Classification

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```r
library(tidyverse)
library(caret)
library(MASS)
library(e1071)
library(tree)
library(randomForest)
set.seed(3)
```

Philosophy

In all of the modeling we have done so far, the response variable has been numeric.

- A binomial glm is used when the response is a binary categorical variable, but the response in the model is the probability of observing the level designated success.

What are our options if we wish to predict a categorical response with more than two levels?

- Nearest-neighbor averaging (KNN, `class::knn`)
- Multinomial logistic regression
- Discriminant analysis (linear, quadratic, naive Bayes, ...)
- Classification trees or Random Forests
- Support vector machines, neural networks and other machine learning methods

Binomial GLMs

Consider a binary categorical variable Y with classes 0 and 1.

In a binomial GLM, we model the expected probability $p(x) = P(Y = 1|X = x)$ using

$$\text{logit}(p(x)) = \beta_0 + \beta_1 x_1 + \cdots + \beta_m x_m$$

where

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

Equivalently

$$p(x) = \frac{e^{\beta_0+\beta_1 x_1+\cdots+\beta_m x_m}}{1 + e^{\beta_0+\beta_1 x_1+\cdots+\beta_m x_m}}.$$

When Y is a categorical variable with more than 2 levels, it continues to be useful to model the probabilities that it takes each individual level.

Multinomial regression

This technique seems like it doesn't get used as much. If you are interested, the tools that do it are `glmnet::glmnet` with `family=multinomial` or `nnet::multinom`.

`glmnet` also does Lasso and Ridge Regression, which do something like dimension reduction by feature selection. See Chapter 6 of James et al. (2013).

Discriminant Analysis

Model the distribution of X for each class, then apply Bayes' theorem. We'll follow James et al. (2013) and use the following notation:

- $f_k(x) = P(X = x|Y = k)$ is the distribution of X for class k.
- $\pi_k = P(Y = k)$ is the prior probability for class k.
- $p_k(x) = P(Y = k|X = x)$ is the posterior probability for class k.

Bayes' theorem says

$$p_k(x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}.$$

Given $X = x$, we can choose the class k for Y such that $p_k(x)$ is largest. Alternatively, we may wish to report all of the probabilities $p_k(x)$.

Linear Discriminant Analysis

Two strong assumptions make finding the largest $p_k(x)$ much easier.

- The distributions $f_k(x)$ are normal. $f_k(x) = \frac{1}{\sigma_k\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma_k}\right)^2}$
- The variance is the same for all classes: $\sigma_k = \sigma$.

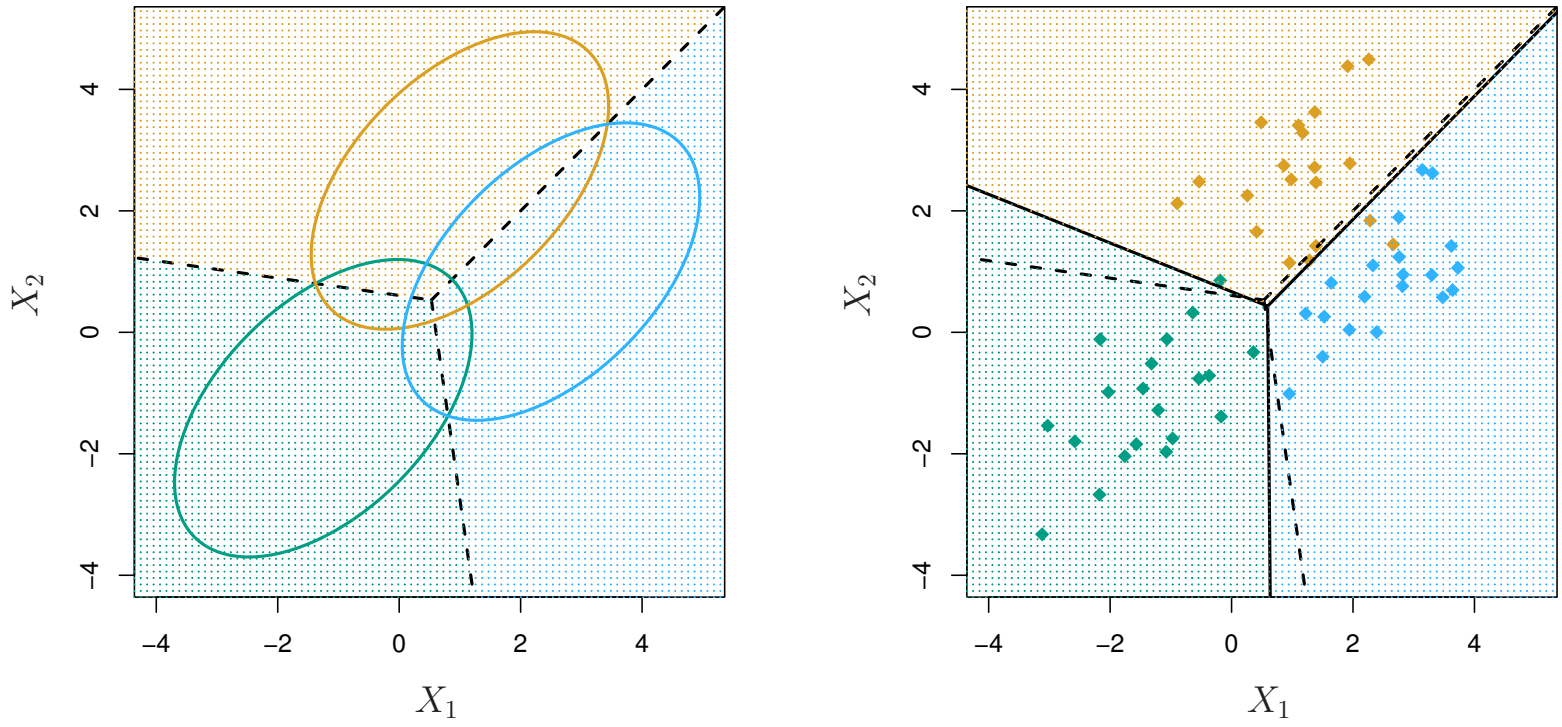
Taking logs of the resulting formulas for $p_k(x)$ and discarding terms that don't depend on k gives the *discriminant*:

$$\delta_k(x) = x\frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k).$$

This is a linear function of x. It is easy to compute and $p_k(x)$ is greatest when $\delta_k(x)$ is greatest. Find the *decision boundary* between class j and class k by solving $\delta_j(x) = \delta_k(x)$.

- The above is written assuming that there is only a single predictor x. For multiple predictors, the math is similar, with x replaced by the vector of predictors and σ by the covariance matrix. Decision boundaries are linear.

LDA illustration

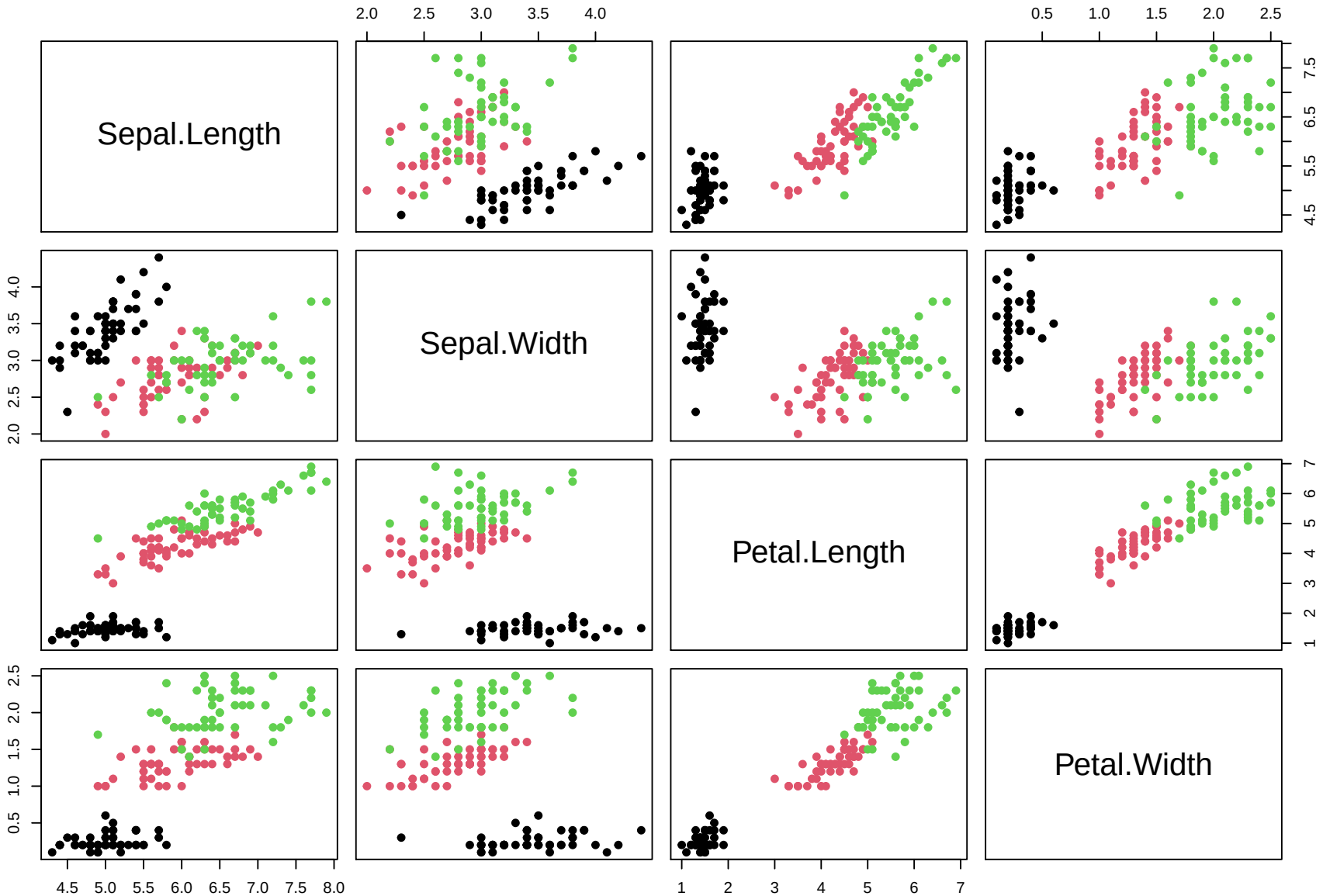


This graphic is from James et al. (2013). It shows simulated data from Gaussian distributions indicated by the ovals. Dotted lines are optimal decision boundaries. Solid lines are decision boundaries from LDA.

LDA example

We'll study Fisher's iris data.

```
pairs(iris[,1:4], col=iris$Species, pch=19)
```



LDA example (model fitting)

The `lda` command from `MASS` performs LDA. The LD1 and LD2 vectors make a nice basis for the plane spanned by the centroids of the 3 species.

```
lda.mod <- lda(Species~., data = iris)
lda.mod
```

```
## Call:
## lda(Species ~ ., data = iris)
##
## Prior probabilities of groups:
##     setosa versicolor  virginica
##  0.3333333  0.3333333  0.3333333
##
## Group means:
##            Sepal.Length Sepal.Width Petal.Length Petal.Width
## setosa            5.006       3.428        1.462       0.246
## versicolor        5.936       2.770        4.260       1.326
## virginica         6.588       2.974        5.552       2.026
##
## Coefficients of linear discriminants:
##                     LD1         LD2
## Sepal.Length  0.8293776  0.02410215
## Sepal.Width   1.5344731  2.16452123
## Petal.Length -2.2012117 -0.93192121
## Petal.Width  -2.8104603  2.83918785
##
## Proportion of trace:
##    LD1    LD2
## 0.9912 0.0088
```

LDA example (model evaluation)

The model is correct in all but 3 cases.

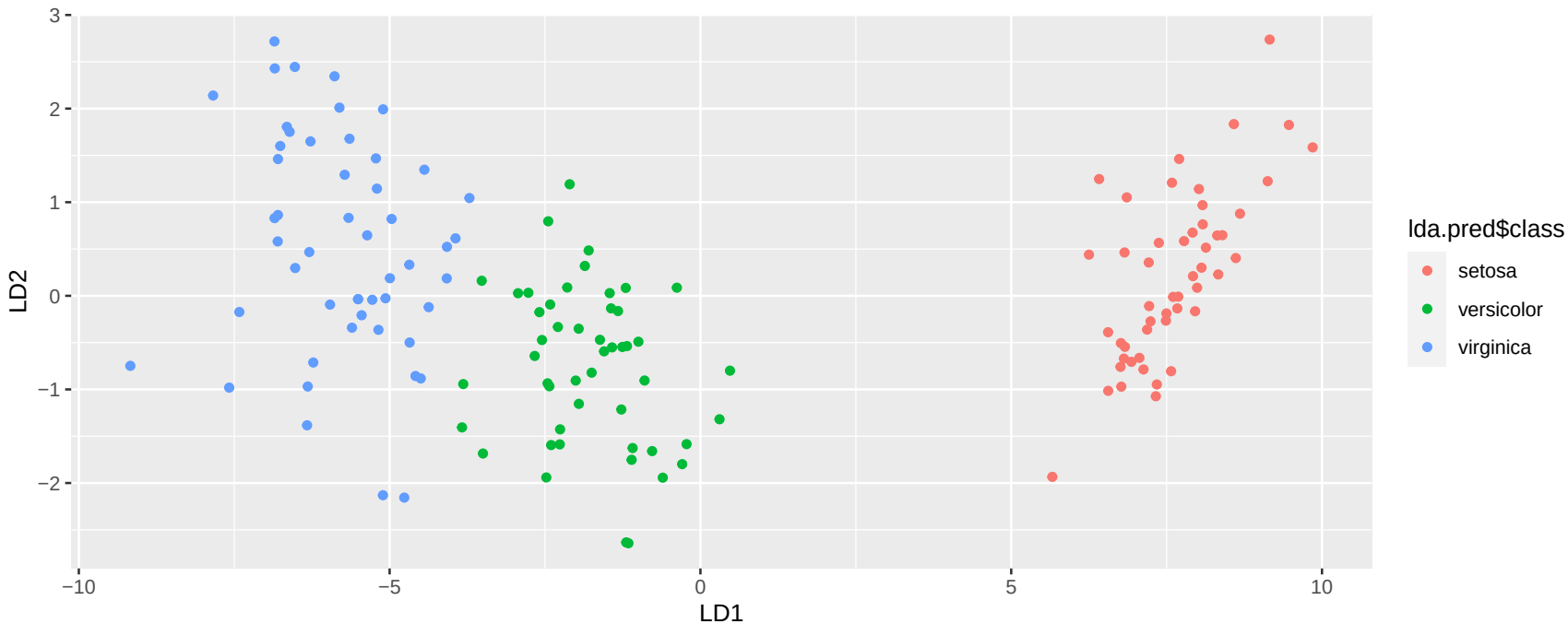
```
lda.pred <- predict(lda.mod)
mean(lda.pred$class==iris$Species)
```

```
## [1] 0.98
```

```
sum(lda.pred$class!=iris$Species)
```

```
## [1] 3
```

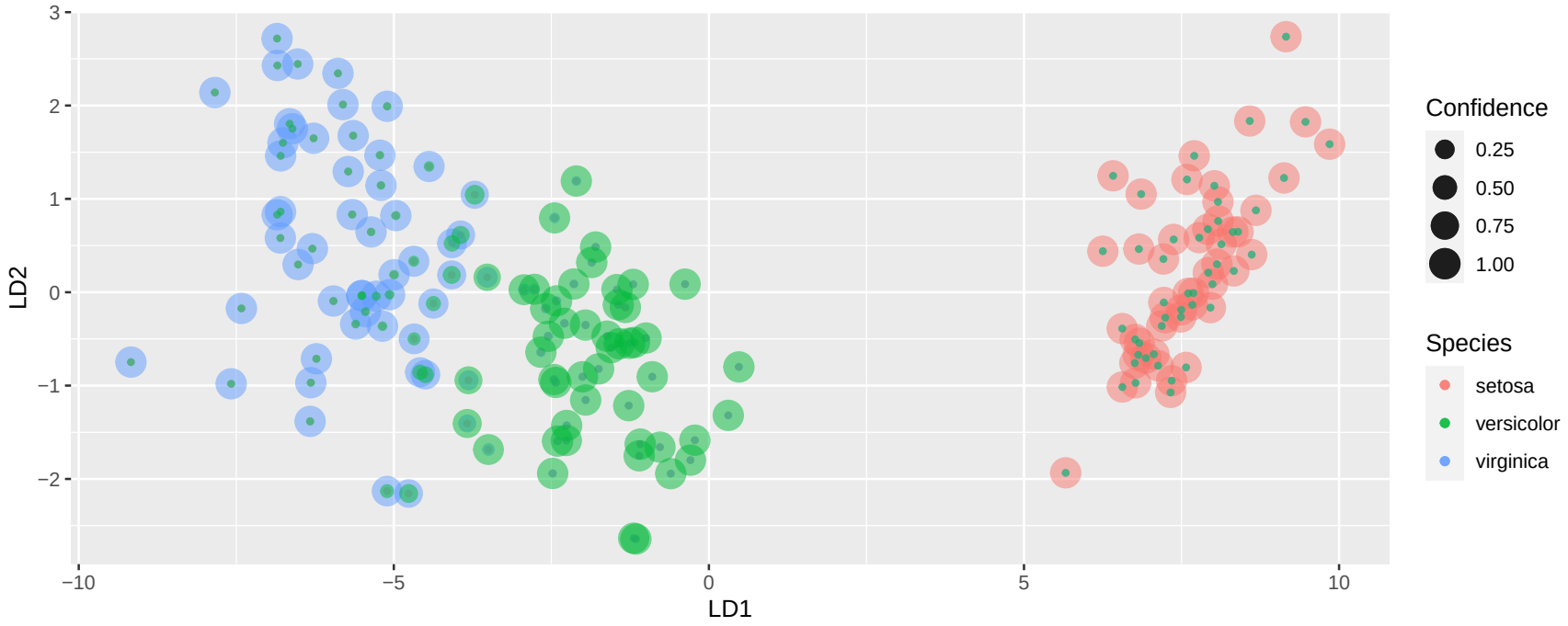
```
lda.obs <- as.data.frame(lda.pred$x)
ggplot(lda.obs, aes(LD1, LD2, color=lda.pred$class))+geom_point()
```



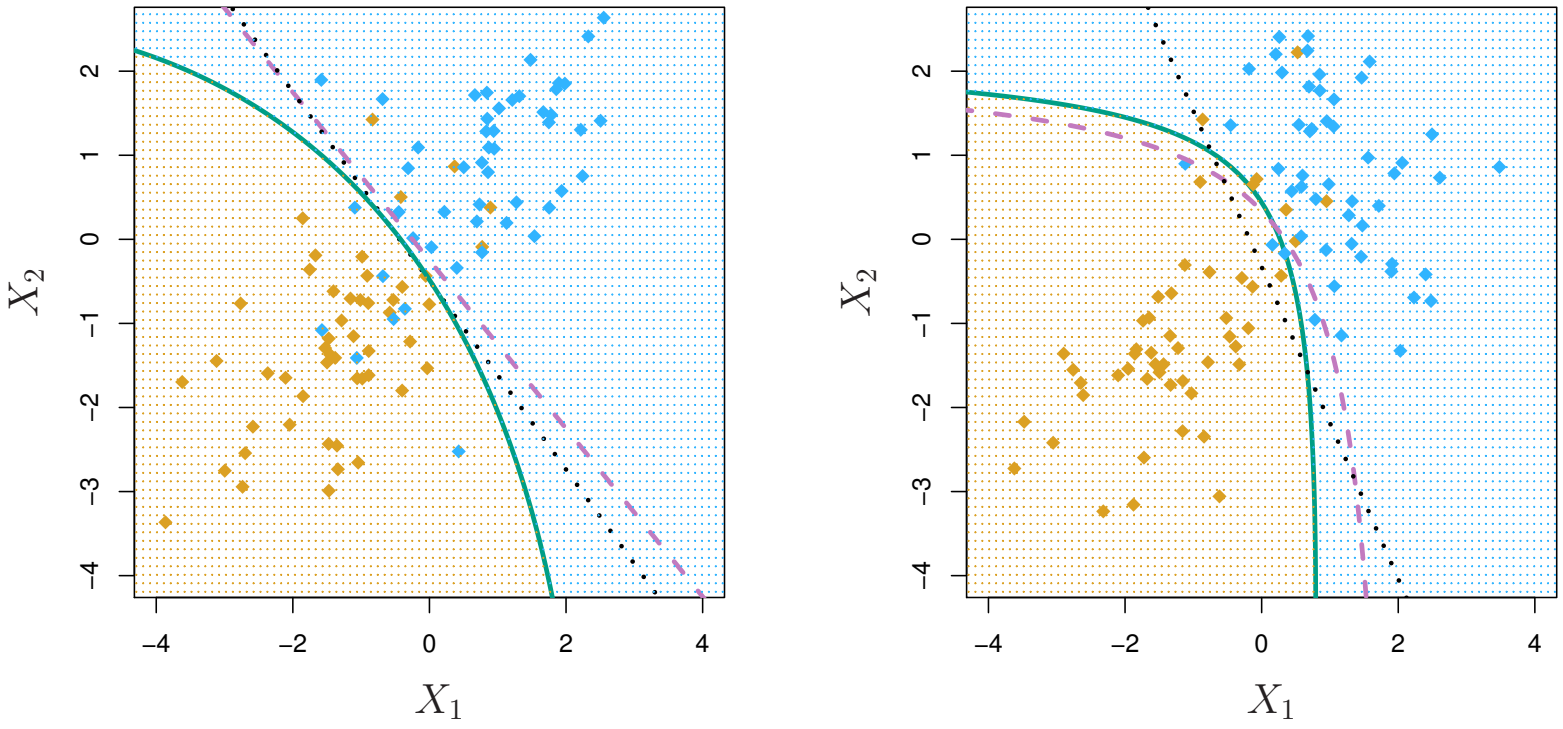
LDA example (posterior probabilities)

Posterior probabilities are also available from `predict.lda`.

```
lda.post <- as.data.frame(lda.pred$posterior)
ggplot(lda.obs, aes(LD1, LD2))+
  geom_point(aes(size=lda.post$setosa, color="setosa"), alpha=0.5)+
  geom_point(aes(size=lda.post$virginica, color="virginica"), alpha=0.5)+
  geom_point(aes(size=lda.post$versicolor, color="versicolor"), alpha=0.5)+
  labs(size="Confidence", color="Species")
```



Quadratic Discriminant Analysis



Keeping the normality assumption but relaxing the condition that all of the variances are equal leads to *quadratic discriminant analysis*. The decision boundaries are quadratic instead of linear.

- Smaller data sets do better with LDA.

QDA example (model fitting)

QDA doesn't do dimension reduction as a byproduct like LDA.

```
qda.mod <- qda(Species~., data = iris)
qda.mod
```

```
## Call:
## qda(Species ~ ., data = iris)
##
## Prior probabilities of groups:
##     setosa versicolor  virginica
##  0.3333333  0.3333333  0.3333333
##
## Group means:
##            Sepal.Length Sepal.Width Petal.Length Petal.Width
## setosa            5.006       3.428        1.462       0.246
## versicolor        5.936       2.770        4.260       1.326
## virginica         6.588       2.974        5.552       2.026
```

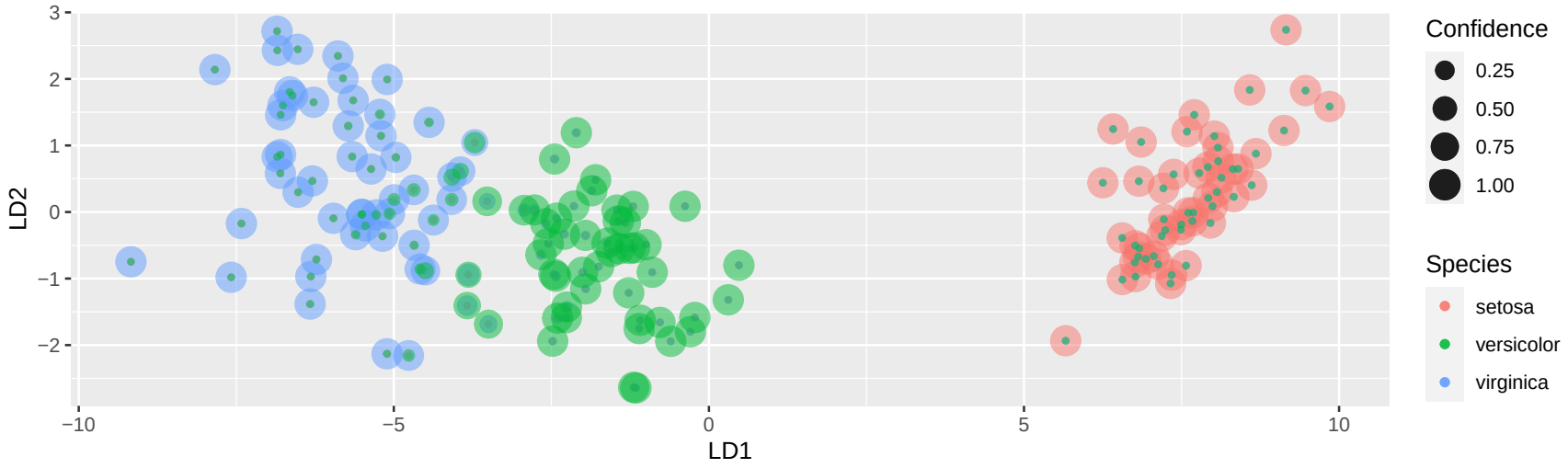
QDA example (model evaluation)

The predictions from QDA are the same as LDA on these data.

```
qda.pred <- predict(qda.mod)
sum(qda.pred$class!=iris$Species)
```

```
## [1] 3
```

```
qda.post <- as.data.frame(qda.pred$posterior)
ggplot(lda.obs, aes(LD1, LD2))+
  geom_point(aes(size=qda.post$setosa, color="setosa"), alpha=0.5)+
  geom_point(aes(size=qda.post$virginica, color="virginica"), alpha=0.5)+
  geom_point(aes(size=qda.post$versicolor, color="versicolor"), alpha=0.5)+
  labs(size="Confidence", color="Species")
```



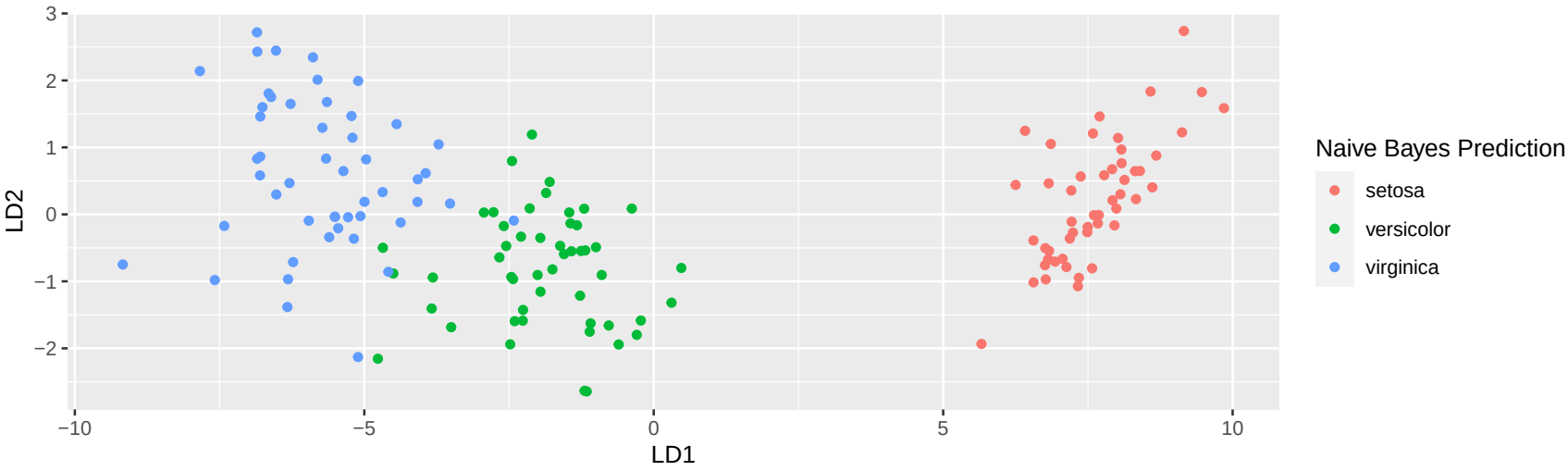
Naive Bayes

With multiple predictors $x = (x_1, \ldots, x_m)$, assuming that the distribution $f_k(x)$ is a product of terms involving only one x_i at a time gives a form for $\delta_k(x)$ that is useful for large numbers of predictors. $(m >> 0)$

```
nb.mod <- naiveBayes(Species~., data=iris)
nb.pred <- predict(nb.mod, newdata = iris)
sum(nb.pred!=iris$Species)
```

```
## [1] 6
```

```
ggplot(lda.obs, aes(LD1, LD2, color=nb.pred))+geom_point()+
  labs(color="Naive Bayes Prediction")
```



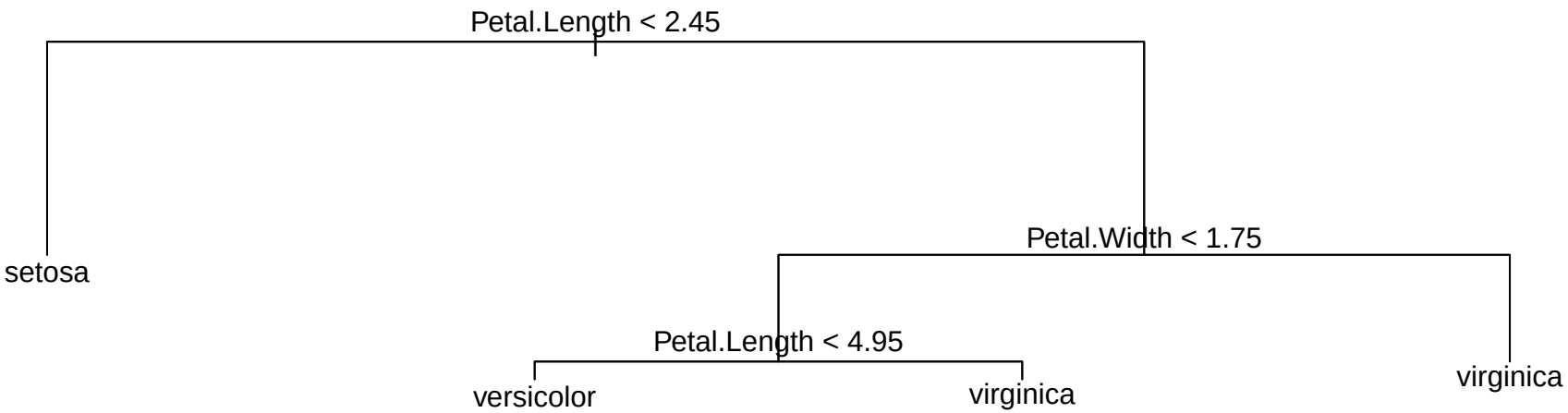
Trees

Decision trees are very intuitive.

```
tree.iris=prune.tree(tree(Species~.,iris), best=4); summary(tree.iris)
```

```
##
## Classification tree:
## snip.tree(tree = tree(Species ~ ., iris), nodes = c(7L, 12L))
## Variables actually used in tree construction:
## [1] "Petal.Length" "Petal.Width"
## Number of terminal nodes:  4
## Residual mean deviance:  0.1849 = 26.99 / 146
## Misclassification error rate: 0.02667 = 4 / 150
```

```
plot(tree.iris); text(tree.iris,pretty=0)
```



Tree Building

Building a tree consists of recursively splitting the data into regions using thresholds on the predictors.

The process is *top-down* and *greedy*.

- Top-down because we start with unlabeled data and perform the best split.
- Greedy because we don't look ahead and make any sub-optimal split that will then allow for better splits further down the tree.

After building a tree, we need to prune it back to avoid overfitting. The degree of pruning is a parameter that can be tuned using cross validation.

Tree Building Details

To determine the best split, we use *Gini index* or *cross-entropy*. Both are defined for a region (subset of the data domain) corresponding to a node/leaf of the tree.

- The Gini index:

$$G = \sum_{k=1}^{K} \hat{p}_k (1 - \hat{p}_k)$$

  where $\hat{p}_k$ is the proportion of training observations in the region that are from the kth class.
- The cross-entropy:

$$D = -\sum_{k=1}^{K} \hat{p}_k \log \hat{p}_k$$

These two measures are similar numerically. Small values indicate that the region in question is homogeneous.

Unfortunately . . .

Single trees do poorly at predicting compared to the other methods we have studied.

Random Forests and Bagging

By building a lot of trees, adding noise to the process as we do so, and then aggregating the predictions we can build very effective predictive models.

- *Bagging* (bootstrap aggregation) in a general technique for building many models and averaging them. Bootstrap samples of the data are used to create replicates of the data for training models.
- The *Random Forest* algorithm builds trees on bootstrapped training samples, but at each step, only a random subset of the predictors are considered as options for defining a split.
- These additions of noise result in models with lower variance and higher predictive power.

Random Forest Example

```
west_fork <- read.csv("data/FieldPlots_WithSpatial.csv")
west_fork$bc_sqrt_7 <- factor(west_fork$bc_sqrt_7)
rf.mod <- randomForest(bc_sqrt_7~.,
                       data = west_fork[, c(4,8:32)], importance=TRUE)

accuracy <- function(tab)sum(sapply(1:nrow(tab),
                                    function(x)tab[x,x]))/(sum(tab))
rf.tab <- table(predict(rf.mod),west_fork$bc_sqrt_7)
rf.tab
```

```
##
##      1  2  3  4  5  6  7
##   1  8  0  4  0  0  3  2
##   2  0 89  4 19 10  4  0
##   3 20 10 60  9  0  3 17
##   4  0 10  6 19  2  0  3
##   5  0  2  1  0  4  0  0
##   6  0  0  0  0  0  0  0
##   7  0  0  1  1  0  0  1
```

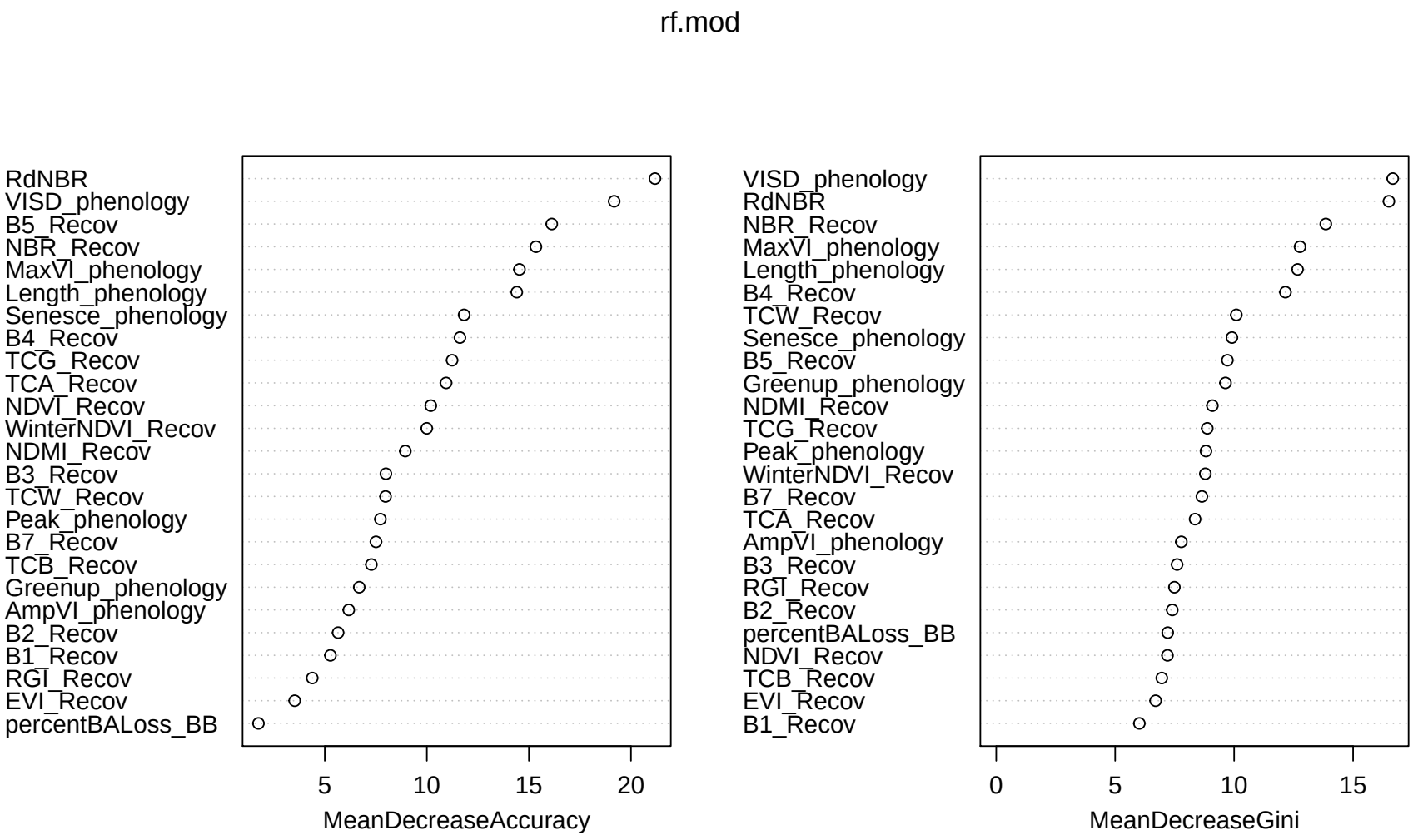
```
accuracy(rf.tab)
```

```
## [1] 0.5801282
```

Variable Importance

Interpretation of a Random Forest is challenging, but we can get relative levels of variable importance by looking at decreases in the Gini index over all the splits where a particular variable is used.

```
varImpPlot(rf.mod)
```



References

James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani. 2013. *An Introduction to Statistical Learning: With Applications in R*. Springer. https://faculty.marshall.usc.edu/gareth-james/ISL/.