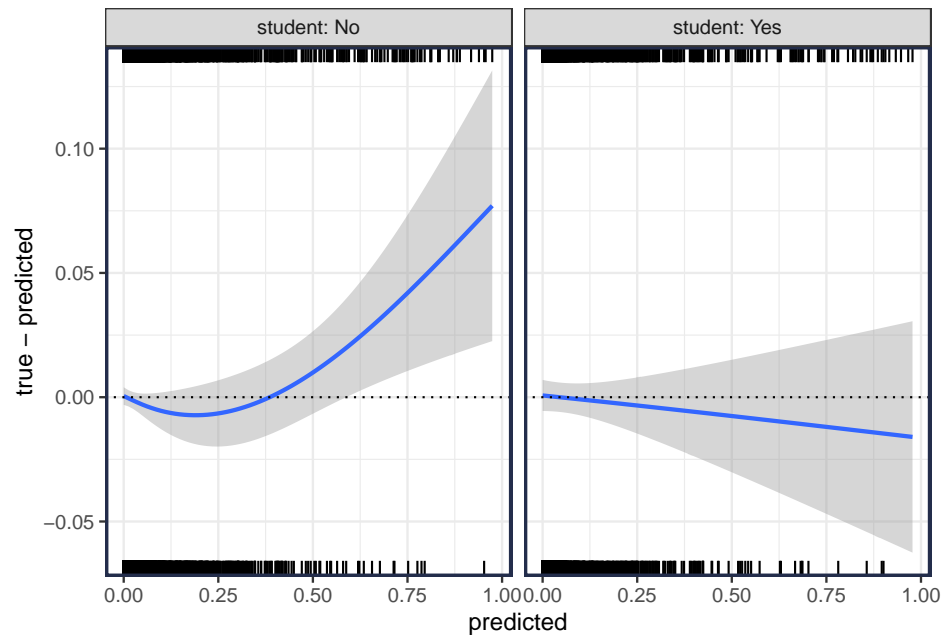
A risk model is said to be *calibrated* if the predicted probabilities are equal to the true risk (probabilities).

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



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.

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



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))

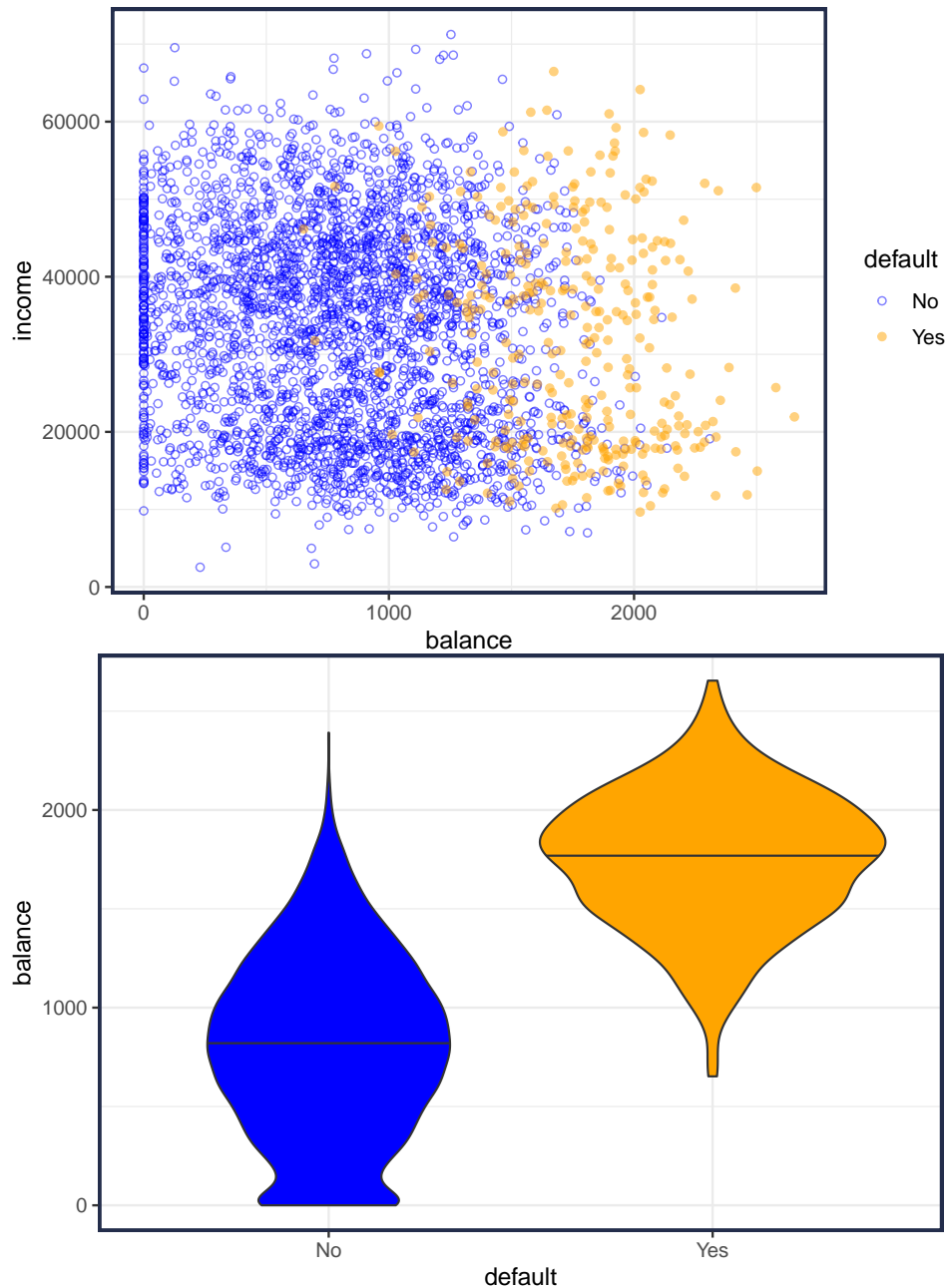
ggplot(Default, aes(default, balance, fill=default)) +
  geom_violin(draw_quantiles=.5) + #alternative: geom_boxplot() +
  scale_fill_manual(values=plot_cols, guide=FALSE)
#> Warning: The 'guide' argument in 'scale_*()' cannot be 'FALSE'. This was deprecated in
#> ggplot2 3.3.4.
#> i Please use "none" instead.
#> This warning is displayed once every 8 hours.
#> Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was
#> generated.

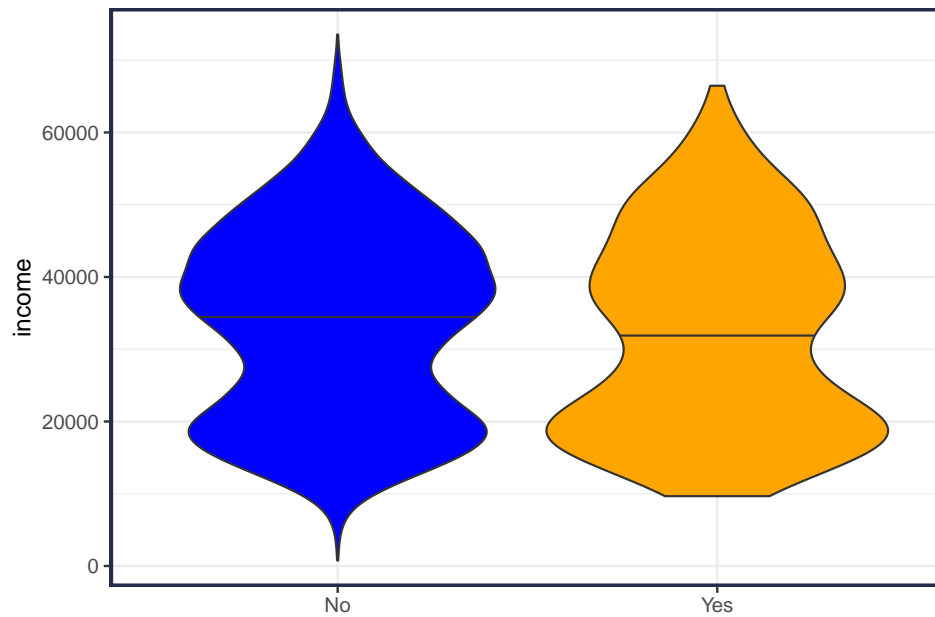
ggplot(Default, aes(default, income, fill=default)) +
  geom_violin(draw_quantiles=.5) +
  scale_fill_manual(values=plot_cols, guide=FALSE)

count(Default, default, student) %>%
  group_by(student) %>% mutate(p=n/sum(n)) %>%
  filter(default == "Yes") %>%
  ggplot(aes(student, p, fill=default)) +

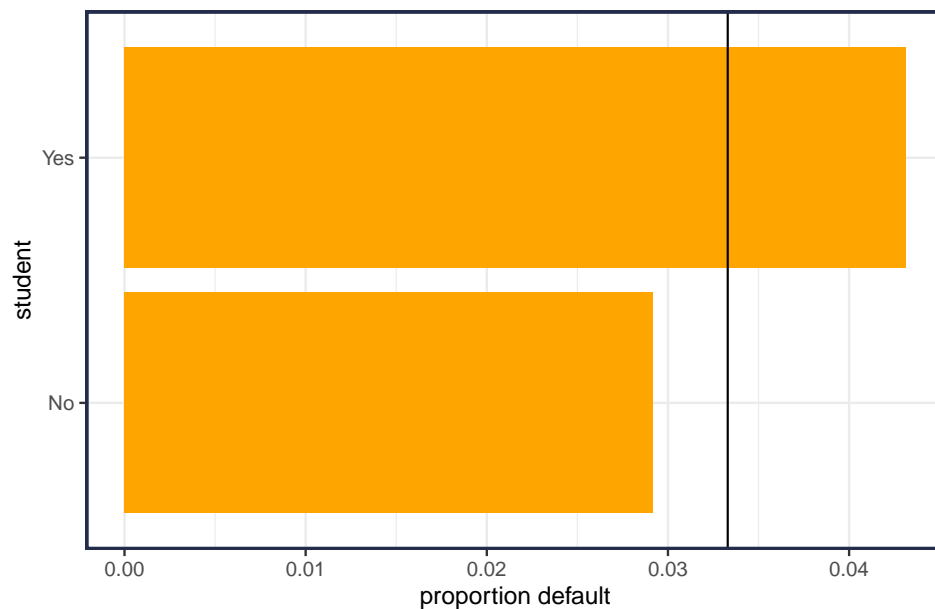
```

```
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(), composition = "data.frame")
# 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)
```

Logistic Regression

```
# More details in ISL_v2 4.7.2

# Fit logistic regression model
fit.lr = glm(y ~ student + balance + income, data=Default,
  family="binomial")

## 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=FALSE)

```



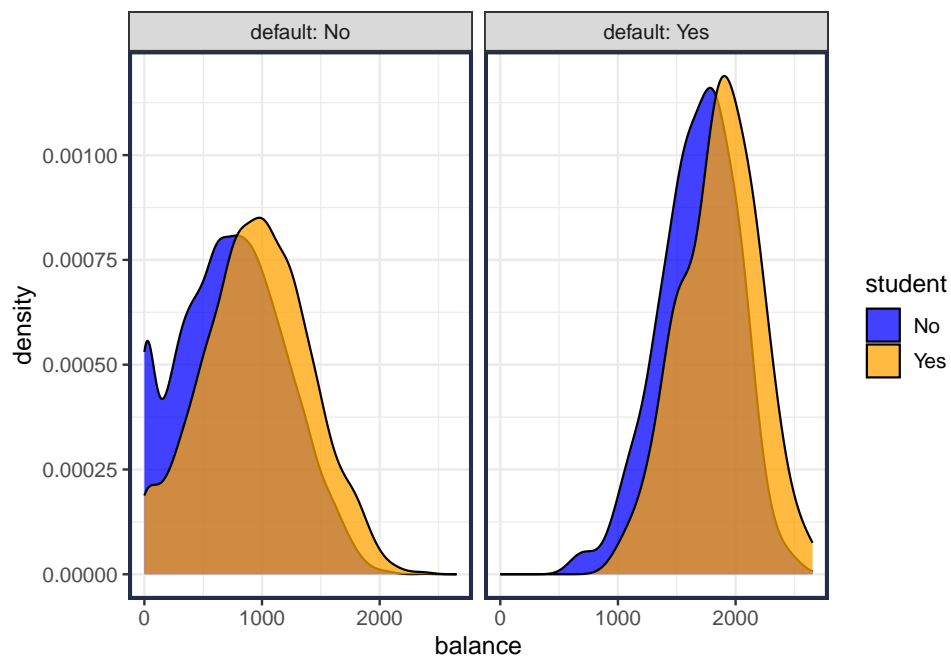
```

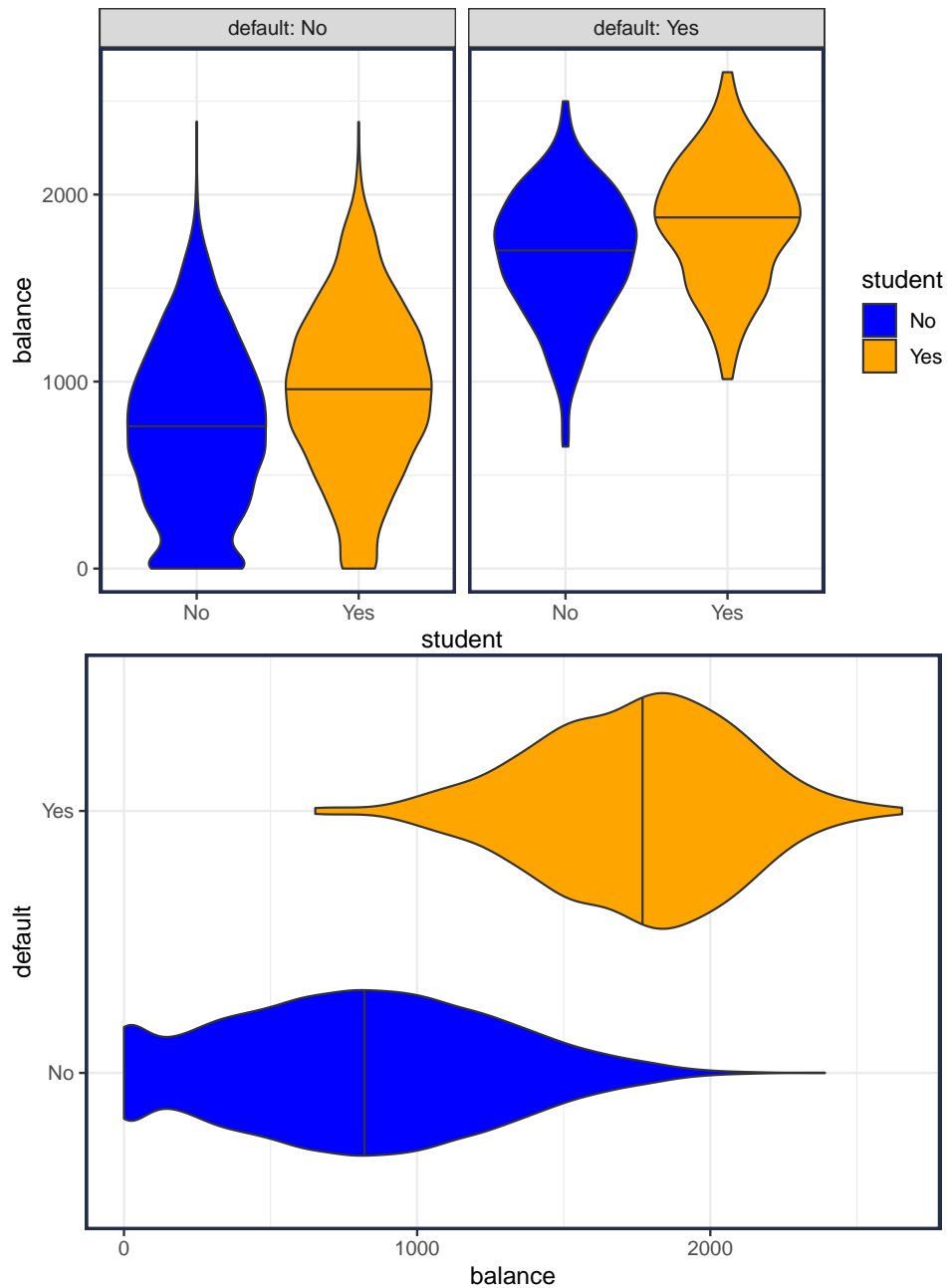
Default %>%
  group_by(default) %>% summarize(avg_balance = mean(balance))
#> # A tibble: 2 x 2
#>   default avg_balance
#>   <fct>     <dbl>
#> 1 No       804.
#> 2 Yes     1748.

# 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.lrr) %>%
  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
fmla = as.formula(y ~ student + balance + income)
vars = fmla %>% terms() %>% labels()
```

```

#-----#
#: Option 1: 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

#-----#
#: Option 2: using tidymodels()
#-----#
# Note: tidymodels is a collection of useful modeling packages (like tidyverse)
library(tidymodels)
# This code only uses the recipe() package
# recipe() sets the variables: predictor, outcome, case_weight, or ID
# prep() performs (i.e., fits) the pre-processing/transformations; set training=data_train
# bake() applies the pre-processing to new data
rec = recipe(fmla, 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.test = bake(rec, new_data = test, all_predictors(), composition="matrix")

#-----#
#: Option 3: using hardhat::mold()
#-----#
obj = hardhat::mold(fmla, data=Default)
X.train = obj$predictors
Y.train = obj$outcomes
# X.test = hardhat::mold(fmla, data=test)$predictors

#-----#
#: Option 4: 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 5: using glmnet::makeX
#-----#
X.train = glmnet::makeX(select(Default, !!vars))
# if test data is available
# X = glmnet::makeX(train = select(Default, -y), test = select(train, -y))
# X.train = X$x
# X.test = X$xtest

```

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'.
#> 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")

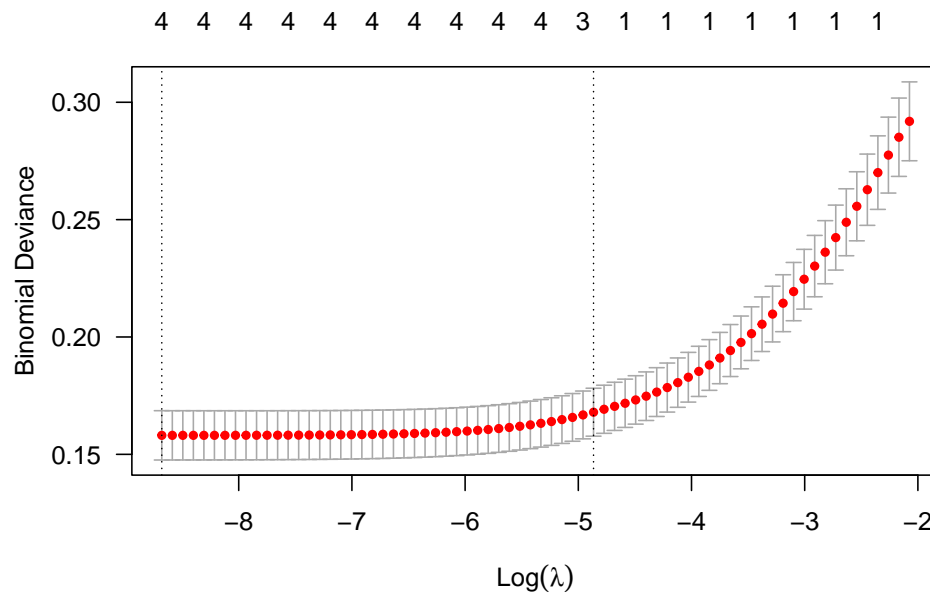
# : CV performance plot
plot(fit_enet, las=1)

# : 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")

library(yardstick)

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") %>%
  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
```