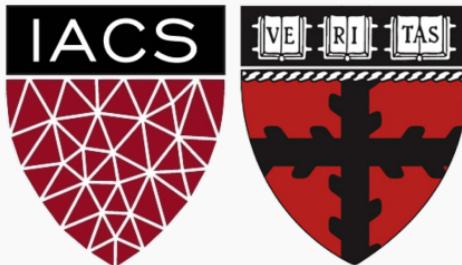


Lecture 17: Logistic Regression II

CS109A Introduction to Data Science
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Lecture Outline

- Interpreting interactions in logistic regression
- Classification Boundaries
- Regularization in Logistic Regression
- Bayes Theorem and Misclassification Rates
- ROC Curves



Interactions in Multiple Logistic Regression

Just like in linear regression, interaction terms can be considered in logistic regression.

An **interaction terms** is incorporated into the model the same way, and the interpretation is very similar (on the log-odds scale of the response of course).

Write down the model for the Heart data for the 2 predictors plus the interactions term based on the output on the next slide.



Interpreting Multiple Logistic Regression: an Example

The results for the multiple logistic regression model are:

```
df_heart['Age_Sex'] = df_heart.Age*df_heart.Sex  
data_x = df_heart[['Age', 'Sex', 'Age_Sex']]  
logit3 = LogisticRegression(penalty='none', max_iter = 1000)  
logit3.fit(data_x, df_heart['AHD'])  
  
print("Logistic Regression Estimated Betas (B0,B1,B2,B3):",  
      np.round(logit3.intercept_,4),np.round(logit3.coef_,5))
```

Logistic Regression Estimated Betas (B0,B1,B2,B3): [-4.2742] [[0.05654 0.77549 0.01273]]

$$\ln \left(\frac{P(Y=1)}{P(Y=0)} \right) = -4.274 + 0.0565(\text{Age}) + 0.775(\text{Sex}) + 0.0127(\text{Age} * \text{Sex})$$

Sex=1
for males

"log-odds"



Some questions

A50

Logistic Regression Estimated Betas (B_0, B_1, B_2, B_3): [-4.2742] [[0.05654 0.77549 0.01273]]

1. Write down the complete model. Break this down into the model to predict log-odds of heart disease (HD) based on Age for women and the same model for men.

For females (Sex = 0)

$$\text{log-odds} = \beta_0 + \beta_1 \text{Age} = -4.274 + 0.0565 \text{Age}$$

For males (Sex = 1)

$$\text{log-odds} = \beta_0 + \beta_1 \text{Age} + \beta_2 \text{Sex} + \beta_3 (\text{Age} * \text{Sex})$$

$$\rightarrow (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \text{Age} = -3.50 + 0.0693 \text{Age}$$



Some questions

Logistic Regression Estimated Betas (B0,B1,B2,B3): [2.90173899] [[-0.0265903 5.41531302 -0.02707269]]

2. Interpret the results of this model. What does the coefficient for the interaction term represent?

$\hat{\beta}$ represents the "additional" association of Age to AHD comparing men to women.

3. Estimate the odds ratio of HD comparing men to women using this model [trick question].

The relationship with "Sex" depends on Age

Do it at various values of Age



Classification Boundaries



Classification boundaries

Recall that we could attempt to purely classify each observation based on whether the estimated $P(Y = 1)$ from the model was greater than 0.5.

Recall, the logistic regression model statement from last week:

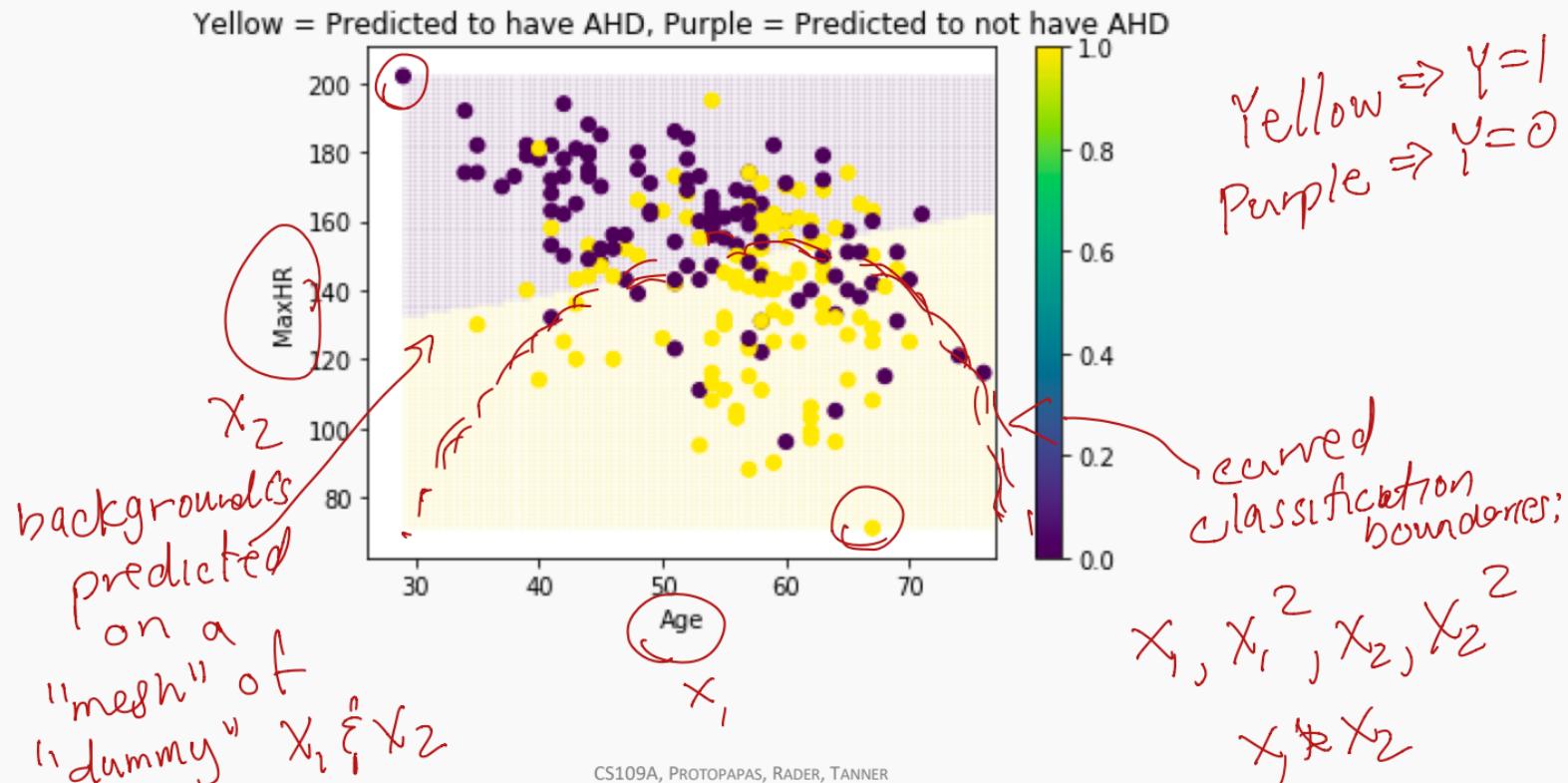
$$\ln\left(\frac{P(Y = 1)}{P(Y = 0)}\right) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

If $P(Y = 1) = 0.5$, then the odds is 1, and the log-odds is 0. Thus the classification boundary that separates the estimated probabilities above 0.5 from below 0.5 is defined when we set $\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p = 0$.

Thus logistic regression is said to lead to a **linear classification boundary**. There is actually a lot more freedom in logistic regression's classification boundary (the **geometry** is defined by the parameterization of your predictors!)



Linear Classification Boundary Example



Classification Boundary: a complicated example

Logistic Regression Estimated Betas (B0,B1,B2,B3): [-4.2742] [[0.05654 0.77549 0.01273]]

4. Using the results of the model above, at what ages will males be predicted to have a heart attack in a classification? At what ages will females be predicted to have a heart attack?

For females: $\text{log-odds} = -4.274 + 0.0565(\text{Age})$ set $= 0$

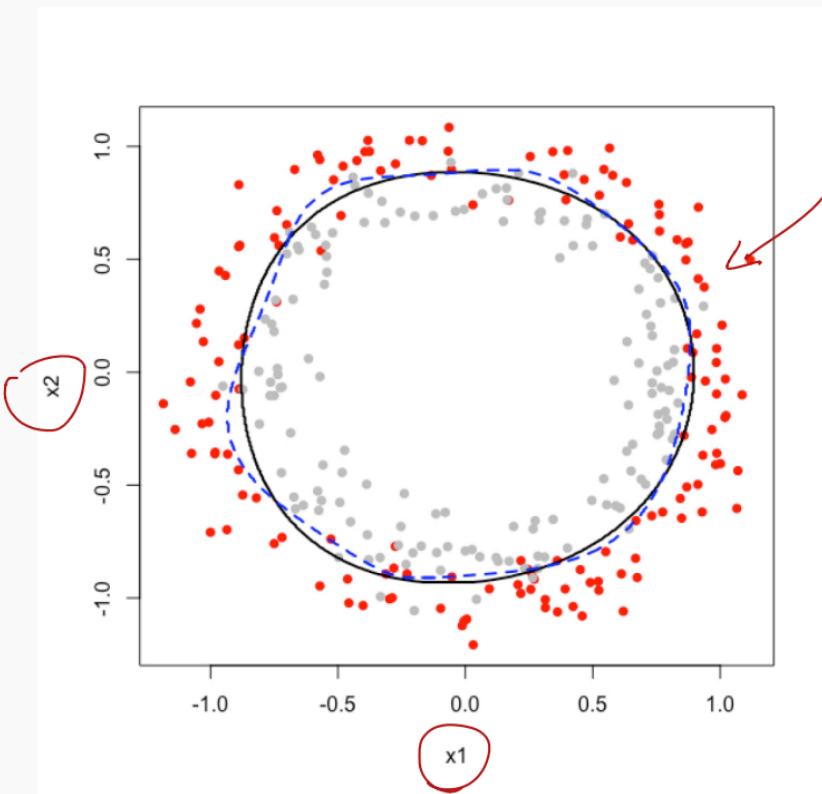
$$\text{Age} = \frac{-4.274}{0.0565}$$
$$= 75.6$$

For males: $\text{log-odds} = -3.5 + 0.0693(\text{Age})$ set $= 0$

$$\text{Age} = \frac{3.5}{0.0693} = 50.5$$



Geometry of 2D Classification in Logistic Regression: an Example



"circle": 2nd order polynomial

"wavy-circle": 5th-order polynomial

2D Classification in Logistic Regression: an Example

Would a logistic regression model perform well in classifying the observations in this example?

What would be a good logistic regression model to classify these points?

Based on these predictors, two separate logistic regression model were considered that were based on different ordered polynomials of X_1, X_2 and their interactions. The 'circles' represent the boundary for classification.

How can the classification boundary be calculated for a logistic regression?

Regularization in Logistic Regression



Review: Regularization in Linear Regression

Based on the Likelihood framework, a loss function can be determined based on the log-likelihood function.

We saw in linear regression that maximizing the log-likelihood is equivalent to minimizing the sum of squares error:

$$\arg \min \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \arg \min \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_{1i} + \dots + \beta_p x_{pi}))^2$$



Review: Regularization in Linear Regression

And a regularization approach was to add a penalty factor to this equation. Which for Ridge Regression becomes:

$$\arg \min \left[\sum_{i=1}^n \left(y_i - \left(\beta_0 + \sum_{j=1}^p \beta_j x_{ji} \right) \right)^2 + \lambda \sum_{j=1}^p \beta_j^2 \right]$$

penalty term +
penalize target
betas
⇒ "shrink"
beta estimates
compared to OLS

Note: this penalty *shrinks* the estimates towards zero, and had the analogue of using a Normal prior centered at zero in the Bayesian paradigm.



Recall: Loss function in Logistic Regression

A similar approach can be used in logistic regression. Here, maximizing the log-likelihood is equivalent to minimizing the following loss function:

$$\underset{\beta_0, \beta_1, \dots, \beta_p}{\operatorname{argmin}} \left[- \sum_{i=1}^n (y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i)) \right]$$

minimizing
negative
log-likelihood

$$\text{where } p_i = \frac{1}{1 - e^{-(\beta_0 + \beta_1 x_{1,i} + \dots + \beta_p x_{p,i})}}$$

Why is this a good loss function to minimize? Where does this come from?

The log-likelihood for independent $Y_i \sim \text{Bern}(p_i)$.

$$p_i = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \dots)}}$$

Regularization in Logistic Regression

penalty term
to the loss
function

A penalty factor can then be added to this loss function and results in a new loss function that penalizes large values of the parameters:

$$\operatorname{argmin}_{\beta_0, \beta_1, \dots, \beta_p} \left[-\sum_{i=1}^n (y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i)) + \lambda \sum_{j=1}^p \beta_j^2 \right]$$

The result is just like in linear regression: shrink the parameter estimates towards zero.

In practice, the intercept is usually not part of the penalty factor.

Note: the sklearn package uses a different tuning parameter: instead of λ they use a constant that is essentially $C = \frac{1}{\lambda}$.

$$\lambda \sum_{j=1}^p |\beta_j|$$



Regularization in Logistic Regression: an Example

Let's see how this plays out in an example in logistic regression.

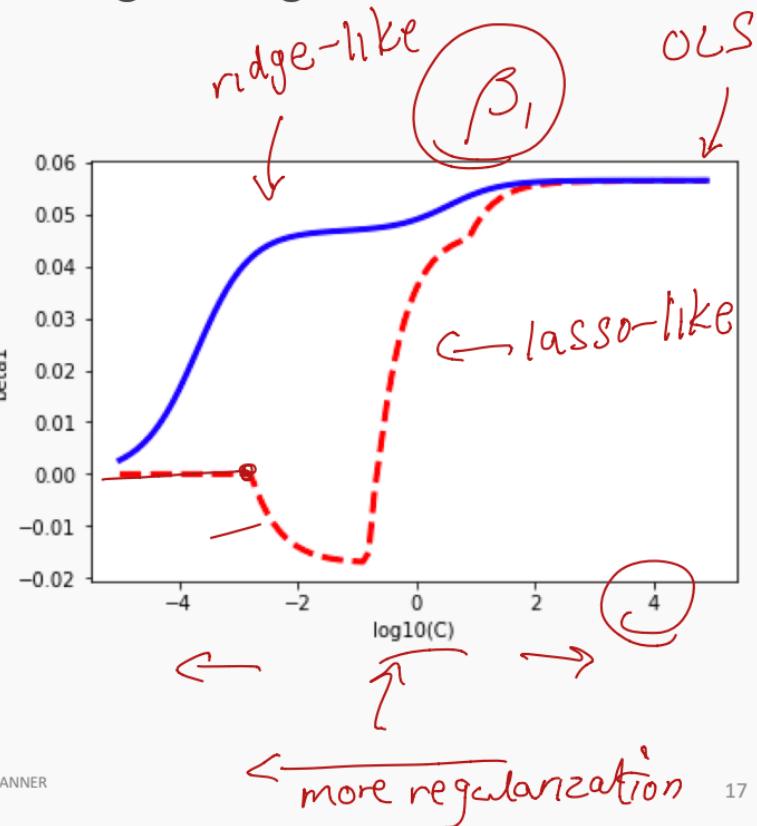
```
beta1_11 = []
beta1_12 = []
Cs = np.power(10,np.arange(0,10,0.1))/np.power(10,5)

data_x = df_heart[['Age', 'Sex', 'Age_Sex']]
data_y = df_heart['AHD']

for C in Cs:
    logitm_11 = LogisticRegression(C = C, penalty = "l1",
                                    solver='liblinear', max_iter=200)
    logitm_11.fit (data_x, data_y)
    logitm_12 = LogisticRegression(C = C, penalty = "l2",
                                    solver='lbfgs', max_iter=200)
    logitm_12.fit (data_x, data_y)
    beta1_11.append(logitm_11.coef_[0][0])
    beta1_12.append(logitm_12.coef_[0][0])

plt.plot(np.log10(Cs), beta1_11, "--", color='red', lw=3)
plt.plot(np.log10(Cs), beta1_12, color='blue', lw=3)
plt.xlabel ("log10(C)")
plt.ylabel("beta1")
plt.show()
```

lasso-like
ridge-like



Regularization in Logistic Regression: tuning λ

Just like in linear regression, the shrinkage factor must be chosen. How should we go about doing this?

Through building multiple training and test sets (hooray, cross-validation!), we can select the best shrinkage factor to mimic out-of-sample prediction.

How could we measure how well each model fits the validation sets?

We could measure this based on some loss function (more coming later)!

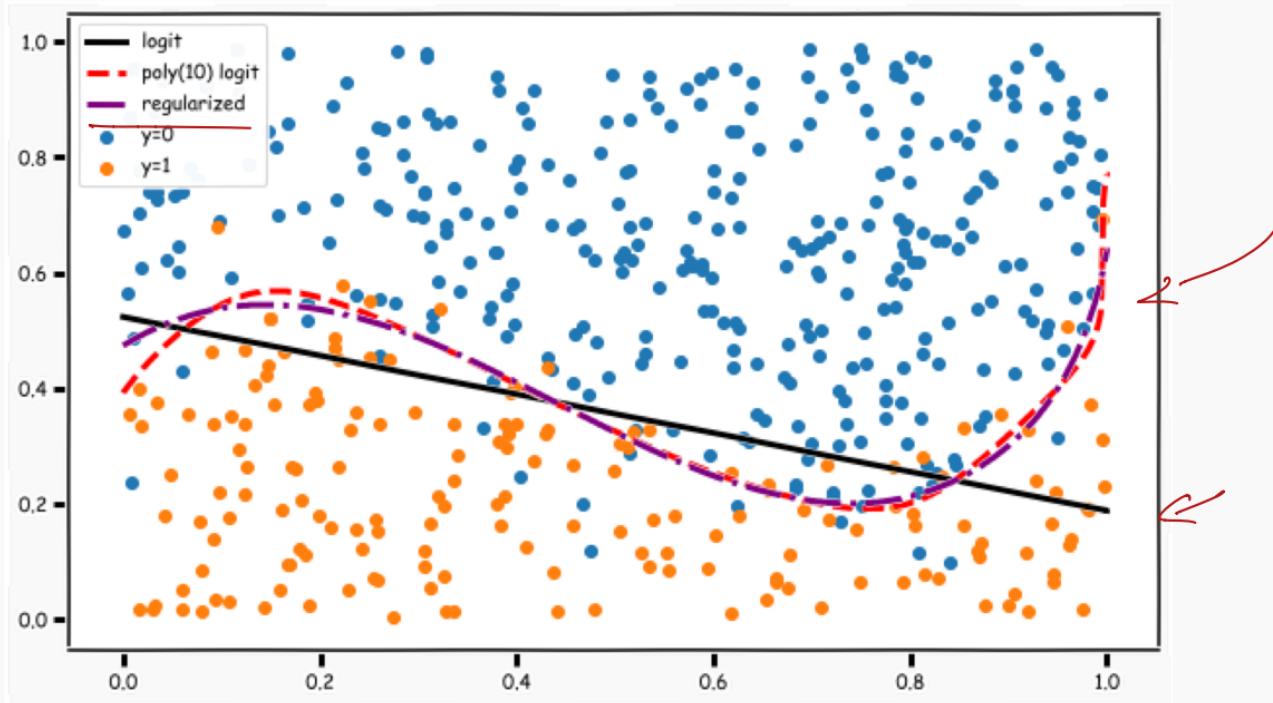
linear: MSE
logistic: classification accuracy?
 \sim log-likelihood

"entropy"

a different metric
in classification problem



Regularized Decision Boundaries



head over to exercises : Ex. 1 :

- classification boundaries
- regularization

Bayes Theorem, Misclassification Rates, False Positives and Negatives



Bayes' Theorem

We defined conditional probability as:

$$P(B|A) = P(B \text{ and } A)/P(A)$$

And using the fact that $P(B \text{ and } A) = P(A|B)P(B)$ we get the simplest form of Bayes' Theorem:

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$

Another version of Bayes' Theorem is found by substituting in the Law of Total Probability (LOTP) into the denominator:

$$P(B|A) = \frac{P(A|B)P(B)}{P(A|B)P(B) + P(A|B^C)P(B^C)}$$

Where have we seen Bayes' Theorem before? Why do we care?



Diagnostic Testing

In the diagnostic testing paradigm, one cares about whether the results of a test (like a classification test) matches truth (the true class that observation belongs to). The simplest version of this is trying to detect disease ($D+$ vs. $D-$) based on a diagnostic test ($T+$ vs. $T-$).

Medical examples of this include various screening tests: breast cancer screening through (i) self-examination and (ii) mammography, prostate cancer screening through (iii) PSA tests, and Colo-rectal cancer through (iv) colonoscopies.

These tests are a little controversial because of poor predictive probability of the tests.



Diagnostic Testing (cont.)

Bayes' theorem can be rewritten for diagnostic tests:

$$P(D+|T+)=\frac{P(T+|D+)P(D+)}{P(T+|D+)P(D+)+P(T+|D-)P(D-)}$$

These probability quantities can then be defined as:

- *Sensitivity*: $P(T+|D+)$
- *Specificity*: $P(T-|D-)$
- *Prevalence*: $P(D+)$
- *Positive Predictive Value*: $P(D+|T+)$
- *Negative Predictive Value*: $P(D-|T-)$

How do positive and negative predictive values relate? Be careful...



Diagnostic Testing

We mentioned that these tests are a little controversial because of their poor predictive probability. When will these tests have poor positive predictive probability?

balance across classes

When the disease is not very prevalent, then the number of 'false positives' will overwhelm the number of true positive. For example, PSA screening for prostate cancer has sensitivity of about 90% and specificity of about 97% for some age groups (men in their fifties), but prevalence is about 0.1%.

What is positive predictive probability for this diagnostic test?



Why do we care?

As data scientists, why do we care about diagnostic testing from the medical world? (hint: it's not just because Kevin is a trained biostatistician!)

Because classification can be thought of as a diagnostic test. Let $Y_i = k$ be the event that observation i truly belongs to category k , and let $\hat{Y}_i = k$ the event that we correctly predict it to be in class k . Then Bayes' rule states that our Positive Predictive Value for classification is:

$$P(\underline{Y_i = k} | \underline{\hat{Y}_i = k}) = \frac{P(\hat{Y}_i = k | Y_i = k) P(Y_i = k)}{P(\hat{Y}_i = k | Y_i = k) P(Y_i = k) + P(\hat{Y}_i = k | Y_i \neq k) P(Y_i \neq k)}$$

Thus the probability of a predicted outcome truly being in a specific group depends on what? The proportion of observations in that class!



Error in Classification

There are 2 major types of error in classification problems based on a binary outcome. They are:

False positives: incorrectly predicting $\hat{Y} = 1$ when it truly is in $Y = 0$.

False negative: incorrectly predicting $\hat{Y} = 0$ when it truly is in $Y = 1$.

The results of a classification algorithm are often summarized in two ways: (1) a confusion matrix, sometimes called a contingency table, or a 2x2 table (more generally $(k \times k)$ table) and (2) a receiver operating characteristics (ROC) curve.

↑ compiling lots of confusion matrices



Confusion matrix

Classification compared to $\pi = 0.5$ $\logit.\text{predict}(x)$

When a classification algorithm (like logistic regression) is used, the results can be summarized in a $(k \times k)$ table as such:

	Predicted no AHD ($\hat{Y} = 0$)	Predicted AHD ($\hat{Y} = 1$)
Truly no AHD ($Y = 0$)	110	54
Truly AHD ($Y = 1$)	53	86

The table above was a classification based on a logistic regression model to predict AHD based on “3” predictors: X_1 = Age, X_2 = Sex, and X_3 = interaction between Age and Sex.

What are the false positive and false negative rates for this classifier?

Bayes' Classifier Choice

A classifier's error rates can be tuned to modify this table. How?

The choice of the Bayes' classifier level will modify the characteristics of this table.

If we thought it was more important to predict AHD patients correctly (fewer false negatives), what could we do for our Bayes' classifier level?

We could classify instead based on:

$$\hat{P}(Y = 1) > \underline{\pi}$$

and we could choose π to be some level other than 0.50.

Let's see what the table looks like if π were 0.40 or 0.60 instead. What should happen to the False Positive and False Negative frequencies?

$\pi = 0.40 \Rightarrow$ classify more individuals as $\hat{Y} = 1$



Other Confusion tables

Based on $\pi = 0.4$:

	Predicted no AHD ($\hat{Y} = 0$)	Predicted AHD ($\hat{Y} = 1$)
Truly no AHD ($Y = 0$)	93	71
Truly AHD ($Y = 1$)	38	101

What has improved? What has worsened?

Based on $\pi = 0.6$:

	Predicted no AHD ($\hat{Y} = 0$)	Predicted AHD ($\hat{Y} = 1$)
Truly no AHD ($Y = 0$)	138	26
Truly AHD ($Y = 1$)	74	65

Which should we choose? Why? If "errors" are not equal.



ROC Curves and Area-Under-the-Curve



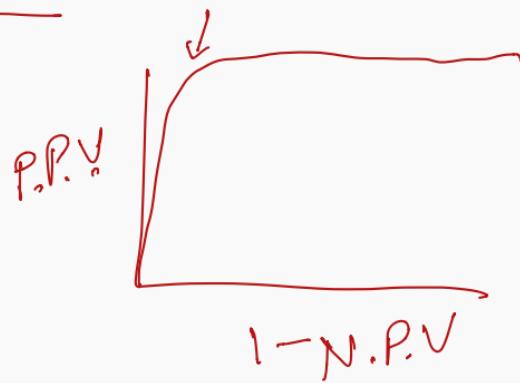
ROC Curves

The Radio Operator Characteristics (ROC) curve illustrates the trade-off for all possible thresholds chosen for the two types of error (or correct classification).

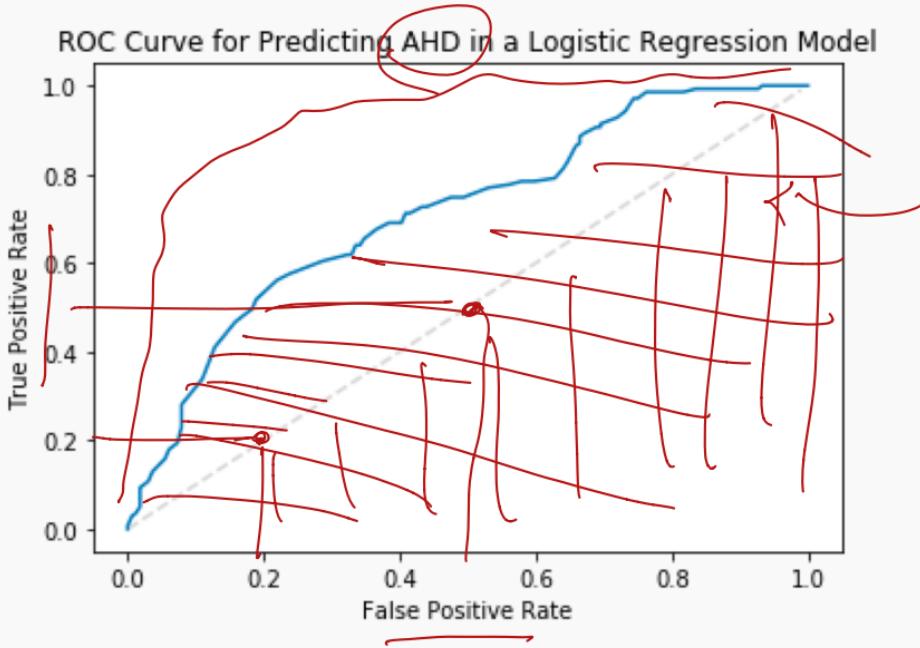
The vertical axis displays the true positive predictive value and the horizontal axis depicts the true negative predictive value.

What is the shape of an ideal ROC curve?

See next slide for an example.



ROC Curve Example



"biased worst case scenario" model

Area under the ROC curve (A.U.C.)

AUC $\approx 0.7 - 0.8$

(A.U.C. =)
(0.5)

AUC for measuring classifier performance

The overall performance of a classifier, calculated over all possible thresholds, is given by the **area under the ROC curve** (AUC).

An ideal ROC curve will hug the top left corner, so the larger the AUC the better the classifier.

What is the worst case scenario for AUC? What is the best case? What is AUC if we independently just flip a [biased] coin to perform classification?

This AUC then can be used to compare various approaches to classification: Logistic regression, k -NN, Decision Trees (to come), etc.

