Lecture 4: Classification

Part I: Classification methods
Part II: Assessing classifier performance

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95-791: Data Mining

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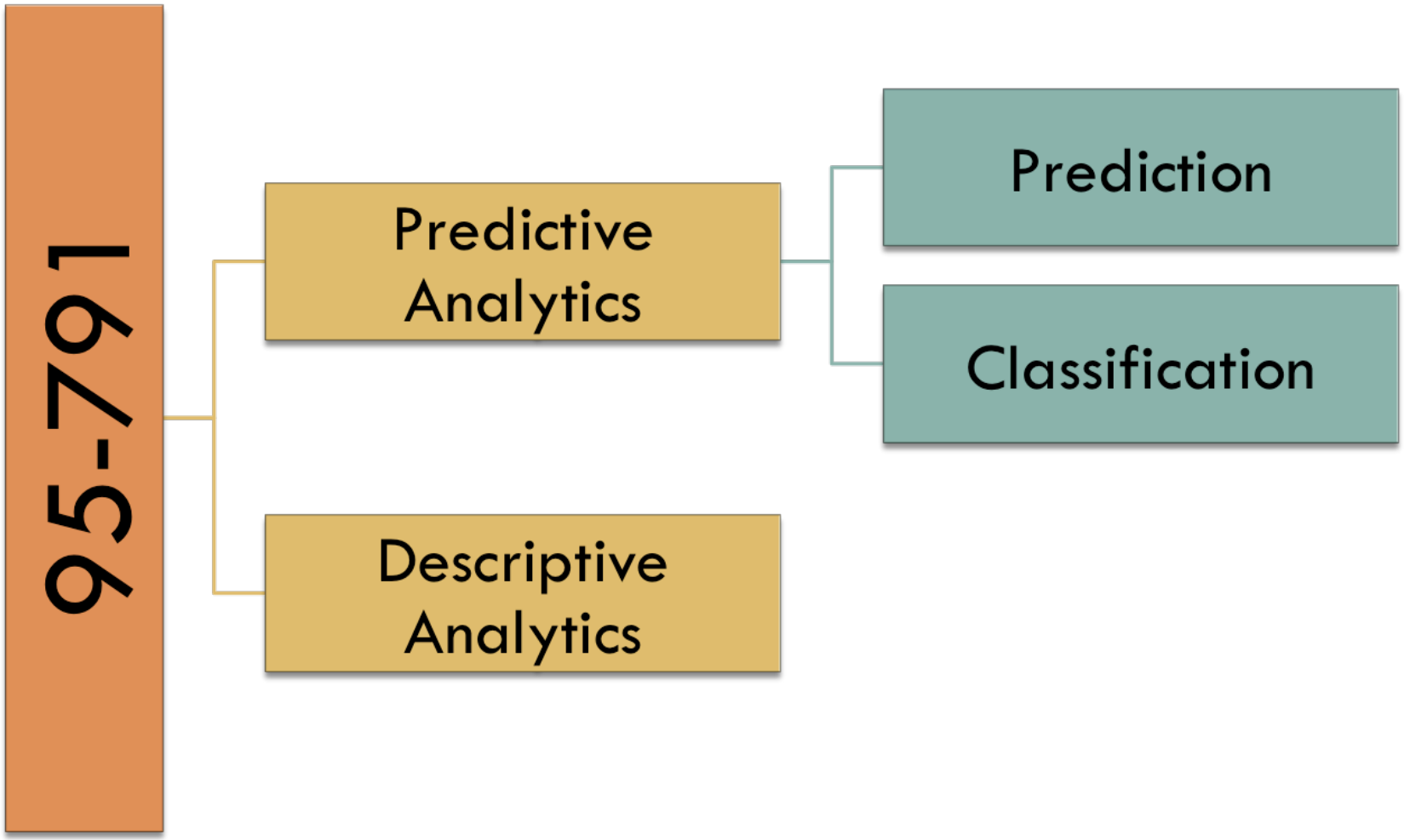
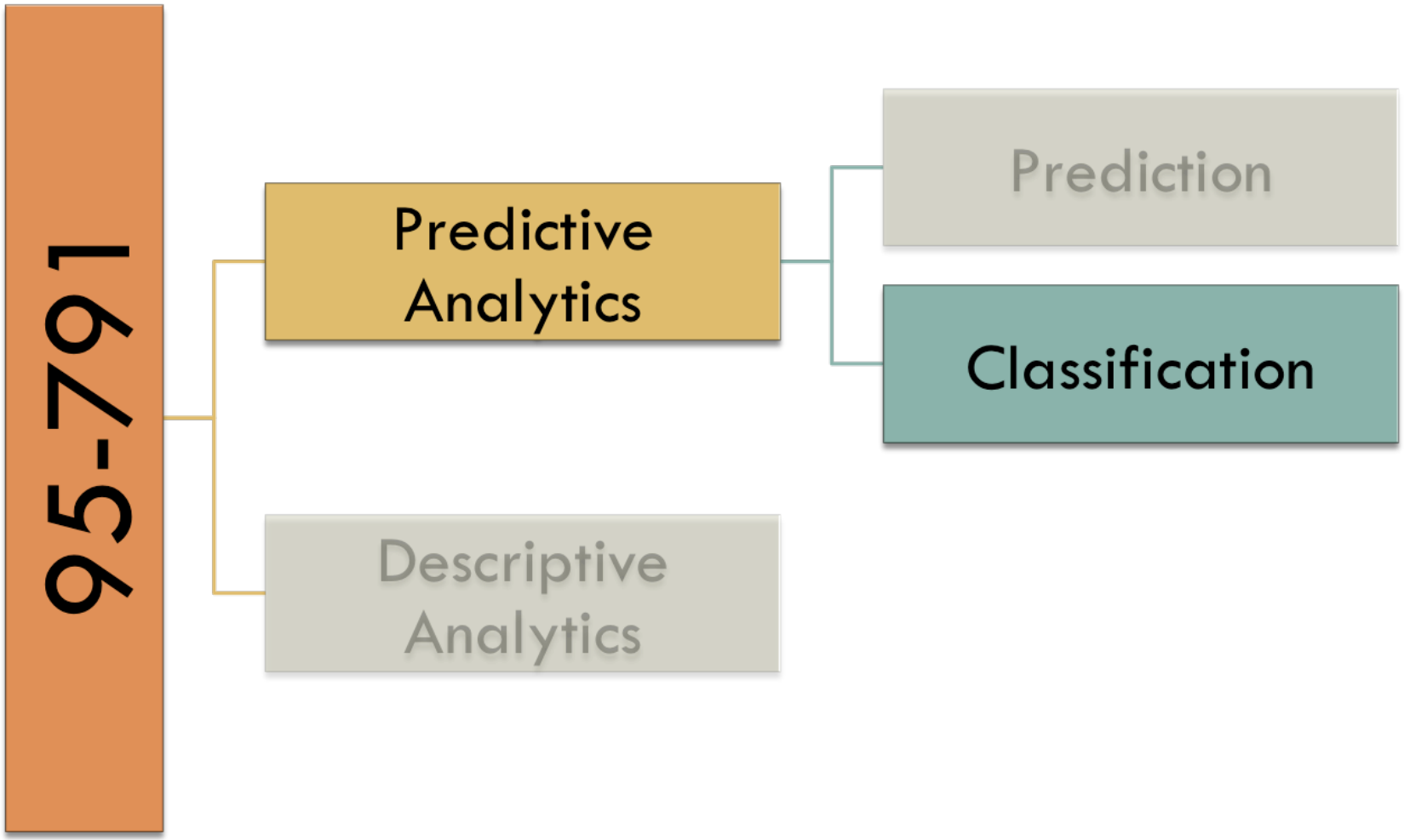
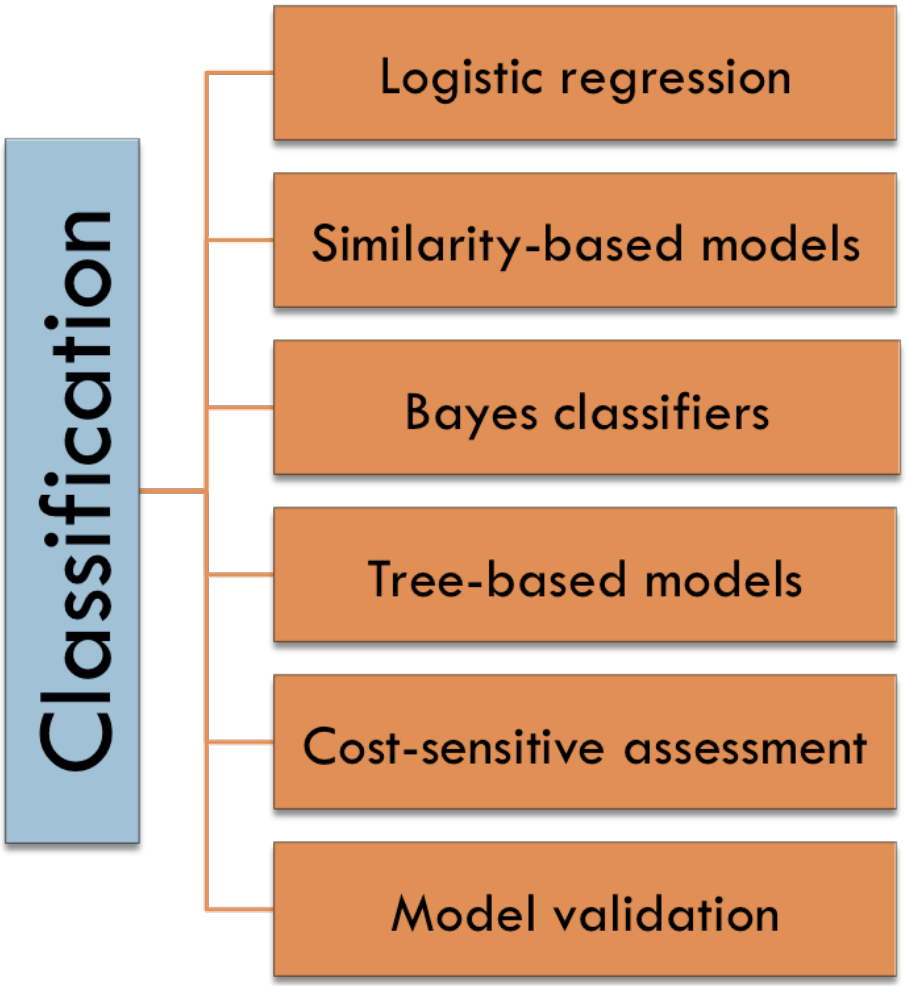
Course Roadmap



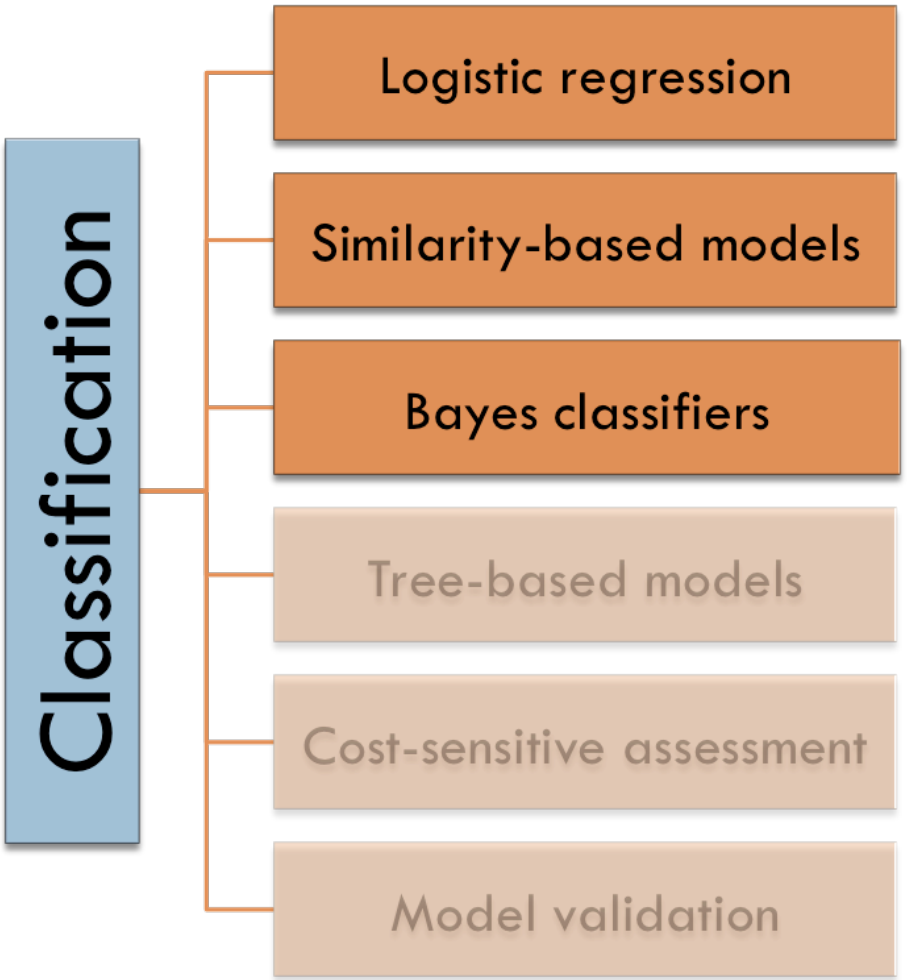
Course Roadmap



Prediction topics



Prediction topics



Agenda for Part I

- **Decision Boundary for Logistic Regression**
- **Nearest-Neighbours methods**
- **Bayes Methods**

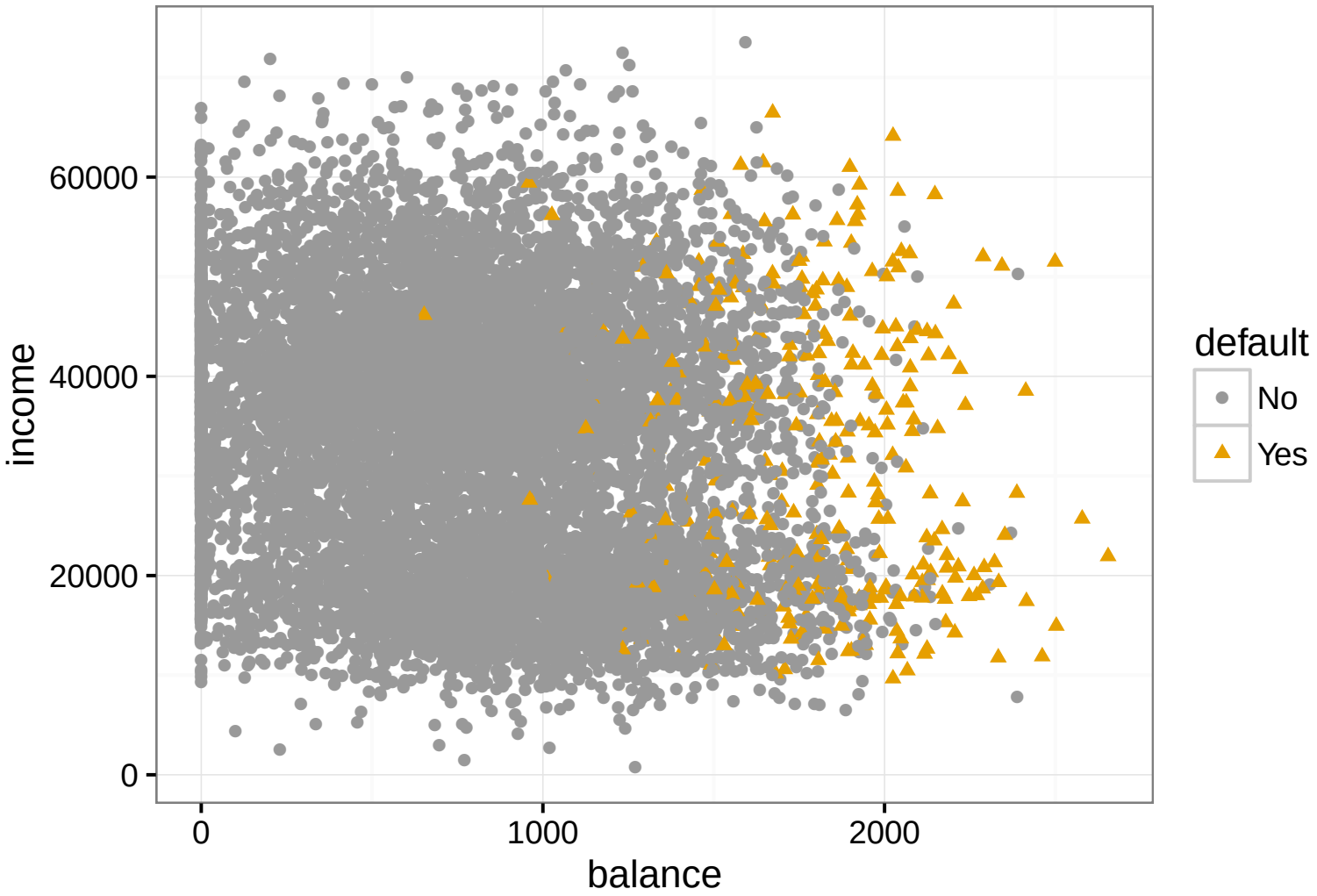
Logistic regression as a classifier

- Last class we saw how to *interpret* logistic regression
- But what does it look like as a classifier?
- i.e., What does the decision rule

$$\hat{Y} = \begin{cases} 1 & \text{if } \frac{e^{\hat{\beta}_0+\hat{\beta}_1 \texttt{balance}+\hat{\beta}_2 \texttt{income}}}{1+e^{\hat{\beta}_0+\hat{\beta}_1 \texttt{balance}+\hat{\beta}_2 \texttt{income}}} > \alpha \\ 0 & \text{otherwise} \end{cases}$$

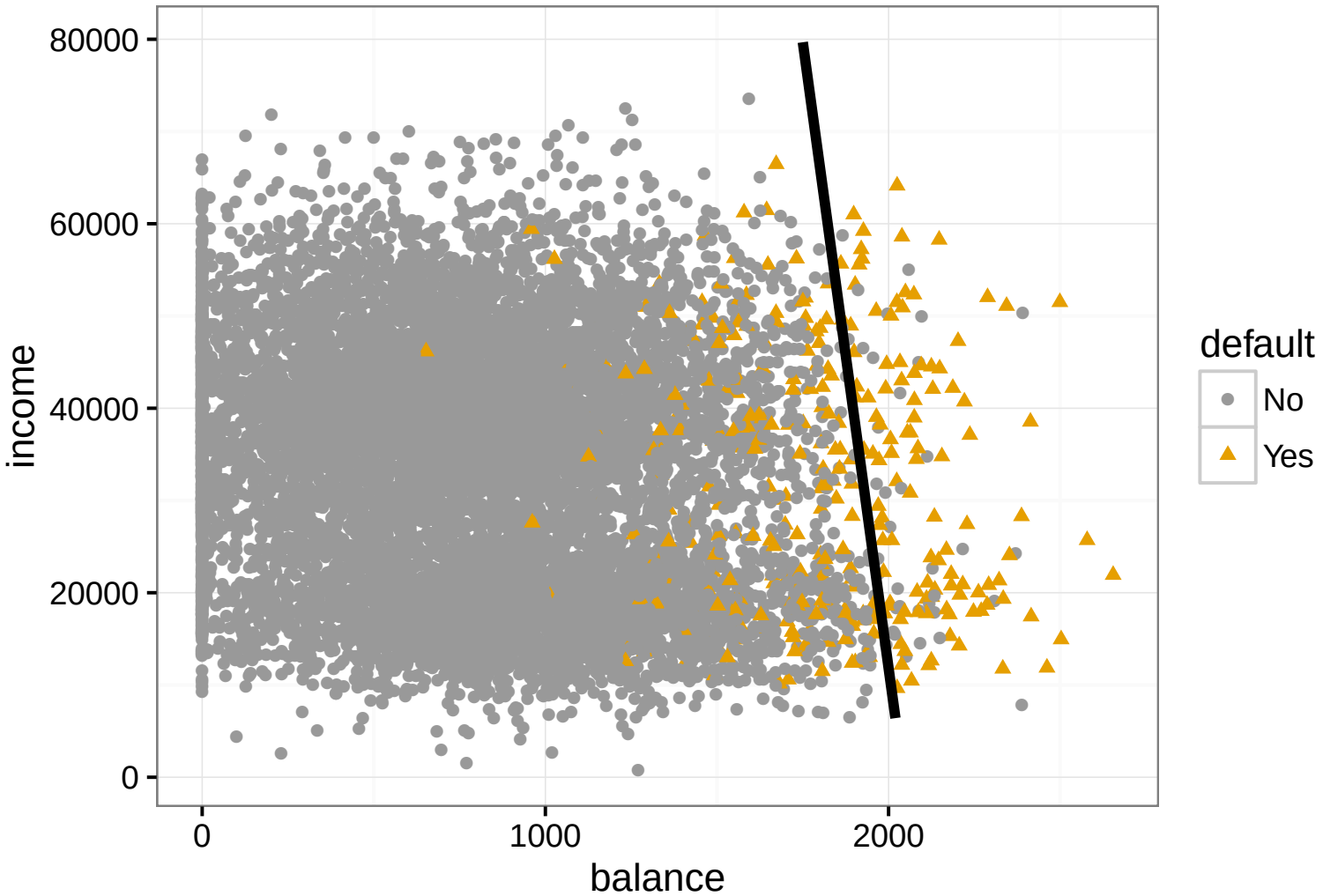
actually look like for various choices of the cutoff α?

Logistic regression: Decision boundary



This is what the data actually looks like (previous scatterplot *undersampled* the `default = No` group.)

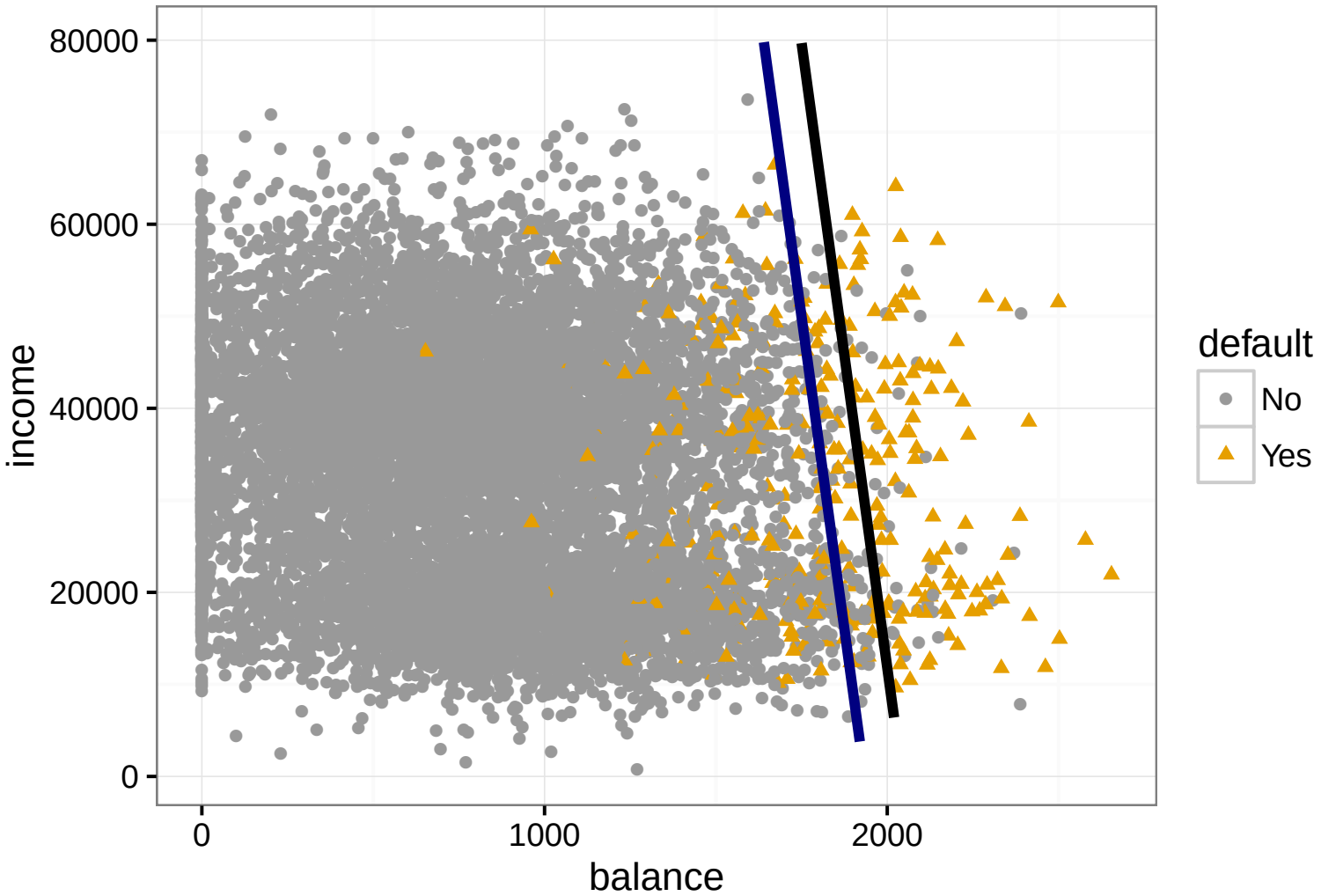
Logistic regression: Decision boundary



Black line shows decision boundary for the rule: $\hat{Y} = 1$ if $\hat{p}(x) > 0.5$

Points to the right of the boundary get classified as `default = Yes`

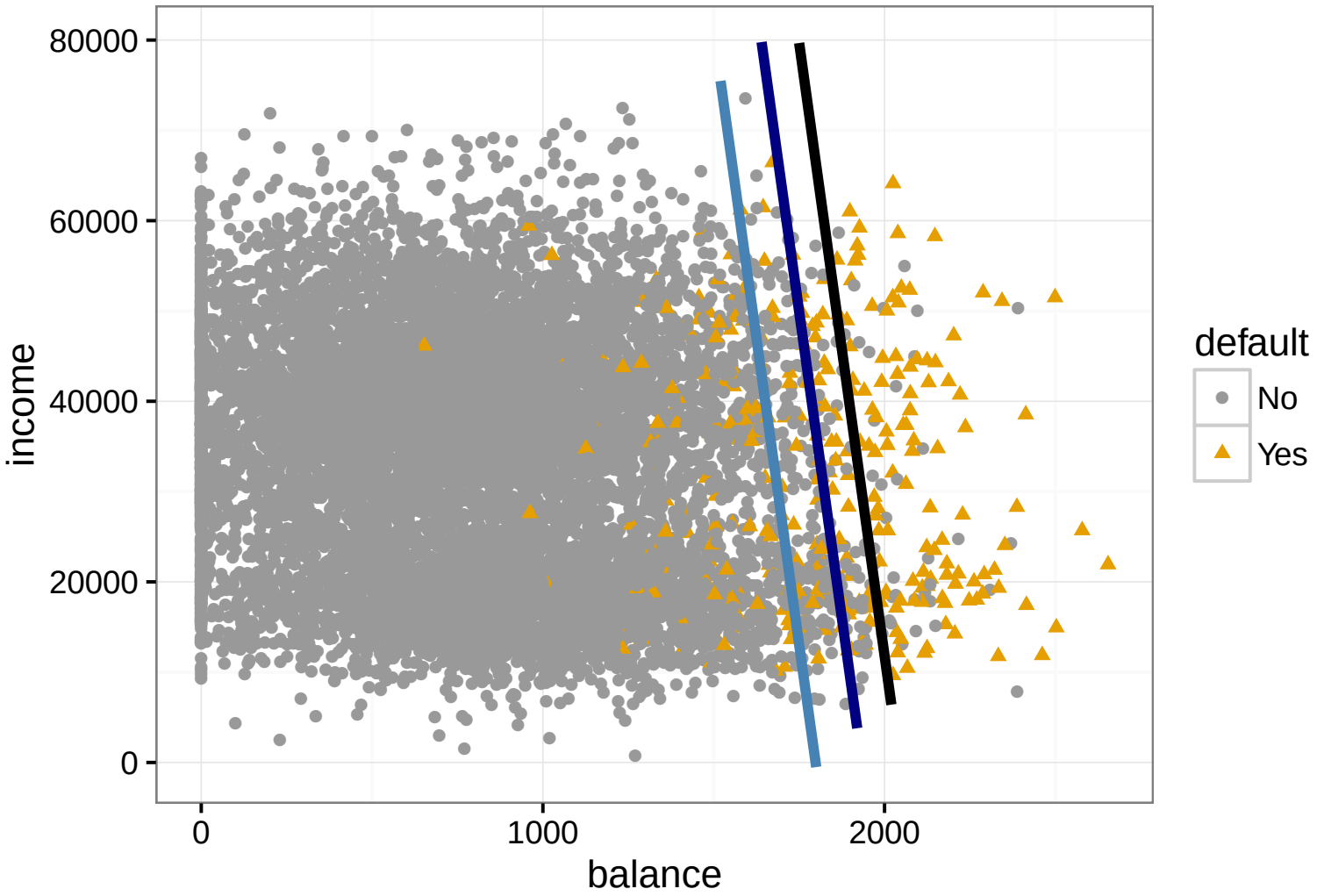
Logistic regression: Decision boundary



Navy line shows decision boundary for the rule: $\hat{Y} = 1$ if $\hat{p}(x) > 0.35$

Points to the right of the boundary get classified as `default = Yes`

Logistic regression: Decision boundary



Blue line shows decision boundary for the rule: $\hat{Y} = 1$ if $\hat{p}(x) > 0.2$

Points to the right of the boundary get classified as `default = Yes`

More general decision boundaries

- We see that the decision boundary provided by logistic regression turns out to be linear:
  - Points on one side of the boundary get classified as $\hat{Y} = 1$
  - Points on the other side get classified as $\hat{Y} = 0$

- When we have $p > 2$ covariates, instead of getting a line, we get a (hyper)-plane

- Just as we don't think that linear models are accurate representations of numeric outcomes, we may not believe that a linear decision boundary is the best way to classify points

- Let's look at one method that results in non-linear decision boundaries

k-Nearest Neighbours Classifier

- Setup: Data (x_i, y_i), $x_i \in \mathbb{R}^p$ vector of inputs, $y_i \in \{0, 1\}$.
- k-Nearest Neighbours (k-NN) classification is an example of a non-parametric "lazy learning" (memory-based) method
- Unlike the methods we've seen before[1], which estimate parameters in some model, k-NN looks at the training data each time it is queried to make a classification[2]
- Let $\mathcal{N}_k(x)$ denote the k training points that are *closest* to x
- If we want to classify a new individual with covariates $X = x$, we simply classify it to the majority class of the points in $\mathcal{N}_k(x)$
- As an estimator of the conditional probability, we can think of k-NN as

$$\hat{p}_{\text{kNN}}(x) = \frac{1}{k} \sum_{x_i \in \mathcal{N}_k(x)} y_i$$

[1] With the exception of local regression, which also has these properties.
[2] k-NN also works for prediction, though we didn't discuss it at the time

k-Nearest Neighbours Classifier: 3-NN example

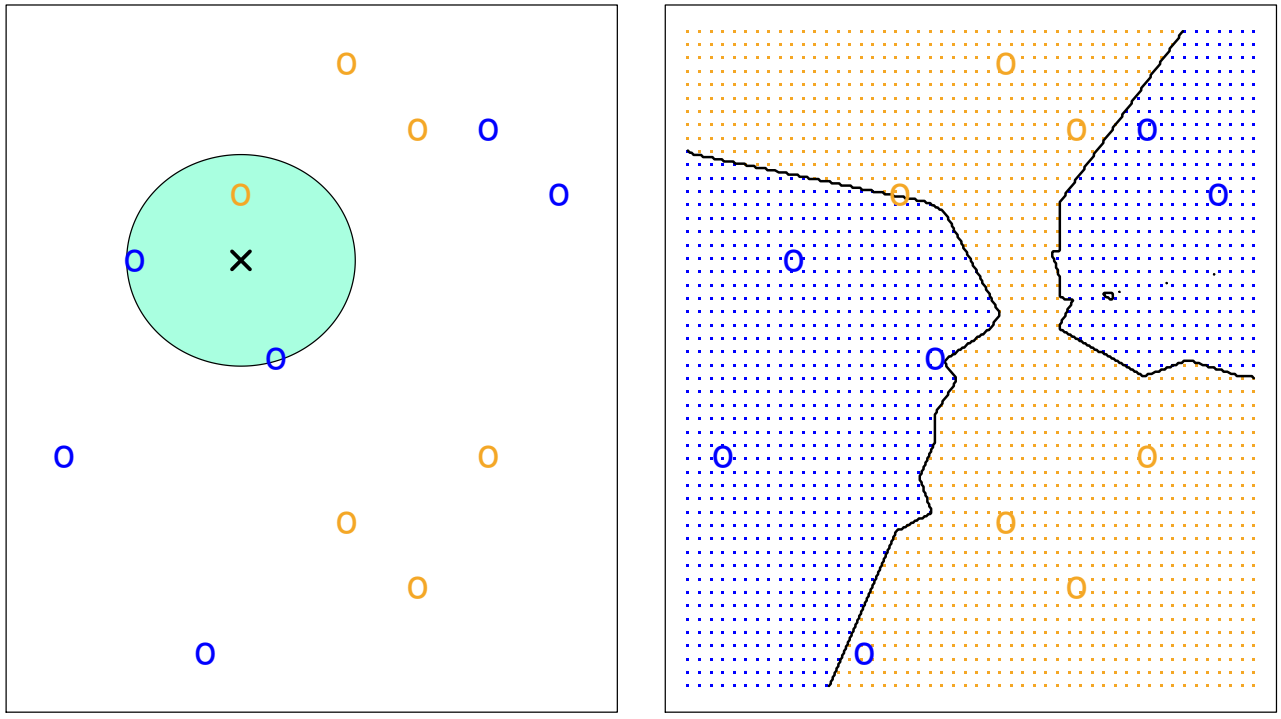


Figure: 2.14 from ISL. Axes represent $p = 2$ predictors.

- *Left*: We have two classes: $Y \in \{\text{orange, blue}\}$. 3-NN is used to classify the $\times$ as a blue point. 2 of $\times$'s 3 nearest neighbours are blue, one is orange, so blue wins.
- *Right*: The decision boundary. Any point in the orange shaded region gets classified by 3-NN as orange. Any point in the blue shaded region area gets classified by 3-NN as blue.

k-Nearest Neighbours: Simulated data

- When we discussed prediction, we relied a lot on simulation experiment to see how well our estimates $\hat{f}(x)$ approximated the true regression function $f(x)$
- The next few slides demonstrate how well k-NN works on a simulated data set where the true Bayes classifier decision boundary is non-linear

k-Nearest Neighbours: Simulated data

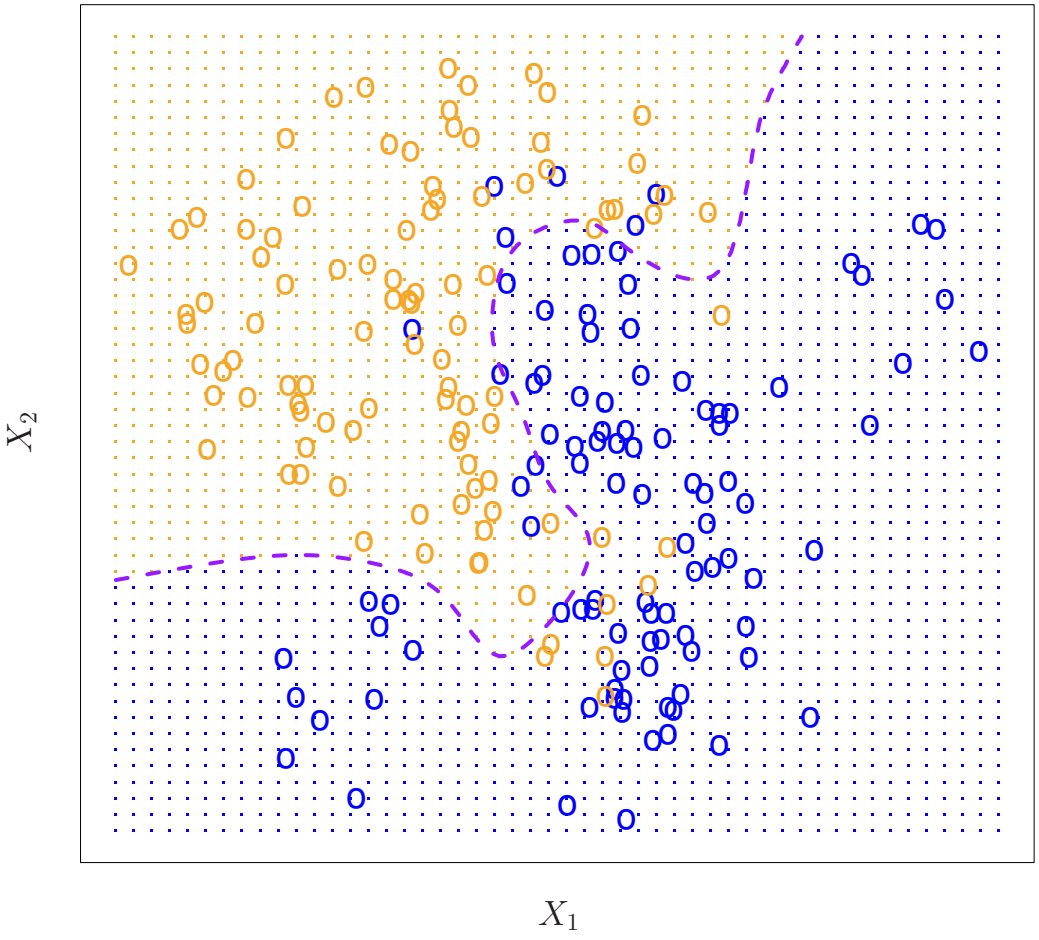


Figure 2.15 from ISL. Dashed purple line is the Bayes classifier "optimal" decision boundary.

k-Nearest Neighbours: Simulated data

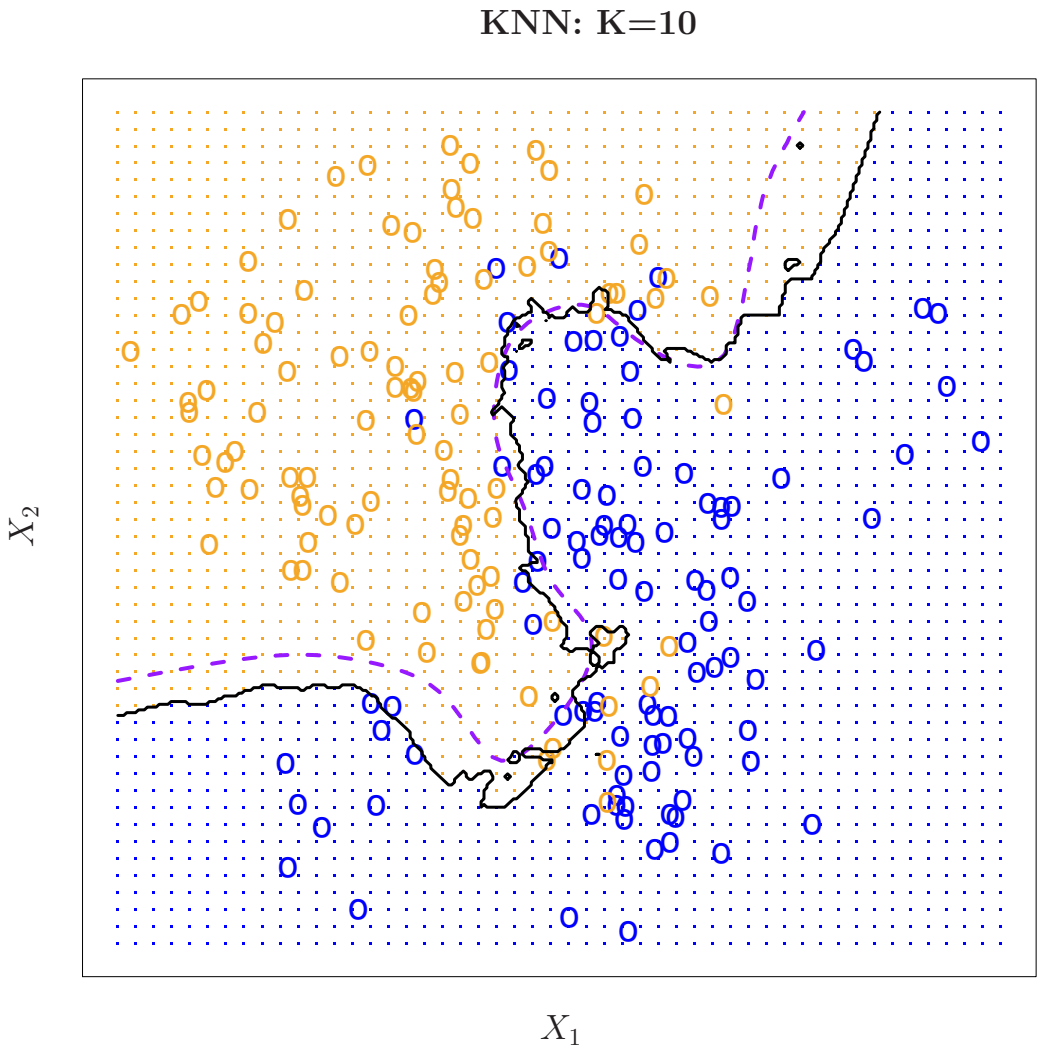


Figure 2.15 from ISL. Dashed purple line is the Bayes classifier "optimal" decision boundary. Solid black line is 10-NN decision boundary.

k-Nearest Neighbours: Simulated data

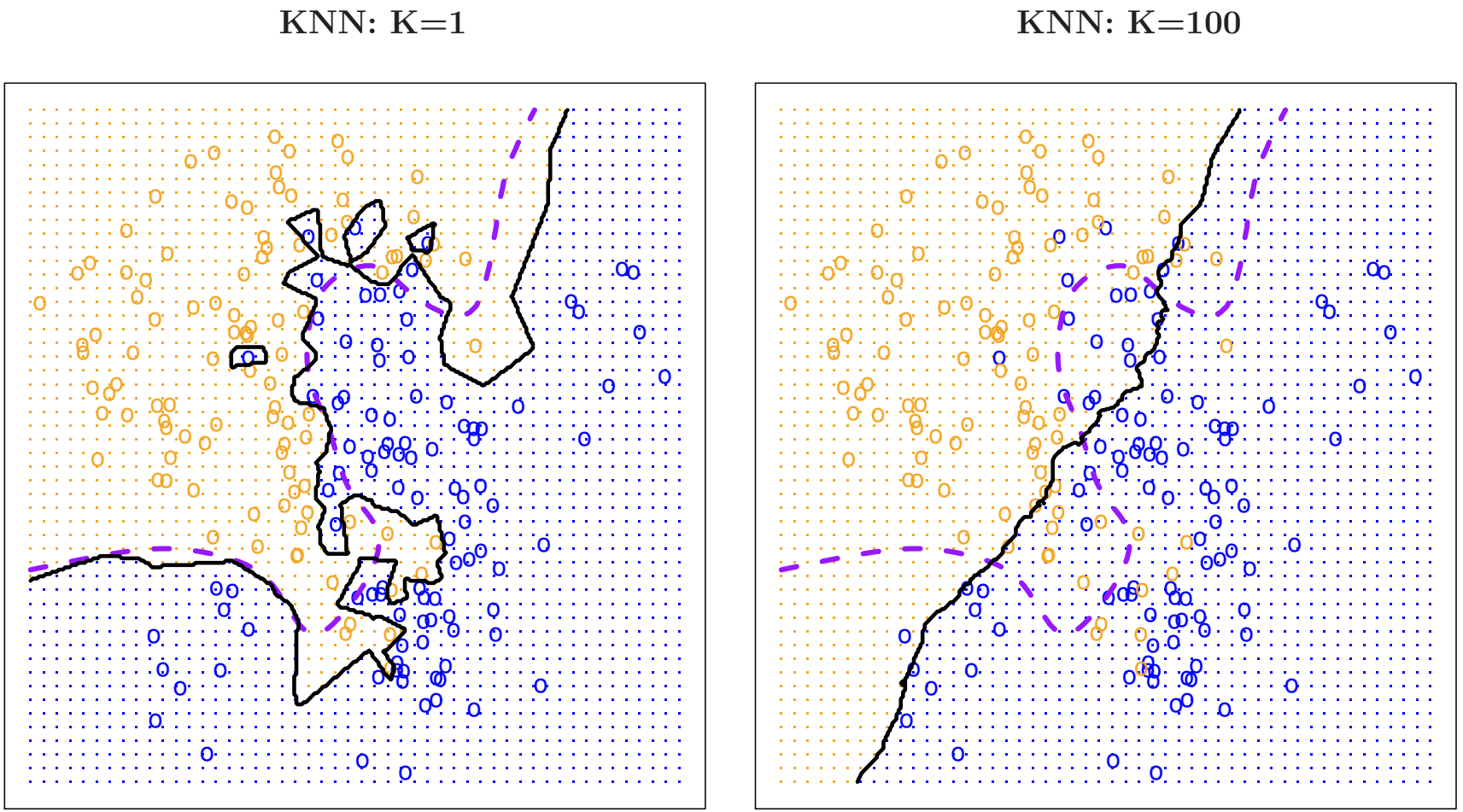


Figure 2.15 from ISL. Dashed purple line is the Bayes classifier "optimal" decision boundary. Solid black lines are 1-NN and 100-NN classifiers.

Can we get non-linear boundaries from Logistic regression?

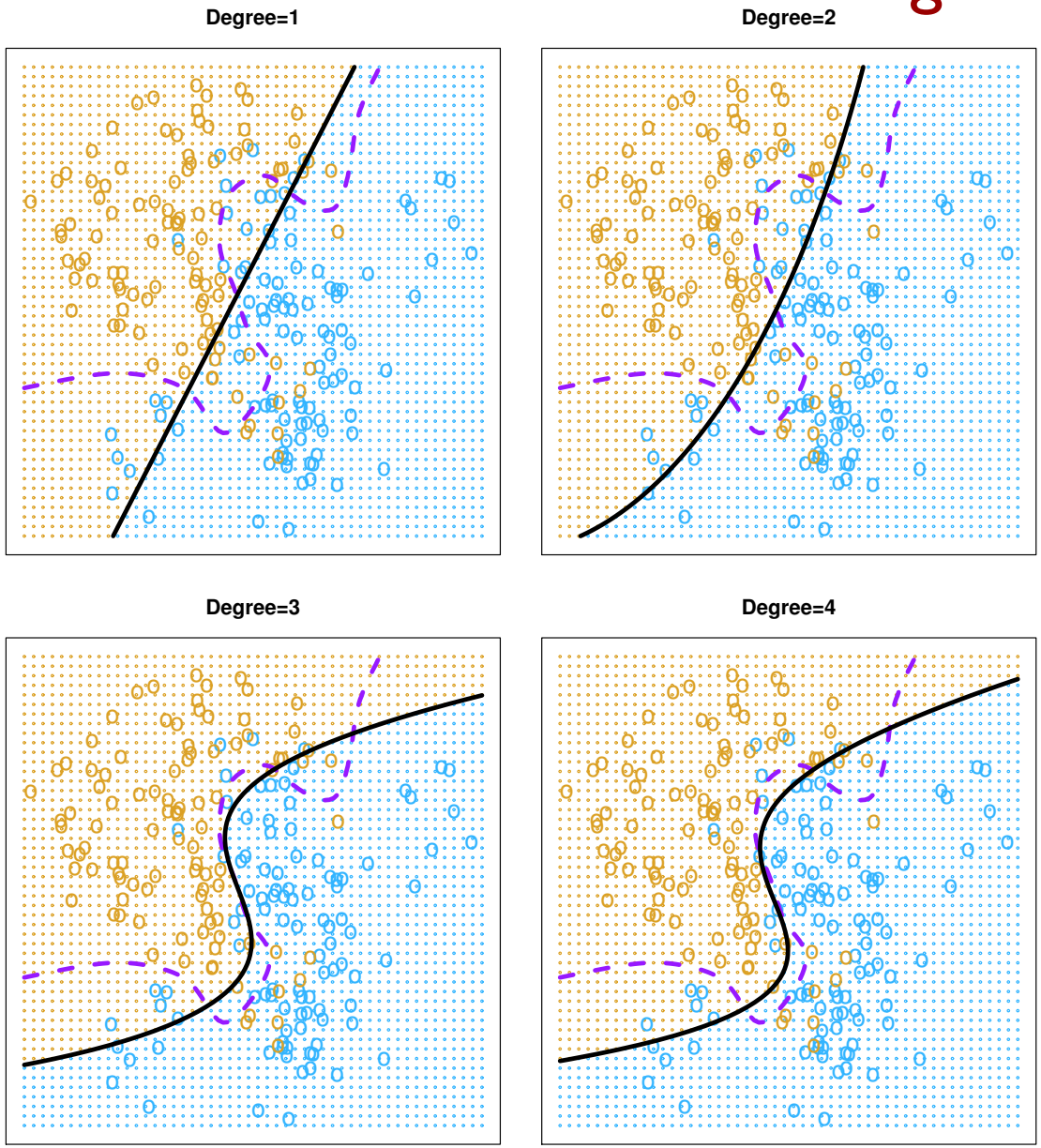
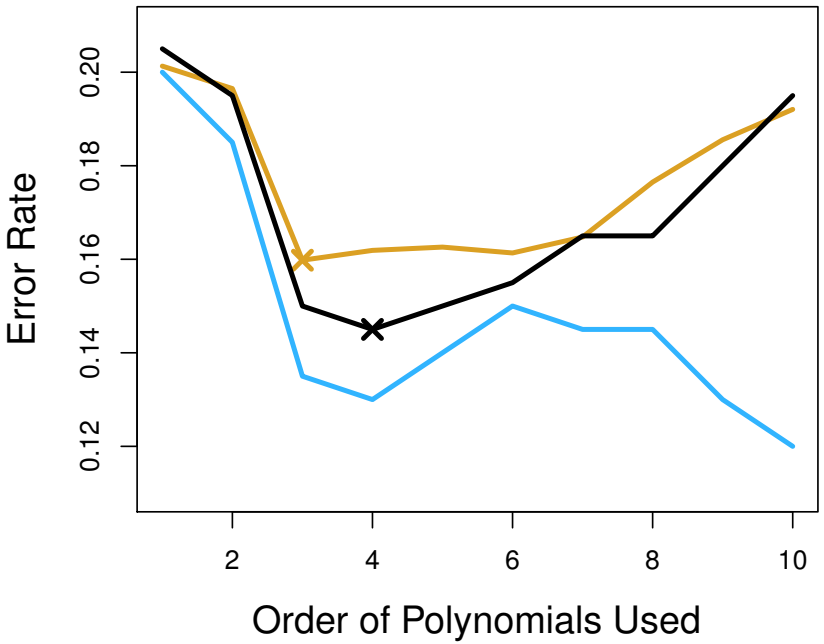


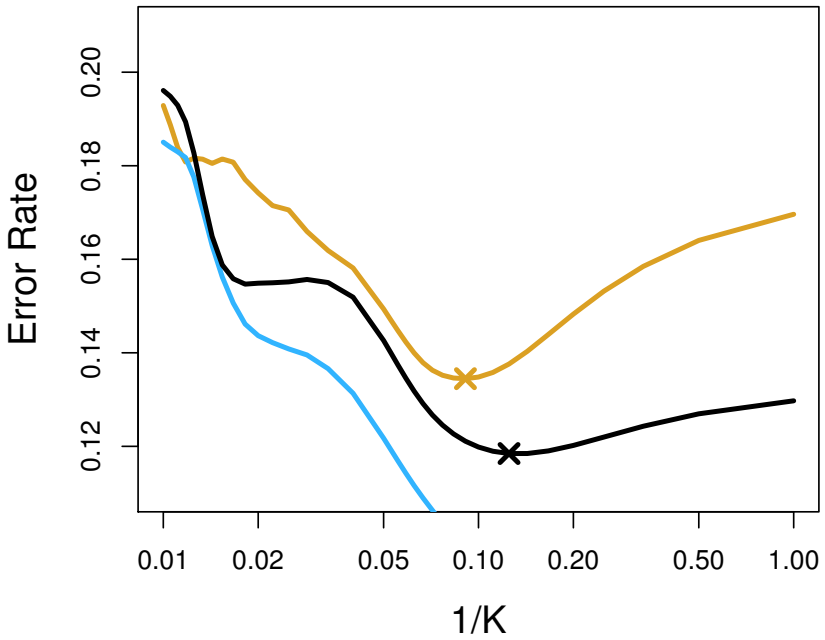
Figure 5.7 from ISL. Decision boundaries are obtained by running logistic polynomial regression for various choices of degree.

Choosing k: Logistic polynomial regression, k-NN

Logistic regression



K-Nearest Neighbours



- Error rate: $\frac{1}{n}\sum_{i=1}^{n} I(y_i \neq \hat{y}_i)$
- Test error (computed through simulation)
- Training error
- Cross-validation error estimate

Other extensions of logistic regression

- When we discussed Linear models, we saw that we could easily extend them to Additive models and Regularized regression models
- The same is true of Logistic regression
- To fit Additive Logistic models:
  Specify `family = binomial()` in a `gam()` command
- To fit ℓ-1 regularized Logistic regression:
  Specify `family = "binomial"` in a `glmnet` command
- Indeed, Google famously uses *massive* regularized logistic regressions as a core component of their AdClick prediction system. This system is trained on many *billions* of observations, with potentially *millions* of predictors

Multi-class classification

- The examples we have considered thus far have all been cases of binary classification
- Y could take on one of *two* possible values: $\{0, 1\}$, {orange, blue}, etc.
- Going forward, it will be just as straightforward to consider the multi-class case where we have $J \geq 2$ classes
- Our goal is to use inputs $X = x$ to classify Y to one of $\{1, 2, \ldots, J\}$, seeing to minimize the (test) error rate (aka misclassification rate)

$$\frac{1}{n} \sum_{i=1}^{n} I(y_i \neq \hat{y}_i)$$

- As we said earlier, the best *any classifier whatsoever* could do is to classify to the group j that has the largest value of

$$\mathbb{P}(Y = j \mid X = x)$$

Multi-class classification

- We can now think of our intermediate goal as getting good estimates of the conditional probability functions

$$\mathbb{P}(Y = j \mid X = x)$$

- There is a multi-class version of Logistic regression, which typically goes by the name Multinomial regression

- We will not discuss this method here, because it's not a particularly popular approach

- For k-NN, there's really no generalization that needs to take place to go from $J = 2$ classes to $J \geq 2$ classes
  - We find that k closest points to x, and classify to the plurality class: the class that appears most often among x's k nearest neighbours

Multi-class classification: Generative models

- Logistic regression is an example of what is called a Discriminative model
- Such models estimate $\mathbb{P}(Y = j \mid X = x)$, but do not try to model the *joint distribution* between the inputs and the response Y
- Since the Bayes classifier itself only uses $\mathbb{P}(Y = j \mid X = x)$, it may seem that to model anything beyond that is *too much work* and seemingly *unnecessary*
- However, there are some nice classification methods that *do* proceed by modeling the joint distribution of $(Y, X_1, \ldots, X_p)$.
- Such methods are called Generative models

Generative models: A toy example

- We're now going to take a look at some examples of Generative models
- To whet your appetite, let's look at a simple toy example
- Canadians and Americans keep insisting that they're "different people", but you can't tell them apart
- Lately, though, you've noticed that Canadian men tend to be somewhat *shorter* than American men
- Sure enough, some internet browsing reveals that:
  - American men are on average 178.2cm tall (St Dev = 4.2cm)
  - Canadian men are on average 173cm tall (St Dev = 3.3cm)
  - Heights are generally Normally distributed

Canadian or American?

- Neil, the next "American sounding" guy you come across, turns out to be 171cm tall.
- **Question**: Is Neil American or Canadian?
- Let H denote a man's height. From your internet search, you found that:

$$H \mid \text{American} \sim \text{Normal}(178.2, \sigma = 4.2)$$
$$H \mid \text{Canadian} \sim \text{Normal}(173, \sigma = 3.3)$$

- But we want: $\mathbb{P}(\text{American} \mid H = 171)$…Hmmm…
- Luckily an 18th century Presbyterian minister tells you that

$$\mathbb{P}(\text{American} \mid H = 171) = \frac{\mathbb{P}(H = 171 \mid \text{American})\mathbb{P}(\text{American})}{\mathbb{P}(H = 171)}$$

$$\mathbb{P}(\text{American} \mid H = 171) = \frac{\mathbb{P}(H = 171 \mid \text{American})\mathbb{P}(\text{American})}{\mathbb{P}(H = 171)}$$

- Since $H \mid \text{American} \sim \text{Normal}(178.2, \sigma = 4.2)$, we can calculate that

$$\mathbb{P}(H = 171 \mid \text{American}) = 0.022$$

- How about $\mathbb{P}(\text{American})$? This is the proportion of "American sounding" males on campus who are actually American. You do more research, and find that this proportion is 0.85.

- Finally, the *Law of Total Probability* tells us that

$$\begin{aligned}\mathbb{P}(H = 171) &= \mathbb{P}(H = 171 \mid A) \cdot \mathbb{P}(A) + \mathbb{P}(H = 171 \mid C) \cdot \mathbb{P}(C) \\ &= 0.022 \cdot 0.85 + 0.10 \cdot 0.15 \\ &= 0.0337\end{aligned}$$

- So according to the minister's rule,
$\mathbb{P}(\text{American} \mid H = 171) = 0.022 \times 0.85/0.0337 = 0.554 = 55.4\%$

- So chances are, Neil is just a short American!

A closer look at Bayes theorem

- Suppose we have an outcome $Y \in \{1, 2, \ldots, K\}$ and an input vector $X = (X_1, \ldots, X_p)$
- Bayes theorem tells us that

$$\mathbb{P}(Y = k \mid X = x) = \frac{\mathbb{P}(X = x \mid Y = k)\mathbb{P}(Y = k)}{\mathbb{P}(X = x)}$$

- $\mathbb{P}(X = x \mid Y = k)$ is the density for X in class k
- $\mathbb{P}(Y = k)$ is the prior probability of class k
- Bayes theorem gives us a way of combining prior beliefs about the likelihood that $Y = k$ with the new evidence that we observed $X = x$.
- $\mathbb{P}(Y = k \mid X = x)$ is often called the posterior probability of class k

Bayes theorem for discriminant analysis

$$\mathbb{P}(Y = k \mid X = x) = \frac{\mathbb{P}(X = x \mid Y = k)\mathbb{P}(Y = k)}{\mathbb{P}(X = x)}$$

- Let $f_k(x) = \mathbb{P}(X = x \mid Y = k)$ denote the density of X in class k
- Let $\pi_k = \mathbb{P}(Y = k)$ denote the prior probability of class k
- By the *Law of total probability*,

$$\mathbb{P}(X = x) = \sum_{\ell=1}^{K} \pi_\ell f_\ell(x)$$

and so we can rewrite Bayes theorem as

$$\mathbb{P}(Y = k \mid X = x) = \frac{\pi_k f_k(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)}$$

How do we use this as a classifier?

$$\mathbb{P}(Y = k \mid X = x) = \frac{\pi_k f_k(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)}$$

- To minimize the misclassification rate, we should classify an observation with inputs x_0 to the class with the highest posterior probability

$$\hat{y}_0 = \underset{k=1,\ldots,K}{\operatorname{argmax}} \frac{\pi_k f_k(x_0)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x_0)}$$

- Note that the denominator term is exactly the same for each term (it depends on x, but not on k).
- Thus the above rule is the same as the simpler rule:

$$\hat{y}_0 = \underset{k=1,\ldots,K}{\operatorname{argmax}} \pi_k f_k(x_0)$$

Why is this interesting?

$$\hat{y}_0 = \underset{k=1,\ldots,K}{\operatorname{argmax}} \frac{\pi_k f_k(x_0)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x_0)} = \underset{k=1,\ldots,K}{\operatorname{argmax}} \pi_k f_k(x_0)$$

- Prior to collecting data, we generally don't know what any of the π_k or $f_k(x)$ should be.
- Thus we must estimate the π_k's and the densities $f_k(x)$ from the data
- The π_k are easy:

$$\hat{\pi}_k = \frac{\#\{i : y_i = k\}}{n}$$

- The $f_k(x)$ are *harder* and *more interesting* to estimate
- Different ways of estimating $f_k(x)$ give us different classifiers!

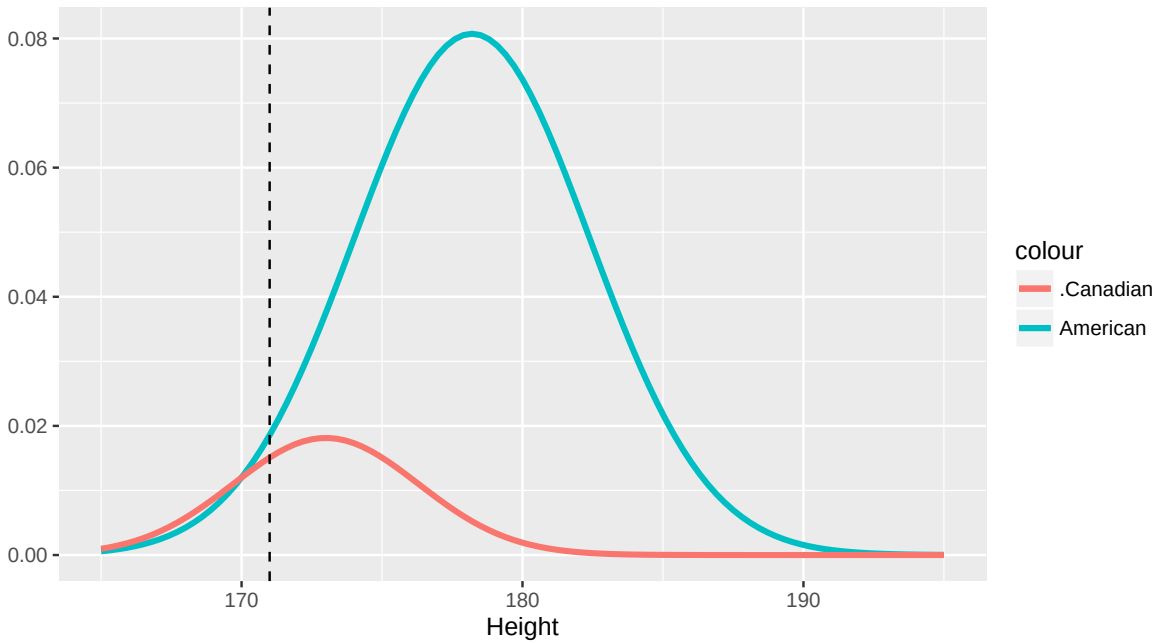
The Canadian vs American example

- In the Toy example we looked at earlier, we knew in advance that

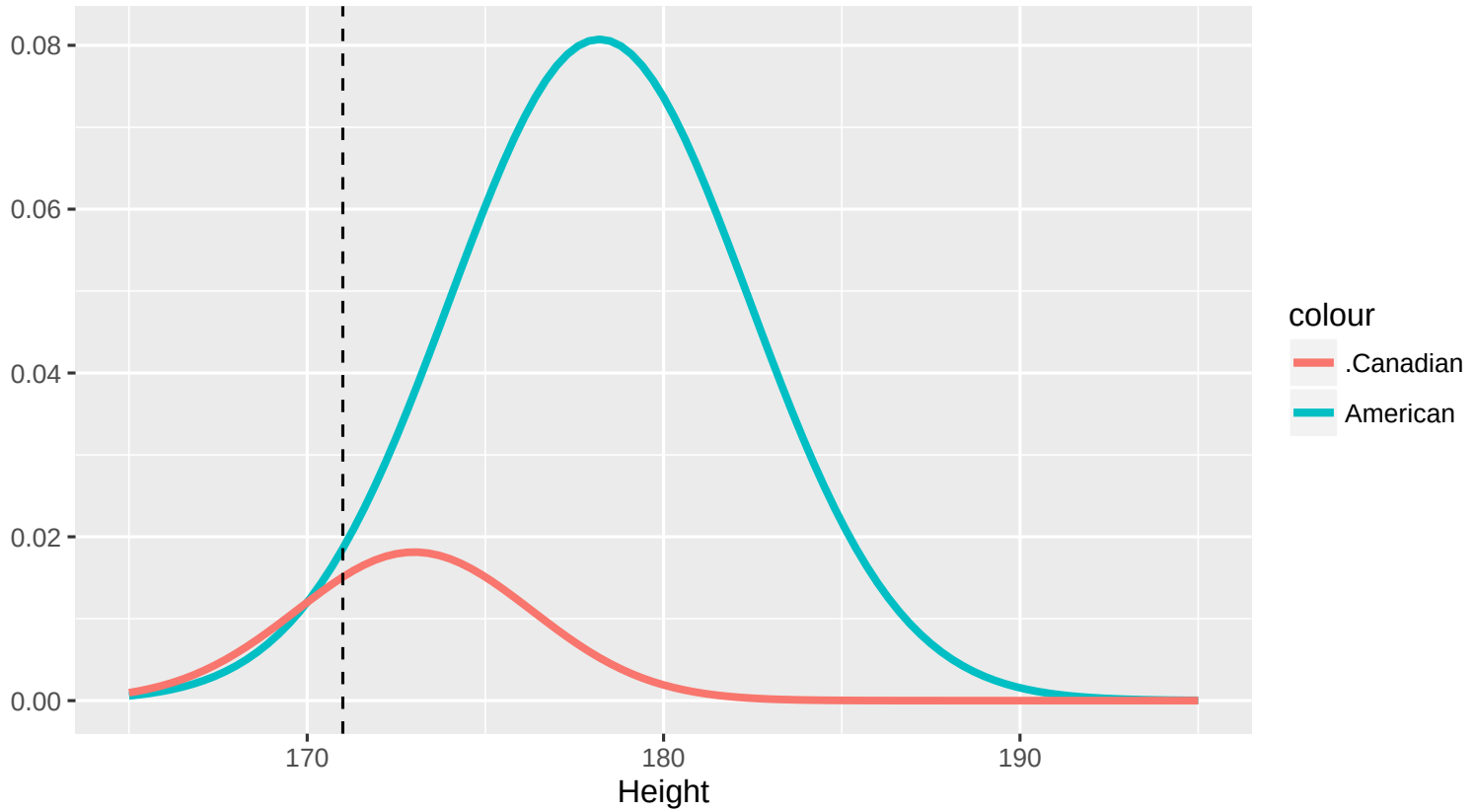
$$H \mid \text{American} \sim \text{Normal}(178.2, \sigma = 4.7) = f_A(x)$$
$$H \mid \text{Canadian} \sim \text{Normal}(173, \sigma = 3.3) = f_C(x)$$

  and $\pi_A = 0.85$, $\pi_C = 0.15$

- Plot below shows value of $\pi_k f_k(x)$ for $k =$ Canadian and American



Plot below shows value of $\pi_k f_k(x)$ for $k =$ Canadian and American



- If $\pi_A f_A(x) > \pi_C f_C(x)$: Classify as American
- If $\pi_A f_A(x) < \pi_C f_C(x)$: Classify as Canadian
- $\pi_A = 0.85$, $\pi_C = 0.15$ so we have a *very* high prior that any "American sounding" male we encounter is actually American
- So there's a very small height range where we would classify someone as Canadian

Linear discriminant analysis

$$\hat{y}_0 = \underset{k=1,\ldots,K}{\operatorname{argmax}} \frac{\pi_k f_k(x_0)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x_0)} = \underset{k=1,\ldots,K}{\operatorname{argmax}} \pi_k f_k(x_0)$$

- Linear discriminant analysis (LDA)[3] assumes all the $f_k(x)$ are Multivariate Normal(μ_k, Σ)
  - Different means, *same* covariance matrix

[3] Not to be confused with Latent Dirichlet Allocation... also abbreviated LDA

What is a Multivariate Normal?

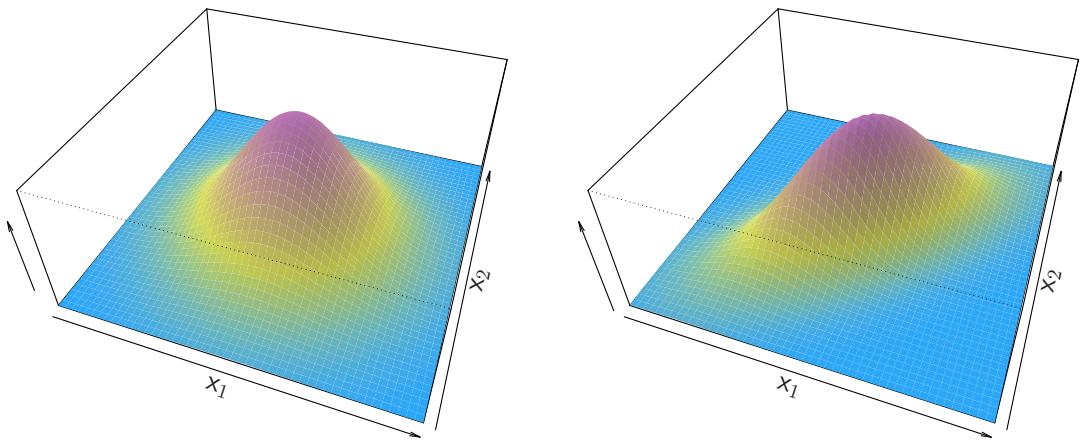
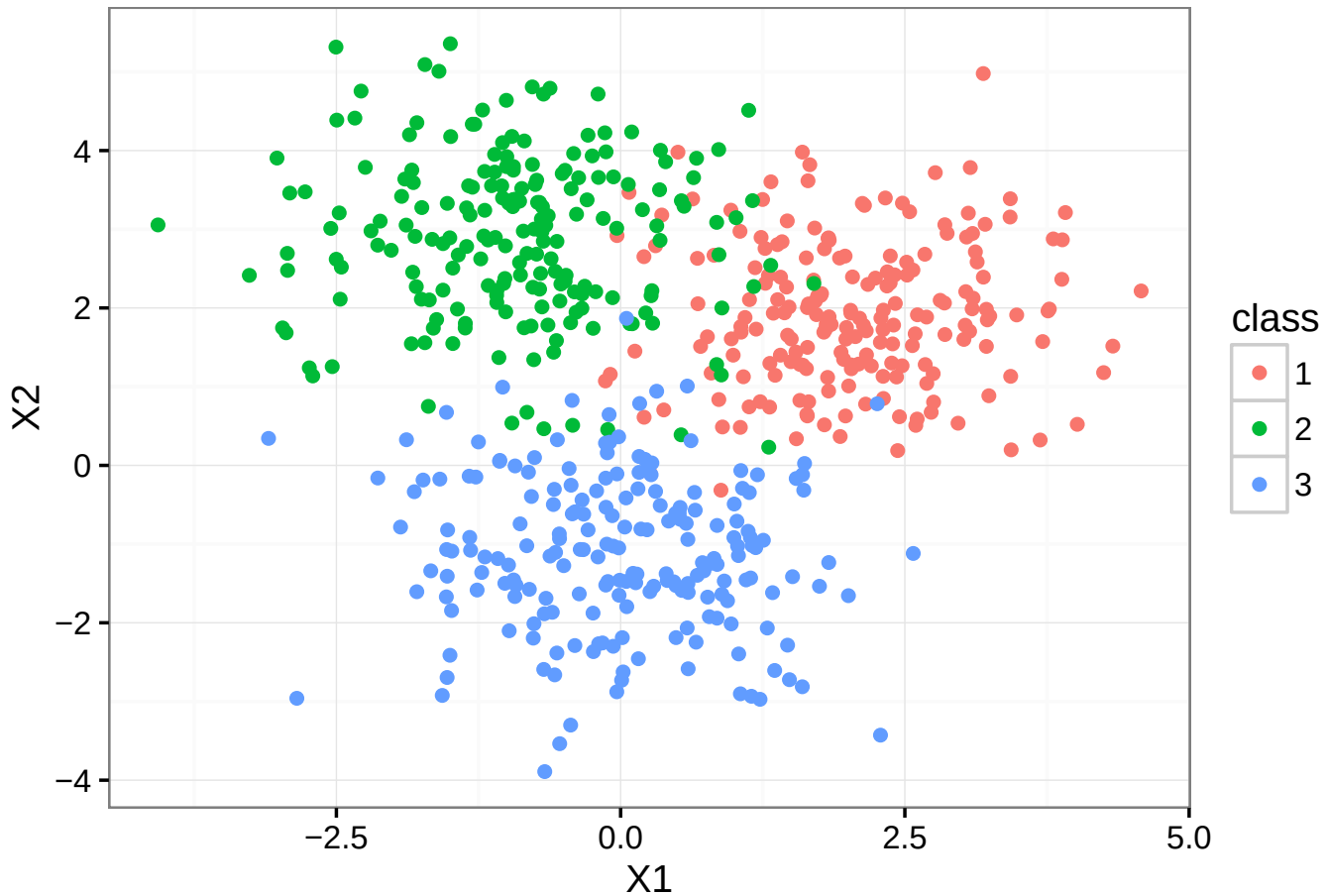
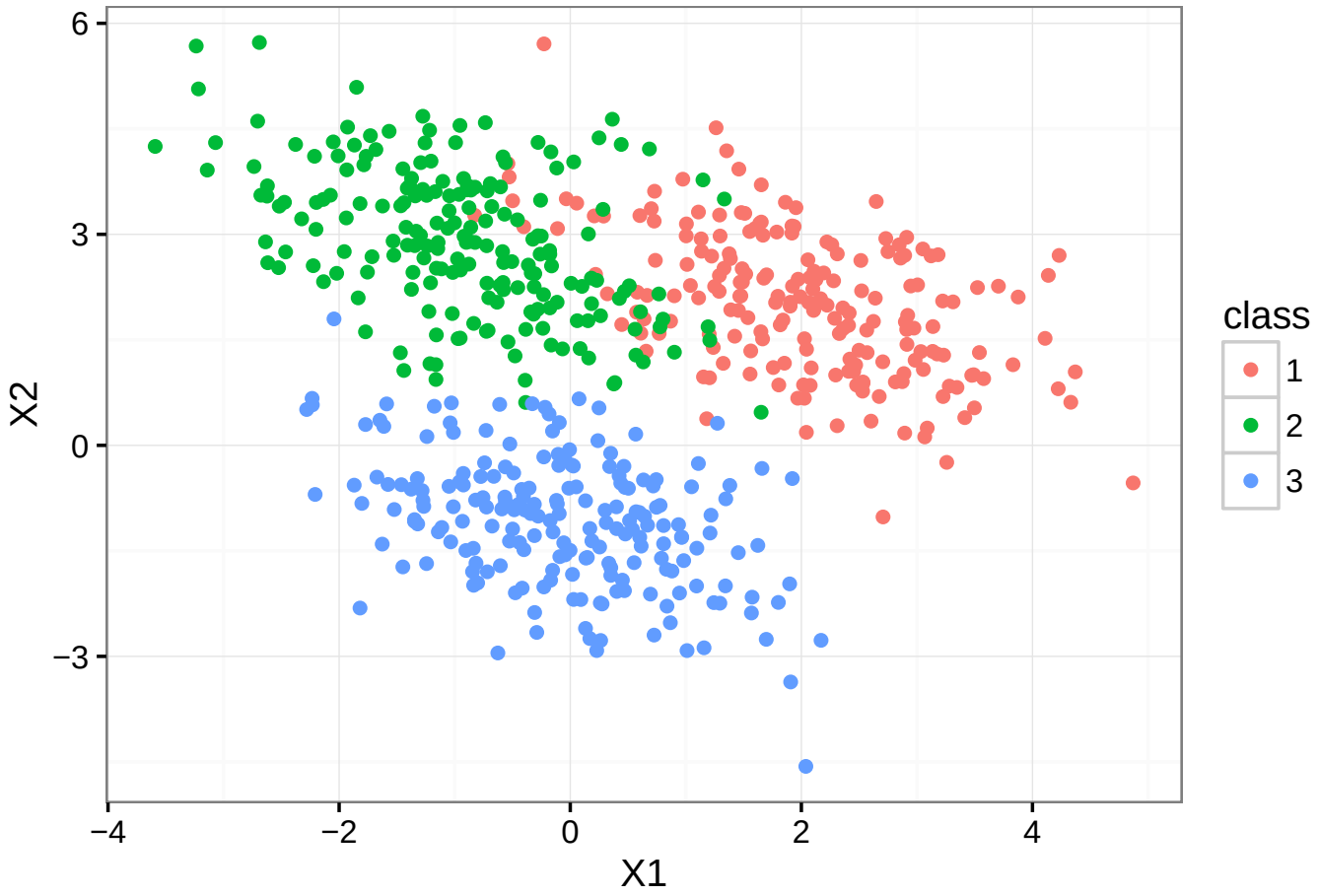


Figure 4.5 from ISL. Bivariate normal density for two choices of Σ.



Covariance matrix $\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

	Class 1	Class 2	Class 3
$\mu_k =$	$(2, 2)$	$(-1, 3)$	$(0, -1)$



Covariance matrix $\Sigma = \begin{pmatrix} 1 & -0.5 \\ -0.5 & 1 \end{pmatrix}$

	Class 1	Class 2	Class 3
$\mu_k =$	$(2, 2)$	$(-1, 3)$	$(0, -1)$

Linear discriminant analysis

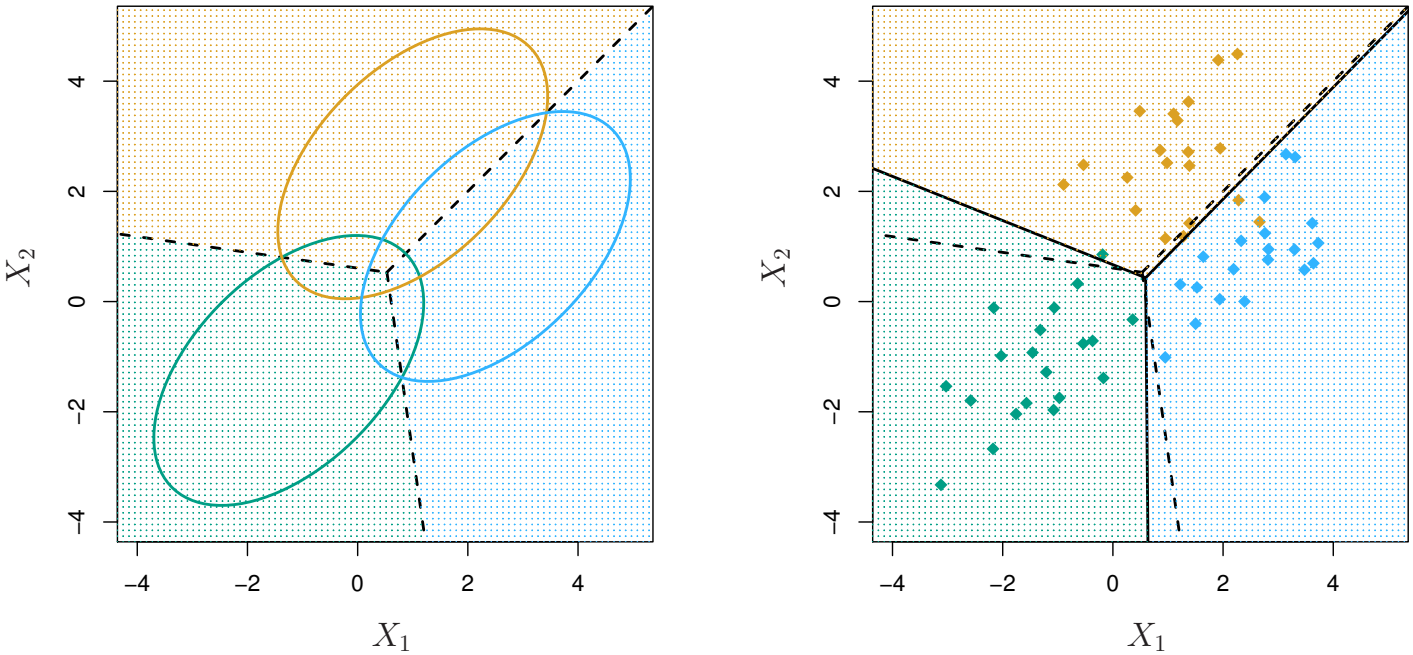


Figure 4.6 from ISL

- **Left**: $K = 3$ classes. True f_k are Bivariate Normal. Ovals represent 95% density contours for each class (95% of points generated from a class will fall into the ellipse). Dashed lines are the LDA boundary from the true f_k
- **Right**: 20 points are observed from each class. Solid lines are the estimated LDA decision boundaries. We had to estimate μ_k and Σ from the data.

Linear discriminant analysis

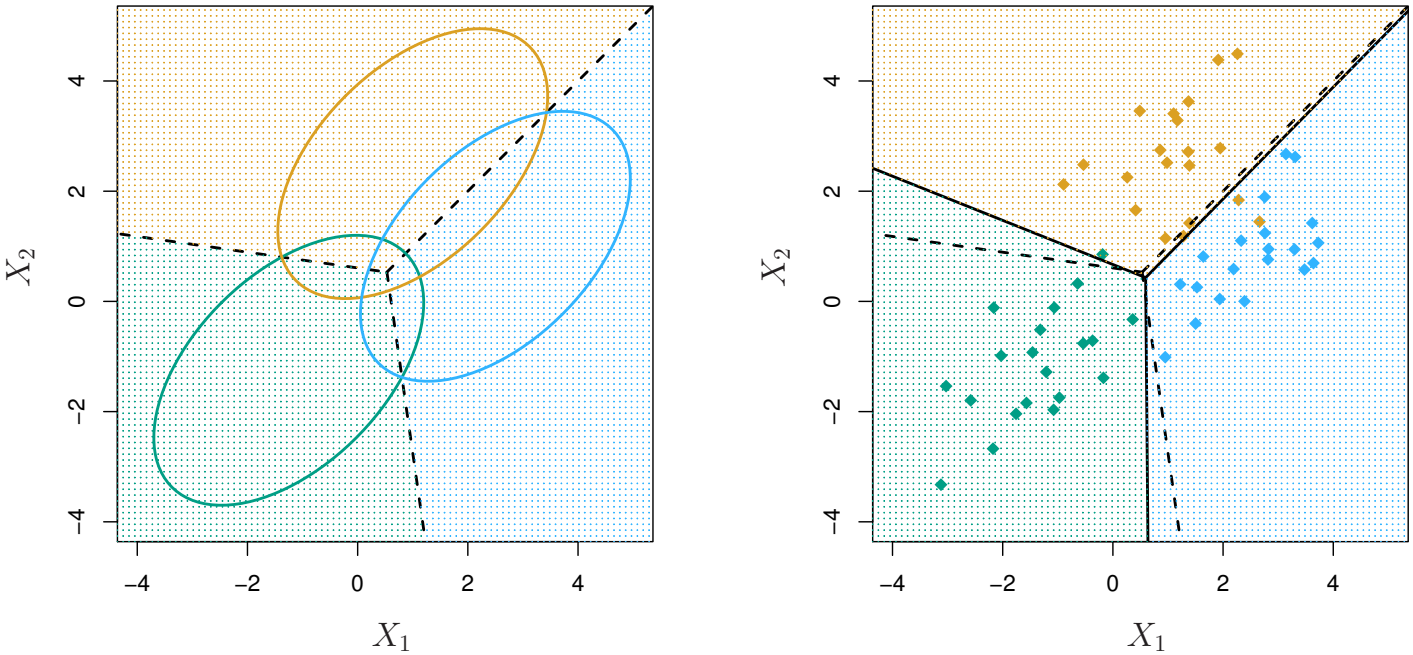


Figure 4.6 from ISL

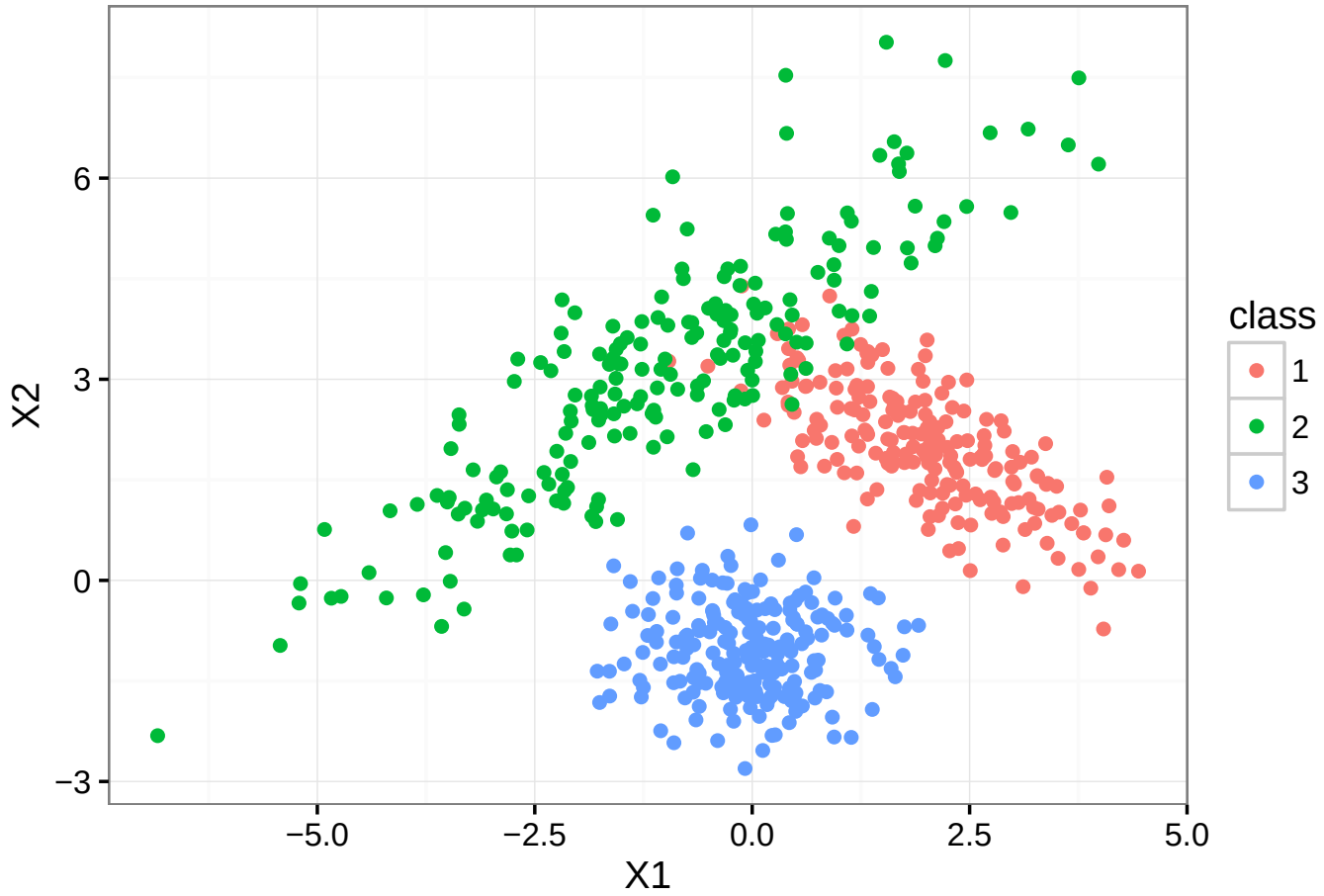
- It's called Linear discriminant analysis because the choice $f_k = \mathrm{MVN}(\mu_k, \Sigma)$ always results in *linear decision boundaries*
- The LDA rule amounts to classifying x_0 to the class with the highest value of the discriminant function δ_k :

$$\delta_k(x_0) = x_0^T \hat{\Sigma}^{-1} \hat{\mu}_k - \frac{1}{2} \hat{\mu}_k^T \hat{\Sigma}^{-1} \hat{\mu}_k + \log(\hat{\pi}_k)$$

Quadratic discriminant analysis

- Quadratic discriminant analysis (QDA) models $f_k(x)$ as MVN(μ_k, Σ_k): it relaxes LDA's assumption that all the covariance matrices are the same

- This produces *quadratic* decision boundaries



$$\Sigma_1 = \begin{pmatrix} 1 & -0.7 \\ -0.7 & 1 \end{pmatrix} \Sigma_2 = \begin{pmatrix} 3 & 2.5 \\ 2.5 & 3 \end{pmatrix} \Sigma_3 = \begin{pmatrix} 0.5 & 0 \\ 0 & 0.5 \end{pmatrix}$$

	Class 1	Class 2	Class 3
$\mu_k =$	$(2, 2)$	$(-1, 3)$	$(0, -1)$

Quadratic discriminant analysis

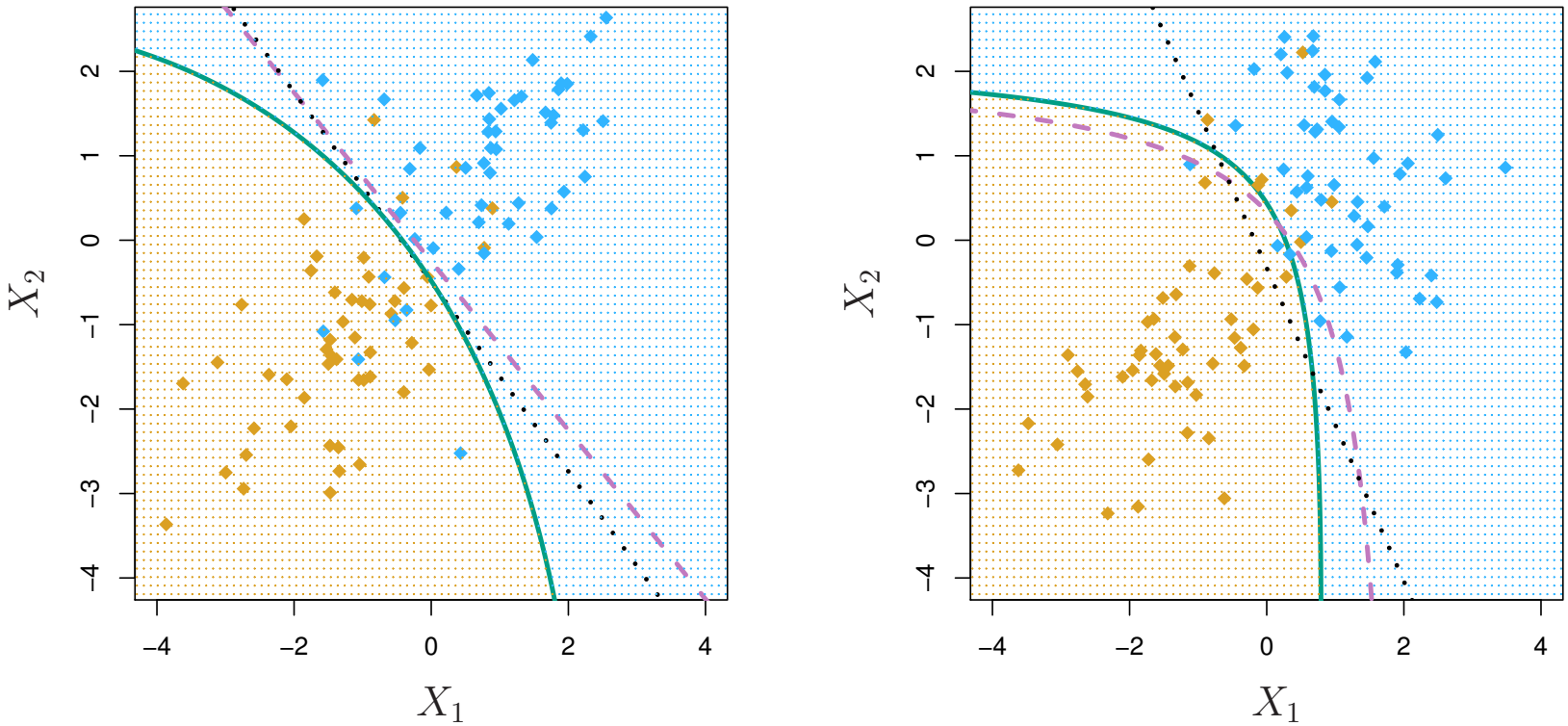


Figure 4.9 from ISL. Dashed purple curve is the Bayes classifier decision boundary. Solid green curve is QDA, dotted black line is LDA.
Left: True boundary is linear. Right: True boundary is quadratic.

Logistic regression vs. Linear discriminant analysis

- When the classes are *well separated*, Logistic regression coefficient estimates are really unstable. LDA does not have this problem.

- LDA makes assumptions on the distribution of $X \mid Y = k$
  - When the assumptions hold (or approximately hold), LDA can produce better, *more stable* decision boundaries, even when n is small

- When we have $K = 2$ classes, Logistic regression can be extended in all kinds of ways (additive models, regularized models, etc.), and is highly interpretable

- Logistic regression gets hard to interpret for $K > 2$ classes. LDA is essentially the same regardless of how many classes we have.

Naive Bayes

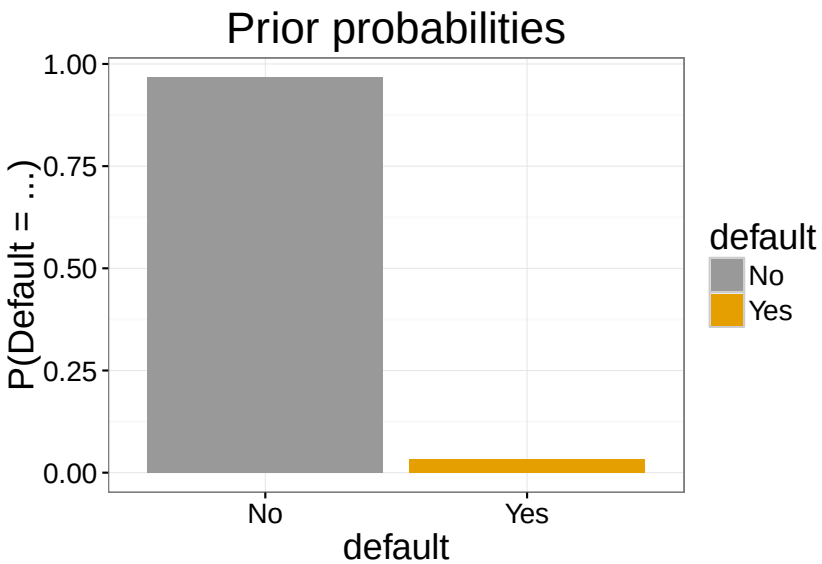
- Naive Bayes is a popular simple classifier in cases where we have a lot of predictors p
- Imagine $p = 1000$ and $n = 2000$. It's going to be *extremely difficult* to accurately estimate $f_k(x)$ without *really strong assumptions* on f_k
- Naive Bayes says: Let's *assume* that all components of $X = (X_1, X_2, \ldots, X_p)$ are independent[4]
- Under the independence assumption, $f_k(x)$ simplifies to:

$$\begin{aligned} f_k(x) &= P(X_1 = x_1, \ldots, X_p = x_p \mid Y = k) \\ &= P(X_1 = x_1 \mid Y = k) \times \cdots \times P(X_p = x_p \mid Y = k) \\ &= \prod_{j=1}^{p} P(X_j = x_j \mid Y = k) \end{aligned}$$

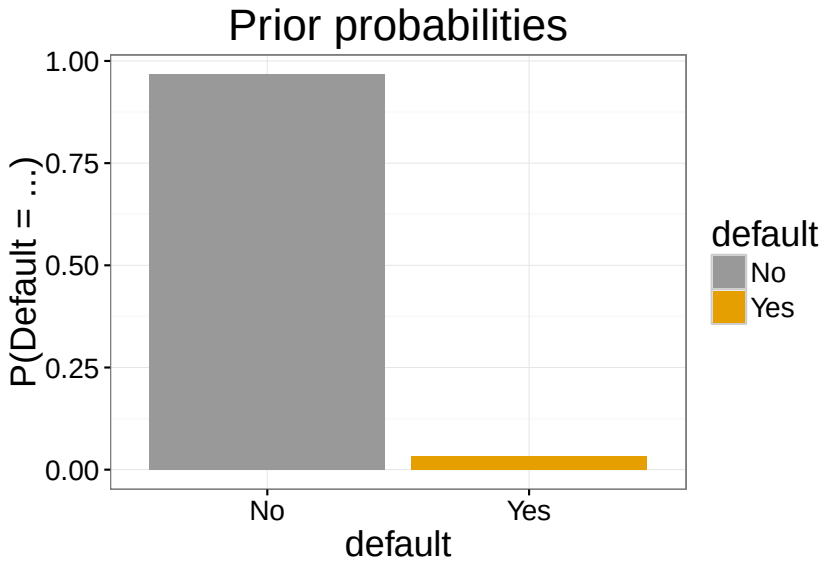
- So now to estimate $f_k(x)$ we just need to estimate p univariate densities: $f_k(x_j) = P(X_j = x_j \mid Y = k)$

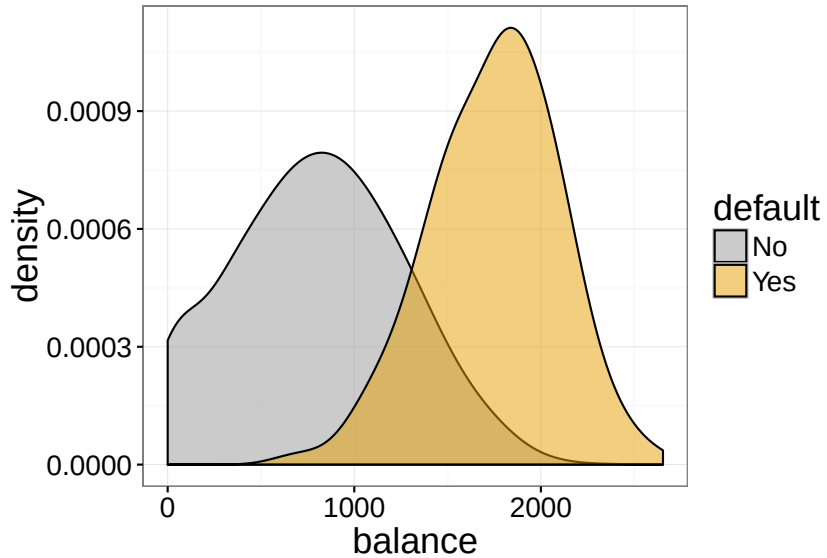
[4] We're actually assuming *conditional independence*: The inputs are independent *given the class labels*

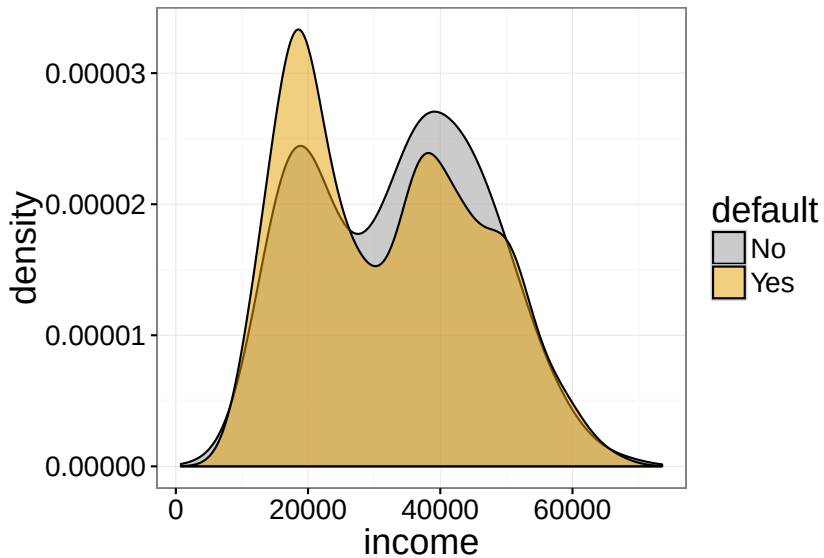
Naive Bayes with the Default Data

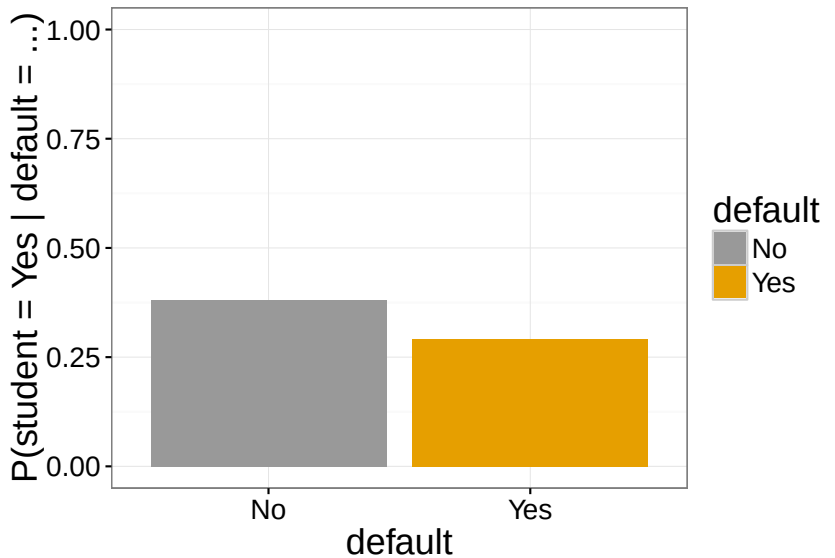


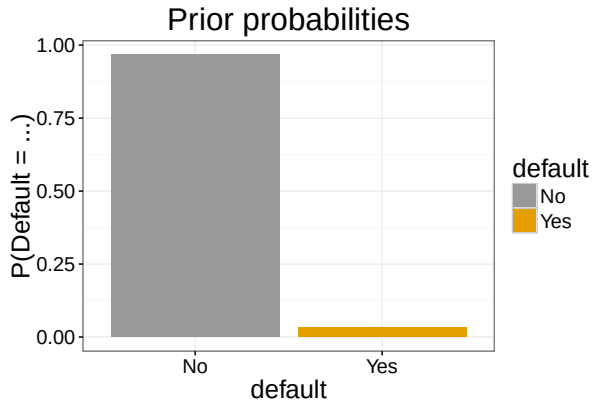
Naive Bayes with the Default Data

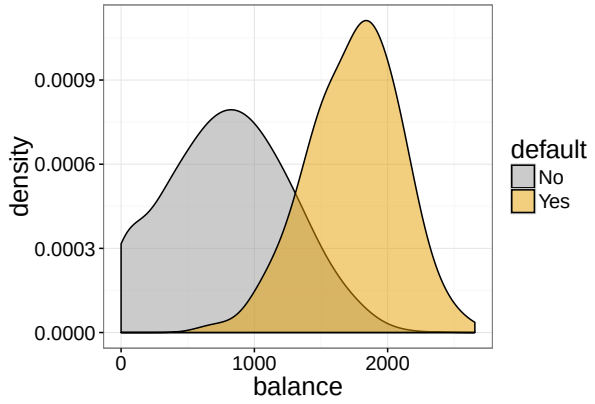


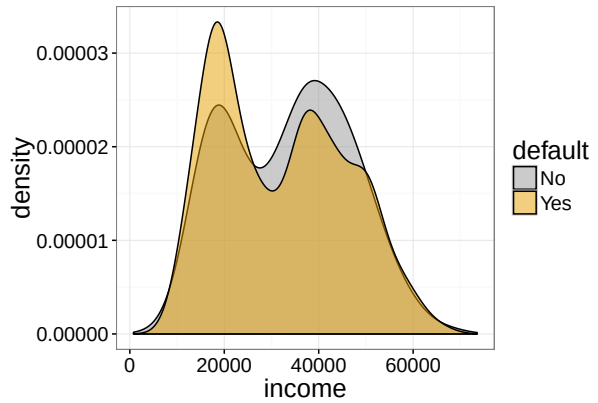


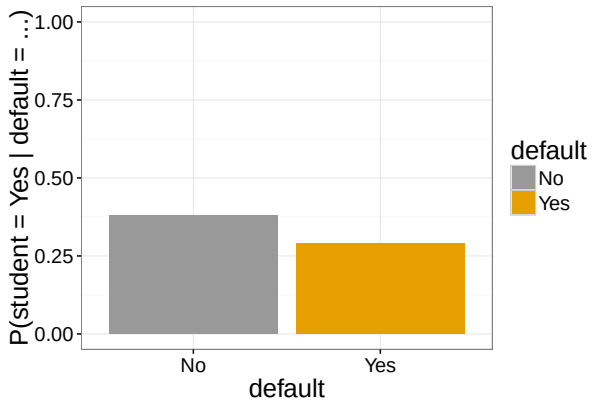












Calculate:

$$\hat{f}_{Yes}(\texttt{i},\texttt{b},\texttt{s}) = \hat{f}_{Yes}(\texttt{income}) \times \hat{f}_{Yes}(\texttt{balance}) \times \hat{f}_{Yes}(\texttt{student})$$

$$\hat{f}_{No}(\texttt{i},\texttt{b},\texttt{s}) = \hat{\pi}_{No}\hat{f}_{No}(\texttt{income}) \times \hat{f}_{No}(\texttt{balance}) \times \hat{f}_{No}(\texttt{student})$$

Naive Bayes posterior probability estimate of `default = Yes`:

$$\hat{\mathbb{P}}(\texttt{default = Yes} \mid \texttt{i},\texttt{b},\texttt{s}) = \frac{\hat{\pi}_{Yes}\hat{f}_{Yes}(\texttt{i},\texttt{b},\texttt{s})}{\hat{\pi}_{Yes}\hat{f}_{Yes}(\texttt{i},\texttt{b},\texttt{s}) + \hat{\pi}_{No}\hat{f}_{No}(\texttt{i},\texttt{b},\texttt{s})}$$

Naive Bayes vs. LDA vs. QDA

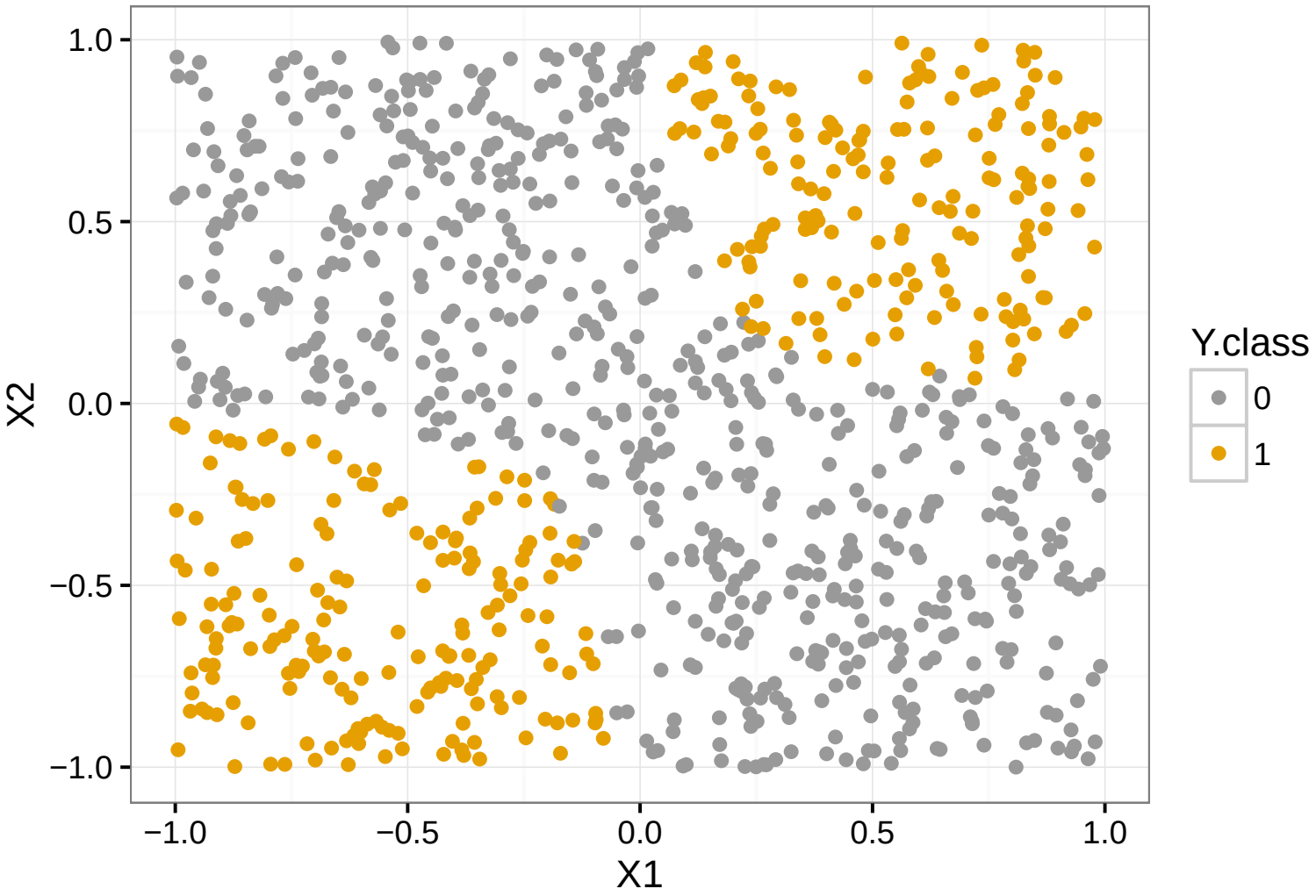
- Naive Bayes scales well to problems where p is large
  - If you have enough data to estimate the univariate density of each predictor (i.e., enough to form a *nice* histogram), you can apply Naive Bayes

- In LDA, we have to estimate $K \times p$ parameters to get $\hat{\mu}_k$'s and another $\frac{1}{2}p(p+1)$ parameters to estimate the $p \times p$ covariance matrix $\hat{\Sigma}$.

- In QDA, we have to estimate the means and K $p \times p$ covariance matrices. That's $\frac{1}{2}Kp(p+1)$ parameters!

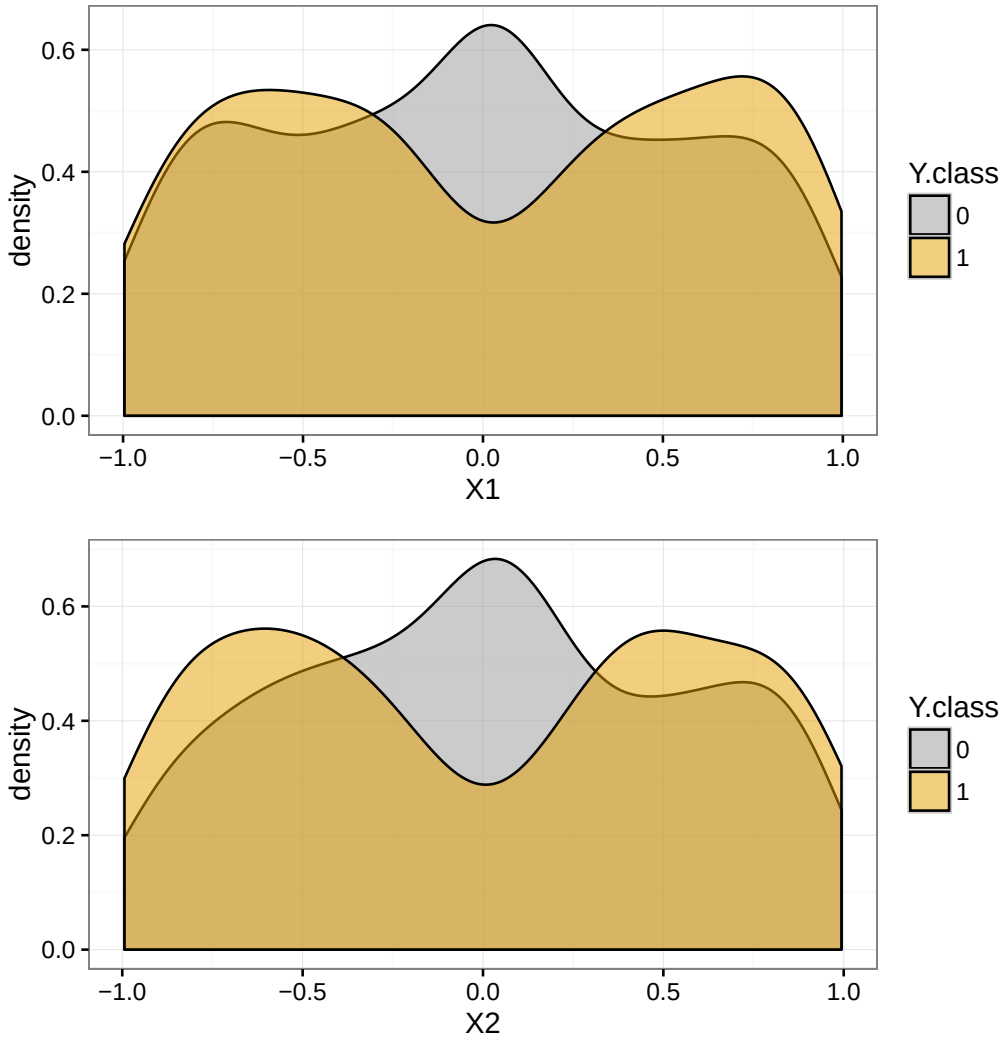
- So why do even bother with methods like LDA or QDA?
  - They can capture meaningful interactions. Naive Bayes cannot.

An example where Naive Bayes fails



This is not a difficult classification problem. Logistic regression with formula `y ~ X1 * X2` gives a perfect classifier.

What does Naive Bayes see on this problem?



Naive Bayes views $X1$ and $X2$ independently, and *cannot* produce the rule: "If $X1$ and $X2$ are both small or both large, classify as $\hat{Y} = 1$"

End of Part I

10 minute break

Assessing the performance of Classifiers

Agenda for Part II

Assessing performance of classification models

- Calibration plots
- Confusion matrices
- Sensitivity, Specificity, Accuracy, Precision, Recall
- Cost-based criteria
- ROC curves

Assessing Classifier Performance

- We now have a bunch of different ways of estimating the conditional probability (aka posterior probability, if we take a Bayes approach)

$$p_k(x) = \mathbb{P}(Y = k \mid X = x)$$

- Now we can start asking questions about whether the estimate $\hat{p}_k(x)$ is a good one, and whether it results is a good decision rule

- Let's start with the question:

Is $\hat{p}_k(x)$ a good estimate of $p_k(x)$?

Are we doing a good job of estimating $p_k(x)$?

Is $\hat{p}_k(x)$ a good estimate of $p_k(x)$?

- Why do we care?
  - An email whose spam probability is $\hat{p}_k(x) = 0.52$ will get classified to spam the same as an email whose spam probability is $\hat{p}_k(x) = 0.999$. But one email is borderline, while the other is extremely likely to be spam. This is important information.
  - Whether to pursue suspicious insurance claim may depend on the estimated probability that it's fraudulent and various cost-related factors
  - Customer Lifetime Value (CLV) calculations require an estimate of the probability that a customer will make a purchase

Calibration plots

1. Bin the data according to $\hat{p}_k(x)$: E.g., bins could be $[0, 0.1], (0.1, 0.2], \ldots, (0.9, 1]$.
2. For each bin, calculate the proportion of observations in bin b that had class $Y = k$
3. Plot the midpoints of the bins on the x-axis and the proportions from Step 2. on the y-axis

- **Note**: Certain methods are obviously poorly calibrated. E.g., we saw that linear regression can return *negative values*
- In such cases, a popular approach is to use the softmax transformation

$$\hat{p}_k^* = \frac{e^{\hat{y}_k}}{\sum_{\ell=1}^{K} \hat{e}^{y_\ell}}$$

These values at least all lie in $[0, 1]$ and sum to 1

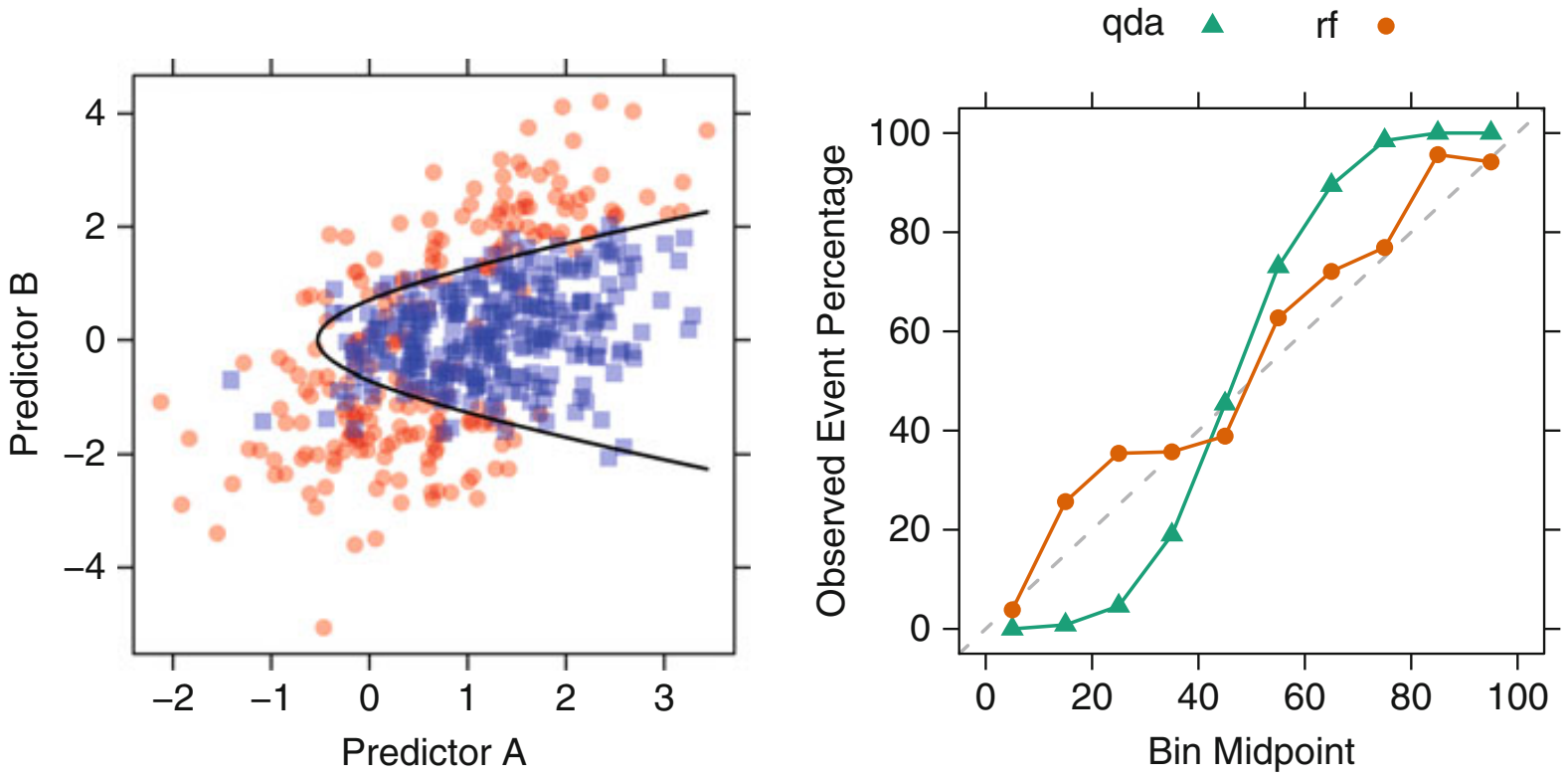


Fig. 11.1: *Left*: A simulated two-class data set with two predictors. The *solid black line* denotes the 50 % probability contour. *Right*: A calibration plot of the test set probabilities for random forest and quadratic discriminant analysis models

The RF is well-calibrated. The QDA model underestimates the true probability when it's low, and overestimates it when it's high.

[source: Applied Predictive Modeling]

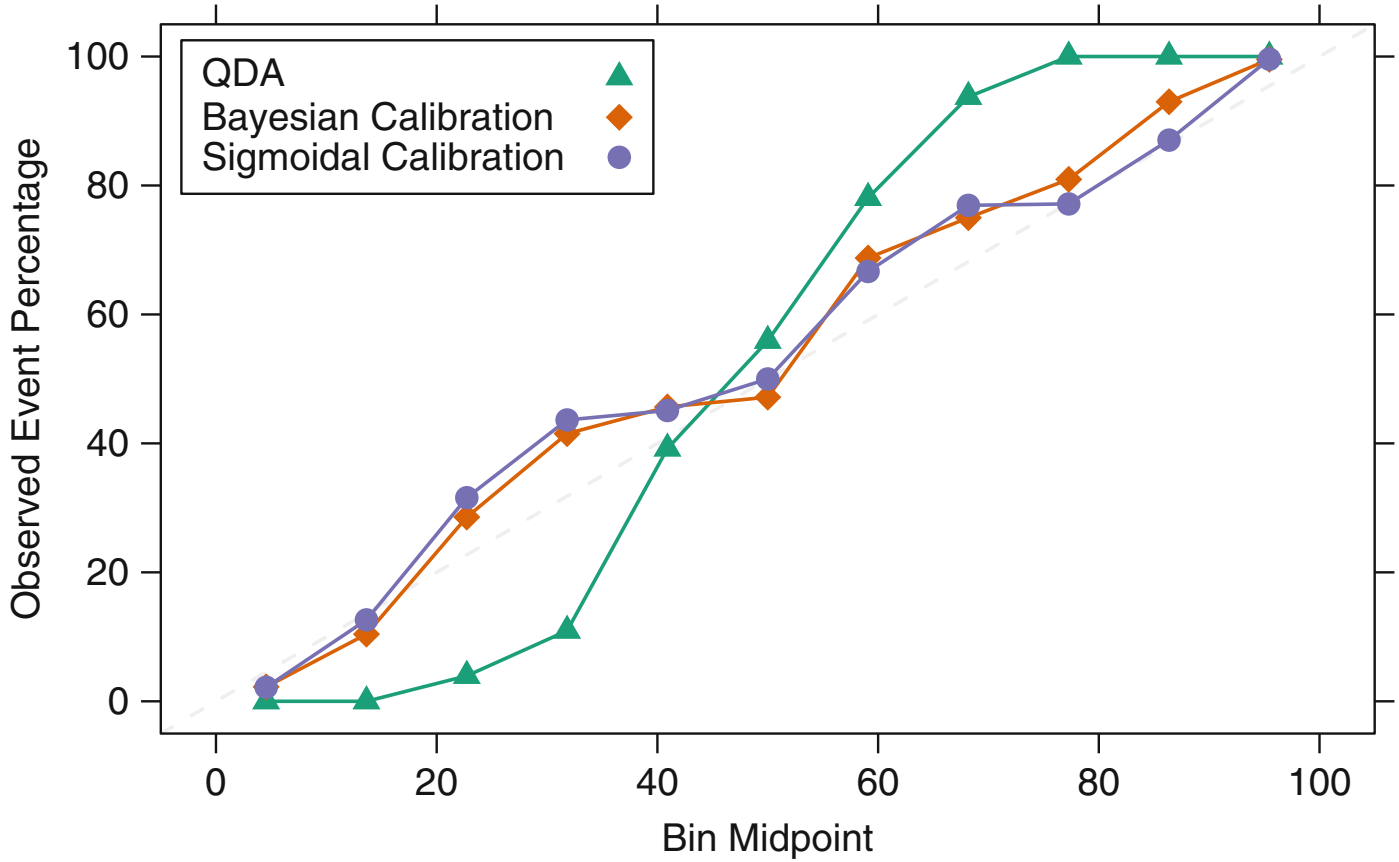


Fig. 11.2: The original QDA class probabilities and recalibrated versions using two different methodologies

The QDA calibration curve looks S-shaped. The technical term to describe this shape is: *sigmoidal*. We can try recalibrating by feeding the $\hat{p}(x)$ into a logistic regression to predict y_i, and then use the resulting probabilities. In some cases this actually works.

[source: Applied Predictive Modeling]

Evaluating Classifications

- Let's focus again on the binary classification setting:
  - $Y = 1$: if the event happened
  - $Y = 0$: if the event did not happen
- The primary building block of essentially all approaches to evaluating a Classifier is the confusion matrix

Table 11.1: The confusion matrix for the two-class problem ("events" and "nonevents." The table cells indicate number of the true positives (TP), false positives (FP), true negatives (TN), and false negatives (FN)

Predicted	Observed	
	Event	Nonevent
Event	TP	FP
Nonevent	FN	TN

[source: Applied Predictive Modeling]

Evaluating Classifications

Table 11.1: The confusion matrix for the two-class problem ("events" and "nonevents." The table cells indicate number of the true positives (TP), false positives (FP), true negatives (TN), and false negatives (FN)

Predicted	Observed	
	Event	Nonevent
Event	TP	FP
Nonevent	FN	TN

- In **R** (and often in practice), it's more natural to form confusion matrices with the Non-event and Event labels swapped.

		Observed	
		No	Yes
Predicted	No	TN	FN
	Yes	FP	TP

[source: Applied Predictive Modeling]

The Confusion Matrix

Table 11.1: The confusion matrix for the two-class problem ("events" and "nonevents." The table cells indicate number of the true positives (TP), false positives (FP), true negatives (TN), and false negatives (FN)

Predicted	Observed	
	Event	Nonevent
Event	TP	FP
Nonevent	FN	TN

- Each cell is a count. The cells in total add up to n
- The diagonal entries are correct classifications
- The off-diagonal entries are classification errors

[source: Applied Predictive Modeling]

What does it mean to have a good classifier?

Predicted	Observed	
	Event	Nonevent
Event	TP	FP
Nonevent	FN	TN

- Accuracy $= (TP + TN)/n$
- Misclassification rate $= (FN + FP)/n = 1 -$ Accuracy
- If FP and FN have the same cost, then our goal is to minimize the Misclassification rate
- E.g., if $Y \in$ {cat photo, dog photo}, we don't care if our error was mistaking a cat for a dog or vice versa
- If $Y \in$ {fraud, not fraud}, the cost of a FN (failing to catch fraud) is typically *much higher* than the cost of a FP (further investigating a false lead)

What does it mean to have a good classifier?

- Suppose I tell you my classifier has 97% accuracy. Are you impressed?
- Well, what if $Y \in$ {wins lottery, does not win}?
  - The chances that a ticket wins the Powerball lottery are *way* smaller than 1% (they're 1 in 175,000,000)
  - By classifying all tickets as "does not win", we'd have an accuracy of $1 - 1/175{,}000{,}000 = 0.99999\ldots$
  - So a 97% accuracy in this case is actually really bad
- We must take the baseline probabilities (i.e., prior probabilities) of each class into account when assessing performance

Sensitivity, Specificity

- We're now going to look at ways of quantifying the performance of a classifier that go beyond the simple notion of Accuracy
- Sensitivity: aka Recall

$$= \frac{\#\text{observations correctly classified to have the event}}{\#\text{observations that had the event}}$$

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

- Specificity: aka True Negative Rate (TNR)

$$= \frac{\#\text{observations correctly classified as non-events}}{\#\text{observations that did not have the event}}$$

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

Sensitivity - Specificity trade-off

- A classifier with high Sensitivity is desirable when False Negatives (e.g., failing to detect fraud) are more costly than False Positives (flagging a case that turns out to be non-fraudulent)

- A classifier with high Specificity is desirable when False Positives (convicting an innocent person of a crime) are more costly than False Negatives (failing to convict a guilty person of a crime)

- Sensitivity and Specificity tend to move in opposite directions
  - To increase Sensitivity, we can always flag more cases as potentially fraudulent. But this would decrease Specificity because more non-fraud cases would now be misclassified as fraud.

An example: Marketing data

- The Marketing data set contains information on bank customers who were contacted by marketers wanting them to open an account
- $Y =$ "Yes" if the customer opened an account when contacted, "No" otherwise
- Here's a confusion matrix obtained from fitting a logistic regression model, and classifying $Y = 1$ if $\hat{p}(x) \geq 0.25$

		Observed	
		Yes	No
Predicted	Yes	121	234
	No	916	7771

- $n = 121 + 234 + 916 + 7771 = 9042$
- Accuracy $= (121 + 7771)/n = 87\%$
- Misclassification rate $= (234 + 916)/n = 13\%$
- Prevalence $= (121 + 916)/n = 11.5\%$

Marketing data

		Observed	
		Yes	No
Predicted	Yes	121	234
	No	916	7771

- $n = 121 + 234 + 916 + 7771 = 9042$
- Accuracy $= (121 + 7771)/n = 87$
- Misclassification rate $= (234 + 916)/n = 13\%$
- Prevalence $= (121 + 916)/n = 11.5\%$
- Sensitivity (Recall) $= 121/(121 + 916) = 11.6\%$
- Specificity $= 7771/(7771 + 234) = 97.1\%$
- So at the cutoff, $\hat{p}(x) \geq 0.25$, our classifier has *low* Sensitivity and *high* Specificity
- This is not a good setting for marketing.

Some other measures of performance

- Here are some other quantities that people have names for
- Positive Predictive Value (PPV):

$$= \frac{\#\text{observations correctly classified to have the event}}{\#\text{observations classified to have the event}}$$

$$= \frac{TP}{TP + FP}$$

- Suppose you take a diagnostic test for a disease. The PPV of the diagnostic is the probability that you actually have disease when you test positive.
- Negative Predictive Value: (NPV)

$$= \frac{\#\text{observations correctly classified as non-events}}{\#\text{observations classified as non-events}}$$

$$= \frac{TN}{TN + FN}$$

- Suppose you take a pregnancy test. The NPV is the probability that you actually aren't pregnant given that the test comes up negative.

Cost-Based Criteria

- All of the criteria we've discussed so far take the form of counts and proportions
- But many real world problems have real costs and benefits
- We may be interested in:
  - Predicting which investments to make to maximize return
  - Improving customer satisfaction through market segmentation
  - Minimize costs associated with fraudulent transactions
- Suppose you work for a clothing retailer and are tasked with mailing out promotional offers
  - It costs you $\$2.00$ to mail a promotion
  - A customer who *Responds* to the promotion yields you an average gain of $\$28.40$
- We can use the confusion matrix now to calculate profit

Simple profit calculation

Table 11.4: Left: A hypothetical test confusion matrix for a predictive model with a sensitivity of 75 % and a specificity of 94.4 %. Right: The confusion matrix when a mass mailing is used for all customers

Predicted	Observed		Observed	
	Response	Nonresponse	Response	Nonresponse
Response	1,500	1,000	2,000	18,000
Nonresponse	500	17,000	0	0

- It costs you $2.00 to mail a promotion
- A customer who *Responds* to the promotion yields you an average gain of $28.40. This is a *net gain* of $26.40 (benefit of a TP).
- A customer who *would have Responded* but who you did not reach out to thus loses you $28.40 (cost of a FN)
- Thus the strategy for the Left confusion matrix gives us a profit of:

$$\text{profit} = \$26.40TP - \$2.00FP - \$28.40FN = \$23{,}400$$

- If we mailed *everyone* (strategy on right), the profit would be $16,800

[source: Applied Predictive Modeling]

Probabilities as ranking functions

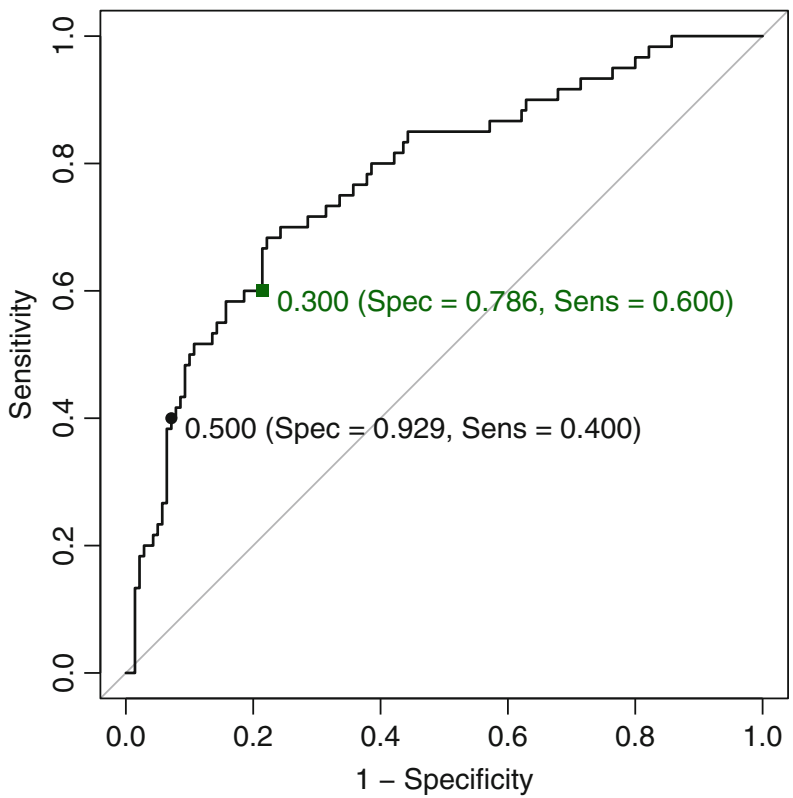
- Suppose we have a probability estimate $\hat{p}(x)$
- We can use $\hat{p}(x)$ to order the observations from *most likely to have the Event* to *least likely*

i	$\hat{p}(x_i)$	y_i
45	0.975	1
12	0.824	0
191	0.762	1
77	0.754	1
$\vdots$	$\vdots$	$\vdots$

- We can think about how well $\hat{p}(x)$ performs by asking: When we order the y_i according to $\hat{p}(x)$, do most of the observations with $y_i = 1$ appear at the top of the list?
- A perfect ranking function will score all of the observations where $y_i = 1$ higher than those where $y_i = 0$
- We're now going to discuss various approaches for visualizing how well $\hat{p}(x)$ does at ranking observations

ROC Curves

- As we vary our probability cutoff α, we get different classification rules and hence different values of all of our performance metrics
- You can think of getting a different confusion matrix at each α
- It's useful to plot the values of various performance metrics as you vary the cutoff α
- Perhaps the most widely used plot is the ROC Curve



[source: Applied Predictive Modeling]

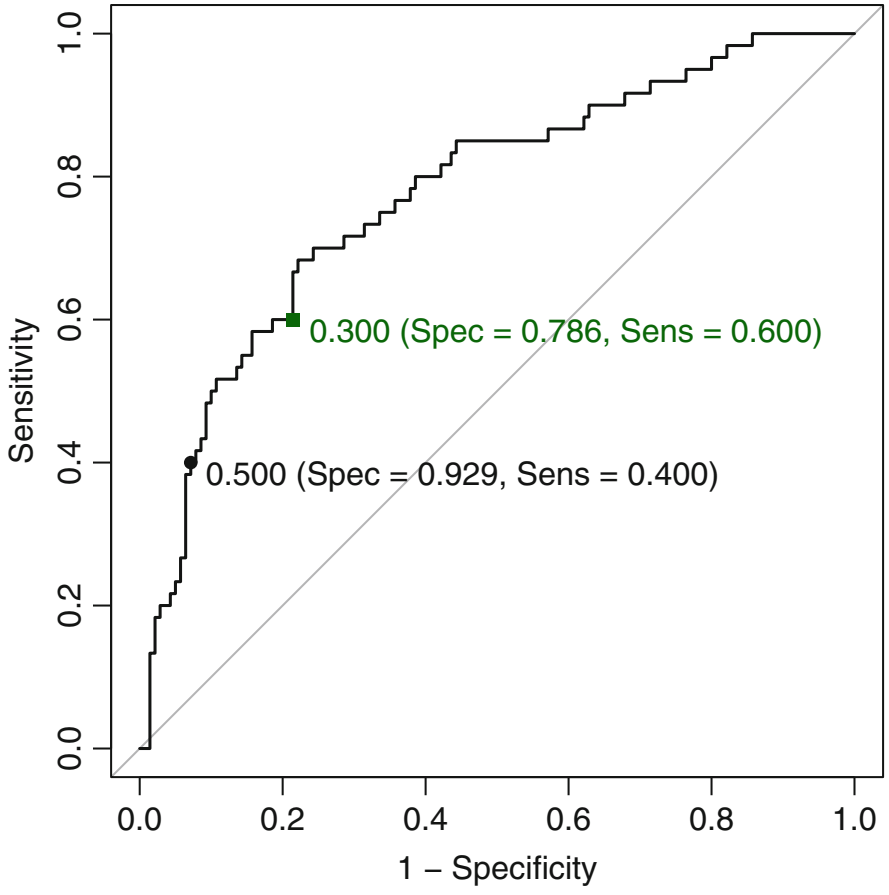
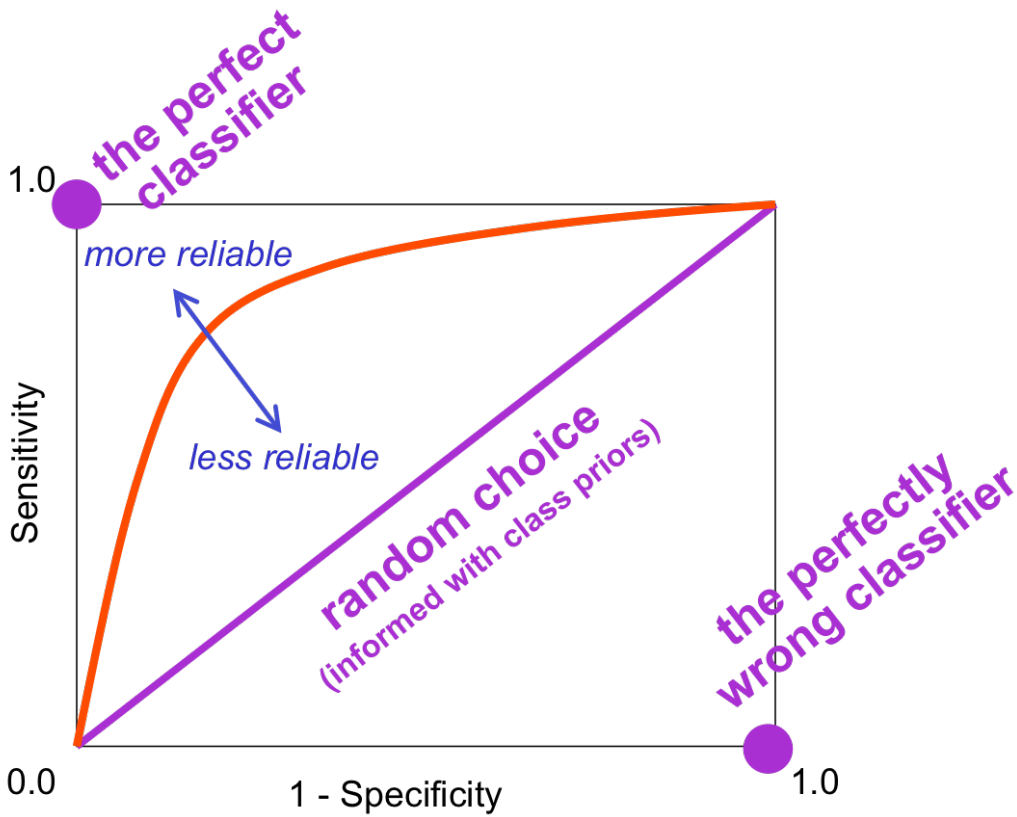


Fig. 11.6: A receiver operator characteristic (ROC) curve for the logistic regression model results for the credit model. The dot indicates the value corresponding to a cutoff of 50 % while the green square corresponds to a cutoff of 30 % (i.e., probabilities greater than 0.30 are called events)

Each point on the curve corresponds to the value of (1−Specificity, Sensitivity) calculated at a particular choice of cutoff α

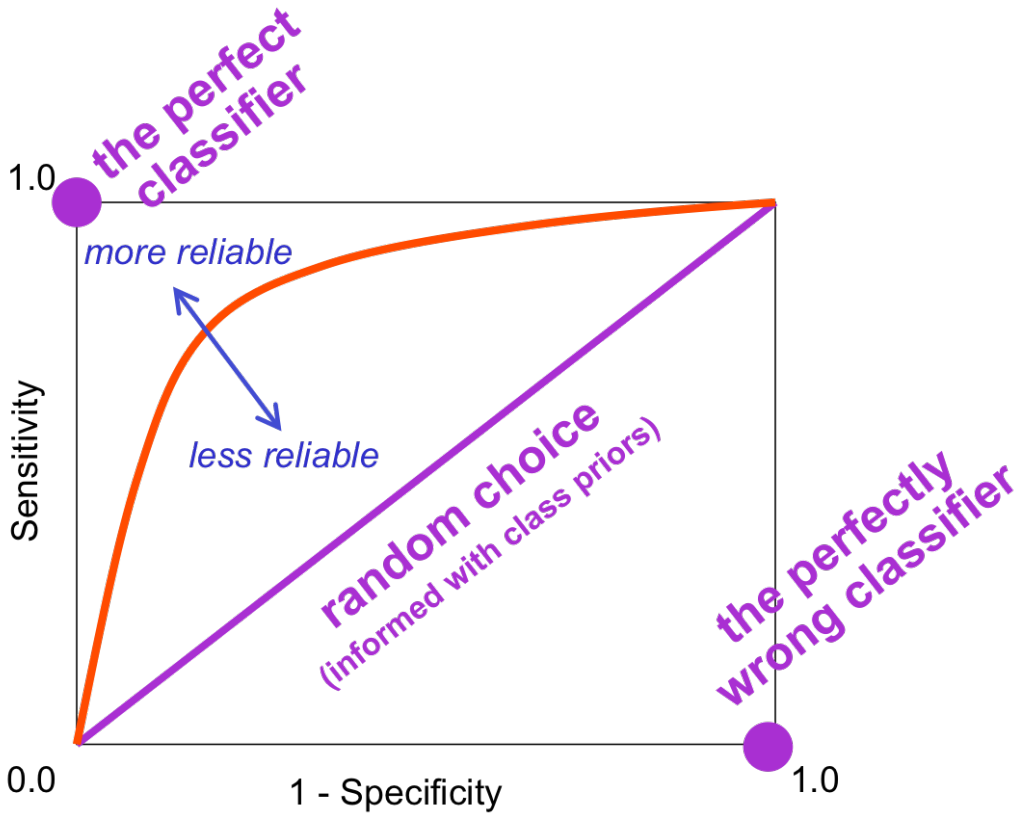
[source: Applied Predictive Modeling]

ROC



- The diagonal is the ROC you would get from randomly picking proportion π_k of the observations to classify to class k
- Higher ROC is better
- The perfect classifier has $(1 - \text{Specificity}, \text{Sensitivity}) = (0, 1)$

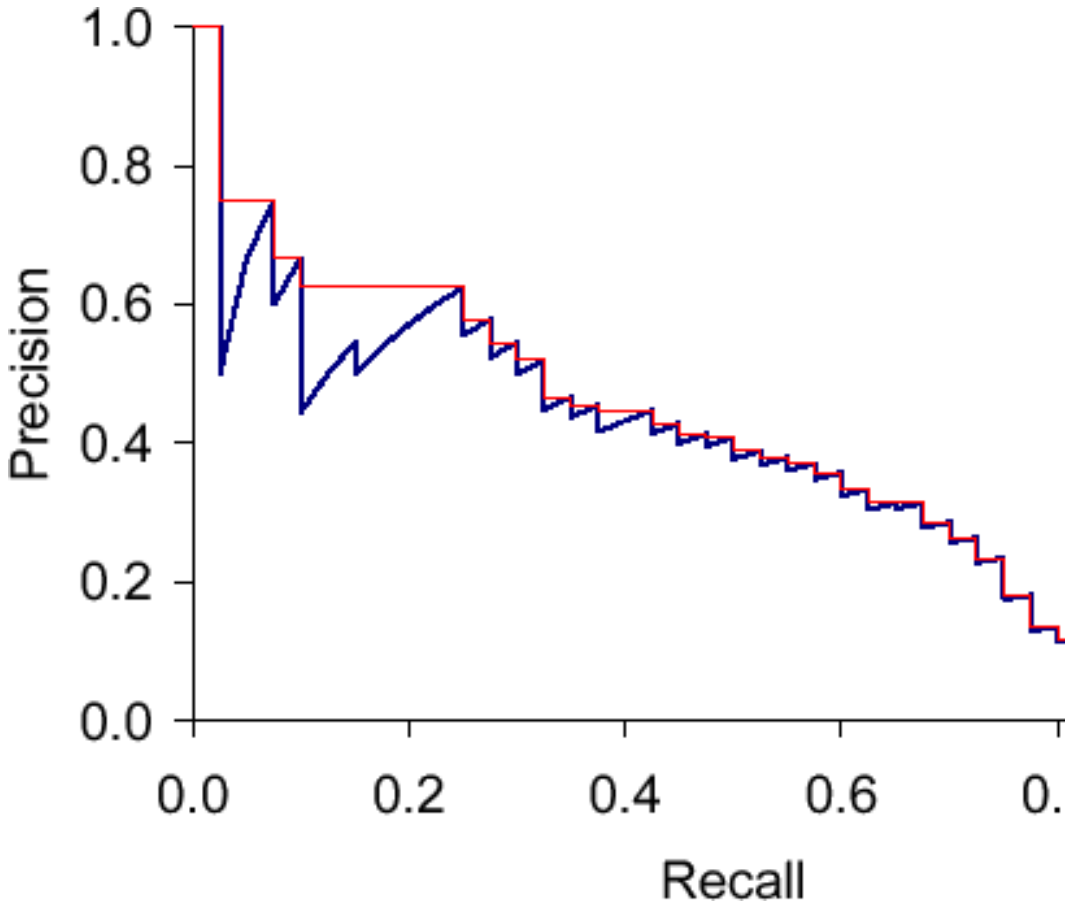
Area under the curve



- The AUC is the *area under the ROC curve*

- AUC has a nice interpretation: The AUC is the probability that the classifier will rank a *randomly selected* observation where $y_i = 1$ higher than a *randomly selected* observation where $y_i = 0$

Precision-Recall curves



- Precision: $TP/(TP+FP)$ (aka, PPV)
- Recall: $TP/(TP+FN)$ (aka, Sensitivity)
- Precision @50% Recall is a common performance metric

[source: Introduction to Information Retrieval, Manning et al.]

Lift charts

- Lift charts are kind of like ROC curves, but may be more useful depending on the application

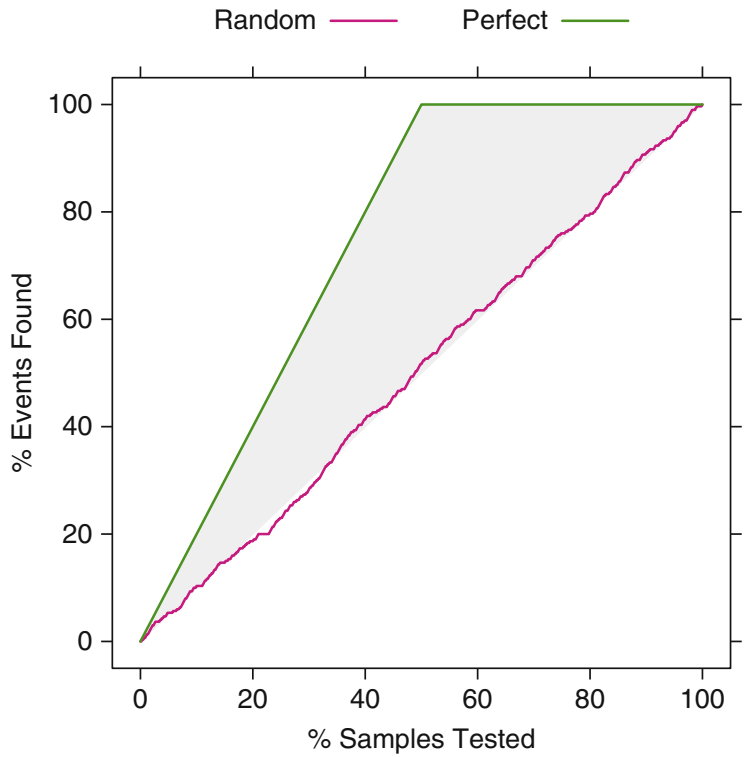
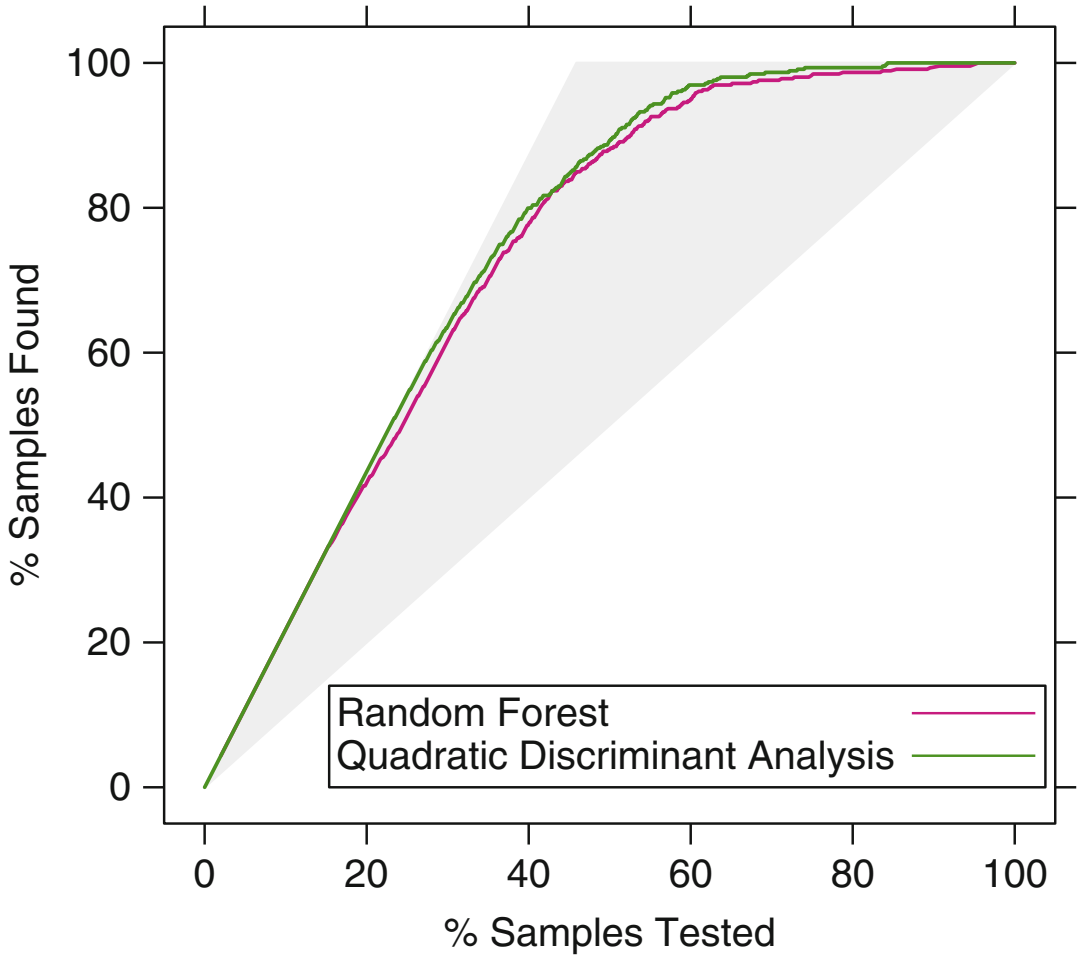


Fig. 11.7: An example lift plot with two models: one that perfectly separates two classes and another that is completely non-informative

- y-axis: Recall (Sensitivity)
- x-axis: $\#\{i : \hat{p}(x_i) > \alpha\}/n = (FP + TP)/n$

[source: Applied Predictive Modeling]

Lift charts

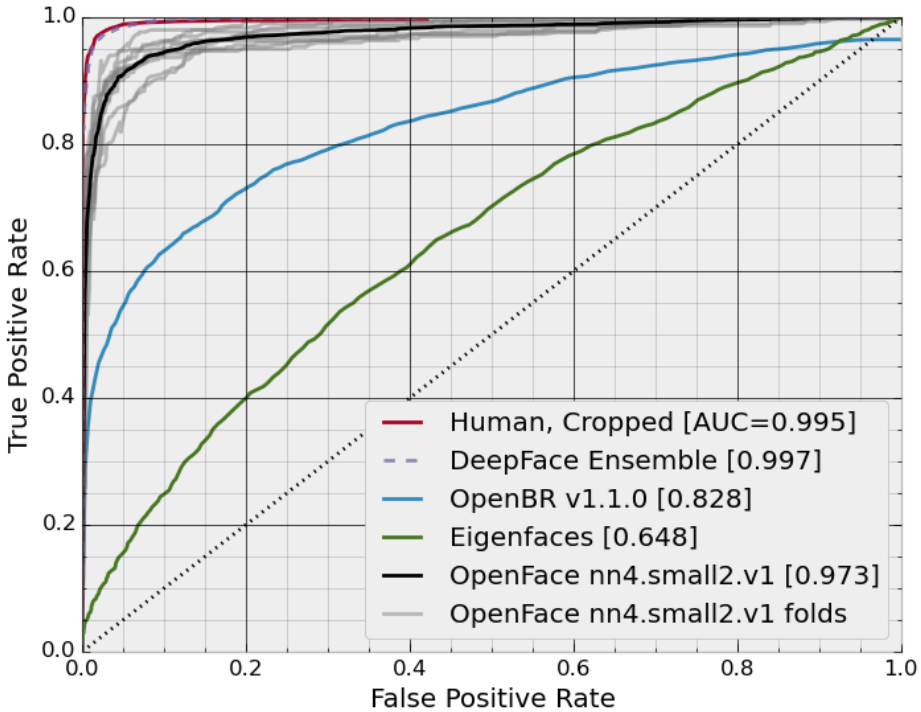


- In this example, of the top 40% of observations ordered according to $\hat{p}(x)$, essentially all of them have $y_i = 1$. This is great!

[source: Applied Predictive Modeling]

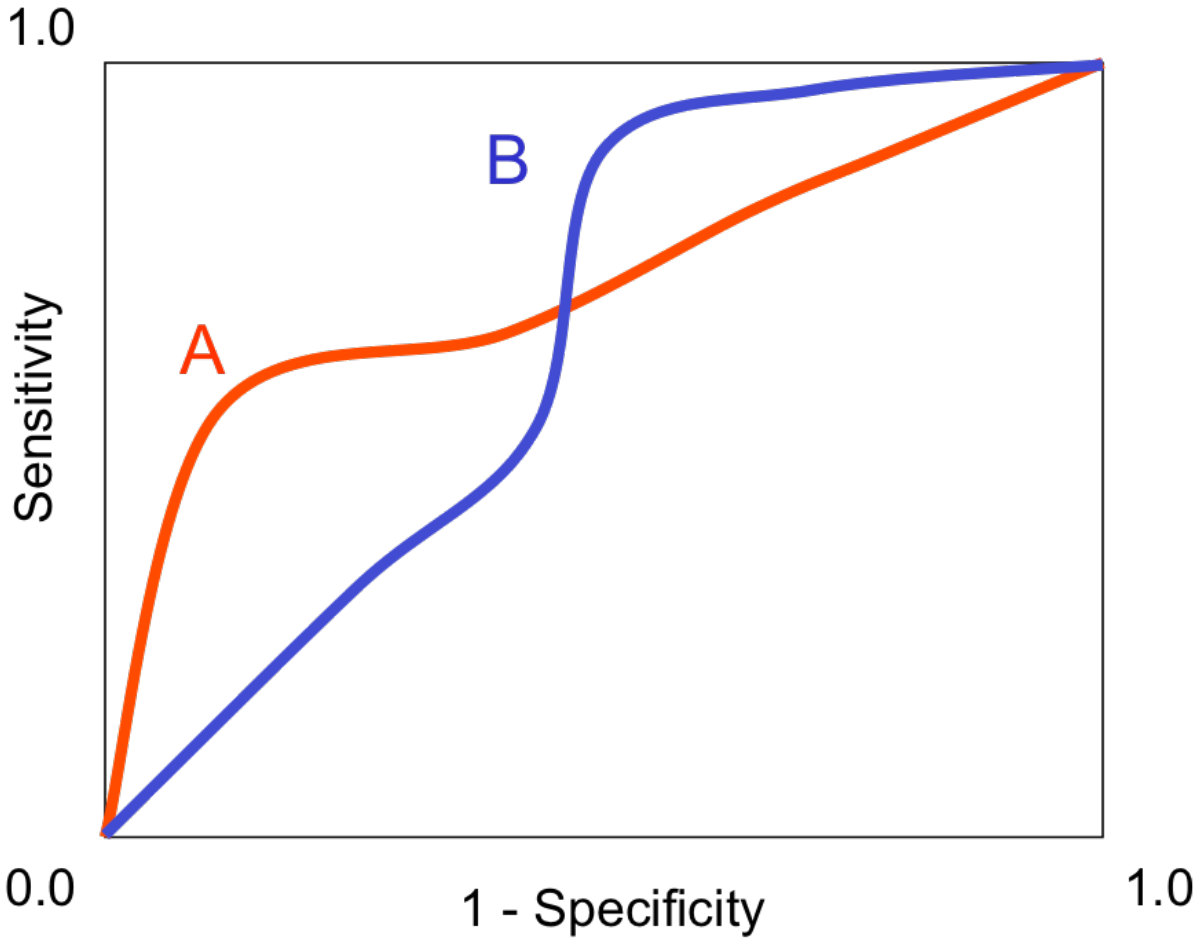
How do we pick the best classifier?

You can overlay the ROC curves from a bunch of different methods.
Here's a facial recognition example. [source: cmusatyalab/openface GitHub]



- The DeepFace Ensemble method is amazing
- The proposed method, OpenFace nn4.small2.v1 does really well. Its ROC curve is the solid black line.
  - 10 grey curves are Test Fold ROC curves from 10-Fold CV

Now which one is better?



It depends on what region of the curve you care most about.

Example: Cancer diagnosis

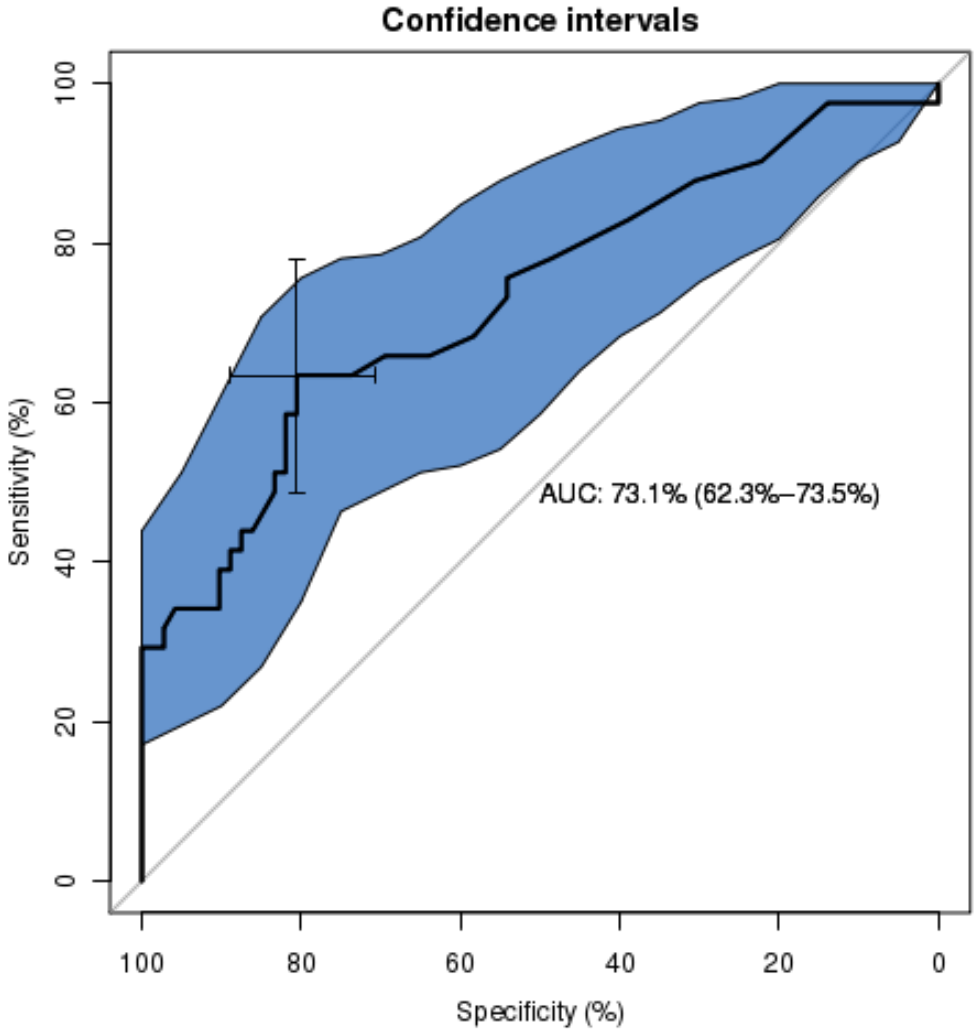
We can think of two settings: Screening, and Referred examinations

- Screening: E.g., we want annual screening of all people above age 40
  - Most people we test will *not* have cancer (high ratio of non-Events to Events)
  - Cost(False positives)/Cost(False negatives) moderate or high
  - Focus on: performance at High Specificity (small x-axis values)

- Referred examination: E.g., you're exhibiting symptoms and your doctor feels a bump under your skin, and refers you for a biopsy to get it tested for cancer
  - Many referred individuals *will* have cancer (*low* or *equal* ratio of non-Events to Events)
  - False negatives are really costly
  - Focus on: performance at High Sensitivity (high y-axis values)

Putting confidence bands on ROC curves

- We like putting standard error bars on our curves so that we can visually discern which trends/differences are *statistically significant*



Using Cross-validation

- In the Prediction setting, we focussed entirely on MSE as our performance metric

- To validate our model, we would use K-Fold CV to estimate the Test MSE

- In the Classification setting, there are *many* metrics out there. The set I presented is by no means exhaustive.

- To estimate Test performance:
  1. Pick a metric (E.g., Accuracy, profit, AUC, Sensitivity @x% Specificity, Precision @x% Recall, etc.)
  2. Calculate the metric on each fold of K-fold CV
  3. Average over all of the folds

- For ROC and Precision-Recall curves, you may want to show the curve you get from each Test fold. This gives a visual representation of the variability of the curve estimates.

Takeaways

- In the Prediction setting, we focussed entirely on MSE as our performance metric
- There are other options out there, but MSE is by the far the most widely accepted
- In the Classification setting, there are *many* metrics out there. The set I presented is by no means exhaustive.
- Whatever criterion it is we wish to maximize (e.g., Accuracy, profit, Sensitivity @x% Specificity, Precision @x% Recall, etc.), we can use Cross-validation to estimate the Test set performance according to this metric

Main takeaway:

Classification is way more interesting than Prediction.

Acknowledgements

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- 36-462/36-662 Lecture notes (Prof. Tibshirani, Prof. G'Sell, Prof. Shalizi)
- 95-791 Lecture notes (Prof. Dubrawski)
- *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani
- *Applied Predictive Modeling*, (Springer, 2013), Max Kuhn and Kjell Johnson