More Classification: ISL 4

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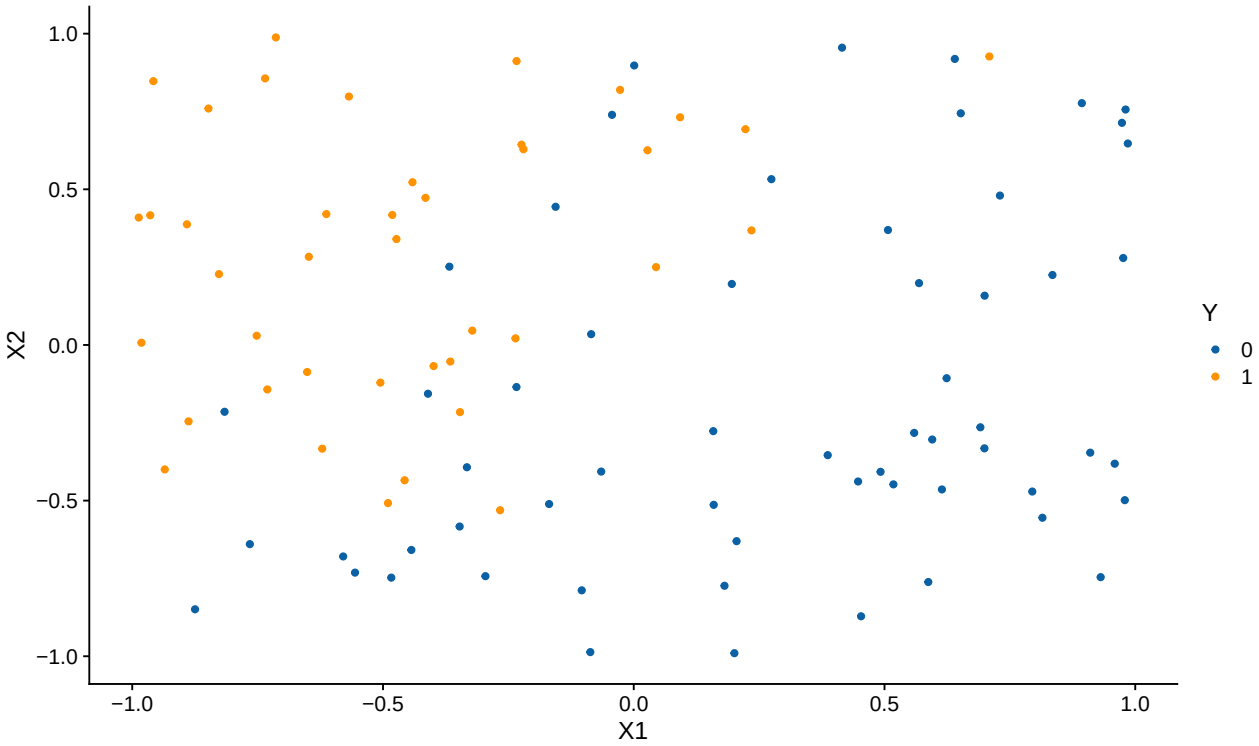
Linear classifiers

Logistic regression

- Logistic regression is one example of a ~~linear classifier~~.
- It produces a line (or plane or hyperplane) which ~~separates~~ the two classes.

```
g <- ggplot(df, aes(X1,X2,color=Y)) + geom_point() +
  scale_color_manual(values=c(blue,orange)) + theme_cowplot(14)
g
```




```
log.lm = glm(Y~.,data=df, family='binomial')
summary(log.lm)
```

```
##
## Call:
## glm(formula = Y ~ ., family = "binomial", data = df)
```

```
##
## Deviance Residuals:
##      Min        1Q    Median        3Q       Max
## -1.99245  -0.37843  -0.08709   0.42603   1.96120
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -1.1986     0.3975  -3.015  0.00257 **
## X1           -4.6102     0.9934  -4.641 3.47e-06 ***
## X2            3.3806     0.8180   4.133 3.59e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 135.372  on 99  degrees of freedom
## Residual deviance:  62.308  on 97  degrees of freedom
## AIC: 68.308
##
## Number of Fisher Scoring iterations: 6
```

What is the line?

- Suppose we decide "Predict `1` if `predict(log.lm) > 0.5`".
- This means "For which combinations of `x1` and `x2` is

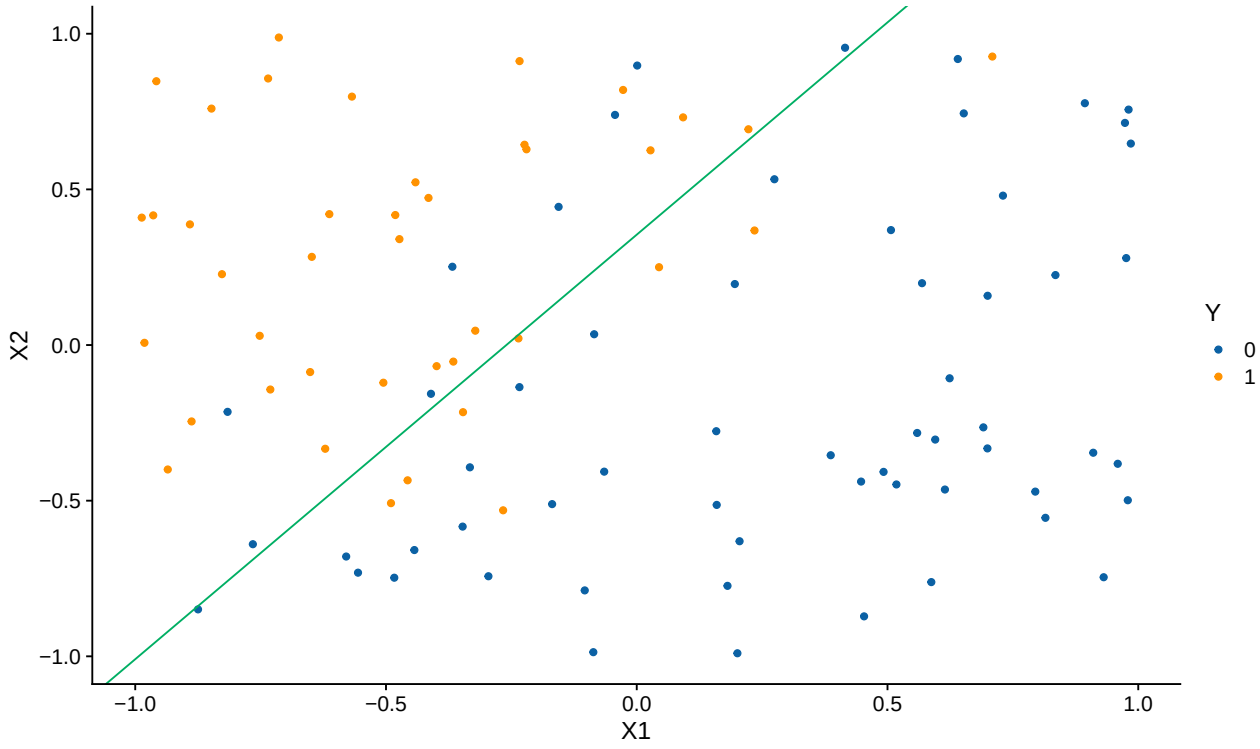
$$\frac{\exp\left(\widehat{\beta}_0 + \widehat{\beta}_1 x_1 + \widehat{\beta}_2 x_2\right)}{1 + \exp\left(\widehat{\beta}_0 + \widehat{\beta}_1 x_1 + \widehat{\beta}_2 x_2\right)} > 0.5?"$$

- Solving this gives

$$\widehat{\beta}_0 + \widehat{\beta}_1 x_1 + \widehat{\beta}_2 x_2 > \log(.5) - \log(1 - .5) \Rightarrow x2 > -\frac{\widehat{\beta}_0 + \widehat{\beta}_1 x_1}{\widehat{\beta}_2}.$$

- That's just a line. Let's plot it:

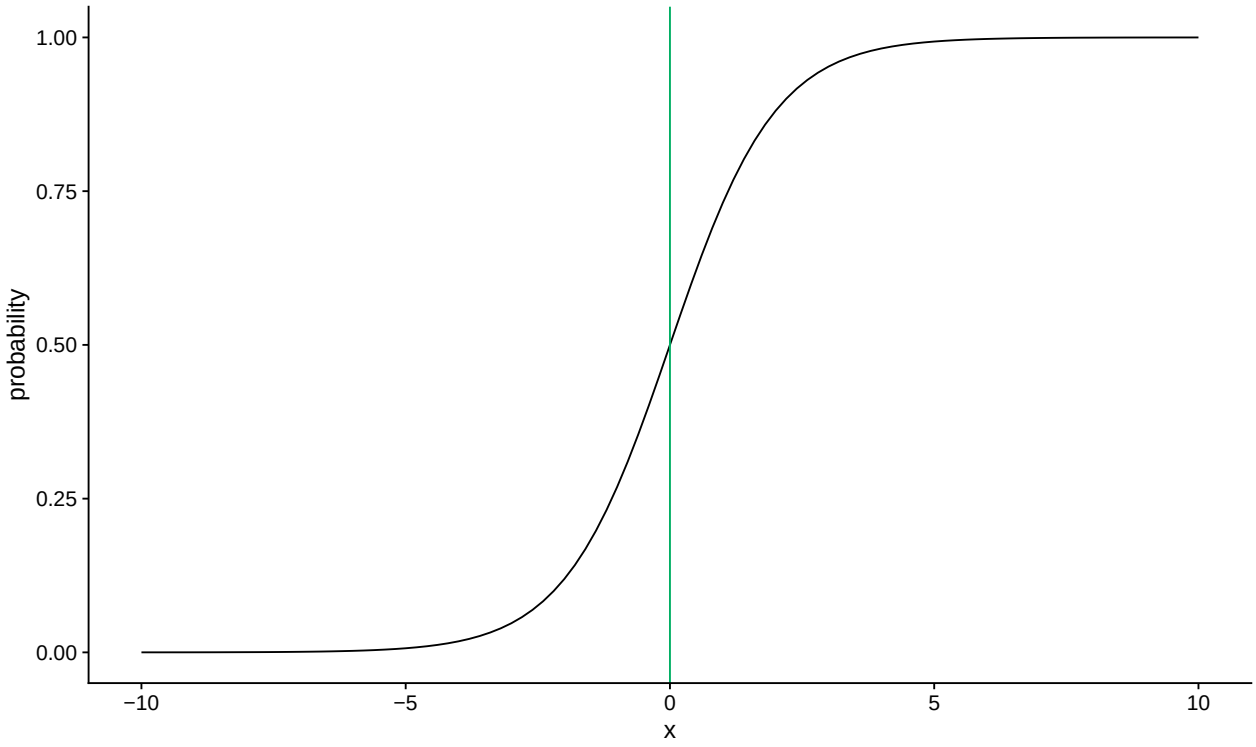
```
cc = coefficients(log.lm)
g + geom_abline(intercept = -cc[1]/cc[3], slope = -cc[2]/cc[3], color=green)
```



Classification boundary

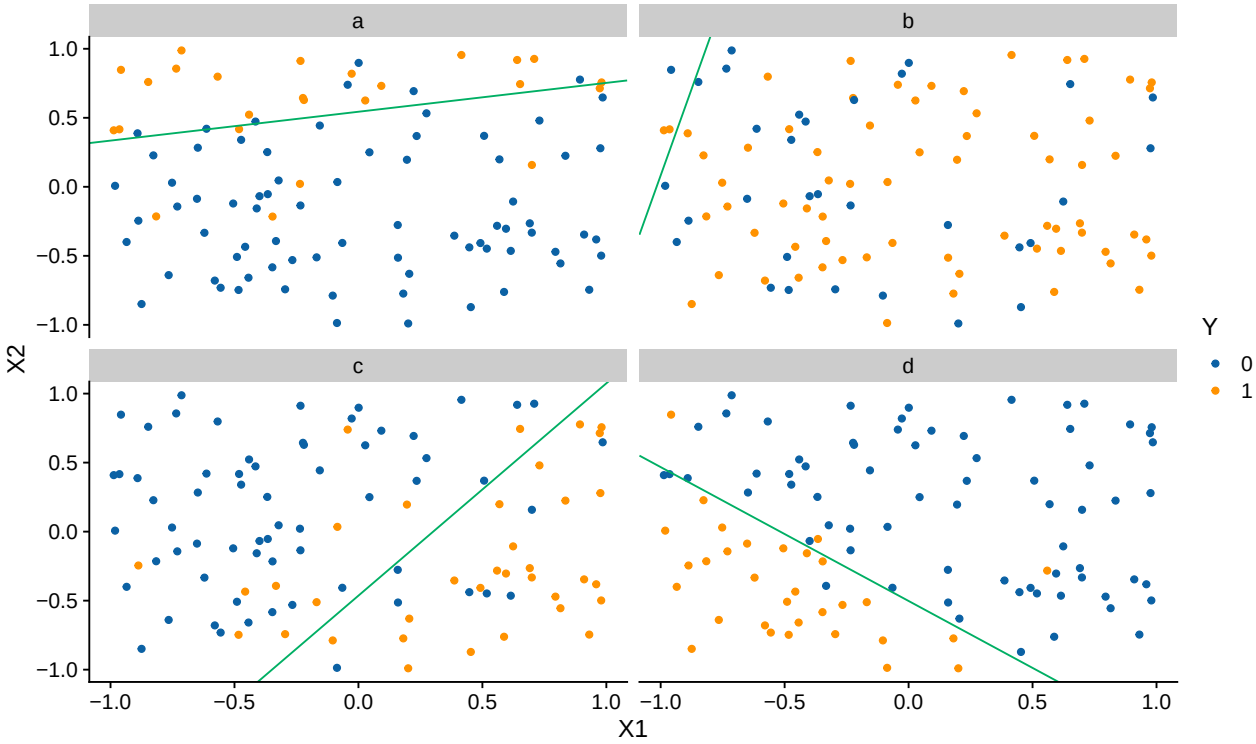
- We call that line the "classification boundary"
- The `ilogit` function looks like a ramp:

```
ggplot(data.frame(x=c(-10,10)), aes(x)) + stat_function(fun=ilogit) +
  geom_vline(xintercept = 0, color=green) + ylab('probability') + theme_cowplot()
```



- Again, solving for where the equation crosses 0.5, gives us a "line".
- Logistic regression always produces "linear" classification boundaries, so we call it a "linear classifier"

Lots of different boundaries



index	intercept	slope
a	0.54	0.21
b	5.10	5.02
c	-0.46	1.54
d	-0.50	-0.97

Linear discriminant analysis

LDA

(Not to be confused with Latent Dirichlet Allocation, also abbrev. LDA)

- Suppose $X_i \mid Y_i = 1 \sim N(\mu_1, \Sigma)$
- And $X_i \mid Y_i = 0 \sim N(\mu_0, \Sigma)$
- Note that these share Σ.
- Suppose that $P(Y_i = 1) = \pi_1$

~~Bayes Rule:~~

$$P(Y_i = 1 \mid X_i = x) = \frac{P(X_i \mid Y_i = 1)\pi_1}{P(X_i \mid Y_i = 1)\pi_1 + P(X_i \mid Y_i = 0)\pi_0}$$

- So if we know $\pi_1, \mu_1, \mu_0, \Sigma$, then we can find $P(Y_i = 1 \mid X)$

Simplification

$$\begin{aligned}
\frac{P(X_i \mid Y_i = 1)\pi_1}{P(X_i \mid Y_i = 1)\pi_1 + P(X_i \mid Y_i = 0)\pi_0} &= \frac{\pi_1 \frac{1}{(2\pi|\Sigma|)^{p/2}} \exp\left(-\frac{1}{2}(x-\mu_1)^\top \Sigma^{-1}(x-\mu_1)\right)}{\sum_{j=0,1} \pi_j \frac{1}{(2\pi|\Sigma|)^{p/2}} \exp\left(-\frac{1}{2}(x-\mu_j)^\top \Sigma^{-1}(x-\mu_j)\right)} \\
&= (\text{take logs}) \\
&= \dots \\
&= x^\top \Sigma^{-1}\mu_1 - \frac{1}{2}\mu_1^\top \Sigma^{-1}\mu_1 + \log \pi_1 \\
&=: \delta_1
\end{aligned}$$

- If this is bigger than δ_0, we predict $\ddagger$ else θ.

Why is this linear?

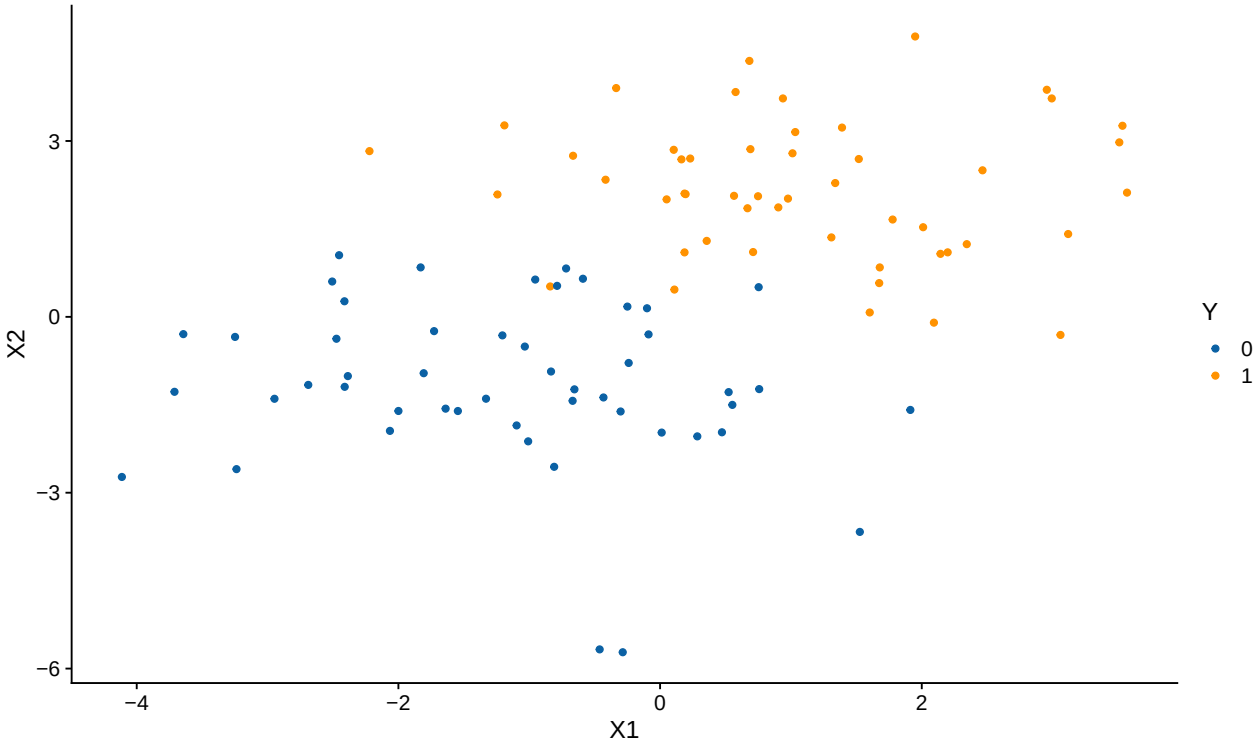
- We are indifferent when $\delta_1 = \delta_0$

$$\begin{aligned}
&\delta_1 = \delta_0 \\
&\Rightarrow x^\top \Sigma^{-1}\mu_1 - \frac{1}{2}\mu_1^\top \Sigma^{-1}\mu_1 + \log \pi_1 = x^\top \Sigma^{-1}\mu_0 - \frac{1}{2}\mu_0^\top \Sigma^{-1}\mu_0 + \log \pi_0 \\
&\Rightarrow x^\top \Sigma^{-1}(\mu_1 - \mu_0) - \frac{1}{2}\left(\mu_1^\top \Sigma^{-1}\mu_1 - \mu_0^\top \Sigma^{-1}\mu_0\right) + \log \pi_1 - \log \pi_0 = 0
\end{aligned}$$

- The slope is $(\mu_1 - \mu_0)^\top \Sigma^{-1}$
- The intercept is $-\frac{1}{2}\left(\mu_0^\top \Sigma^{-1}\mu_0 - \mu_1^\top \Sigma^{-1}\mu_1\right) + \log \pi_1 - \log \pi_0$

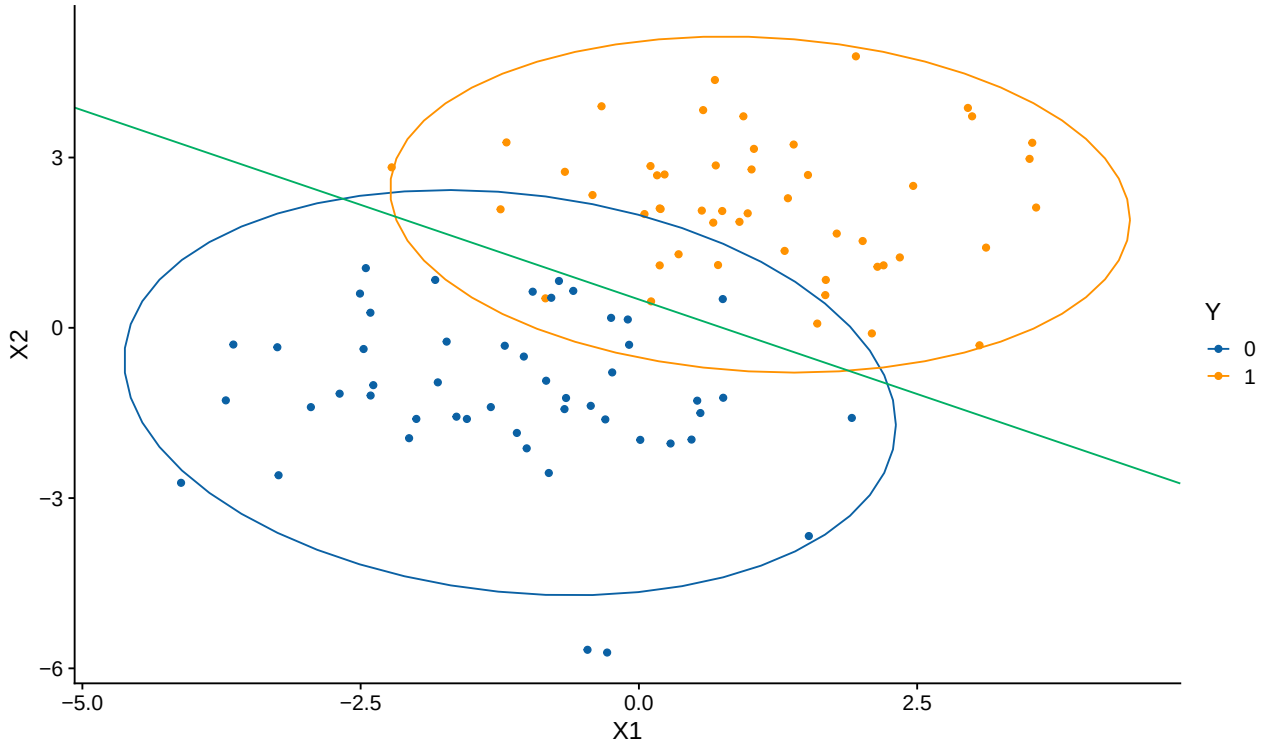
Example

```
library(mvtnorm)
lda_gen <- function(n1, n0=n1, mu1=0, mu0=m1, Sigma=2*diag(2)){
  plist = list(n1=n1,n0=n0,pi1=n1/(n0+n1),mu1=mu1,mu0=mu0,Sigma=Sigma)
  X1 = rmvnorm(n1, mu1, Sigma)
  X2 = rmvnorm(n0, mu0, Sigma)
  X = rbind(X1,X2)
  Y = factor(c(rep(1,n1),rep(0,n0)))
  df = data.frame(Y,X)
  Sinv = solve(Sigma)
  b = t(mu1-mu0) %*% Sinv
  b0 = 0.5*(t(mu0) %*% Sinv %*% mu0 - t(mu1) %*% Sinv %*% mu1) +
    log(plist$pi1) - log(1-plist$pi1)
  return(
    list(df=df, plist=plist,
         slint=tibble(slope=-b[1]/b[2], int=-b0/b[2]))
         )
}
dat = lda_gen(50, mu1=c(1,2), mu0=c(-1,-1))
g <- ggplot(dat$df, aes(X1,X2,color=Y)) + geom_point() +
  scale_color_manual(values=c(blue,orange)) + theme_cowplot(14)
g
```



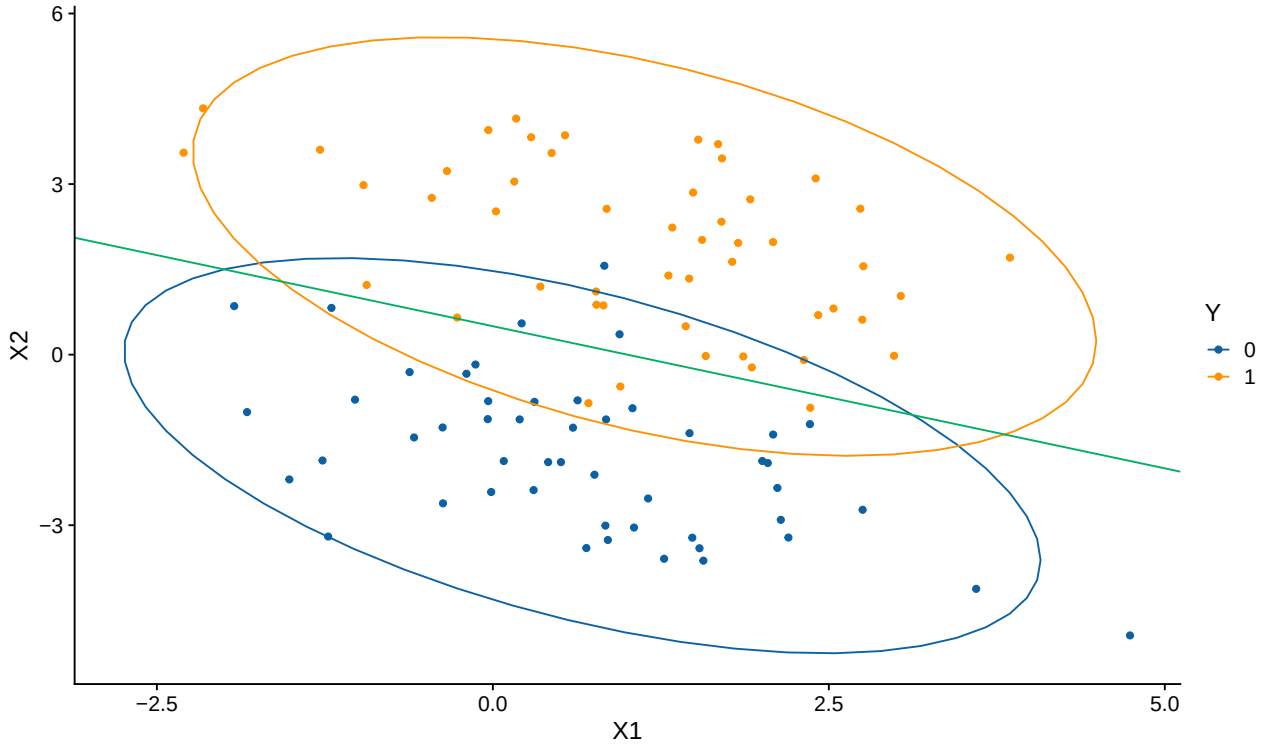
The distributions and the classifier

```
g + stat_ellipse(type='norm') + # these are estimated, not the truth
  geom_abline(data = dat$slint, aes(intercept = int, slope = slope), color=green)
```



Try another one

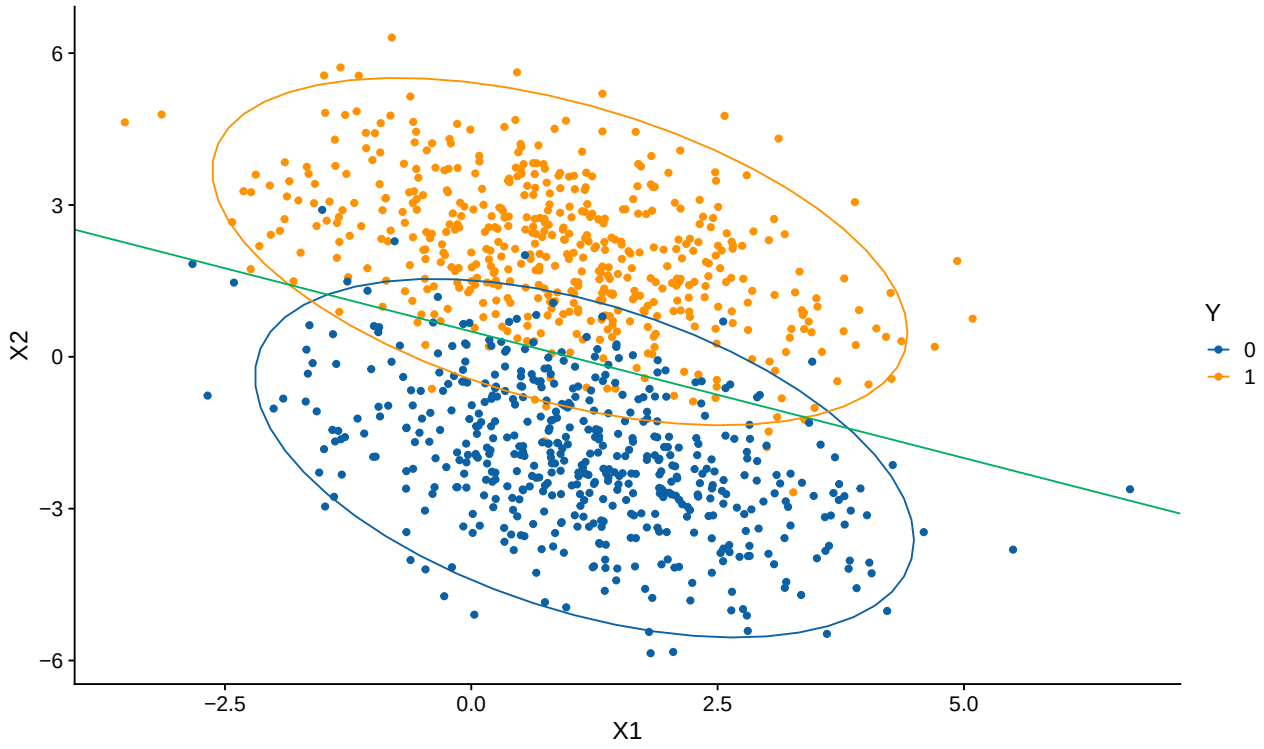
```
dat = lda_gen(50, mu1=c(1,2), mu0=c(1,-2), Sigma=2*matrix(c(1,-.5,-.5,1),2))
ggplot(dat$df, aes(X1,X2,color=Y)) + geom_point() +
  scale_color_manual(values=c(blue,orange)) +
  stat_ellipse(type='norm') + theme_cowplot(14) +
  geom_abline(data = dat$slint, aes(intercept = int, slope = slope), color=green)
```



- Note: here there is a single Σ, but I don't know how to plot ellipses in `ggplot`. So these are estimated.

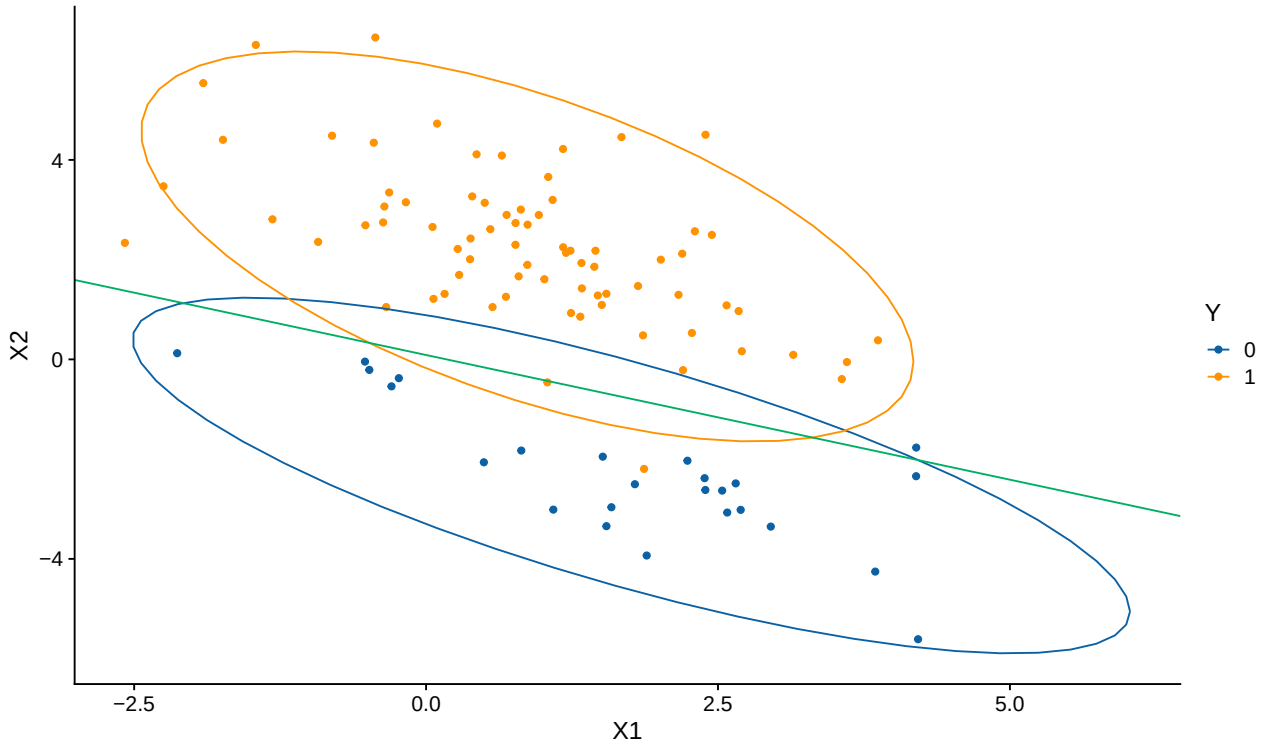
Same one, but make n big

```
dat = lda_gen(500, mu1=c(1,2), mu0=c(1,-2), Sigma=2*matrix(c(1,-.5,-.5,1),2))
ggplot(dat$df, aes(X1,X2,color=Y)) + geom_point() +
  scale_color_manual(values=c(blue,orange)) +
  stat_ellipse(type='norm') + theme_cowplot() +
  geom_abline(data = dat$slint, aes(intercept = int, slope = slope), color=green)
```



Same one, but change P(Y=1)

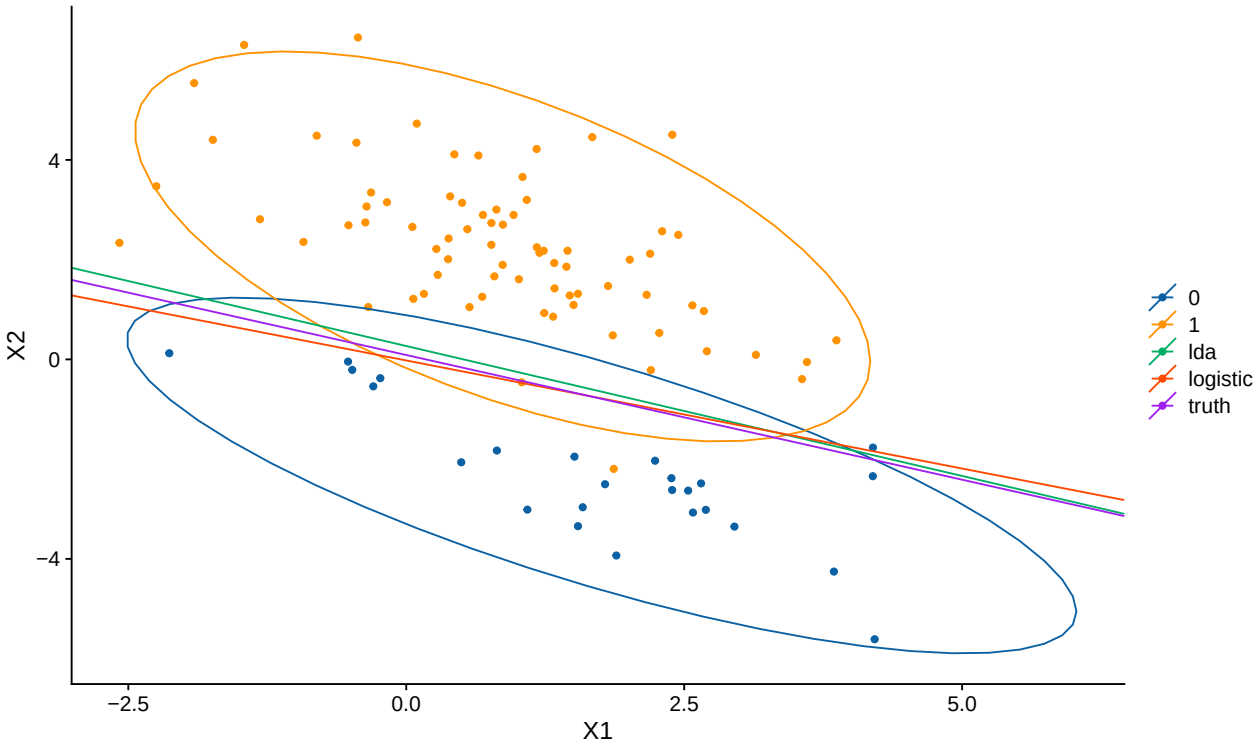
```
dat = lda_gen(n1=75,n0=25, mu1=c(1,2), mu0=c(1,-2), Sigma=2*matrix(c(1,-.5,-.5,1),2))
ggplot(dat$df, aes(X1,X2,color=Y)) + geom_point() +
  scale_color_manual(values=c(blue,orange)) +
  stat_ellipse(type='norm') + theme_cowplot() +
  geom_abline(data = dat$slint, aes(intercept = int, slope = slope), color=green)
```



Ok, how do you do it?

- Estimate everything with sample analogues
- $\widehat{\pi}_1 = n_1/(n_1 + n_0)$
- $\widehat{\mu}_1 = \frac{1}{n_1} \sum X_i I(Y_i = 1)$. Same for $\widehat{\mu}_0$.
- $\widehat{\Sigma} = \frac{1}{n} \sum_{ij} I(Y_i = j)(X_i - \widehat{\mu}_j)^\top (X_i - \widehat{\mu}_j)$

```
library(MASS)
lda.fit = lda(Y~X1+X2, data=dat$df)
sl.int = lda.disc(lda.fit,dat$df)
log.bd = decision.boundary(dat$df)
truth = data.frame(intercept=dat$slint$int, slope=dat$slint$slope)
dfa = bind_rows(sl.int,log.bd,truth)
dfa$discriminant = c('lda','logistic','truth')
ggplot(dat$df, aes(X1,X2,color=Y)) + geom_point() +
  stat_ellipse(type='norm') + theme_cowplot() +
  scale_color_manual(values=c(blue,orange,green,red,"purple")) +
  geom_abline(mapping=aes(intercept=intercept, slope=slope,color=discriminant),data=dfa) +
  theme(legend.title = element_blank())
```



Comparing LDA and Logistic regression

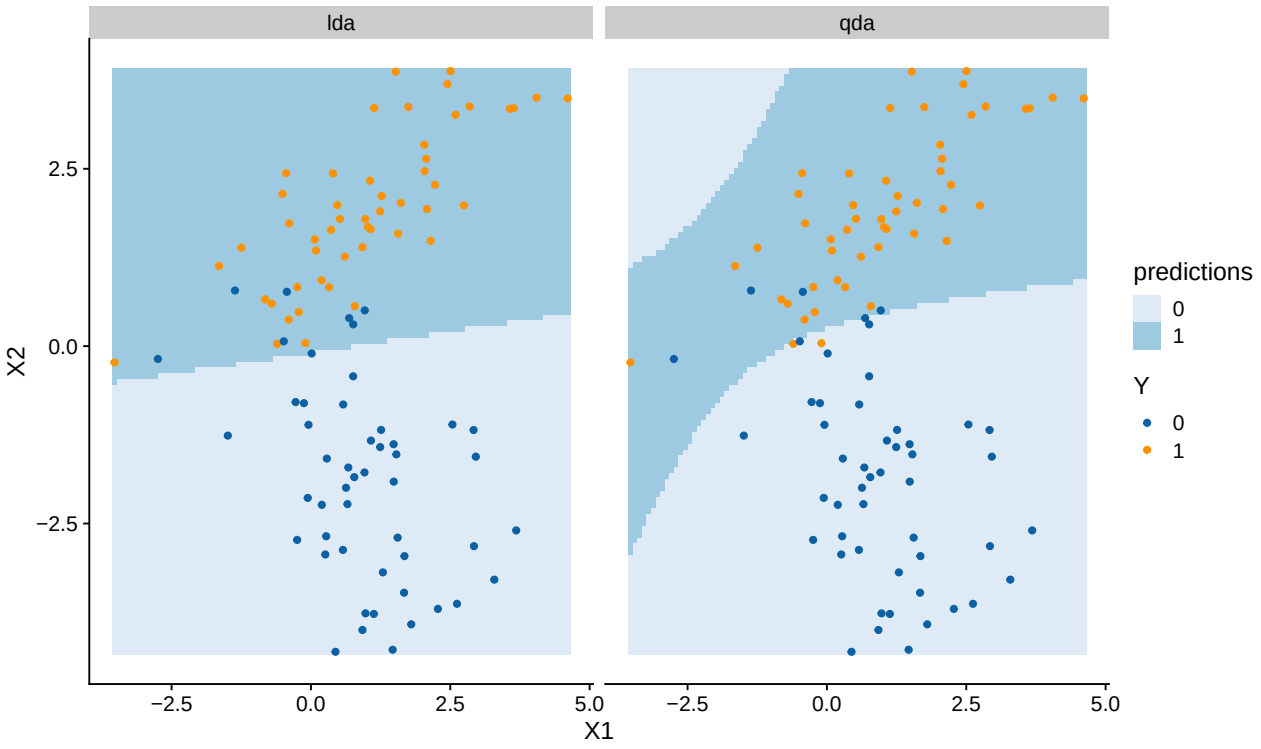
- Both are linear in x:
  - LDA$\longrightarrow \alpha_0 + \alpha_1^\top x$
  - Logit$\longrightarrow \beta_0 + \beta_1^\top x$.
- But the parameters are estimated differently.
- Examine the joint distribution of (X, y):
  - LDA $\prod_i f(x_i, y_i) = \underbrace{\prod_i f(X_i|y_i)}_{\text{Gaussian}} \underbrace{\prod_i f(y_i)}_{\text{Bernoulli}}$
  - Logistic $\prod_i f(x_i, y_i) = \underbrace{\prod_i f(y_i|X_i)}_{\text{Logistic}} \underbrace{\prod_i f(X_i)}_{\text{Ignored}}$
- LDA estimates the joint, but Logistic estimates only the conditional distribution. But this is really all we need.
- So logistic requires fewer assumptions.
- But if the two classes are perfectly separable, logistic crashes (and the MLE is undefined)
- LDA works even if the conditional isn't normal, but works poorly if any X is qualitative

QDA

- Start like LDA, but let $\Sigma_1 \neq \Sigma_0$.
- This gives a "quadratic" decision boundary (it's a curve).

- If we have many columns in X (p)
  - Logistic estimates $p+1$ parameters
  - LDA estimates $2p + p(p+1)/2 + 1$
  - QDA estimates $2p + p(p+1) + 1$
- If $p = 50$,
  - Logistic: 51
  - LDA: 1376
  - QDA: 2651
- QDA doesn't get used much: there are better nonlinear versions with way "fewer" parameters (SVMs)
- LDA only really depends on $\Sigma^{-1}(\mu_1 - \mu_0)$ and $(\mu_1 + \mu_0)$, so it has $< 2p$ parameters.

```
n1=50; n0=50
Sigma1 = matrix(c(2,.8,.8,1),2)
Sigma0 = matrix(c(1,-.5,-.5,2),2)
X1 = rmvnorm(n1, dat$plist$mu1, Sigma1)
X2 = rmvnorm(n0, dat$plist$mu0, Sigma0)
X = rbind(X1,X2)
Y = factor(c(rep(1,n1),rep(0,n0)))
df = data.frame(Y,X)
qda.fit = qda(Y~X1+X2, data=df)
lda.fit = lda(Y~X1+X2, data=df)
pred.grid = expand.grid(X1=seq(min(df$X1),max(df$X1),len=100),
                        X2=seq(min(df$X2),max(df$X2),len=100))
pred.grid$qda = predict(qda.fit, newdata=pred.grid)$class
pred.grid$lda = predict(lda.fit, newdata=pred.grid)$class
pg = pivot_longer(pred.grid,names_to ='key',values_to ='predictions',-c(X1,X2))
ggplot(pg, aes(X1,X2)) + geom_raster(aes(fill=predictions)) +
  facet_wrap(~key) + scale_fill_brewer()+
  geom_point(data=df,mapping=aes(X1,X2,color=Y)) +
  scale_color_manual(values=c(blue,orange)) + theme_cowplot(14)
```

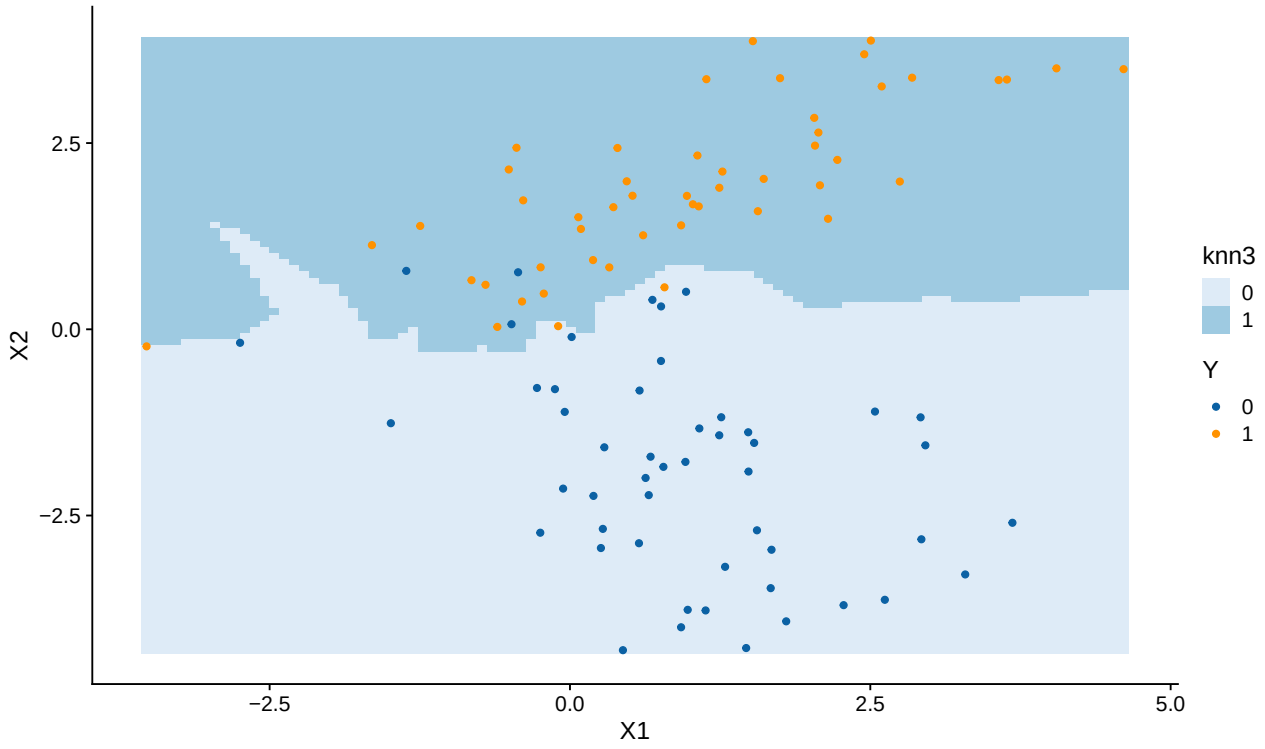


KNN

Re-entry

- We saw k-nearest neighbors at the very beginning of the course.

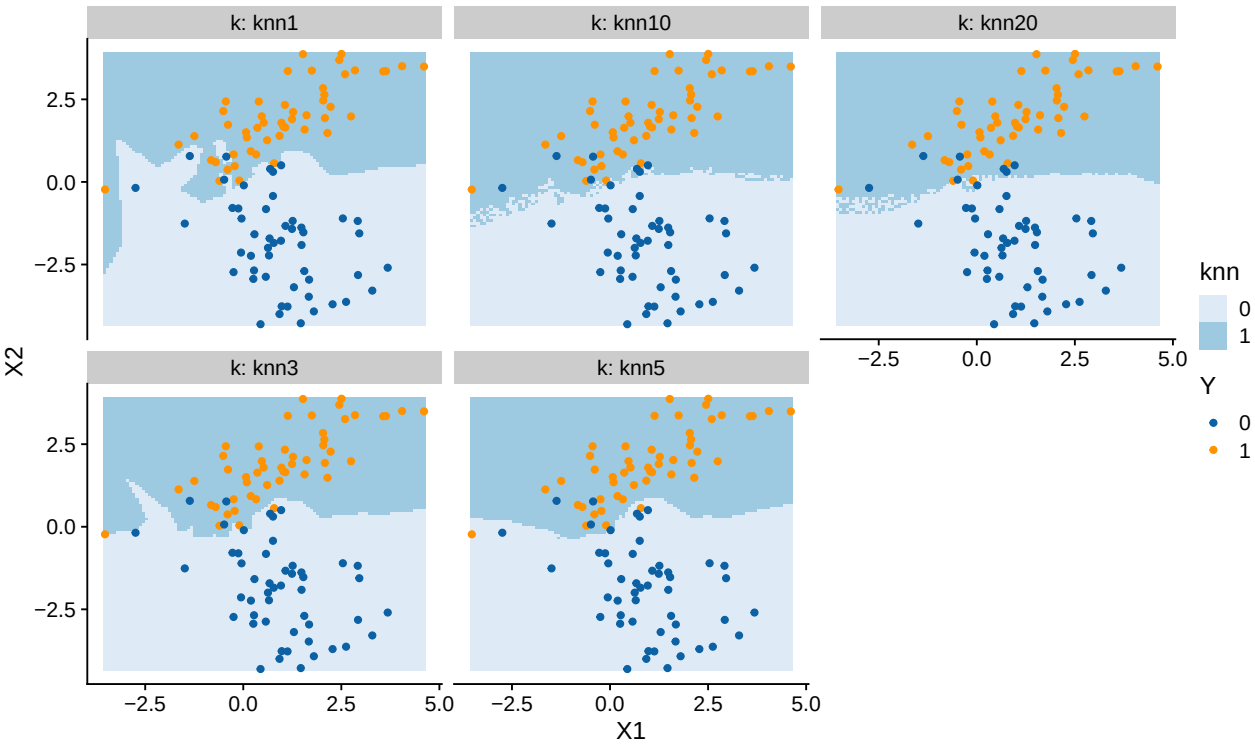
```
library(class)
pred.grid = expand.grid(X1=seq(min(df$X1),max(df$X1),len=100),
                        X2=seq(min(df$X2),max(df$X2),len=100))
pred.grid$knn3 = knn(df[,-1], pred.grid, df$Y, k=3)
ggplot(pred.grid, aes(X1,X2)) + geom_raster(aes(fill=knn3)) +
  scale_fill_brewer() + geom_point(data=df,mapping=aes(X1,X2,color=Y)) +
  scale_color_manual(values=c(blue,orange)) + theme_cowplot(14)
```



Choosing k

- Choosing k is very important.

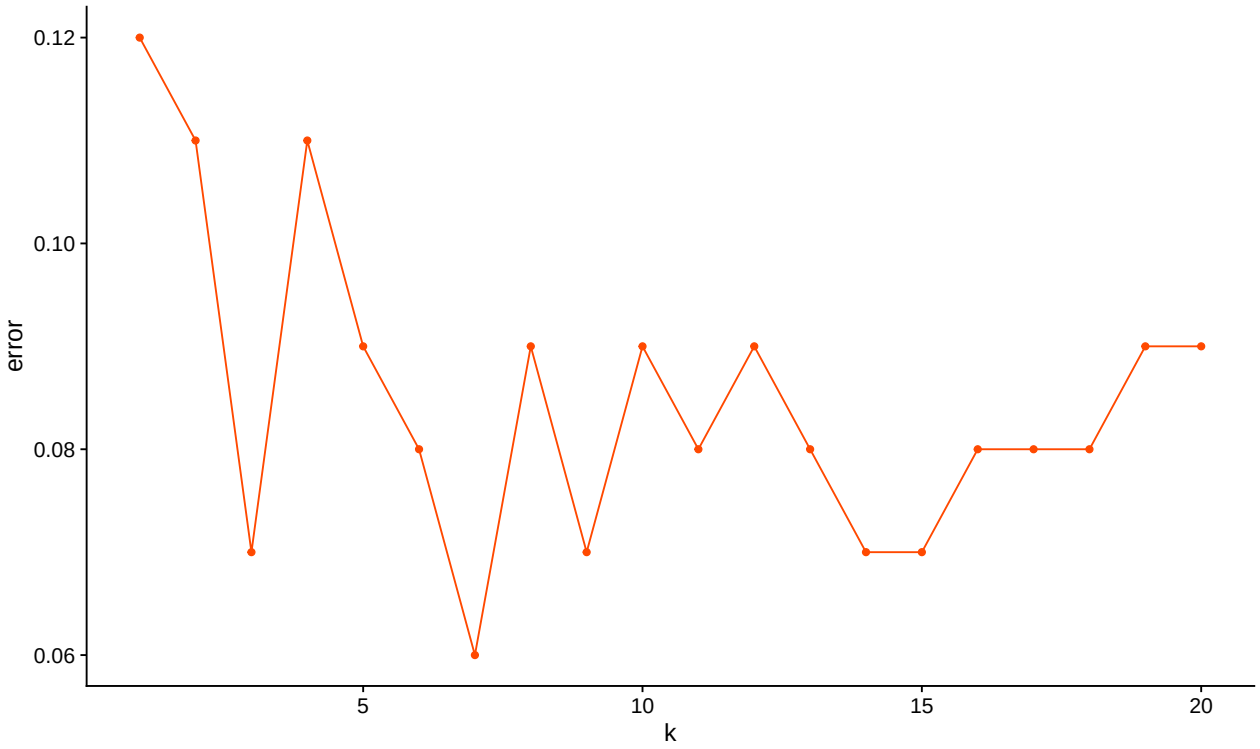
```
pred.grid$knn1 = knn(df[,-1], pred.grid[,1:2], df$Y, k=1)
pred.grid$knn5 = knn(df[,-1], pred.grid[,1:2], df$Y, k=5)
pred.grid$knn10 = knn(df[,-1], pred.grid[,1:2], df$Y, k=10)
pred.grid$knn20 = knn(df[,-1], pred.grid[,1:2], df$Y, k=20)
pg = pivot_longer(pred.grid, names_to='k',values_to = 'knn',-c(X1,X2))

ggplot(pg, aes(X1,X2)) + geom_raster(aes(fill=knn)) +
  facet_wrap(~k,labeller = label_both) + scale_fill_brewer()+
  geom_point(data=df,mapping=aes(X1,X2,color=Y)) +
  scale_color_manual(values=c(blue,orange)) + theme_cowplot(14)
```



- How should we choose k?
- Scaling is also very important. The nearest neighbors are determined by their distance, so better to standardize your data first.

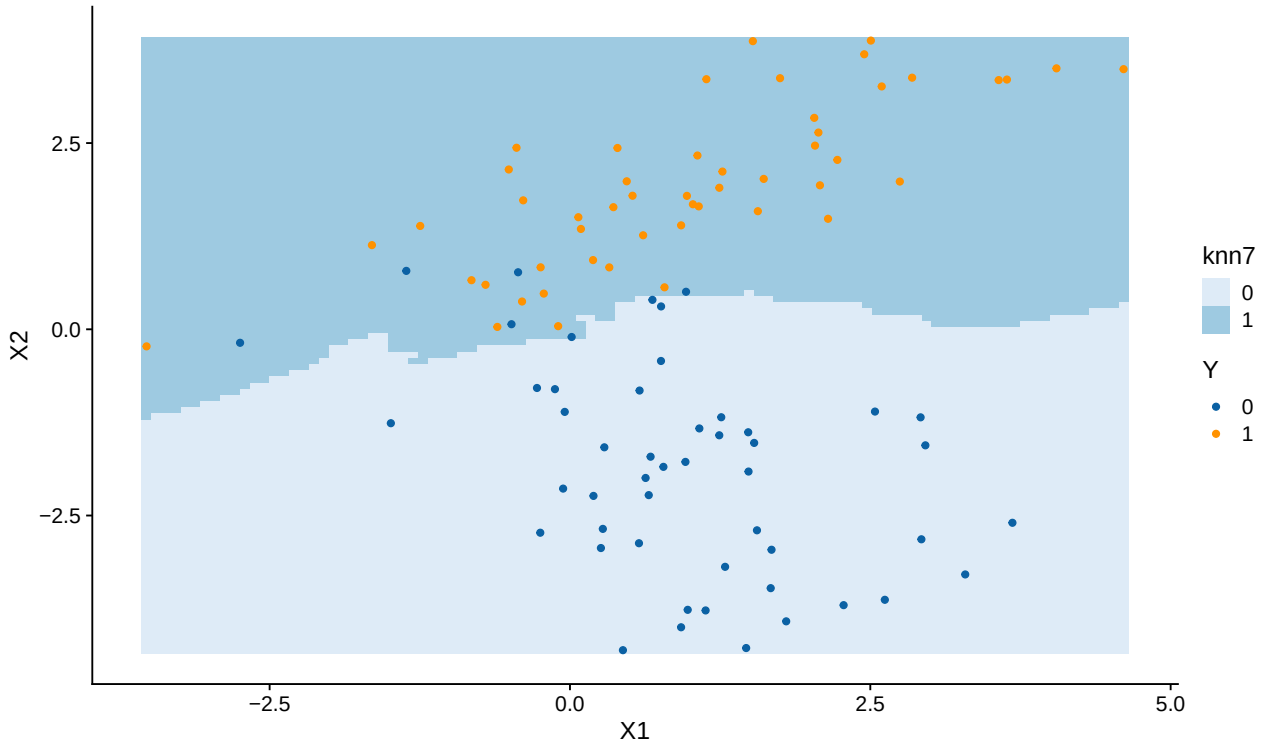
knn.cv

```
kmax = 20
err = double(kmax)
for(ii in 1:kmax){
  pk = knn.cv(df[,-1],df$Y, k=ii) # does leave one out CV
  err[ii] = mean(pk != df$Y)
}
ggplot(data.frame(k=1:kmax,error=err), aes(k,error)) + geom_point(color=red) +
  geom_line(color=red) + theme_cowplot(14)
```



- I would use the ~~largest~~ k that is close to the minimum. This produces simpler, smoother, decision boundaries.

```
pred.grid$knn7 = knn(df[,-1], pred.grid[,1:2], df$Y, k=7)
ggplot(pred.grid, aes(X1,X2)) + geom_raster(aes(fill=knn7)) +
  scale_fill_brewer() + geom_point(data=df,mapping=aes(X1,X2,color=Y)) +
  scale_color_manual(values=c(blue,orange)) + theme_cowplot(14)
```




```
(tt <- table(knn(df[,-1],df[,-1],df$Y,k=7),df$Y,dnn=c('predicted','truth')))
```

```
##           truth
## predicted  0  1
##         0 44  0
##         1  6 50
```

```
1-sum(diag(tt))/sum(tt) # misclassification rate
```

```
## [1] 0.06
```

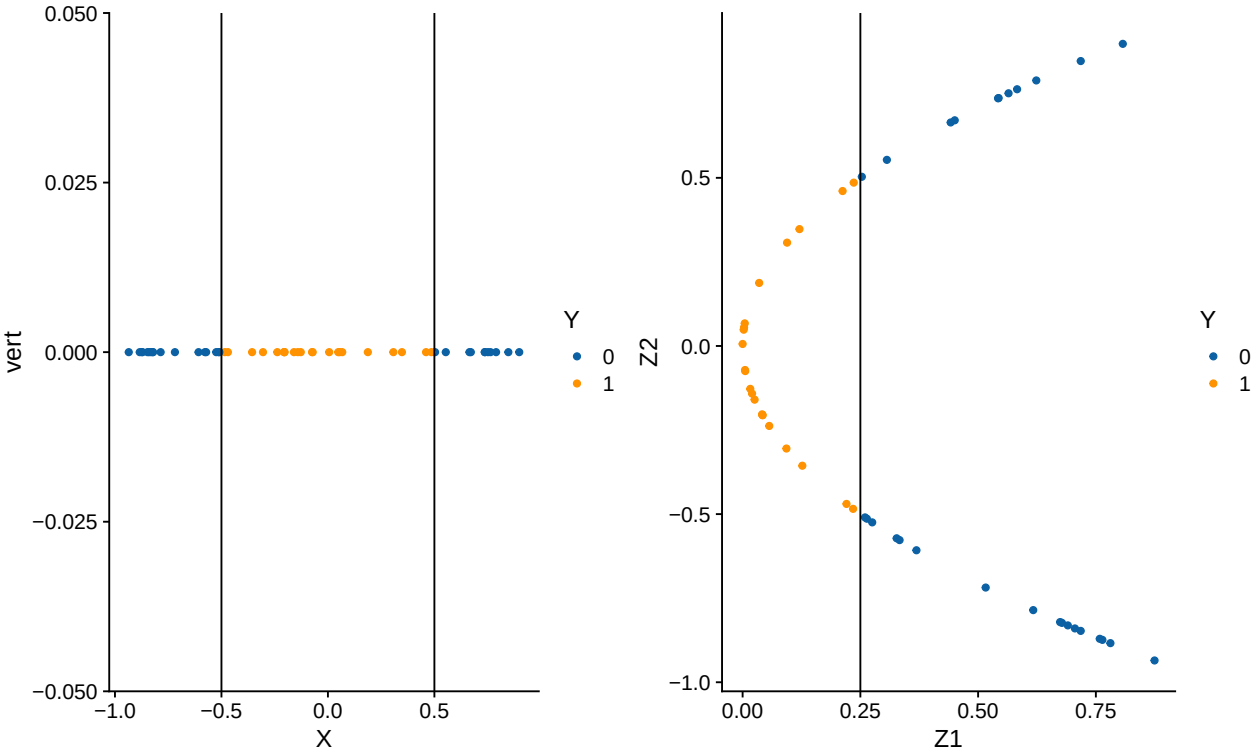
Kernelization

Other non-linear classifiers

- We already saw that knn produces non-linear decision boundaries.
- Next week, we'll see trees, which are also non-linear.
- "Kernelization" is a way of turning linear classifiers (or linear regression) into non-linear classifiers.
- You've already seen this happen when you add interactions or quadratic terms to linear models

The idea

- Suppose X_i takes values in some space $\mathcal{X}$.
- Find a mapping $\phi : \mathcal{X} \to \mathcal{Z}$.
- Apply a linear classifier on $\mathcal{Z}$.
- Example: $\mathcal{X} = \mathbb{R}$, $\mathcal{Z} = \mathbb{R}^2$, $\phi(x) = (z_1, z_2) = (x, x^2)$



- A linear classifier in the higher-dimensional space corresponds to a non-linear classifier in low dimensions.
- Of course, if $\dim(\mathcal{Z})$ is too big, then there will be too many parameters to estimate well.

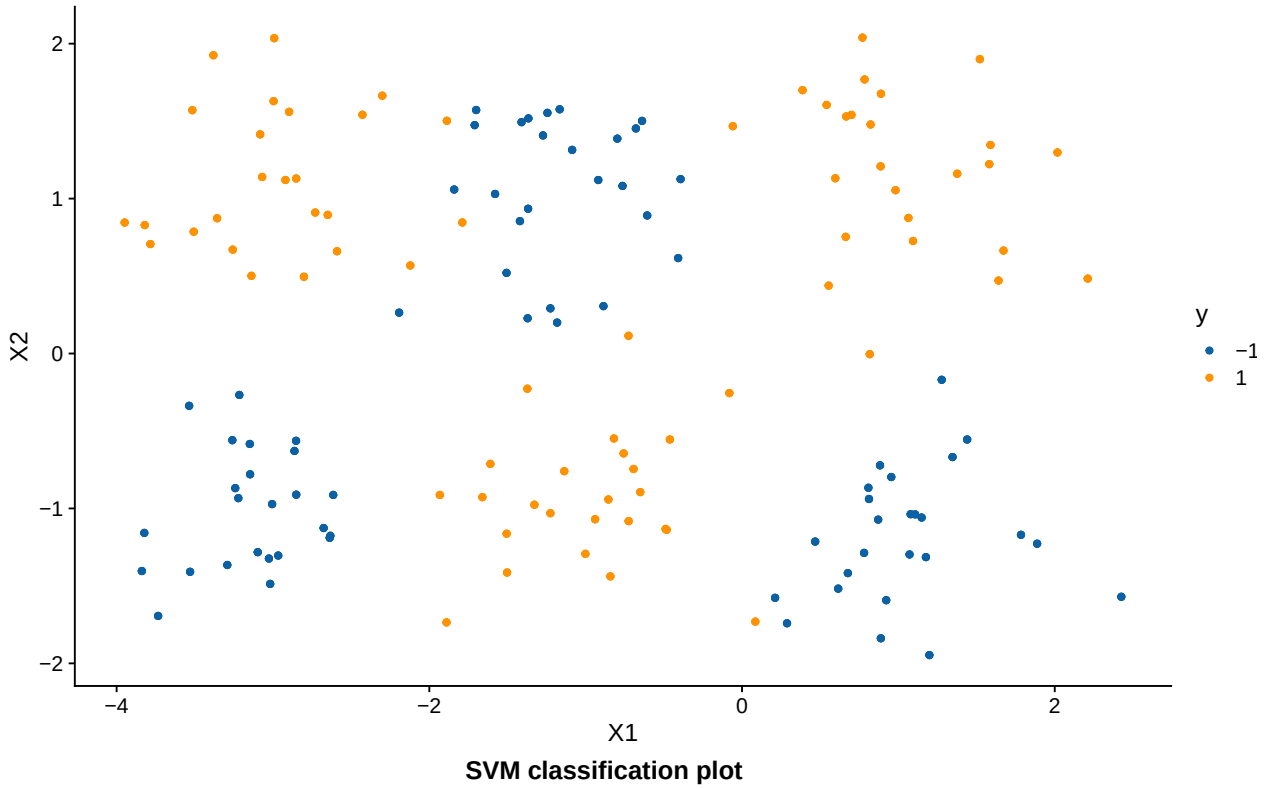
The trick

If:

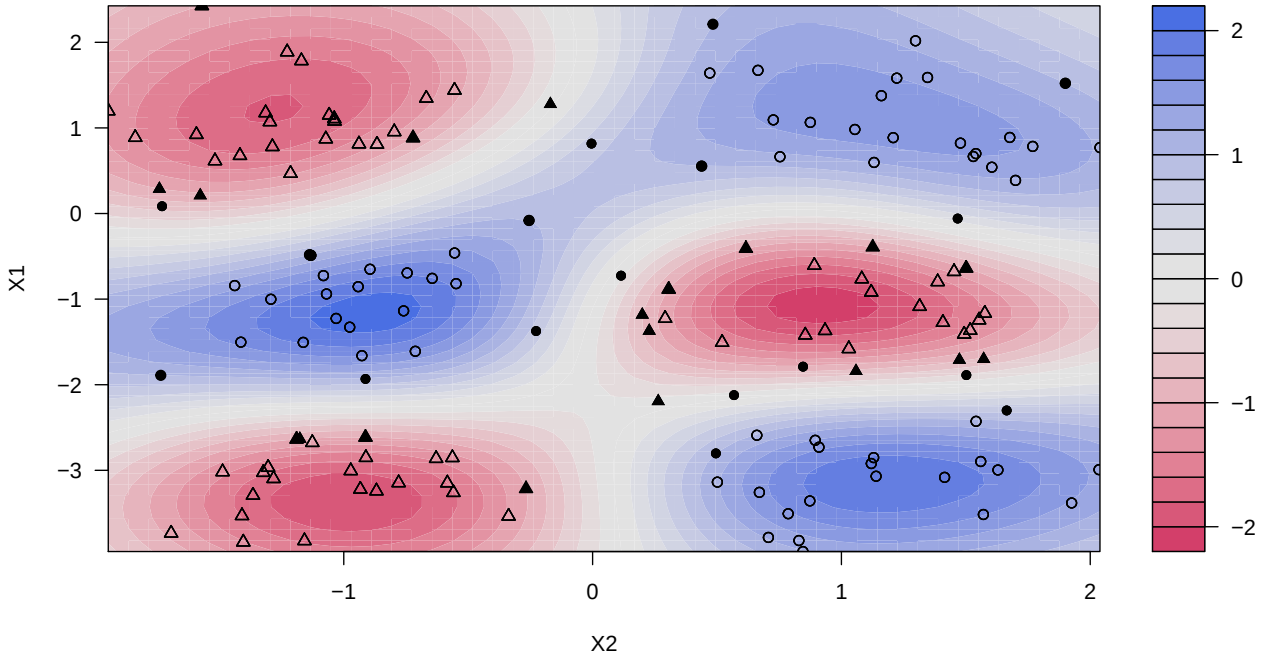
1. There is a mapping $\phi : \mathcal{X} \to \mathcal{Z}$
2. Your classifiers of choice only needs the ~~inner product~~ between observations, not the observations themselves. (logistic regression, LDA, and SVMs work)
3. There is a function K such that $K(x, x') = \langle \phi(x), \phi(x') \rangle$ (Mercer's theorem gives this)

Then, we can just replace all inner products $\langle x, x' \rangle$ with $K(x, x')$.

- This produces a nonlinear classifier based on a linear classifier.
- We don't actually need x or ϕ, just $K(x, x')$ (this is an $n \times n$ matrix)
- $\mathcal{Z}$ can be infinite dimensional.



SVM classification plot



Here, filled in triangles/circles are called “support vectors”, they are the points that determine the boundary.