Lecture 8: Discriminant Analysis, PCA, and Dealing with Missingness

S-109A Introduction to Data Science

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Lecture Outline

- Discriminant Analysis
  - LDA for one predictor
  - LDA for $p > 1$
  - QDA
- Comparison of Classification Methods (so far)
- High Dimensionality and PCA
- Dealing with Missingness

Recall the Heart Data (for classification)

response variable ***Y*** is Yes/No

Age	Sex	ChestPain	RestBP	Chol	Fbs	RestECG	MaxHR	ExAng	Oldpeak	Slope	Ca	Thal	AHD
63	1	typical	145	233	1	2	150	0	2.3	3	0.0	fixed	No
67	1	asymptomatic	160	286	0	2	108	1	1.5	2	3.0	normal	Yes
67	1	asymptomatic	120	229	0	2	129	1	2.6	2	2.0	reversable	Yes
37	1	nonanginal	130	250	0	0	187	0	3.5	3	0.0	normal	No
41	0	nontypical	130	204	0	2	172	0	1.4	1	0.0	normal	No

Discriminant Analysis for Classification

Linear Discriminant Analysis (LDA)

Linear discriminant analaysis (LDA) takes a different approach to classification than logistic regression. Rather than attempting to model the conditional distribution of Y given X, $P(Y = k|X = x)$, LDA models the distribution of the predictors X given the different categories that Y takes on, $P(X = x|Y = k)$.

In order to flip these distributions around to model $P(X = x|Y = k)$ an analyst uses Bayes' theorem.

In this setting with one feature (one X), Bayes' theorem can then be written as:

$$P(Y = k|X = x) = \frac{f_k(x)\pi_k}{\sum_{j=1}^{K} f_j(x)\pi_j}$$

What does this mean?

LDA (cont.)

$$P(Y = k|X = x) = \frac{f_k(x)\pi_k}{\sum_{j=1}^{K} f_j(x)\pi_j}$$

The left hand side, $P(Y = k|X = x)$, is called the *posterior* probability and gives the probability that the observation is in the kth category given the feature, X, takes on a specific value, x. The numerator on the right is conditional distribution of the feature within category k, $f_k(x)$, times the *prior* probability that observation is in the kth category.

The *Bayes' classifier* is then selected. That is the observation assigned to the group for which the posterior probability is the largest.

Inventor of LDA: R.A. Fisher

The 'Father' of Statistics. More famous for work in genetics (statistically concluded that Mendel's genetic experiments were 'massaged').

Novel statistical work includes:

- Experimental Design
- ANOVA
- *F*-test (why do you think it's called the *F*-test?)
- Exact test for 2 x 2 tables
- Maximum Likelihood Theory
- Use of α = 0.05 significance level: “The value for which P = .05, or 1 in 20, is 1.96 or nearly 2; it is convenient to take this point as a limit in judging whether a deviation is to be considered significant or not”.
- And so much more...

LDA for one predictor

LDA has the simplest form when there is just one predictor/feature (p = 1). In order to estimate $f_k(x)$, we have to assume it comes from a specific distribution. If X is quantitative, what distribution do you think we should use?

One common assumption is that $f_k(x)$ comes from a Normal distribution:

$$f_k(x) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$$

In shorthand notation, this is often written as $(X|Y=k) \sim N(\mu_k, \sigma_k^2)$, meaning, the distribution of the feature X within category k is Normally distributed with mean μ_k and variance σ_k^2.

LDA for one predictor (cont.)

An extra assumption that the variances are equal,

$\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_K^2$ will simplify are lives.

Plugging this assumed likelihood into the Bayes' formula (to get the posterior) results in:

$$P(Y = k|X = x) = \frac{\pi_k \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma^2}\right)}{\sum_{j=1}^{K} \pi_j \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu_j)^2}{2\sigma^2}\right)}$$

The Bayes classifier will be the one that maximizes this over all values chosen for *x*. How should we maximize?

So we take the log of this expression and rearrange to simplify our maximization...

LDA for one predictor (cont.)

So we maximize the following simplified expression:

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

How does this simplify if we have just two classes (*K = 2*) and if we set our prior probabilities to be equal?

This is equivalent to choosing a decision boundary for *x* for which

$$x = \frac{\mu_1^2 - \mu_2^2}{2(\mu_1 - \mu_2)} = \frac{\mu_1 + \mu_2}{2}$$

Intuitively, why does this expression make sense? What do we use in practice?

LDA for one predictor (cont.)

In practice we don't know the true mean, variance, and prior. So we estimate them with the classical estimates, and plug-them into the expression:

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$$

and

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$$

where n is the total sample size and n_k is the sample size within class k (thus, $n = \sum n_k$).

LDA for one predictor (cont.)

This classifier works great if the classes are about equal in proportion, but can easily be extended to unequal class sizes.

Instead of assuming all priors are equal, we instead set the priors to match the 'prevalence' in the data set:

$$\hat{\pi}_k = \hat{n}_k / n$$

Note: we can use a prior probability from knowledge of the subject as well; for example, if we expect the test set to have a different prevalence than the training set.

How could we do this in the Dem. vs. Rep. data set?

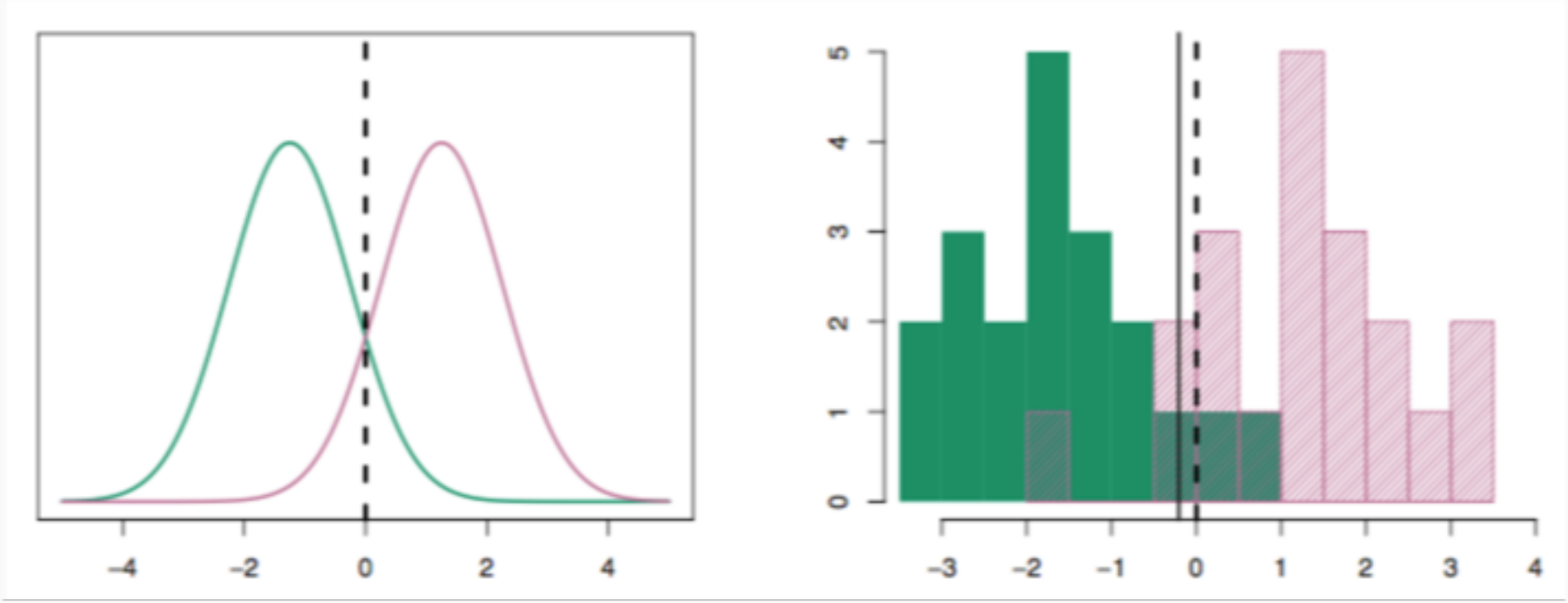
LDA for one predictor (cont.)

Plugging all of these estimates back into the original logged maximization formula we get:

$$\hat{\delta}_k(x) = x\frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log \hat{\pi}_k$$

Thus this classifier is called the linear discriminant classifier: this discriminant function is a linear function of *x*.

Illustration of LDA when $p = 1$



LDA when $p > 1$

LDA when $p > 1$

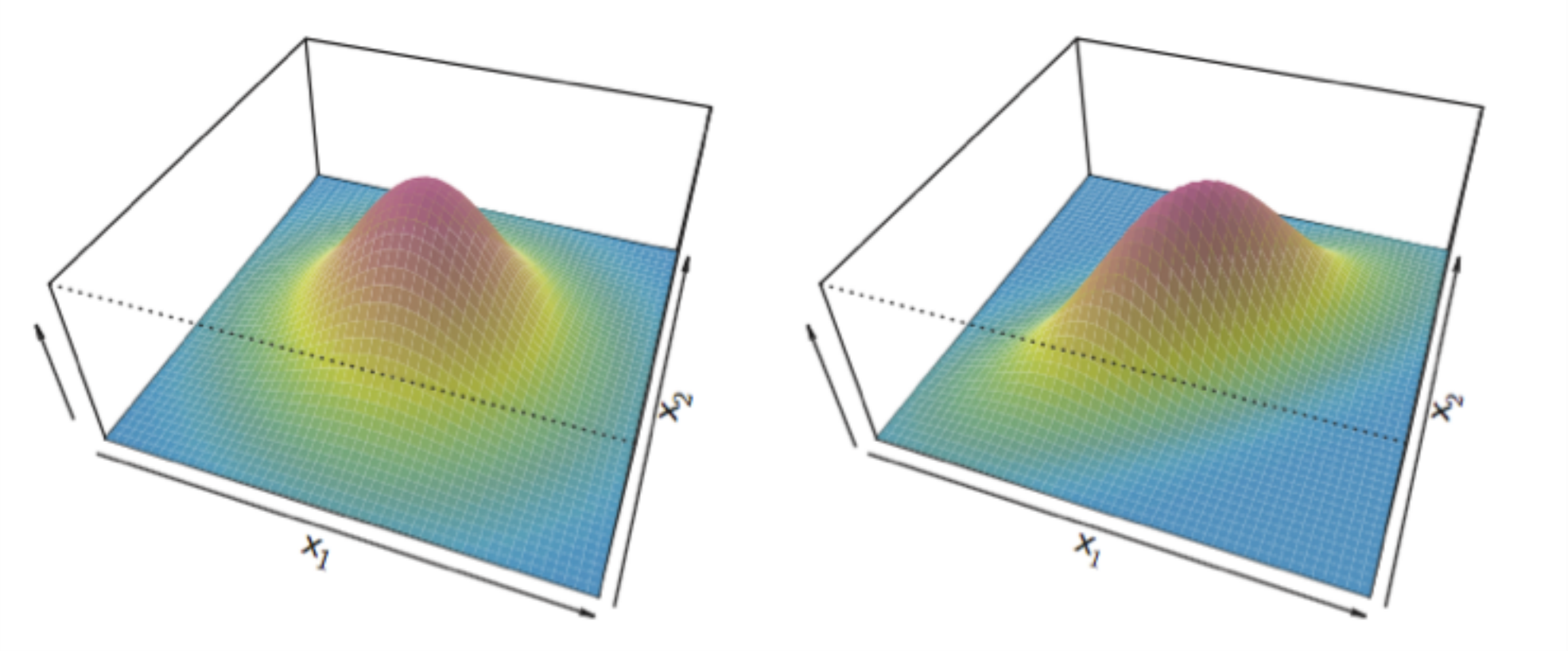
LDA generalizes 'nicely' to the case when there is more than one predictor.

Instead of assuming the one predictor is Normally distributed, it assumes that the set of predictors for each class is 'multivariate normal distributed' (shorthand: MVN). What does that mean? \pause

This means that the vector of X for an observation has a multidimensional normal distribution with a mean vector, μ, and a covariance matrix, $\mathbf{\Sigma}$.

Multivariate Normal Distribution

Here is a visualization of the Multivariate Normal distribution with 2 variables:



MVN Distribution

The joint PDF of the Multivariate Normal distribution, $\vec{X} \sim MVN(\vec{\mu}, \Sigma)$, is:

$$f(\vec{x}) = \frac{1}{2\pi^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T\Sigma^{-1}(\vec{x}-\vec{\mu})\right)$$

where $\vec{X}$ is a *p* dimensional vector and $|\Sigma|$ is the determinant of the *p* x *p* covariance matrix.

Let's do a quick dimension analysis sanity check...

What do $\vec{X}$ and Σ look like?

LDA when $p > 1$

Discriminant analysis in the multiple predictor case assumes the set of predictors for each class is then multivariate Normal: $\vec{X} \sim MVN(\vec{\mu}, \Sigma)$

Just like with LDA for one predictor, we make an extra assumption that the covariances are equal in each group, $\Sigma_1 = \Sigma_2 = \cdots = \Sigma_K$. in order to simplify our lives.

Now plugging this assumed likelihood into the Bayes' formula (to get the posterior) results in:

$$P(Y = k|\vec{X} = \vec{x}) = \frac{\pi_k \frac{1}{2\pi^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu}_k)^T \Sigma^{-1} (\vec{x} - \vec{\mu}_k)\right)}{\sum_{j=1}^{K} \frac{1}{2\pi^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu}_j)^T \Sigma^{-1} (\vec{x} - \vec{\mu}_j)\right)}$$

LDA when $p > 1$ (cont.)

Then doing the same steps as before (taking log and maximizing), we see that the classification will for an observation based on its predictors, $\vec{x}$, will be the one that maximizes (maximum of *K* of these $\delta_k(\vec{x})$):

$$\delta_k(\vec{x}) = \vec{x}^T \Sigma^{-1} \vec{\mu}_k - \frac{1}{2} \vec{\mu}_k^T \Sigma^{-1} \vec{\mu}_k + \log \pi_k$$

Note: this is just the vector-matrix version of the formula we saw earlier in lecture:

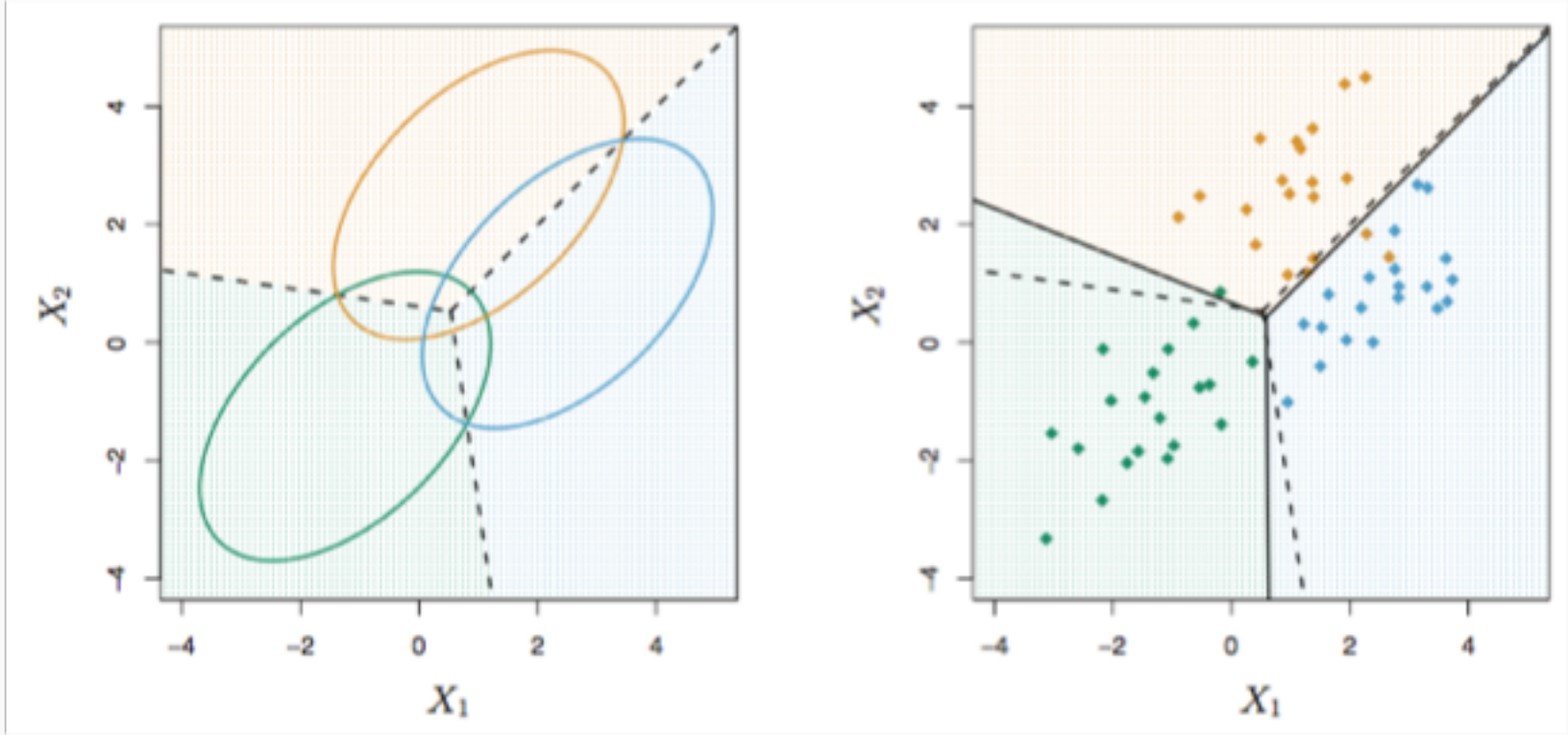
$$\delta_k(x) = x \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log \pi_k$$

What do we have to estimate now with the vector-matrix version? How many parameters are there?

There are *pK* means, *pK* variances, *K* prior proportions, and $\binom{p}{2} = \frac{p(p-1)}{2}$ covariances to estimate.

LDA when $K > 2$

The linear discriminant nature of LDA still holds not only when $p > 1$, but also when $K > 2$ for that matter as well. A picture can be very illustrative:



Quadratic Discriminant Analysis (QDA)

Quadratic Discriminant Analysis (QDA)

A generalization to linear discriminant analysis is quadratic discriminant analysis (QDA).

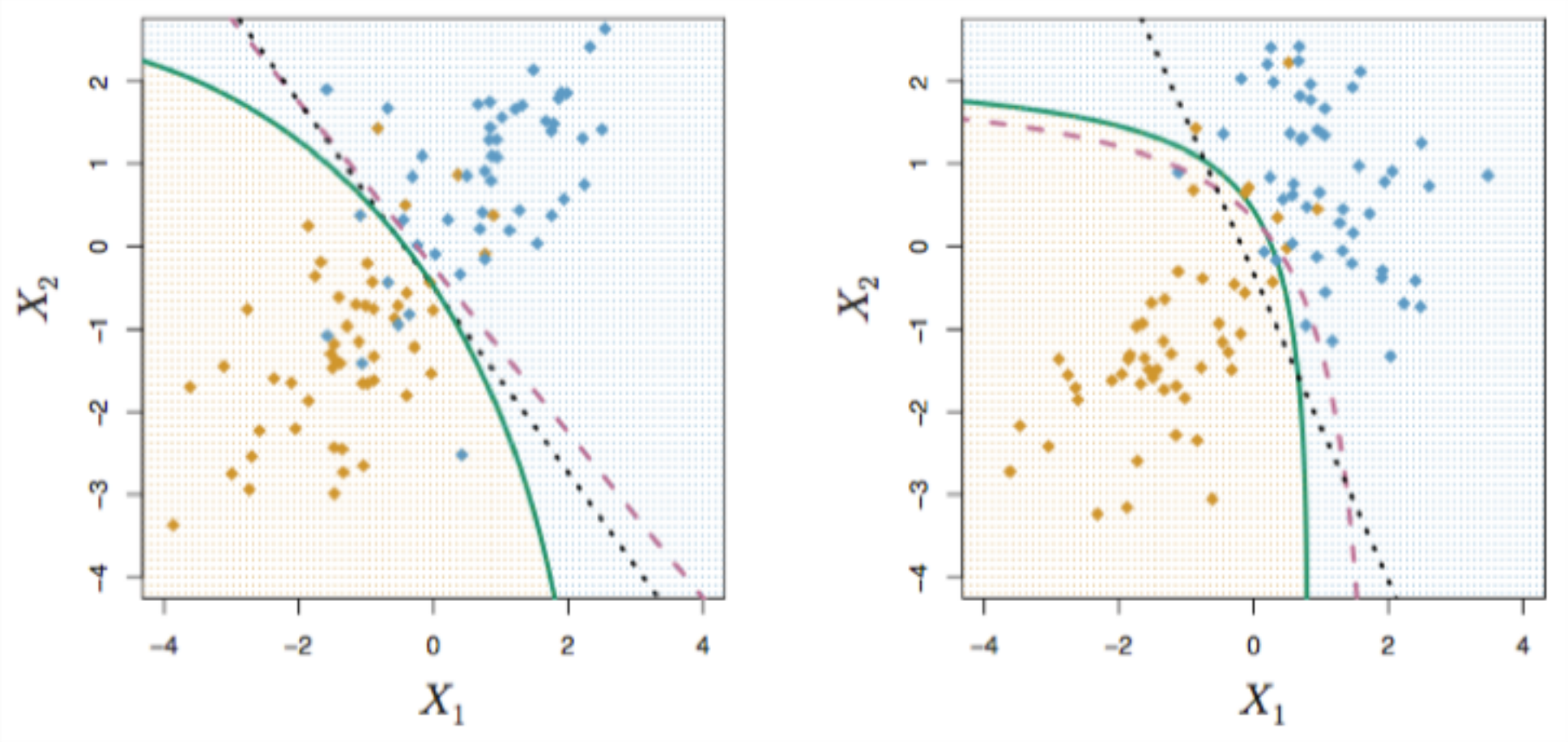
Why do you suppose the choice in name?

The implementation is just a slight variation on LDA. Instead of assuming the covariances of the MVN distributions within classes are equal, we instead allow them to be different.

This relaxation of an assumption completely changes the picture...

QDA in a picture

A picture can be very illustrative:



QDA (cont.)

When performing QDA, performing classification for an observation based on its predictors $\vec{x}$ is equivalent to maximizing the following over the *K* classes:

$$\delta_k(\vec{x}) = -\frac{1}{2}\vec{x}^T\Sigma_k^{-1}\vec{x} + \vec{x}^T\Sigma_k^{-1}\vec{\mu}_k - \frac{1}{2}\vec{\mu}_k^T\Sigma_k^{-1}\vec{\mu}_k - \frac{1}{2}\log|\Sigma_k| + \log\pi_k$$

Notice the `quadratic form' of this expression. Hence the name QDA.

Now how many parameters are there to be estimated?

There are *pK* means, *pK* variances, *K* prior proportions, and $\binom{p}{2}K = \left(\frac{p(p-1)}{2}\right)K$ covariances to estimate. This could slow us down very much if *K* is large...

Discriminant Analysis in Python

LDA is already implemented in Python via the `sklearn.discriminant_analysis` package through the `LinearDiscriminantAnalysis` function.

QDA is in the same package and is the `QuadraticDiscriminantAnalysis` function.

It's very easy to use. Let's see how this works

Discriminant Analysis in Python (cont.)

```
#read in the GSS data
gssdata = pd.read_csv("gsspartyid.csv")
print(gssdata[1:5])
```

```
  politicalparty  income  educ  abortion  republican
1     Republican     906     6         0           1
2       Democrat    1373     6         0           0
3       Democrat    1941     4         0           0
4       Democrat     355     7         0           0
```

```
LDA = da.LinearDiscriminantAnalysis()
X = gssdata[["income","educ","abortion"]]
model_LDA = LDA.fit(X,gssdata['republican'])
print("Specificity is",np.mean(model_LDA.predict(X[gssdata['republican']==0])))
print("Sensitivity is",1-np.mean(model_LDA.predict(X[gssdata['republican']==1])))
print("False positive rate is",np.mean(gssdata['republican'][model_LDA.predict(X)==1]))
print("False negative rate is",1-np.mean(gssdata['republican'][model_LDA.predict(X)==0]))
```

```
Specificity is 0.388387096774
Sensitivity is 0.374060150376
False positive rate is 0.5252365930599369
False negative rate is 0.7043090638930163
```

QDA vs. LDA

So both QDA and LDA take a similar approach to solving this classification problem: they use Bayes' rule to flip the conditional probability statement and assume observations within each class are multivariate Normal (MVN) distributed.

QDA differs in that it does not assume a common covariance across classes for these MVNs. What advantage does this have? What disadvantage does this have?

QDA vs. LDA (cont.)

So generally speaking, when should QDA be used over LDA? LDA over QDA?

The extra covariance parameters that need to be estimated in QDA not only slow us down, but also allow for another opportunity for overfitting. Thus if your training set is small, LDA should perform better for `out-of-sample prediction`, aka, predicting future observations (how do we mimic this process?)

Comparison of Classification Methods (so far)

Quadratic Discriminant Analysis (QDA)

We have seen 3 major methods for doing classification:\pause

- Logistic Regression
- *k*-NN
- Discriminant Analysis (LDA and QDA)

For a specific problem, which approach should be used?

Well of course, it depends on the nature of the data. So how should we decide?

Visualize the data!

Six Classification Models We'll Compare

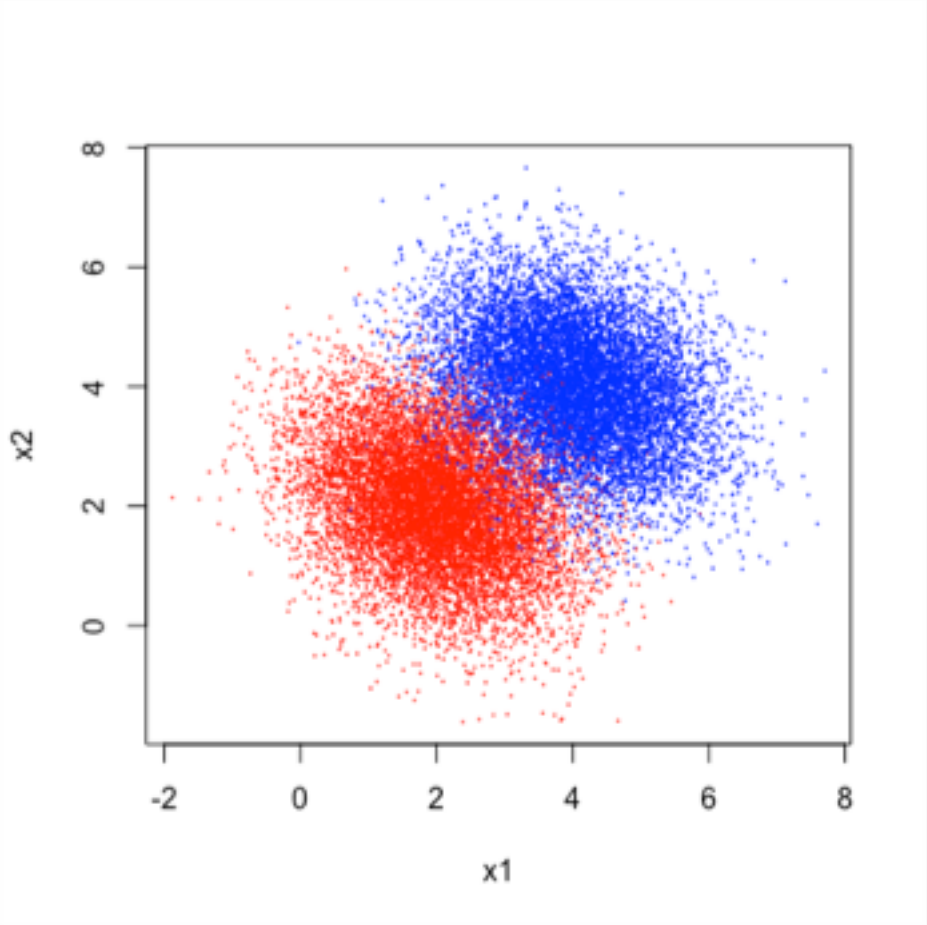
Let's investigate which method will work the best (as measured by lowest overall classification error rate), by considering 6 different models for 4 different data sets (each data set as a pair of predictors...you can think of them as the first 2 PCA components...to come later in the lecture). The 6 models to consider are:

- A logistic regression with only 'linear' main effects}
- A logistic regression with only 'linear' and 'quadratic' effects}
- LDA
- QDA
- *k*-NN where *k* = 3
- *k*-NN where *k* = 25

What else will also be important to measure (besides error rate)?

Which method should perform better? #1

$n = 20{,}000,\ p = 2,\ K = 2,\ \pi_1 = \pi_2 = 0.5$



method	misclass rate	run time (ms)
logit1	0.04410	417.95
logit2	0.04405	229.71
lda	0.04425	50.63
qda	0.04410	49.08
knn3	0.05225	1856.11
knn25	0.04500	2166.57

Notice anything fishy about our answers? What did Kevin do? What should he have done?

Easy to implement in Python

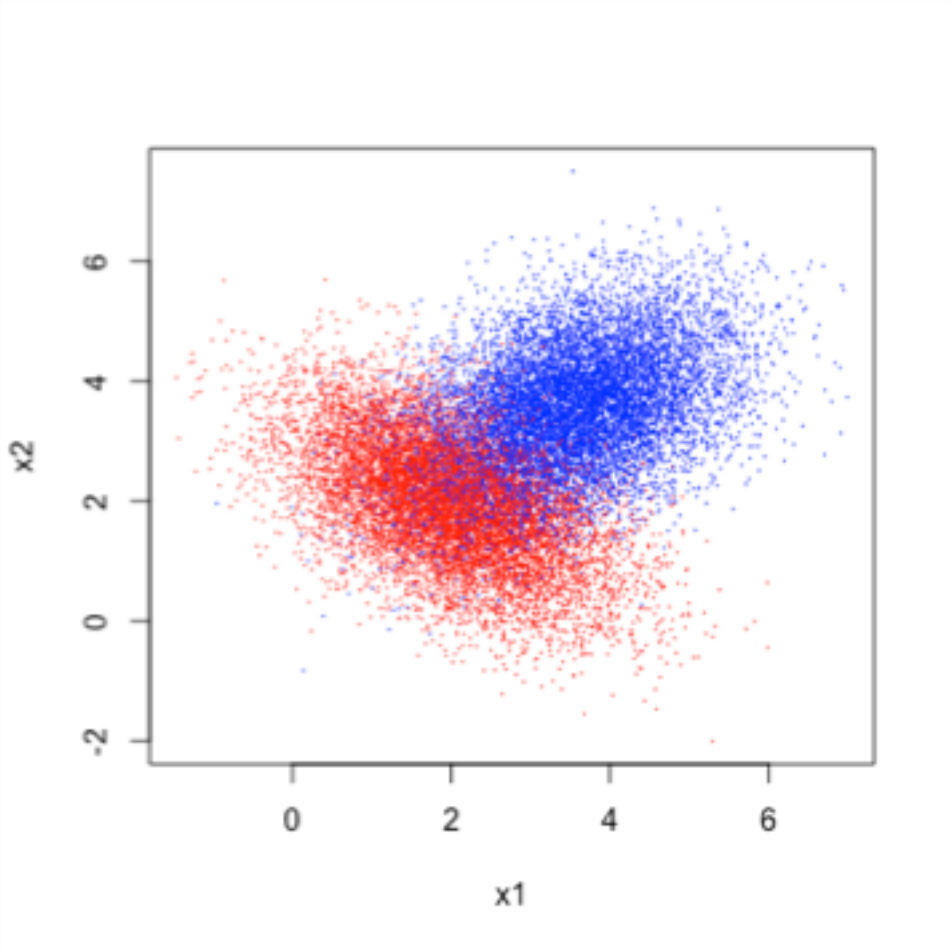
```
lda = da.LinearDiscriminantAnalysis()
qda = da.QuadraticDiscriminantAnalysis()
lda.fit(X,y)
qda.fit(X,y)
logit2 = sk.linear_model.LogisticRegression(C = 1000000)
logit1 = sk.linear_model.LogisticRegression(C = 1000000)
logit1.fit(X,y)
logit2.fit(X2,y)

print("Overall misclassification rate of Logit1 is",(1-logit1.score(X,y)))
print("Overall misclassification rate of Logit2 is",(1-logit2.score(X2,y)))
print("Overall misclassification rate of LDA is",(1-lda.score(X,y)))
print("Overall misclassification rate of QDA is",(1-qda.score(X,y)))
```

```
Overall misclassification rate of Logit1 is 0.0441
Overall misclassification rate of Logit2 is 0.0441
Overall misclassification rate of LDA is 0.04425
Overall misclassification rate of QDA is 0.0441
```

Which method should perform better? #2

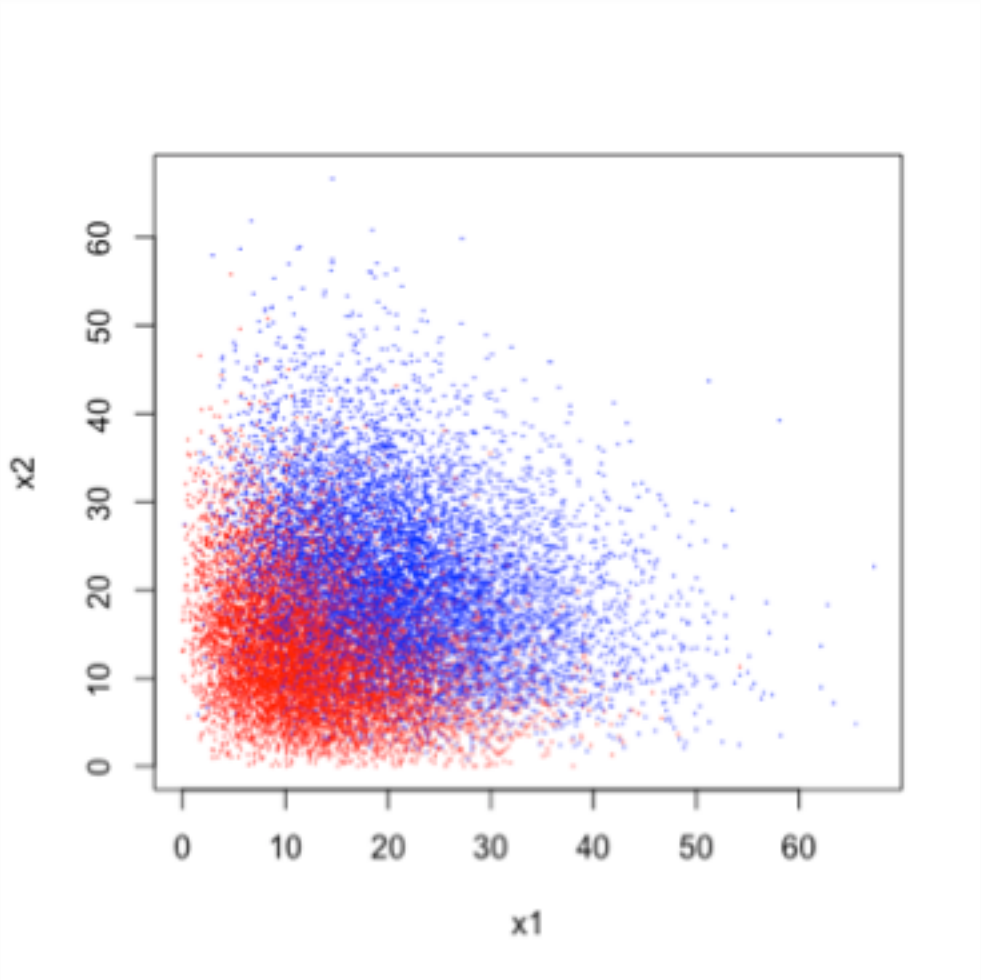
$n = 20{,}000$, $p = 2$, $K = 2$, $\pi_1 = \pi_2 = 0.5$



method	misclass rate	run time (ms)
logit1	0.12230	169.53
logit2	0.11860	196.42
lda	0.12215	47.93
qda	0.11445	47.03
knn3	0.14380	1861.90
knn25	0.12015	2223.13

Which method should perform better? #3

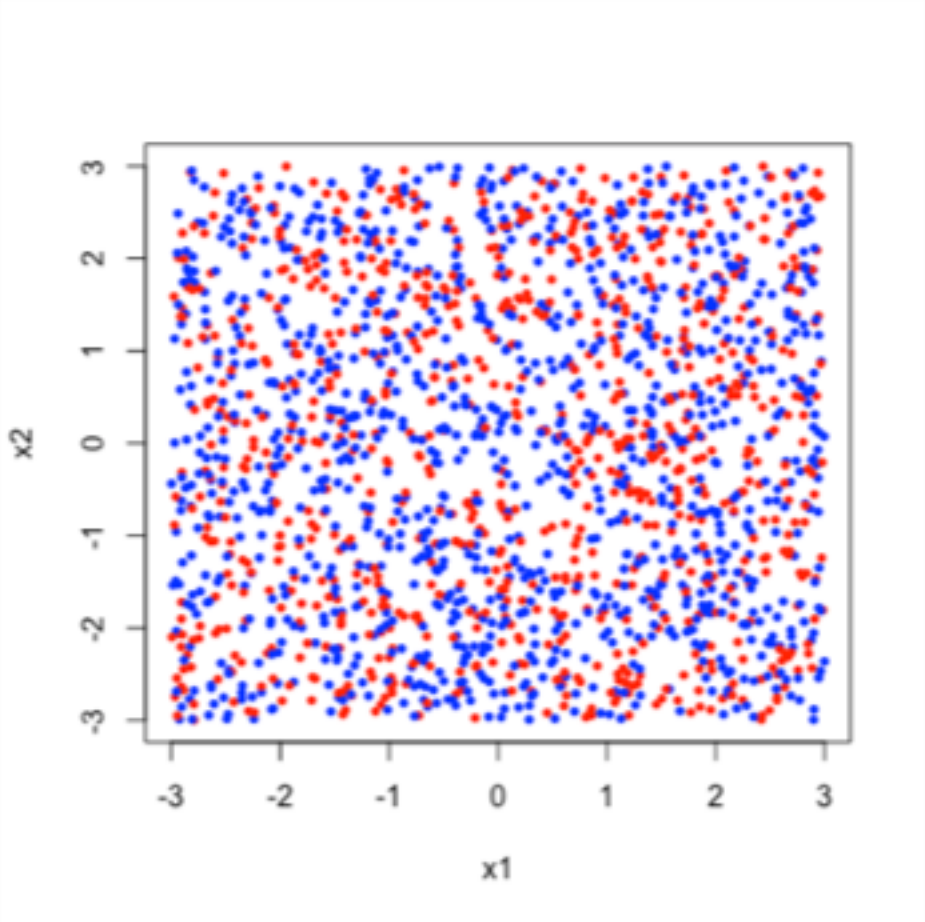
$n = 20{,}000$, $p = 2$, $K = 2$, $\pi_1 = \pi_2 = 0.5$



method	misclass rate	run time (ms)
logit1	0.20260	1234.35
logit2	0.19535	192.99
lda	0.20320	49.08
qda	0.21450	60.61
knn3	0.23300	1869.44
knn25	0.20270	2166.77

Which method should perform better? #4

$n = 20{,}000$, $p = 2$, $K = 2$, $\pi_1 = \pi_2 = 0.5$



method	misclass rate	run time (ms)
logit1	0.45690	1181.44
logit2	0.37880	147.95
lda	0.45770	51.06
qda	0.40705	44.04
knn3	0.34820	1835.42
knn25	0.30655	2126.38

Summary of Results

Generally speaking:

- LDA outperforms Logistic Regression if the distribution of predictors is reasonably MVN (with constant covariance).
- QDA outperforms LDA if the covariances are not the same in the groups.
- k-NN outperforms the others if the decision boundary is extremely non-linear.
- Of course, we can always adapt our models (logistic and LDA/QDA) to include polynomial terms, interaction terms, etc... to improve classification (watch out for overfitting!)
- In order of <u>computational speed</u> (generally speaking, it depends on K, p, and n of course):

LDA > QDA > Logistic > k-NN

High Dimensionality

When Does High Dimensionality Occur?

The problem of high dimensionality can occur when the number of parameters exceeds or is close to the number of observations. This can occur when we consider lots of interaction terms, like in our previous example. But this can also happen when the number of main effects is high.

For example:

- When we are performing polynomial regression with a high degree and a large number of predictors.
- When the predictors are genomic markers in a computational biology problem.
- When the predictors are the counts of all English words appearing in a text.

A Framework For Dimensionality Reduction

One way to reduce the dimensions of the feature space is to create a new, smaller set of predictors by taking linear combinations of the original predictors.

We choose $Z_1, Z_2, \ldots, Z_m$, where $m < p$ and where each Z_i is a linear combination of the original p predictors

$$Z_i = \sum_{j=1}^{p} \phi_{ji} X_j$$

for fixed constants ϕ_{ji}. Then we can build a linear regression regression model using the new predictors

$$Y = \beta_0 + \beta_1 Z_1 + \ldots + \beta_m Z_m + \epsilon.$$

Notice that this model has a smaller number ($m < p$) of parameters.

A Framework For Dimensionality Reduction (cont.)

A method of dimensionality reduction includes 2 steps:

- Determine a optimal set of new predictors $Z_1, \ldots, Z_m$, for $m < p$.
- Express each observation in the data in terms of these new predictors. The transformed data will have m columns rather than p.

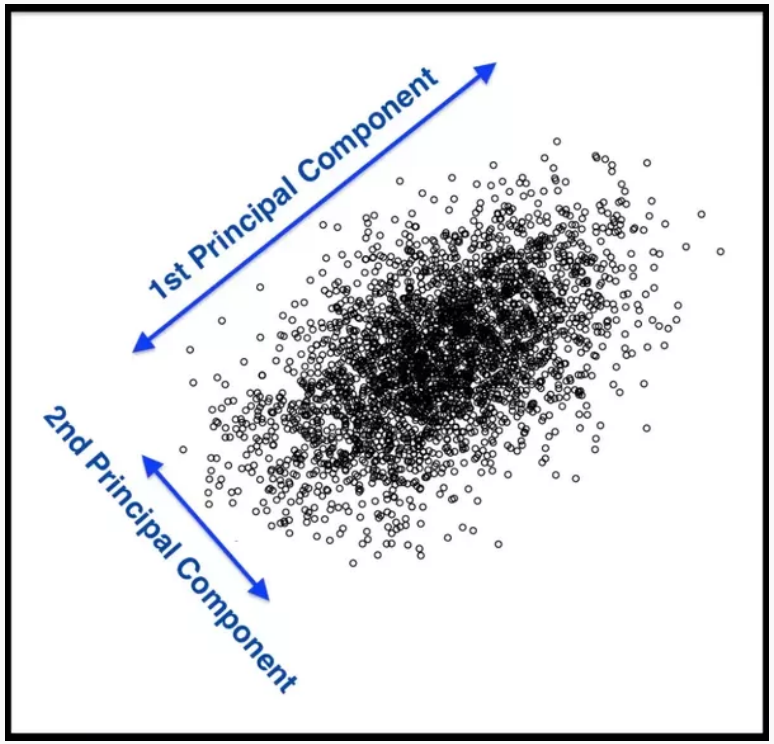
Thereafter, we can fit a model using the new predictors.

The method for determining the set of new predictors (what do we mean by an optimal predictors set) can differ according to application. We will explore a way to create new predictors that captures the variations in the observed data.

Principal Components Analysis (PCA)

Principal Components Analysis (PCA)

Principal Components Analysis (PCA) is a method to identify a new set of predictors, as linear combinations of the original ones, that captures the `maximum amount' of variance in the observed data.



PCA (cont.)

Principal Components Analysis (PCA) produces a list of *p principle components* $Z_1,\ldots, Z_p$ such that

- Each Z_i is a linear combination of the original predictors, and it's vector norm is 1
- The Z_i's are pairwise orthogonal
- The Z_i's are ordered in decreasing order in the amount of captured observed variance.

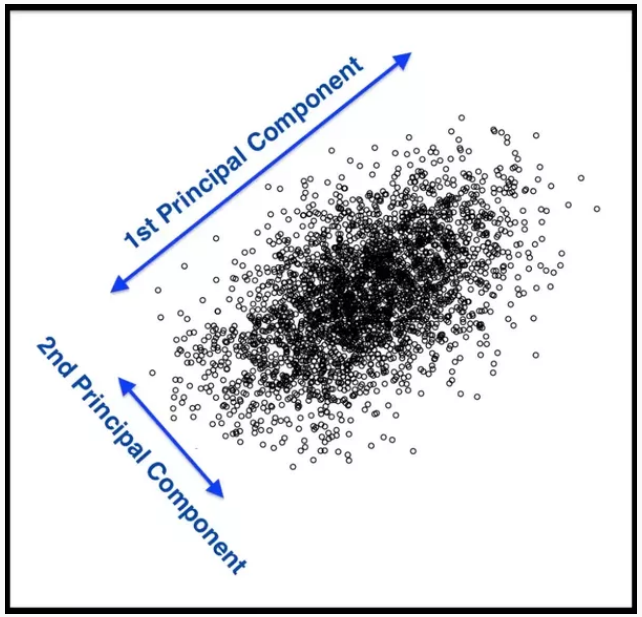
That is, the observed data shows more variance in the direction of Z_1 than in the direction of Z_2.

To perform dimensionality reduction we select the top *m* principle components of PCA as our new predictors and express our observed data in terms of these predictors.

The Intuition Behind PCA

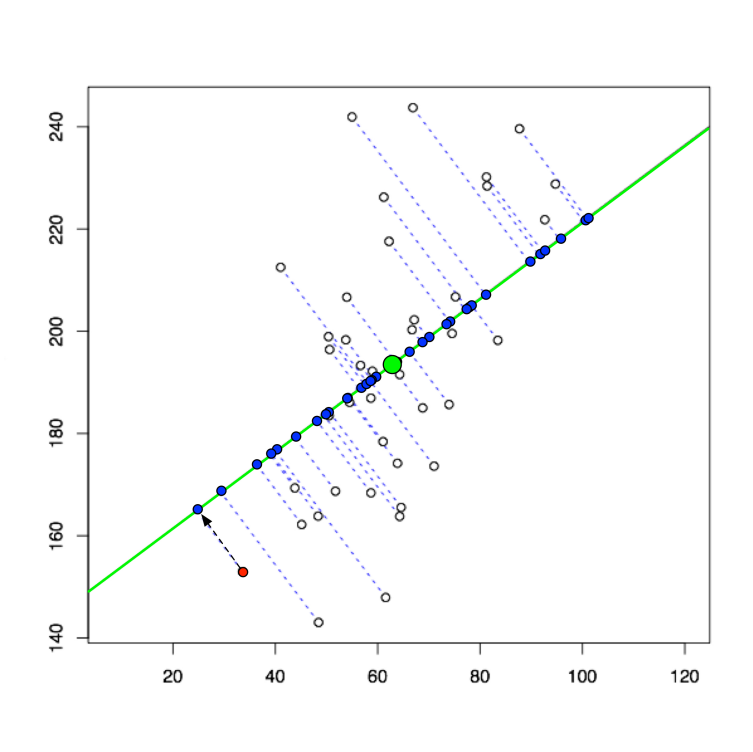
Top PCA components capture the most of amount of variation (interesting features) of the data.

Each component is a linear combination of the original predictors - we visualize them as vectors in the feature space.



The Intuition Behind PCA (cont.)

Transforming our observed data means projecting our dataset onto the space defined by the top *m* PCA components, these components are our new predictors.



The Math behind PCA

PCA is a well-known result from linear algebra. Let **Z** be the n x p matrix consisting of columns $Z_1,\ldots, Z_p$ (the resulting PCA vectors), **X** be the n x p matrix of $X_1,\ldots, X_p$ of the original data variables (each re-centered to have mean zero, and without the intercept), and let **W** be the p x p matrix whose columns are the eigenvectors of the square matrix $\mathbf{X}^T\mathbf{X}$ then

$$\mathbf{Z}_{n\times p} = \mathbf{X}_{n\times p}\mathbf{W}_{p\times p}$$

Implementation of PCA using linear algebra

To implement PCA yourself using this linear algebra result, you can perform the following steps:

- Subtract off the mean for each of your predictors (so they each have mean zero).
- Calculate the eigenvectors of the $\mathbf{X}^T\mathbf{X}$ matrix and create the matrix with those columns, **W**, in order from largest to smallest eigenvalue.
- Use matrix multiplication to determine $\mathbf{Z} = \mathbf{X}\mathbf{W}$.

Note: this is not efficient from a computational perspective. This can be sped up using Cholesky decomposition.

However, PCA is easy to perform in Python using the `decomposition.PCA` function in the `sklearn` package.

PCA for Regression (PCR)

PCA for Regression (PCR)

PCA is easy to use in Python, so how do we then use it for regression modeling in a real-life problem?

If we use all p of the new Z_j, then we have not improved the dimensionality. Instead, we select the first M PCA variables, $Z_1,\ldots,Z_M$, to use as predictors in a regression model.

The choice of M is important and can vary from application to application. It depends on various things, like how collinear the predictors are, how truly related they are to the response, etc...

What would be the best way to check for a specified problem?

Train and Test!!!

Dealing with Missingness

What is missing data?

Often times when data is collected, there are some missing values apparent in the dataset. This leads to a few questions to consider:

- How does this show up in pandas?
- How does pandas and sklearn handle these NaNs?
- How does this effect our modeling?

Naively handling missingness

What is the simplest way to handle missing data?

- Impute the mean (if quantitative) or most common class (if categorical) for all missing values.
- How does pandas and sklearn handle these NaNs?

What are some consequences in handling missingness in this fashion?

Types of Missingness

Sources of Missingness

Missing data can arise from various places in data:

- A survey was conducted and values were just randomly missed when being entered in the computer.
- A respondent chooses not to respond to a question like `Have you ever done cocaine?'.
- You decide to start collecting a new variable (like Mac vs. PC) partway through the data collection of a study.
- You want to measure the speed of meteors, and some observations are just 'too quick' to be measured properly.

The source of missing values in data can lead to the major types of missingness:

Types of Missingness

There are 3 major types of missingness to be concerned about:

1. **Missing Completely at Random (MCAR)** - the probability of missingness in a variable is the same for all units. Like randomly poking holes in a data set.
2. **Missing at Random (MAR)** - the probability of missingness in a variable depends only on available information (in other predictors).
3. **Missing Not at Random (MNAR)** - the probability of missingness depends on information that has not been recorded and this information also predicts the missing values.

What are examples of each these 3 types?

Missing completely at random (MCAR)

Missing Completely at Random is the best case scenario, and the easiest to handle:

- Examples: a coin is flipped to determine whether an entry is removed. Or when values were just randomly missed when being entered in the computer.
- Effect if you ignore: there is no effect on inferences (estimates of beta).
- How to handle: lots of options, but best to impute (more on next slide).

Missing at random (MAR)

Missing at random is still a case that can be handled.

- Example(s): men and women respond to the question "have you ever felt harassed at work?" at different rates (and may be harassed at different rates).
- Effect if you ignore: inferences are biased (estimates of beta) and predictions are usually worsened.
- How to handle: use the information in the other predictors to build a model and `impute' a value for the missing entry.

Key: we can fix any biases by modeling and imputing the missing values based on what is observed!

Missing Not at Random (MNAR)

Missing Not at Random is the worst case scenario, and impossible to handle:

- Example(s): patients drop out of a study because they experience some really bad side effect that was not measured. Or cheaters are less likely to respond when asked if you've ever cheated.
- Effect if you ignore: there is no effect on inferences (estimates of beta) or predictions.
- How to handle: you can 'improve' things by dealing with it like it is MAR, but you [likely] may never completely fix the bias.

What type of missingness is present?

Can you ever tell based on your data what type of missingness is actually present?

Since we asked the question, the answer must be no.

It generally cannot be determined whether data really are missing at random, or whether the missingness depends on unobserved predictors or the missing data themselves. The problem is that these potential “lurking variables” are unobserved (by definition) and so can never be completely ruled out.

In practice, a model with as many predictors as possible is used so that the `missing at random' assumption is reasonable.

Imputation Methods

Handling Missing Data

When encountering missing data, the approach to handling it depends on:

1. whether the missing values are in the response or in the predictors. Generally speaking, it is much easier to handle missingness in predictors.
2. whether the variable is quantitative or categorical.
3. how much missingness is present in the variable. If there is too much missingness, you may be doing more damage than good.

Generally speaking, it is a good idea to attempt to **impute** (or `fill in') entries for missing values in a variable (assuming your method of imputation is a good one).

Imputation Methods

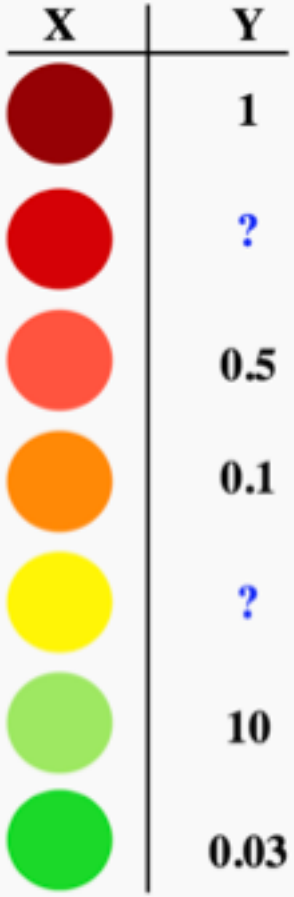
There are several different approaches to imputing missing values:

1. Plug in the mean or median (quantitative) or most common class (categorical) for all missing values in a variable.
2. Create a new variable that is an indicator of missingness, and include it in any model to predict the response (also plug in zero or the mean in the actual variable).
3. Hot deck imputation: for each missing entry, randomly select an observed entry in the variable and plug it in.
4. Model the imputation: plug in predicted values ($\hat{y}$) from a model based on the other observed predictors.
5. Model the imputation with uncertainty: plug in predicted values plus randomness ($\hat{y} + \epsilon$) from a model based on the other observed predictors.

What are the advantages and disadvantages of each approach?

Schematic: imputation through modeling

How do we use models to fill in missing data?

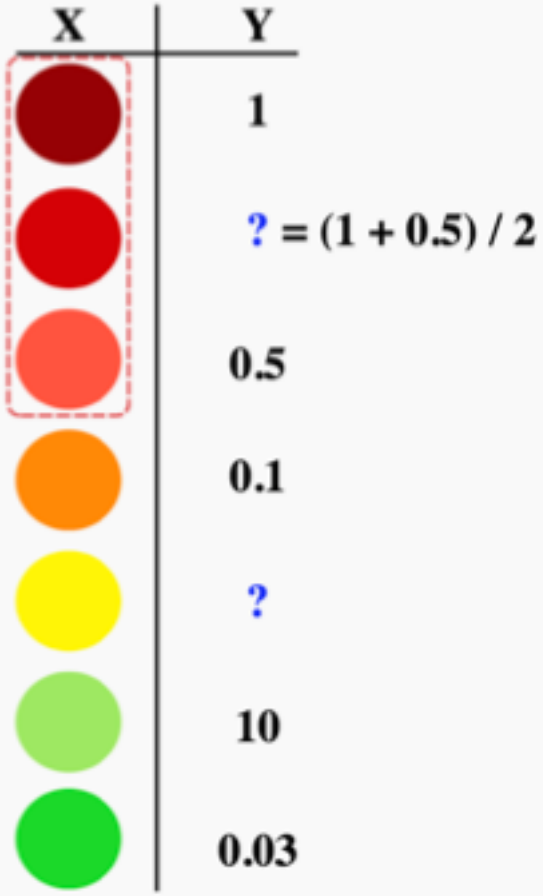


Schematic: imputation through modeling

How do we use models to fill in missing data?

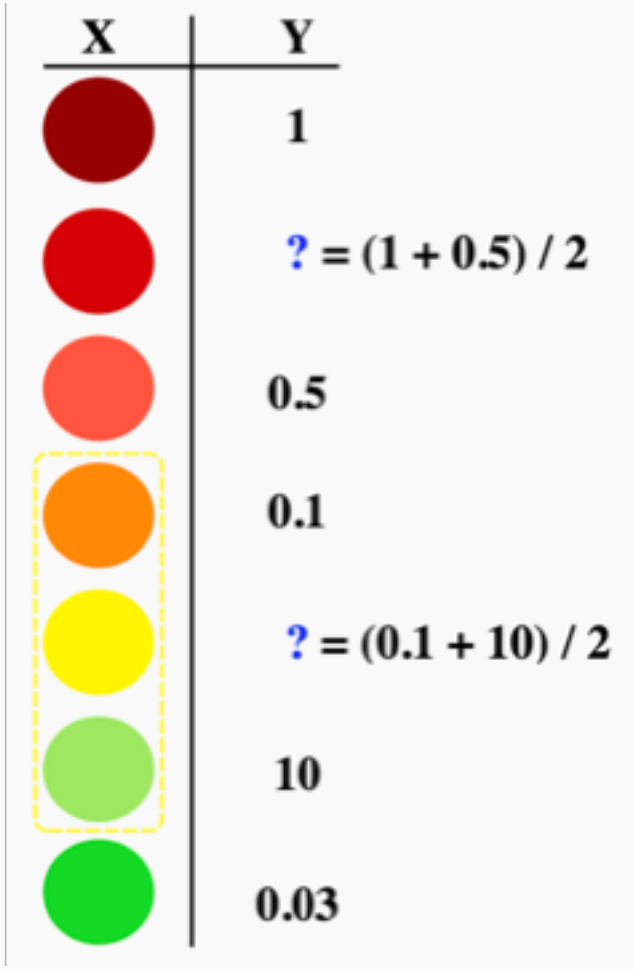
Schematic: imputation through modeling

How do we use models to fill in missing data? Using *k*-NN for *k* = 2?



Schematic: imputation through modeling

How do we use models to fill in missing data? Using *k*-NN for *k* = 2?



Schematic: imputation through modeling

How do we use models to fill in missing data? Using linear regression?

Where *m* and *b* are computed from the observations (rows) that do not have missingness (we should call them $b = \beta_0$ and $m = \beta_1$).

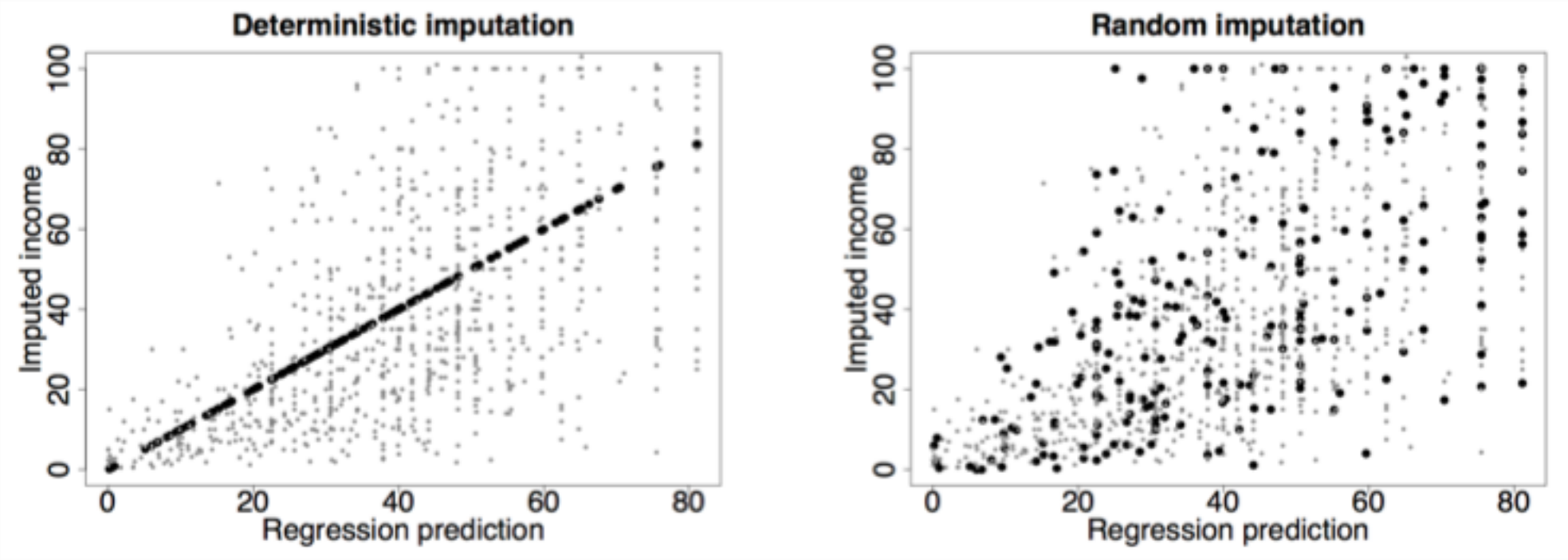
Imputation through modeling with uncertainty

The schematic in the last few slides ignores the fact of imputing with uncertainty. What happens if you ignore this fact and just use the 'best' model to impute values solely on $\hat{y}$?

The distribution of the imputed values will be too narrow and not represent real data (see next slide for illustration). The goal is to impute values that include the uncertainty of the model.

How can this be done in practice in *k*-NN? In linear regression? In logistic regression?

Imputation through modeling with uncertainty: an illustration



Imputation through modeling with uncertainty: an illustration

Recall the probabilistic model in linear regression:

$$Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \varepsilon$$

where $\epsilon \sim N(0, \sigma^2)$. How can we take advantage of this model to impute with uncertainty?

It's a 3 step process:

1. Fit a model to predict the predictor variable with missingness from all the other predictors.
2. Predict the missing values from the model in the previous part.
3. Add in a measure of uncertainty to this prediction by randomly sampling from a $N(0, \sigma^2)$ distribution, where σ^2 is the mean square error (MSE) from the model.

Imputation through modeling with uncertainty: *k*-NN regression

How can we use *k*-NN regression to impute values that mimic the error in our observations?

Two ways:

- Use $k = 1$.
- Use any other k, but randomly select from the nearest neighbors in $\mathcal{N}_0$. This can be done with equal probability or with some weighting (inverse to the distance measure used).

Imputation through modeling with uncertainty: classifiers

For classifiers, this imputation with uncertainty/randomness is a little easier process. How can it be implemented?

If a classification model (logistic, *k*-NN, etc...) is used to predict the variable with missingness on the observed predictors, then all you need to do is flip a 'biased coin' (or multi-sided die) with the probabilities of coming up for each class equal to the predicted probabilities from the model.

Warning: do not just classify blindly using the predict command in sklearn!

Imputation across multiple variables

If only one variable has missing entries, life is easy. But what if all the predictor variables have a little bit of missingness (with some observations having multiple entries missing)? How can we handle that?

It's an iterative process. Impute X_1 based on X_2, ..., X_p. Then impute X_2 based on X_1 and X_3, ..., X_p. And continue down the line.

Any issues? Yes, not all of the missing values may be imputed with just one 'run' through the data set. So you will have to repeat these 'runs' until you have a completely filled in data set.

Multiple imputation: beyond this class

What is an issue with treating your now ‘complete’ data set (a mixture of actually observed values and imputed values) as simply all observed values?

Any inferences or predictions carried out will be tuned and potentially overfit to the random entries imputed for the missing entries. How can we prevent this phenomenon?

By performing **multiple imputation**: rerun the imputation algorithm many times, refit the model on the response many times (one time each), and then ’average’ the predictions or estimates of β coefficients to perform inferences (also incorporating the uncertainty involved).

Note: this is beyond what we would expect in this class. But it generally a good thing to be aware of.