INTRO TO DATA SCIENCE
IMBALANCED CLASSES/EVALUATION METRICS

DATA SCIENCE IN THE NEWS

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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.
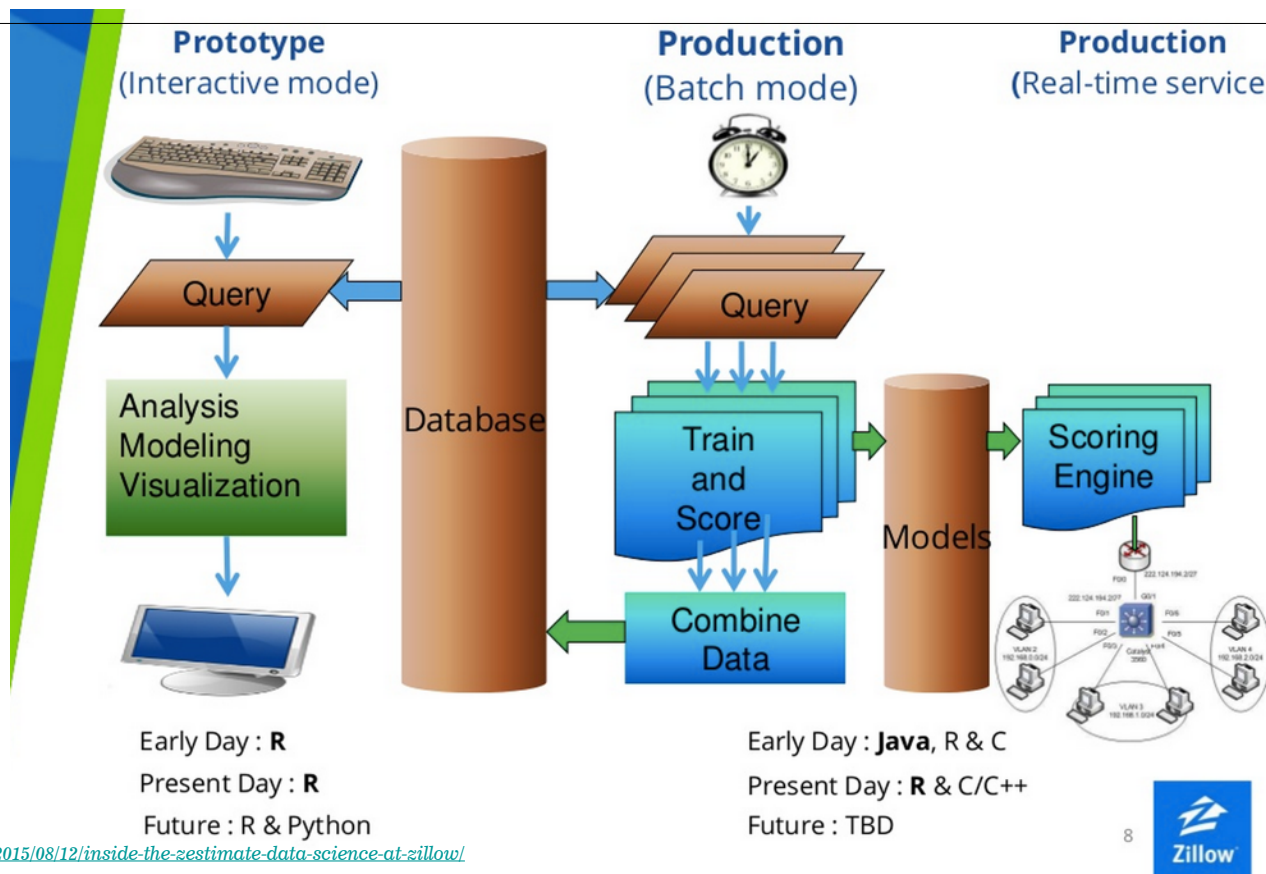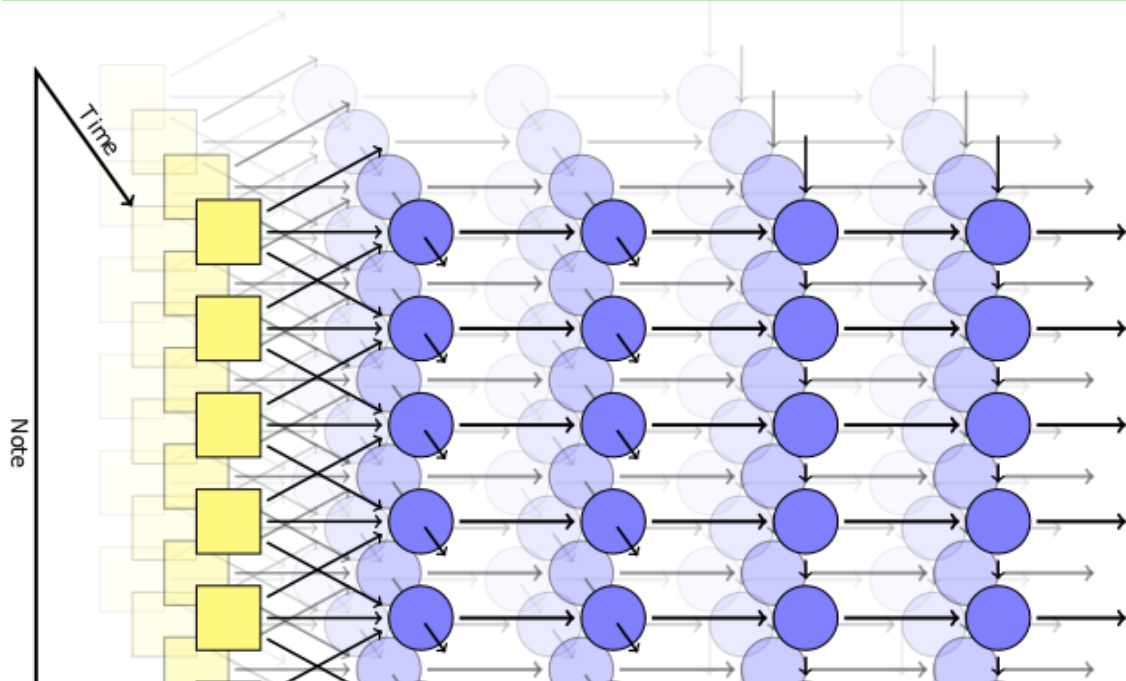
LAST TIME:

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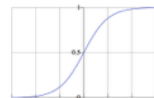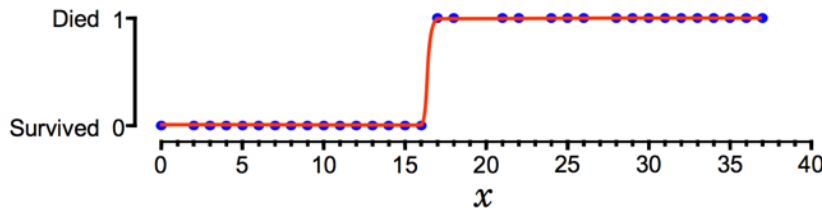# II. OUTCOME VARIABLES
III. ERROR TERMS
IV. INTERPRETING RESULTS

LAB: IMPLEMENTING LOGISTIC REGRESSION IN PYTHON

QUESTIONS?

QUESTIONS?

WHAT WAS THE MOST INTERESTING THING YOU LEARNT?

WHAT WAS THE HARDEST TO GRASP?

I. IMBALANCED CLASSES

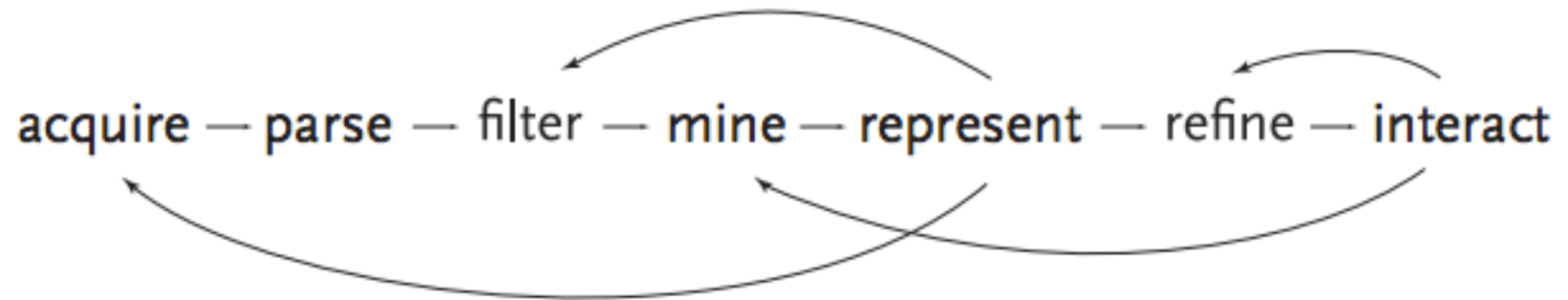II. ERROR RATES
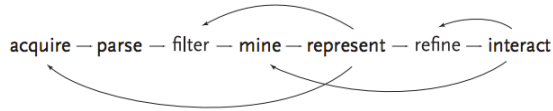
III. ROC CURVES

IV. EVALUATION METRICS

V. COST FUNCTION

VI. VALIDATION CURVES AND LEARNING CURVES

KEY OBJECTIVES

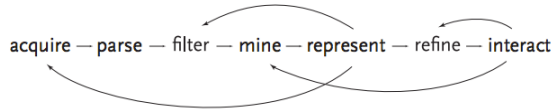- RECOGNIZE IMBALANCED CLASSES

- 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

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

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

	Continuous	Categorical
Supervised	regression ✓	classification ✓
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Regression & Regularization

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

	Continuous	Categorical
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Regression & Regularization

3 Classification methods

KNN

Women age 40

A   B

Naïve Bayes

Logistic Regression

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

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Regression & Regularization

3 Classification methods

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Logistic Regression

Train - Test Split

training set

test set

dataset

new data

model

predictions

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

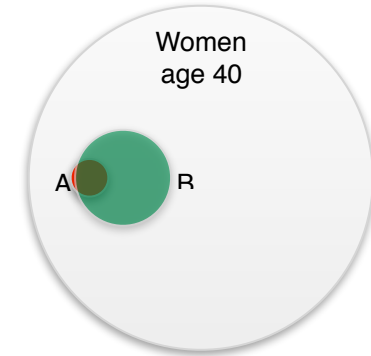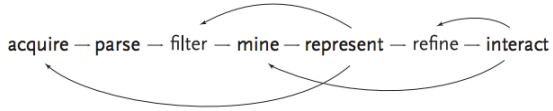|	**Continuous**	**Categorical**
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3 Classification methods

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predictions

Cross Validation

1. Randomly split training instances into *K* equal-sized subsets

fold 1
fold 2
...
fold i
...
fold K

Features & **Target**

For i in 1:K

training: all folds except fold i

fold i

model

2. Train a ML **model** on the *training* subset

ignore Target when predicting

3. Make **predictions** on *fold i* subset

fold i predictions

4. Store *fold i* **predictions** in the **CV predictions** array

CV predictions

fold i predictions

5. Compare **CV predictions** to **Target** to assess accuracy

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

	Continuous	*Categorical*
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Regression & Regularization
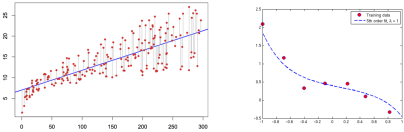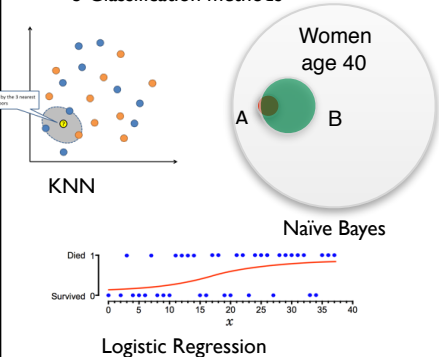
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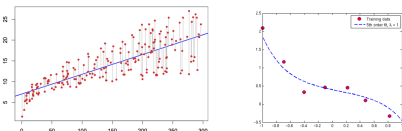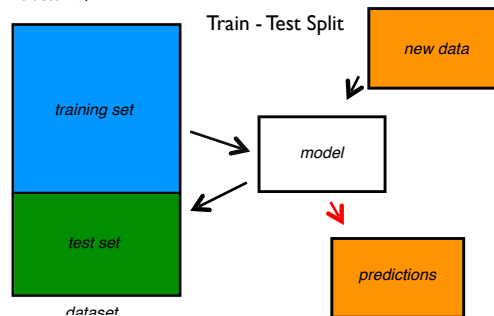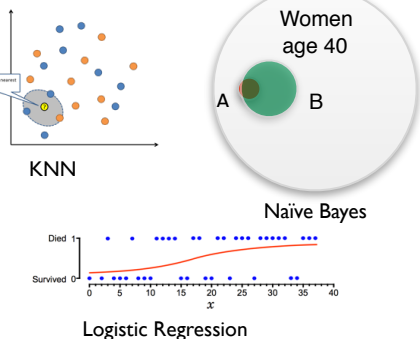
KNN

Women age 40

A   B

Naïve Bayes

Died 1

Survived 0

Logistic Regression

Train - Test Split

training set

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new data

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predictions

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2. Train a ML model on the training subset

model

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3. Make predictions on fold i subset

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CV predictions   fold i predictions

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What else?

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

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Regression & Regularization

3 Classification methods
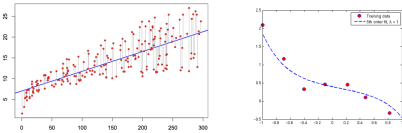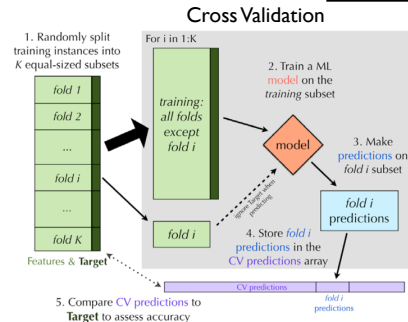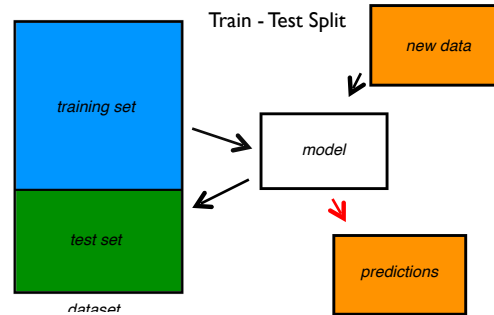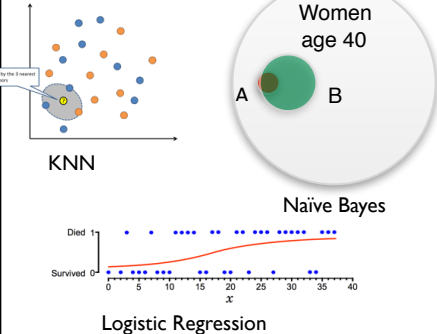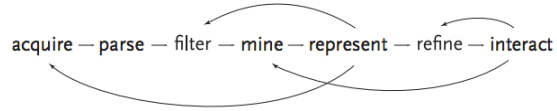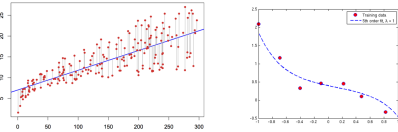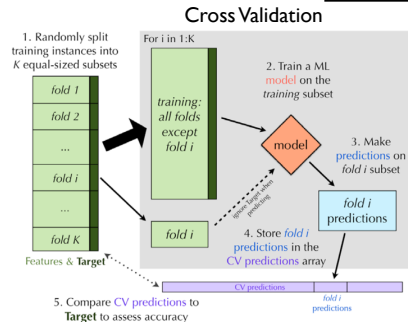
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CV predictions

fold i predictions

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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

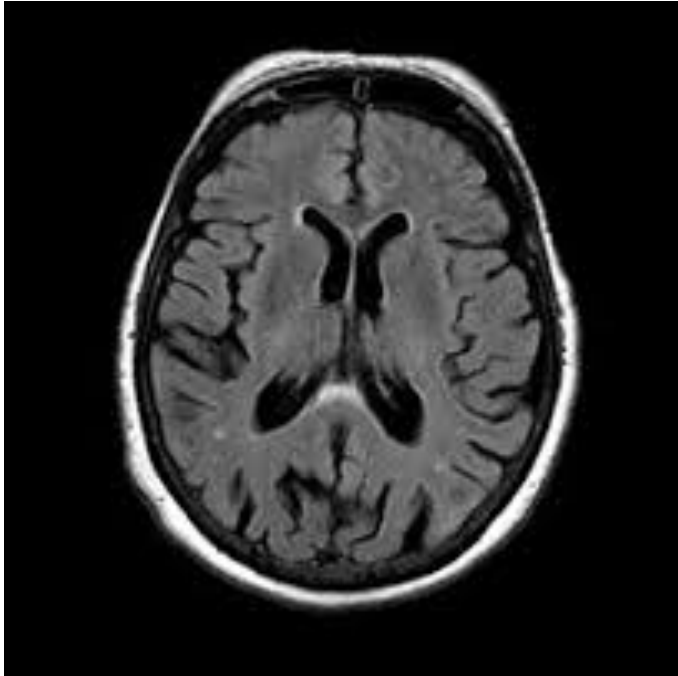- Imbalance confuses classifiers => only perform well on dominant class
- Situation is very common in other fields (e.g. fraud detection)
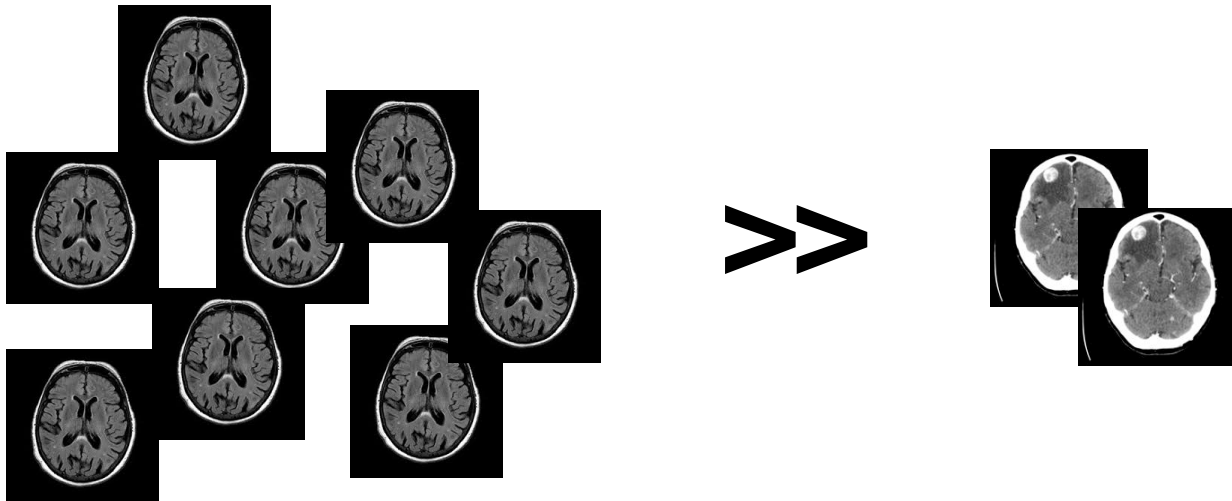
ISSUE 2: Not all errors are equal…
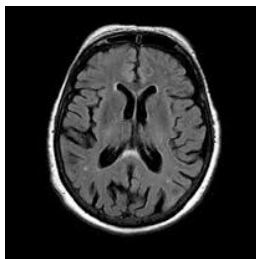
Error 1   Classifier Label: Cancerous   Permissable, because a physician will review it
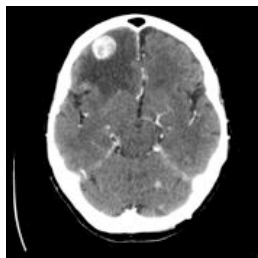
Error 2   Classifier Label: Non-Cancerous   Not permissable, because this data will be discarded

IMBALANCED CLASSES

Imbalanced classes can be re-balanced in several ways
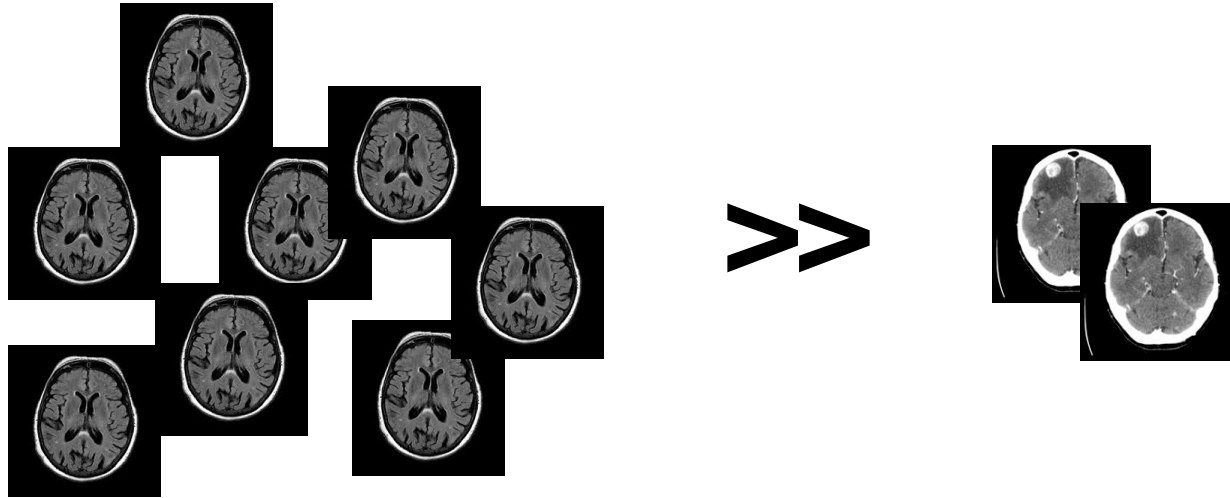
Imbalanced classes can be re-balanced in several ways

1. **Undersampling** the dominant class - remove some the majority class so it has less weight

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3. **Hybrid** - doing both

Imbalanced classes can be re-balanced in several ways

1. **Undersampling** the dominant class - remove some the majority class so it has less weight

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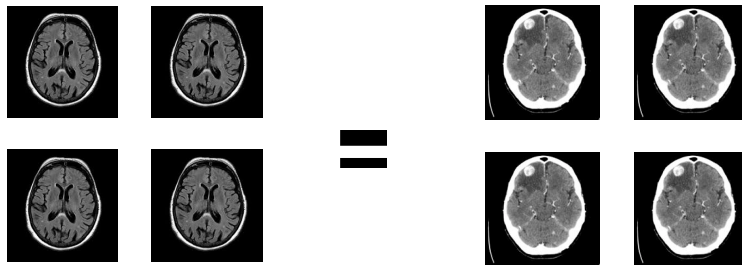
3. **Hybrid** - doing both

Undersampling

Randomly remove elements from the majority class.
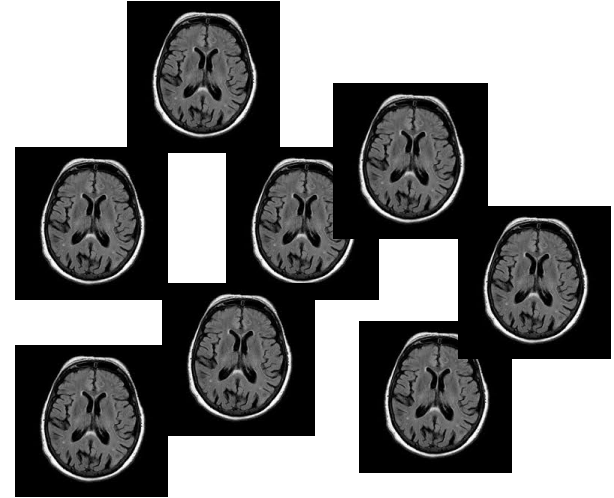
Undersampling

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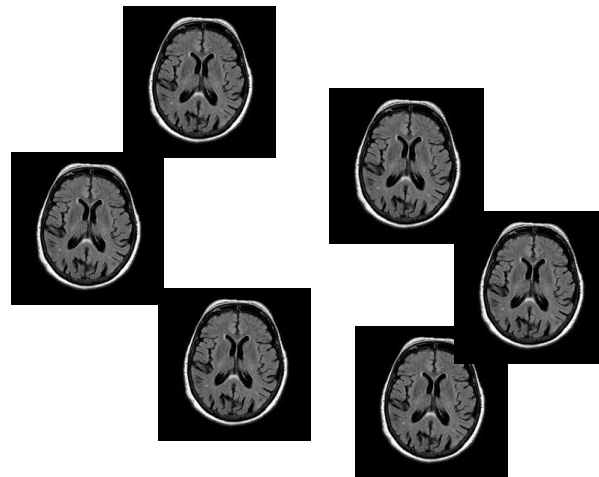
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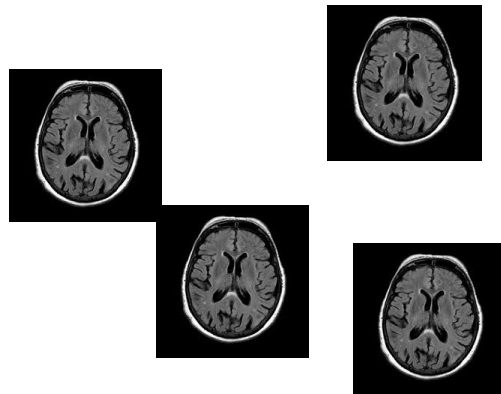
Undersampling

Randomly remove elements from the majority class.

Drawback: Removing data points could lose important information
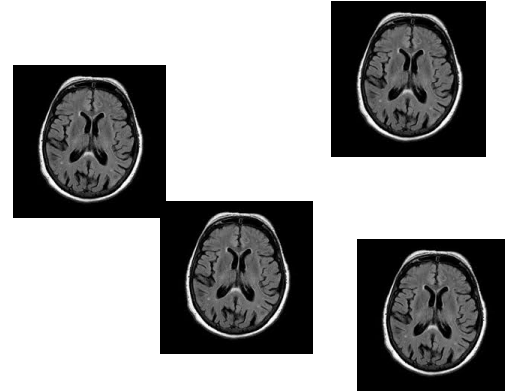
Oversampling

Duplicate elements of your minority class

Oversampling

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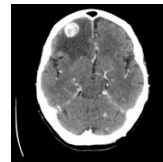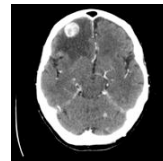
Oversampling

Duplicate elements of your minority class
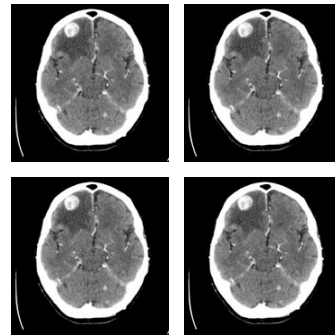
Oversampling

Duplicate elements of your minority class
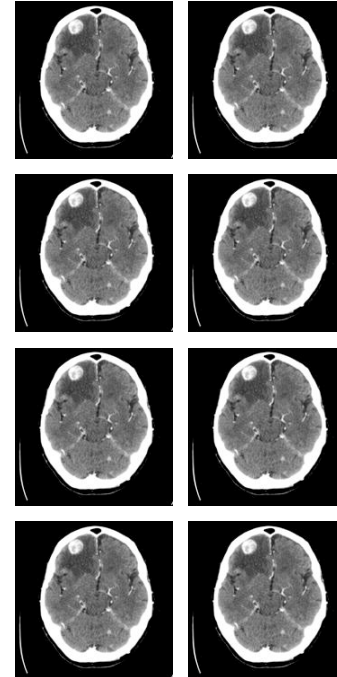
Oversampling

Duplicate elements of your minority class

Drawback: Just replicating randomly minority classes could cause overfit
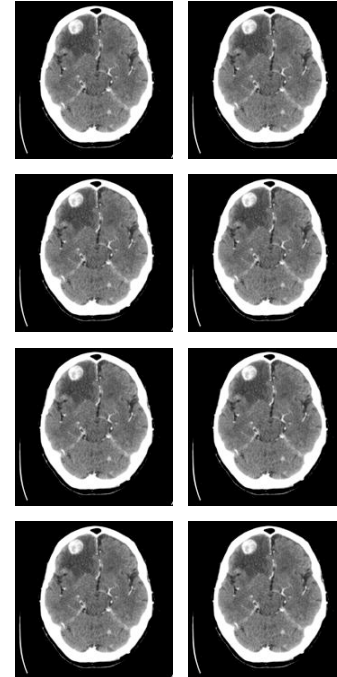
SMOTE: generate synthetic minority examples
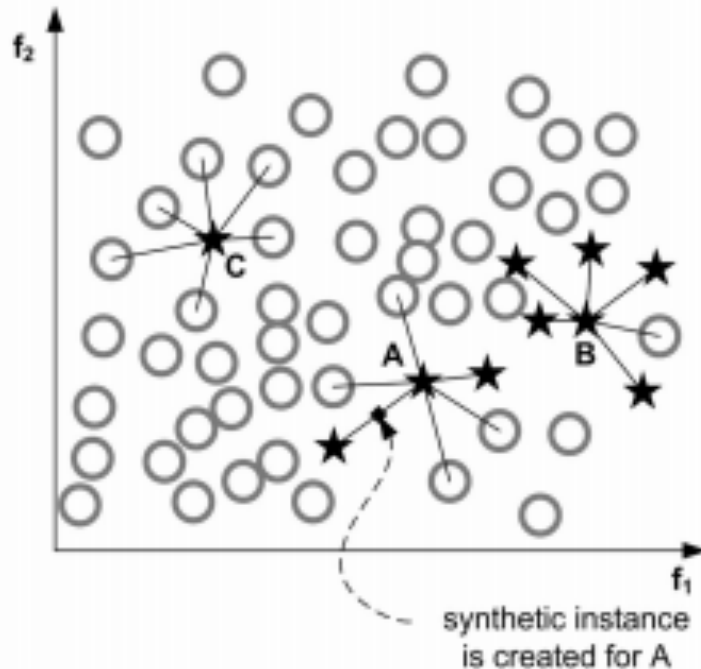
http://egr.uri.edu/wp-uploads/he/learning-from-imbalanced-data.pdf

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.

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**
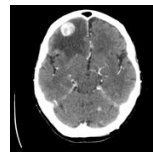
Label:
positive

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**
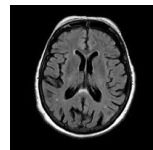
Label: **negative**

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**
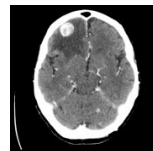
Label: **negative**

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")			
Test outcome	Total population	Condition positive	Condition negative	Prevalence $= \frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	
	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

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

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

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

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

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Test Positive	100	10
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Precision:
When test is positive, how often is prediction correct?
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When actual value is positive, how often is prediction correct?
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F score

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

Confusion matrix
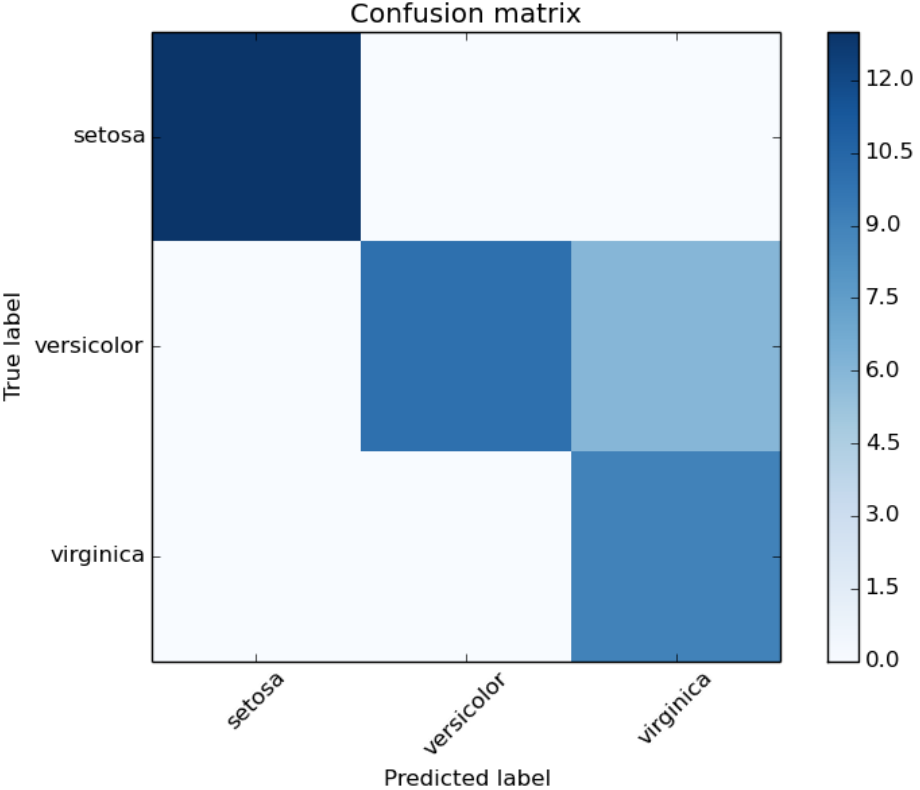
ROC CURVES
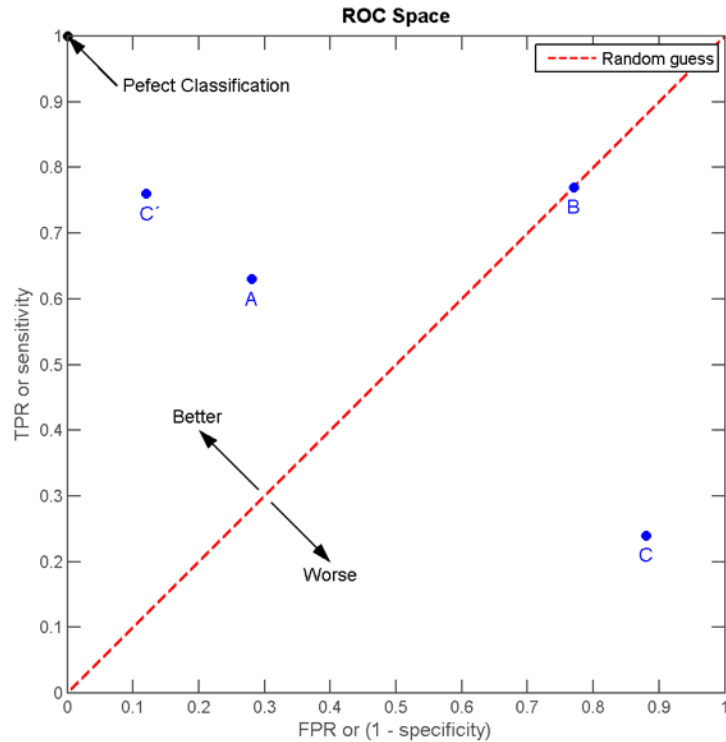
TP Rate = True Positives / All positives

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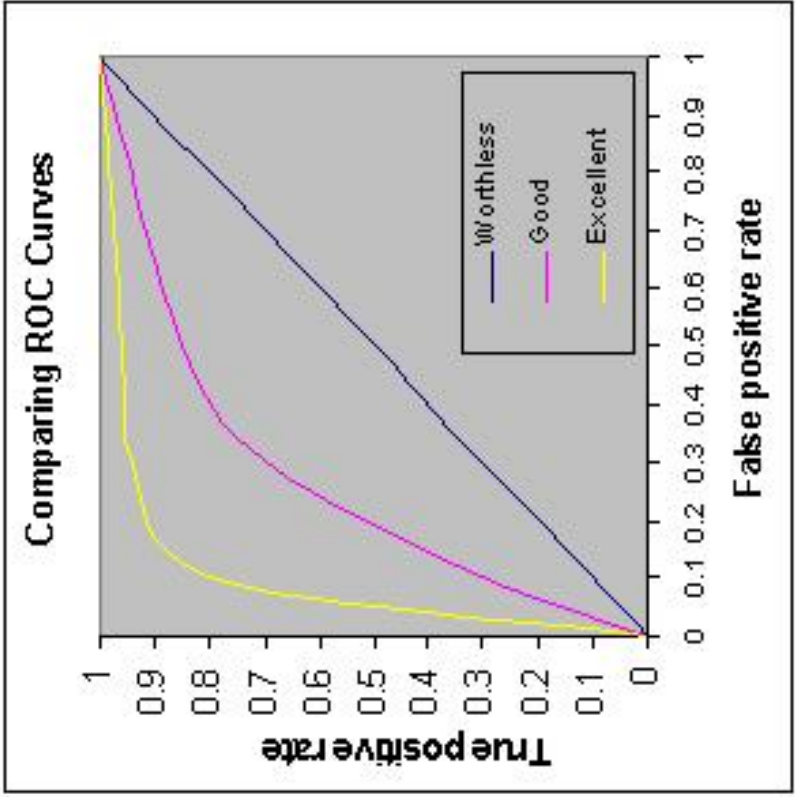
Cut off	TPR (y)	FPR (x)	Cut off	TPR (y)	FPR (x)
0	1	1	0.50	0.75	0.25
0.05	1	0.75	0.65	0.5	0
0.15	1	0.5	0.85	0.25	0
0.25	1	0.25	1	0	0

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

Comparing ROC Curves

— Worthless
— Good
— Excellent

True positive rate

False positive rate

Comparing ROC Curves

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

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

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

RMSE

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

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

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

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

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

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

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

Particularly interesting because it's robust to outliers.

Classification Metrics

Accuracy Score

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

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
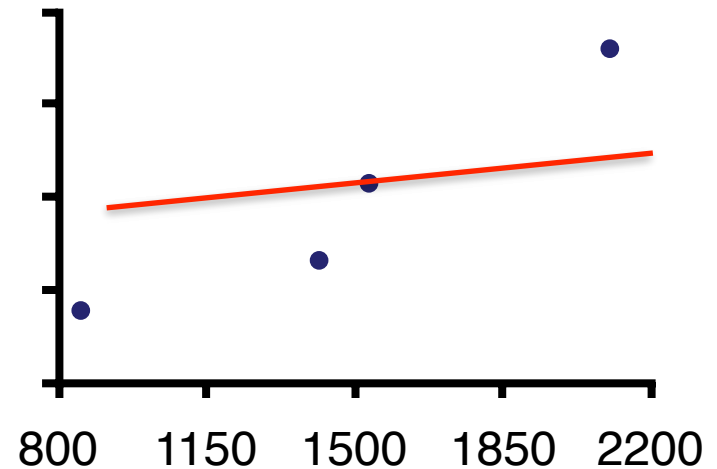
Linear Regression Example

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

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Hypothesis

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

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How do I determine the βs?

Linear Regression Example

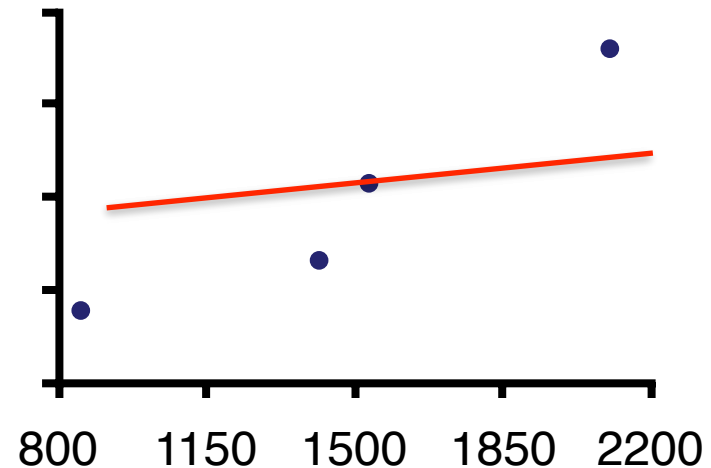| Size in feet² (x)	Price in 1000$ (y)
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Hypothesis

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How do I determine the βs?

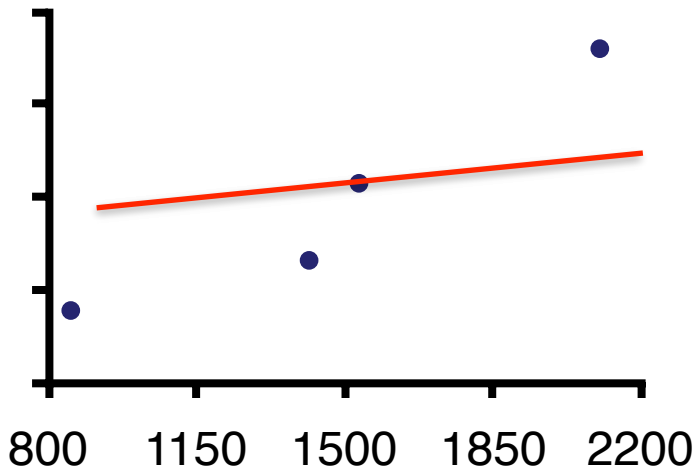IDEA: choose the βs to minimize distance of h(x) from training data (x, y)

Linear Regression Example

In this case the distance used is
the Squared Error

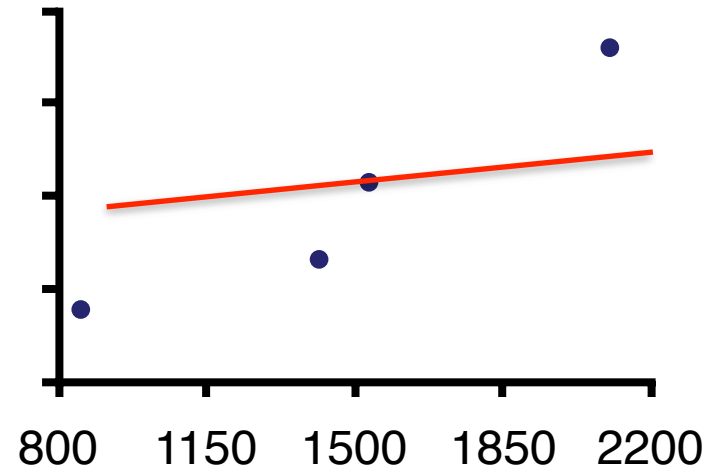| Size in feet² (x)	Price in 1000$ (y)
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Linear Regression Example

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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...	...

800   1150   1500   1850   2200
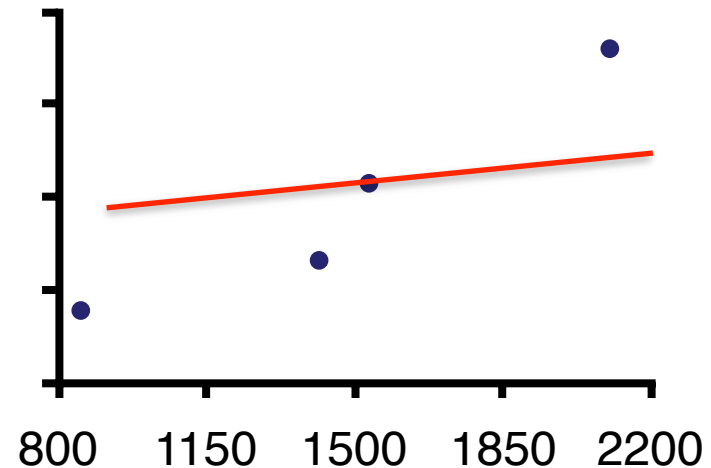
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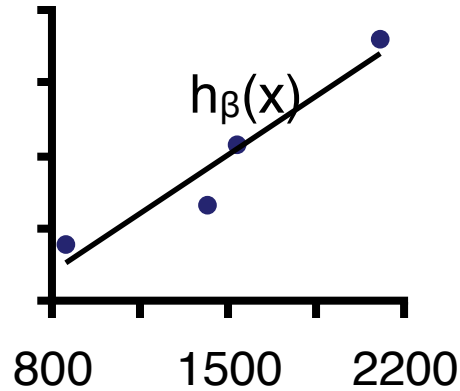
Which is just an example of

COST FUNCTION

Size in feet² (x)	Price in 1000$ (y)
2104	460
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1534	315
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...	...

We can generalize and say:

Training set : (x, y)

Hypothesis Function : $h_\beta(x)$

$h_\beta(x)$

800   1500   2200

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Training set : (x, y)

Hypothesis Function : $h_\beta(x)$

$h_\beta(x)$

800   1500   2200

$J(\beta)$

β

Cost Function: $J(\beta)$

GOAL
Find the values for the parameters β that minimize
the cost function over the set of training data
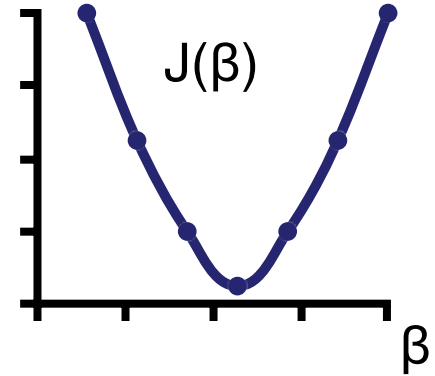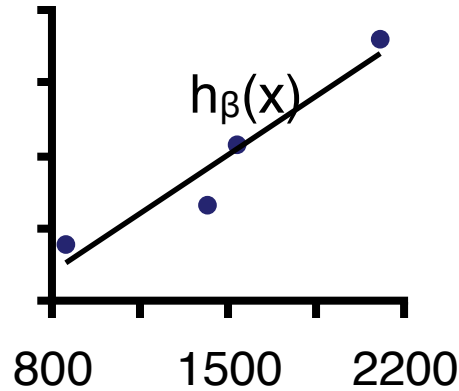
We can generalize and say:

Training set : (x, y)

Hypothesis Function : $h_\beta(x)$

Cost Function: $J(\beta)$

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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Hyperparameters

Not the βs, but e.g.
regularization strength

ML models depend on
Hyperparameters
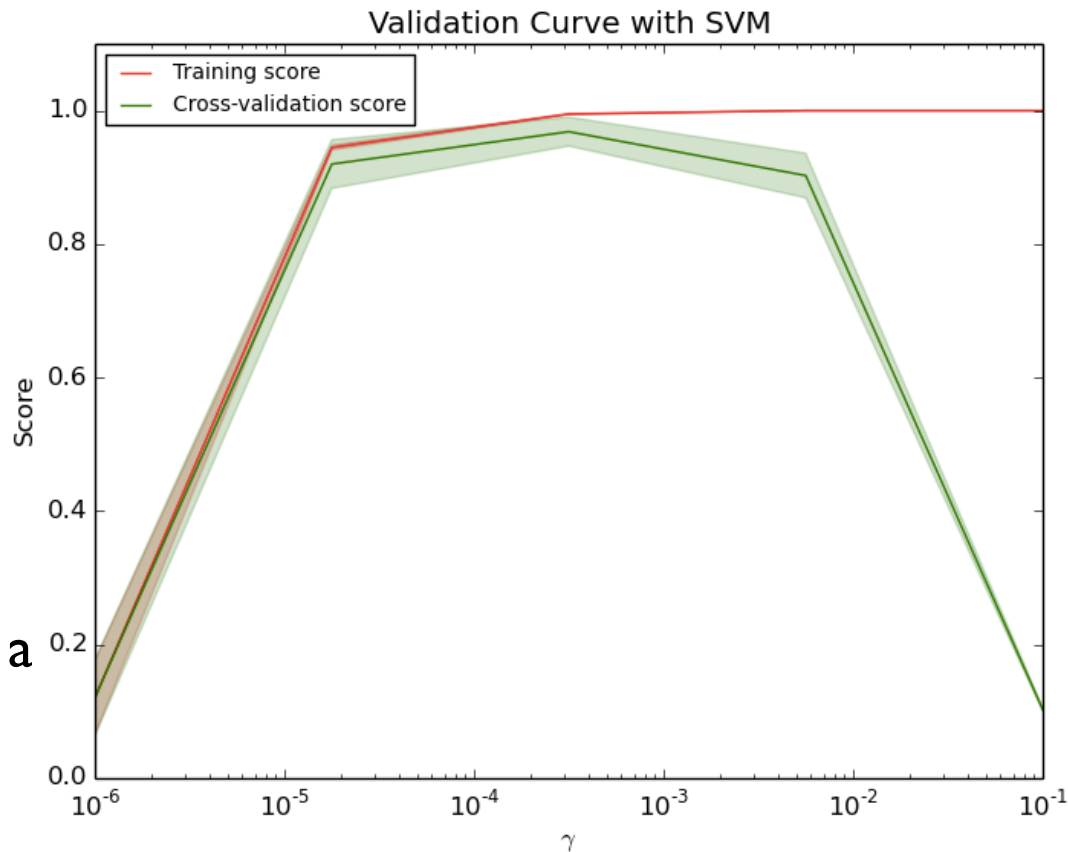
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How do I tune them? What
value to choose?

ML models depend on
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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?

How do I know if I have enough data?

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