Linear Models for Regression

Problem Definition

Given features: x_1, x_2, \ldots, x_n

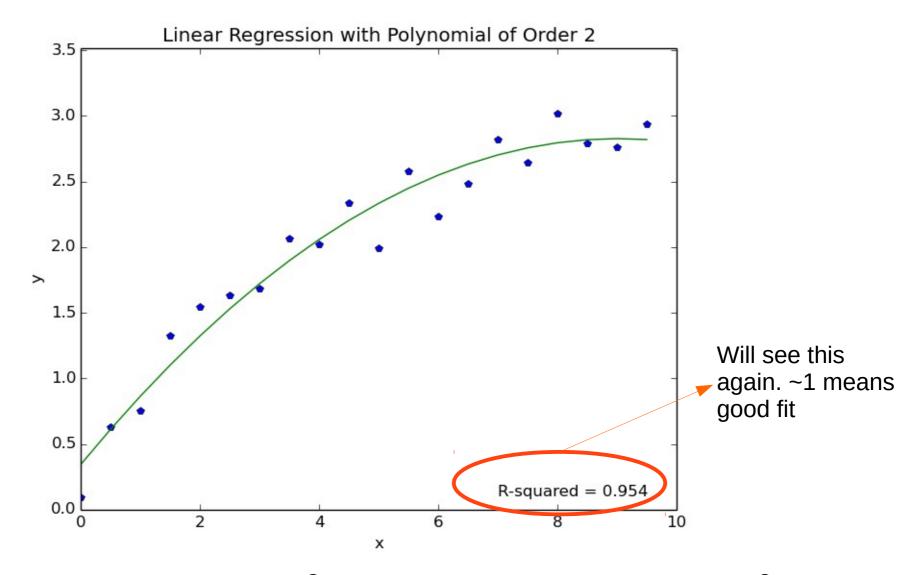
predict real number y

Simplest Guess

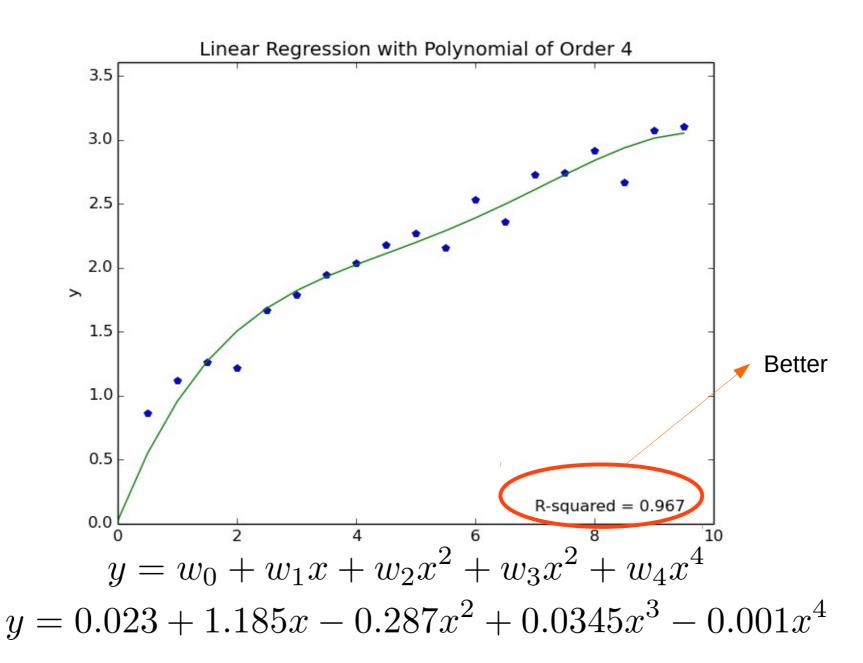
$$y = w_0 + w_1 x_1 + \ldots + w_n x_n$$

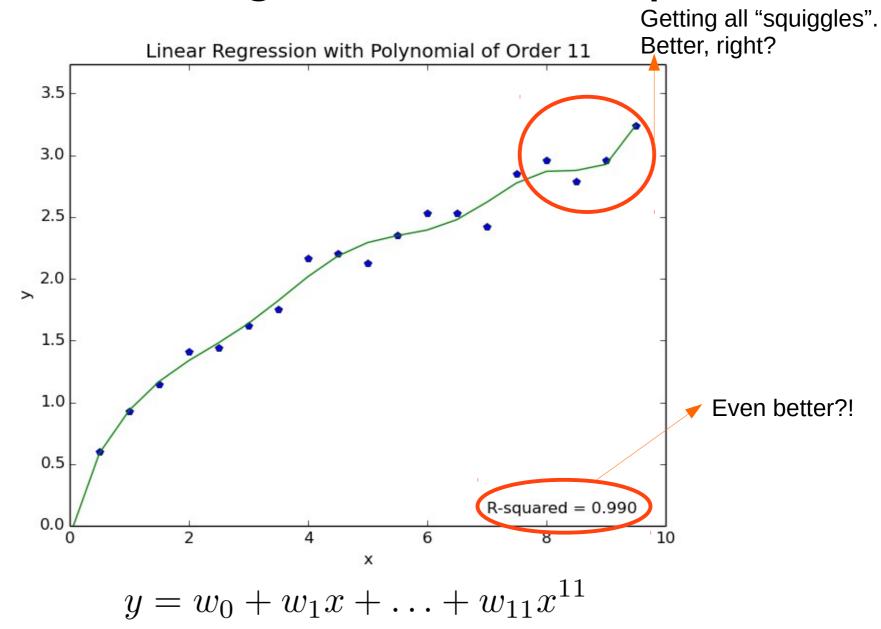
Linear in weights, **NOT** features

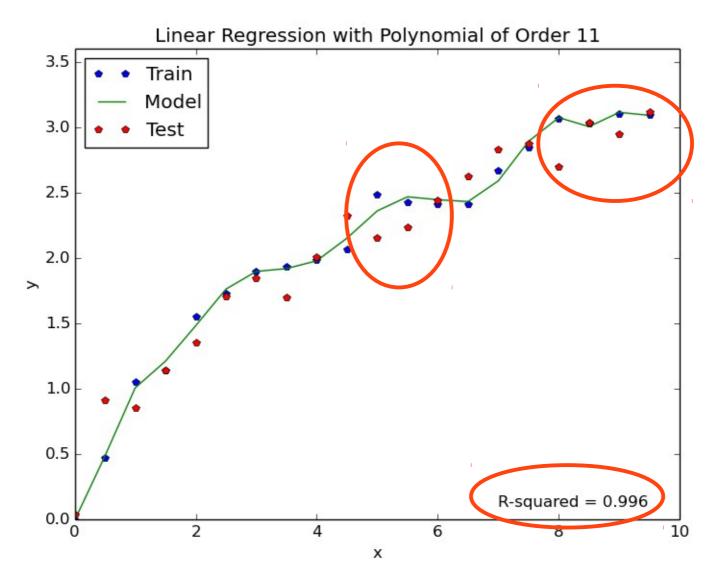
For example, maybe $x_1 = x$ and $x_n = x^n, n > 1$ Definitely not linear in features x, but linear in weights w_i



$$y = w_0 + w_1 x + w_2 x^2 = 0.344 + 0.551x - 0.031x^2$$







Overfitting: Model too complex and fits too well to training data. Does badly when applied to new data.

Define cost function to minimize:

$$C(w_0, w_1, \dots, w_n) = \sum_{i=1}^{M} C_i(w_0, w_1, \dots, w_n)$$

Total Cost

Cost for each training example

What should we choose for $C_i(w_0, w_1, \ldots, w_n)$?

What should we choose for $C_i(w_0, w_1, \ldots, w_n)$?

One choice:
$$C_i = (y_i - p_i)^2$$

 $y_i = \text{Known value for example i}$

 $p_i = \text{Predicted value for example i}$

$$p_i = w_0 + w_1 x_1^i + \ldots + w_n x_n^i$$
 Example i

Minimize cost function: $C(w_0, w_1, \ldots, w_n)$

Solve:
$$\frac{\partial C}{\partial w_i} = 0, i = 0, \dots, n$$

$$C = \sum_{i=1}^{M} (y_i - (w_0 + w_1 x_1^i + \dots + w_n x_n^i))^2$$

$$\Sigma_{i=1}^{M}(y_i - w_0 - w_1 x_1^i - \dots - w_n x_n^i).1 = 0$$

$$\Sigma_{i=1}^{M}(y_i - w_0 - w_1 x_1^i - \dots - w_n x_n^i).x_1^i = 0$$

$$\vdots$$

$$\Sigma_{i=1}^{M}(y_i - w_0 - w_1 x_1^i - \dots - w_n x_n^i).x_n^i = 0$$

Define:

$$Y \equiv \sum_{ex=1}^{M} y_{ex}$$

$$X_{i,j} \equiv \sum_{ex=1}^{M} x_i^{ex} x_j^{ex}$$

$$Z_i \equiv \Sigma_{ex=1}^M y_{ex} x_i^{ex}$$

$$X_{i,0} = X_{0,i} \equiv \Sigma_{ex=1}^{M} x_i^{ex}$$

$$X_{0,0} = \sum_{i=1}^{M} 1 = M$$

$$w_0 X_{0,0} + w_1 X_{0,1} + \dots + w_n X_{0,n} = Y$$

$$w_0 X_{1,0} + w_1 X_{1,1} + w_2 X_{1,2} + \dots + w_n X_{1,n} = Z_1$$

$$w_0 X_{n,0} + w_1 X_{n,1} + \ldots + w_n X_{n,n} = Z_n$$

$$w_0 X_{0,0} + w_1 X_{0,1} + \ldots + w_n X_{0,n} = Y$$

$$w_0 X_1 + w_1 X_{1,1} + w_2 X_{1,2} + \ldots + w_n X_{1,n} = Z_1$$

$$w_0 X_{n,0} + w_1 X_{n,1} + \ldots + w_n X_{n,n} = Z_n$$

Invert matrix to solve for weights

$$\begin{pmatrix} X_{0,0} & X_{0,1} & \dots & X_{0,n} \\ X_{1,0} & X_{1,1} & \dots & X_{1,n} \\ \vdots & \vdots & \vdots & \vdots \\ X_{n,0} & X_{n,1} & \dots & X_{n,n} \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} Y \\ Z_1 \\ \vdots \\ Z_n \end{pmatrix}$$

Linear Regression: Assumptions

Data:
$$y = w_0 + w_1 x_1 + ... + w_n x_n + \mathcal{N}(0, \sigma^2)$$

Gaussian Noise

Linear relationship between y and x_m , $\forall m$ where all other x_n are fixed

 $\mathcal{N}(0, \sigma^2)$: Gaussian noise with 0 mean and constant variance Might consist of many noise terms

They should be independent, Gaussian with constant variance

Linear Regression: Priors

No assumptions made about values that weights take

Minimizing Least Squares Error



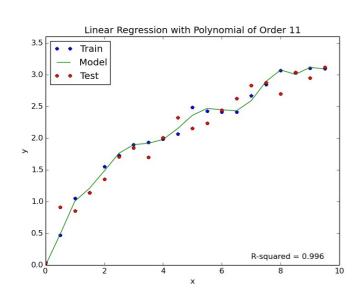
Maximizing Likelihood assuming Gaussian predictions

Likelihood, LL =
$$\prod_{i=1}^{M} \frac{1}{2\pi\sigma^2} e^{-\frac{(y_i - w_0 - w_1 x_1 - \dots - w_n x_n)^2}{2\sigma^2}}$$

Probability, under a Gaussian distribution, that the model will predict the values observed.

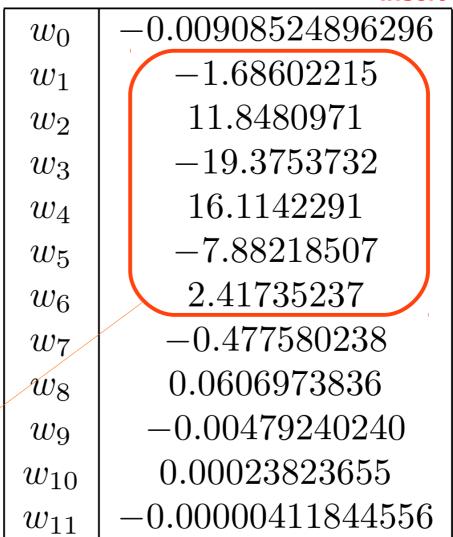
Linear Regression: Priors

Insert variances



Recall overfitting example

Large, alternating weights to account for "squiggliness"



Please excuse significant figures!

Linear Regression: L2 Regularization (Ridge)

Assumption about weights: follow Gaussian distribution.

$$\frac{1}{2\pi\tau^2}e^{-\frac{w_i^2}{2\tau^2}}, i = 1, \dots, n$$

Penalty on weights away from 0

$$LL = \prod_{i=1}^{M} \frac{1}{2\pi\sigma^{2}} e^{-\frac{(y_{i}-w_{0}-w_{1}x_{1}-...-w_{n}x_{n})^{2}}{2\sigma^{2}}} \prod_{i=1}^{n} \frac{1}{2\pi\tau^{2}} e^{-\frac{w_{i}^{2}}{2\tau^{2}}}$$

Maximizing Likelihood

Minimizing new cost function

$$C = \sum_{i=1}^{M} (y_i - (w_0 + w_1 x_1^i + \dots + w_n x_n^i))^2 + \frac{\sigma^2}{\tau^2} \sum_{i=1}^{n} w_i^2$$

Prevents overfitting

Linear Regression: L1 Regularization (Lasso)

Assumption about weights: follow Laplace distribution.

$$\frac{\lambda}{2}e^{-\lambda|w_i|}, i = 1, \dots, n$$

Penalty on weights away from 0

$$LL = \prod_{i=1}^{M} \frac{1}{2\pi\sigma^2} e^{-\frac{(y_i - w_0 - w_1 x_1 - \dots - w_n x_n)^2}{2\sigma^2}} \prod_{i=1}^{n} \frac{\lambda}{2} e^{-\lambda |w_i|}$$

$$\prod_{i=1}^{n} \frac{\lambda}{2} e^{-\lambda |w_i|}$$

Maximizing Likelihood

Prevents overfitting

Minimizing new cost function

Minimizing new cost function
$$C = \sum_{i=1}^{M} (y_i - (w_0 + w_1 x_1^i + ... + w_n x_n^i))^2 + 2\lambda \sigma^2 \sum_{i=1}^{n} |w_i|$$

$$2\lambda\sigma^2\Sigma_{i=1}^n|w_i|$$

Linear Regression: Python Code

```
from sklearn import linear_model
model = linear_model.LinearRegression() #create instance of linear regression model
model.fit(x_values, y_values) #train model

#DONE!!!
model.predict(new_x_values) #predict result on new inputs
model.coef_ #see weights
model.score(x_values, y_values) #we'll see this soon. Compute R2
```

Linear Regression: Python Code

```
model = linear_model.Ridge(alpha = 0.5) #"Ridge" regression with one free parameter model = linear_model.Lasso(alpha = 0.5) #"Lasso" regression with one free parameter
```

Use these instead of linear model used previously Prevent overfitting (coming up soon)

Also, it's very enlightening to look at source code if interested

Linear Regression: Scaling

Generally, features x_m can have different ranges they take values in

Good to normalized each feature to have mean = 0 and standard deviation = 1

Mean across all examples

$$x_m o rac{x_m - \mu(x_m)}{\sigma(x_m)}$$

Standard dev. across all examples

Mean = 0 helps with convergence of algorithms too

according to influence on output

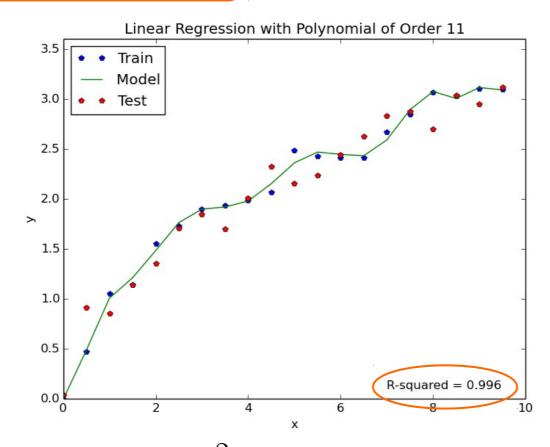
Variance
$$\equiv \sum_{i=1}^{N} (y_i - \bar{y})^2$$

Unexplained Variance Ratio
$$=\frac{\text{Residual}}{\text{Variance}}$$

$$R^2 \equiv 1 - \frac{\text{Residual}}{\text{Variance}}$$
 — Close to 1 = Good(*)

$$R^2 \equiv 1 - \frac{\text{Residual}}{\text{Variance}}$$

Close to 1 but might be overfitting



Compare R^2 between train and test sets!!!!!

Simpler model is better

 R_{Adjusted}^2 penalizes model with many parameters

$$R^2 \equiv 1 - \frac{\text{Residual}}{\text{Variance}}$$
 $R_{\text{Adjusted}}^2 \equiv 1 - \frac{\frac{\text{Residual}}{df_e}}{\frac{\text{Variance}}{df_t}}$

$$df_t \equiv n-1$$
 "Degrees of freedom for variance"
$$df_e \equiv n-p-1$$
 "Degree of freedom for model"

n = Number of examplesp = number of weights (excluding constant term)

Look at distribution of residuals: $y_i - f(x_i)$

Should be Gaussian with constant variance

Linear Models for Classification: Logistic "Regression"

Problem Definition

Given features: x_1, x_2, \ldots, x_n

predict class or label, y = 0 or 1

First Stab

Group together all distinct values of tuples (x_1, x_2, \ldots, x_n)

For each distinct group, count number of entries with y = 0 and y = 1

Now have
$$\text{Prob}[y = 0 \mid (x_1, x_2, ..., x_n)]$$

 $Prob[y = 0 \mid (x_1, x_2, ..., x_n)] > P \rightarrow label = 0$
 $Prob[y = 0 \mid (x_1, x_2, ..., x_n)] \leq P \rightarrow label = 1$

P tuning parameter, e.g., 0.5

Problems with First Stab

 x_1, x_2, \ldots, x_n continuous - can't count!

Solution: bucket/bin continuous variables in intervals

Receive new features: (x_1, x_2, \dots, x_n) NOT in training set

Have no data on $Prob[y = 0 | (x_1, x_2, ..., x_n)]!!!$

Solution: Find closest (x_1, x_2, \ldots, x_n) that exists in training set and use it as a proxy

Linear Model

Can we map:

$$(x_1, x_2, \dots, x_n)$$

$$\downarrow$$

$$Prob[y|(x_1, x_2, \dots, x_n)]$$

using some other method?

Linear Model

How about:

$$(x_1, x_2, \dots, x_n)$$

$$\downarrow w_0 + w_1 x_1 + w_2 x_2 + \dots + w_n x_n$$
Linear combination:
$$\downarrow ?$$

$$[0, 1]$$

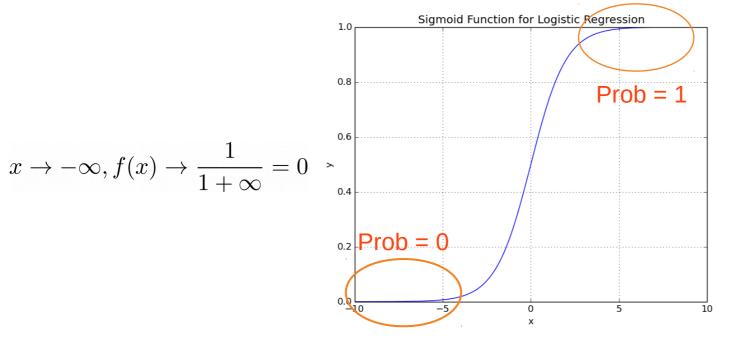
Logistic/Sigmoid Function

Want to map real number to [0,1]

One possible solution:
$$f(x) = \frac{1}{1 + e^{-x}}$$

$$x \to \infty, f(x) \to \frac{1}{1+0} = 1$$
$$x \to -\infty, f(x) \to \frac{1}{1+\infty} = 0$$
$$x = 0, f(x) = 0.5$$

Logistic/Sigmoid Function



$$x \to \infty, f(x) \to \frac{1}{1+0} = 1$$

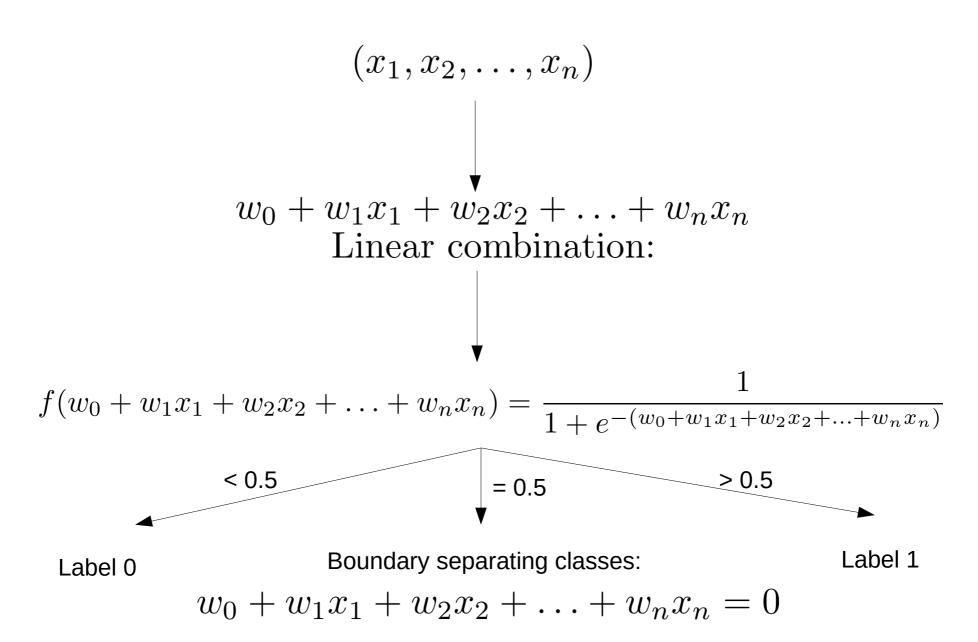
Probability

Want to map real number to [0,1]

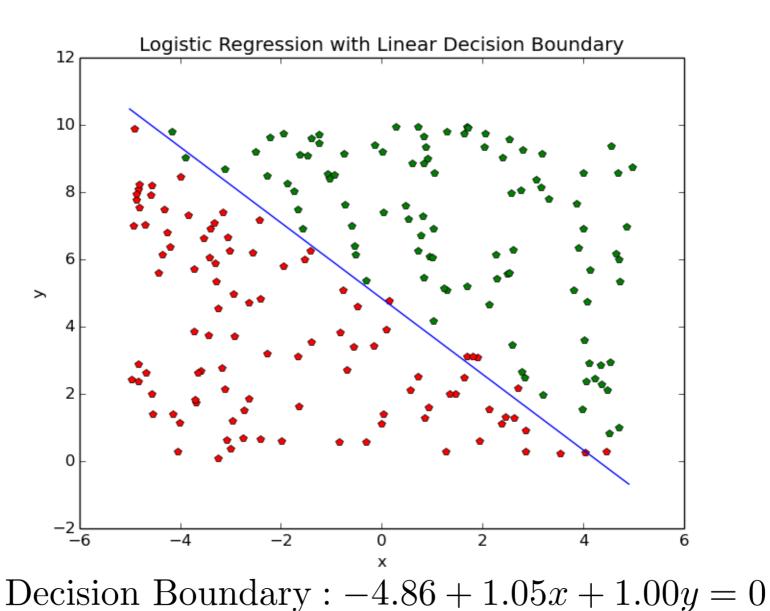
One possible solution:
$$f(x) = \frac{1}{1 + e^{-x}}$$

$$x=0, f(x)=0.5$$
 — "Boundary" or "Threshold"

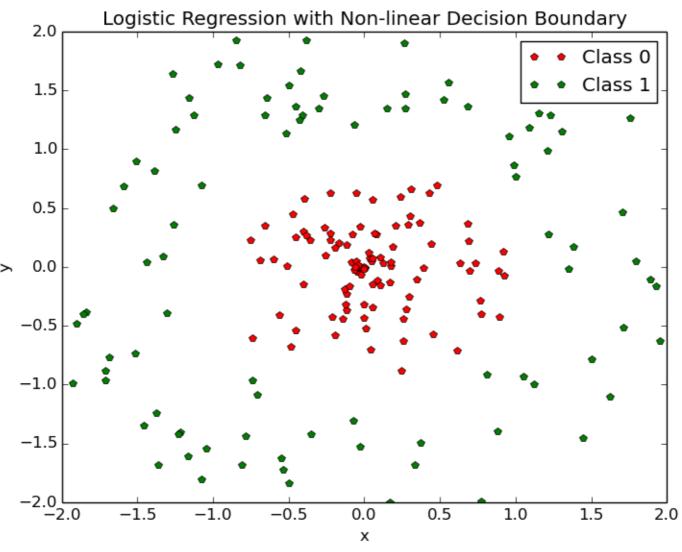
Logistic Regression



Logistic Regression Example 1

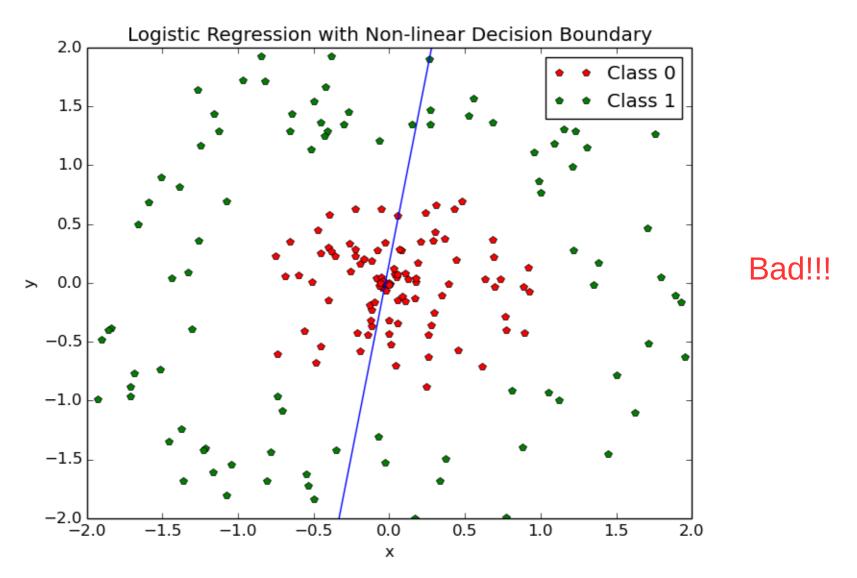


Logistic Regression Example 2



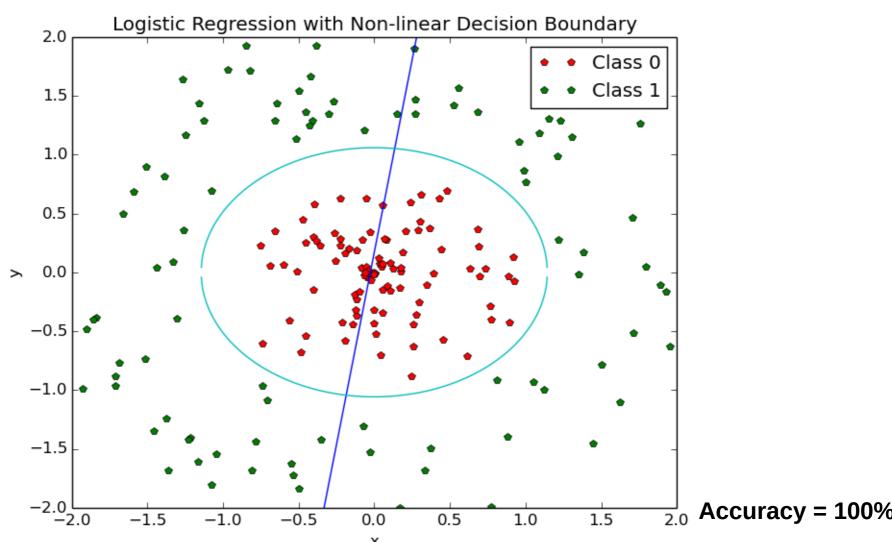
Features are:(x, y)

Accuracy = 64%



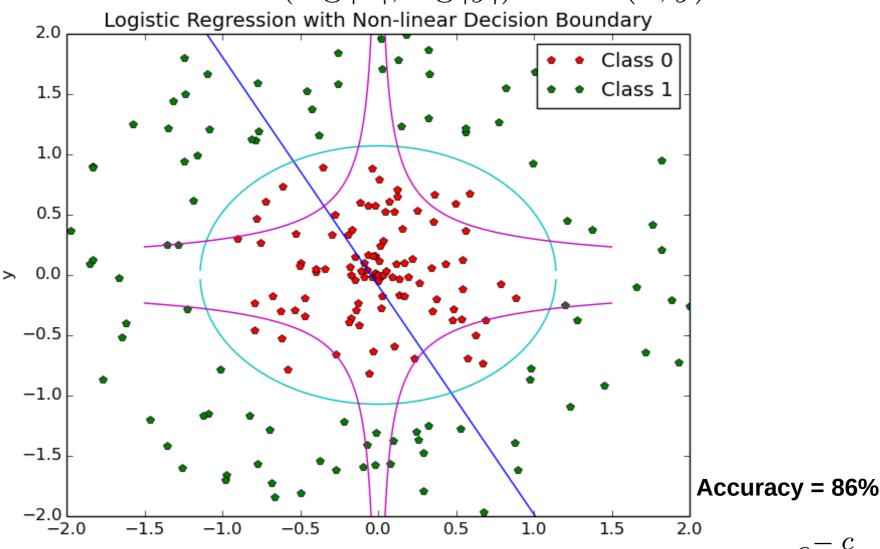
Decision Boundary: $w_0 + w_1 x + w_2 y = 0 \implies \text{Straight Line}$

Features are: (x^2, y^2) NOT (x, y)



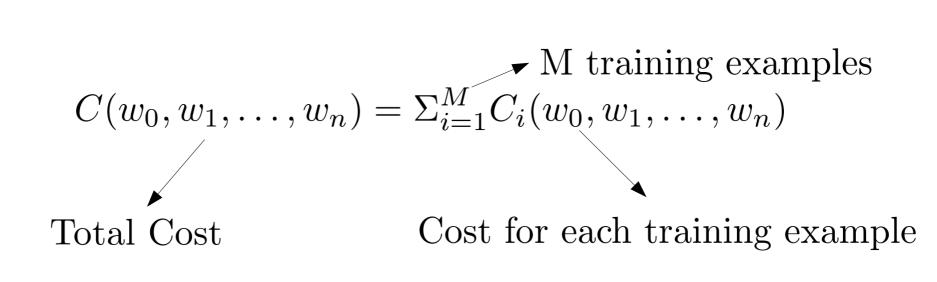
Decision Boundary: $w_0 + w_1 x^2 + w_2 y^2 = 0 \implies \text{Ellipse (in this case at least)}$

Features are: $(\log |x|, \log |y|)$ NOT (x, y)



Decision Boundary: $a \log |x| + b \log |y| + c = 0 \implies y = \pm \frac{e}{|x|^{\frac{a}{b}}}$

Define cost function to minimize:



What should we choose for $C_i(w_0, w_1, \ldots, w_n)$?

What should we choose for $C_i(w_0, w_1, \ldots, w_n)$?

One choice:
$$C_i = (y_i - p_i)^2$$

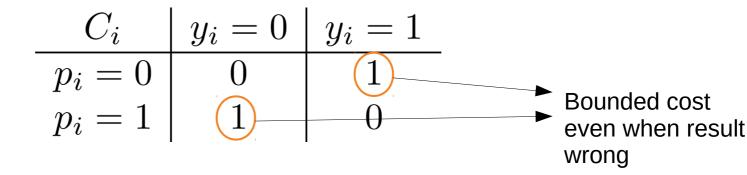
 $y_i = \text{Known class of example i} \in \{0, 1\}$

 p_i = Predicted class of example $i \in \{0, 1\}$

Could also try:

$$p_i = \text{Predicted probability of example i} = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + \dots + w_n x_n)}}$$

One choice:
$$C_i = (y_i - p_i)^2$$



Unlike linear regression, in logistic regression, the result is binary: right or wrong.

Want to impose high cost for wrong and no cost for right.

Let's try something else.

Different Choice:
$$C_i = -y_i \log p_i - (1 - y_i) \log (1 - p_i)$$

where:

 $y_i = \text{Known class of example i} \in \{0, 1\}$

$$p_i = \text{Predicted probability of example i} = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + \dots + w_n x_n)}}$$

Why this C_i ?!!!

$$y_i = 0 p_i = 0$$

$$C_i = 0?$$

$$y_i = 0$$

$$p_i = 0$$

$$C_i = 0$$
?

$$C_i = -0\log 0 - (1 - 0)\log(1 - 0)$$
$$= 0 - \log 1 = 0$$

$$y_i = 1 p_i = 1$$

$$C_i = 0$$
?

$$y_i = 1$$

$$C_i = 0$$

$$C_i = -1 \log 1 - (1 - 1) \log(1 - 1)$$
$$= -\log 1 - 0 \log 0 = 0$$

$$y_i = 1 p_i = 0$$

$$C_i = \text{large?}$$

$$y_i = 1 p_i = 0$$

$$C_i = \text{large?}$$

$$C_i = -1\log 0 - (1-1)\log (1-0)$$

$$\log 0 = -\infty$$

$$C_i = \infty$$

$$y_i = 0 p_i = 1$$

$$C_i = \text{large?}$$

$$y_i = 0 p_i = 1$$

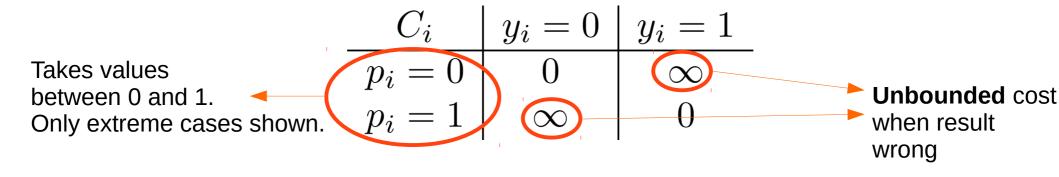
$$C_i = \text{large?}$$

$$C_i = -0 \log 1 - (1 - 0) \log (1 - 1)$$

$$\log 0 = -\infty$$

$$C_i = \infty$$

Different Choice:
$$C_i = -y_i \log p_i - (1 - y_i) \log (1 - p_i)$$



More appropriate for binary classification

Cost function measures "entropy"

Also, equivalent to negative log likelihood

Minimize:

$$C(w_0, w_1, \dots, w_n) = \sum_{i=1}^{M} C_i(w_0, w_1, \dots, w_n)$$

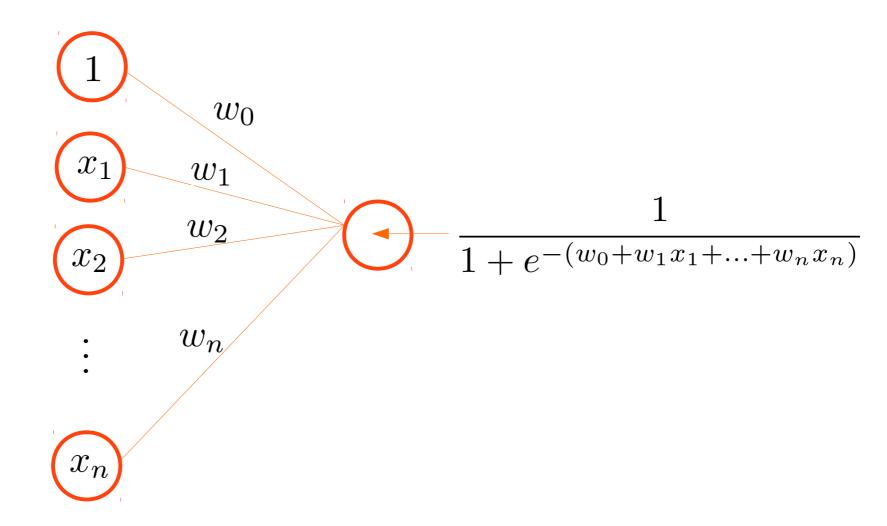
$$C_i = -y_i \log p_i - (1 - y_i) \log (1 - p_i)$$

$$p_i = \text{Predicted probability of example i} = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + \dots + w_n x_n)}}$$

with respect to:

$$w_0, w_1, \ldots, w_n$$

Logistic Regression: Visualization



This kind of structure will occur again when we look at neural networks

Logistic Regression: Python Code

```
from sklearn import linear_model

model = linear_model.LogisticRegression()
model.fit(features, labels) #train the model

model.predict(test_features) #make predictions (0/1)
model.predict_proba(test_features) #predict probabilities
```

Have data with binary labels, built a logistic regression model.

How good is the model? How to evaluate its performance?

$$C_i$$
 $pred = 0$ $pred = 1$
 $label = 0$ $0 \rightarrow 0$ $0 \rightarrow 1$
 $label = 1$ $1 \rightarrow 0$ $1 \rightarrow 1$

Good Bad

=

	C_{i}	pred = 0	pred = 1
•	label = 0	True Negatives	False Positives
	label = 1	False Negatives	True Positives

Some metrics to measure on the test set

$$\frac{(0 \to 0) + (1 \to 1)}{(0 \to 0) + (1 \to 1) + (0 \to 1) + (1 \to 0)}$$

=

examples predicted correctly total examples

known as **Accuracy**

Accuracy =
$$\frac{(0 \to 0) + (1 \to 1)}{(0 \to 0) + (1 \to 1) + (0 \to 1) + (1 \to 0)}$$

What if 98% of examples are labeled 0 and 2% labeled 1?

Build "dumb" model that predicts 0 for every examples

Accuracy = 98% (Get everything labeled 0 correct)

Bad measure if population of labeled classes very uneven

Sensitivity/Recall =
$$\frac{(1 \to 1)}{(1 \to 1) + (1 \to 0)}$$

Ideally, Recall = 1

In previous example, Recall = 0

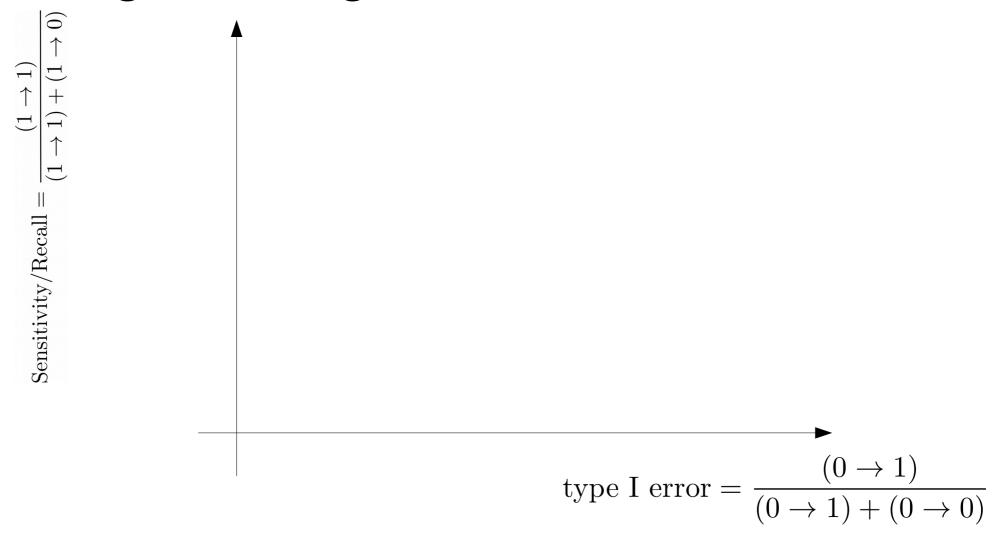
Sensitivity/Recall =
$$\frac{(1 \to 1)}{(1 \to 1) + (1 \to 0)}$$

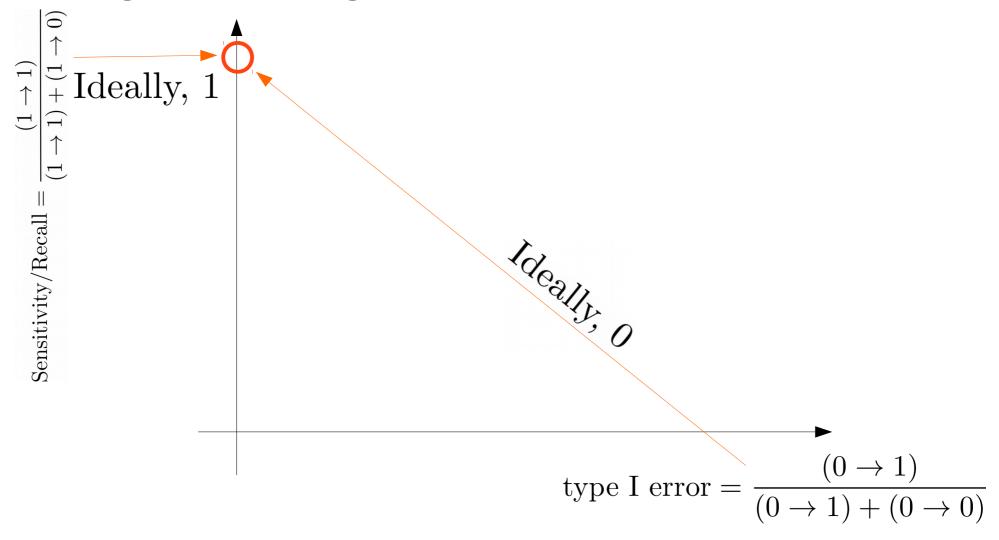
Specificity =
$$\frac{(0 \to 0)}{(0 \to 0) + (0 \to 1)}$$

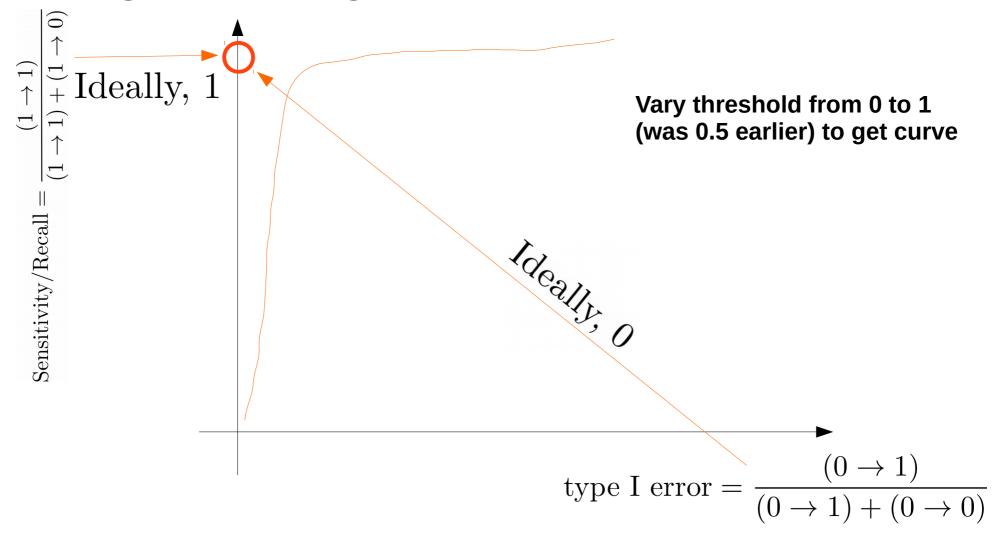
Class labels arbitrary
Symmetry under: $0 \leftrightarrow 1$ Sensitivity/Recall \leftrightarrow Specificity
Ideally, both are 1

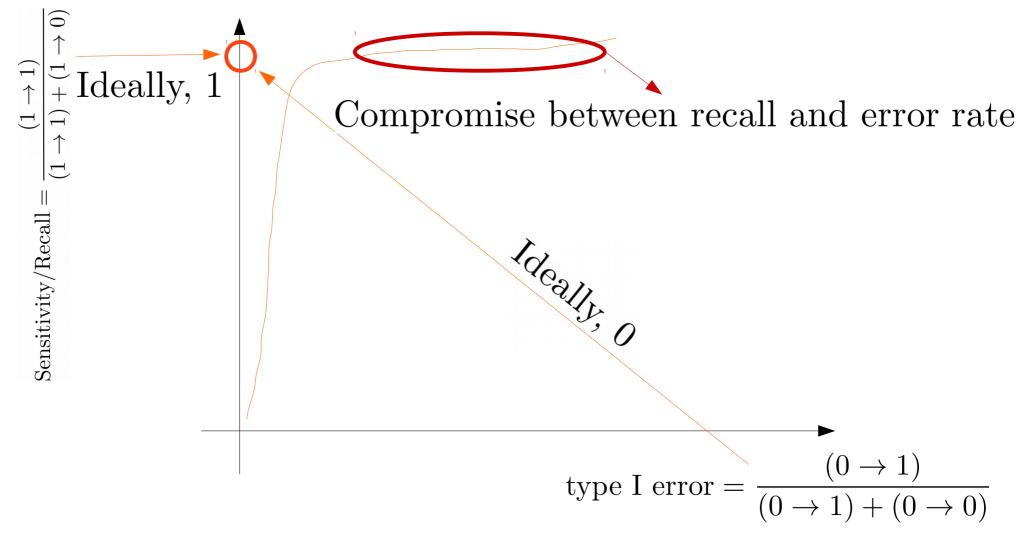
type I error =
$$\frac{(0 \to 1)}{(0 \to 1) + (0 \to 0)}$$
$$0 \leftrightarrow 1 \updownarrow$$
type II error =
$$\frac{(1 \to 0)}{(1 \to 0) + (1 \to 1)}$$

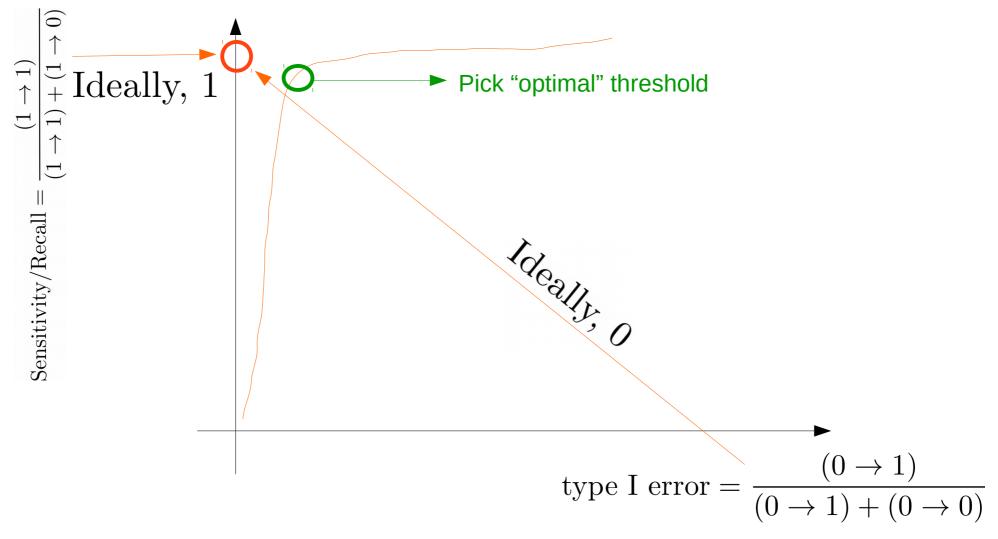
Ideally, both are 0

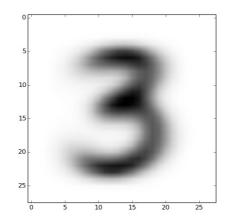












Hand-written digits dataset: 28 x 28 pixels

Let's try logistic regression to identify the digit 3 (label = 1) from other digits (label = 0)

Test Set: # of examples with label 1 = 1,301

Test Set: # of examples with label 0 = 11,299

Assign every test example to label = 0:

Accuracy =
$$\frac{11,299}{1,301+11,299} = 89.7\%$$

Accuracy =
$$\frac{12,229}{12,600} = 97.1\%$$

Sensitivity/Recall =
$$\frac{(1 \to 1)}{(1 \to 1) + (1 \to 0)}$$

Assign every test example to label = 0:

Sensitivity/Recall =
$$\frac{0}{0+1301} = 0$$

Sensitivity/Recall =
$$\frac{1,077}{1,077 + 224} = 82.7\%$$

Specificity =
$$\frac{(0 \to 0)}{(0 \to 0) + (0 \to 1)}$$

Assign every test example to label = 0:

Specificity =
$$\frac{11,299}{11,299+0} = 100\%$$

Specificity =
$$\frac{11,152}{11,152+147} = 98.7\%$$

type I error =
$$\frac{(0 \to 1)}{(0 \to 1) + (0 \to 0)}$$

Assign every test example to label = 0:

type I error =
$$\frac{0}{0+11,299} = 0\%$$

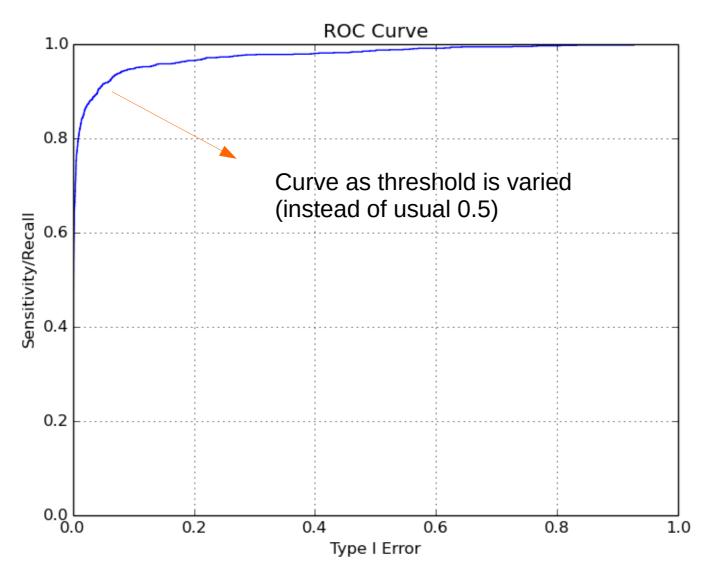
type I error =
$$\frac{147}{147 + 11,152} = 1.3\%$$

type II error =
$$\frac{(1 \to 0)}{(1 \to 0) + (1 \to 1)}$$

Assign every test example to label = 0:

type II error =
$$\frac{1,301}{1,301+0} = 100\%$$

type II error =
$$\frac{224}{224 + 1,077} = 17.2\%$$



Area under curve, AUC = 0.975

Questions?

Questions?