Risk Modeling and Classification

Logistic Regression, ROC Curves, Generalized Additive models (GAM)

DS 6030 | Fall 2022

classification.pdf

Contents

1 Risk 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.

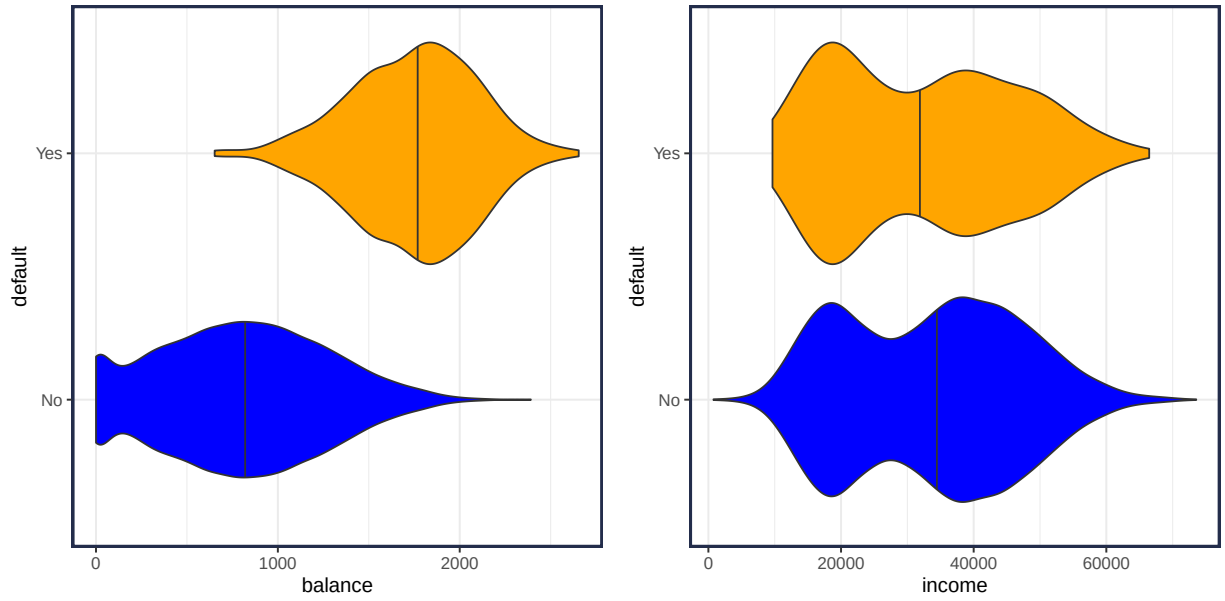
```
data(Default, package="ISLR")
```

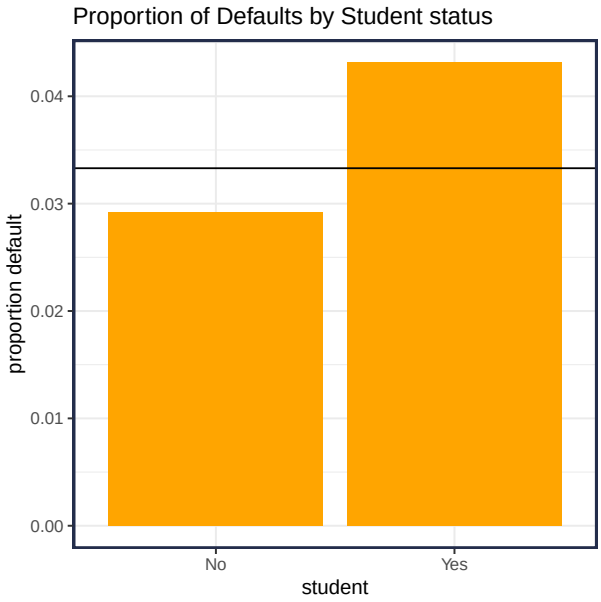
The variables are:

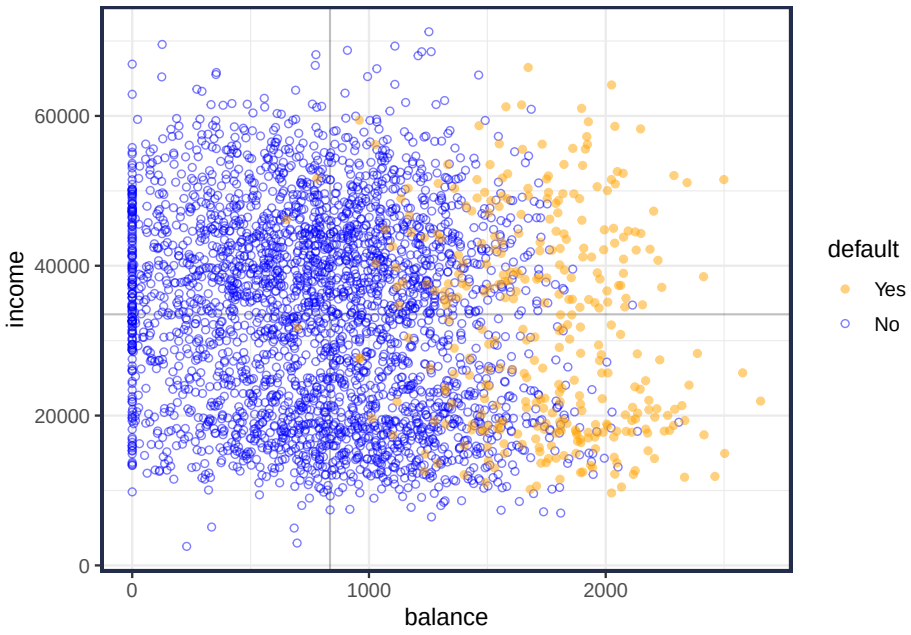
- *outcome variable* is categorical (factor) `Yes` and `No`, (`default`)
- the categorical (factor) variable (`student`) is either `Yes` or `No`
- the average balance a customer has after making their monthly payment (`balance`)
- the customer's income (`income`)

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
```




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
Yes
No

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: $\mathcal{G} = \{\text{"Yes", "No"}\}$
  - Medical Diagnosis Example: $\mathcal{G} = \{\text{"stroke", "heart attack", "drug overdose", "vertigo"}\}$
- 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 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

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?

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

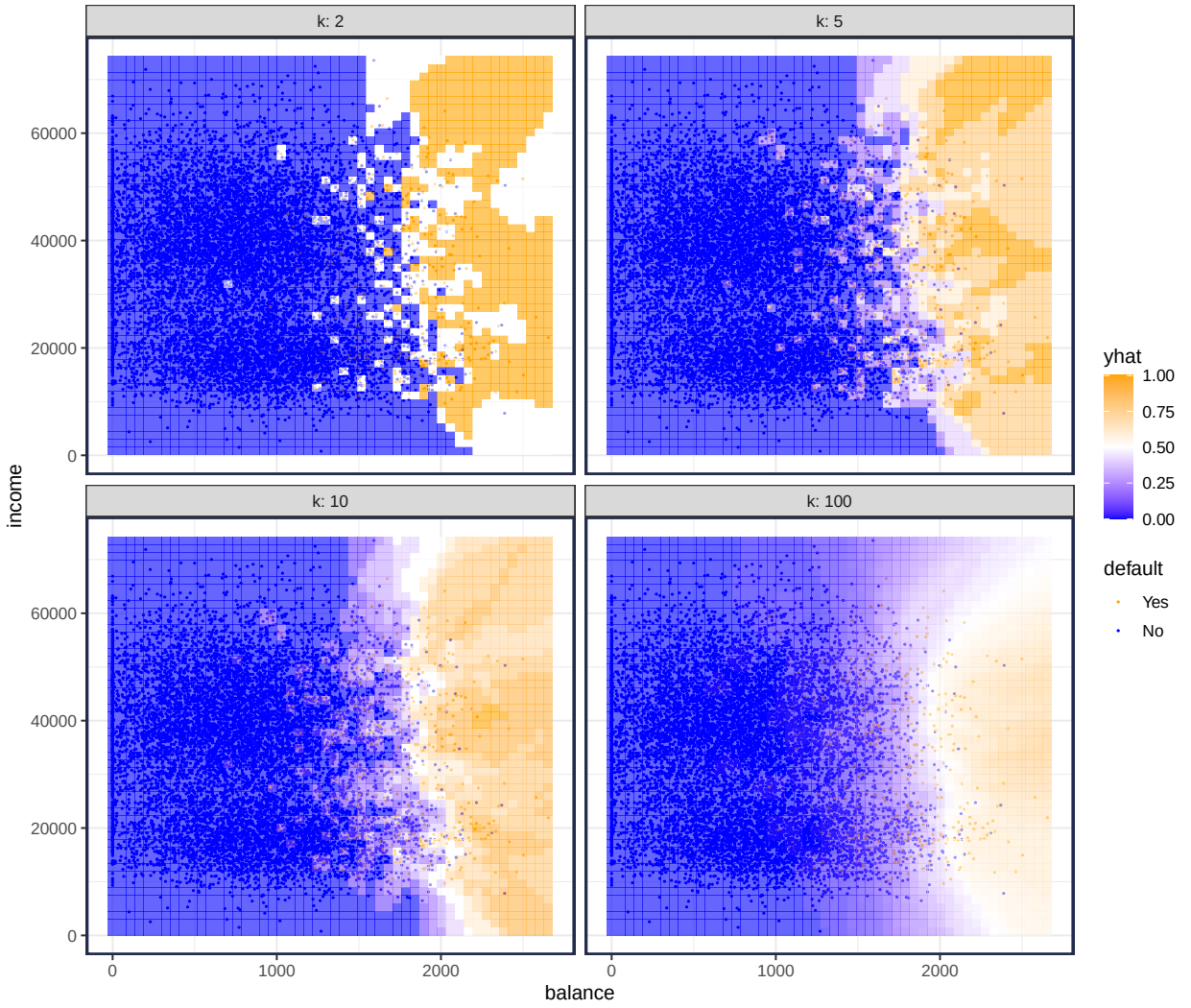
1.3.2 k-nearest neighbor (kNN)

- 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

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



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

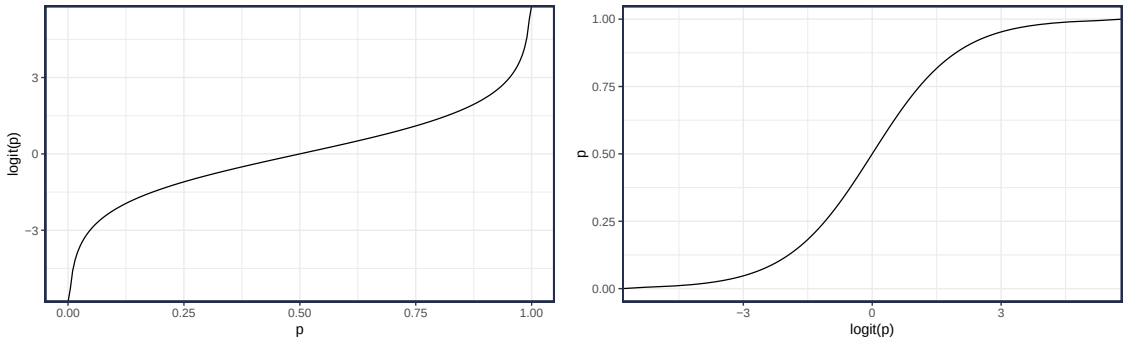
2.1 Basics

- 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*. Let $f = \text{logit(p)}$, then

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



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

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

- Alternatively, Logistic Regression models

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

and thus,

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

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

$$L(\beta) = \prod_{i=1}^{n} p_i(\beta)^{y_i}(1 - p_i(\beta))^{1-y_i}$$

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

- 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., $C = 1/n$

- This view facilitates *penalized logistic regression*

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

Ridge Penalty	$P(\beta) = \|\beta\|_2^2 = \sum_{j=1}^{p} \|\beta_j\|^2 = \beta^\mathsf{T}\beta$
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, data = Default,
             family="binomial")
```

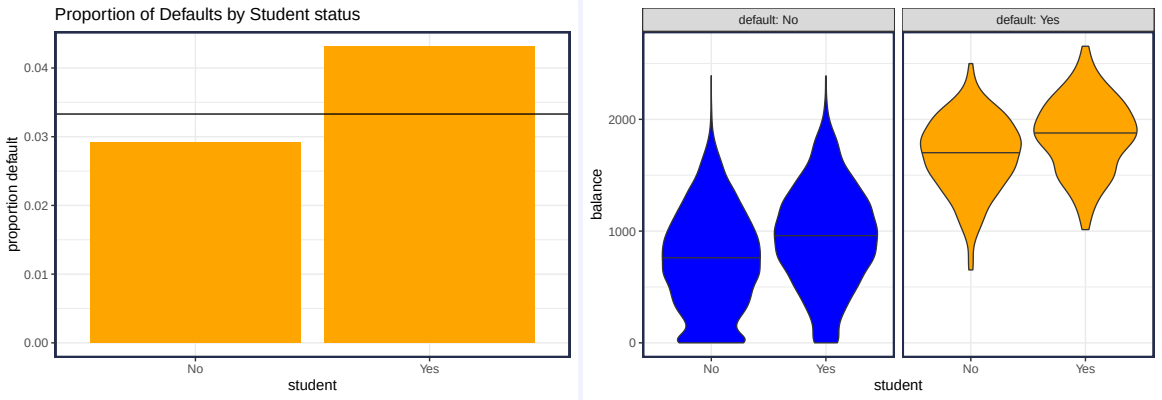
term	estimate	std.error	statistic	p.value
(Intercept)	-10.869	0.492	-22.080	0.000
studentYes	-0.647	0.236	-2.738	0.006
balance	0.006	0.000	24.738	0.000
income	0.000	0.000	0.370	0.712

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?

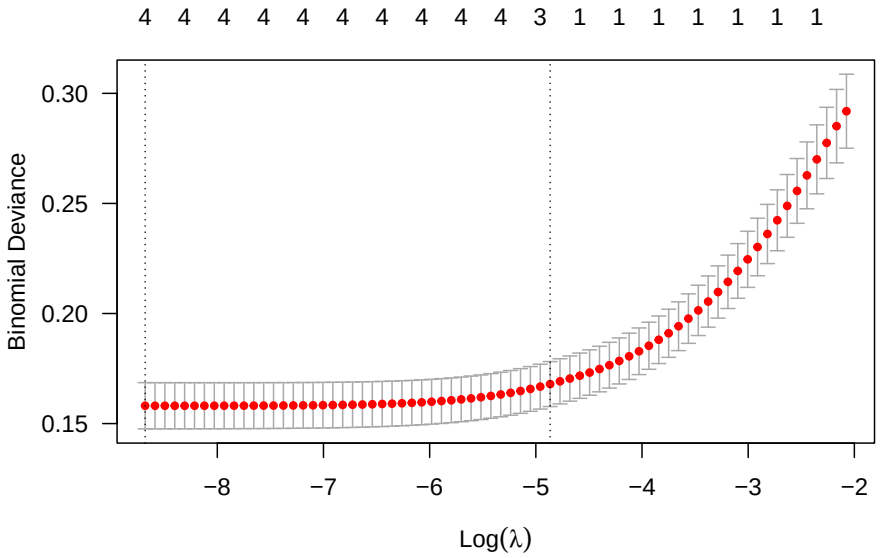
3. Why does `student=Yes` appear to lower risk of default, when the plot of student status vs. default appears to increase risk?



2.3.1 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(select(Default, 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

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

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 $\hat{p}(x) \in \{0, 1\}$.
  - Call $\hat{p}(x)$ the *risk score*
- **Brier Score / Squared Error**

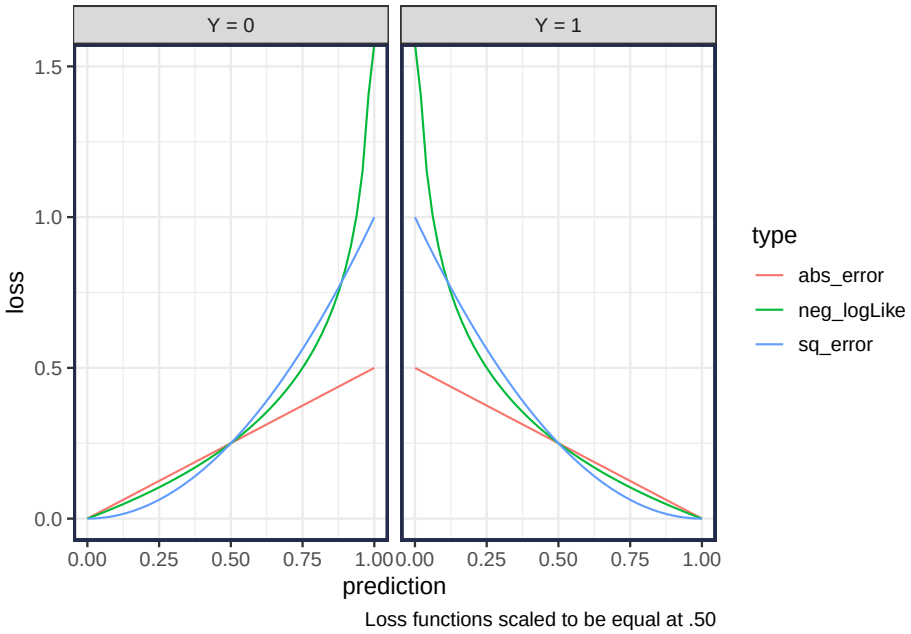
$$\begin{aligned} L(y, \hat{p}) &= (y - \hat{p})^2 \\ &= \begin{cases} (1 - \hat{p})^2 & y = 1 \\ \hat{p}^2 & y = 0 \end{cases} \end{aligned}$$

- **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)**
  - This is the loss function for Logistic Regression

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



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))
  )
}
```

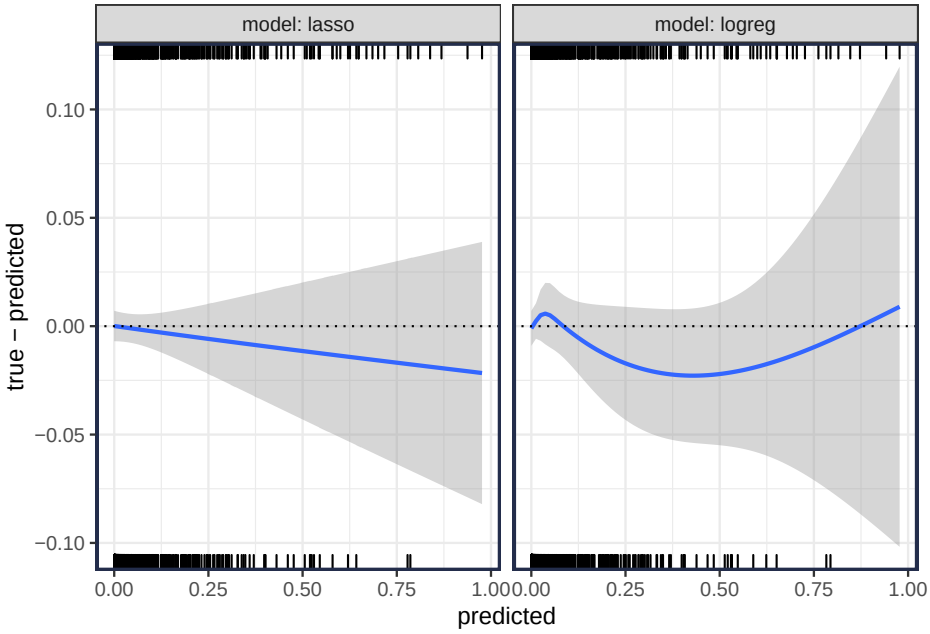
```
#: train/test split
set.seed(2019)
test = sample(nrow(Default), size=2000)
train = -test
```

```
#: 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 Calibration

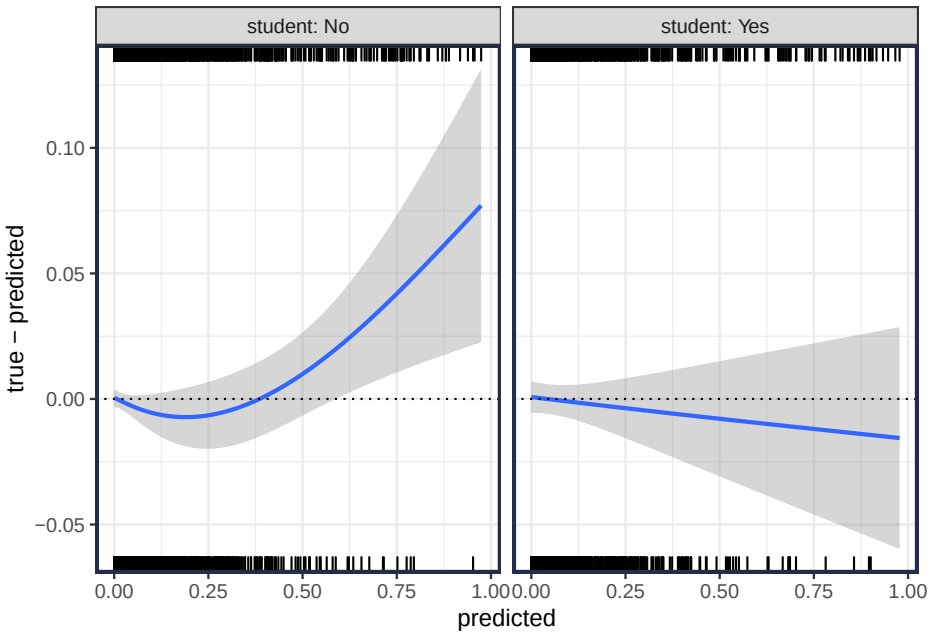
A risk model is said to be *calibrated* if the predicted probabilities are equal to the true risk (probabilities).

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



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.

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



3.3.1 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 revisit calibration when we cover Support Vector Machines (SVM) to convert a generic score to a probability.

- Platt Scaling
- Isotonic Regression
- Calibration: the Achilles heel of predictive analytics
  - Article on clinical decision-making
- The Measure and Mismeasure of Fairness: A Critical Review of Fair Machine Learning

3.4 Area under the ROC curve (AUC or AUROC)

The AUC 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.

$$\text{AUC} = \Pr(\hat{p}(x_1) > \hat{p}(x_0))$$

- where x_k is a randomly chosen example from class $Y = k$.

4 Risk Scoring vs. Classification

Most of the models we will encounter can output a predicted probability $\hat{p}_k(x) = \widehat{\Pr}(Y = k \mid X = x)$ for every class $k \in \mathcal{G}$.

Sometimes a *hard classification* needs to be made, i.e., decide on single label/class to assign the observation.

1. Hard Classification:
   - Use training data to estimate the *label* $\hat{G}(X)$
   - The loss/cost $L(G, \hat{G}(X))$ is the loss incurred by estimating G with $\hat{G}$
2. Risk Scoring (Soft-Classification):
   - Use training data to estimate the *probability* $\hat{p}_k(X)$
   - The loss/cost $L(G, \hat{p}(X))$ is the loss incurred by estimating G with $\hat{p}_k(X)$, where $\hat{p}(X) = [\hat{p}_1(X), \ldots, \hat{p}_K(X)]$

4.0.1 Example: Recidivism Prediction

Recently the National Institute of Justice hosted a Recidivism Forecasting Challenge which challenged contestants to predict if a parolee would be arrested for another offense within the next few years. The motivation is not to determine who should be released on parole, but rather which parolees should get additional assistance/supervision.

Objective	Model Output
Classification	Predict {Yes, No} if person will re-offend
Scoring	Predict probability that person will re-offend

Your Turn #6 : Recidivism Prediction

1. How could you use the probability/score to make a hard classification?
2. Do you think a hard classification or probability/score is better for this scenario?
3. If there were limited resources (e.g., only N parolees could get extra assistance), which type of model output would be more useful?

5 Binary Classification

5.1 Decision Theory

- We are considering *binary* outcomes, so the outcomes $G \in \{0, 1\}$
- Let $p(x) = \Pr(G = 1 \mid X = x)$
- Loss Function: $L(\text{True Label}, \text{Estimated Label}) = L(G, \hat{G})$
- A model's *Expected Prediction Error (EPE)* (also called *Risk*) at input X is the expected loss on new data with input X.
- The EPE (for a binary outcome) is:

$$\begin{aligned}\text{EPE}_x(g) &= \text{E}_{G|X=x}\left[L(G, \hat{G}(x) = g) \mid X = x\right] \\ &= L(1, g)\Pr(G = 1 \mid X = x) + L(0, g)(1 - \Pr(G = 1 \mid X = x)) \\ &= L(1, g)p(x) + L(0, g)(1 - p(x))\end{aligned}$$

- Hard Decision ($\hat{G}(x) \in \{0, 1\}$): choose $\hat{G}(x) = 1$ if

$$\begin{aligned}\text{EPE}_x(1) &< \text{EPE}_x(0) \\ L(1,1)p(x) + L(0,1)(1 - p(x)) &< L(1,0)p(x) + L(0,0)(1 - p(x)) \\ p(x)\left(L(1,1) - L(1,0)\right) &< (1 - p(x))\left(L(0,0) - L(0,1)\right) \\ p(x)\left(L(1,0) - L(1,1)\right) &\geq (1 - p(x))\left(L(0,1) - L(0,0)\right) \qquad \textit{(multiply both sides by -1)} \\ \frac{p(x)}{1 - p(x)} &\geq \frac{L(0,1) - L(0,0)}{L(1,0) - L(1,1)}\end{aligned}$$

Note

In most cases, there will be no loss/cost for making a correct classification. Thus it is convention to set $L(0, 0) = L(1, 1) = 0$ in these scenarios.

5.1.1 Example: Cancer Diagnosis

- Say we have a goal of estimating if a patient has cancer using medical imaging
  - Let $G = 1$ for cancer and $G = 0$ for no cancer
- Suppose we have solicited a loss function with the following values
  - $L(G = 0, \hat{G} = 0) = 0$: There is no loss for correctly diagnosis a patient without cancer.
  - $L(G = 1, \hat{G} = 1) = 0$: There is no loss (for our model) for correctly diagnosis a patient with cancer.
  - $L(G = 0, \hat{G} = 1) = C_{\text{FP}}$: There is a cost of C_{FP} units if the model issues a *false positive*, estimating the patient has cancer when they don't.
  - $L(G = 1, \hat{G} = 0) = C_{\text{FN}}$: There is a cost of C_{FN} units if the model issues a *false negative*, estimating the patient does not have cancer when they really do.
  - In these scenarios C_{FN} is often much larger than C_{FP} ($C_{\text{FN}} >> C_{\text{FP}}$) because the the effects of not promptly treating (or further testing, etc) a patient is more severe than starting a treatment path for patients that don't actually have cancer.

- The optimal decision is to issue a positive indication for cancer if $\text{EPE}_x(1) < \text{EPE}_x(0)$. This occurs when

$$\frac{p(x)}{1-p(x)} \geq \frac{C_{\text{FP}}}{C_{\text{FN}}} \quad \text{OR} \quad p(x) \geq \frac{C_{\text{FP}}}{C_{\text{FP}}+C_{\text{FN}}} \quad \text{OR} \quad \log\left(\frac{p(x)}{1-p(x)}\right) \geq \log\left(\frac{C_{\text{FP}}}{C_{\text{FN}}}\right)$$

- The ratio of C_{FP} to C_{FN} is all that matters for the decision. Let's say that $C_{\text{FP}} = 1$ and $C_{\text{FN}} = 10$. Then if $p(x) \geq 1/11$, our model will diagnose cancer.
  - Note: $p(x) = \Pr(Y = 1|X = x)$ is affected by the class prior $\Pr(Y = 1)$ (e.g., the portion of the population tested who have cancer), which is usually going to be small.

5.1.2 Optimal Threshold

- Recall, the optimal *hard classification* decision is to choose $\hat{G} = 1$ if:

$$\frac{p(x)}{1-p(x)} \geq \frac{L(0,1)-L(0,0)}{L(1,0)-L(1,1)}$$

- It can be convenient to use model output other than $p(x)/(1-p(x))$ to make decisions
- Some models directly output $\hat{p}(x)$
- Other models, like GLMs, naturally work with the link function (linear part)
  - Denote $\gamma(x)$ as the *logit* of $p(x)$:

$$\gamma(x) = \log\frac{p(x)}{1-p(x)} = \log\frac{\Pr(G=1 \mid X=x)}{\Pr(G=0 \mid X=x)}$$

- Table of equivalent representations:

Score	Threshold	Threshold (simplified)
$\dfrac{p(x)}{1-p(x)}$	$\dfrac{L(0,1)-L(0,0)}{L(1,0)-L(1,1)}$	$\dfrac{C_{\text{FP}}}{C_{\text{FN}}}$
$\gamma(x) = \log\dfrac{p(x)}{1-p(x)}$	$\log\left(\dfrac{L(0,1)-L(0,0)}{L(1,0)-L(1,1)}\right)$	$\log\left(\dfrac{C_{\text{FP}}}{C_{\text{FN}}}\right)$
$p(x)$	$\log\left(\dfrac{L(0,1)-L(0,0)}{L(0,1)-L(0,0)+L(1,0)-L(1,1)}\right)$	$\dfrac{C_{\text{FP}}}{C_{\text{FP}}+C_{\text{FN}}}$

The *Threshold (simplified)* assumes $L(0,0) = L(1,1) = 0$

5.1.3 Using estimated values

- We will never have the actual $p(x)$ or $\gamma(x)$, so replace them with the estimated values.
- For a given threshold t and input x, the hard classification rule is $\hat{G}_t(x) = \mathbb{1}(\hat{\gamma}(x) \geq t)$

Note

Because we have to estimate $\hat{p}(x)$ or $\hat{\gamma}(x)$, the best threshold t^* may differ from the theoretical optimal and need to be estimated. (more info about this below)

5.2 Common Binary Loss Functions

- Suppose we are going to estimate a binary outcome $G \in \{0, 1\}$ with a predicted label $\hat{G}(x)$
- **Mis-Classification Cost**

$$L(G, \hat{G}(x)) = \begin{cases} C_{\text{FP}} & G = 0, \hat{G}(x) = 1 \\ C_{\text{FN}} & G = 1, \hat{G}(x) = 0 \\ 0 & \text{otherwise} \end{cases}$$

  - Requires that a *hard classification* is made
  - The optimal prediction is $G^*(x) = \mathbb{1}(p(x) > C_{\text{FP}}/(C_{\text{FP}} + C_{\text{FN}}))$.
- **0-1 Loss** or **Misclassification Error**

$$L(G, \hat{G}(x)) = \mathbb{1}(y \neq \hat{G}(x)) = \begin{cases} 0 & G = \hat{G}(x) \\ 1 & G \neq \hat{G}(x) \end{cases}$$

  - This assumes $L(0, 1) = L(1, 0)$ (i.e., false positive costs the same as a false negative)
  - Requires that a *hard classification* is made
  - The optimal prediction is $G^*(x) = \mathbb{1}(p(x) > 1 - p(x))$ which is equivalent to $\mathbb{1}(p(x) > 0.50)$

5.3 Performance Metrics

5.3.1 Confusion Matrix

- Given a threshold t, we can make a *confusion matrix* to help analyze our model's performance on data
  - Data = $\{(X_i, G_i)\}_{i=1}^N$ (ideally this is hold-out/test data)
  - N_k is number of observations from class k ($N_0 + N_1 = N$)

		True Outcome		
		$G = 1$	$G = 0$	**total**
Model Outcome	$\hat{G}_t = 1$	True Positive (TP)	False Positive (FP)	$\hat{N}_1(t)$
	$\hat{G}_t = 0$	False Negative (FN)	True Negative (TN)	$\hat{N}_0(t)$
	total	N_1	N_0	N

Table from: https://tex.stackexchange.com/questions/20267/how-to-construct-a-confusion-matrix-in-latex

To illustrate a confusion table in practice let's go back to the `Default` data and see how the basic logistic regression models performs.

- In order to evaluate on hold-out data, split the data into train/test (used 8000 training, 2000 testing), fit a logistic regression model on training data, and make predictions on the test data

- Note that only 3.3% of the data is default.
  - Using a threshold of $\hat{p}(x) \geq 0.10$ to make a hard classification.
  - Equivalent to $\hat{\gamma}(x) \geq \log(.10) - \log(1 - .10) = -2.1972$

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

#: fit model on training data
fit.lm = glm(y~student + balance + income, family='binomial',
             data=Default[train, ])

#: Get predictions (of p(x)) on test data
p.hat = predict(fit.lm, Default[test, ], type='response')

#: Make Hard classification (use .10 as cut-off)
G.hat = ifelse(p.hat >= .10, 1, 0)

#: Make Confusion Table
G.test = Default$y[test]  # true values

table(predicted=G.hat, truth = G.test) %>% addmargins()
#>           truth
#> predicted    0    1  Sum
#>       0   1805   17 1822
#>       1    128   50  178
#>       Sum 1933   67 2000
```

5.3.2 Metrics

There are lots of common evaluation metrics that can be calculated from the confusion matrix:

Metric	Definition	Estimate
Risk/Exp.Cost	$\sum_{i=0}^{1}\sum_{j=0}^{1} L(i,j)P_X(G(X)=i, \hat{G}_t(X)=j)$	$\frac{1}{N}\sum_{i=1}^{N} L(G_i, \hat{G}_t(x_i))$
Mis-classification Rate	$P_{XG}(\hat{G}_t(X) \neq G(X)) =$ $P_X(\hat{G}_t(X)=0, G(X)=1) +$ $P_X(\hat{G}_t(X)=1, G(X)=0)$	$\frac{1}{N}\sum_{i=1}^{N} \mathbb{1}(\hat{G}_t(x_i) \neq G_i)$
False Positive Rate (FPR) {1-*Specificity*}	$P_X(\hat{G}_t(X)=1 \mid G(X)=0)$	$\frac{1}{N_0}\sum_{i:G_i=0} \mathbb{1}(\hat{G}_t(x_i)=1)$
True Positive Rate (TPR) {*Hit Rate, Recall, Sensitivity*}	$P_X(\hat{G}_t(X)=1 \mid G(X)=1)$	$\frac{1}{N_1}\sum_{i:G_i=1} \mathbb{1}(\hat{G}_t(x_i)=1)$
Precision TP/(TP + FP)	$P_X(G(X)=1 \mid \hat{G}_t(X)=1)$	$\frac{1}{\hat{N}_1(t)}\sum_{i:\hat{G}(x_i)=1} \mathbb{1}(G_i=1)$

- Note: Performance estimates are best carried out on *hold-out* data!
- See Wikipedia Page: Confusion Matrix for more metrics:

		Predicted condition			
	Total population = P + N	**Positive (PP)**	**Negative (PN)**	Informedness, bookmaker informedness (BM) = TPR + TNR − 1	Prevalence threshold (PT) = $\frac{\sqrt{TPR \times FPR} - FPR}{TPR - FPR}$
Actual condition	**Positive (P)**	**True positive (TP),** **hit**	**False negative (FN),** **type II error, miss, underestimation**	True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power = $\frac{TP}{P}$ = 1 − FNR	False negative rate (FNR), miss rate = $\frac{FN}{P}$ = 1 − TPR
	Negative (N)	**False positive (FP),** **type I error, false alarm, overestimation**	**True negative (TN),** **correct rejection**	False positive rate (FPR), probability of false alarm, fall-out = $\frac{FP}{N}$ = 1 − TNR	True negative rate (TNR), specificity (SPC), selectivity = $\frac{TN}{N}$ = 1 − FPR
	Prevalence = $\frac{P}{P+N}$	Positive predictive value (PPV), precision = $\frac{TP}{PP}$ = 1 − FDR	False omission rate (FOR) = $\frac{FN}{PN}$ = 1 − NPV	Positive likelihood ratio (LR+) = $\frac{TPR}{FPR}$	Negative likelihood ratio (LR−) = $\frac{FNR}{TNR}$
	Accuracy (ACC) = $\frac{TP + TN}{P + N}$	False discovery rate (FDR) = $\frac{FP}{PP}$ = 1 − PPV	Negative predictive value (NPV) = $\frac{TN}{PN}$ = 1 − FOR	Markedness (MK), deltaP (Δp) = PPV + NPV − 1	Diagnostic odds ratio (DOR) = $\frac{LR+}{LR-}$
	Balanced accuracy (BA) = $\frac{TPR + TNR}{2}$	F_1 score = $\frac{2PPV \times TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes–Mallows index (FM) = $\sqrt{PPV \times TPR}$	Matthews correlation coefficient (MCC) = $\sqrt{TPR \times TNR \times PPV \times NPV} - \sqrt{FNR \times FPR \times FOR \times FDR}$	Threat score (TS), critical success index (CSI), Jaccard index = $\frac{TP}{TP + FN + FP}$

Sources: [13][14][15][16][17][18][19][20] view • talk • edit

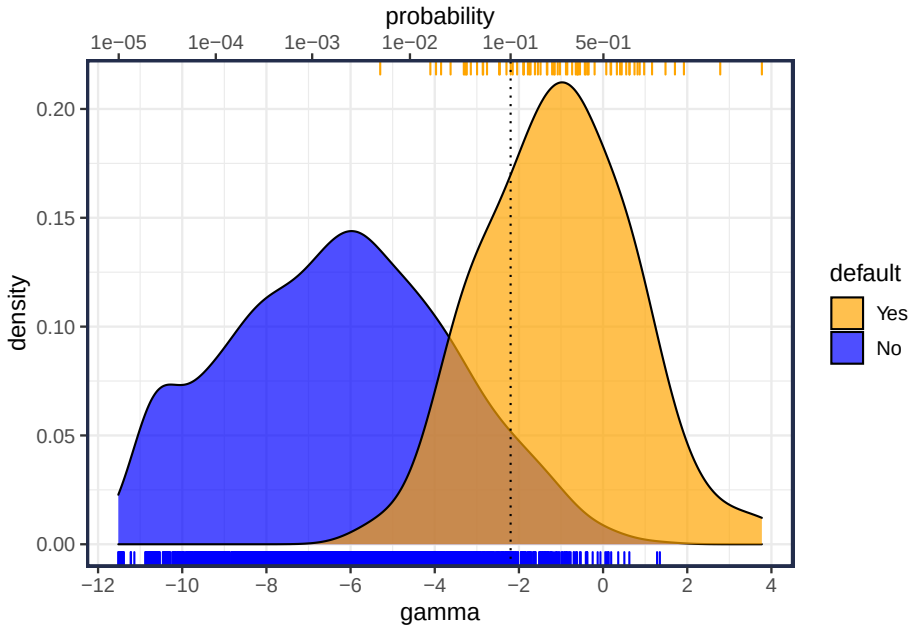
5.4 Performance over a range of thresholds

In the previous example, a hard classification was made using a threshold of $\hat{p}(x) \geq 0.10$. But performance varies as we adjust the threshold. Let's explore!

I'll use $\hat{\gamma}(x)$ instead of $\hat{p}(x)$ for this illustration.

```
#: Get predictions (of gamma(x)) on test data
gamma = predict(fit.lm, Default[test,], type='link')
```

- The model is unable to perfectly discriminate between groups, but the *defaults* do get scored higher in general:
  - As a reference point, note that $\gamma(x) = 0 \rightarrow \Pr(Y = 1 \mid X = x) = 1/2$
  - $\gamma(x) = \log p(x)/(1 - p(x))$



- We can calculate performance over a range of thresholds.
  - Unless the test data is too large, use all unique values of the training data as the thresholds. If too large, manually create threshold sequence.

```
#: Get performance data (by threshold)
perf = tibble(truth = G.test, gamma, p.hat) %>%
  #- group_by() + summarize() in case of ties
  group_by(gamma, p.hat) %>%
  summarize(n=n(), n.1=sum(truth), n.0=n-sum(truth)) %>% ungroup() %>%
  #- calculate metrics
  arrange(gamma) %>%
  mutate(FN = cumsum(n.1),     # false negatives
         TN = cumsum(n.0),     # true negatives
         TP = sum(n.1) - FN,   # true positives
         FP = sum(n.0) - TN,   # false positives
         N = cumsum(n),        # number of cases predicted to be 1
         TPR = TP/sum(n.1), FPR = FP/sum(n.0)) %>%
  #- only keep relevant metrics
```

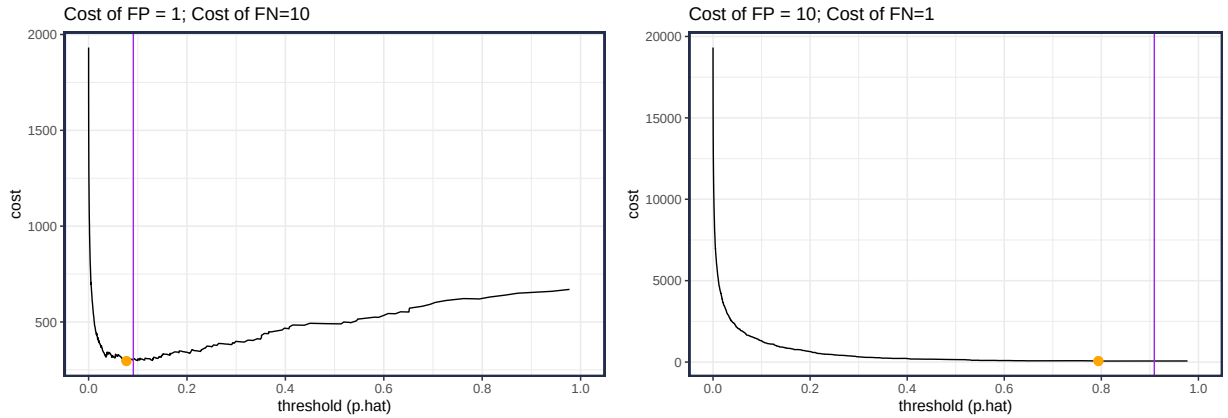
```
  select(-n, -n.1, -n.0, gamma, p.hat)
```

gamma	p.hat	FN	TN	TP	FP	N	TPR	FPR
-11.52	0	0	1	67	1932	1	1	0.999
-11.51	0	0	2	67	1931	2	1	0.999
-11.49	0	0	3	67	1930	3	1	0.998
-11.49	0	0	4	67	1929	4	1	0.998
-11.48	0	0	5	67	1928	5	1	0.997
-11.47	0	0	6	67	1927	6	1	0.997

- Note: the `perf` object is *only based on the rank order* of the predictions. This means that the same results would be obtained if we used $\hat{\gamma}(x)$ or $\hat{p}(x)$ to do the ranking.
  - This is because there is a one-to-one monotone relationship between $\hat{\gamma}(x)$ and $\hat{p}(x)$.
  - The `perf` object grouped by both `gamma` and `p.hat` so both thresholds are available. But we can switch back and forth from the relationship $\log(p/(1-p)) = \gamma$, so its easy to switch between the two depending on what is most convienient.

5.4.1 Cost Curves

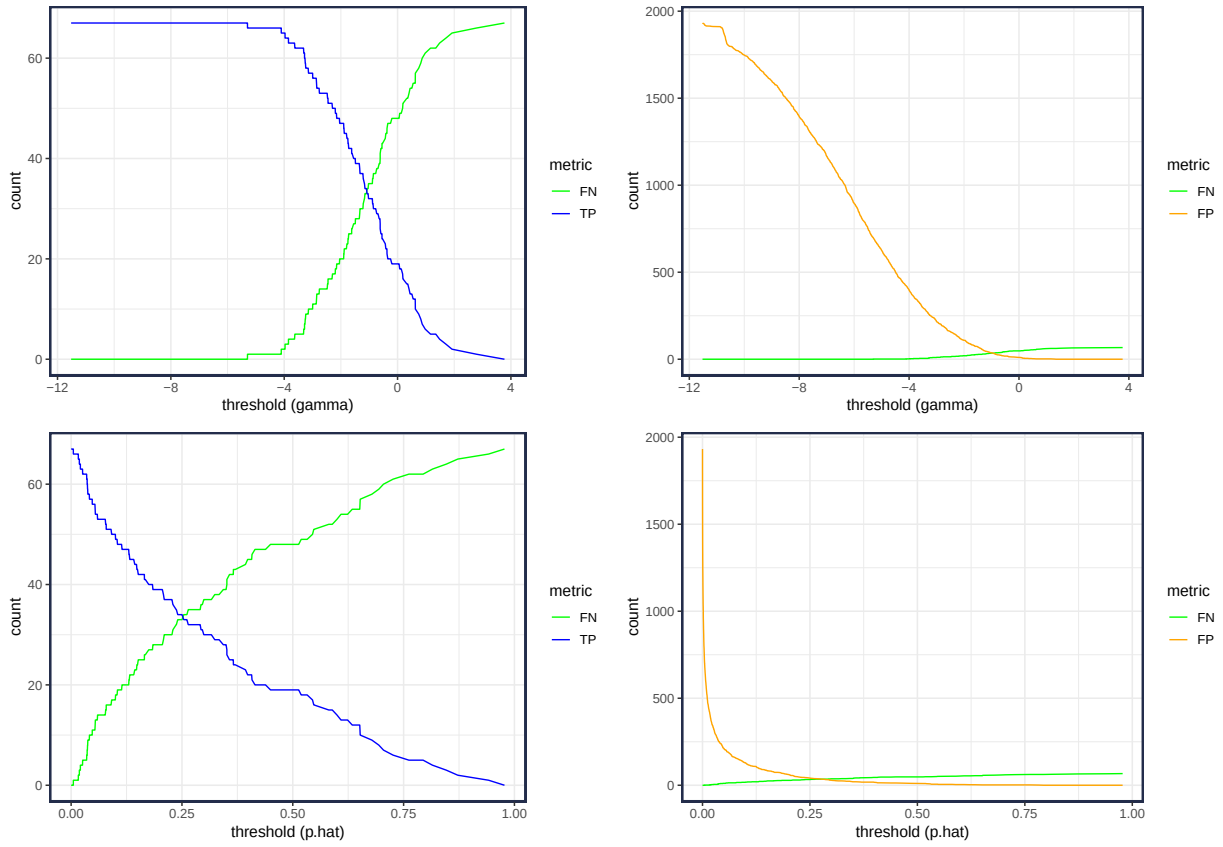
- Under the usual scenario where $L(0,0) = L(1,1) = 0$, the cost only depends on the ratio of false positive costs (C_{FP}) to false negative costs (C_{FN}).
- note: the purple is the *theoretical* optimal threshold (using $t^* = \log C_{\text{FP}}/C_{\text{FN}}$ for $\hat{\gamma}(x)$ and $C_{\text{FP}}/(C_{\text{FP}} + C_{\text{FN}})$ for $\hat{p}(x)$) and the orange point is at the optimal value using the model



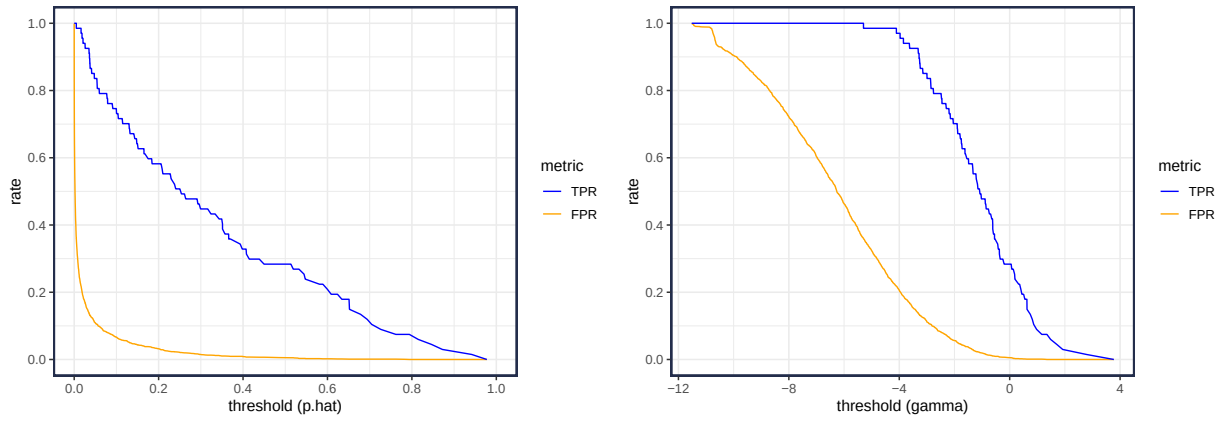
Optimal Threshold

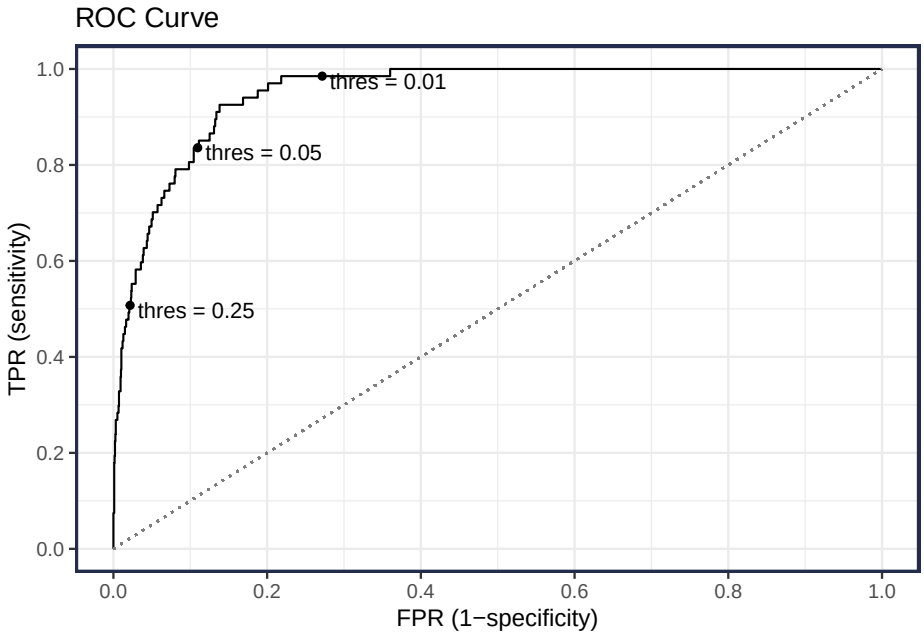
- The *theoretically* optimal threshold is based on the *true* $\gamma(x) = \log \frac{p(x)}{1-p(x)}$ (for a given cost ratio of FP to FN)
- The observed optimal threshold will differ when the model's estimate $\hat{\gamma}(x) \neq \gamma(x)$
  - Hopefully, they are close and it won't make much difference which one you use. But I'd take the estimated threshold if I had sufficient data.
- Note that the estimated values depend on the prior class probabilities. If you suspect these may differ in the future, then you should adjust the threshold.

5.4.2 General Performance as function of threshold (select metrics)



5.4.3 ROC Curves (Receiver Operating Characteristic)



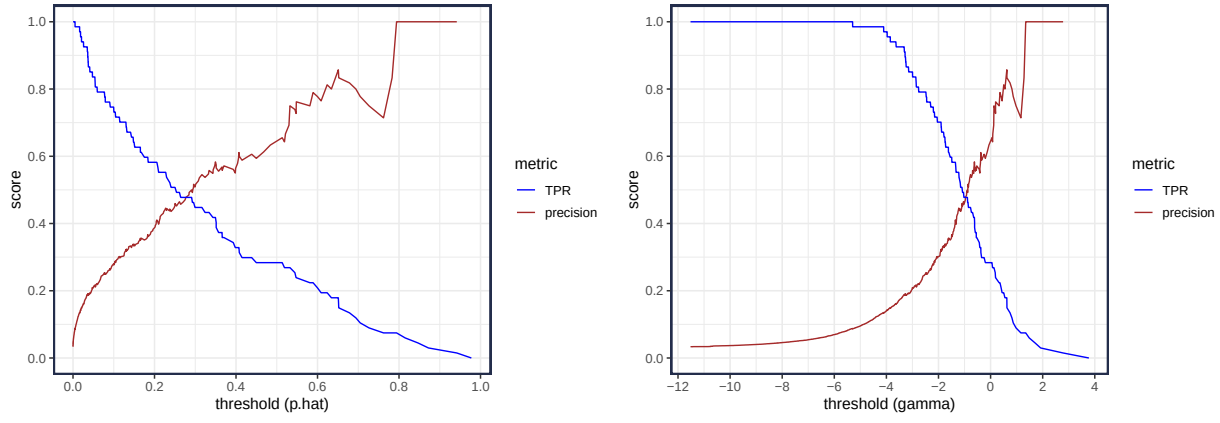


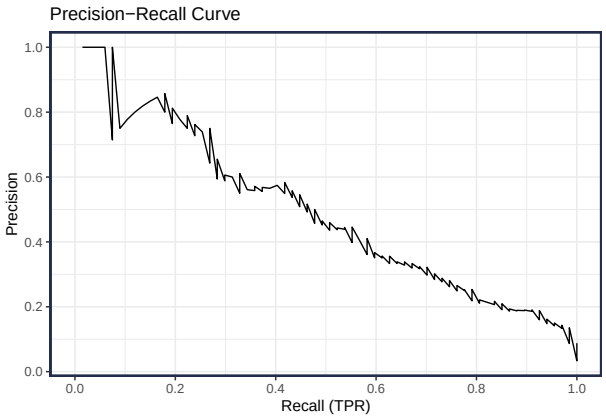
AUROC

- The *area under the ROC curve* (AUROC or AUC) is a popular performance metric
- I don't think it is a great way to compare classifiers for several reasons
  - The main reason is that in a real application you can almost always come up with an estimated cost/loss for the different decisions
  - To say it another way, comparisons should be made at a single point on the curve; the entire FPR region should not factor into the comparison.
- The AUROC is equal to the probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one.
  - AUROC is proportional to the Mann-Whitney U statistic

5.4.4 Precision Recall Curves

- Popular for information retrieval/ranking
- The *precision* metric is not monotonic wrt threshold, hence the sawteeth pattern.



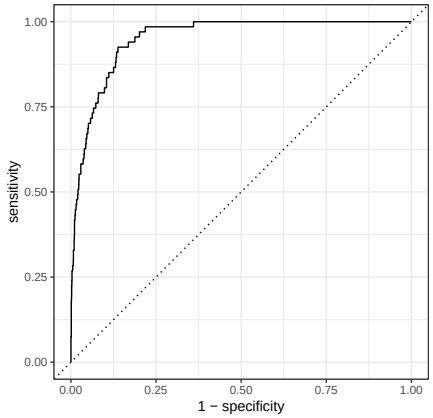


5.4.5 R Code

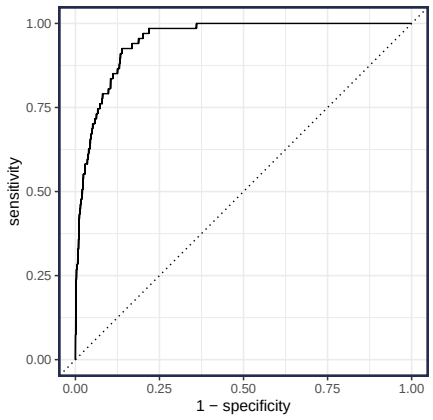
Once we have the FP, TP, TN, FN values for a set of thresholds (like what is in the `perf` object), then we have everything we need to calculate any metric (e.g., gain, lift, F1, . . .).

- But I will mention the `yardstick` R package which offers some functionality you may find convenient
- List of the metrics included in the `yardstick` package

```
library(yardstick)  # for evaluation functions

#: ROC plots
ROC = tibble(truth = factor(G.test, levels=c(1,0)), gamma) %>%
  yardstick::roc_curve(truth, gamma)

autoplot(ROC)  # autoplot() method
```




```
ROC %>%         # same as autoplot()
  ggplot(aes(1-specificity, sensitivity)) + geom_line() +
  geom_abline(lty=3) +
  coord_equal()
```




```
#: Area under ROC (AUROC)
tibble(truth = factor(G.test, levels=c(1,0)), gamma) %>%
  roc_auc(truth, gamma)
#> # A tibble: 1 x 3
#>   .metric .estimator .estimate
#>   <chr>   <chr>          <dbl>
#> 1 roc_auc binary         0.951

roc_auc_vec(factor(G.test, 1:0), gamma)
#> [1] 0.9505
```

5.5 Summary of Classification Evaluation

- Ask yourself: do I really need to make a hard classification? Or are risk scores/probabilities better for end user?
- Use cost! The other metrics are probably not going to give you what you really want.
  - Resist the pressure to use AUROC, Accuracy, F1.
  - If you don't know cost(FP)/cost(FN) ratio, then report performance for a reasonable range of values.
- For Binary Classification Problems, the optimal decision is to choose $\hat{G}(x) = 1$ if

$$\frac{p(x)}{1-p(x)} \geq \frac{L(0,1) - L(0,0)}{L(1,0) - L(1,1)} = \frac{\text{FP} - \text{TN}}{\text{FN} - \text{TP}}$$

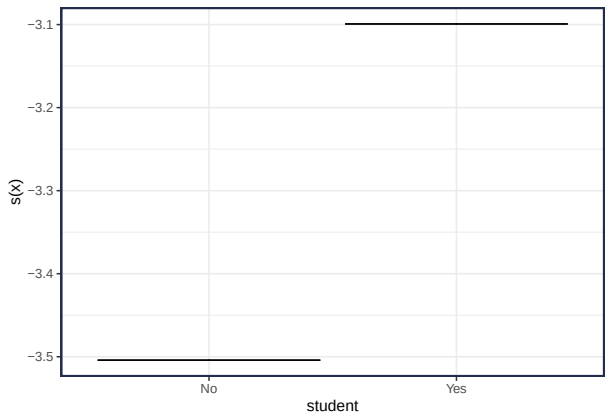
- Consider the connection to Decision Theory, make the decision that maximizes *expected utility*. The losses define the utility.
- In practice, we need to use an *estimated* $\hat{p}(x)$ or $\hat{\gamma}(x)$ and *estimated* threshold.
- Model parameters are usually estimated with a different metric than what's used for evaluation.
  - E.g., Estimate logistic regression parameters by minimizing Log-loss (i.e., maximum likelihood)
  - E.g., Hinge Loss for Support Vector Machines (SVM)
  - But Total Cost, MAE, F1, AUROC are used for evaluation (and tuning parameter estimation).
  - Reason: its difficult to estimate model parameters with such loss functions (e.g., non-differentiable, non-unique, etc.)

6 Generalized Additive Models (GAM)

In our discussion of Basis Expansions, we covered how the relationship between a single raw predictor x and the outcome could be made more complex with basis expansions.

- **Example 1: Categorical Predictor One-Hot Encoded**

```
#: One-hot Basis
X1 = model.matrix(~student-1, data=Default)
head(X1, 4)
#>   studentNo studentYes
#> 1         1          0
#> 2         0          1
#> 3         1          0
#> 4         1          0

#: Fit
fit.1 = glm(y ~ student-1, family="binomial", data=Default)

#: Plot
Default %>%
  mutate(pred = predict(fit.1, newdata=Default, type="link")) %>%
  distinct(student, pred) %>%
  ggplot(aes(student, pred)) + geom_errorbar(aes(ymin=pred, ymax=pred)) +
  labs(y="s(x)")
```



- **Example 2: Continuous Predictor with Polynomial Basis**

```
#: Fit linear
fit.lm = glm(y~income, data=Default, family="binomial")

#: Polynomial Basis
X2 = model.matrix(y~poly(income, degree=4)-1, data=Default)
head(X2, 4)
#>   poly(income, degree = 4)1 poly(income, degree = 4)2 poly(income, degree = 4)3
#> 1                  0.008132                 -0.003807                 -0.0080610
#> 2                 -0.016055                  0.016202                 -0.0138049
#> 3                 -0.001312                 -0.009300                  0.0057123
#> 4                  0.001640                 -0.009414                  0.0009502
#>   poly(income, degree = 4)4
#> 1                 0.0006076
#> 2                 0.0052431
#> 3                 0.0063483
#> 4                 0.0083087
```

```
#: Polynomial Model (edf=5)
fit.2 = glm(y~poly(income, degree=4), family="binomial", data=Default)
# equivalent to:  glm(y~X2, family="binomial", data=Default)
```

- **Example 3: Continuous Predictor with Binning (Regressograms)**

```
#: Binning Basis
X3 = model.matrix(~cut(income, 5)-1, data=Default)
head(X3, 4)
#>   cut(income, 5)(699,1.53e+04] cut(income, 5)(1.53e+04,2.99e+04]
#> 1                            0                                  0
#> 2                            1                                  0
#> 3                            0                                  0
#> 4                            0                                  0
#>   cut(income, 5)(2.99e+04,4.44e+04] cut(income, 5)(4.44e+04,5.9e+04]
#> 1                                 1                                0
#> 2                                 0                                0
#> 3                                 1                                0
#> 4                                 1                                0
#>   cut(income, 5)(5.9e+04,7.36e+04]
#> 1                                0
#> 2                                0
#> 3                                0
#> 4                                0

#: Binning Model (edf=5)
fit.3 = glm(y~cut(income, 5)-1, data=Default, family="binomial")
# equivalent to:  glm(y~X3-1, family="binomial", data=Default)
```

- **Example 4: Continuous Predictor with B-Splines Basis**

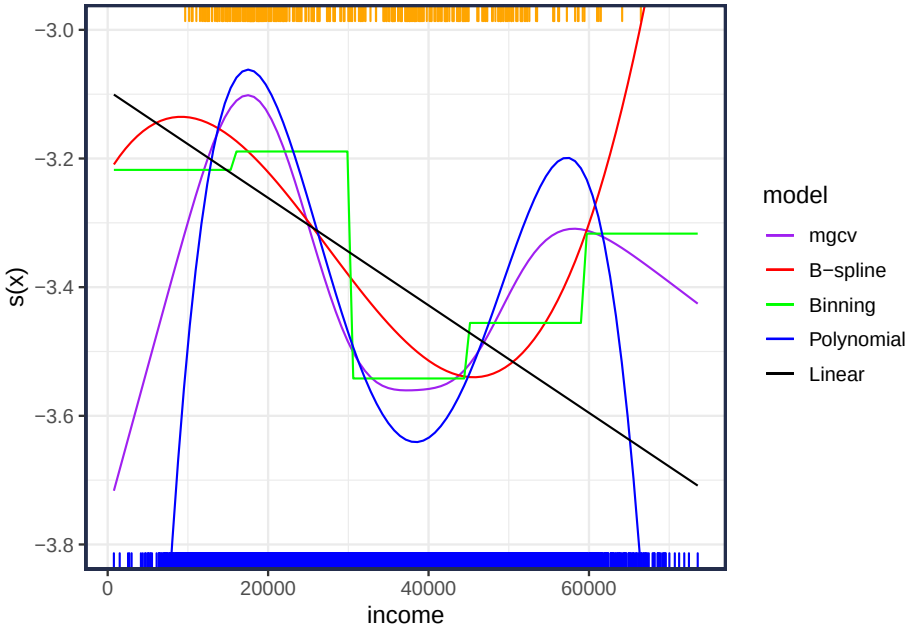
```
library(splines) # for bs() function

#: B-spline Basis
X4 = model.matrix(~bs(income, df=4)-1, data=Default)
head(X4, 4)
#>   bs(income, df = 4)1 bs(income, df = 4)2 bs(income, df = 4)3
#> 1              0.1204              0.4351             0.428565
#> 2              0.5755              0.1229             0.008137
#> 3              0.3521              0.4809             0.166404
#> 4              0.2625              0.4994             0.238160
#>   bs(income, df = 4)4
#> 1           1.591e-02
#> 2           0.000e+00
#> 3           0.000e+00
#> 4           2.576e-05

#: Binning Model (edf=5)
fit.4 = glm(y~bs(income, df=3), data=Default, family="binomial")
# equivalent to:  glm(y~X4, family="binomial", data=Default)
```

- **Example 5: Continuous Predictor with Penalized Spline**

```
library(mgcv)
#: Fit penalized spline, it will select best edf
#    specify smooth with s()
fit.5 = gam(y~s(income), data=Default, family="binomial")
summary(fit.5)
#>
```

```
#> Family: binomial
#> Link function: logit
#>
#> Formula:
#> y ~ s(income)
#>
#> Parametric coefficients:
#>             Estimate Std. Error z value Pr(>|z|)
#> (Intercept)  -3.3819     0.0564     -60   <2e-16 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> Approximate significance of smooth terms:
#>            edf Ref.df Chi.sq p-value
#> s(income) 4.31   5.37   10.8    0.06 .
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> R-sq.(adj) =  0.00098   Deviance explained = 0.466%
#> UBRE = -0.70823  Scale est. = 1         n = 10000
```

```
#: Plot of Fit
Default %>%
  ggplot(aes(income)) +
  geom_rug(data=. %>% filter(y==1), aes(color=default), sides="t", color = plot_cols[["Yes"]]) +
  geom_rug(data=. %>% filter(y==0), aes(color=default), sides="b", color = plot_cols[["No"]]) +
  scale_color_manual(values=c(mgcv = "purple", `B-spline`="red" ,
                              Binning="green", Polynomial="blue", Linear="black"), name="model") +
  coord_cartesian(ylim=c(-3.8, -3)) +
  labs(y="s(x)") +
  geom_function(fun = ~predict(fit.5, newdata=tibble(income=.)), aes(color="mgcv")) +
  geom_function(fun = ~predict(fit.4, newdata=tibble(income=.)), aes(color="B-spline")) +
  geom_function(fun = ~predict(fit.3, newdata=tibble(income=.)), aes(color="Binning")) +
  geom_function(fun = ~predict(fit.2, newdata=tibble(income=.)), aes(color="Polynomial")) +
  geom_function(fun = ~predict(fit.lm, newdata=tibble(income=.)), aes(color="Linear"))
```



6.1 Generalized Additive Models (GAMs)

All of the above models are for a *single* predictor. The extension to multiple predictors is called **Generalized Additive Models (GAMs)**.

Instead of the linear form

$$f(\mathbf{x}) = \beta_0 + \sum_j \beta_j x_j,$$

use non-linear bases for each predictor

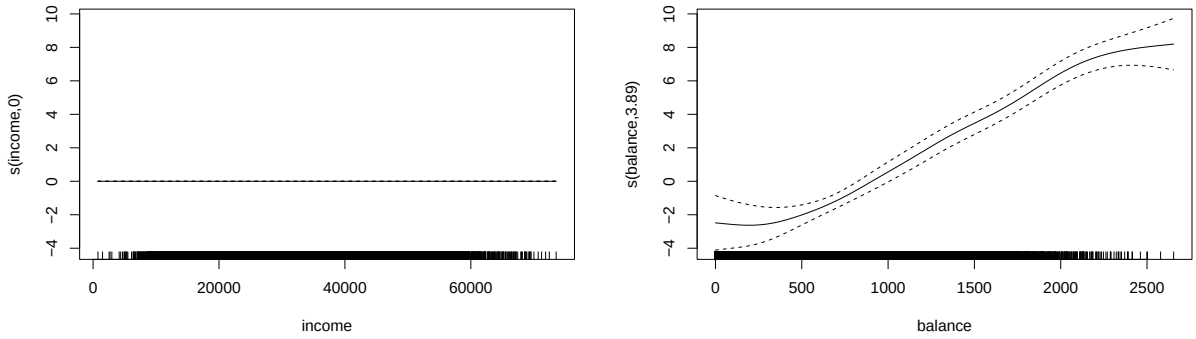
$$f(\mathbf{x}) = \beta_0 + \sum_j s_j(x_j)$$

where $s_j(x_j)$ can allow non-linear (e.g., smooth) forms, like B-splines.

- For binary classification setting: $\text{logit} p(\mathbf{x}) = f(\mathbf{x})$
- These are *additive* models because each term adds its contribution, although potentially in a non-linear way
  - But interactions can still be accommodated using `s(x1, x2)` or `s(x1, by=fac)`
- These are *generalized* models following the GLM notation. You can use different distributions with the `family=` argument
- GAMs retain the interpretability of a linear additive model (linear regression, logistic regression), but can add complexity to predictors where needed
  - Drawback: can be slow, especially for high dimensional data
- In **R**, the `mgcv` package is excellent for implementing GAM models.
  - It used Generalized Cross-validation to select optimal smoothing for each component
  - It also has a `select=TRUE` argument to further shrink entire components toward 0
  - Can handle low dimension interactions (even factor-continuous)
- See ISL 7.7 or ESL 9.1 for more details

```
library(mgcv)

fit.gam = gam(y ~ student + s(income) + s(balance),  # smooth main effects
              select = TRUE,                         # shrink components toward 0
              family="binomial", data=Default)

summary(fit.gam)
#>
#> Family: binomial
#> Link function: logit
#>
#> Formula:
#> y ~ student + s(income) + s(balance)
#>
#> Parametric coefficients:
#>             Estimate Std. Error z value Pr(>|z|)
#> (Intercept)   -5.611      0.318  -17.62  < 2e-16 ***
#> studentYes    -0.711      0.149   -4.78  1.7e-06 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
#>
#> Approximate significance of smooth terms:
#>                edf Ref.df Chi.sq p-value
#> s(income)  0.000806      9      0    0.85
#> s(balance) 3.888128      9    641  <2e-16 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> R-sq.(adj) =  0.339   Deviance explained = 46.3%
#> UBRE = -0.84185  Scale est. = 1         n = 10000
plot(fit.gam)
```



6.2 Estimating $\hat{s}_j(x_j)$ with Backfitting

The smooth terms of a GAM model can be estimating using an iterative approach called *backfitting*.

Algorithm: Backfitting for GAM (Squared Error Loss / Linear Regression)

Model: $\hat{y}(\mathbf{x}) = \beta_0 + \sum_{j=1}^{p} \hat{s}_j(x_j)$

1. Start with intercept-only model. All smooth terms set to zero: $s_j(x_j) = 0$.
2. Iterate over all p predictor variables:
   a. Construct *partial residuals* $r_i = y_i - \hat{\beta}_0 - \sum_{k \neq j} \hat{s}_k(x_{ik})$ holding out the jth predictor
   b. Fit jth smoother to residuals: Estimate $\hat{s}(x_j)$ from $\{(r_i, x_{ij})\}_{i=1}^{n}$
3. Repeat many times stopping when converged (i.e., smooth fits no longer changing very much)

Note: There are more details (see ESL 9.1), but this is the main (and simple) idea.