GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

IMBALANCED CLASSES/EVALUATION METRICS

DATA SCIENCE IN THE NEWS

DATA SCIENCE IN THE NEWS

August 12, 2015

Inside the Zestimate: Data Science at Zillow

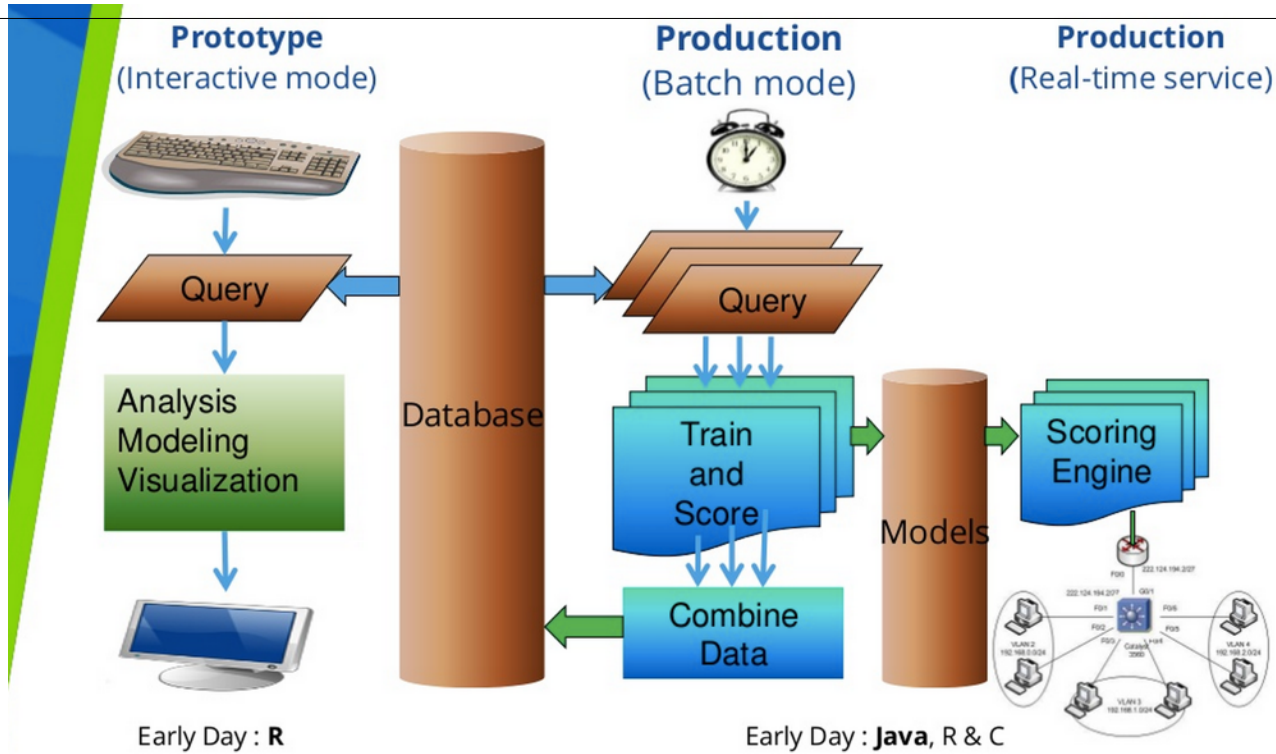
Alex Woodie

If you're like most homeowners, you probably sneak a peek at your 'Zestimate' from time to time to see how your home's value might have changed. Getting a Zestimate is very easy and straightforward for users, but behind the scenes, there's a hefty amount of data science that goes into the equation.

The Zestimate is a core part of Zillow's offering, and is critical for the company's business model. The figure is an estimated market value that's based on a number of public and user-submitted data, including physical attributes, like location, lot size, square footage, and number of bedrooms and bathrooms. Historical data like real-estate transfers and tax information is also factored in, as are sales of comparable houses in a neighborhood.

http://www.datanami.com/2015/08/12/inside-the-zestimate-data-science-at-zillow/

DATA SCIENCE IN THE NEWS



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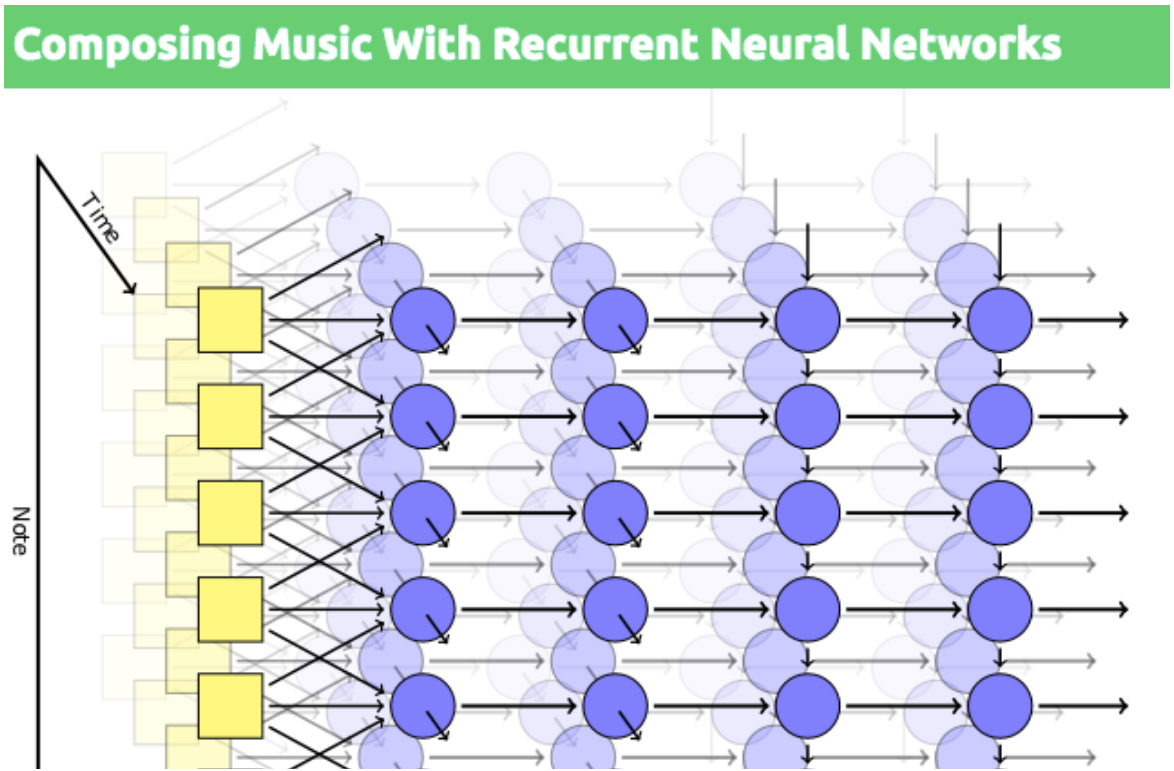
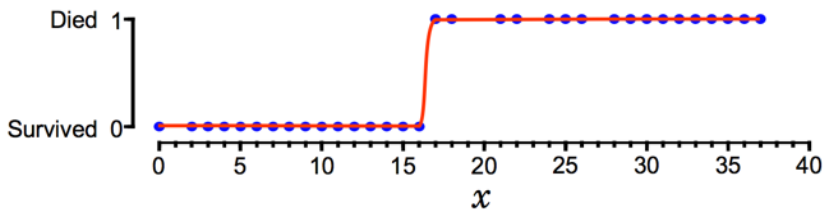
Zillow

DATA SCIENCE IN THE NEWS

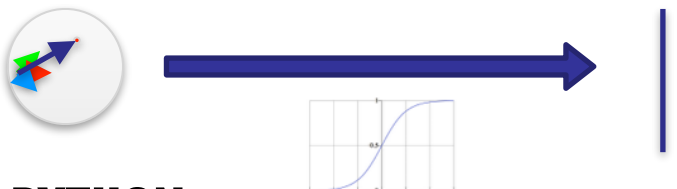


http://www.hexahedria.com/2015/08/03/composing-music-with-recurrent-neural-networks/

LAST TIME:



I. LOGISTIC REGRESSION
II. OUTCOME VARIABLES
III. ERROR TERMS
IV. INTERPRETING RESULTS



LAB: IMPLEMENTING LOGISTIC REGRESSION IN PYTHON

QUESTIONS?

QUESTIONS?

WHAT WAS THE MOST INTERESTING THING YOU LEARNT?

WHAT WAS THE HARDEST TO GRASP?

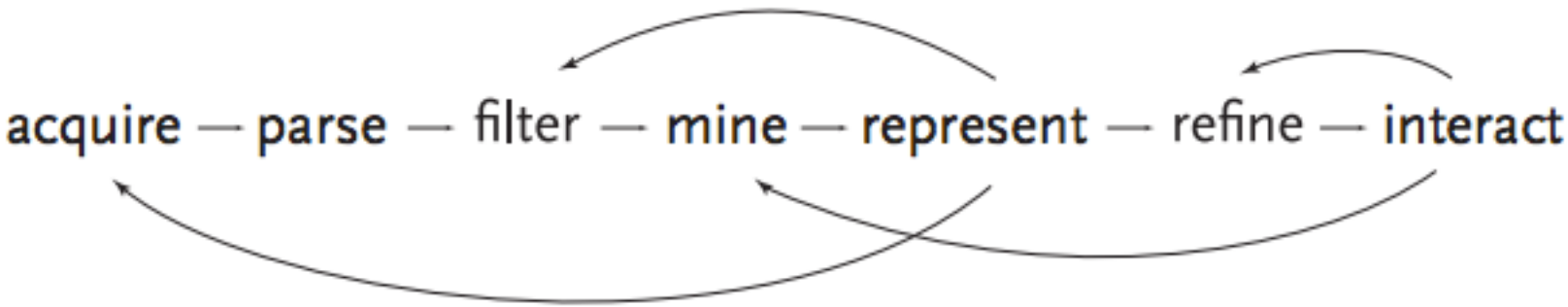
AGENDA

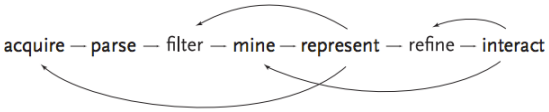
I. IMBALANCED CLASSES
II. ERROR RATES
III. ROC CURVES
IV. EVALUATION METRICS
V. COST FUNCTION
VI. VALIDATION CURVES AND LEARNING CURVES

KEY OBJECTIVES

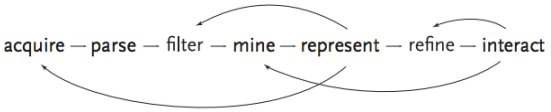
- RECOGNIZE IMBALANCED CLASSES
- TREAT DATASETS INVOLVING IMBALANCED CLASSES
- KNOW VARIOUS EVALUATION METRICS FOR REGRESSION AND CLASSIFICATION
- USE DIFFERENT EVALUATION METRICS TO JUDGE QUALITY OF A MODEL
- UNDERSTAND AND USE ROC CURVES IN BINARY CLASSIFICATION PROBLEMS
- UNDERSTAND AND USE LEARNING CURVES
- GENERALIZE ML PROCESS USING COST FUNCTION FRAMEWORK
- IMPLEMENT ALL THE ABOVE IN PYTHON

A BRIEF RECAP


acquire — parse — filter — mine — represent — refine — interact

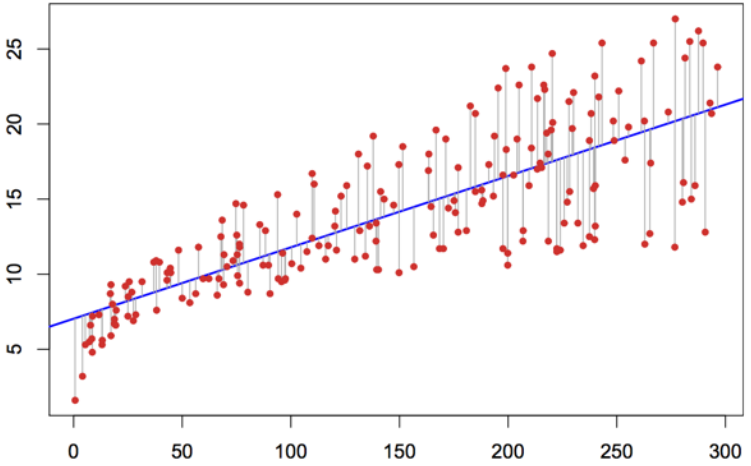


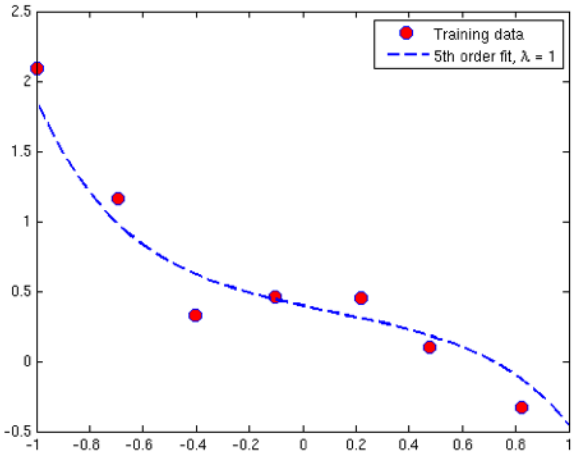
	Continuous	Categorical
Supervised	*regression* ✔	*classification* ✔
Unsupervised	*dimension reduction*	*clustering*

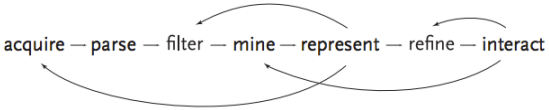


	Continuous	Categorical
Supervised	regression ✓	classification ✓
Unsupervised	dimension reduction	clustering

Regression & Regularization







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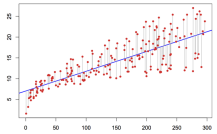
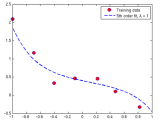
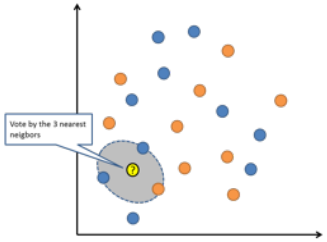
Regression & Regularization

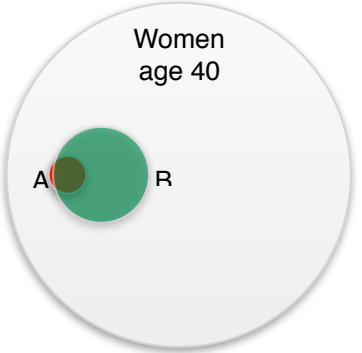




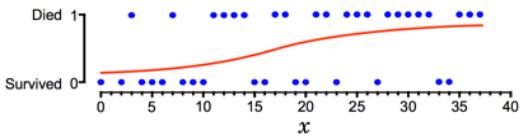
3 Classification methods



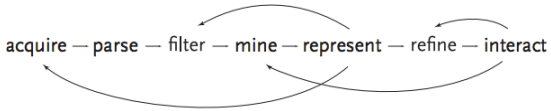
KNN



Naïve Bayes



Logistic Regression



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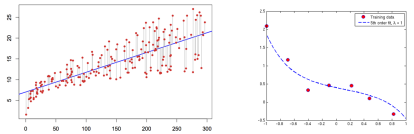
Regression & Regularization



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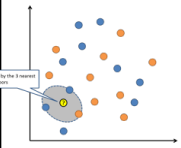

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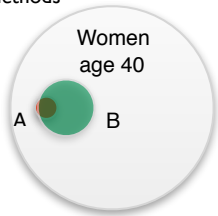

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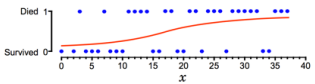

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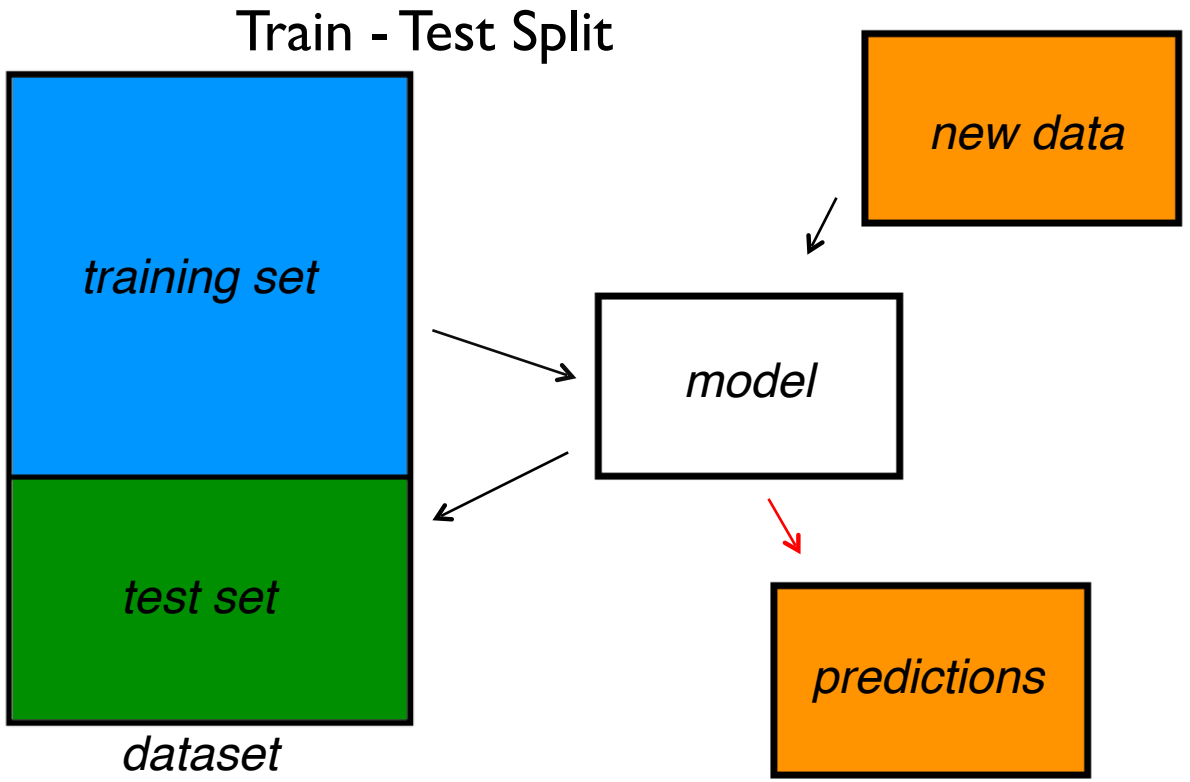

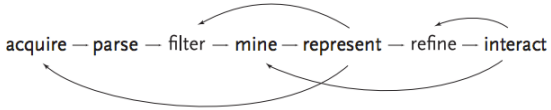

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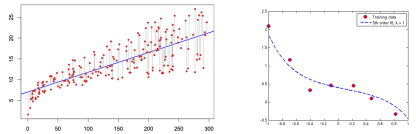

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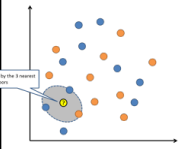

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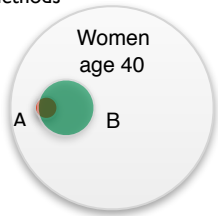

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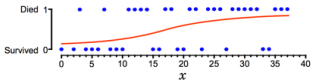
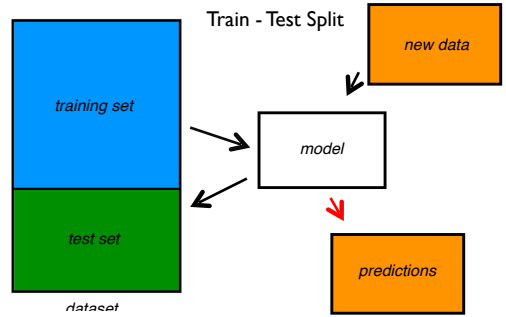
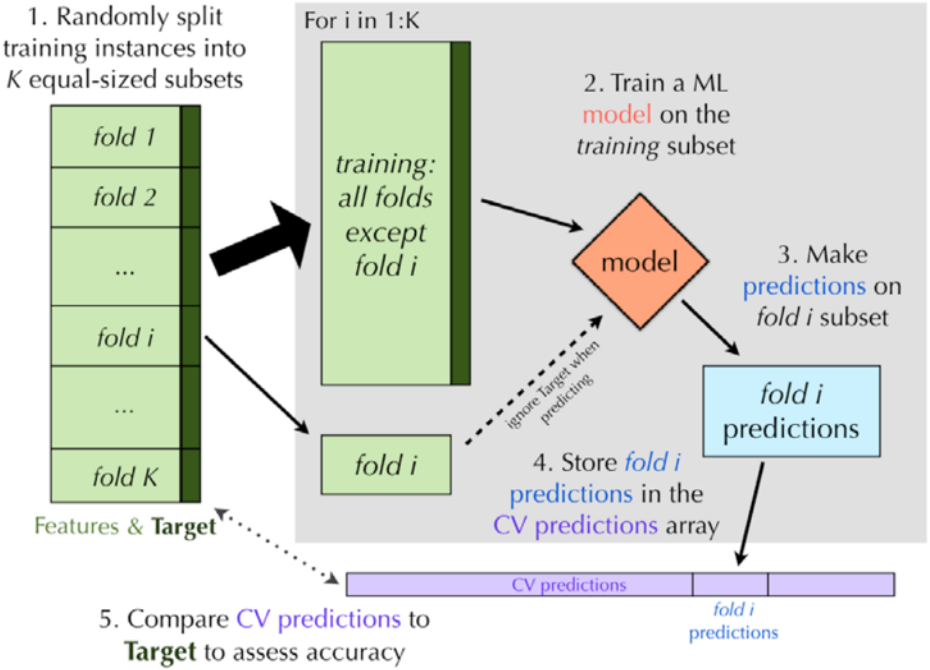


Logistic Regression



Cross Validation



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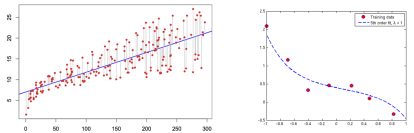
Regression & Regularization



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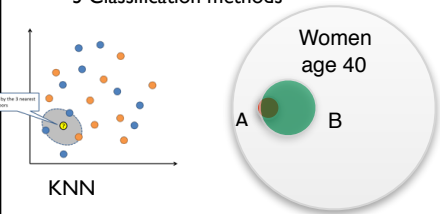

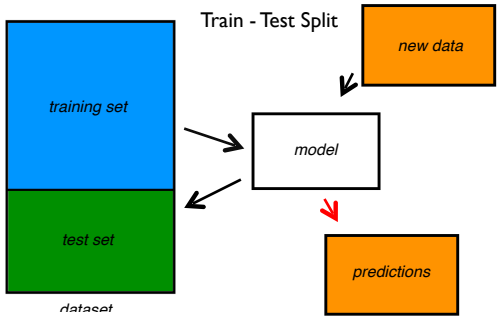

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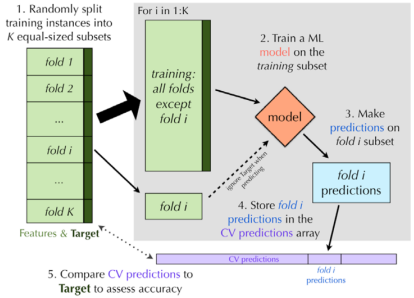

What else?

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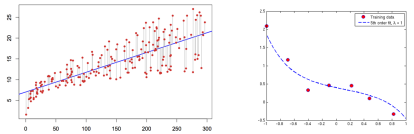
Regression & Regularization



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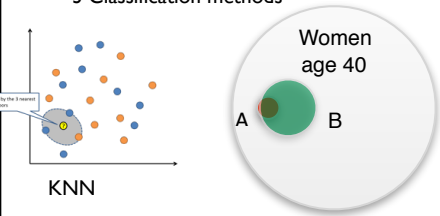
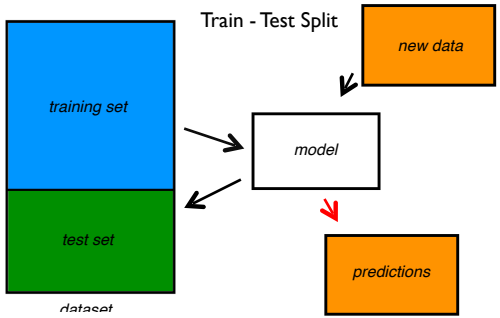
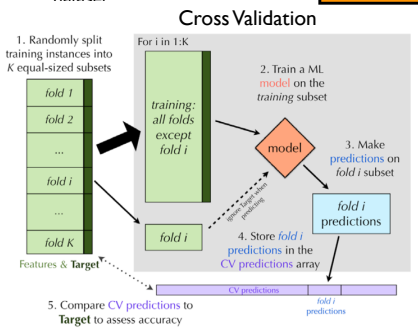






What else?

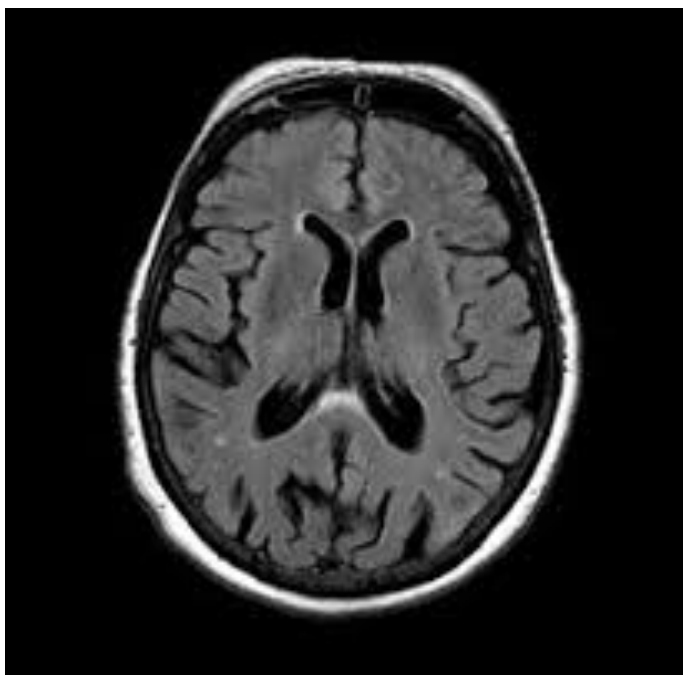
- Probability
- Bayes Theorem
- GLMs
- …

Today we consolidate and expand

A MOTIVATION EXAMPLE

Cancer Screen => classify cancer scans for doctor to review

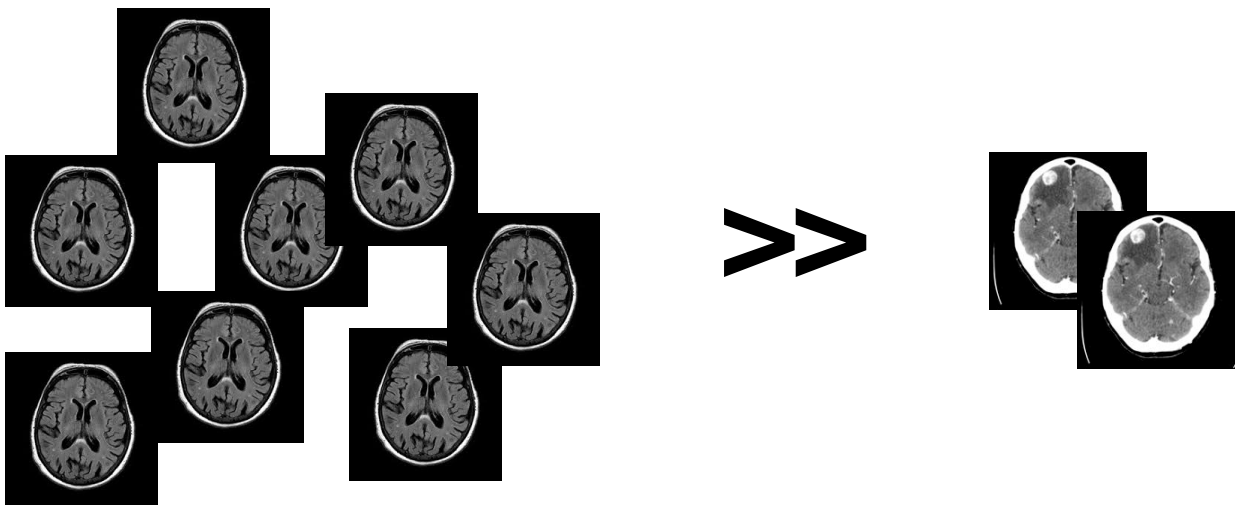
No Cancer



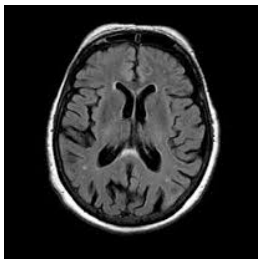
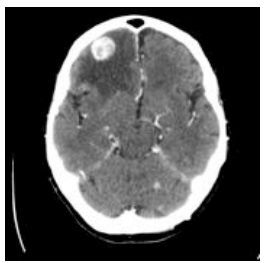
Cancer

ISSUE 1: Many more healthy brain scans

- Imbalance confuses classifiers => only perform well on dominant class
- Situation is very common in other fields (e.g. fraud detection)

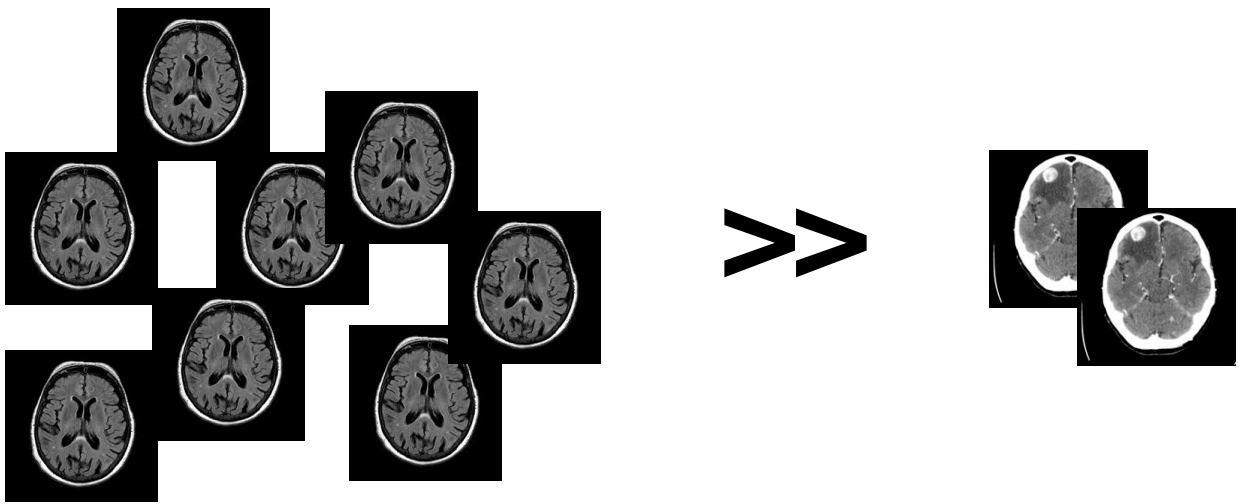


ISSUE 2: Not all errors are equal…

Error 1		Classifier Label: Cancerous	Permissable, because a physician will review it
Error 2		Classifier Label: Non-Cancerous	Not permissable, because this data will be discarded

IMBALANCED CLASSES

Imbalanced classes can be re-balanced in several ways



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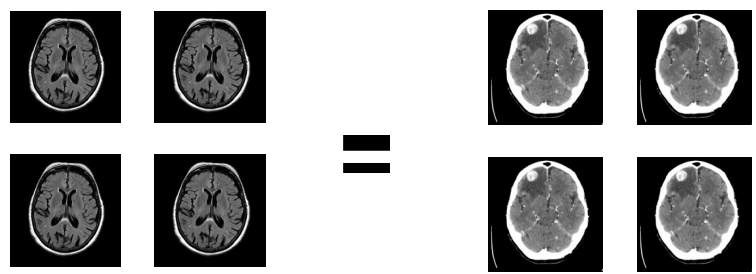
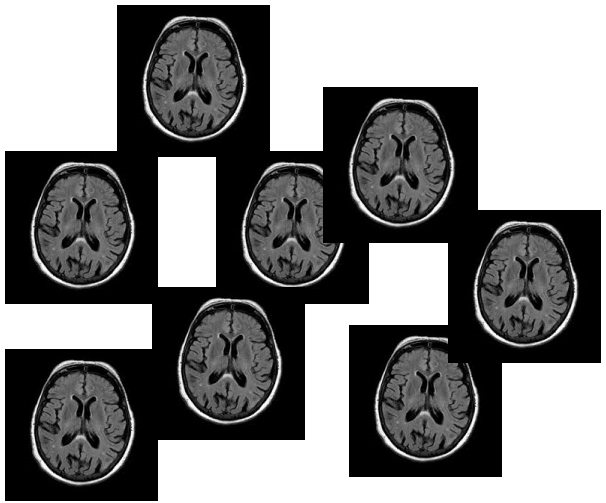
2. **Oversampling** the minority class - add more of the minority class so it has more weight.

3. **Hybrid** - doing both



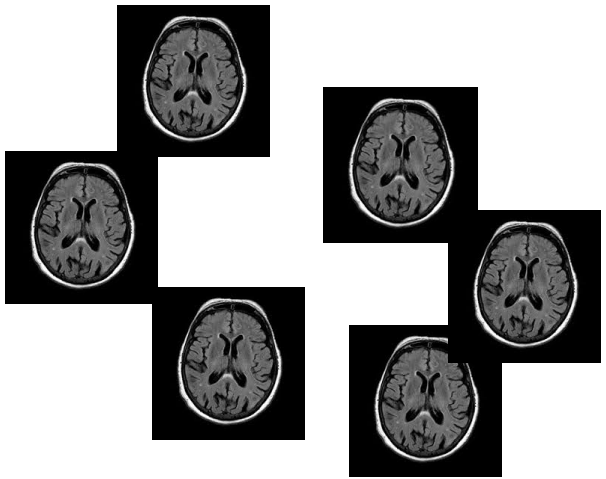
Undersampling

Randomly remove elements from the majority class.



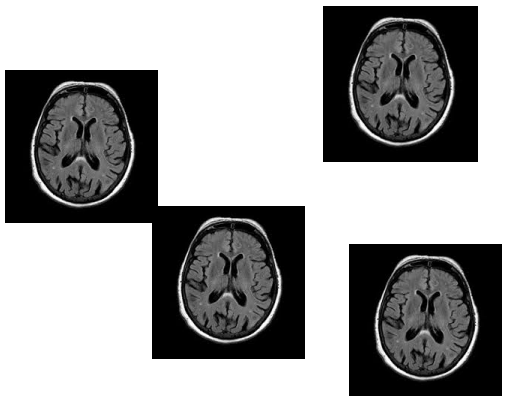
Undersampling

Randomly remove elements from the majority class.



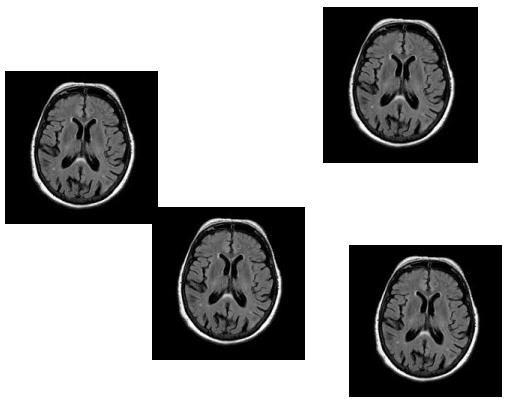
Undersampling

Randomly remove elements from the majority class.



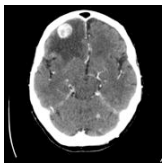
Undersampling

Randomly remove elements from the majority class.



Drawback: Removing data points could lose important information

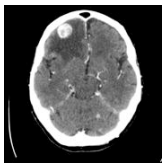
Oversampling

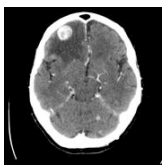


Duplicate elements of your minority class

Oversampling

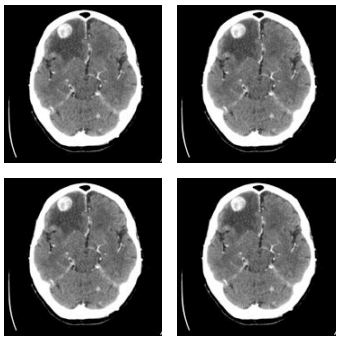
Duplicate elements of your minority class





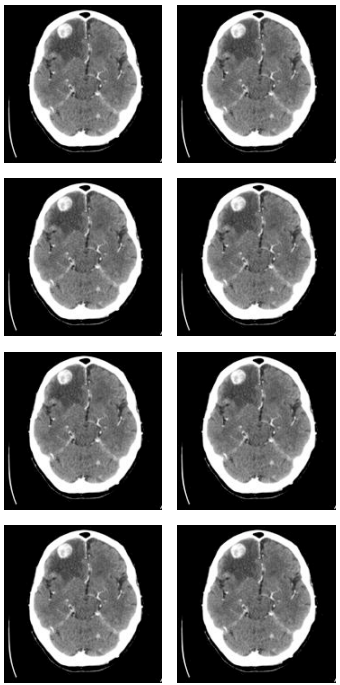
Oversampling

Duplicate elements of your minority class



Oversampling

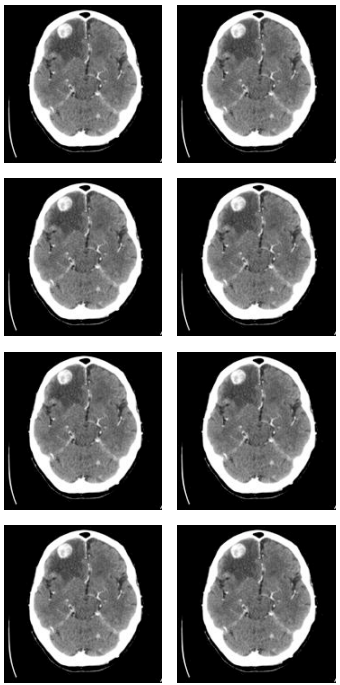
Duplicate elements of your minority class



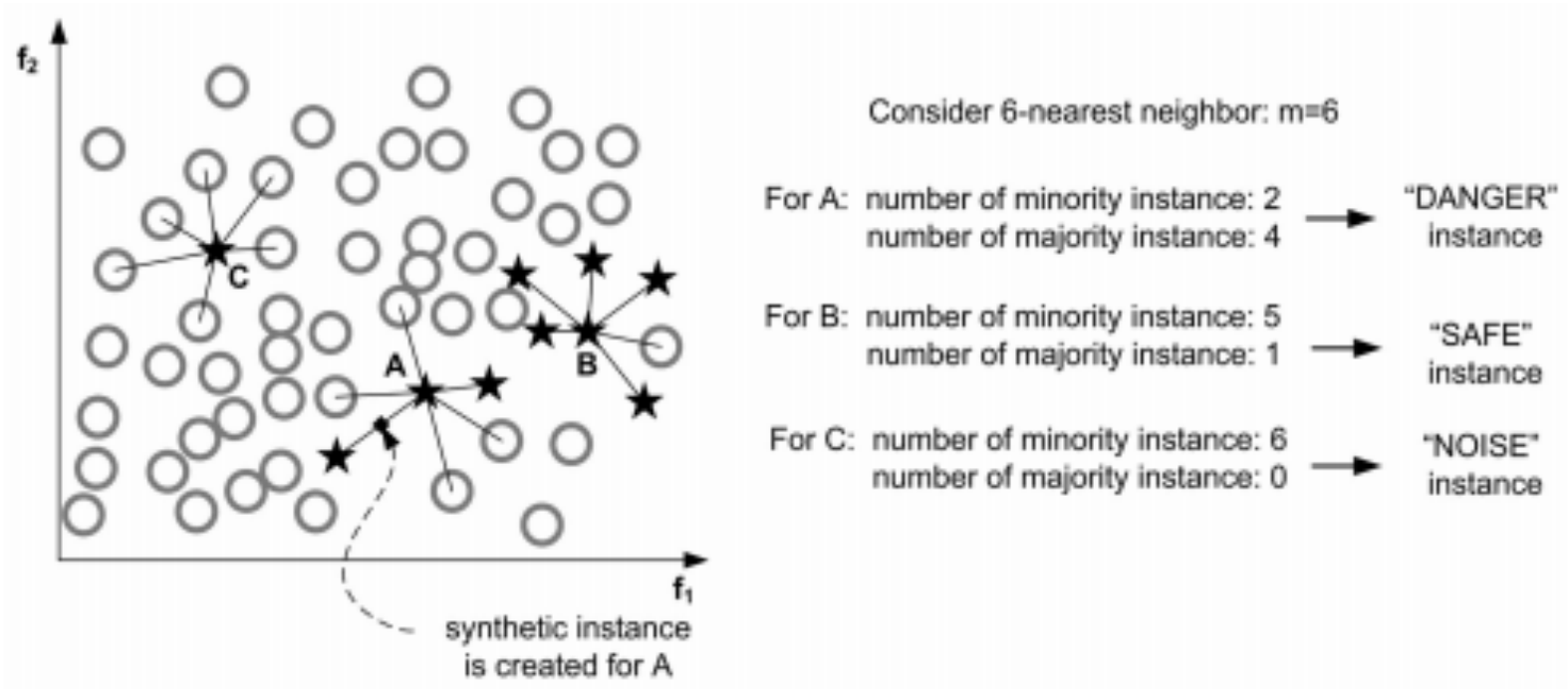
Oversampling

Duplicate elements of your minority class

Drawback: Just replicating randomly minority classes could cause overfit



SMOTE: generate synthetic minority examples



http://egr.uri.edu/wp-uploads/he/learning-from-imbalanced-data.pdf

SMOTE: generate synthetic minority examples

For every minority example:

1) find k nearest neighbors in the minority class
2) randomly select one of these neighbors
3) generate new synthetic examples along the line between the minority example and the selected neighbor.

http://egr.uri.edu/wp-uploads/he/learning-from-imbalanced-data.pdf

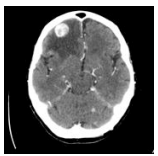
There are even more sophisticated methods, for a review see:

http://egr.uri.edu/wp-uploads/he/learning-from-imbalanced-data.pdf

ERROR RATES

To deal with issue 2 we need a more sophisticated definition of error rates in a binary classification problem

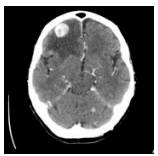
True Positive: An Example that is **positive** and is classified as **positive**



Label: **positive**

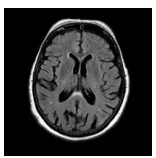
To deal with issue 2 we need a more sophisticated definition of error rates in a binary classification problem

True Positive: An Example that is **positive** and is classified as **positive**



Label: **positive**

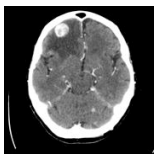
True Negative: An Example that is **negative** and is classified as **negative**



Label: **negative**

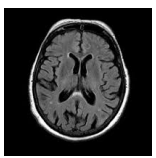
To deal with issue 2 we need a more sophisticated definition of error rates in a binary classification problem

True Positive: An Example that is **positive** and is classified as **positive**



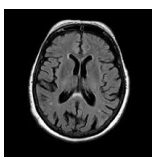
Label: **positive**

True Negative: An Example that is **negative** and is classified as **negative**



Label: **negative**

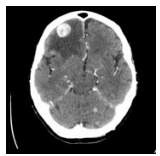
False Positive: An Example that is **negative** and is classified as **positive**



Label: **positive**

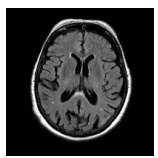
To deal with issue 2 we need a more sophisticated definition of error rates in a binary classification problem

True Positive: An Example that is **positive** and is classified as **positive**



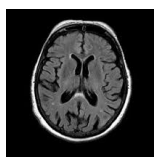
Label: **positive**

True Negative: An Example that is **negative** and is classified as **negative**



Label: **negative**

False Positive: An Example that is **negative** and is classified as **positive**



Label: **positive**

False Negative: An Example that is **positive** and is classified as **negative**

Label: **negative**

Confusion Matrix

	Condition Positive	***Condition Negative***
Test Positive	***TRUE POSITIVE***	***FALSE POSITIVE (Type I error)***
Test Negative	***FALSE NEGATIVE (Type II error)***	***TRUE NEGATIVE***

Confusion Matrix

n = 165	*Condition Positive*	*Condition Negative*
Test Positive	*100*	*10*
Test Negative	*5*	*50*

How many classes are there?
How many patients?
How many times is disease predicted?
How many patients actually have the disease?

Confusion Matrix

		Condition (as determined by "Gold standard")			
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	
Test outcome	Test outcome positive	**True positive**	**False positive** (Type I error)	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Test outcome positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Test outcome positive}}$
	Test outcome negative	**False negative** (Type II error)	**True negative**	False omission rate (FOR) = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Test outcome negative}}$	Negative predictive value (NPV) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Test outcome negative}}$
	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	True positive rate (TPR), Sensitivity, Recall = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) = $\frac{\text{LR+}}{\text{LR−}}$
		False negative rate (FNR), Miss rate = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) = $\frac{\text{FNR}}{\text{TNR}}$	

n = 165	*Condition Positive*	*Condition Negative*
Test Positive	*100*	*10*
Test Negative	*5*	*50*

Accuracy:
Overall, how often is it **correct**?

(TP + TN) / total = 150/165 = 0.91

Precision:
When test is positive, how often is prediction correct?
TP / test yes = 100/110 = 0.91

Sensitivity/Recall/TPR:
When actual value is positive, how often is prediction correct?
TP / actual yes = 100/105 = 0.95

Specificity/TNR:
When actual value is negative, how often is prediction correct?
TN / actual no = 50/60 = 0.83

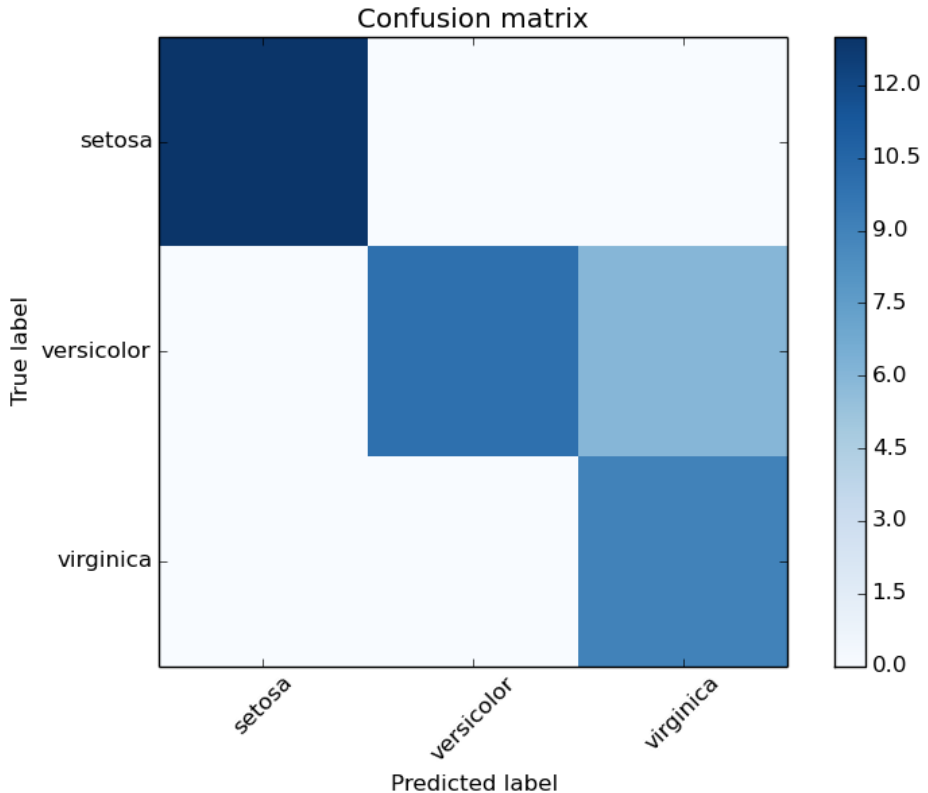
n = 165	*Condition Positive*	*Condition Negative*
Test Positive	*100*	*10*
Test Negative	*5*	*50*

Precision:
When test is positive, how often is prediction correct?
TP / test yes = 100/110 = 0.91

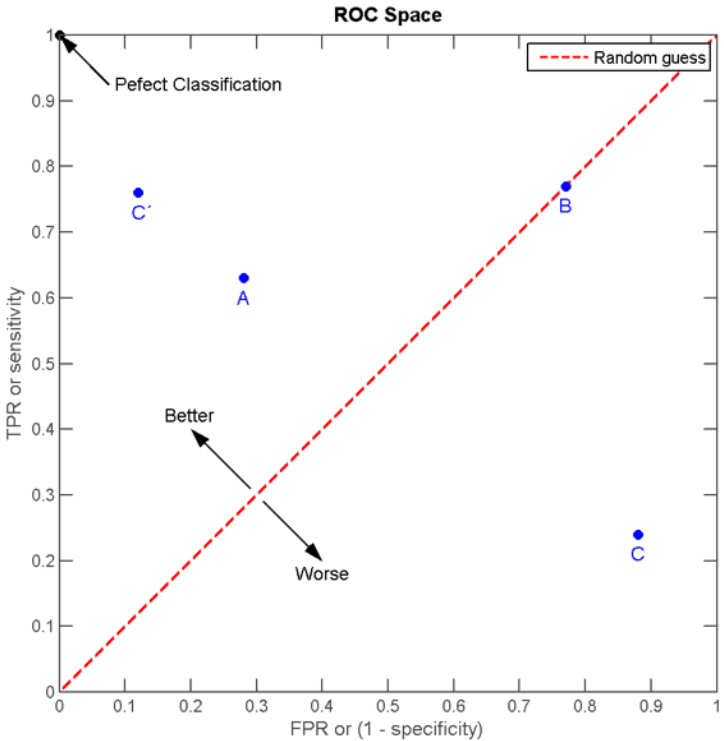
Sensitivity/Recall/TPR:
When actual value is positive, how often is prediction correct?
TP / actual yes = 100/105 = 0.95

F score

$$F = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}$$


Confusion matrix
setosa
versicolor
virginica
True label
setosa
versicolor
virginica
Predicted label
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.0

ROC CURVES



TP Rate = True Positives / All positives

FP Rate = False Positives / All Negatives

Email Number	Score	True Label
5	0.99	Spam
8	0.82	Spam
2	0.60	Spam
1	0.60	Ham
7	0.48	Spam
3	0.22	Ham
4	0.10	Ham
6	0.02	Ham

Every email is assigned a “spamminess” score by our classification algorithm. To actually make our predictions, we choose a numeric cutoff for classifying as spam.

An ROC Curve will help us to visualize how well our classifier is doing without having to choose a cutoff!

Email Number	Score	True Label
5	0.99	Spam
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Every email is assigned a "spamminess" score by our classification algorithm. To actually make our predictions, we choose a numeric cutoff for classifying as spam.

An ROC Curve will help us to visualize how well our classifier is doing without having to choose a cutoff!

Cut off	TPR (y)	FPR (x)	Cut off	TPR (y)	FPR (x)
0			0.50		
0.05			0.65		
0.15			0.85		
0.25			1		

Email Number	Score	True Label
5	0.99	Spam
8	0.82	Spam
2	0.60	Spam
1	0.60	Ham
7	0.48	Spam
3	0.22	Ham
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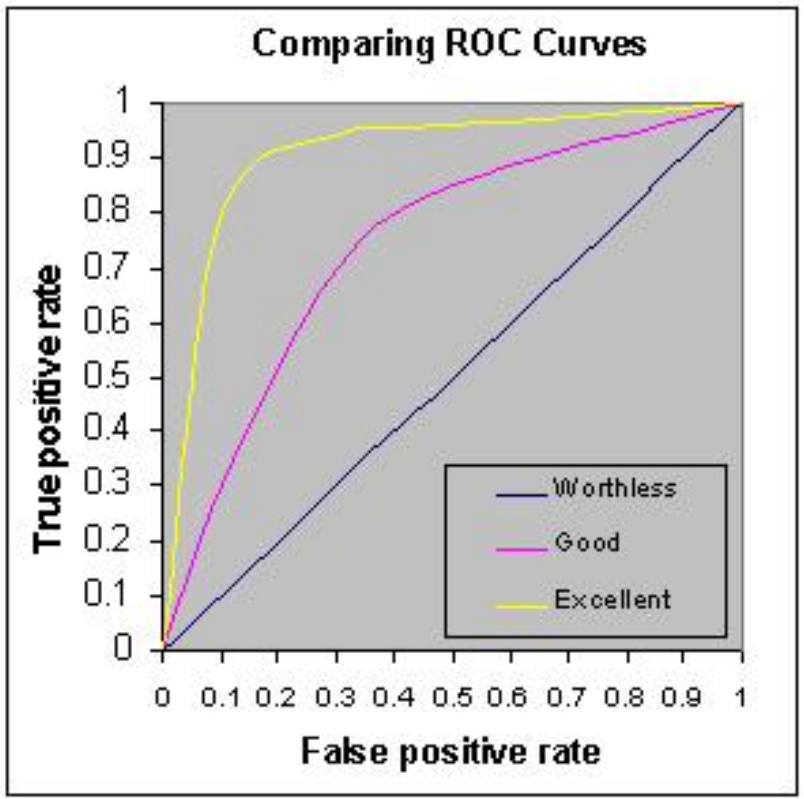
Every email is assigned a "spamminess" score by our classification algorithm. To actually make our predictions, we choose a numeric cutoff for classifying as spam.

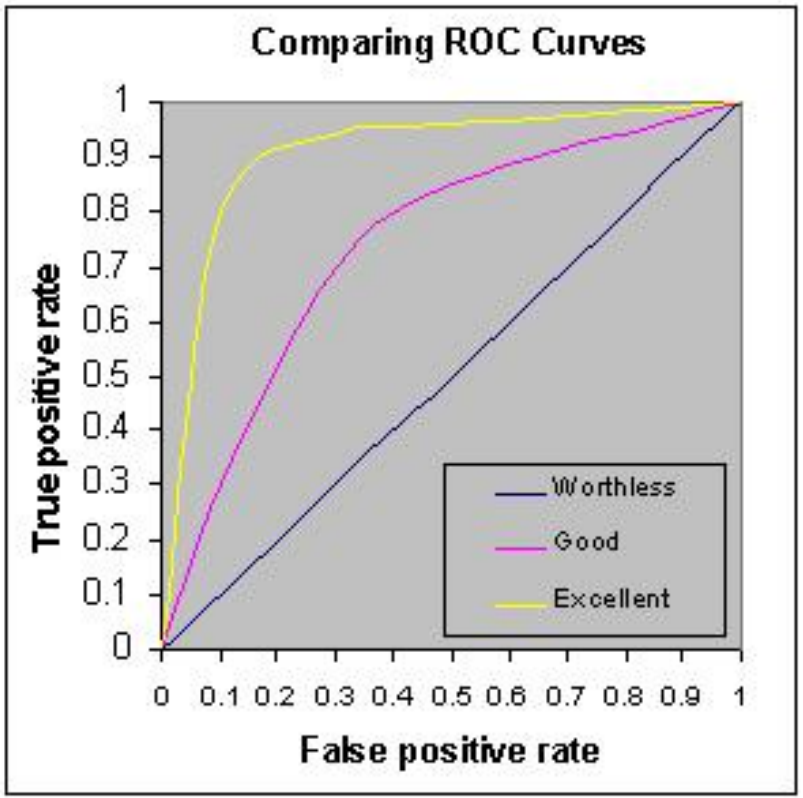
An ROC Curve will help us to visualize how well our classifier is doing without having to choose a cutoff!

Cut off	TPR (y)	FPR (x)	Cut off	TPR (y)	FPR (x)
0	1	1	0.50	0.75	0.25
0.05	1	0.75	0.65	0.5	0
0.15	1	0.5	0.85	0.25	0
0.25	1	0.25	1	0	0



ROC Curves show the relationship between the TP Rate and the FP Rate as we vary the decision threshold for the classifier

Cut off	TPR (y)	FPR (x)	Cut off	TPR (y)	FPR (x)
0	1	1	0.50	0.75	0.25
0.05	1	0.75	0.65	0.5	0
0.15	1	0.5	0.85	0.25	0
0.25	1	0.25	1	0	0



Area Under the Curve (AUC)

We evaluate a classifier by measuring the Area Under the Curve for its ROC curve. The Greater area under the curve, the more effective the classifier.

Then for our chosen classifer, we pick an appropriate decision threshold. In general, we pick the decision threshold that gets us closest to the upper left corner

Q: Would the ROC Curve (and AUC) change if the scores changed but the ordering remained the same?

A: Not at all! The ROC Curve is only sensitive to rank ordering and does not require calibrated scores.

Area Under the Curve (AUC)

We evaluate a classifier by measuring the Area Under the Curve for its ROC curve. The Greater area under the curve, the more effective the classifier.

Then for our chosen classifier, we pick an appropriate decision threshold. In general, we pick the decision threshold that gets us closest to the upper left corner

OTHER EVALUATION METRICS

REGRESSION METRICS

RMSE

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

- Used for regression problems
- Square root of the mean of the squared errors
- Easily interpretable (in the "y" units)
- "Punishes" larger errors

RMSE

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Example:
y_true = [100, 50, 30]
y_preds = [90, 50, 50]
RMSE = np.sqrt((10**2 + 0**2 + 20**2) / 3) = 12.88

EXPLAINED VARIANCE

$$\texttt{explained\_variance}(y, \hat{y}) = 1 - \frac{Var\{y - \hat{y}\}}{Var\{y\}}$$

Example:
y_true = [3, -0.5, 2, 7]
y_pred = [2.5, 0.0, 2, 8]
explained_variance(y_true, y_pred) = 0.957

Mean Absolute Error

$$\mathrm{MAE}(y, \hat{y}) = \frac{1}{n_{\mathrm{samples}}} \sum_{i=0}^{n_{\mathrm{samples}}-1} |y_i - \hat{y}_i| .$$

Example:
y_true = [3, -0.5, 2, 7]
y_pred = [2.5, 0.0, 2, 8]
mean_absolute_error(y_true, y_pred) = 0.5

Median Absolute Error

$$\text{MedAE}(y, \hat{y}) = \text{median}(| \ y_1 - \hat{y}_1 \ |, \ldots, | \ y_n - \hat{y}_n \ |).$$

Particularly interesting because it's robust to outliers.

Classification Metrics

Accuracy Score

$$\texttt{accuracy}(y, \hat{y}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} 1(\hat{y}_i = y_i)$$

i.e. the relative frequency of accurate predictions.

Log Loss

$$L_{\log}(y, p) = -\log \Pr(y|p) = -(y \log p) + (1 - y) \log(1 - p))$$

It is commonly used in (multinomial) logistic regression and neural networks, as well as in some variants of expectation-maximization

COST FUNCTION

Linear Regression Example

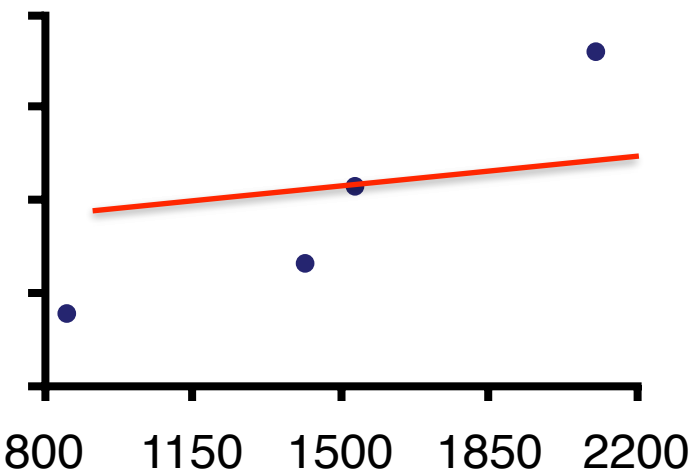
Size in feet^2 (x)	*Price in 1000$ (y)*
2104	*460*
1416	*232*
1534	*315*
852	*178*
…	*…*

Linear Regression Example

Hypothesis

$h(x) = \beta_0 + \beta_1 x$

Size in feet² (x)	Price in 1000$ (y)
2104	460
1416	232
1534	315
852	178
...	...



Linear Regression Example

Size in feet² (x)	Price in 1000$ (y)
2104	460
1416	232
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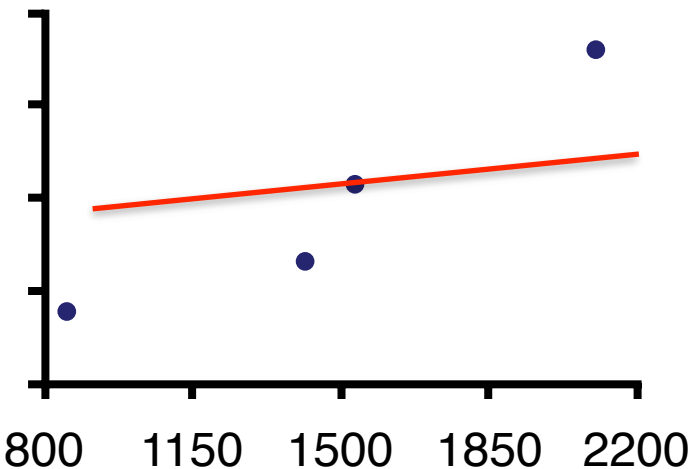
852	178
…	…

Hypothesis

$h(x) = \beta_0 + \beta_1 x$

How do I determine the βs?



Linear Regression Example

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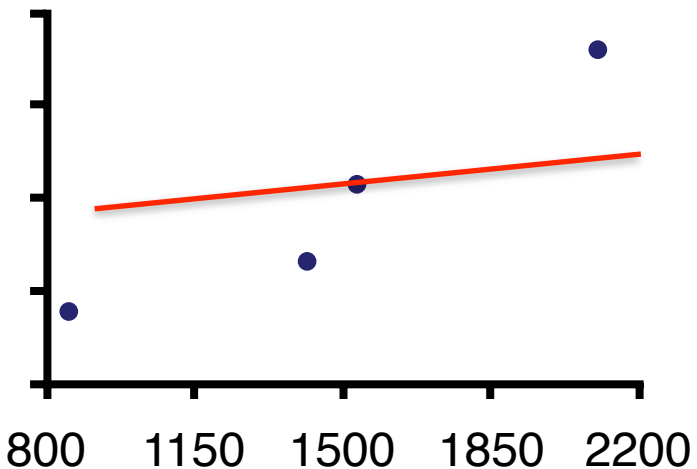
...	...

Hypothesis

$h(x) = \beta_0 + \beta_1 x$

How do I determine the βs?

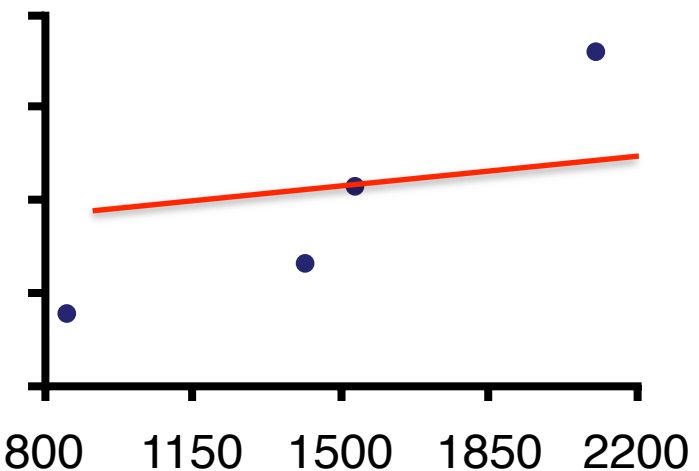
IDEA: choose the βs to minimize distance of h(x) from training data (x, y)



Linear Regression Example

In this case the distance used is the Squared Error

Size in feet² (x)	Price in 1000$ (y)
2104	460
1416	232
1534	315
852	178
…	…



Linear Regression Example

In this case the distance used is the Squared Error:

$$J(\beta_0, \beta_1) = \frac{1}{m} \sum_{i=0}^{m} (h_\beta(x_i) - y_i)^2$$

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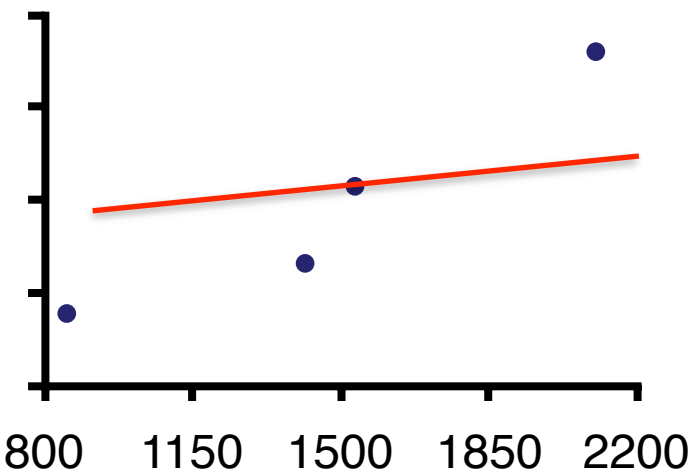

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Which is just an example of

COST FUNCTION

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1534	315
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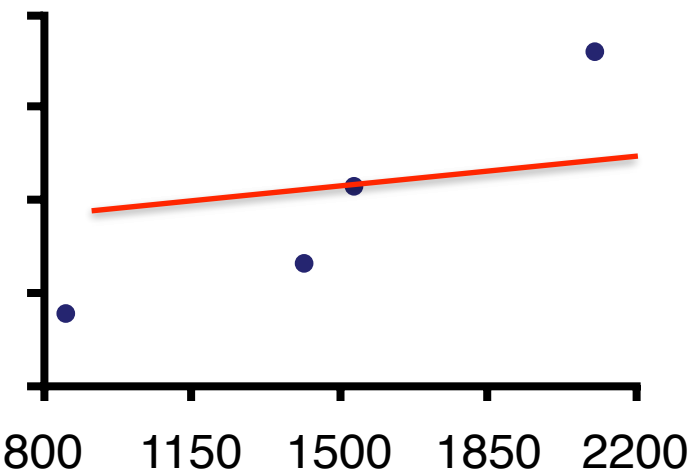
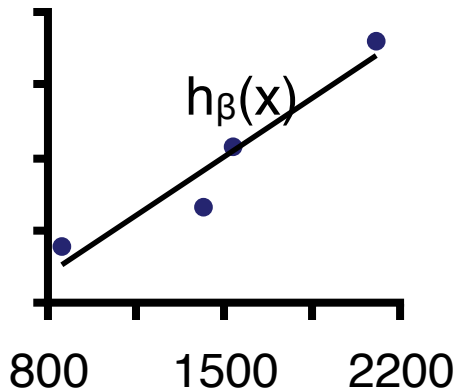


We can generalize and say:

Training set : (x, y)

Hypothesis Function : $h_\beta(x)$



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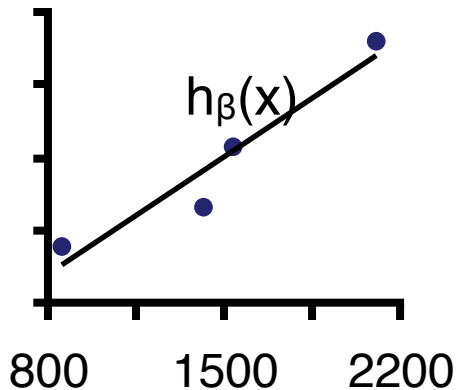

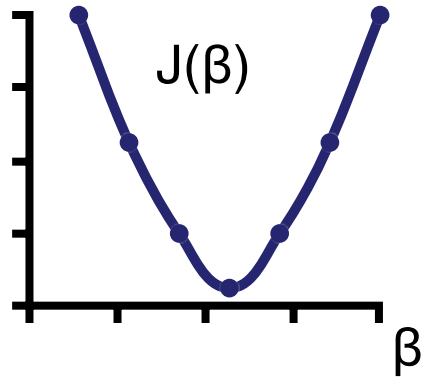

Cost Function: J(β)

GOAL

Find the values for the parameters β that minimize the cost function over the set of training data

We can generalize and say:

Training set : (x, y)

Hypothesis Function : $h_\beta(x)$

Cost Function: J(β)

And this is approach can be generalized to any ML problem, with any dimension and any goal (regression, classification)

GOAL

Find the values for the parameters β that minimize the cost function over the set of training data

Machine learning problems can be re-stated as:

1. Define a hypothesis function over the training set
2. Choose an appropriate cost function that depends on parameters
3. Find the combination of parameters that minimize the cost of the hypothesis over the training set

VALIDATION CURVES AND LEARNING CURVES

ML models depend on Hyperparameters

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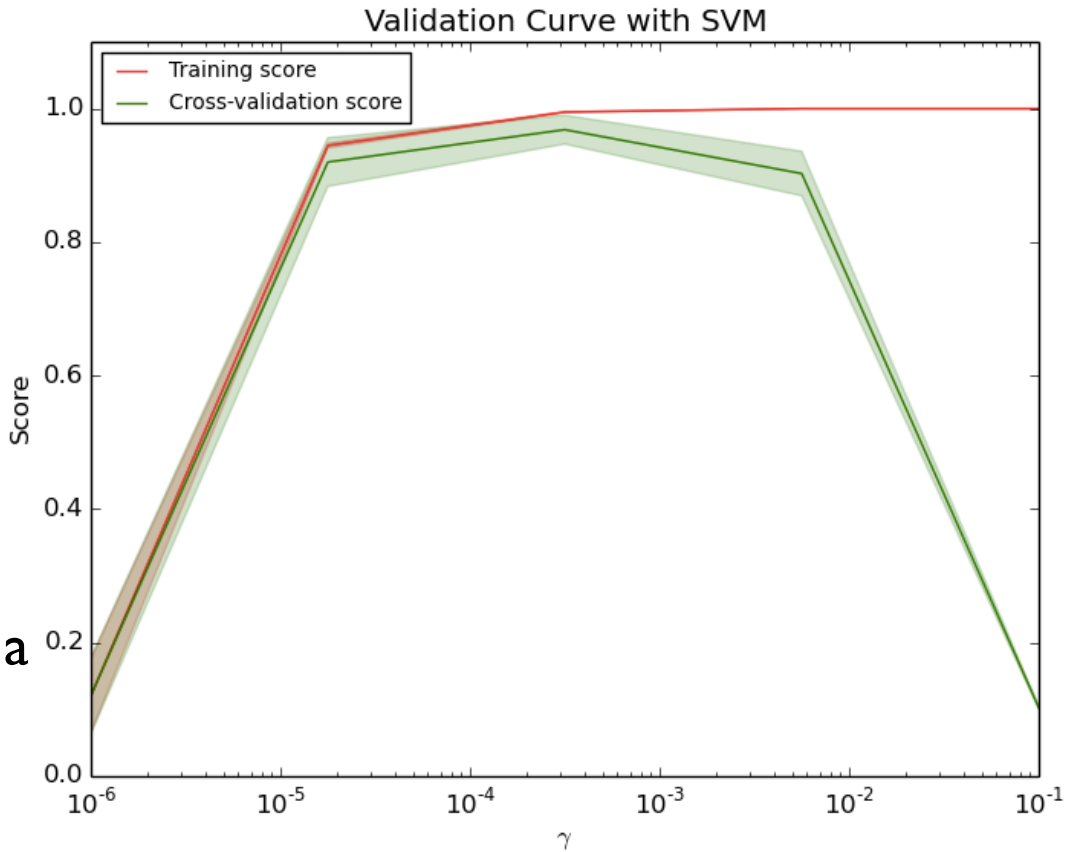
Plot Training and CV score as a function of the Hyper params



How do I know if I have enough data?

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