

Announcements

- HW1 due.
 - Scaling should always be done before test, train split. If you did this (which is more correct) you get full points. If you didn't, you also will get full points since I didn't make the distinction in the question.
- HW0 should be graded by next week. It seems most people did relatively well.
- Sorry the last week or so I've been somewhat unavailable.
- There will be two more homeworks before the final assignment, which will be assigned in April. You will have approximately one month to work on it.

APMA E4990.02: Classification Problems

Lecture 4

Examples of Classification Problems

- User churn for subscription services.
- Acquisition - who is likely to subscribe?
- Who should receive a loan?
- What's a good pickup spot?
- Engagement - Who is likely to click? How do we target them? (later)
- Purchases - will somebody purchase a product? How will they rate it?



Credit Union



Outline

- Logistic regression hypothesis
- Decision Boundary
- Cost function (why we need a new one)
- Gradient Descent and a concrete example in Python
- AUC/ROC and model evaluation.
- Model selection and regularization for classification problems.

Example of a Classification Problem - User Churn

The New York Times

$X_n = \text{['subscription tenure', 'age', 'online activity', 'authors', etc]}$

$y = \text{probability of ending subscription in the next 2 months}$

Question: How do we predict the probability a user will churn?

Example of some of the most predictive features for the churn model at The New York Times

What is a good destination suggestion?

The image displays two side-by-side screenshots from a mobile application, likely Uber or Lyft, illustrating different destination suggestions.

Left Screenshot (Wednesday, November 29):

- Scheduled Pickup:** 3:00 PM
- Dropoff:** The Oaks
- Map Area:** Thousand Oaks, CA (near Newbury Park)
- Destinations:**
 - Near Marty Ct (Thousand Oaks, CA 91320)
 - Near W Hillcrest Dr (Thousand Oaks, CA 91360)
- Estimated earnings:** \$4 - \$6
- Buttons:** Confirm pickup (purple) and Cancel pickup (pink)

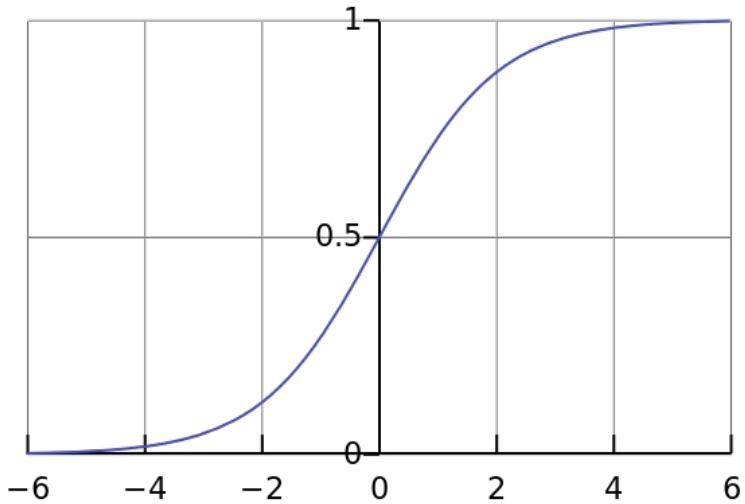
Right Screenshot (Friday, November 24):

- Scheduled Pickup:** 9:00 AM
- Dropoff:** Westlake Village
- Map Area:** Thousand Oaks, CA (near Hidden Valley)
- Destinations:**
 - Near Rancho Conejo Blvd (Thousand Oaks, CA 91320)
 - Near Thousand Oaks Blvd (Westlake Village, CA 91362)
- Text:** BE ONLINE BETWEEN 9:00 AM - 9:10 AM
- Estimated earnings:** \$9 - \$13
- Buttons:** Confirm pickup (purple) and Cancel pickup (pink)

What is the model?

$$\log \frac{p(y = 1)}{1 - p(y = 1)} = \beta \cdot \mathbf{x}$$

- p is the probability of the outcome.
- We compose the output of a linear model with a function which has range between -1 and 1.
- Beta defines a decision boundary in the variable space ($y=1$, $y=0$).

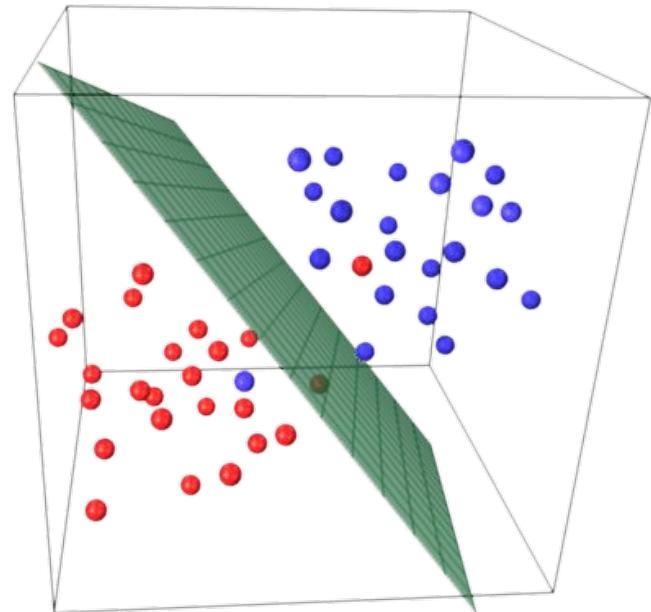


$$p_\beta(\mathbf{x}) = \frac{1}{1 + \exp(-\beta^T \cdot \mathbf{x})}$$

Decision boundary for Logistic Regression

$$p_{\beta}(\mathbf{x}) = \frac{1}{1 + \exp(-\beta^T \cdot \mathbf{x})}$$

- This defines a decision boundary where:
 $\beta^T \cdot \mathbf{x}$
 - Large and positive implies class 1
 - Large and negative implies class 0



Decision boundary for Logistic Regression

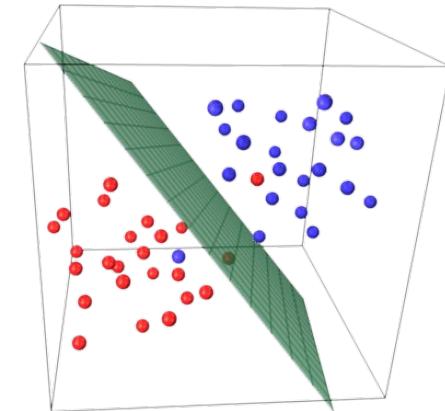
$$p_{\beta}(\mathbf{x}) = \frac{1}{1 + \exp(-\beta^T \cdot \mathbf{x})}$$

Let R denote the red class and B the blue class. Then

If $p_{\beta}(\mathbf{x}) > 0.5$ then $\mathbf{x} \in R$

If $p_{\beta}(\mathbf{x}) \leq 0.5$ then $\mathbf{x} \in B$

Note: The choice of 0.5 here is arbitrary.

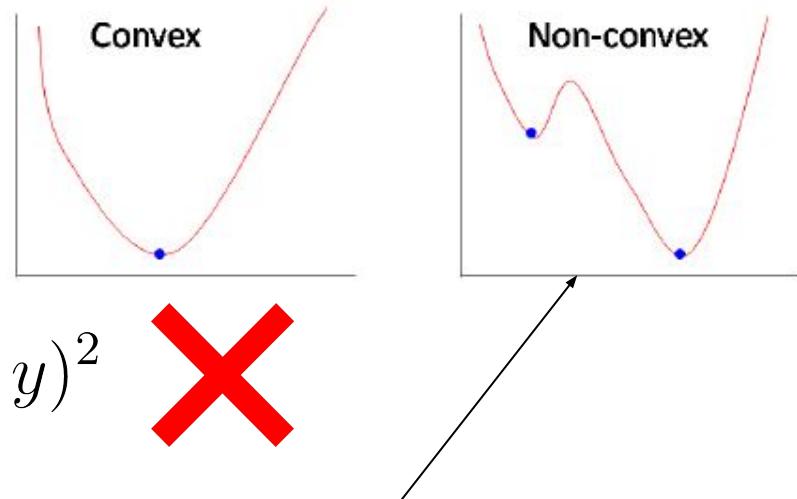


The Logistic Regression Cost Function

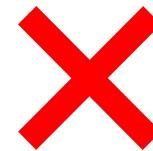
How do we measure distance?

For linear regression, recall we used L^p norms. However for the logit function, when we need a different way to measure performance of our model.

$$p_\beta(\mathbf{x}) = \frac{1}{1 + \exp(-\beta^T \cdot \mathbf{x})}$$



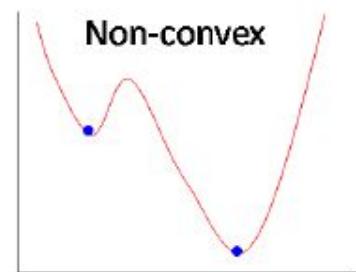
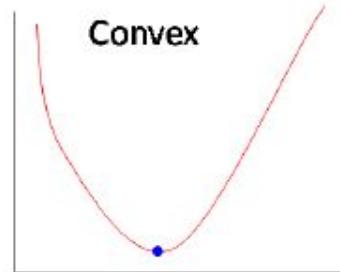
$$\text{Cost}_1(h_\beta(\mathbf{x}), \mathbf{y}) := \frac{1}{N} \sum_{k=1}^N (p_\beta(x) - y)^2$$



We would obtain a **non-convex cost function**. These are **difficult to minimize**. Instead we define another cost function (its derivation will be explained in more detail when we get into probabilistic concepts)

How do we measure distance? The new cost

$$p_\beta(\mathbf{x}) = \frac{1}{1 + \exp(-\beta^T \cdot \mathbf{x})}$$



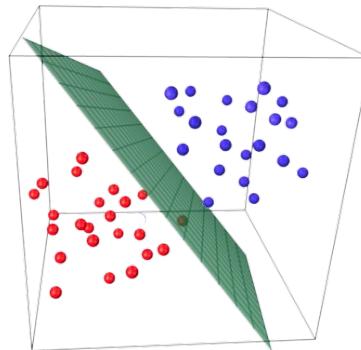
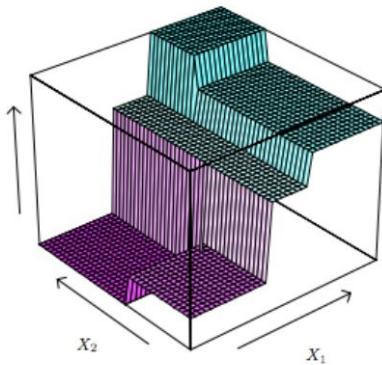
$$\text{Cost}_2(p_\beta(\mathbf{x}), y) = \begin{cases} -\log p_\beta(\mathbf{x}) & \text{if } y \text{ is 1} \\ -\log(1 - p_\beta(\mathbf{x})) & \text{if } y \text{ is 0} \end{cases}$$

- When y is 1, $p_\beta(\mathbf{x})$ tries to be close to 1.
- When y is 0, $p_\beta(\mathbf{x})$ tries to be close to 0.
- It may seem like we pulled this out of thin air, but we didn't. It actually can be **derived naturally from the method of Maximum Likelihood**.

Recall General Goal

More generally, joint random variables (\mathbf{x}, y) with distribution $P(\mathbf{x}, y)$
we want to minimize:

$$\mathcal{L}(\hat{f}) := \mathbb{E}_P L(y, \hat{f}(\mathbf{x})) \sim \frac{1}{N} \sum_{i=1}^N L(y_i, \hat{f}(x_i))$$



How do we choose a good loss function here?.

$$\hat{f}(\mathbf{x}_i) = \mathbf{1}_{R_t(\mathbf{x}_i)}(\mathbf{x}_i) \text{ for } \mathbf{x}_i \in R_{t(i)}$$

$$\hat{f}(\mathbf{x}_i) = \beta \cdot \mathbf{x}_i$$

The probabilistic approach - maximum likelihood.

$$p = \frac{\exp(\beta \cdot \mathbf{x})}{1 + \exp(\beta \cdot \mathbf{x})}$$

We then compute the likelihood function, which is just the conditional probability of the outcome on the data.

$$\mathcal{L}(\beta | x_n, y_n) = \prod_{k=1}^N p^{y_k} (1 - p)^{1-y_k}$$

$$l(\beta | x, y) = \sum_{k=1}^n y_k \log p(x_k) + (1 - y_k) \log(1 - p(x_k))$$

Relating likelihood to our cost

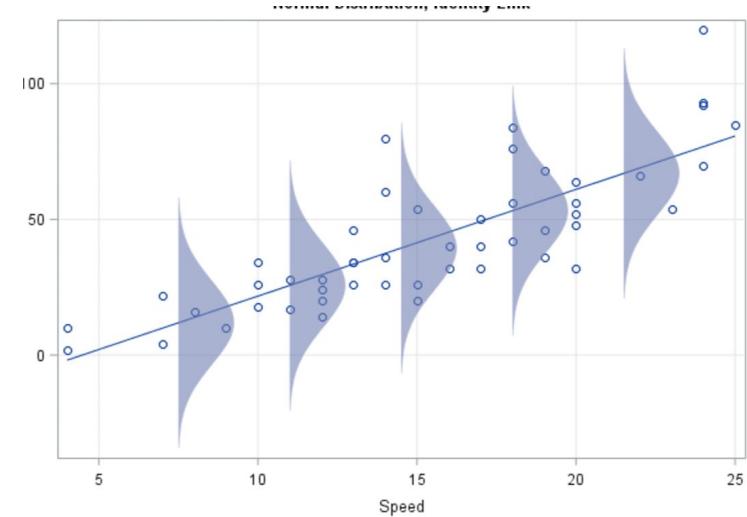
$$\text{Cost}_2(p_\beta(\mathbf{x}), y) = \begin{cases} -\log p_\beta(\mathbf{x}) & \text{if } y \text{ is 1} \\ -\log(1 - p_\beta(\mathbf{x})) & \text{if } y \text{ is 0} \end{cases}$$

$$l(\beta|\mathbf{x}, \mathbf{y}) = \sum_{k=1}^n y_k \log p_\beta(\mathbf{x}_k) + (1 - y_k) \log(1 - p_\beta(\mathbf{x}_k))$$

Regression example

$$p(y_k|x_k, \beta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(y_k - \beta \cdot x_k)^2}{\sigma^2}\right)$$

$$\min_{\beta} - \sum_{k=1}^N \log p(y_k|x_k, \beta)$$



Exercise: Plug in p and see what you get!

Regression Example

$$p(y_k|x_k, \beta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(y_k - \beta \cdot x_k)^2}{\sigma^2}\right)$$

$$\min_{\beta} - \sum_{k=1}^N \log p(y_k|x_k, \beta)$$

Answer: $\min_{\beta} \sum_{k=1}^N (y_k - \beta \cdot x_k)^2$

- Thus ordinary least squares is just maximum likelihood under the assumption that the errors have a Gaussian distribution! (Recall we assumed this in lecture.)
- This makes sense because of CLT.
- More on this in a separate lecture.

General Framework

$$\min_{\beta} - \sum_{k=1}^N \log p(y_k | x_k, \beta)$$

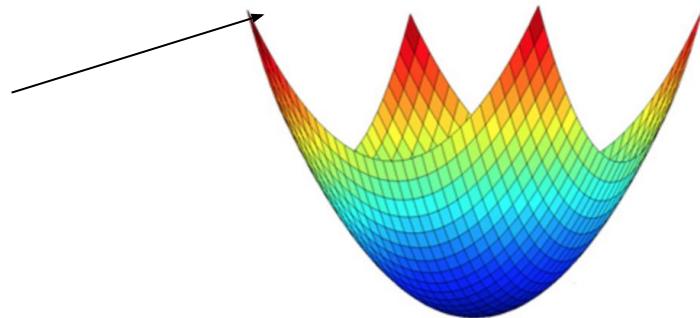
- Our goal before was to minimize an expected loss. This can now be interpreted as maximizing the likelihood of the observations conditioned on x and the parameters.
- This is a very general concept in machine learning. **The L2 norm only came about as a result of the Gaussian assumption with constant variances.**

How do we maximize this?

$$\prod_{k=1}^N p^{y_k} (1-p)^{1-y_k} = \prod_{k=1}^N \frac{\exp(y_k \beta \cdot \mathbf{x})}{1 + \exp(\beta \cdot \mathbf{x})}$$

$$l(\beta|x, y) = \sum_{k=1}^n y_k \log p(x_k) + (1 - y_k) \log(1 - p(x_k))$$

Claim: $\beta \mapsto l(\beta|x, y)$ is convex



Setting up Gradient Descent

$$l(\beta|x, y) = \sum_{k=1}^n y_k \log p(x_k) + (1 - y_k) \log(1 - p(x_k))$$

$$\frac{\partial l}{\partial \beta_i} = \sum_{k=1}^N (y_k - p(x_k)) x_{ki}$$

Notice that when **y is 1, then p should be 1,**
and when **y is 0, p should be 0.**

$$\frac{\partial^2 l}{\partial \beta_i \partial \beta_j} = - \sum_{k=1}^n p(x_k)(1 - p(x_k)) x_{ki} x_{kj}$$

Why we need this?

- This is our first encounter with a **minimization problem that doesn't have an analytical solution** - hence we **need to use gradient descent to reach a minimum**.
- The **method of maximum likelihood is used to solve almost all parametric problems in machine learning**. We will cover this more thoroughly in a few lectures.

Concrete Example

Admission based on test scores

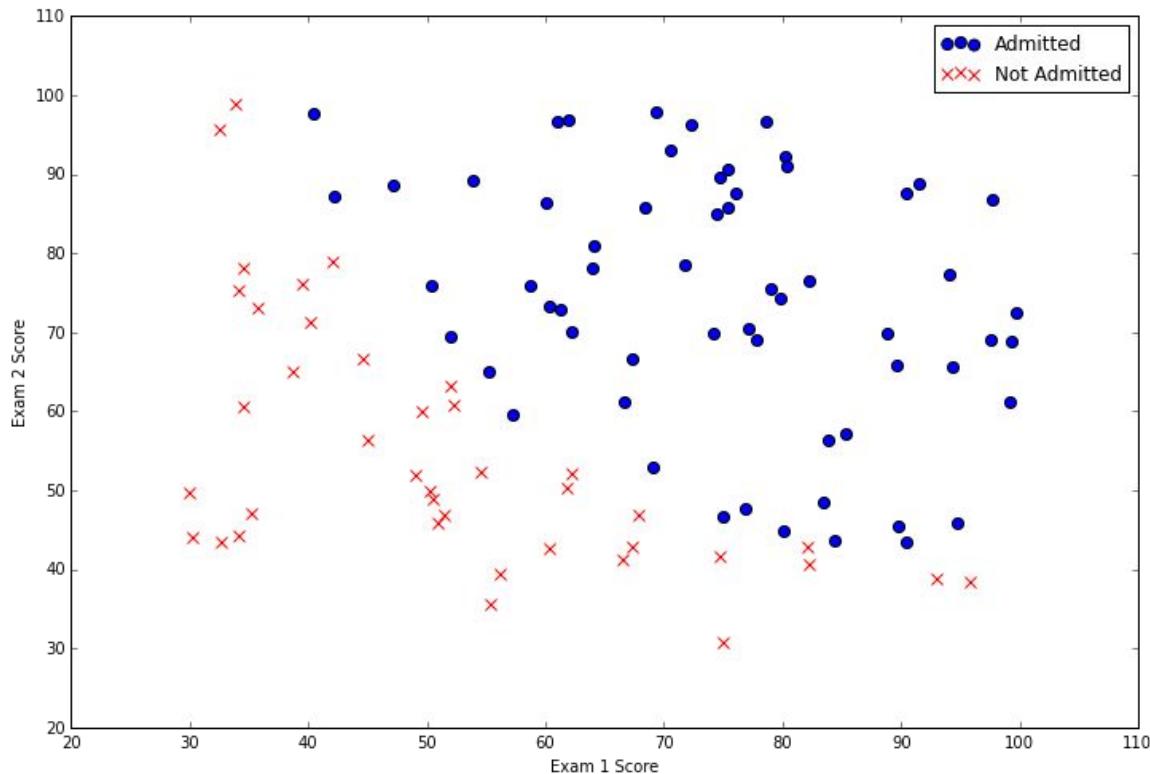
Example - Admission to a doctoral program

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline

import os
path = os.getcwd() + '\data\ex2data1.txt'
data = pd.read_csv(path, header=None, names=['Exam 1', 'Exam 2', 'Admitted'])
data.head()
```

	Exam 1	Exam 2	Admitted
0	34.623660	78.024693	0
1	30.286711	43.894998	0
2	35.847409	72.902198	0
3	60.182599	86.308552	1
4	79.032736	75.344376	1

Scatter plot of admission results



Python code

```
def sigmoid(z):  
    return 1 / (1 + np.exp(-z))
```

```
def cost(theta, X, y):  
    theta = np.matrix(theta)  
    X = np.matrix(X)  
    y = np.matrix(y)  
    first = np.multiply(-y, np.log(sigmoid(X * theta.T)))  
    second = np.multiply((1 - y), np.log(1 - sigmoid(X * theta.T)))  
    return np.sum(first - second) / (len(X))
```

Gradient Calculation

$$\frac{\partial l}{\partial \beta_i} = \sum_{k=1}^N (y_k - p(x_k)) x_{ki}$$

```
def gradient(theta, X, y):
    theta = np.matrix(theta)
    X = np.matrix(X)
    y = np.matrix(y)

    parameters = int(theta.ravel().shape[1])
    grad = np.zeros(parameters)

    error = sigmoid(X * theta.T) - y

    for i in range(parameters):
        term = np.multiply(error, X[:,i])
        grad[i] = np.sum(term) / len(X)

    return grad
```

Minimizing Cost in Python

$$\text{Cost}_2(p_\beta(\mathbf{x}), y) = \begin{cases} -\log p_\beta(\mathbf{x}) & \text{if } y \text{ is 1} \\ -\log(1 - p_\beta(\mathbf{x})) & \text{if } y \text{ is 0} \end{cases}$$

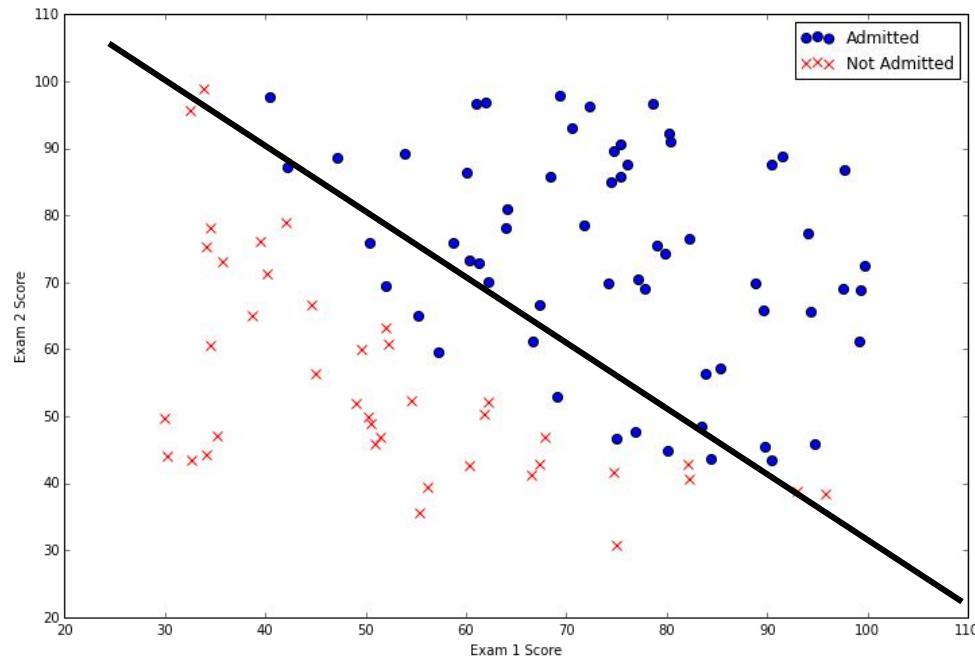
```
import scipy.optimize as opt

result = opt.fmin_tnc(func=cost, x0=theta, fprime=gradient, args=(X, y))

cost(result[0], X, y)
```

0.20357134412164668

Final Decision Boundary



$$p_{\beta}(\mathbf{x}) = \frac{1}{1 + \exp(-\beta^T \cdot \mathbf{x})}$$

How do we measure performance of a classifier?

Accuracy

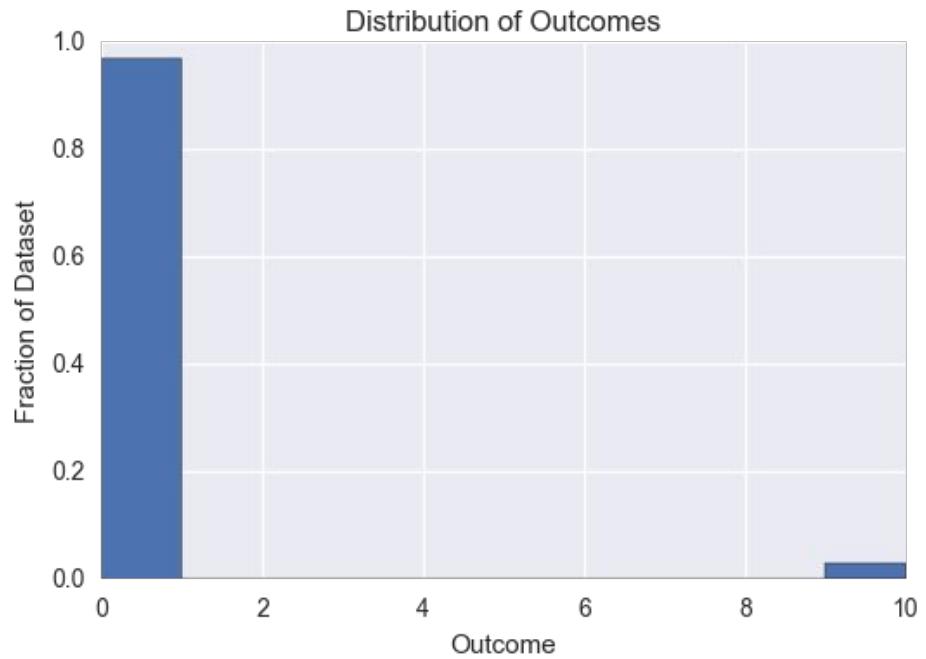
$$\frac{1}{N} \sum_{i=1}^N \mathbf{1}(y_i = f(x_i))$$

- # of correct predictions / # of samples.

Easy to understand, but not a good metric in general. Why?

What would be a good model here?

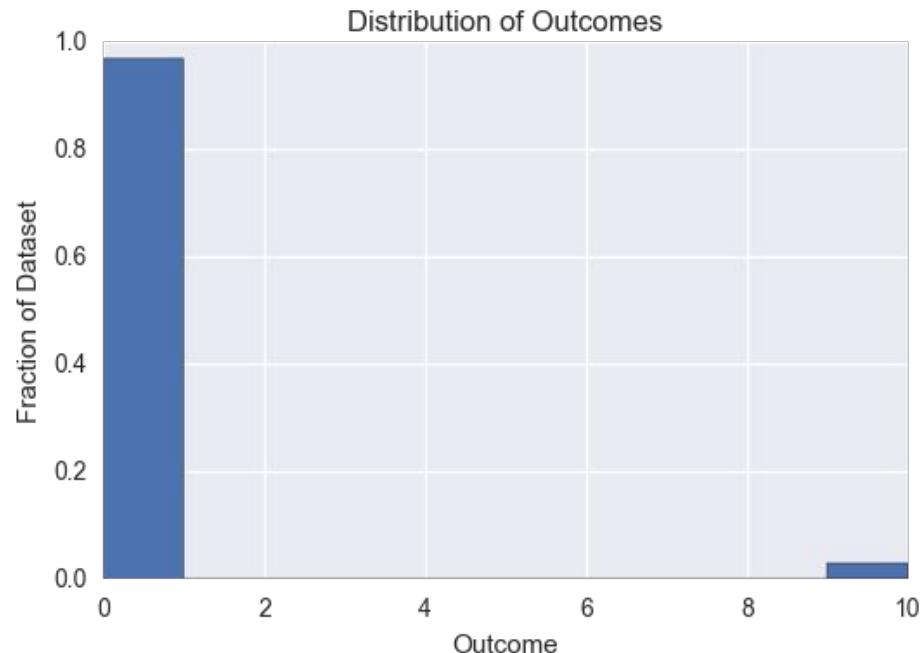
$$\frac{1}{N} \sum_{i=1}^N \mathbf{1}(y_i = f(x_i))$$



What would be a good model here?

$$\frac{1}{N} \sum_{i=1}^N \mathbf{1}(y_i = f(x_i))$$

- If we just set $\mathbf{y} = \mathbf{0}$, we will have **97% accuracy!**
- Accuracy is a useless measure unless you break it into deciles or have a balanced dataset.



What's wrong with accuracy?

- In any scenario I've encountered thus far, datasets are ***heavily*** imbalanced. This means one outcome occurs much more frequently than the alternative. **Examples are:** users subscribing, churning, clicking etc.
- In general, you have **thousands, if not millions of impressions**, but maybe only **1-10% (or less) of the outcome variable** you are interested in.
- If we create a model which simply sets $y=0$, we will have incredible accuracy - what does that mean though?

Primary Methods Used

For measuring the performance of models,

There are two standards:

- AUC ROC (area under ROC curve) .
(good for scientists)
- Accuracy as a function of percentile of propensity.
(good for stakeholders)



AUC ROC and Lift Curves

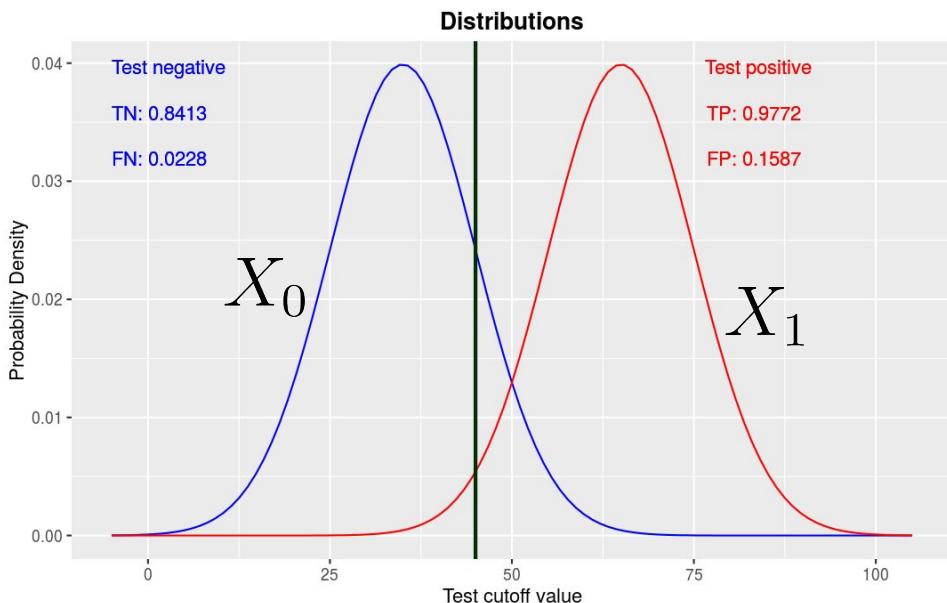
Example - Income Data Set

Question: Does the individual make over \$50k? (yes/no)

Variables:

- **age:** continuous.
- **workclass:** Private, Self-emp-not-inc, Self-emp-inc, Federal-gov, Local-gov, State-gov, Without-pay, Never-worked.
- **education:** Bachelors, Some-college, 11th, HS-grad, Prof-school, Assoc-acdm, Assoc-voc, 9th, 7th-8th, 12th, Masters, 1st-4th, 10th, Doctorate, 5th-6th, Preschool.
- **education-num:** continuous.
- **marital-status:** Married-civ-spouse, Divorced, Never-married, Separated, Widowed, Married-spouse-absent, Married-AF-spouse.
- **occupation:** Tech-support, Craft-repair, Other-service, Sales, Exec-managerial, Prof-specialty, Handlers-cleaners, Machine-op-inspct, Adm-clerical, Farming-fishing, Transport-moving, Priv-house-serv, Protective-serv, Armed-Forces.
- **relationship:** Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried.
- **race:** White, Asian-Pac-Islander, Amer-Indian-Eskimo, Other, Black.
- **sex:** Female, Male.
- **capital-gain:** continuous.
- **capital-loss:** continuous.
- **hours-per-week:** continuous.
- **native-country:**

Plotting a classifier

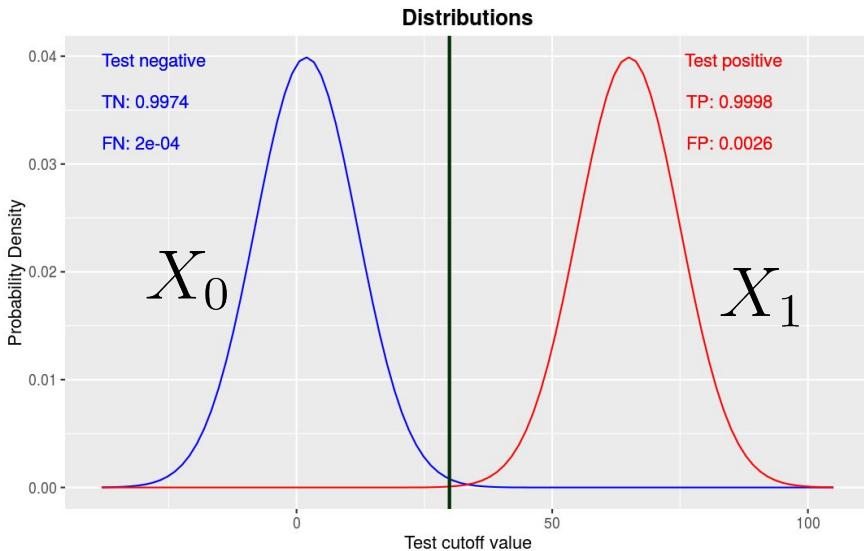


$$X_1 = p_{\beta}(x|y = 1)$$

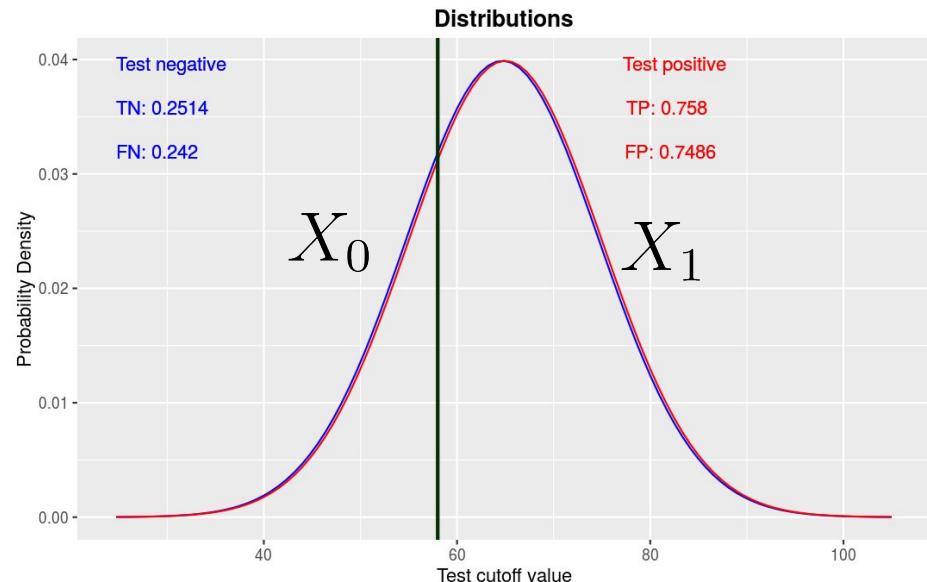
$$X_0 = p_{\beta}(x|y = 0)$$

- Intuitively speaking, we wish to somehow measure **how well our classifier can separate these two distributions.**

Perfect versus Random

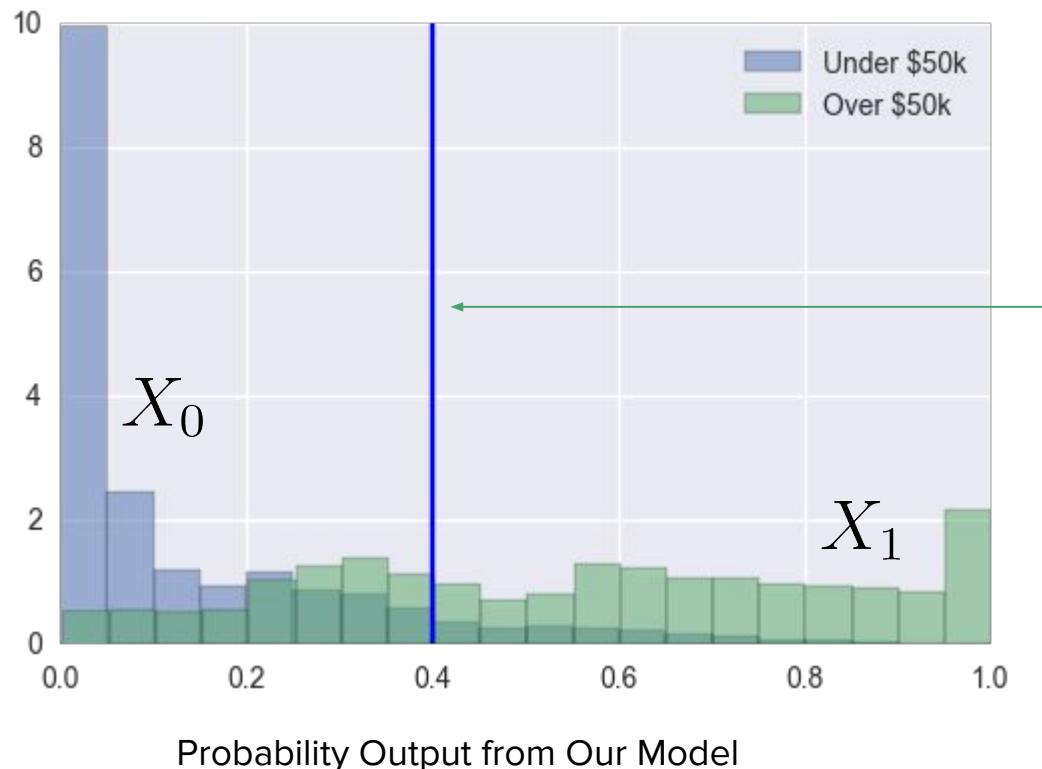


A perfect classifier is able to separate the two classes (1 and 0) completely.



A completely random classifier can't make any distinction.

Adult Data Set Example



- A good classifier is one which separates the two distributions well.
- After assigning ‘scores’, we often want to find a good threshold to separate the classes. How do we do this?

Definitions

- We **predict 0** while we should have the **class is actually 0**: this is called a **True Negative**, i.e. we correctly predict that the class is negative (0). For example, an antivirus did not detect a harmless file as a virus .
- We **predict 0** while we should have the **class is actually 1**: this is called a **False Negative**, i.e. we incorrectly predict that the class is negative (0). For example, an antivirus failed to detect a virus.
- We **predict 1** while we should have the **class is actually 0**: this is called a **False Positive**, i.e. we incorrectly predict that the class is positive (1). For example, an antivirus considered a harmless file to be a virus.
- We **predict 1** while we should have the **class is actually 1**: this is called a **True Positive**, i.e. we correctly predict that the class is positive (1). For example, an antivirus rightfully detected a virus.

Confusion Matrix

		Predicted class	
		Class 1	Class 0
Actual class	Class 1	10 true positives (TP)	2 false negatives (FN)
	Class 0	3 false positives (FP)	35 true negatives (TN)

In this example of a confusion matrix, among the **50 data points** that are classified, **45 are correctly classified** and the **5 are misclassified**.

True positive and False Positive Rates

- True positive rate (**TPR**), aka. sensitivity, hit rate, and recall, which is defined as

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

- Intuitively this metric corresponds to the proportion of positive data points that are correctly considered as positive, with respect to all positive data points. In other words, the higher TPR, the fewer positive data points we will miss.
- False positive rate (**FPR**), aka. fall-out, which is defined as

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

- Intuitively this metric corresponds to the proportion of negative data points that are mistakenly considered as positive, with respect to all negative data points. In other words, the higher FPR, the more negative data points we will misclassified.

An example calculation

		Predicted class	
		Class 1	Class 0
Actual class	Class 1	10 true positives (TP)	2 false negatives (FN)
	Class 0	3 false positives (FP)	35 true negatives (TN)

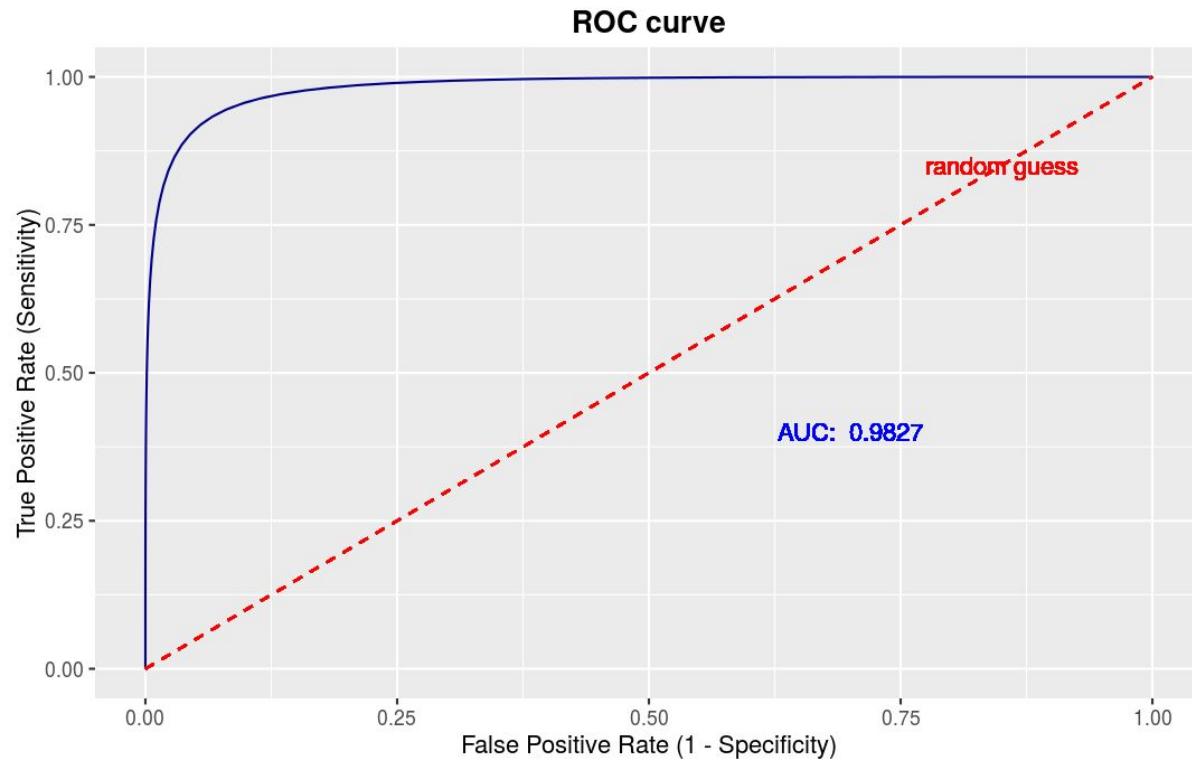
$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}} = \frac{10}{10 + 2}$$

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}} = \frac{3}{3 + 35}$$

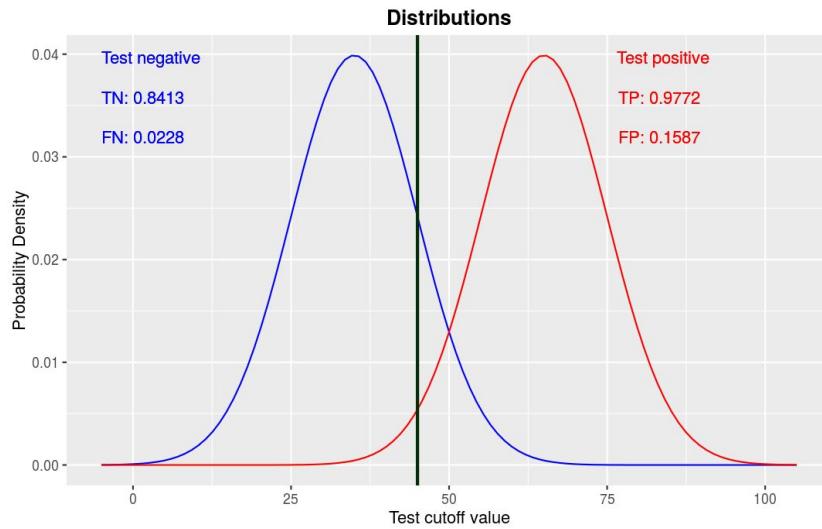
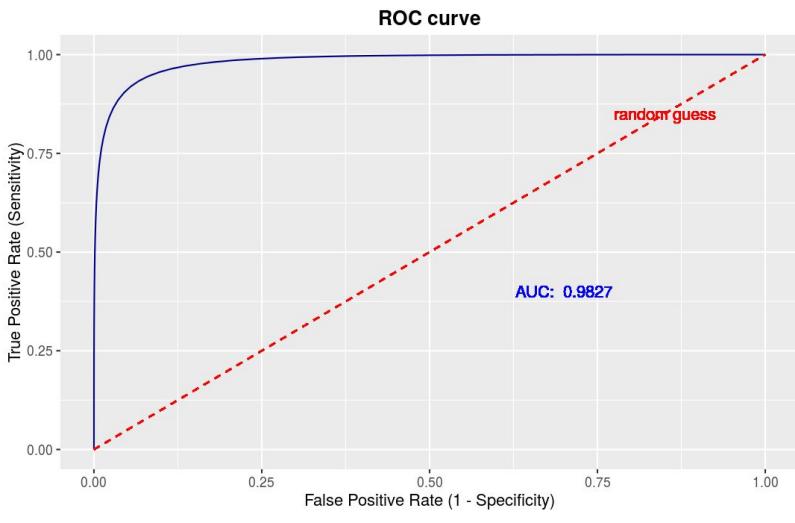
Confusion Matrices

A			B			C			C'		
TP=63	FN=37	100	TP=77	FN=23	100	TP=24	FN=76	100	TP=76	FN=24	100
FP=28	TN=72	100	FP=77	TN=23	100	FP=88	TN=12	100	FP=12	TN=88	100
91	109	200	154	46	200	112	88	200	88	112	200
TPR = 0.63			TPR = 0.77			TPR = 0.24			TPR = 0.76		
FPR = 0.28			FPR = 0.77			FPR = 0.88			FPR = 0.12		
PPV = 0.69			PPV = 0.50			PPV = 0.21			PPV = 0.86		
F1 = 0.66			F1 = 0.61			F1 = 0.22			F1 = 0.81		
ACC = 0.68			ACC = 0.50			ACC = 0.18			ACC = 0.82		

ROC Curve

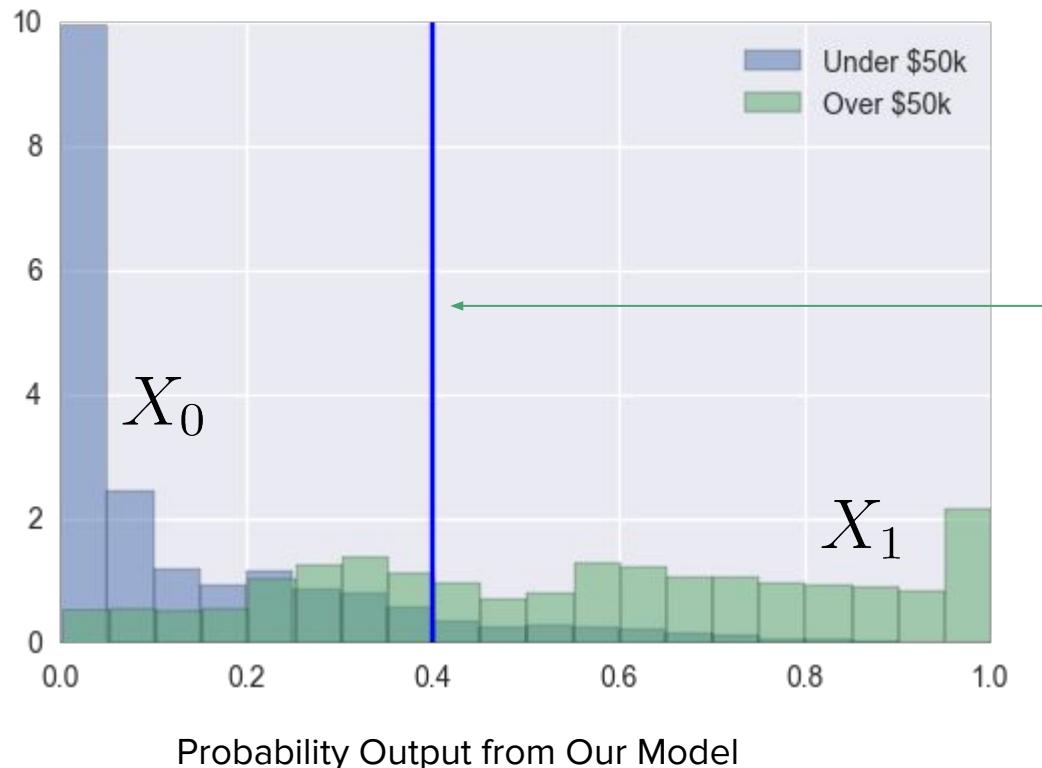


ROC Curve



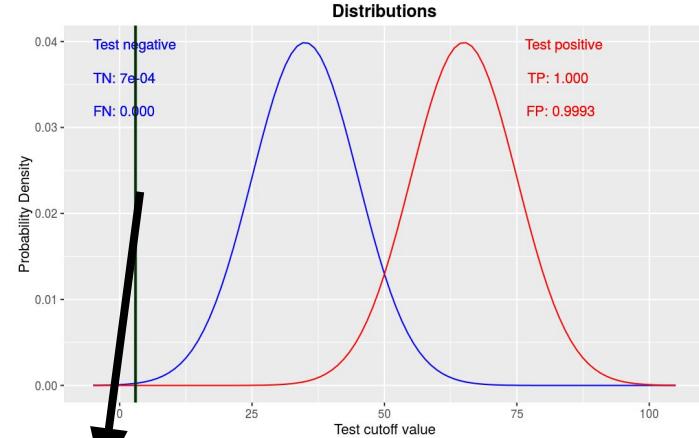
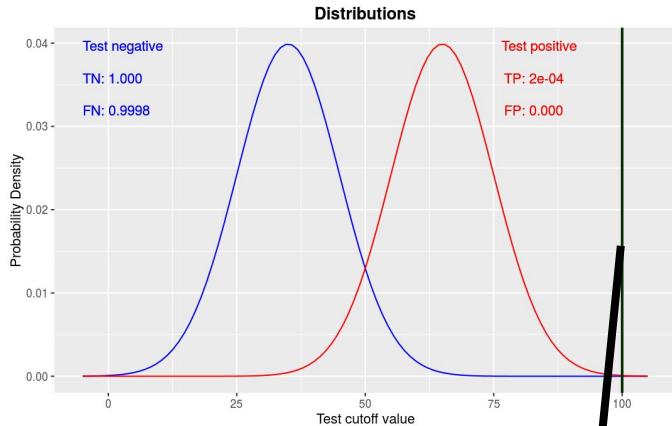
Note: We learn the model on training data. The plot to the right is done on testing data. i.e. The goal of this is to see how well our scores separate the two actual distributions.

Adult Data Set Example

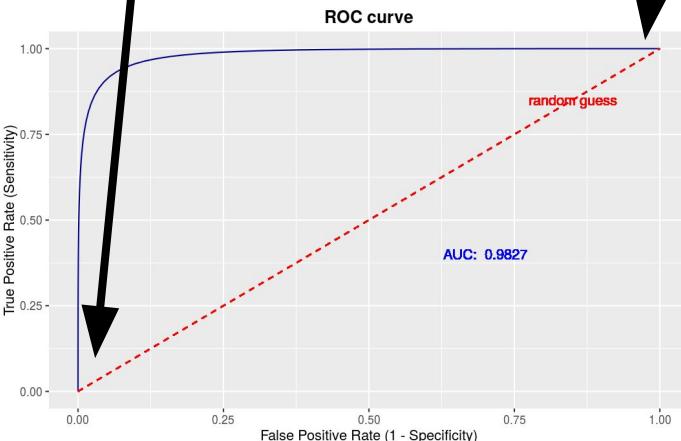


- A good classifier is one which separates the two distributions well.
- This is plotting distributions of scores on testing data (unseen data not used to learn the model), and seeing how well they separate the two outcomes (1 and 0).

Extreme thresholds

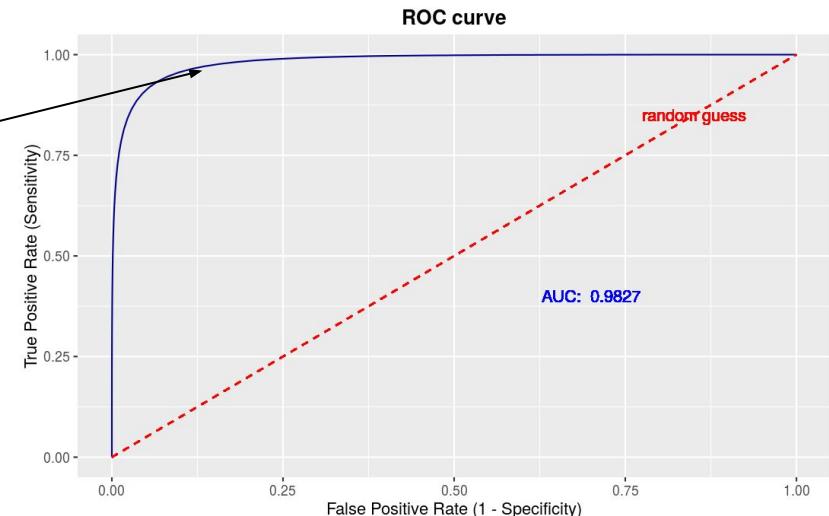
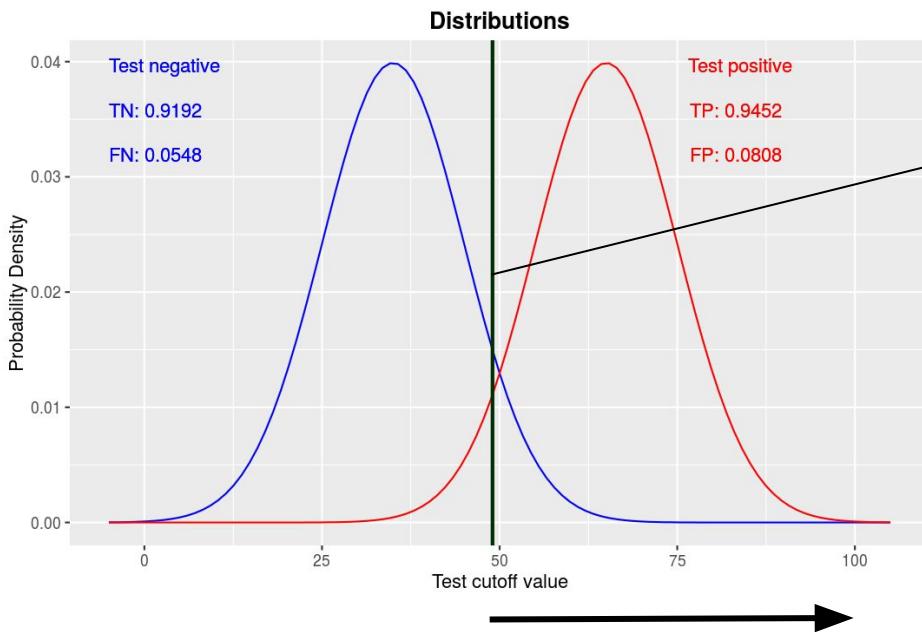


- Need 100% probability to be the red class.
- Assigns 0 to everything.



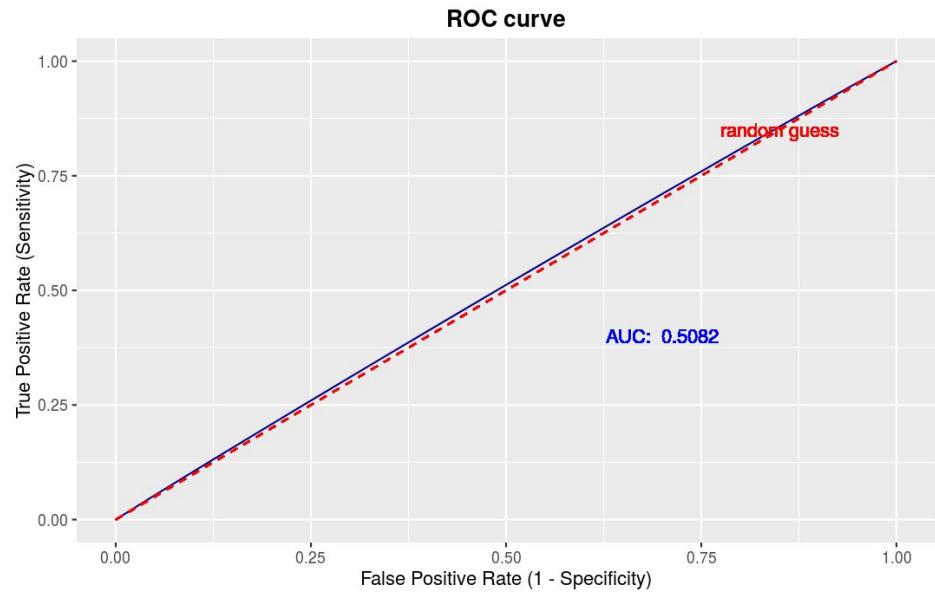
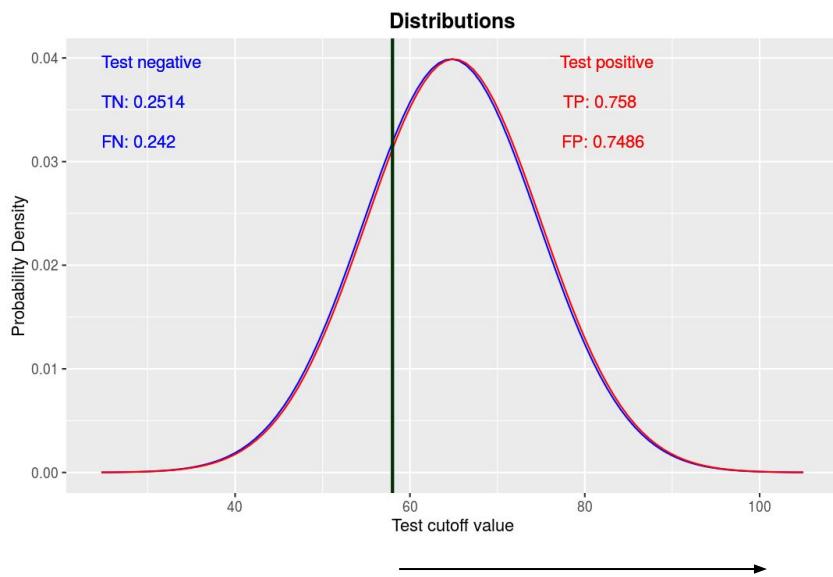
- Need above 0% probability to be in the red class.
- Assigns 1 to everything.

A cut off point



TPR/FPR (Test Cut Off) = (Area To Right Under Blue, Area To Right Under Red)

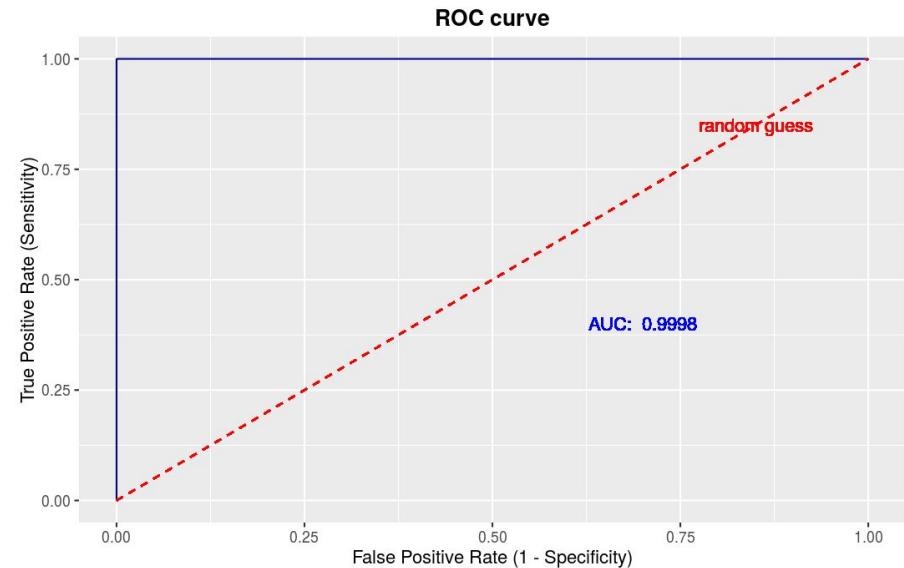
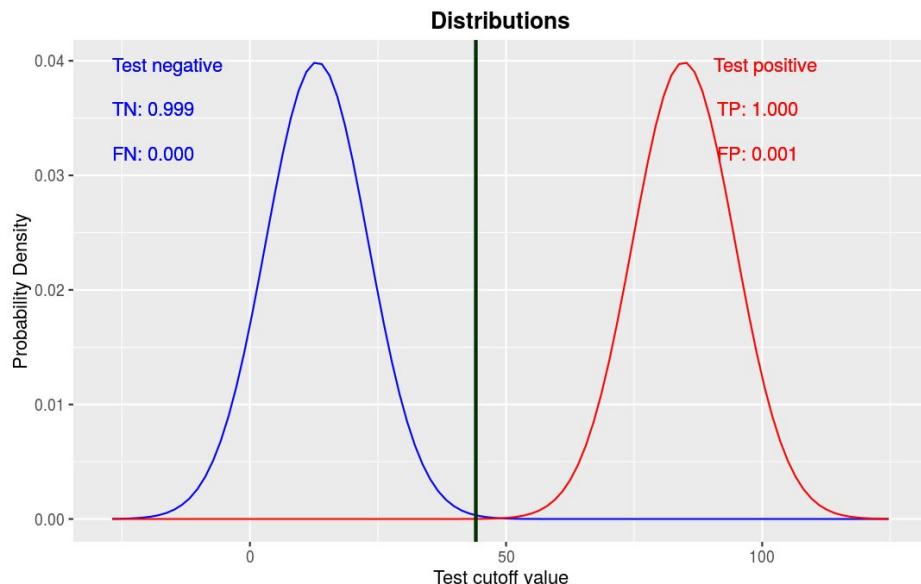
ROC of a Random Classifier



TPR/FPR (Test Cut Off) = (Area To Right Under Blue, Area To Right Under Red) = 0.5

A **random classifier** has an **AUC ROC** of 0.5

ROC of a perfect classifier



TPR/FPR (Test Cut Off) = (Area To Right Under Blue, Area To Right Under Red) = 1.0

A **perfect classifier** has an **AUC ROC of 1**

Python Example

```
from sklearn.datasets import make_classification
from sklearn.linear_model import LogisticRegression
import numpy as np
X, y = make_classification(n_samples=10000, n_features=10, n_c
df_X=pd.DataFrame(X)
y_vals=np.array(y)
Xtrain = X[:9900]
Xtest = X[9900:]
ytrain = y[:9900]
ytest = y[9900:]

clf = LogisticRegression()
clf.fit(Xtrain, ytrain)
```

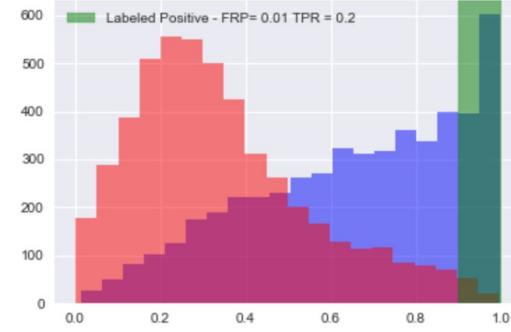
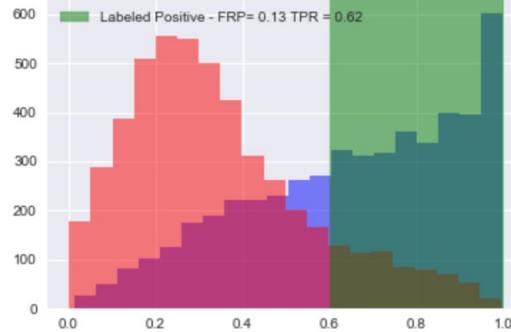
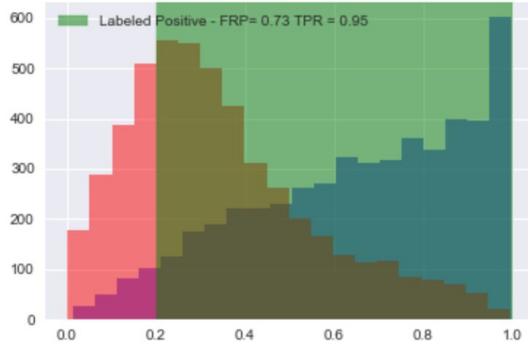
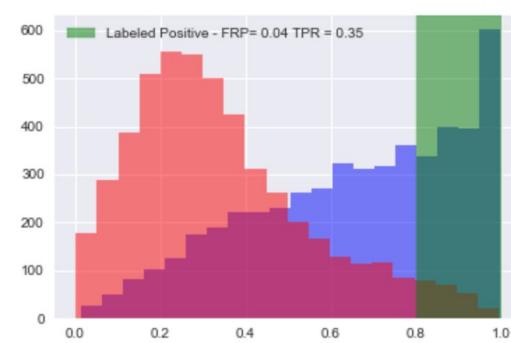
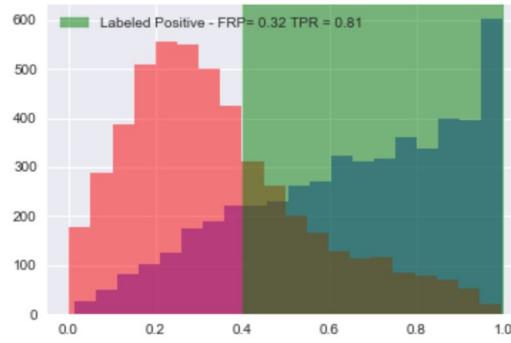
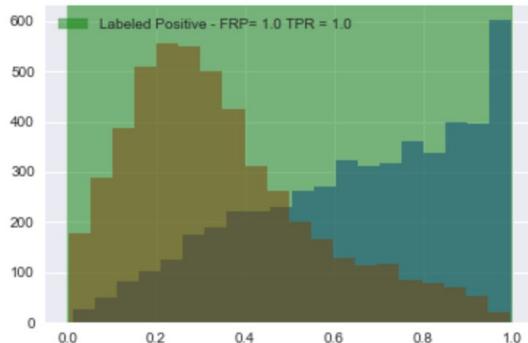
Let's make our predictions now

```
from sklearn import metrics  
import pandas as pd  
%matplotlib inline  
  
df_X=pd.DataFrame(X)  
df_X['score']=clf.predict_proba(df_X)[:,1]  
df_X['outcome']=y_vals
```

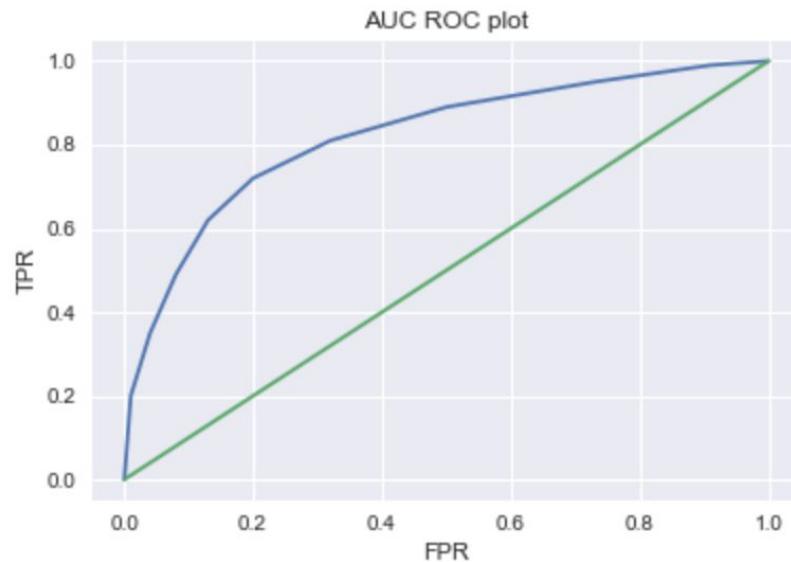
Plot ROC curves

```
import seaborn
import matplotlib.pyplot as plt
fprs=[]
tprs=[]
for i in range(0,11):
    threshold = float(i)/10
    print (threshold)
    fig, ax = plt.subplots()
    df_X[df_X['outcome']==1]['score'].hist(bins=20,color='b',alpha=0.5)
    df_X[df_X['outcome']==0]['score'].hist(bins=20,color='r',alpha=0.5)
    fpr = np.round(len(df_X[(df_X['outcome']==0) & (df_X['score']>threshold)]) / len(df_X[df_X['outcome']==0]),2)
    tpr = np.round(len(df_X[(df_X['outcome']==1) & (df_X['score']>threshold)]) / len(df_X[df_X['outcome']==1]),2)
    fprs.append(fpr)
    tprs.append(tpr)
    ax.axvspan(threshold, 1, alpha=0.5, color='g',label='Labeled Positive - FPR= ' + str(fpr)+ ' TPR = ' + str(tpr))
    plt.legend()
    plt.savefig("../img/roc_" + str(i) + ".png")
    plt.show()
```

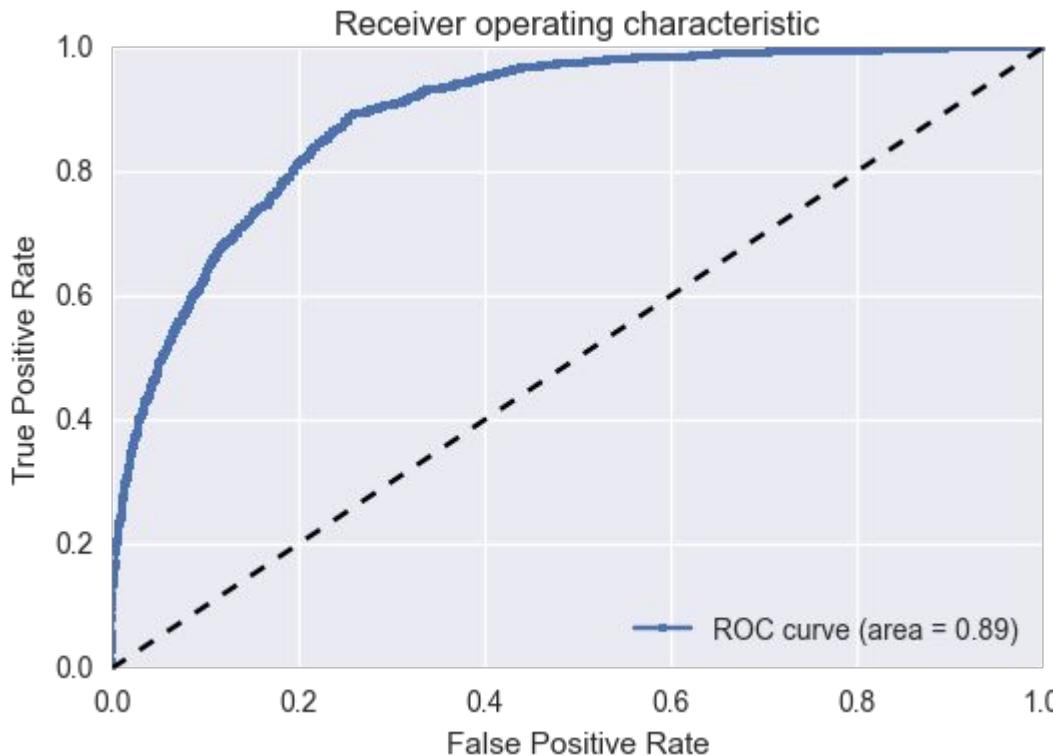
Varying Thresholds



Now that we've calculated all of the true positive rates (TPR) and false positive rates (FPR), let's plot them:

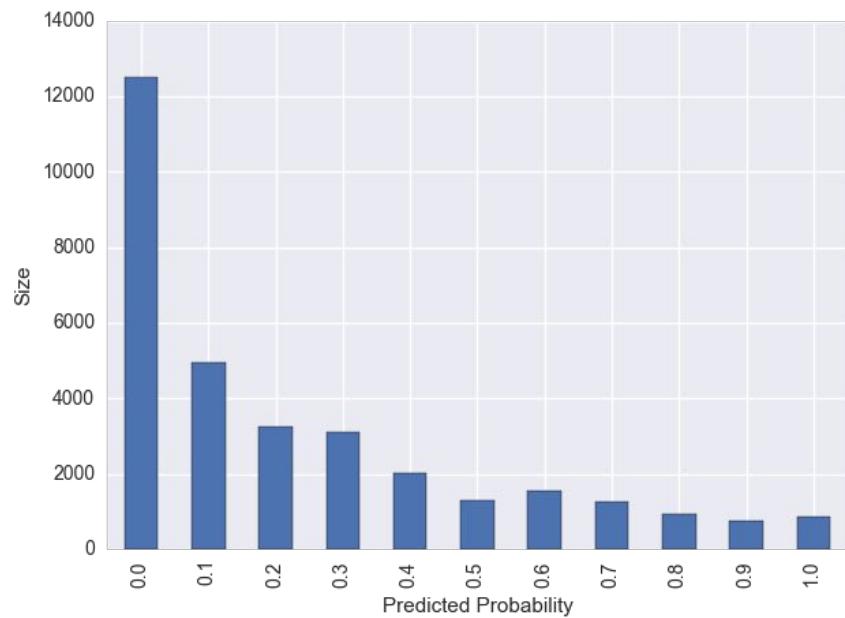
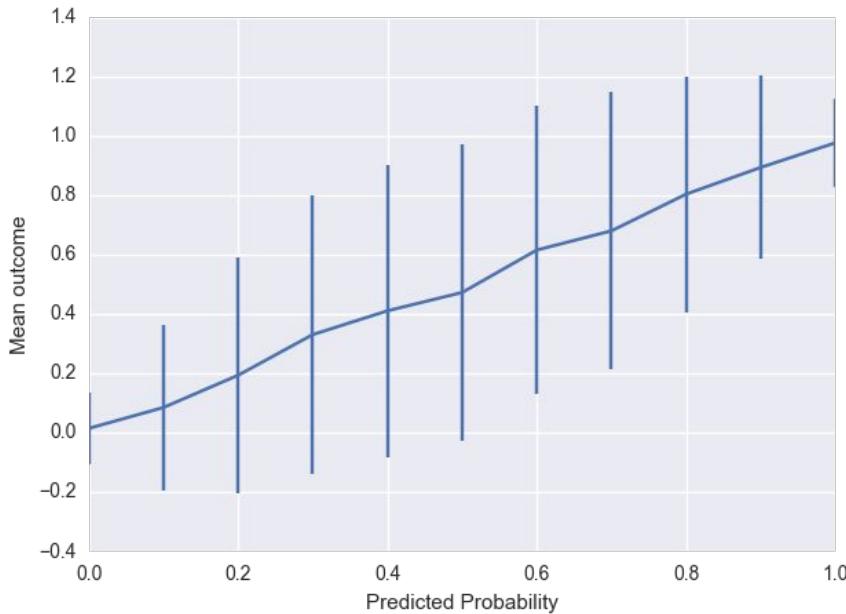


Predicting income over \$50k



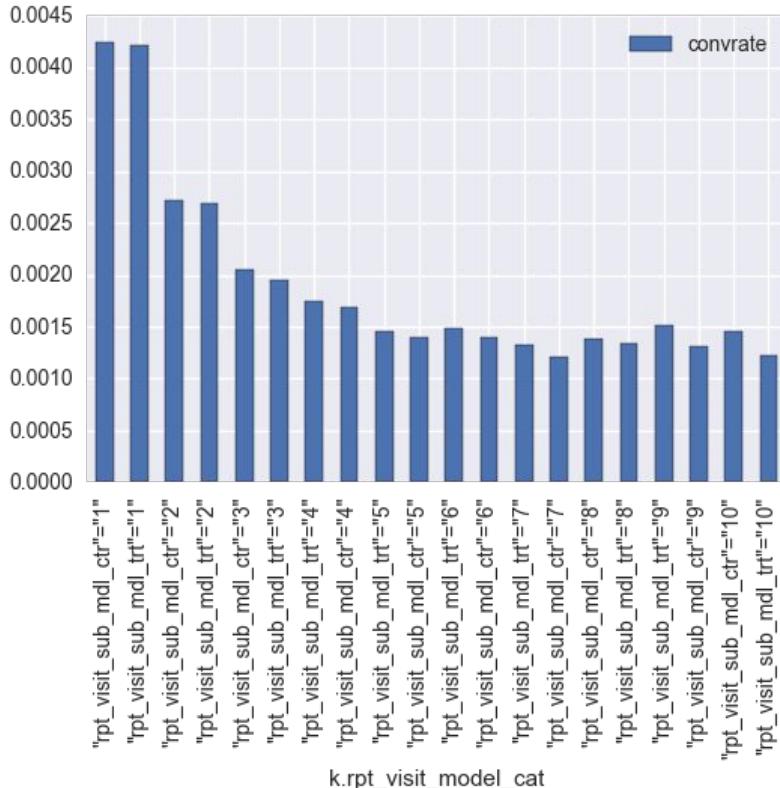
- In the notebook example on Github, we find the AUC ROC is 0.9 which is very good.
- In general, anything over 0.7 is good, anything over 0.8 is amazing, and anything over 0.9 is suspicious (more on this later).

Accuracy as a function of propensity



- These plots are easily understood by non-technical people.
- Also useful when you run experiments to understand the impact of an action on people with a particular propensity.

Example: Acquisition for The New Yorker

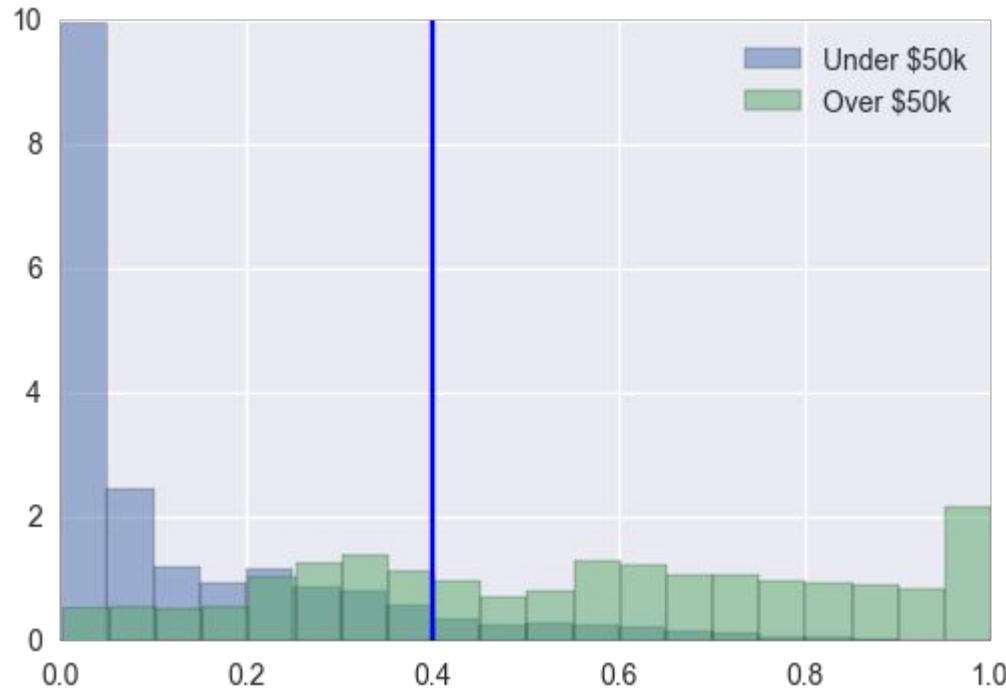


- In practice one often wants to see how an experiment affects different deciles of propensity.
- Before we launch (March 01) we wanted to see if
 - a) Is the model working?
 - b) Are the deciles evenly bucketed?
- **Why?** We want to measure the impact of the experiment on each decile separately. Maybe high propensity users react differently?

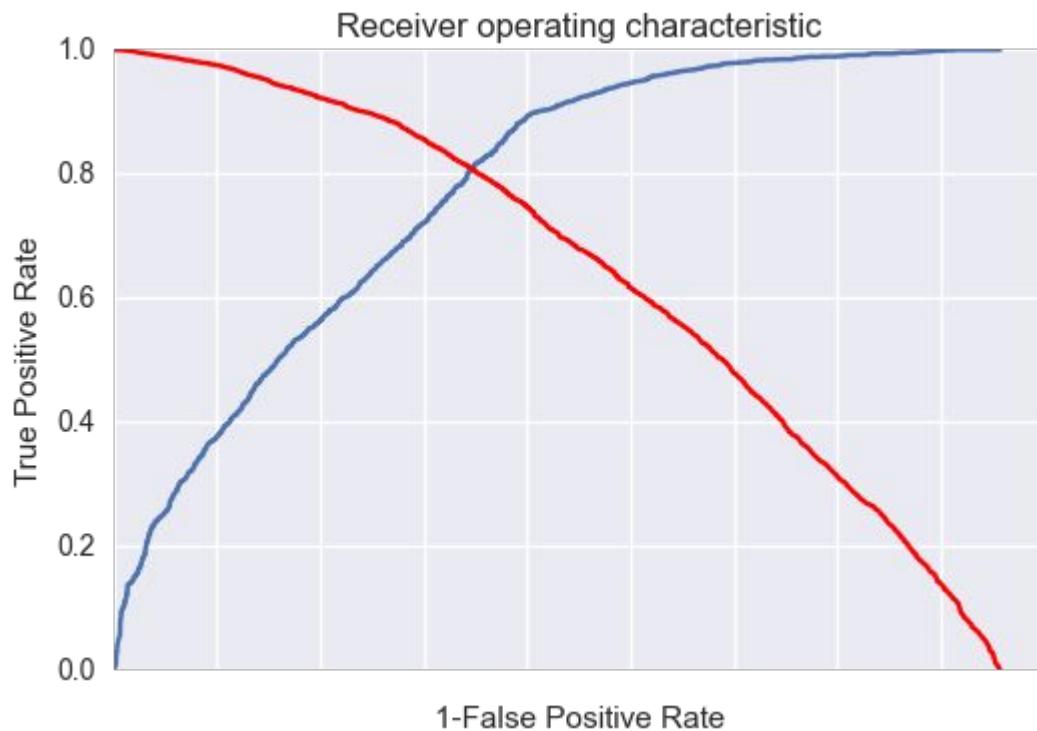
Choosing a cutoff

What is the best cutoff for our model?

What's the best cut off point?



The best cut off



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

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

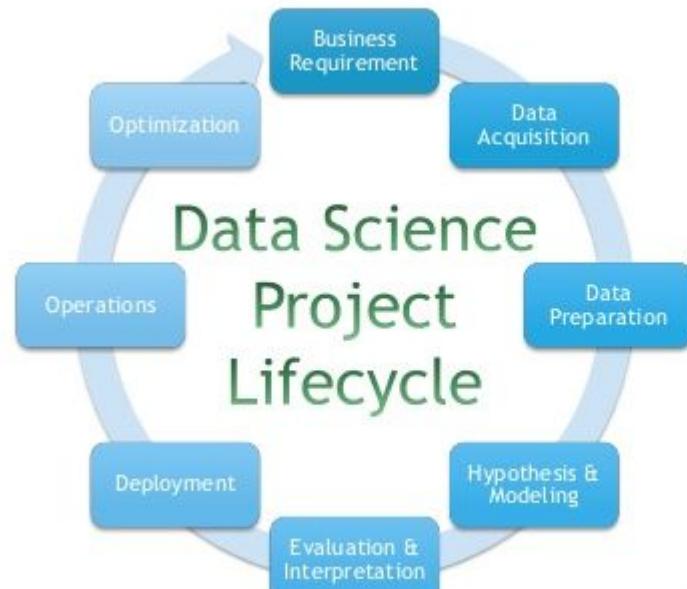
We want TPR to be large and FPR to be small.

How do we evaluate a model? Appendix

		Predicted condition			
Total population		Predicted Condition positive	Predicted Condition negative	Prevalence = $\frac{\sum \text{Condition positive}}{\sum \text{Total population}}$	
True condition	condition positive	True positive	False Negative (Type II error)	True positive rate (TPR), Sensitivity, Recall, probability of detection $= \frac{\sum \text{True positive}}{\sum \text{Condition positive}}$	False negative rate (FNR), Miss rate $= \frac{\sum \text{False negative}}{\sum \text{Condition positive}}$
	condition negative	False Positive (Type I error)	True negative	False positive rate (FPR), Fall-out, probability of false alarm $= \frac{\sum \text{False positive}}{\sum \text{Condition negative}}$	True negative rate (TNR), Specificity (SPC) $= \frac{\sum \text{True negative}}{\sum \text{Condition negative}}$
Accuracy (ACC) = $\frac{\sum \text{True positive} + \sum \text{True negative}}{\sum \text{Total population}}$	Positive predictive value (PPV), Precision $= \frac{\sum \text{True positive}}{\sum \text{Test outcome positive}}$	False omission rate (FOR) $= \frac{\sum \text{False negative}}{\sum \text{Test outcome negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) $= \frac{\text{LR}^+}{\text{LR}^-}$	
	False discovery rate (FDR) $= \frac{\sum \text{False positive}}{\sum \text{Test outcome positive}}$	Negative predictive value (NPV) $= \frac{\sum \text{True negative}}{\sum \text{Test outcome negative}}$	Negative likelihood ratio (LR-) = $\frac{\text{FNR}}{\text{TNR}}$		

~ ~ ~

Project Lifecycle



Optimizing your model

Regularization and feature selection

Model Optimization

- Just as with regression, we risk over fitting our model if we include too many variables.
- We also risk instability and lack of confidence in variables if we have collinear features.
- The same methods are used to optimize models in classification problems, but our metric for evaluating performance is now AUC ROC and not R^2.

Updating Maximum Likelihood Function

$$\mathcal{L}(\beta | (x_1, y_1), \dots, (x_n, y_n)) = \prod_{k=1}^N p(y_k | x_k, \beta) = \prod_{k=1}^N p^{y_k} (1 - p)^{y_k}$$

$$\min_{\beta} - \sum_{k=1}^N \log p(y_k | x_k, \beta)$$

$$\min_{\beta} - \sum_{k=1}^N \log p(y_k | x_k, \beta) + \lambda \sum_{m=1}^M |\beta_m|^p$$

This is our regularization term which we've added to our cost function, just as we did for ordinary least squares regression.

Regularization for Classification

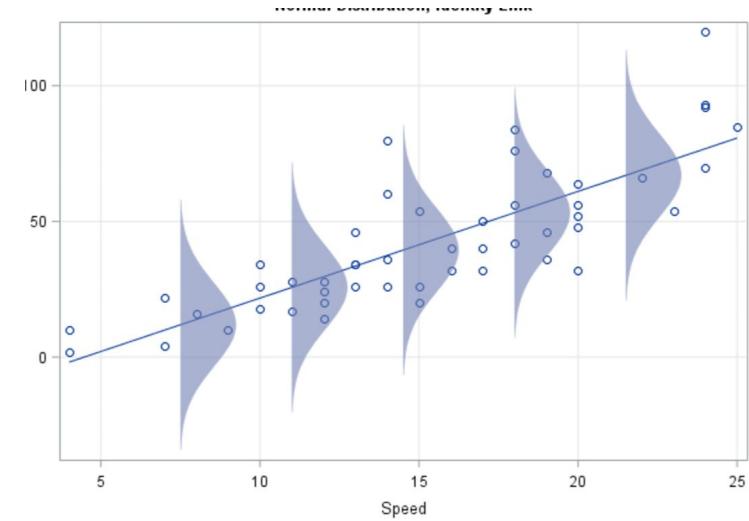
$$\min_{\beta} - \sum_{k=1}^n \log p(y_i | x_i, \beta) + \lambda \sum_{m=1}^M |\beta_m|^p$$

- As before, we want to find the **lambda which results in the best performance on test data.**
- Here though we will use **AUC ROC as our performance metric.**

Regression interpretation

$$p(y_k|x_k, \beta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(y_k - \beta \cdot x_k)^2}{\sigma^2}\right)$$

$$\min_{\beta} - \sum_{k=1}^N \log p(y_k|x_k, \beta)$$



Exercise: Plug in p and see what you get!

Regression interpretation

$$p(y_k|x_k, \beta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(y_k - \beta \cdot x_k)^2}{\sigma^2}\right)$$

$$\min_{\beta} - \sum_{k=1}^N \log p(y_k|x_k, \beta)$$

Answer: $\min_{\beta} \sum_{k=1}^N (y_k - \beta \cdot x_k)^2$

- Thus ordinary least squares is just maximum likelihood under the assumption that the errors have a Gaussian distribution! (Recall we assumed this in lecture.)
- This makes sense because of CLT.
- More on this in a separate lecture.

Example - Income Data Set

Question: Does the individual make over \$50k? (yes/no)

Variables:

- **age:** continuous.
- **workclass:** Private, Self-emp-not-inc, Self-emp-inc, Federal-gov, Local-gov, State-gov, Without-pay, Never-worked.
- **education:** Bachelors, Some-college, 11th, HS-grad, Prof-school, Assoc-acdm, Assoc-voc, 9th, 7th-8th, 12th, Masters, 1st-4th, 10th, Doctorate, 5th-6th, Preschool.
- **education-num:** continuous.
- **marital-status:** Married-civ-spouse, Divorced, Never-married, Separated, Widowed, Married-spouse-absent, Married-AF-spouse.
- **occupation:** Tech-support, Craft-repair, Other-service, Sales, Exec-managerial, Prof-specialty, Handlers-cleaners, Machine-op-inspct, Adm-clerical, Farming-fishing, Transport-moving, Priv-house-serv, Protective-serv, Armed-Forces.
- **relationship:** Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried.
- **race:** White, Asian-Pac-Islander, Amer-Indian-Eskimo, Other, Black.
- **sex:** Female, Male.
- **capital-gain:** continuous.
- **capital-loss:** continuous.
- **hours-per-week:** continuous.
- **native-country:**

Outline

1. Inspect the data, convert categorical variables to new features. Convert string based variables to numerical values.
2. Train the model using Logistic Regression.
3. Evaluate performance using AUC ROC and accuracy vs percentile.
4. Check for collinear features and plot the correlation matrix.
5. Optimize by using L1 and L2 regularization (measuring performance on testing data).

A look at the data

In [272]: df.head()

Out[272]:

	Age	Workclass	Sector	Education	Education-num	Marital-Status	Occupation	Relationship	Race	Sex	Capital-Gain	Capital-Loss	Hours-Per-Week	Native-Country	y
0	39	State-gov	77516	Bachelors	13	Never-married	Adm-clerical	Not-in-family	White	Male	2174	0	40	United-States	<=50K
1	50	Self-emp-not-inc	83311	Bachelors	13	Married-civ-spouse	Exec-managerial	Husband	White	Male	0	0	13	United-States	<=50K
2	38	Private	215646	HS-grad	9	Divorced	Handlers-cleaners	Not-in-family	White	Male	0	0	40	United-States	<=50K
3	53	Private	234721	11th	7	Married-civ-spouse	Handlers-cleaners	Husband	Black	Male	0	0	40	United-States	<=50K
4	28	Private	338409	Bachelors	13	Married-civ-spouse	Prof-specialty	Wife	Black	Female	0	0	40	Cuba	<=50K

Handling nulls/NAs

1. **Get rid of rows that have NAs.** (if there aren't that many NAs overall, or if there are rows consisting of mostly NAs)
2. **Get rid of columns that have NAs** (you may want to do this if a variable is mostly NAs)
3. **Imputation.** A common method is using the mean or median, or most frequent value for a discrete variable.
4. **Actually creating a new value for the nulls:** In some situations (for discrete variables) you might consider that the nulls "mean something". For example, say you have some variable, customer satisfaction after a phone call, and the values are Good (customer is satisfied), Bad (customer is not satisfied), NA (customer did not fill out survey after). In this situation you could choose to interpret the NA as neutral satisfaction. Fix any mislabeled classes that you discovered while summarizing the data.
5. **Remove any duplicate rows**

Prepping discrete variables

- **For regression you need to create dummy variables (also known as one hot encoding).**
 1. **Create binary variables for each category of the categorical variable.** Example: say you have some variable called, “Weather”, and the classes are, [sunny, rainy, cloudy]. The dummy variables will be 3 new variables, “sunny”, “rainy”, and “cloudy” and they each have values [0,1].
 2. **Drop one dummy variable.** Why? Well, its easier to understand it using a binary variable as an example. imagine if you have a binary variable like gender where the classes are [M,F]. If you create two new variables, one for “M” and one for “F” with both containing values [0,1], well then you just created two variables that are perfectly correlated. So you always need to drop one category. Read this for more explanation. To code this in python, you can use this in pandas. Don’t forget to use the drop_first argument.
 3. **Drop the original variable from the data frame**
 - *If you are not doing regression you may not need to create dummy variables. For example, a decision tree doesn’t need to only contain binary splits, although that is how it is most frequently done.*

How do we deal with categorical data?

id	Race	Sex	Capital-Gain
ily	White	Male	2174
	White	Male	0
ily	White	Male	0
	Black	Male	0
	Black	Female	0

- Notice two issues we encounter here:
 - Many of the variables are strings.
 - How can we input categorical features into a model?

$$y = \beta \cdot \text{male} \quad \text{makes no sense!}$$

How do we deal with categorical data?

Solution: Create dummy variables. This is also known as one-hot encoding.

```
In [339]: df_workclass=pd.get_dummies(df['Workclass'])
df_sector=pd.get_dummies(df['Sector'])
df_education=pd.get_dummies(df['Education'])
df_occupation=pd.get_dummies(df['Occupation'])
df_relationship = pd.get_dummies(df['Relationship'])
df_race = pd.get_dummies(df['Sex'])
df_country=pd.get_dummies(df['Native-Country'])
```

```
In [340]: df_final = pd.concat([df[['Age','Capital-Gain','Capital-Loss']],df_workclass,df_education,df_relationship,df_race,df_co
```

For each category (ie. Gender: MALE, FEMALE), we create a new column. The MALE column will be 1 when the person is male, 0 otherwise.

How do we deal with categorical data?

Solution: Create dummy variables. This is also known as one hot encoding.

```
In [565]: df['Sex'].head()
```

```
Out[565]: 0      Male  
1      Male  
2      Male  
3      Male  
4    Female  
Name: Sex, dtype: object
```

```
In [563]: df_final[[u' Female',u' Male']]
```

```
Out[563]:
```

	Female	Male
0	0	1
1	0	1
2	0	1
3	0	1
4	1	0

Convert the outcome variable

We convert the y variable into a binary outcome (do they make over 50k or not)

```
In [279]: def get_y(y):
    if y.find("<=")>-1:
        return 0
    else:
        return 1
```

Now that the **data is processed**, we can **train a model** and **evaluate its performance**.

```
In [9]: # X are features and y is predictive variable - cancelled HD or not.
X = df_final
y = df['y'].apply(lambda y : get_y(y))
```

Train model and compute AUC ROC

1. Split data into **testing** and **training**.
2. Train model using sklearn's **LogisticRegression** on the **training data**.
3. Make **predictions** on the **testing data**.
4. Evaluate performance using AUC ROC.

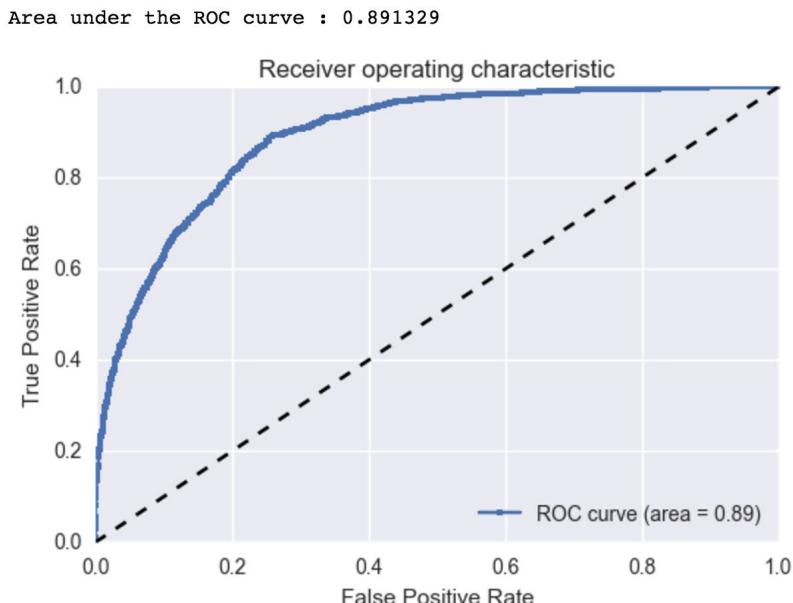
Train model and compute AUC ROC

```
# Computes the AUC ROC of the classifier.
def generate_auc(X,y,clf_class,**kwargs):
    # Construct a kfolds object
    random_state = np.random.RandomState(0)
    # Construct training and testing set.
    X, y = shuffle(X, y, random_state=random_state)
    n_samples, n_features = X.shape
    half = int(n_samples/1.2)
    X_train, X_test = X[:half], X[half:]
    y_train, y_test = y[:half], y[half:]

    # Choose SVC classifier.
    classifier = clf_class(**kwargs)
    probas_ = classifier.fit(X_train, y_train).predict_proba(X_test)

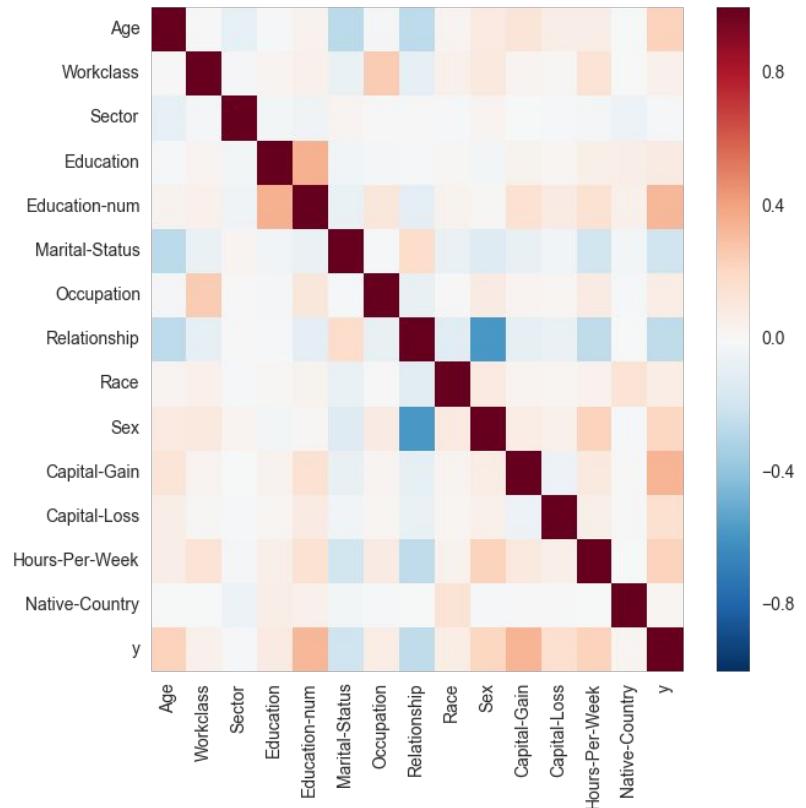
    fpr, tpr, thresholds = roc_curve(y_test, probas_[:, 1])
    roc_auc = auc(fpr, tpr)
    print "Area under the ROC curve : %f" % roc_auc
    return fpr, tpr, roc_auc, thresholds
```

Train model and compute AUC ROC



- Our first model seems pretty good! An **AUC ROC of 0.9**.
- I often just feed everything into a classifier/regression algorithm before I begin optimizing and analyzing the data further.
- Next, we will look at correlation between features, followed by optimizing the complexity of the model.

Correlation of features



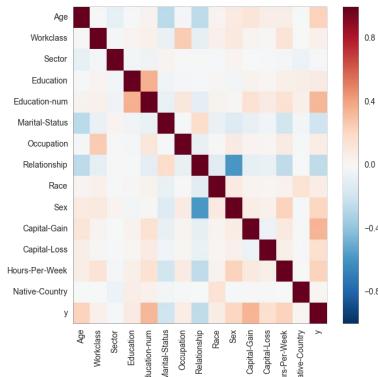
Positive Correlations:

- Capital-Gain and y
- Education-num and y
- Workclass and Occupation
- Education-num and Education

Negative Correlations:

- Sex and Relationship
- Age and Relationship
- Marital status and Age

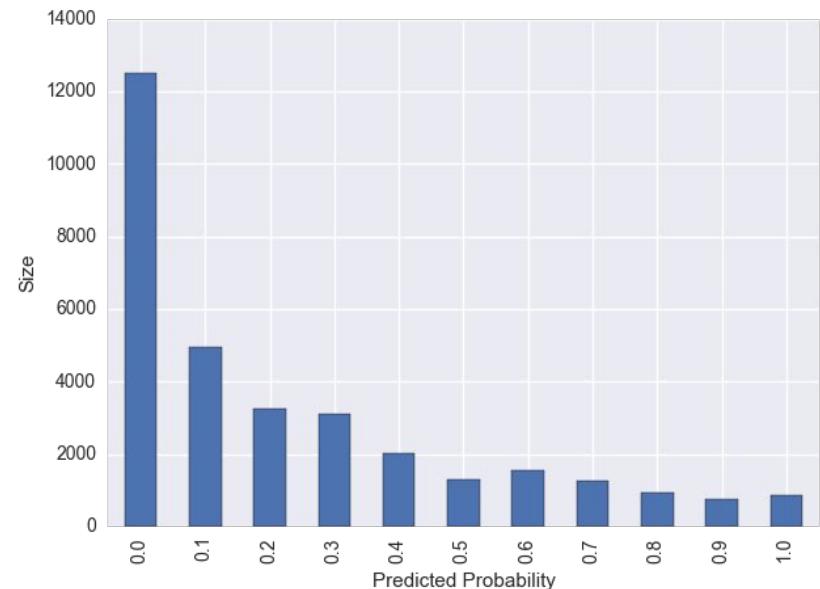
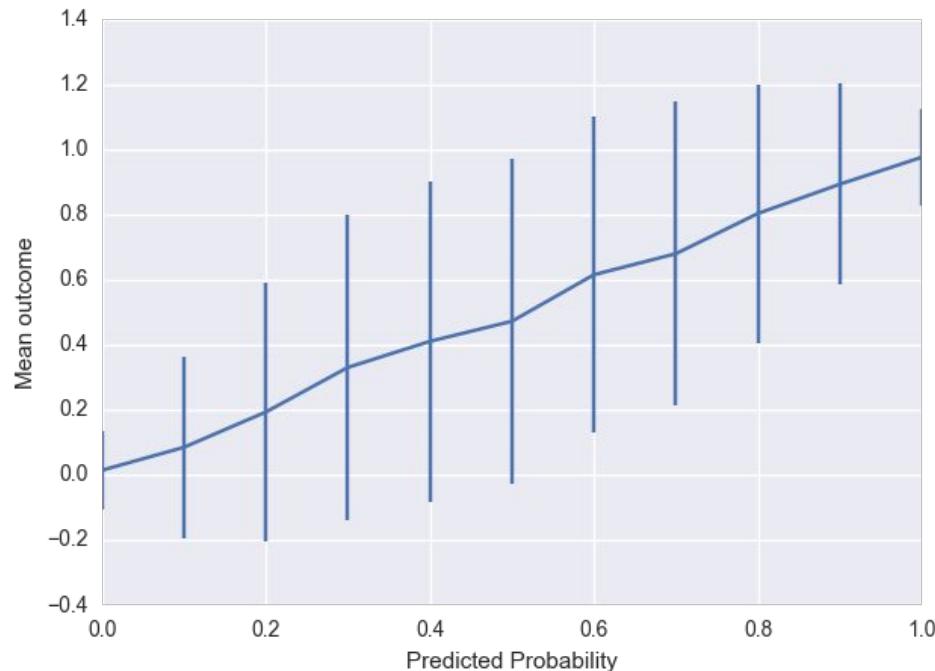
Correlation of features - Removing Them



How to remove correlated features:

- L1 and L2 regularization are the standard methods.
(how we will do this)
- PCA (to be covered soon) also works for this purpose.
- Old School (removing features with large p values manually).

Accuracy vs Percentile



Feature Importance

Regularization and feature selection

Fit the optimal model

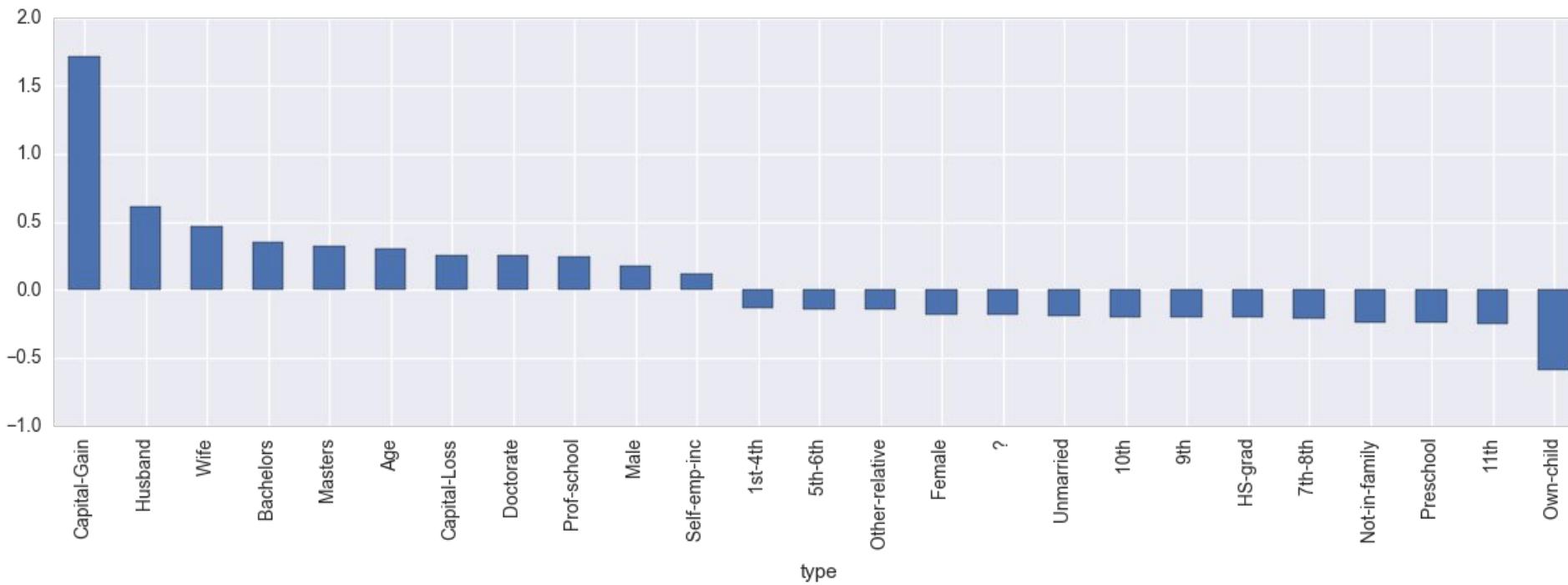
```
In [304]: alpha = alphas[np.argmax(scores)]
```

```
In [356]: regr = LogisticRegression(C=alpha,penalty='l1')
```

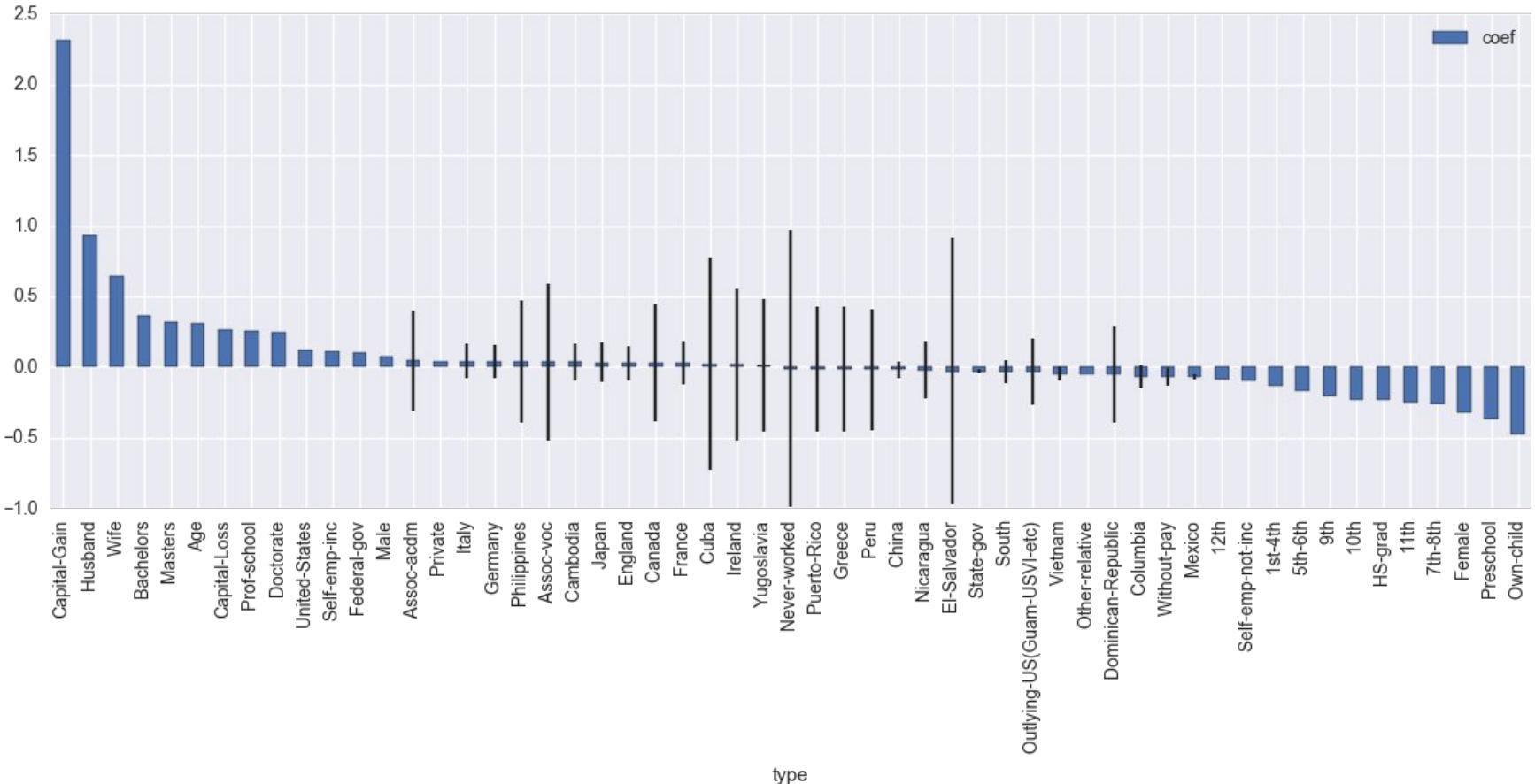
```
# Train the model using the training sets  
regr.fit(X_train, y_train)
```

```
Out[356]: LogisticRegression(C=0.1000000000000001, class_weight=None, dual=False,  
fit_intercept=True, intercept_scaling=1, max_iter=100,  
multi_class='ovr', n_jobs=1, penalty='l1', random_state=None,  
solver='liblinear', tol=0.0001, verbose=0, warm_start=False)
```

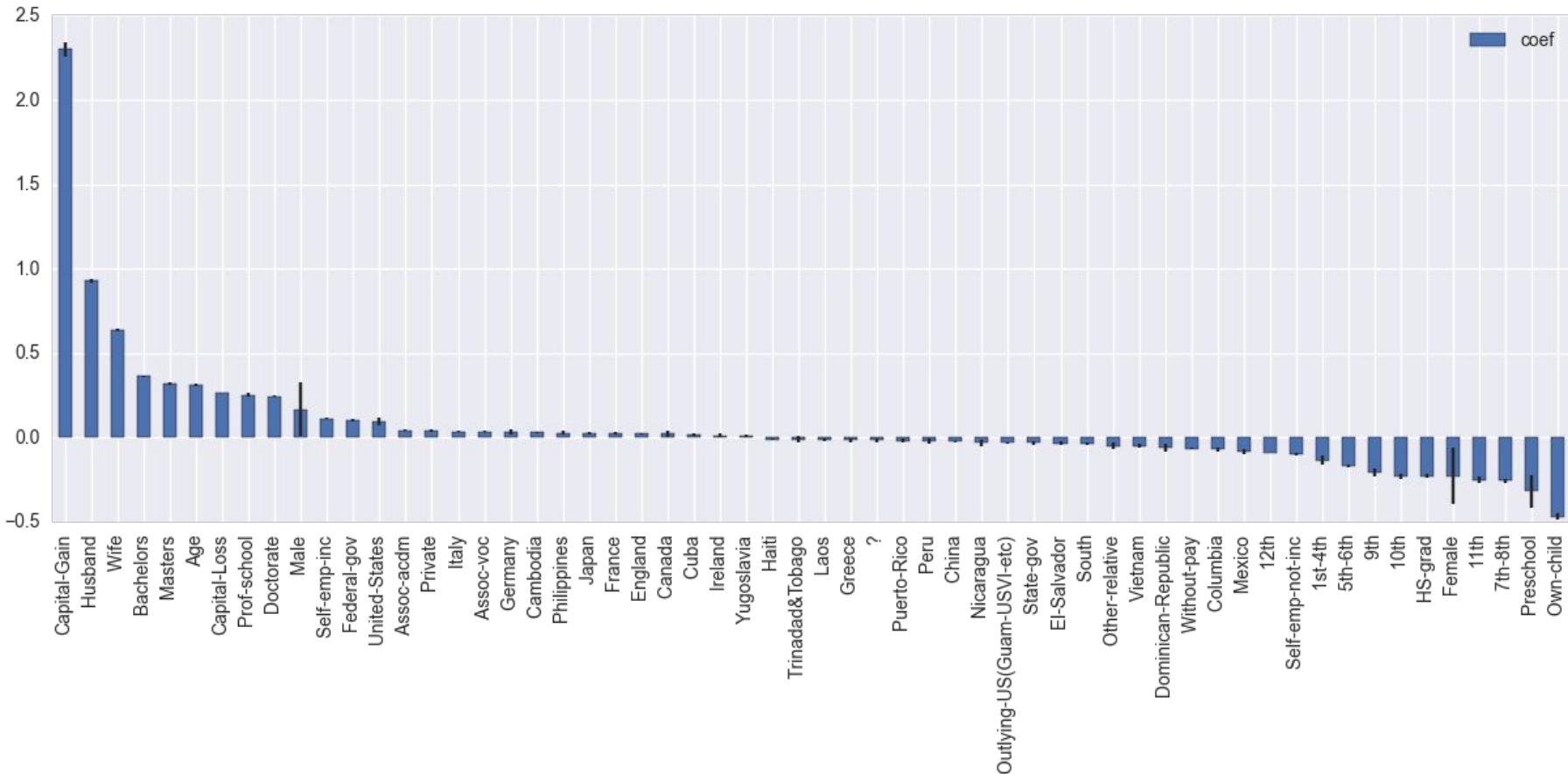
Sort and plot coefficients



Variance of coefficients



Cross Validation



Our final model

$$p_{\beta}(\mathbf{x}) = \frac{1}{1 + \exp(-\beta^T \cdot \mathbf{x})}$$

$$\beta = [2.3, 0.93, 0.64, 0.36, 0.32, 0.31, 0.27, 0.25, 0.24, 0.17]$$

