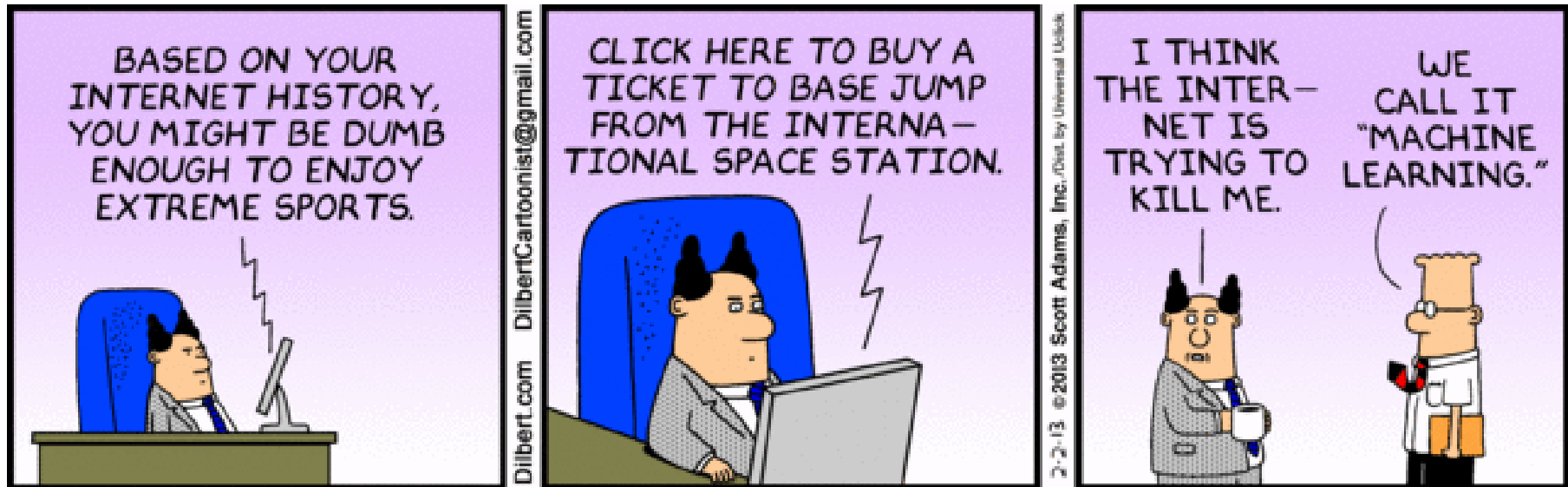
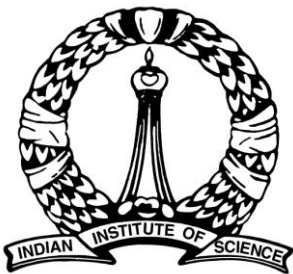




<http://dilbert.com/>

# Harikrishna Narasimhan



Department of Computer Science and Automation  
Indian Institute of Science, Bangalore

Learning from 'Binary Labels':

A Plethora of Performance Measures,

A Plethora of Algorithms Needed

A Software Engineer's Plight to Build a  
Machine Learning System **that Works!**

# Machine Learning

Machine Learning

Data Mining

Machine Learning

Data Mining

Big Data! 😊

Machine Learning

Data Mining

Big Data! 😊

Predictive Analytics

...

# Spam Filter

Google

in:spam



Gmail ▾



Delete forever

Not spam



More ▾

COMPOSE

Time travelers PLEASE HELP!!!!!!

Spam x



Inbox (12)

Chats

Sent Mail

Drafts (229)

Spam (176)

► Circles

Personal

Project K

Work

More ▾

<xxxxxxx@yyy.com>

10:29 PM (1 minute ago) ☆

to me ▾

*If you are a time traveler or alien disguised as human and or have the technology to travel physically through time I need your help!*

*My life has been severely tampered with and cursed!!*

*I have suffered tremendously and am now dying!*

*I need to be able to:*

*Travel back in time.*

Spam or Non-spam?

# Movie Recommendation

**Suggestions to Watch Instantly** See all >



**Inspector Lewis**  
Masterpiece Mystery!:  
Inspector Lewis  
Because you enjoyed:  
Sense and Sensibility

Play

★★★★★

Not Interested



**Drop Dead Diva**  
Because you enjoyed:  
Sex and the City

Play

★★★★★

Not Interested



**That's What I Am**  
Because you enjoyed:  
The Joneses

Play

★★★★★

Not Interested

**Action & Adventure** See all >



**Unstoppable**  
Because you enjoyed:  
Maid in Manhattan

Add

★★★★★

Not Interested



**LOTR: Fellowship of the Ring: Extended Ed.**  
Because you enjoyed:  
Crouching Tiger, Hidden Dragon

Add

★★★★★

Not Interested



**Man on Fire**  
Because you enjoyed:  
The Bone Collector

Add

★★★★★

Not Interested

What rating will user X  
give movie Y?

# Click Prediction

New User? Register | Sign In | Help

Get new Yahoo! Mail apps

MY YAHOO!

Web Images News

Web Search

My Main Tab New Tab

Content Themes Options

Sign in to permanently save changes you make on My Yahoo!

Sign In I'm new here.

Weather 24°C Horoscope Stocks Bookmarks

Quicklinks

Yahoo! Services

- Answers
- Astrology
- Buzz
- Crikoet
- Dainik Jagran
- Finance
- Filokir
- Games
- Groups
- Lifestyle
- Local
- Mail
- Maps
- Messenger
- Mobile
- Movies
- News
- Pulse
- Weather

More Yahoo! Services

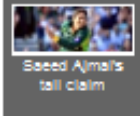
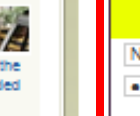
Today

TODAY - August 26, 2013



**'I pushed Aimal called...**

- Sachin retire...
- 15,000-runs summit
- Tendulkar: 100 Not Out

1 of 48

National News | National News Headlines - Yahoo! India News

- BJP wants FIR against Dikshit, ministers in transport 'scam' - 36 minutes ago
- Bengal assembly passes bill for time-bound services - 30 minutes ago
- Judiciary, Politicians, Police responsible for dismal rates of rape conviction: Brinda Karat - 37 minutes ago
- Mumbai police to seek 'maximum punishment' for rape case accused - 37 minutes ago
- VHP yatra not a political agenda, saints have right to go to Ayodhya: Singhal - 37 minutes ago

Bollywood News & Gossips | Regional Movie News Headlines - Yahoo! Movies India

Options

Options

Cricket Scores and Schedules

Live Now Results Upcoming

Aug 24  ZIM vs.  PAK

2nd T20I - Harare - View Scores

PAK lead the match by 49 runs

ZIM 160/6 (20) - 2nd Inn

What is the probability of a user clicking this ad?

Get a **FREE** Equity Trading Account at FundsIndia.com

No Equity Account Opening FEE of **Rs 500** Till August 31st, 2013\*

Name  Email

\*\*\*\*\*  Mobile

**REGISTER NOW**

Disclaimer: FundsIndia collects the information within this form and is solely responsible for their use. Please read their Privacy Policy. FundsIndia does not collect or use this information in any way.

\*Mutual Fund Investment

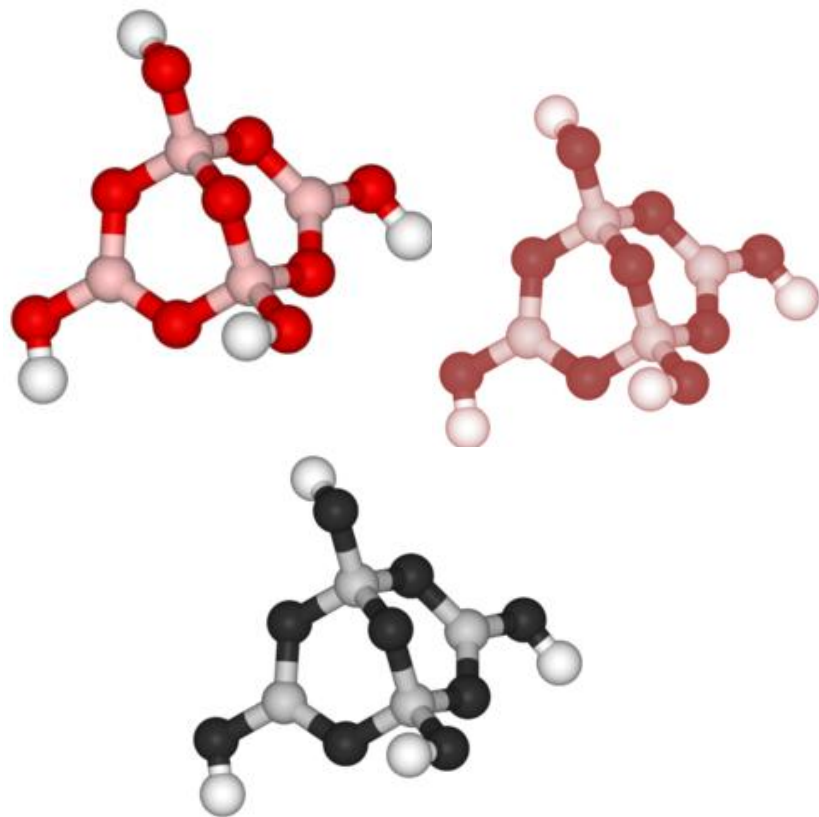
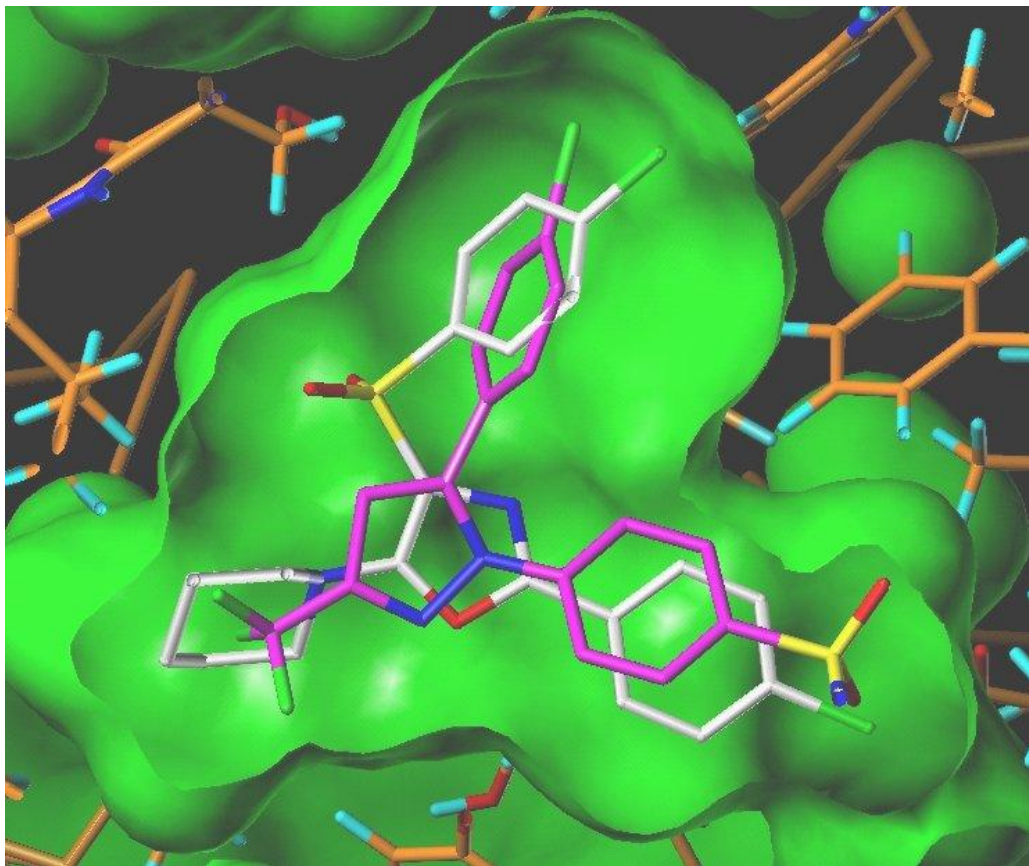
http://in.yahoo.com

# Hospital Readmission

What is the *probability* of a patient being readmitted?

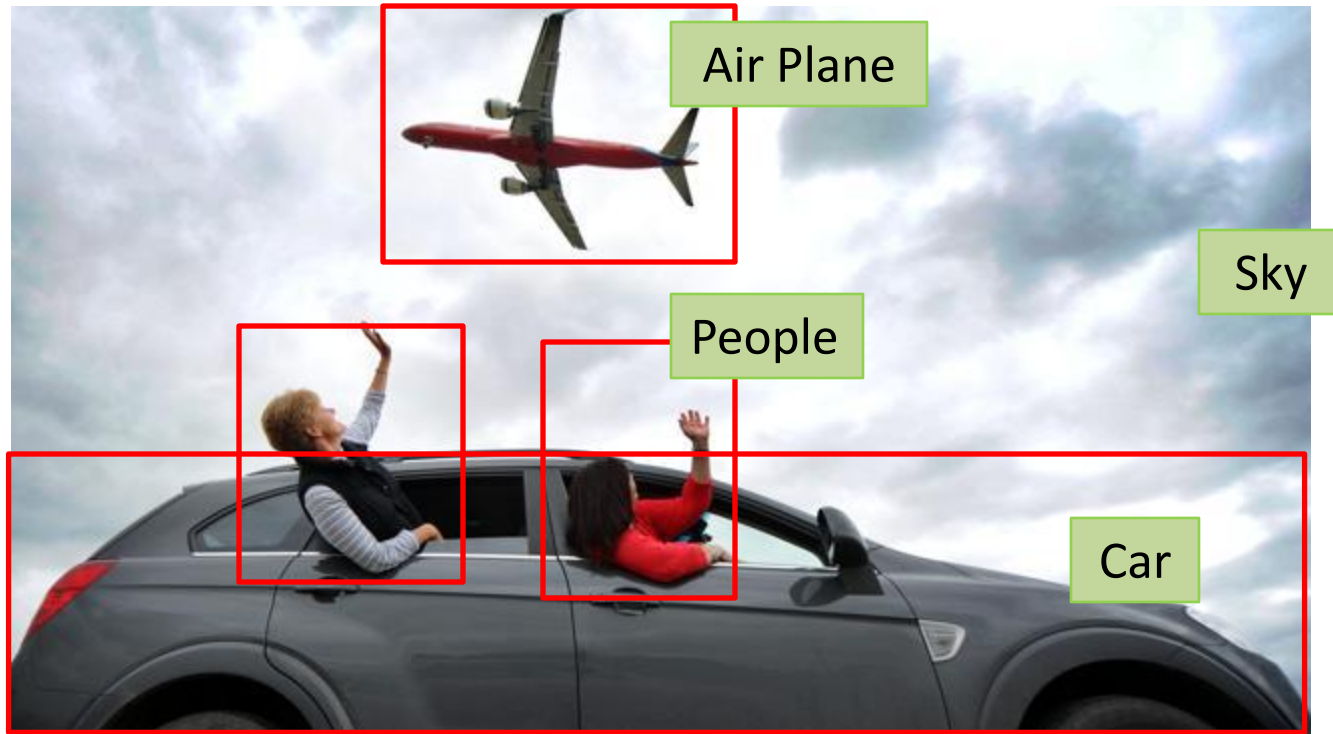


# Drug Discovery

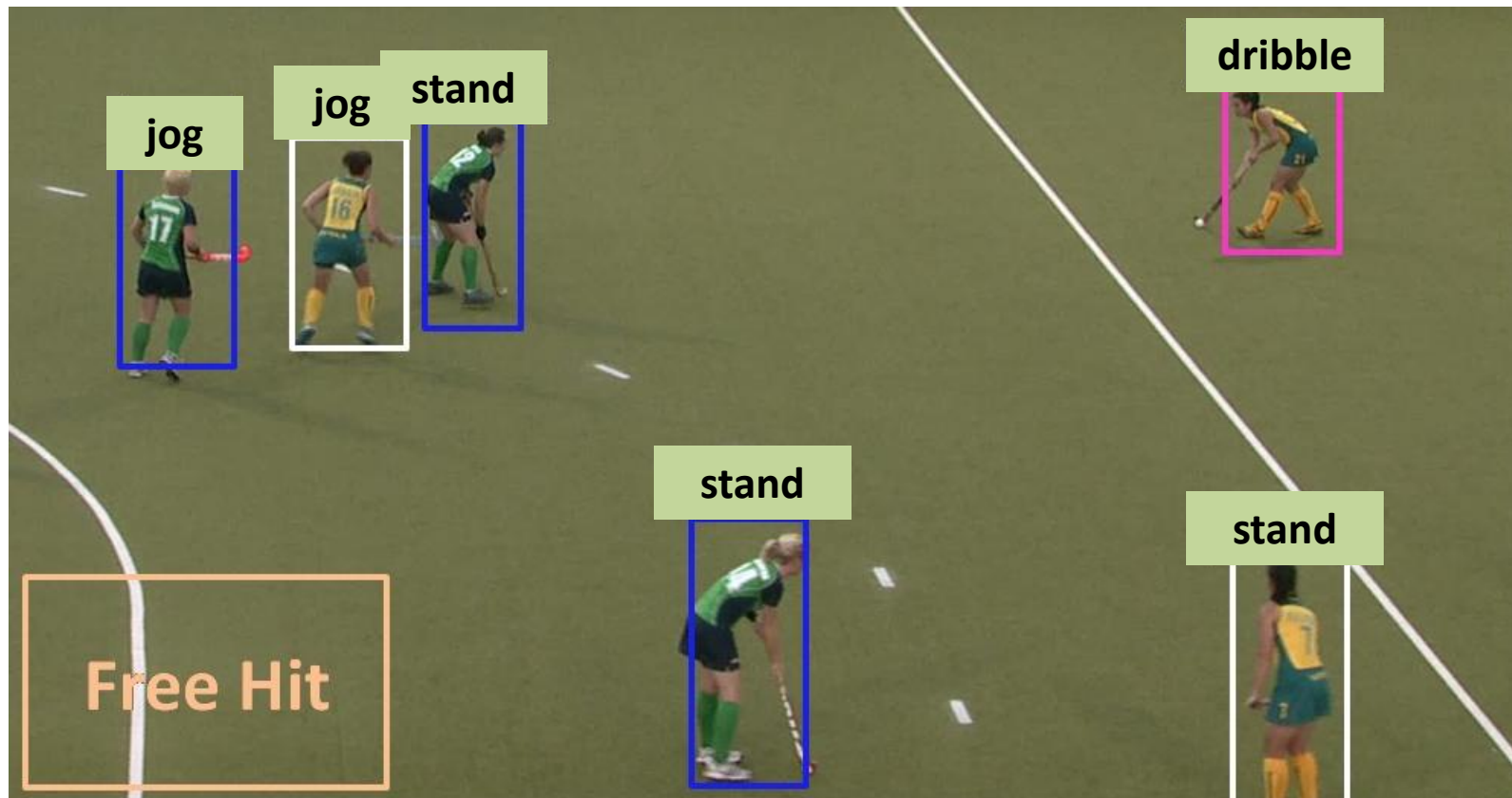


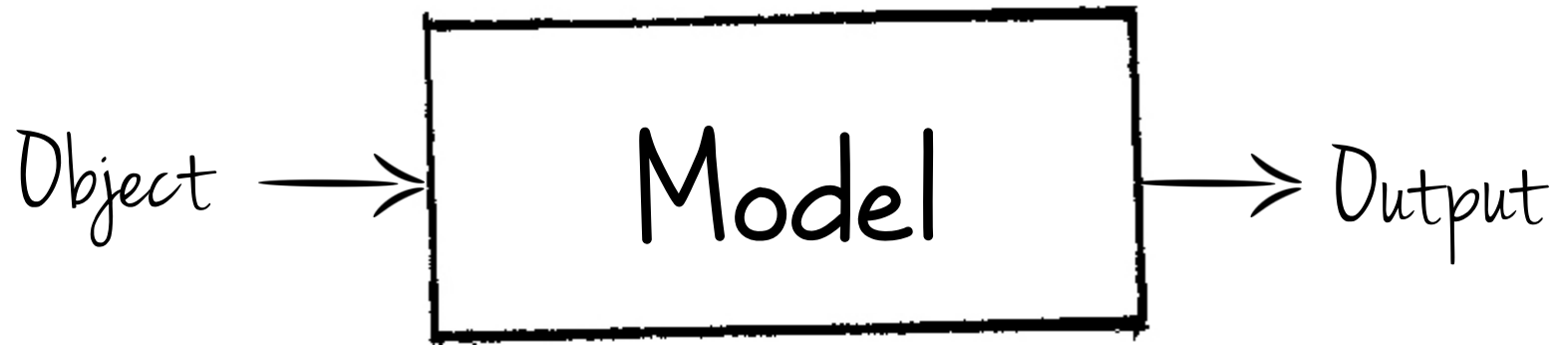
Millions of Chemical Compounds!!

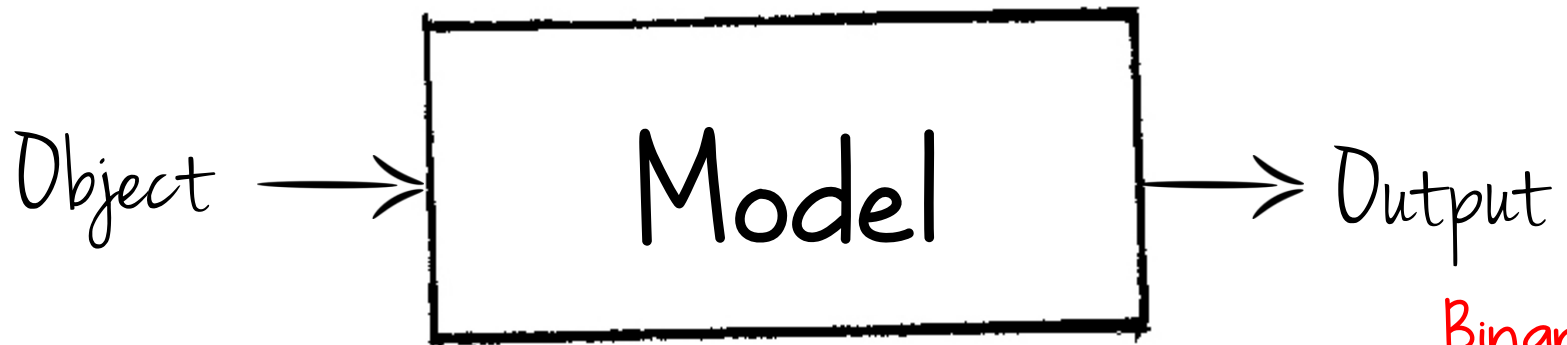
# Image Annotation



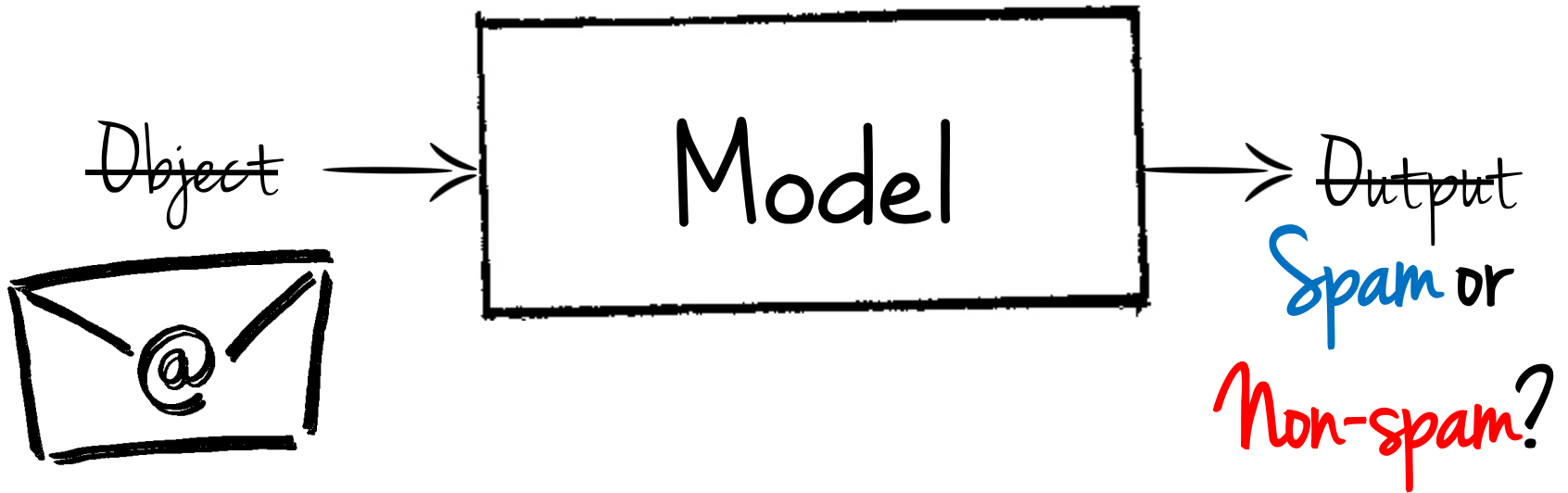
# Activity Recognition







Binary  
Categorical  
Real Valued  
Multi-label  
Structured  
....

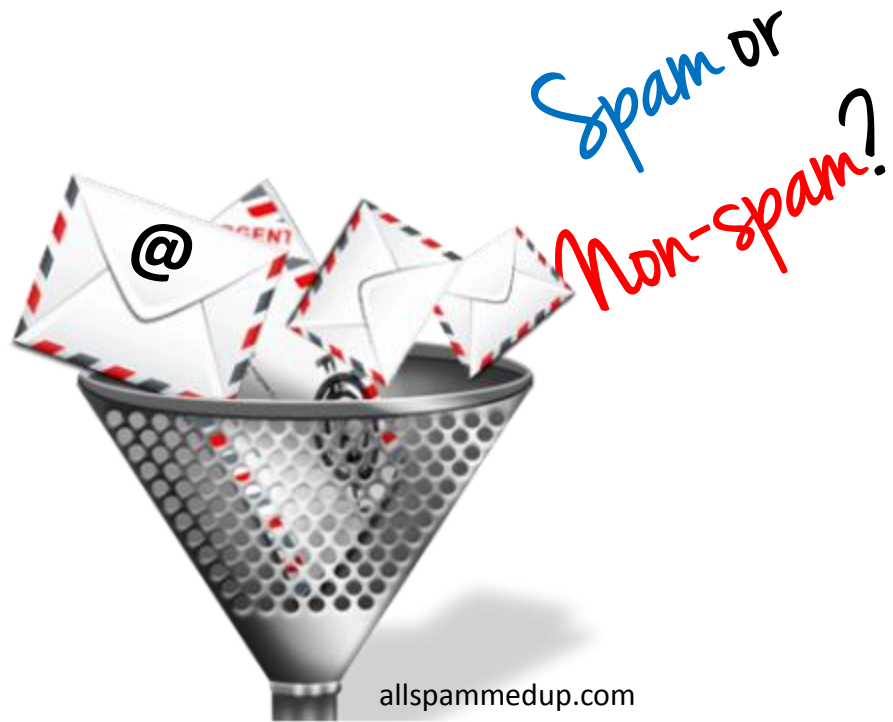


Learning from 'Binary Labels'

Spam or  
Non-spam?



[allspammedup.com](http://allspammedup.com)



Spam or  
Non-spam?



allspammedup.com

Disease or  
No Disease?



pascal-network.org

Relevant or  
Irrelevant?



Google

altavista

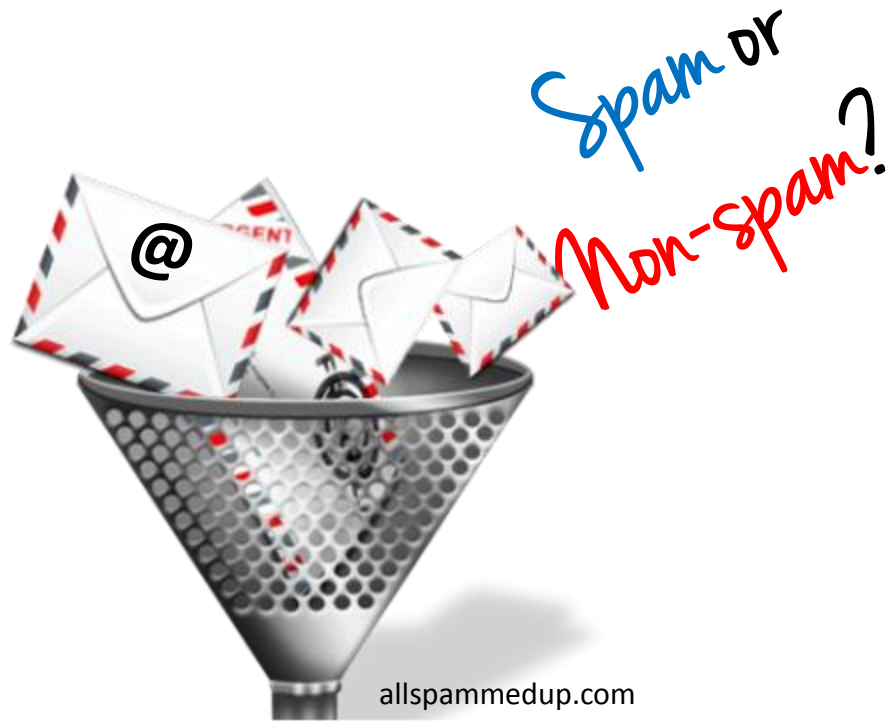
YAHOO!

AOL

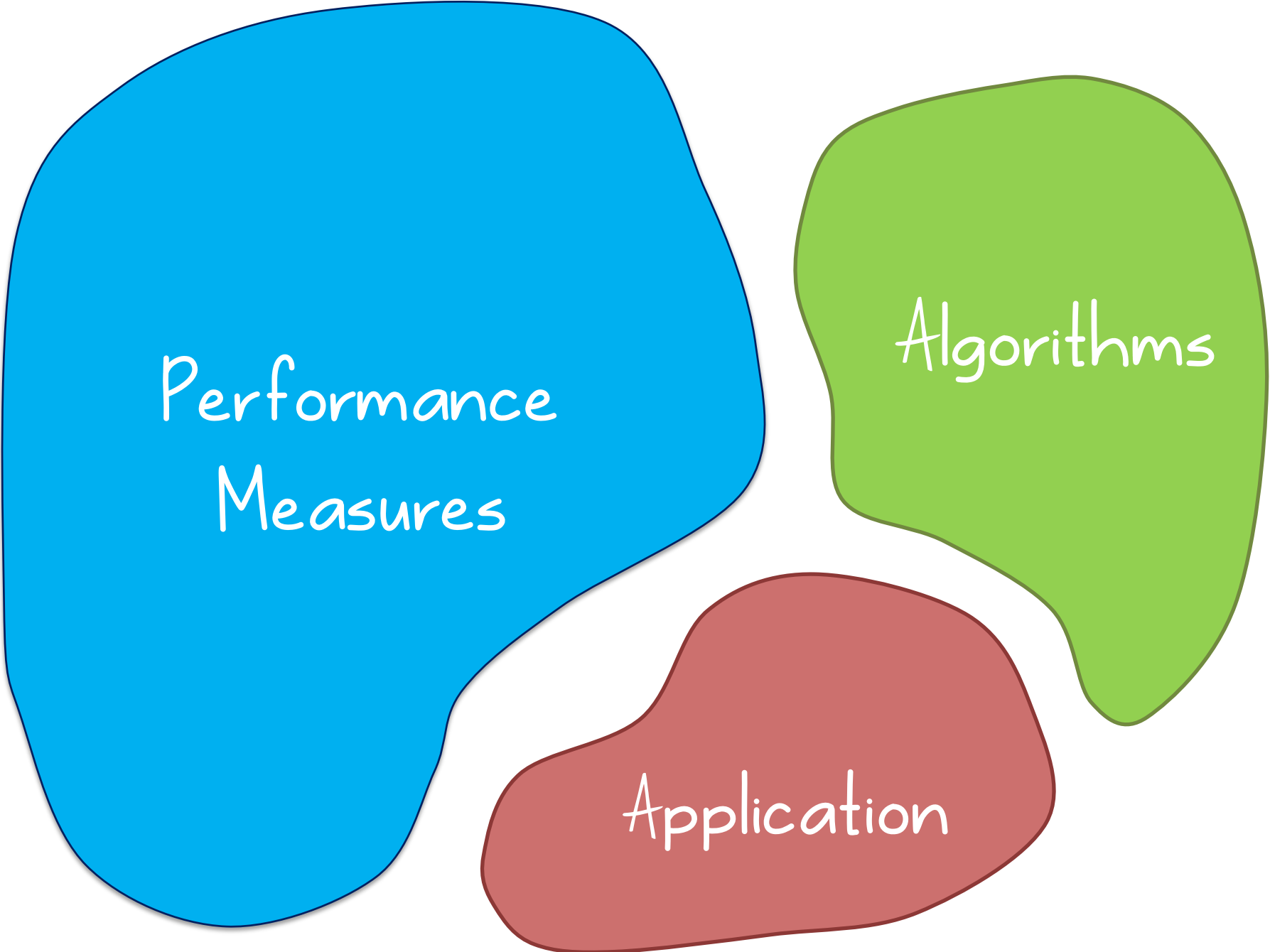
....T...Online...

msn

fusionsedge.com



WTAF-measureAUCCalibrationLossLogLoss  
ParialAUCAccuracy@TopPRBEP MRR  
AM-measureg-mean  
Accuracy@Top MRR StratifiedBS BalancedMPR  
PRBEP  
MAE MPR  
StratifiedBS  
Recall MPR  
BalancedMPR  
AUC  
AM-measure  
TPR  
LogLoss  
BrierScore  
LocalAUC  
FPR  
RefinementLoss  
F-measure  
WeightedAccuracy  
TPR  
Positives@Top  
BrierScore  
Precision  
g-mean  
LocalAUC  
MAE  
Recall  
AveragePrecision  
Positives@Top  
Accuracy  
FPR

A diagram consisting of three irregular, hand-drawn shapes. The largest shape on the left is blue and contains the text 'Performance Measures'. To its right is a green shape containing the text 'Algorithms'. Below the green shape is a red shape containing the text 'Application'.

Performance  
Measures

Algorithms

Application

# Performance Measures

Binary  
Classification

Standard Error  
F1-measure  
G-mean  
...

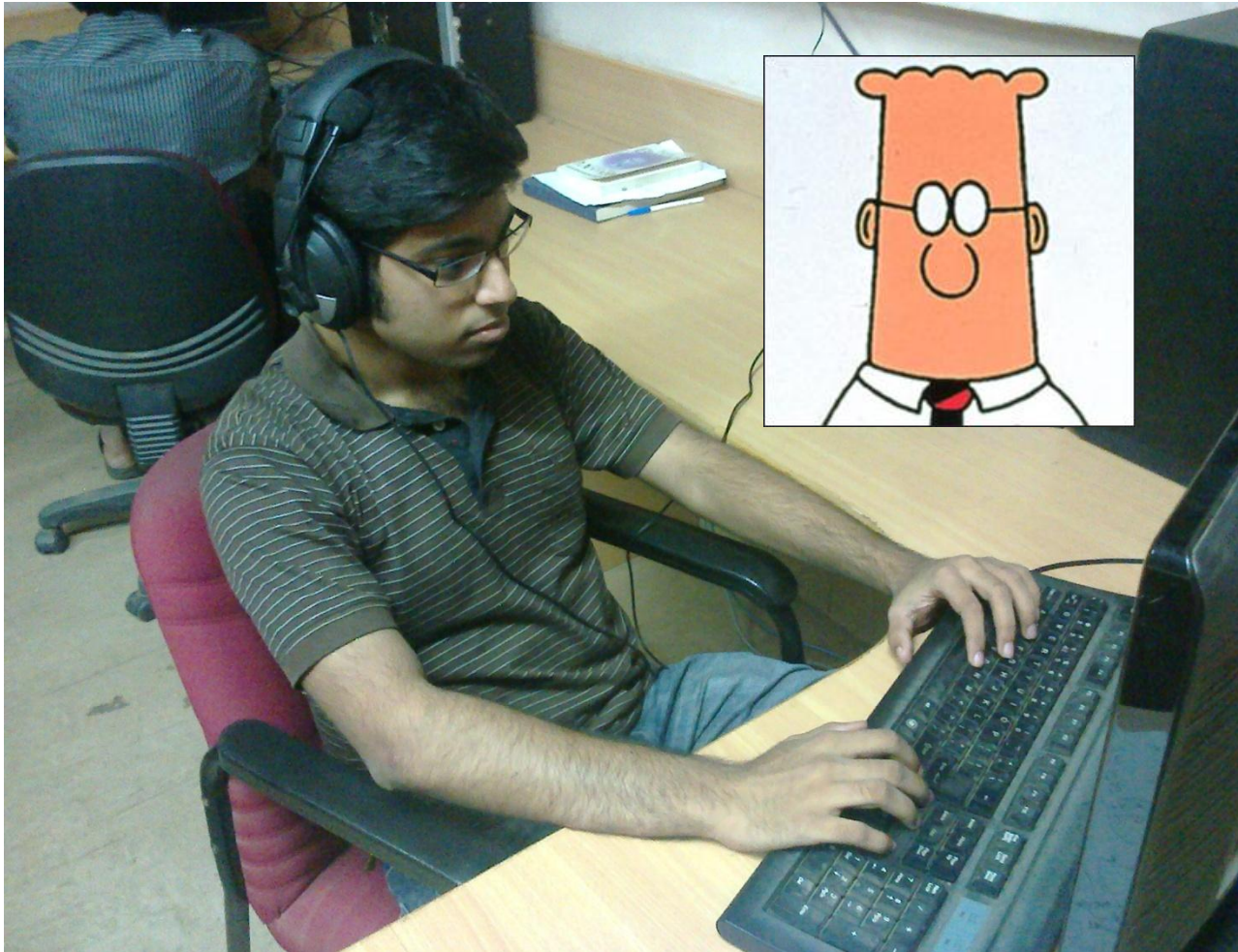
Bipartite  
Ranking

Pair-wise Accuracy  
Precision@K  
Average Precision  
...

Binary  
Class Prob.  
Estimation

logloss  
Squared Error  
...

# Our 'Desi' Dilbert **Then**



# Our 'Desi' Dilbert Now







Genuine



Fraud

.....

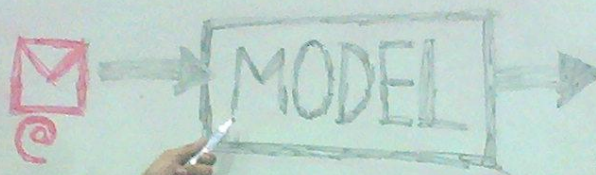


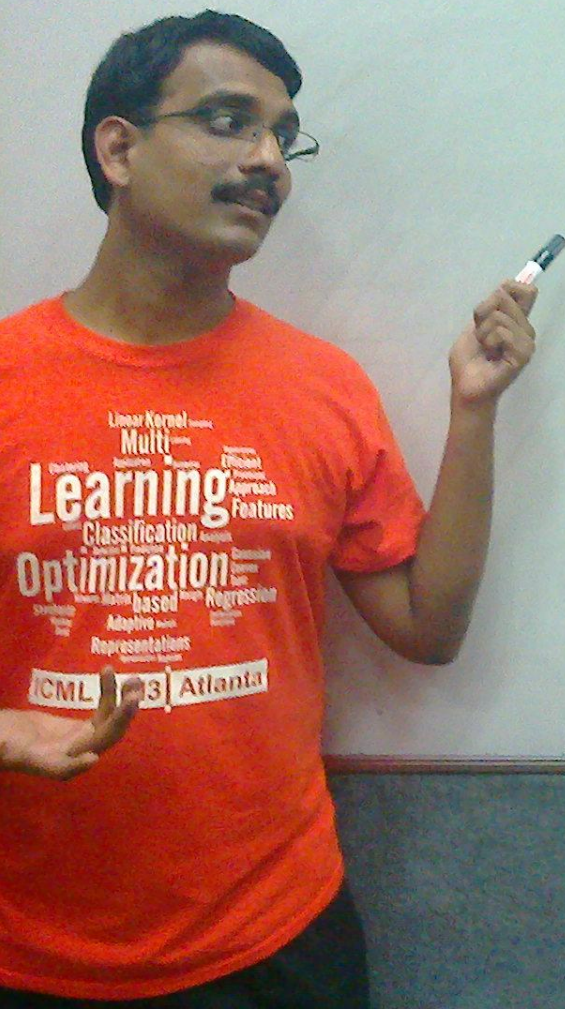
Genuine



Fraud or  
Genuine?

ML



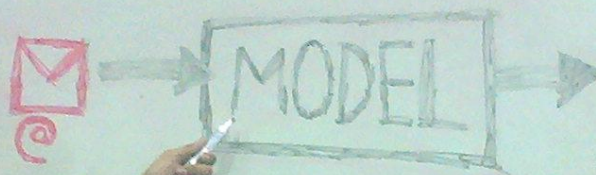


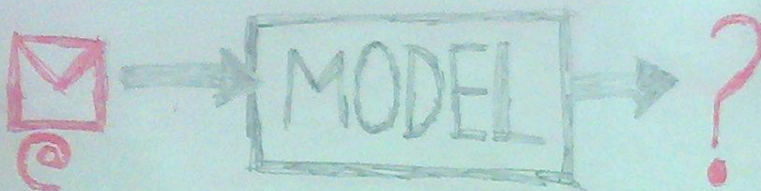
Surrogate Risk Minimization  
with a classification-calibrated  
loss function and appropriate  
regularization



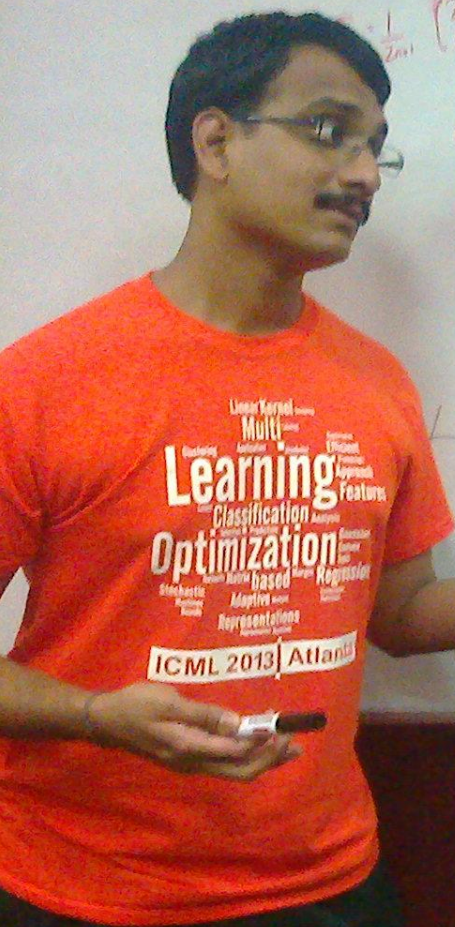


ML





A poster for the ICML 2013 workshop "Learning with Graphs". The poster features a red background with the words "Learning", "Optimization", and "Graphs" in large, white, stylized fonts. Other words like "Generalization", "Efficiency", "Scalability", "Robustness", "Adaptivity", "Representational", "Basis", "Progress", "Theoretical", "Practical", "Foundational", "Computational", "Statistical", "Machine", "Learning", "Data", "Science", "Artificial", "Intelligence", "Computer", "Science", "Mathematics", "Physics", "Chemistry", "Biology", "Medicine", "Engineering", "Finance", "Marketing", "Social", "Networks", "Complex", "Systems", "Information", "Theory", "Game", "Theory", "Economics", "Law", "Education", "Health", "Environment", "Energy", "Transportation", "Infrastructure", "Security", "Privacy", "Ethics", "Policy", "Societal", "Impact", "Future", "Directions", "Challenges", "Opportunities", "Collaboration", "Interdisciplinary", "Research", "Community", "Workshop", "Tutorial", "Course", "Lecture", "Seminar", "Workshop", "Tutorial", "Course", "Lecture", "Seminar" are scattered around the main text. At the bottom, it says "ICML 2013" in a white box.



Whiteboard content:

- Hinge Loss**:  $\frac{1}{2m} \sum_{i=1}^m \max(0, 1 - y_i w^T x_i)$
- SVM**:  $N_\infty(\mathcal{F}, \epsilon)$
- Log Loss**:  $\log(1 + e^{-w^T x})$
- Sigmoid**:  $\sigma(w^T x)$
- Minimization**:  $\xi \geq 0$ ,  $\min f(x)$
- Diagram**:  $I(yf(x) \geq \gamma) \rightarrow \text{MODEL} \rightarrow ?$
- Equations**:
  - $x_{k+1} = x_k - \eta_k \nabla f(x_k)$
  - $\hat{y} = \text{sign}(w^T x + b)$
  - $\|x\|_2^2$
  - $L$ -Lipschitz?  $\nabla f(x)$
  - $\|w\|_1$
  - $w^T [\psi(x, \hat{y}) - \psi(x, y)] \geq 1 - \xi(x, \hat{y})$
  - $L: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$
  - $S \in (\mathcal{X} \times \mathcal{Y})^n$
  - $(xx + \lambda I) x^T y = w^* \cdot \frac{d_k - \tilde{J}_k g_k}{1^T Q g_k}$



$w = \frac{1}{\sqrt{n}}$  Hinge Loss  
 $\log(1 + e^{-w^T x})$   
 $\frac{1}{2} \left( \frac{1}{n} \right)$   
**SVM**  $N_\infty(\mathcal{F}, \epsilon)$   
 $\mathbb{I}(y \neq \hat{y})$    **MODEL**   
 $x_{w^*} = x_0 - \eta \nabla f(x_0)$   $\hat{y} = \text{argmax}(w^T x + b)$   $\|x\|_2^2$   
 $L$ -Lipschitz?  $\nabla f(x)$   $w[f(x, y) - \gamma(x, y)] \geq 1 - \xi(x, y)$   
 $\|w\|_1$   $\mathcal{L}: \mathcal{Y} \times \mathcal{X} \rightarrow \mathbb{R}^+$   $S \in (\mathcal{X} \times \mathcal{Y})^n$   
 $(X^T X + \lambda I)^{-1} X^T y = W^* \frac{d_k - \tilde{y}_k}{N Q \gamma_k}$

**SIGMOID**  
 $\sigma(w^T x)$  ??  
 $\xi \geq 0$   
 $\min f(x)$







$$\phi(n) = n \prod_{q=1}^k \left(1 - \frac{1}{p_q}\right)$$

Hinge Loss!

$$C_n = \frac{1}{2n+1} \binom{2n}{n}$$

$$\log(1 + e^{-w^T x})$$

SVM  $N_\infty(\mathcal{F}, \epsilon)$

SIGMOID

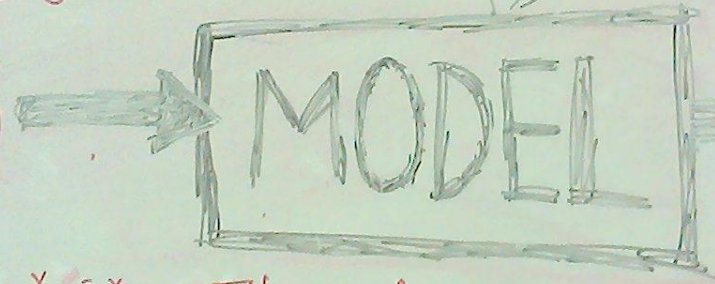
$$\sigma(w^T x) \quad ??$$

$d(x, y), \dots, (x, y_n)$

$$\xi \geq 0$$

$$\min f(x)$$

$$I(y \neq \hat{y})$$



Bayesian Inference

L0-1

$$(\cdot)_+ = ?$$

$$x_{t+1} = x_t - \eta_t \nabla f(x_t) \quad \hat{y} = \text{sign}(w^T x + b)$$

$$\|x\|_*^2$$

L-Lipschitz?  $\nabla f(x)$

$$\|w\|_1$$

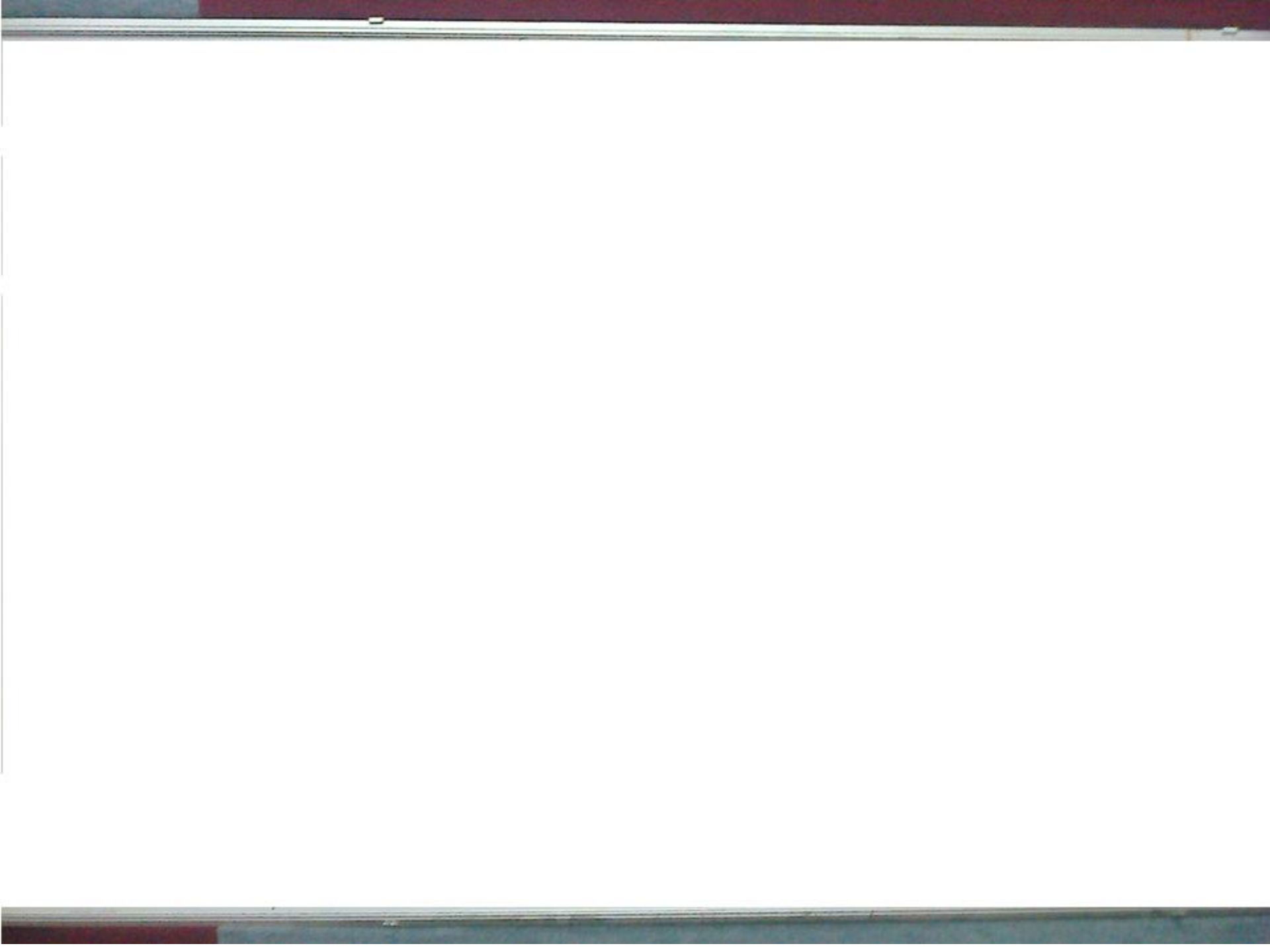
$$w^T [\psi(x, \hat{y}) - \psi(x, y)] \geq 1 - \xi_{\psi}(x, \hat{y})$$

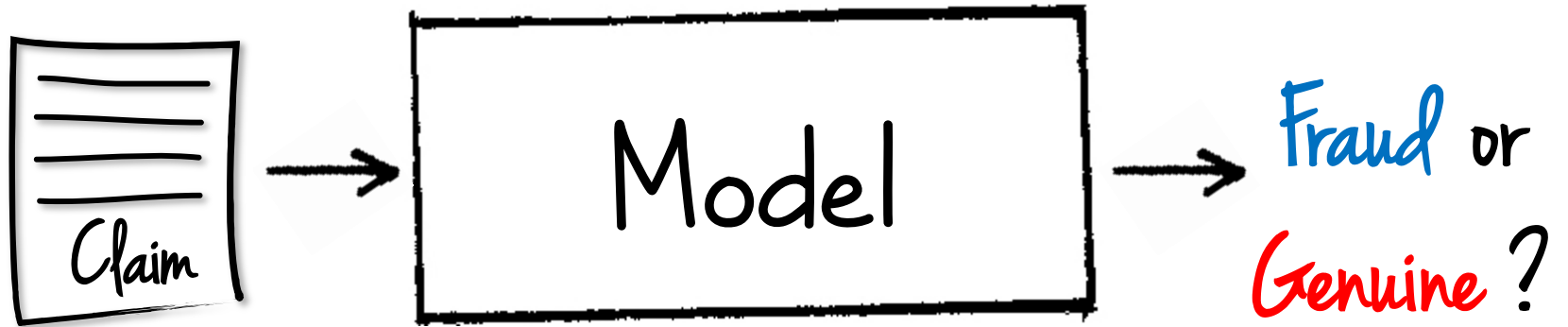
F-measure

$$L: Y \times X \rightarrow \mathbb{R}^+$$

$$S \in (X \times Y)^n$$

$$(X^T X + \lambda I)^{-1} X^T y = w^* \quad d_k = -\frac{j_k^T g_k}{j_k^T Q_k j_k}$$





# Training Set



Genuine



Fraud

.....



Genuine

# Training Set

Goal?

Learn a model with 'minimum error'  
on training set!

Model

Genuine

Claim 1

Fraud

Claim 2

.....

Genuine

Claim N



Age

Injury Type

# of Days in Hospital

Amount Claimed

...

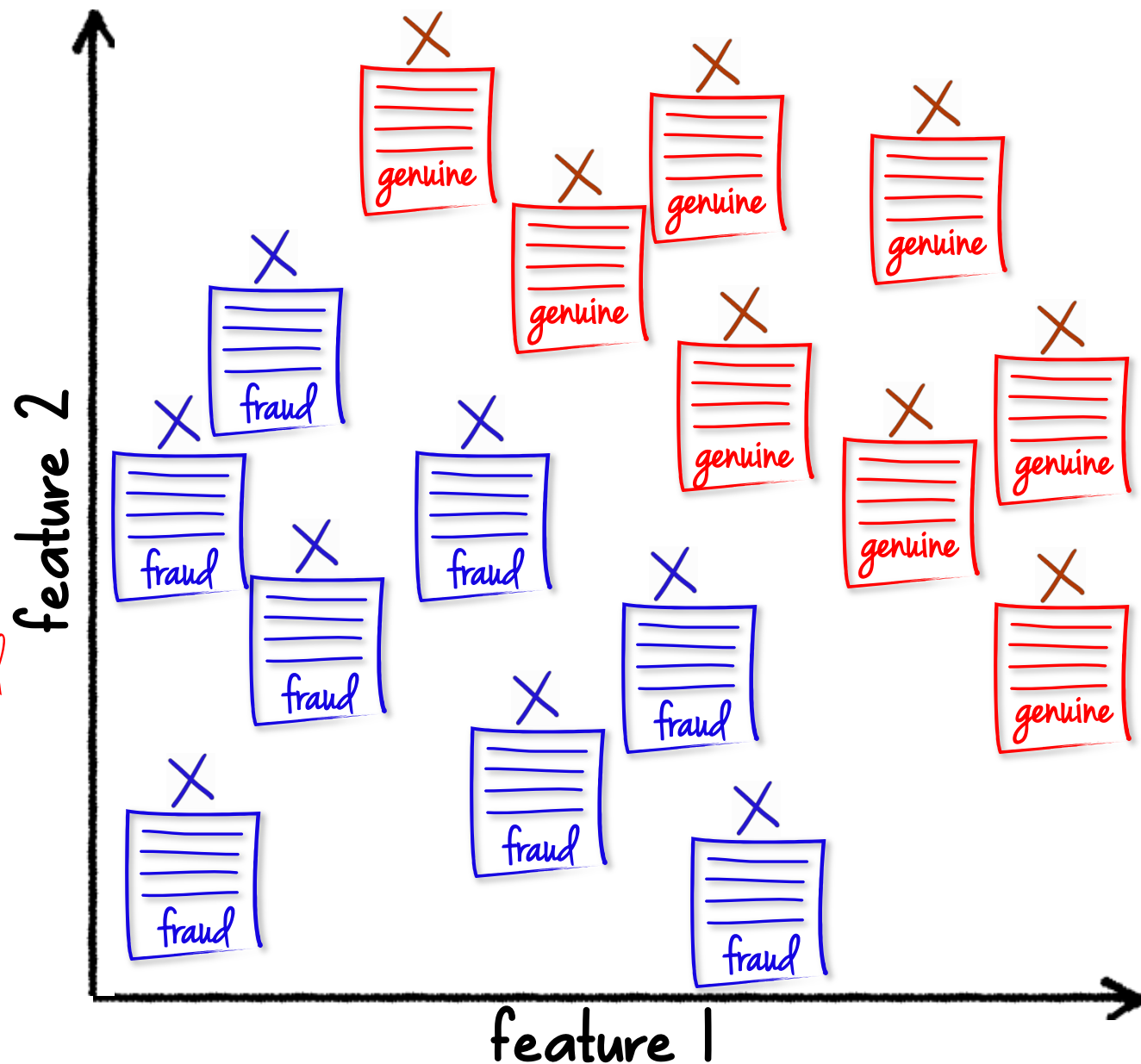
...



Age  
Injury Type  
# of Days in Hospital  
Amount Claimed

...

...

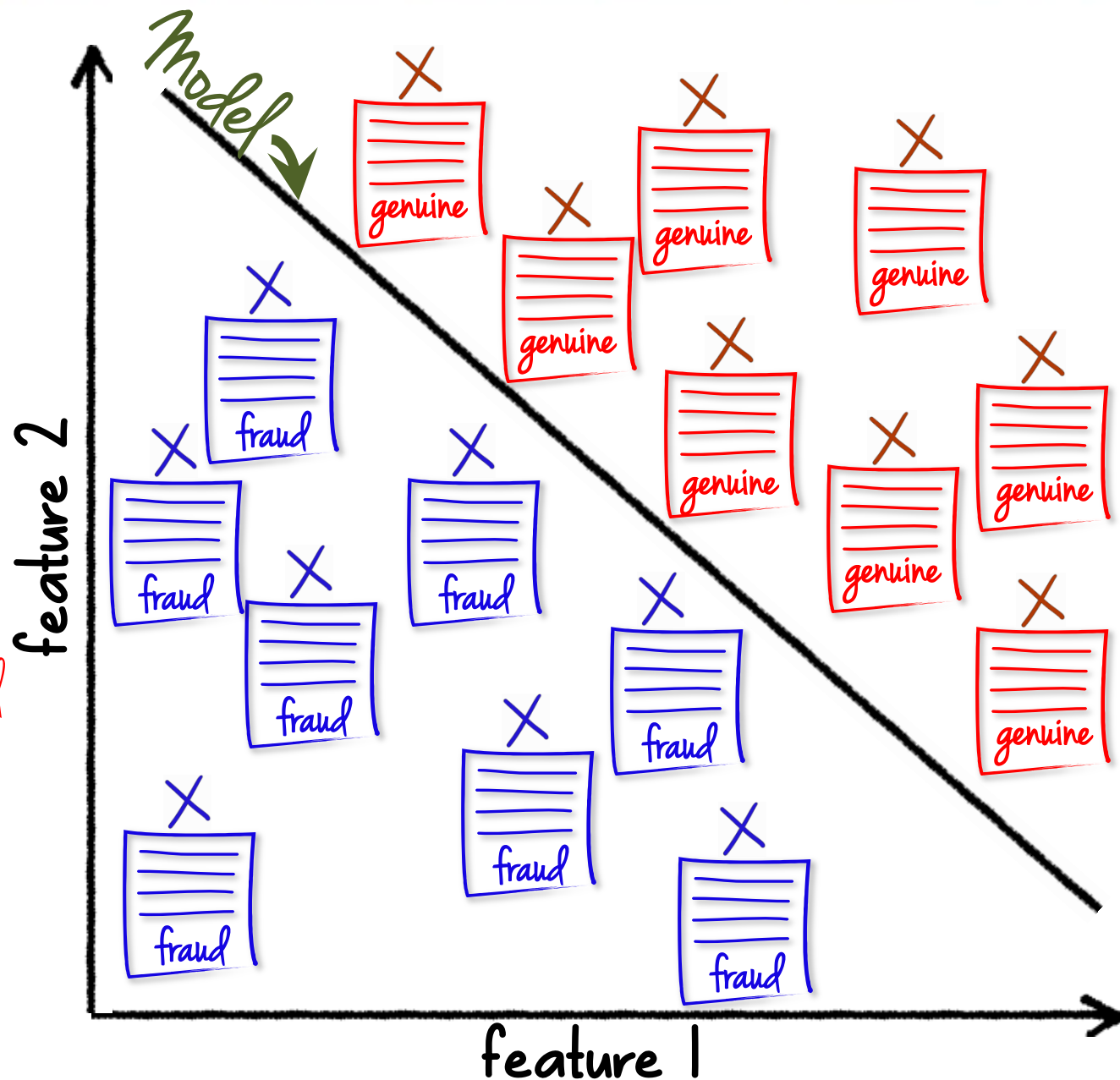




Age  
Injury Type  
# of Days in Hospital  
Amount Claimed

...

...

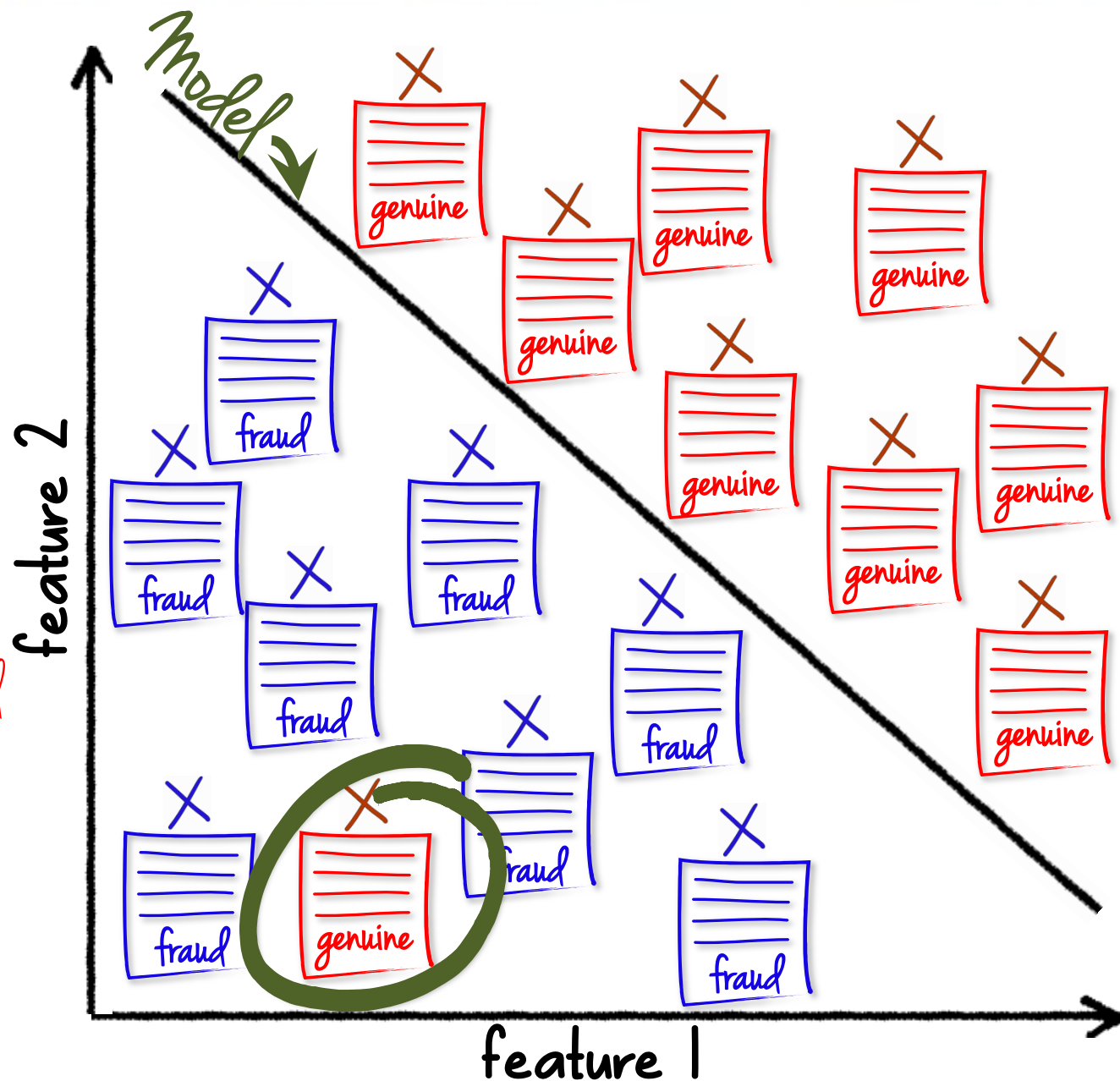




Age  
Injury Type  
# of Days in Hospital  
Amount Claimed

...

...



.....

.....

Model-17

Model-5

Model-19

Model-9

Model-2

Model-6

Model-7

Model-3

Model-7

Model-15

Model-18

Model-10

Model-4

Model-21

Model-15

Bag of  
models

Model-17

68%

Model-5

8%

Model-19

27%

Model-9

22%

Model-2

7%

Model-6

4%

Model-7

33%

Model-3

11%

Model-7

6%

Model-15

12%

Model-18

7%

Model-10

9%

Model-4

44%

Model-21

18%

Model-15

41%

Bag of models

Model-17

68%

Model-5

8%

Model-19

27%

Model-9

22%

Model-2

7%

Model-6

4%

Model-3

11%

Model-7

6%

Model-15

12%

Model-7

33%

Model-18

7%

Model-10

9%

Model-4

44%

Model-21

18%

Model-15

41%

Bag of models

# Optimization Problem

find model with  
'minimum training error'

Intractable /  
Hard

Optimization  
Problem

find model with  
'minimum training error'



Intractable /  
Hard

Optimization  
Problem

find model with  
'minimum training error'



Proxy  
Optimization  
Problem



zation

blem

del with  
aining error'

Logistic Regression  
Support Vector Machine  
AdaBoost  
Neural Network  
Decision Trees

...

Proxy  
Optimization  
Problem

# Binary Classification

E.g. Support Vector Machine



# Training Set



Genuine



Fraud

.....



Genuine

# Training Set



Genuine



Fraud

.....



Genuine

# Test Set



?



?

.....



?



[ Age      Injury Type      # of Days  
in Hospital      ...      ...      Amount  
Claimed ]



# Support Vector Machine

$\begin{bmatrix} 1 & 23 & 9 & \dots & \dots & 24 \\ \text{Age} & \text{Injury Type} & \text{\# of Days} & & & \text{Amount} \\ & & \text{in Hospital} & & & \text{Claimed} \end{bmatrix}$



# Support Vector Machine

[ <sup>7</sup>Age    <sup>23</sup>Injury Type    <sup>9</sup># of Days in Hospital    ...    ...    <sup>24</sup>Amount Claimed ]



Model  
[7, 23, 9, ..., ..., 24]

2%  
training  
error

# Test Set



Model

[7, 23, 9, ..., ..., 24]

Claim 1

Claim 2

.....

Claim M

# Test Set



Model

[7, 23, 9, ..., ..., 24]

??  
??  
??  
??  
??



Genuine



Genuine

.....



Genuine

Only 2% of the  
training examples  
are 'fraud'

?? ? ? ?



## Training Set



Genuine



Fraud

.....

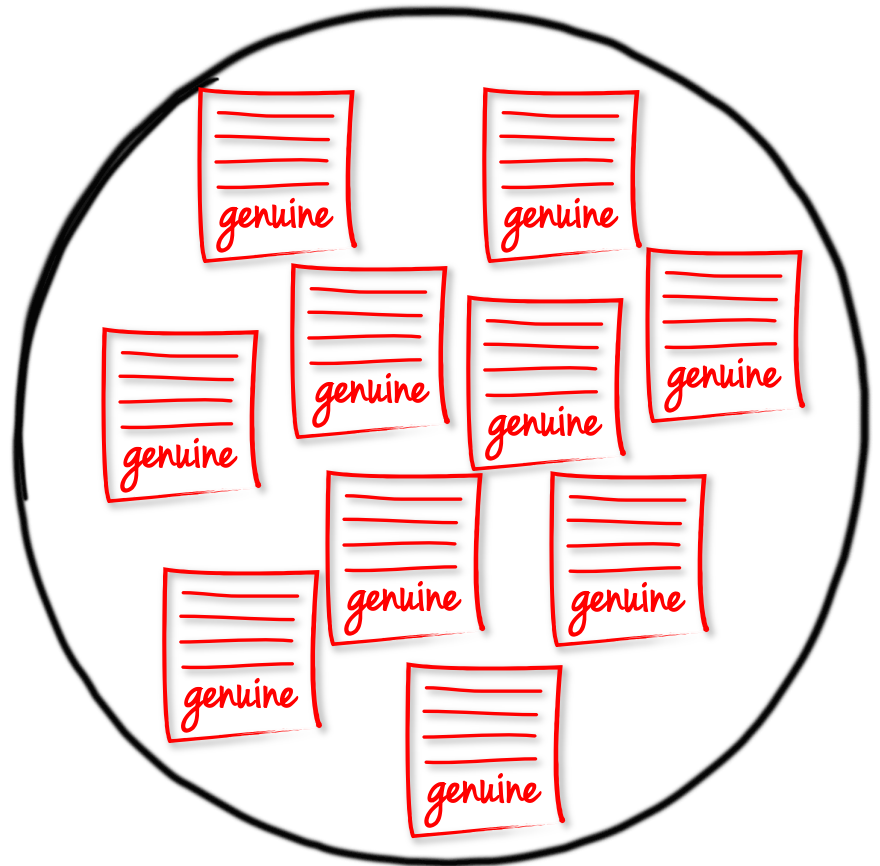


Genuine

# Performance Measure?



# Class Imbalance Problem





Correctly  
predicted **positive**  
examples

Correctly  
predicted **positive**  
examples



Correctly  
predicted **negative**  
examples



True Positive  
Rate

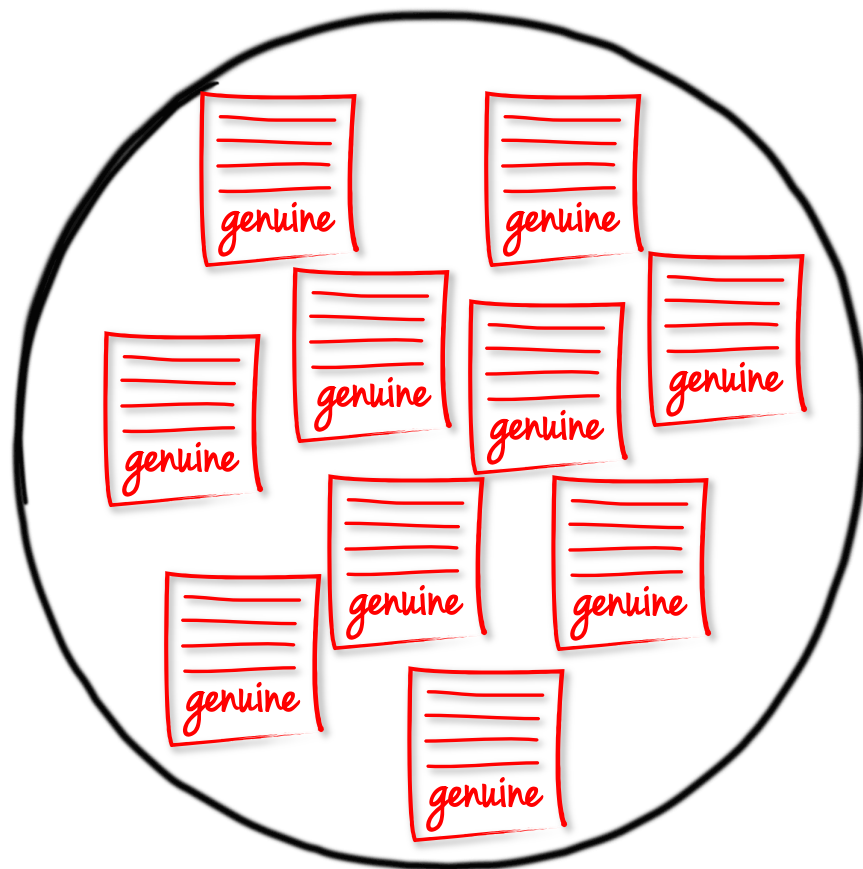
True Negative  
Rate

$$\frac{\text{True Positive Rate} + \text{True Negative Rate}}{2}$$

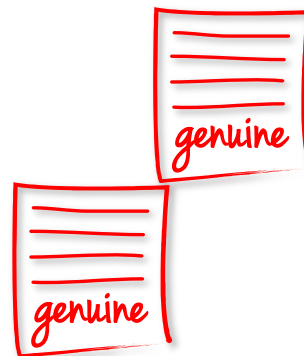
$$\sqrt{\text{True Positive Rate} \times \text{True Negative Rate}}$$

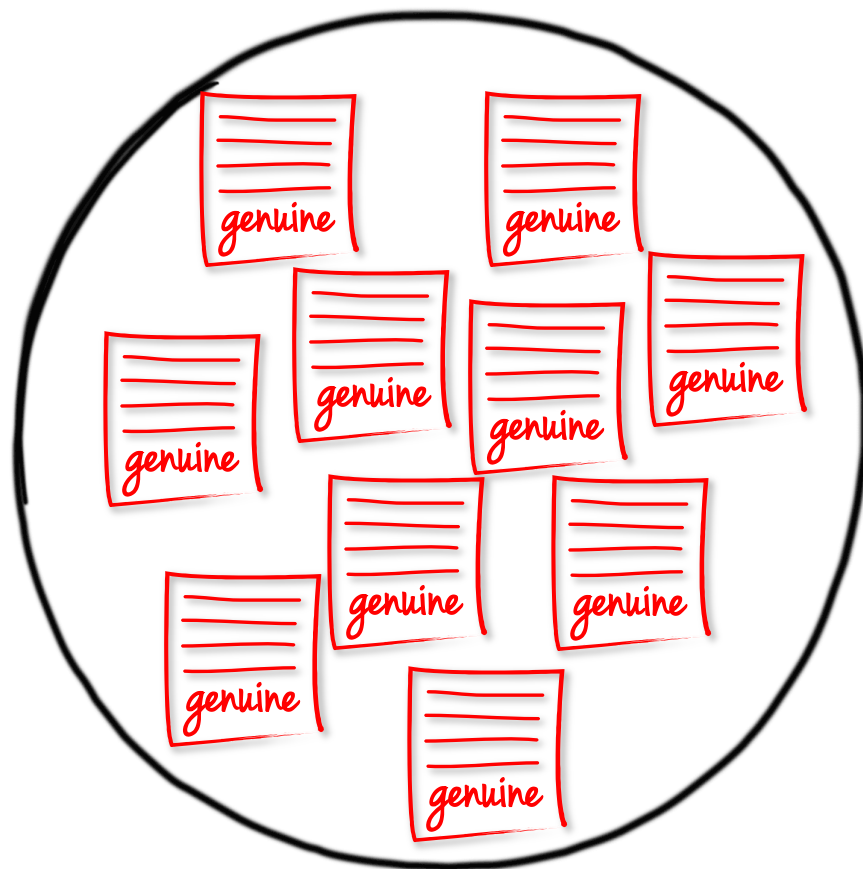
Algorithm?



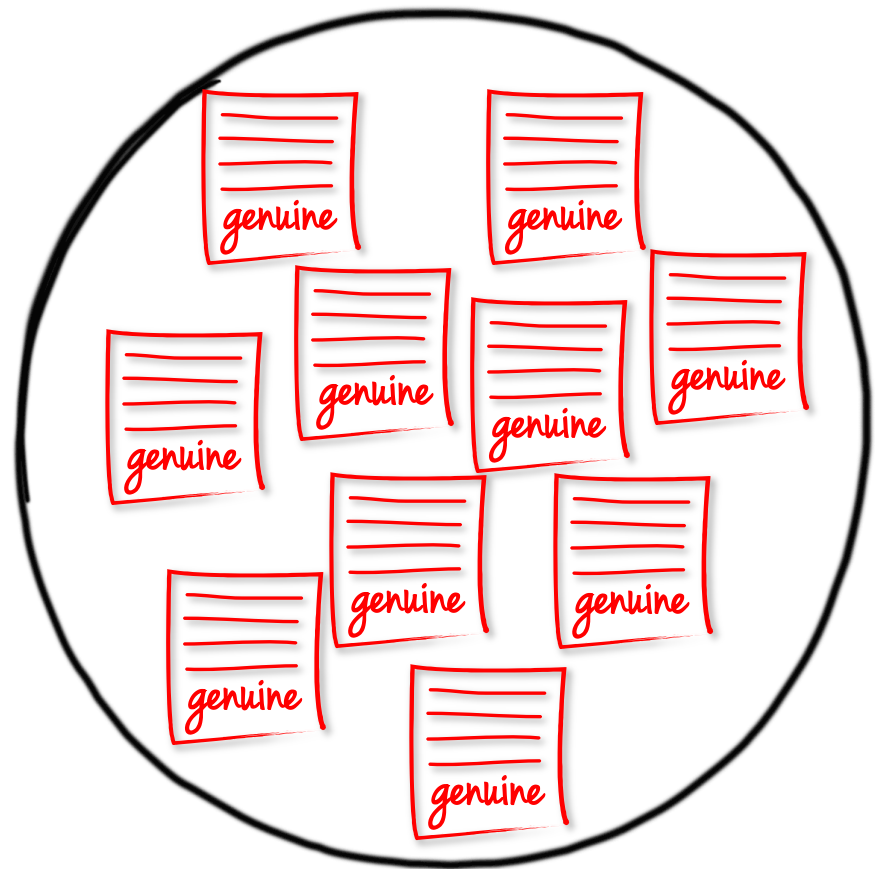
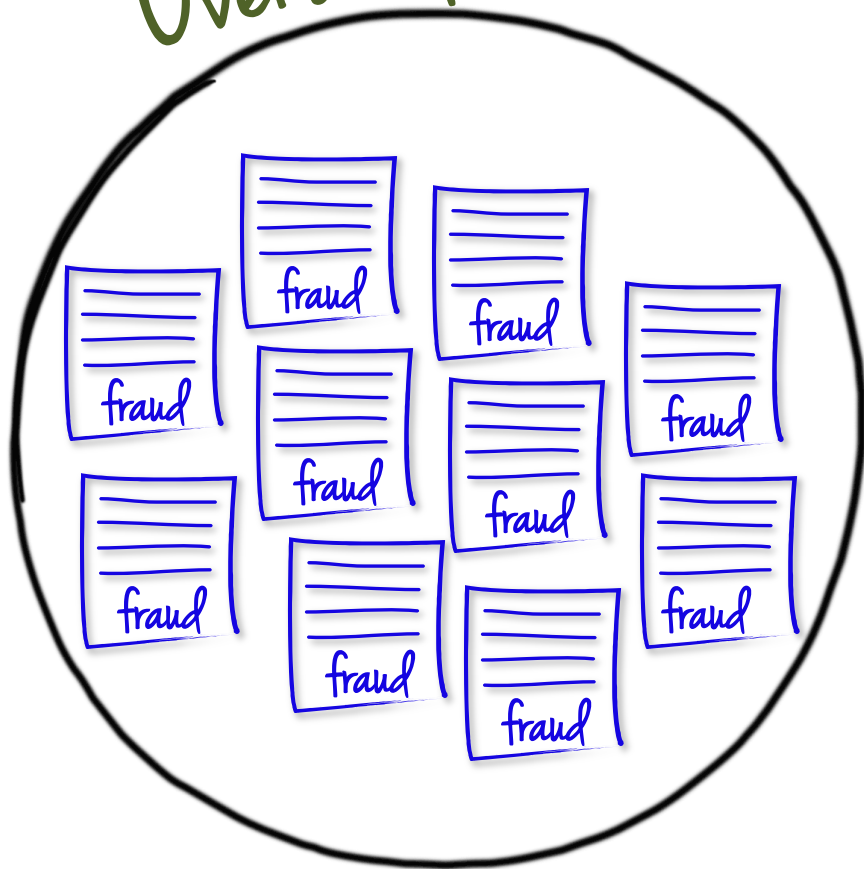


Undersampling





# Oversampling



# Undersampling + Support Vector Machine



# AM-measure

$$\frac{\text{True Positive Rate} + \text{True Negative Rate}}{2}$$



[ Age      Injury Type      # of Days in Hospital      ...      ...      Amount Claimed ]



# Undersampling + Support Vector Machine

[ <sup>19</sup>Age    <sup>12</sup>Injury Type    <sup>21</sup># of Days  
in Hospital    ...    ...    <sup>17</sup>Amount  
Claimed ]



# Undersampling + Support Vector Machine

$$\begin{bmatrix} 19 & 12 & 21 & \dots & \dots & 17 \\ \text{Age} & \text{Injury Type} & \text{\# of Days} & & & \text{Amount} \\ & & \text{in Hospital} & & & \text{Claimed} \end{bmatrix}$$

Model

[19, 12, 21, ..., ..., 17]

94%  
F1-measure  
on training set

# Test Set

Model

[19, 12, 21, ..., ..., 17]

Claim 1

Claim 2

.....

Claim M

# Test Set

Model

[19, 12, 21, ..., ..., 17]



Claim 1

Fraud

Claim 2

Genuine

.....

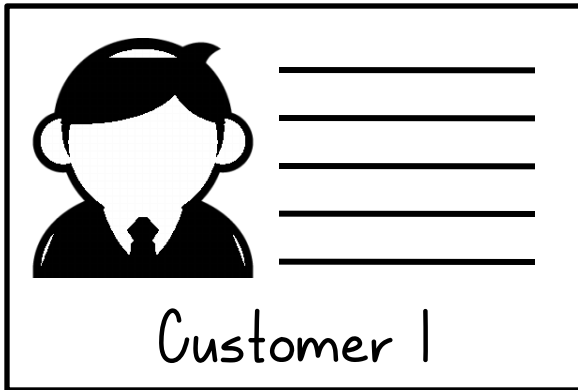
Claim M

Genuine

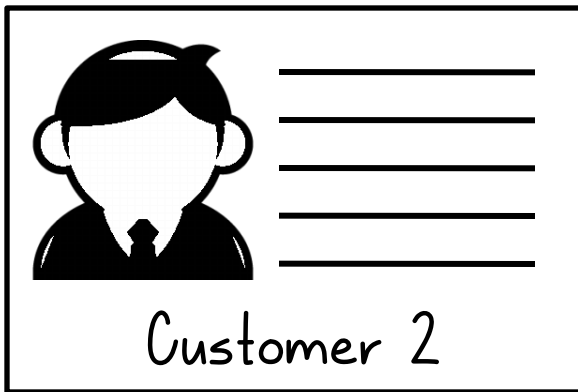
91%  
A/M  
measure







Churn

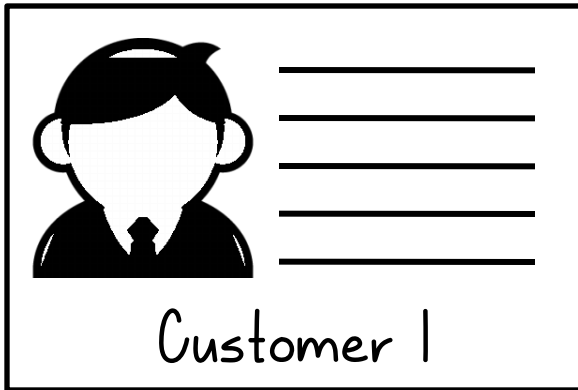


Non-Churn

.....



Churn



Churn



.....



Churn



.....



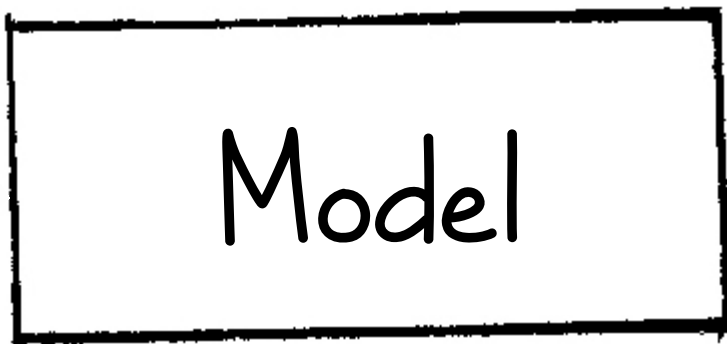


Model



real  
score





real  
score



8



1



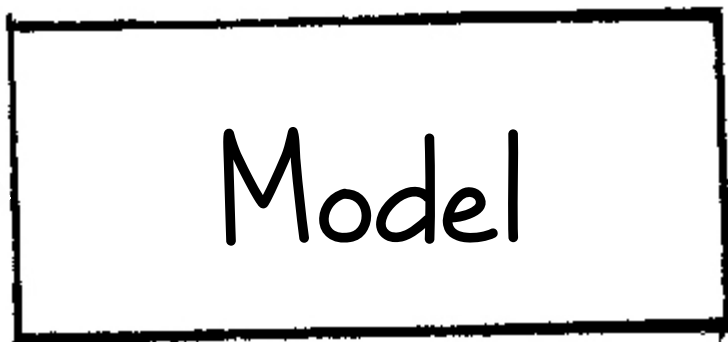
17



-3



2



real  
score



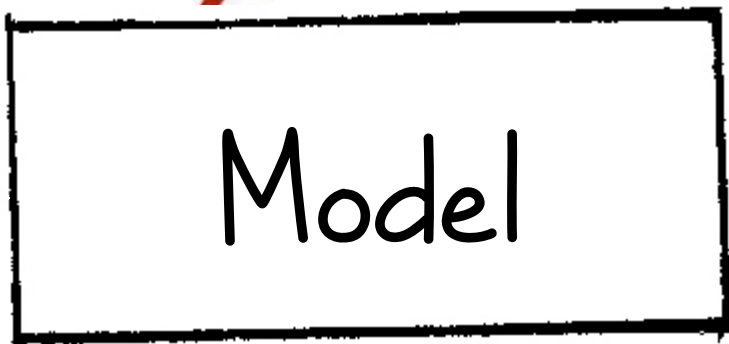
17

8

2

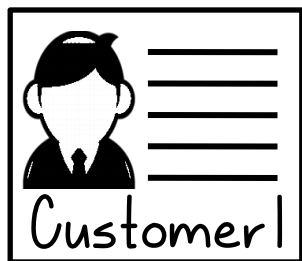
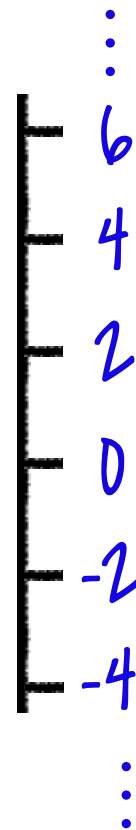
1

-3



real  
score

Performance  
Measure?



17

8

2

1

-3

## A man with glasses and a mustache, wearing an orange t-shirt, is standing in front of a whiteboard. The t-shirt features the text 'Learning Optimization' in a large, stylized font, with 'ICML 2016' and 'Adaptive' visible below it. He is gesturing with his right hand towards the whiteboard, which has the words 'Data Bi' written in red.



>



?



>



?

.....

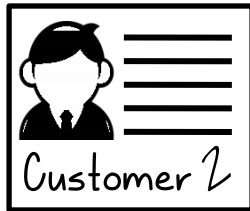
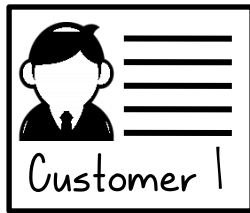


>



?

Pair-wise  
Accuracy



.....



Positives in  
top K positions

Precision@K



Positives in  
top K positions

Average  
Precision

.....  
.....



.....

RankSVM

RankNet

RankBoost

SVM MAP

SVM Perf

...

Binary Classification

Bipartite Ranking

E.g. RankSVM





[ location   Avg. #. of calls   Avg. duration   ...   ...   Mobile  
                    per day            of call                                            Tarrif ]



# RankSVM

[ 9      33      17      ...      ...      41 ]  
location   Avg. #. of calls   Avg. duration   ...   ...   Mobile  
                 per day           of call                                   Tarrif

Model  
[9, 33, 17, ..., ..., 41]

93%  
pair-wise accuracy  
on training set

# Test Set

Model

[9, 33, 17, ..., ..., 41]



Customer 1



Customer 2

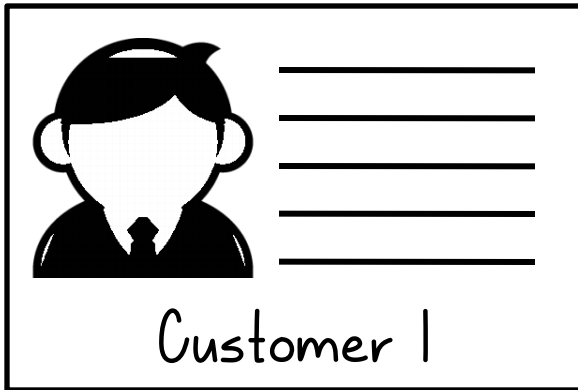
.....



Customer M

90%  
pair-wise  
accuracy





Churn



.....

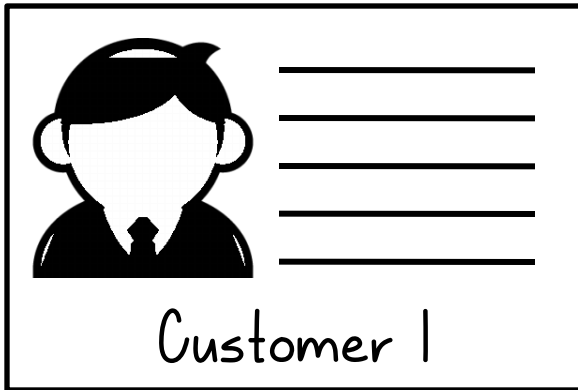


Churn



.....





Churn



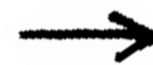
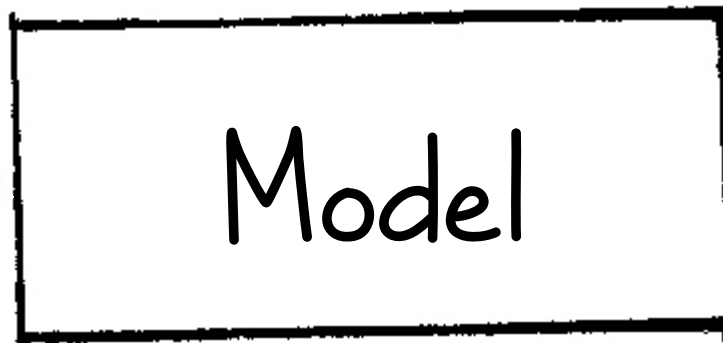
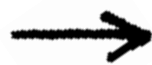
.....



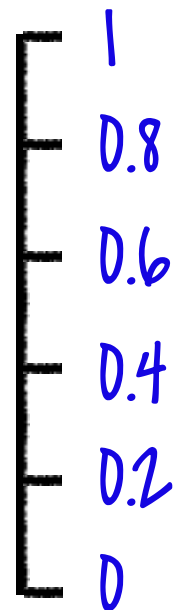
Churn

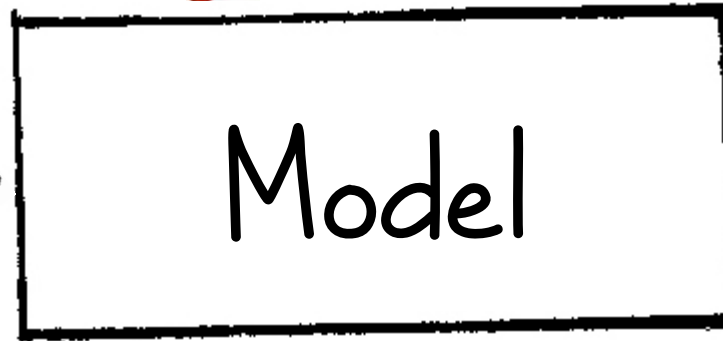
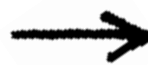


What is the  
probability of  
churn?



probability  
of churn

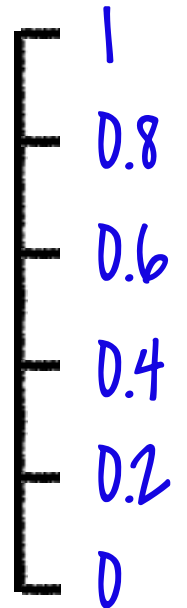




Performance  
Measure?



probability  
of churn

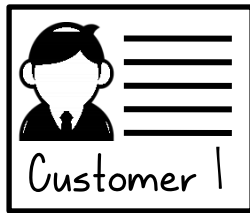


Binary Classification

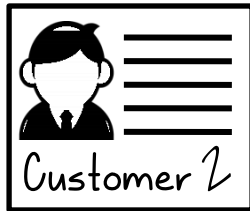
Bipartite Ranking

Binary Class Probability Estimation





0.16



0.23



0.89



0.37

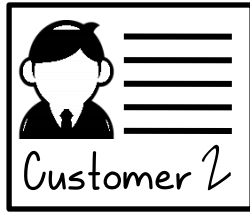


0.93

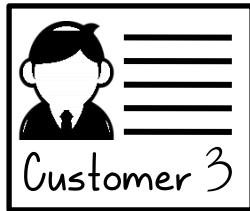
.....



0.16



0.23



0.89



0.37



0.93

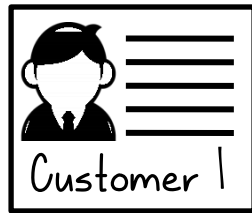
.....

# Performance Measure?

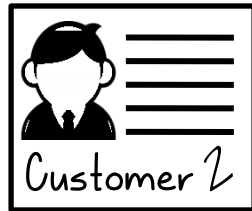
Logloss

Squared Error

...



0.16



0.23



0.89



0.37



0.93

.....

# Performance Measure?

Logloss

Squared Error

...

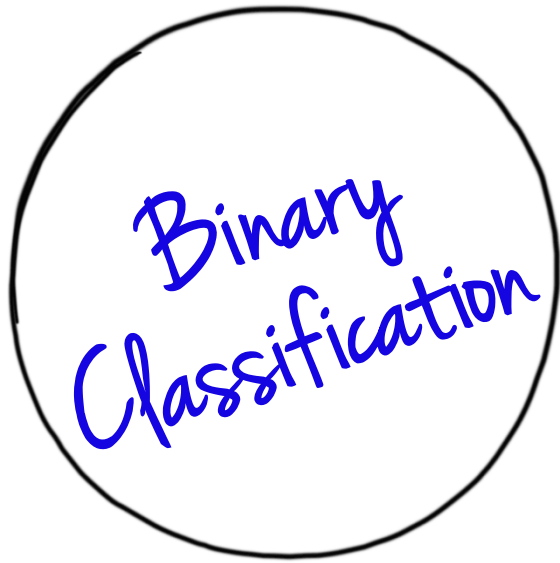
# Algorithms?

Logistic Regression

LogitBoost

...

the story so far ...



the story so far ...

Binary  
Classification

Bipartite  
Ranking

the story so far ...

Binary  
Classification

Bipartite  
Ranking

Binary  
Class Prob.  
Estimation

# the story so far ...

Binary  
Classification

Standard Error

AM-measure

G-mean

...

Bipartite  
Ranking

Pair-wise Accuracy

Precision@K

Average Precision

...

Binary  
Class Prob.  
Estimation

Logloss

Squared Error

...

$F_1$ -measure

Standard Error

Precision@K

Pair-wise Accuracy



Average Precision

G-mean

F-measure

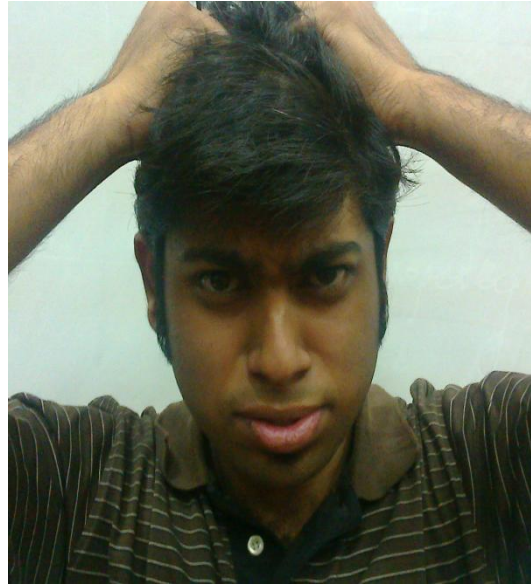
Logloss

Logistic  
Regression

Rank SVM

Support Vector  
Machine

Neural Network

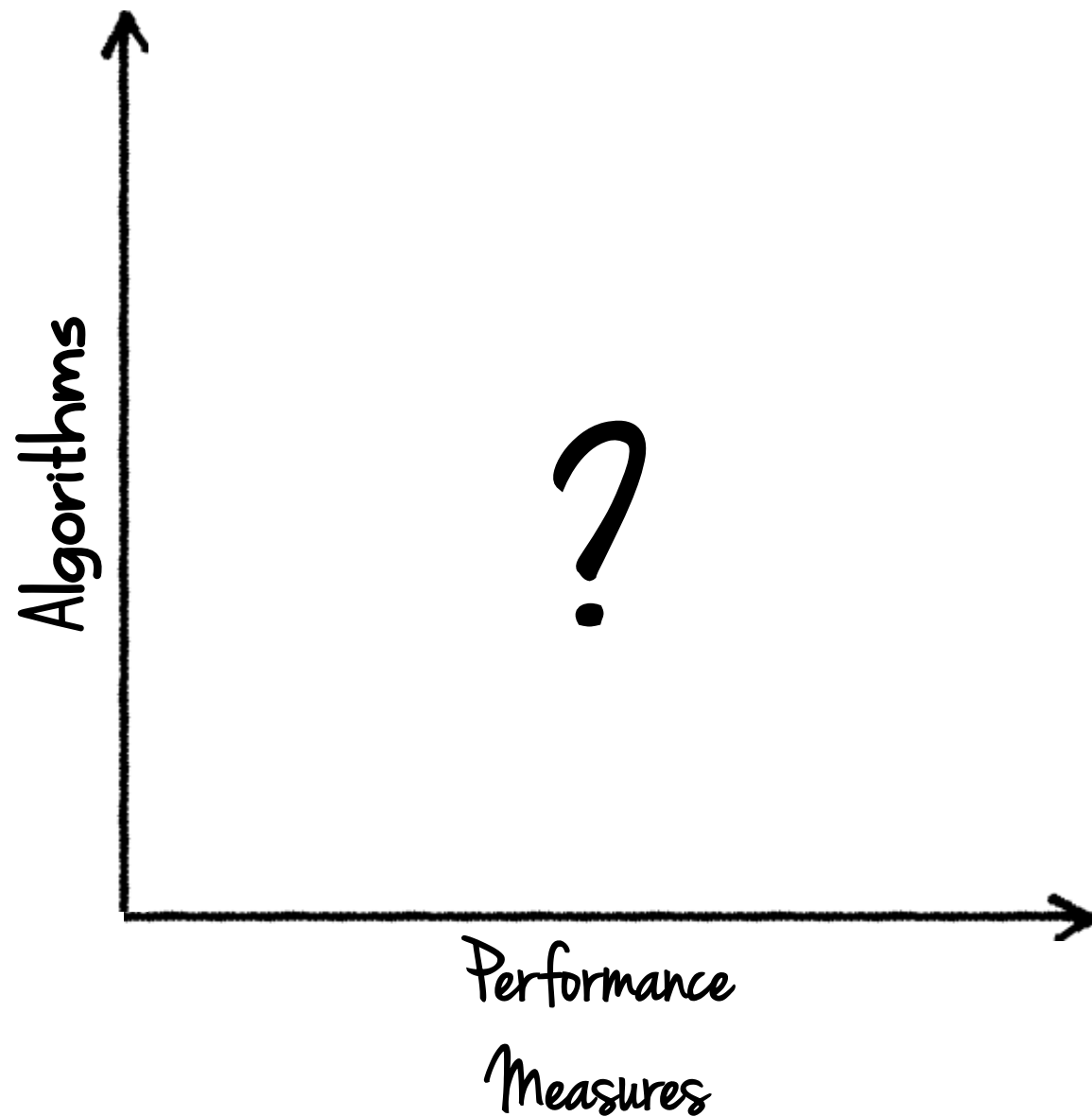


Decision Tree

RankBoost

AdaBoost

RankNet



NAH!



Bipartite  
Ranking



Binary  
Classification

?



Binary  
Class Prob.  
Estimation

Bipartite  
Ranking



May be!



?

Binary  
Classification

Binary  
Class Prob.  
Estimation

Bipartite  
Ranking

?

Binary  
Classification

Binary  
Class Prob.  
Estimation

Plausible!



# Performance Measures

Binary  
Classification

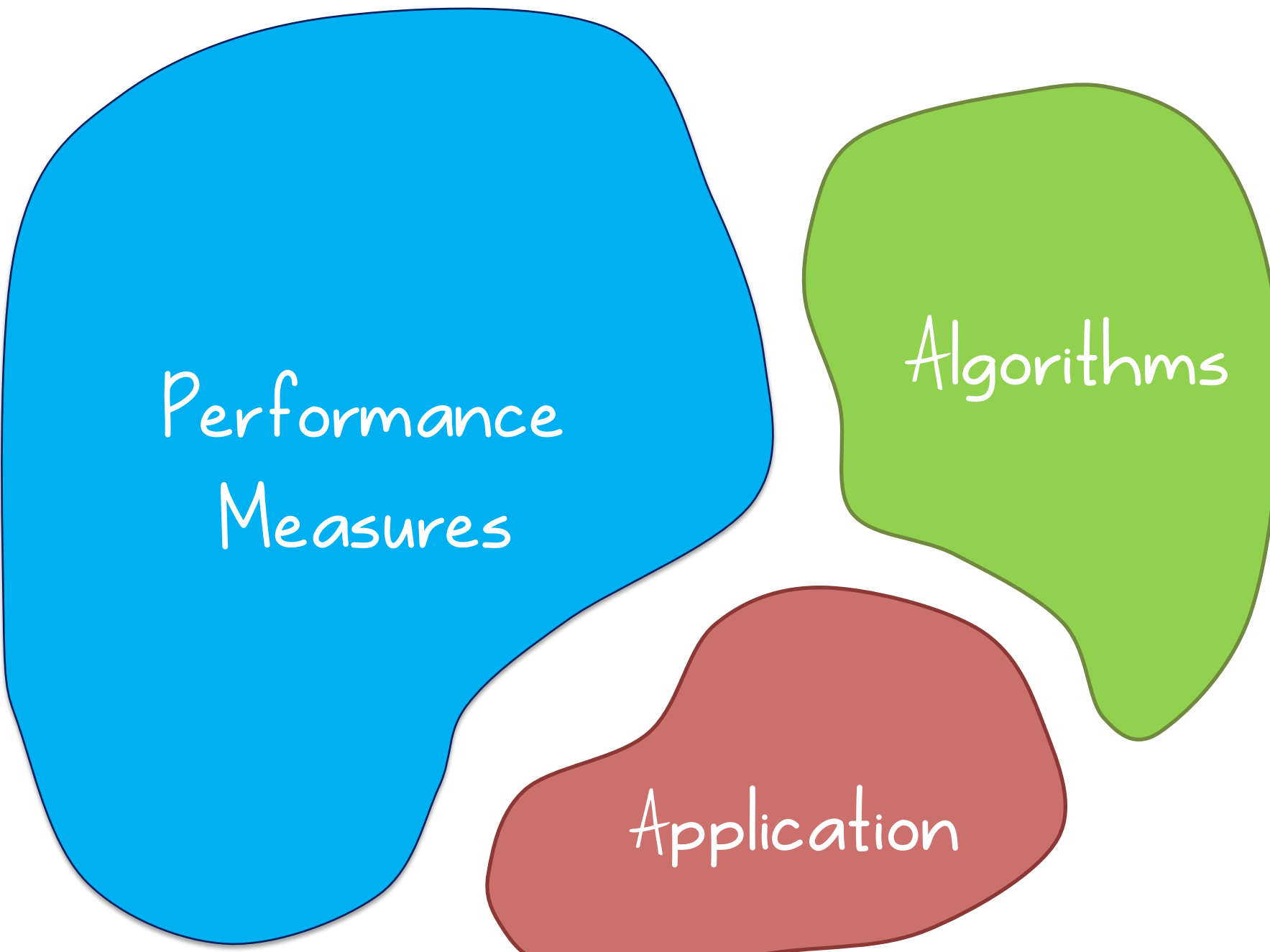
Standard Error  
F1-measure  
G-mean  
...

Bipartite  
Ranking

Pair-wise Accuracy  
Precision@K  
Average Precision  
...

Binary  
Class Prob.  
Estimation

logloss  
Squared Error  
...

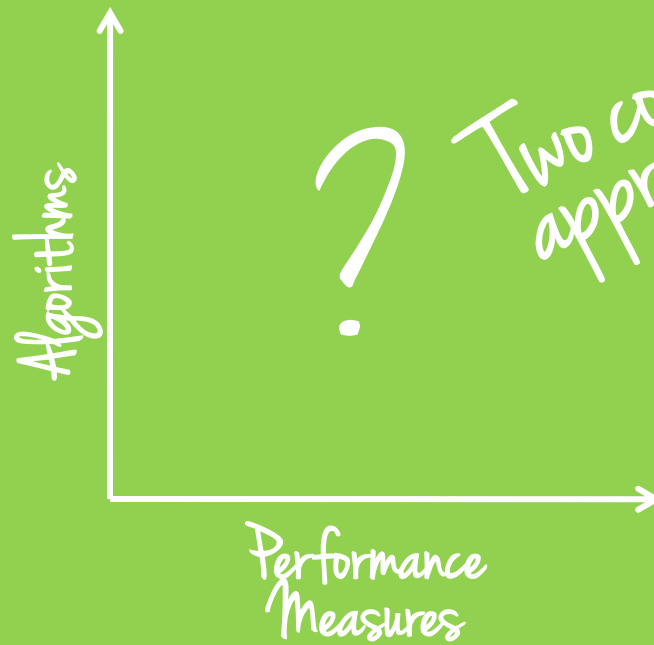


Performance  
Measures

Algorithms

Application

# Algorithms

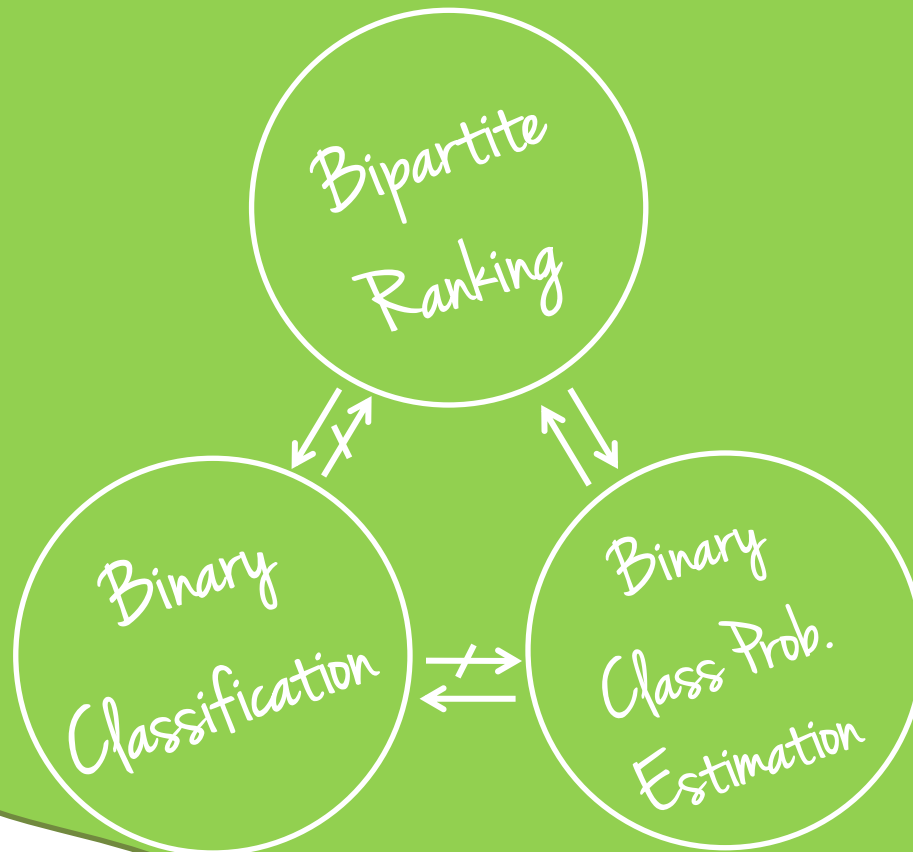


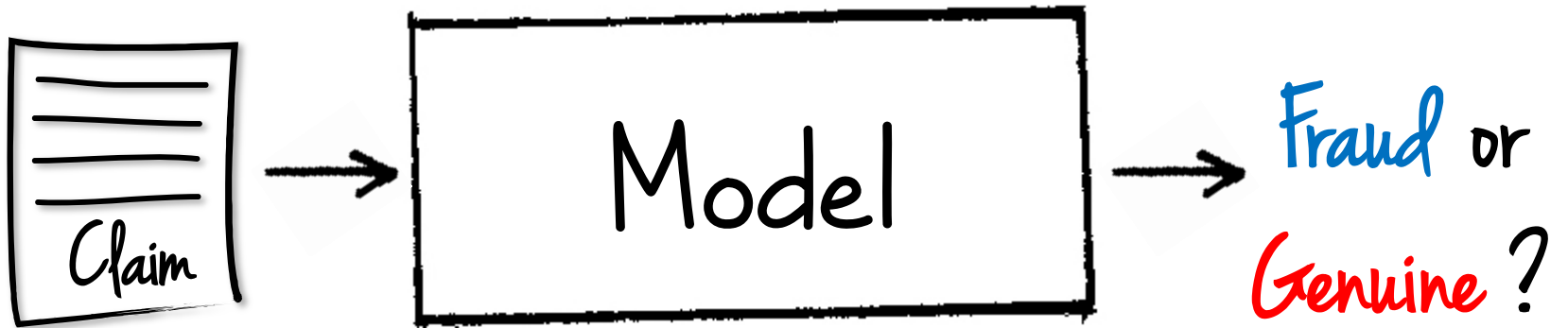
Two common approaches

# Algorithms



# Algorithms

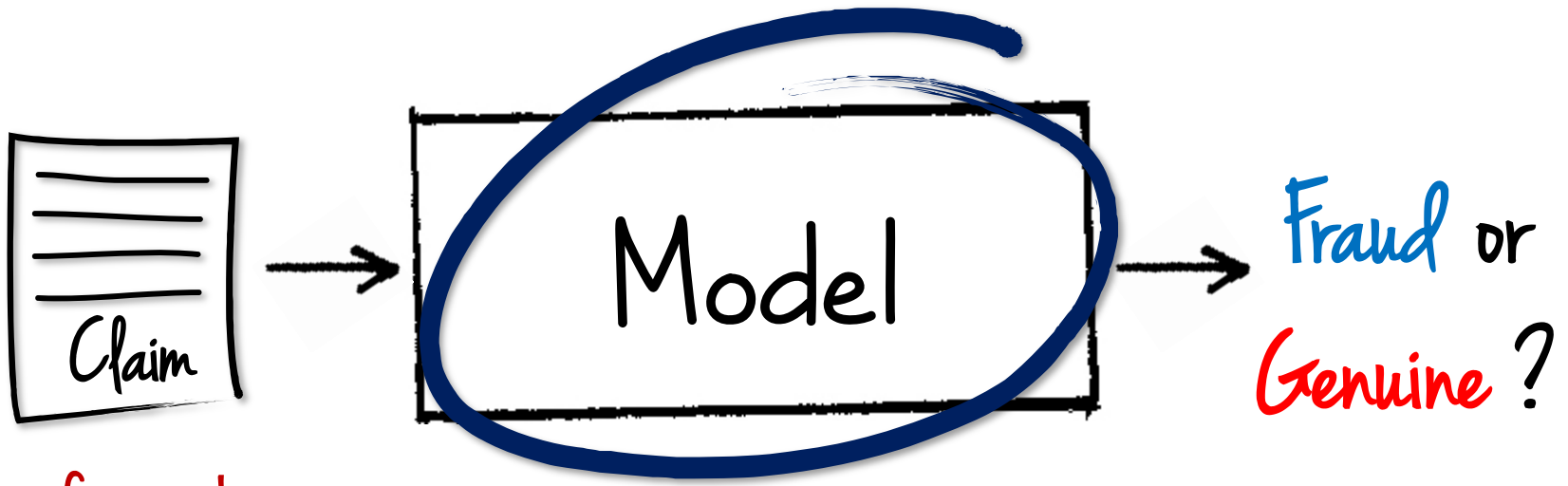




feature 1  
feature 2

...

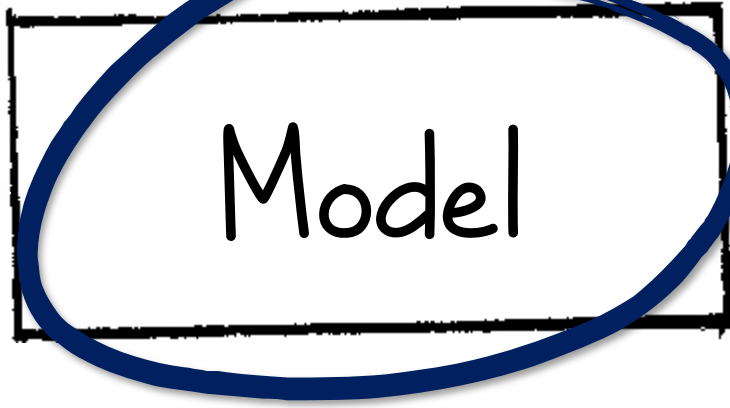
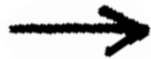
...



feature 1  
feature 2  
...  
...

Maximum value on  
'performance measure' X

Two Common  
Approaches



Fraud or  
Genuine?

feature 1  
feature 2  
...  
...

Maximum value on  
'performance measure' X

Approach 1

# Training Set



Genuine

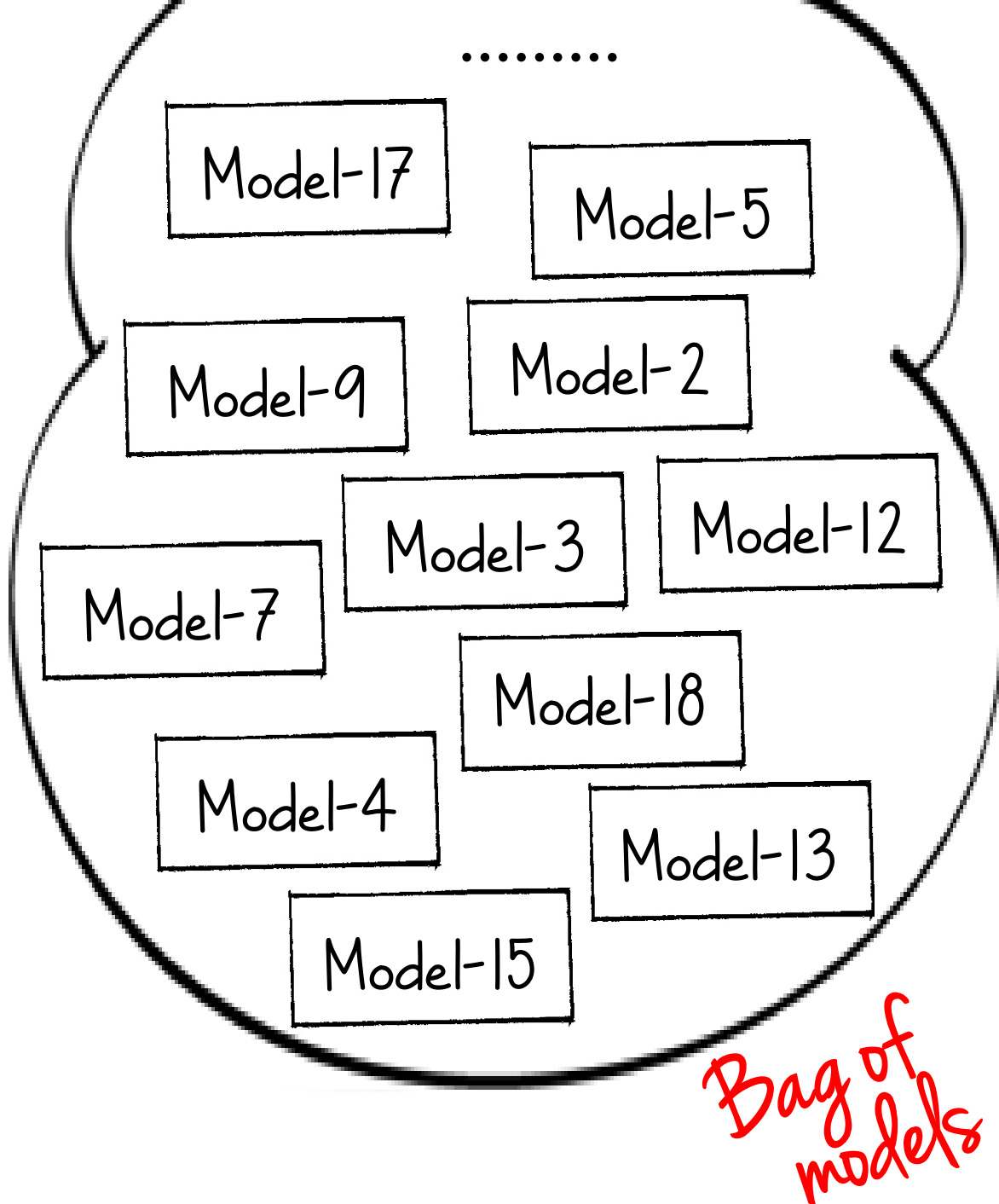


Fraud

.....



Genuine



# Training Set

Claim 1

Genuine

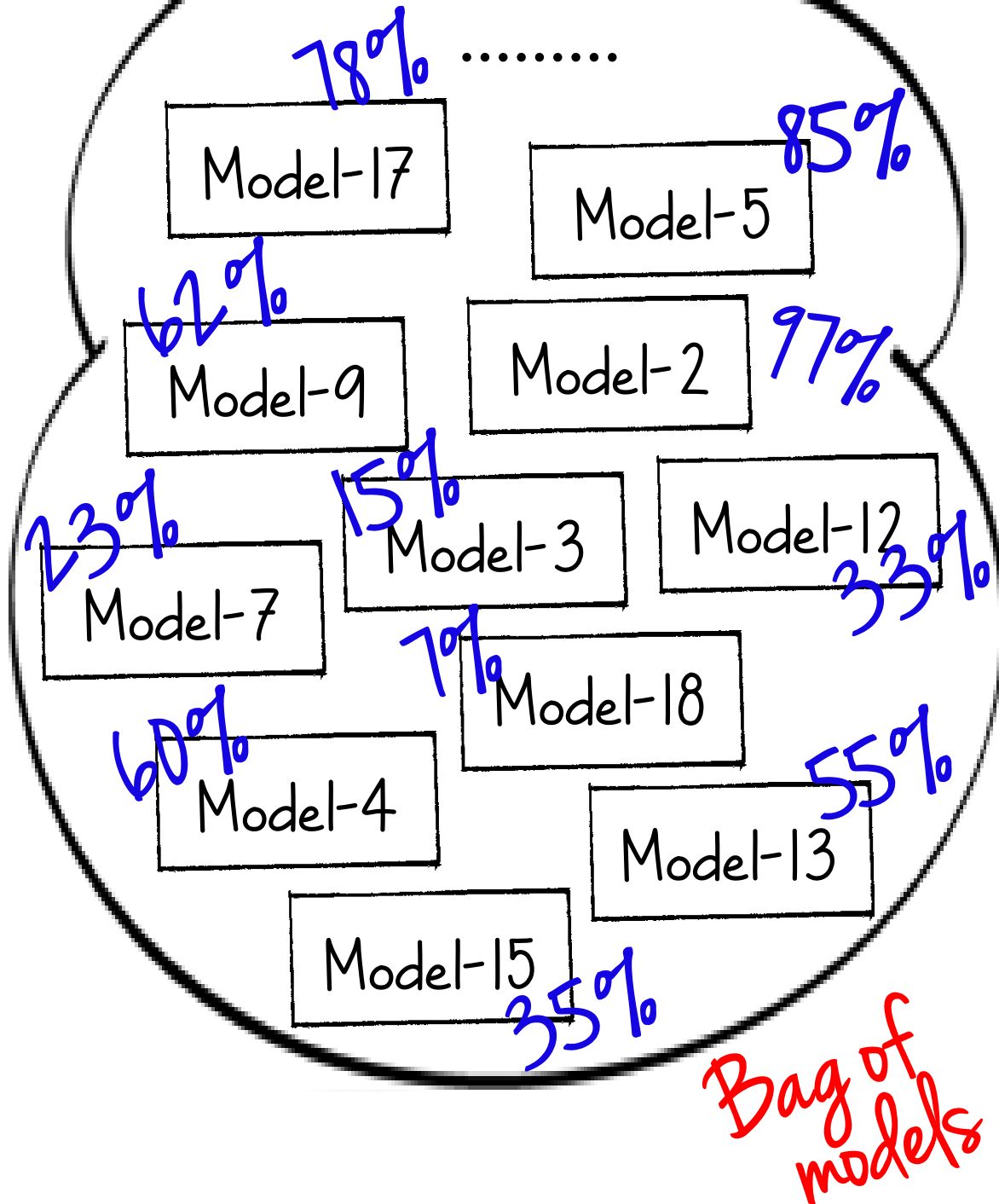
Claim 2

Fraud

.....

Claim N

Genuine



# Training Set

Claim 1

Genuine

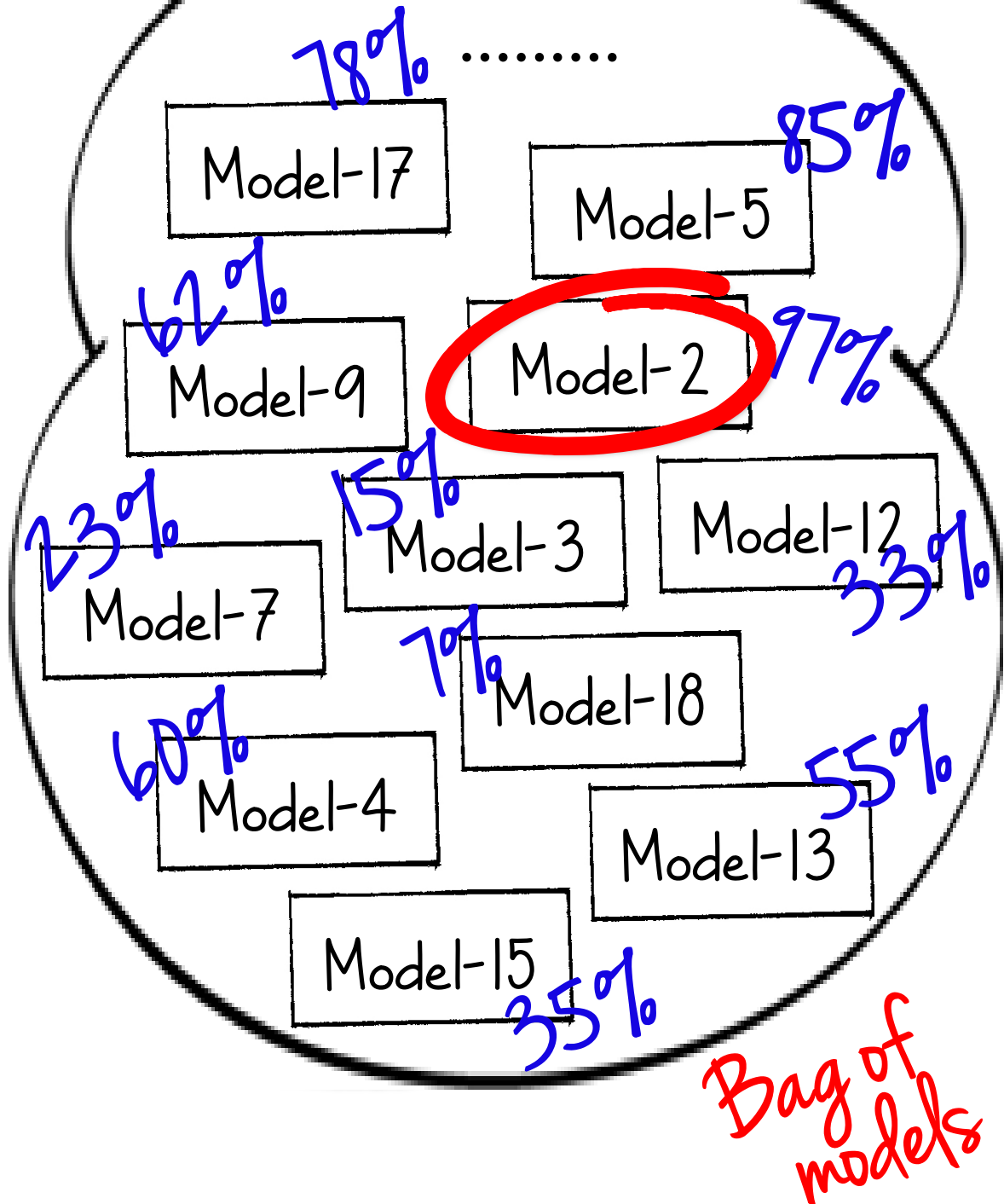
Claim 2

Fraud

.....

Claim N

Genuine



# Optimization Problem

find model with  
maximum value on  
performance measure 'X'

Intractable /  
Hard

Optimization  
Problem

find model with  
maximum value on  
performance measure 'X'

Proxy  
Optimization  
Problem  
(often possible\*)

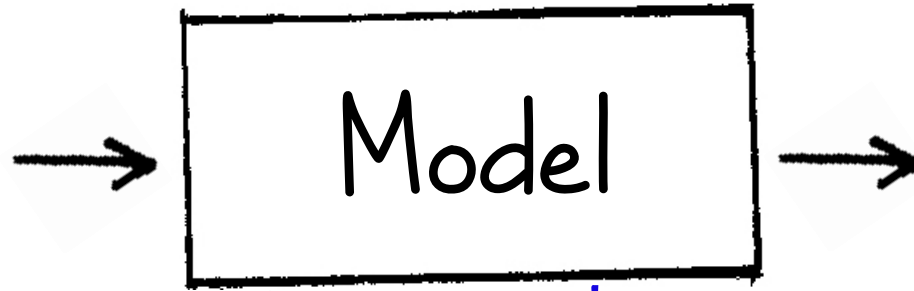
# Approach I

## for different performance measures

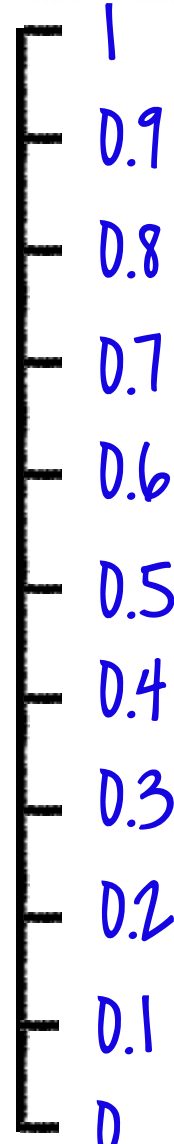
| Performance Measure                | Run-time            | References                                                   |
|------------------------------------|---------------------|--------------------------------------------------------------|
| F-measure<br>PBREP<br>Precision@K  | $O(N^2)$            | Joachims (2005);                                             |
| AUC<br>Partial AUC<br>Pos@Top      | $O(N \log N)$       | Joachims (2005, 2006);<br>Narasimhan & Agarwal<br>(2013 a,b) |
| Average Precision                  | $O(N^2)$            | Yue et al. (2007)                                            |
| Discounted Cumulative Gain (DCG) * | $O(Nk)$             | Chakrabarti et al. (2008)                                    |
| Mean Reciprocal Rank (MRR) *       | $O(N \log N + k^2)$ | Chakrabarti et al. (2008)                                    |

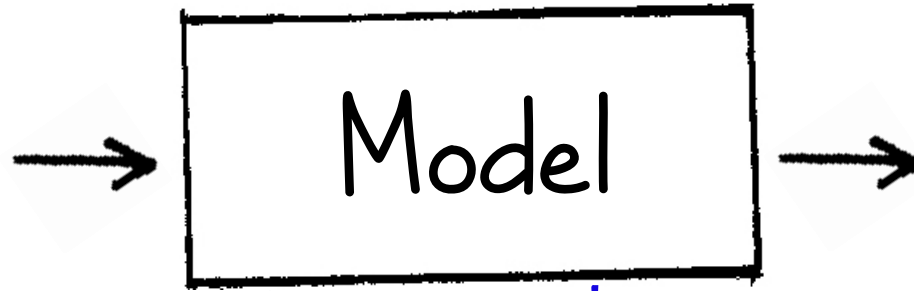
\* performance measure truncated to top 'k' positions

Approach II  
(Plug-in)

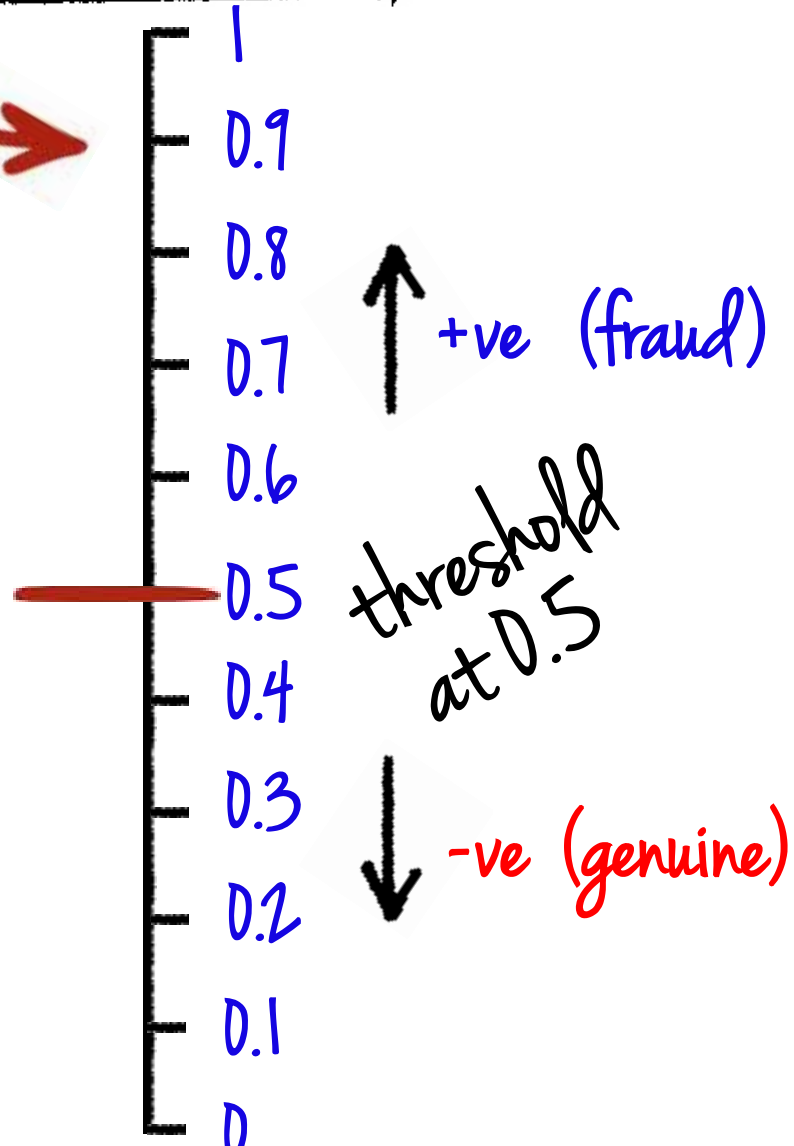


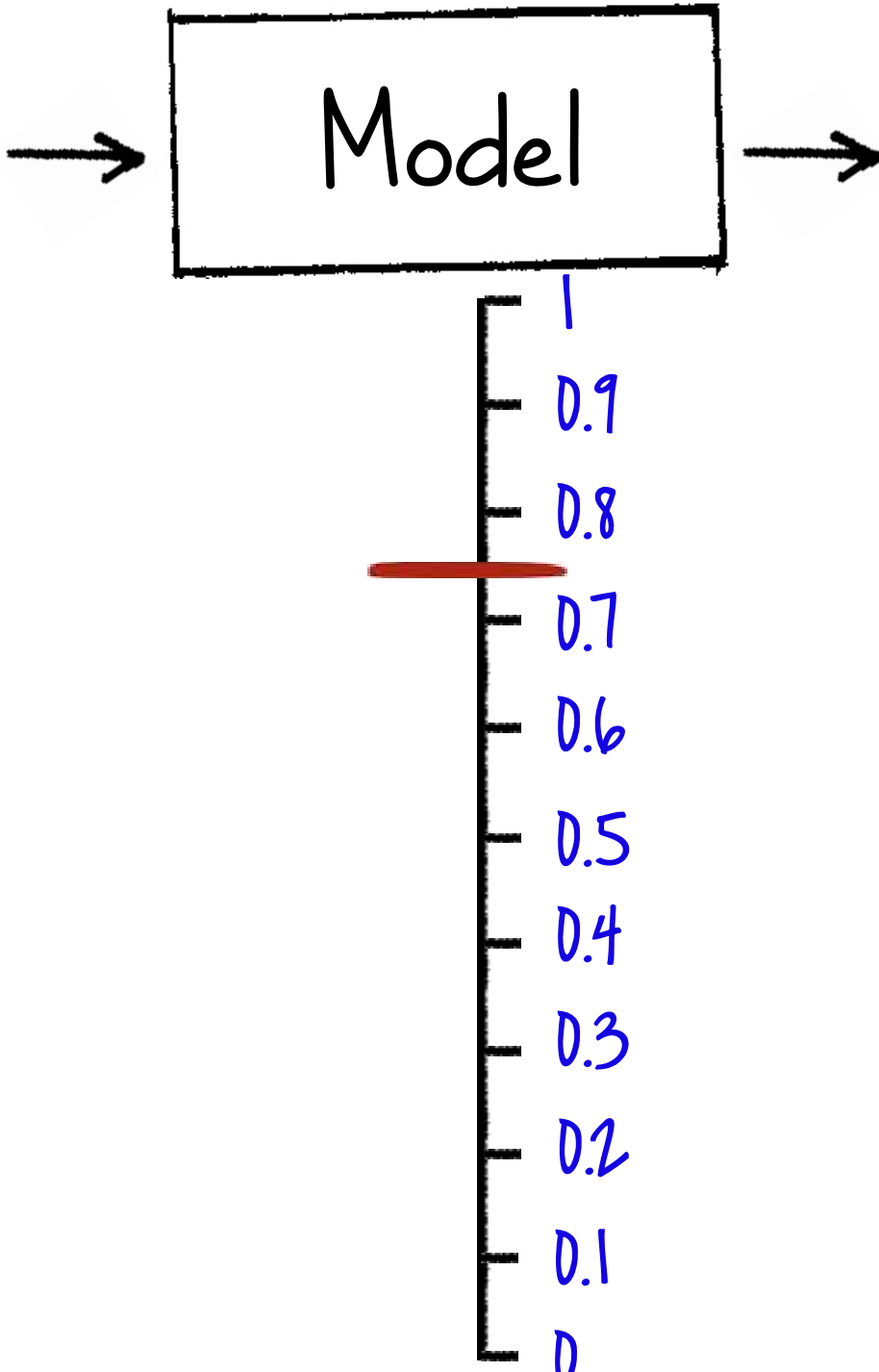
predict  
probability  
of 'fraud'



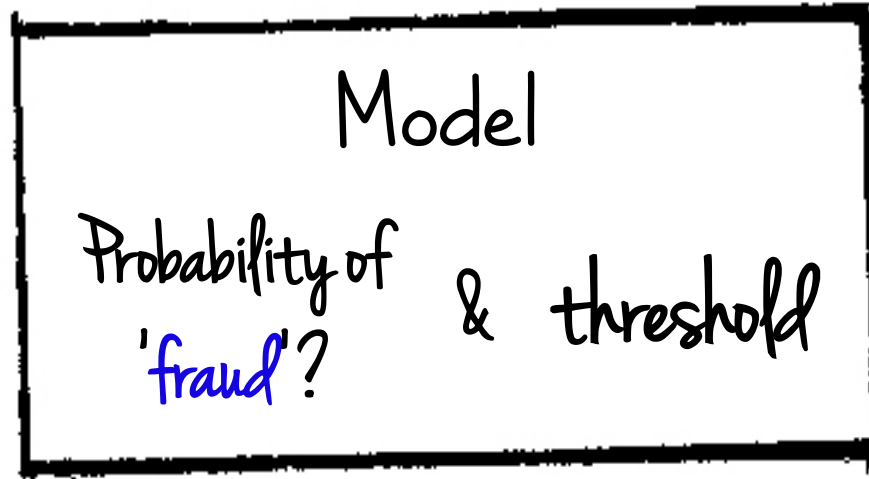
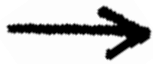


predict  
probability  
of 'fraud'

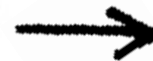
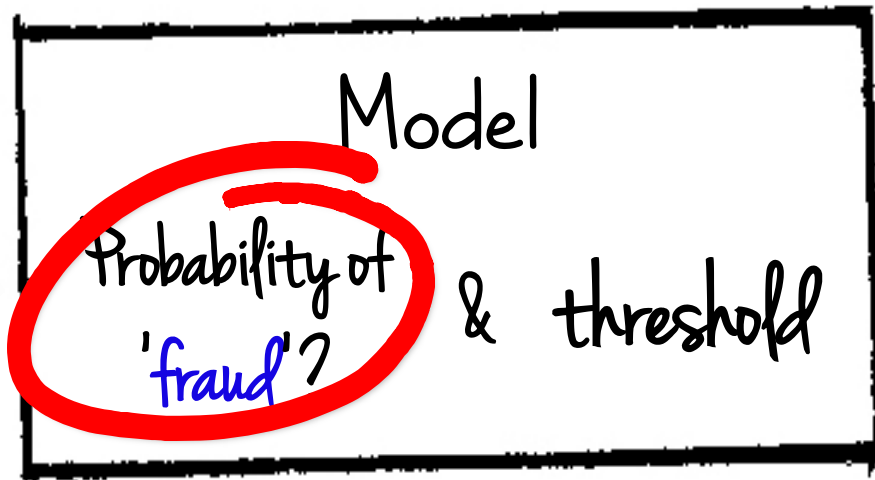
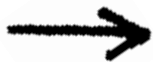




Choose **threshold**  
that maximizes  
'performance measure'  $\chi$



Fraud or  
Genuine?



Fraud or  
Genuine?

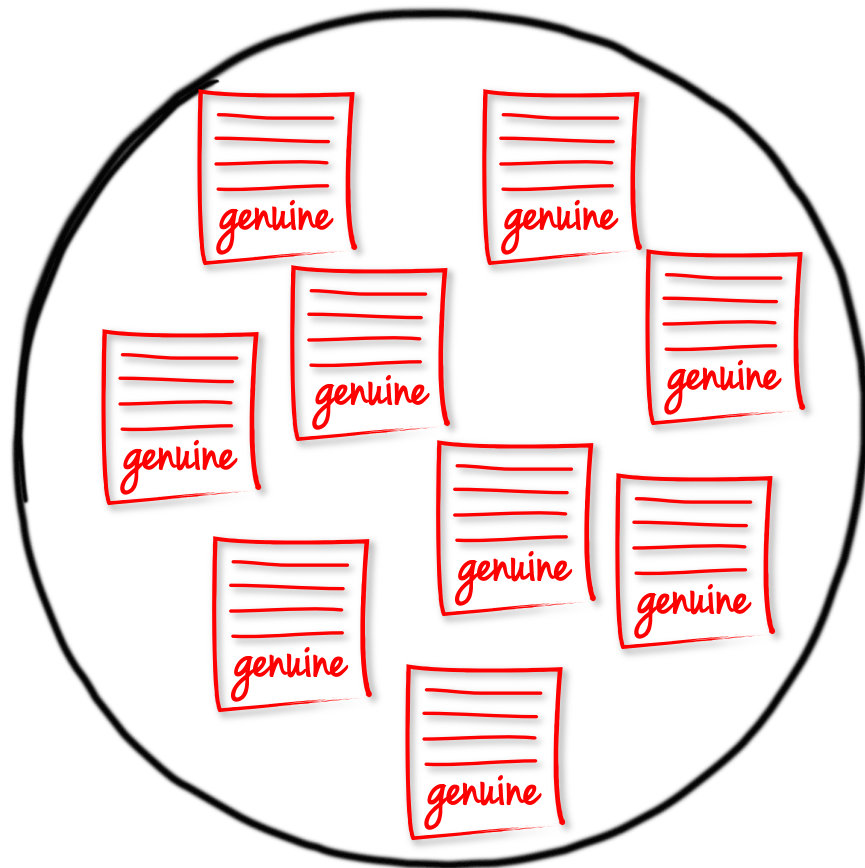
# Example

AM-measure

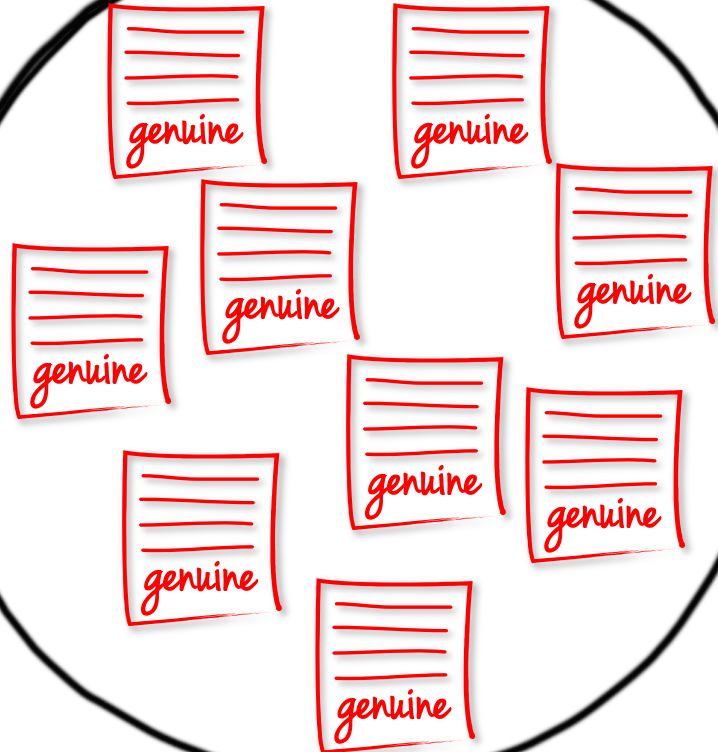
$$\frac{\text{True Positive Rate} + \text{True Negative Rate}}{2}$$

Menon, A., Narasimhan, H., Agarwal, S. and Chawla, S. "On the statistical consistency of algorithms for binary classification under class imbalance", ICML 2013.

# Class Imbalance Problem

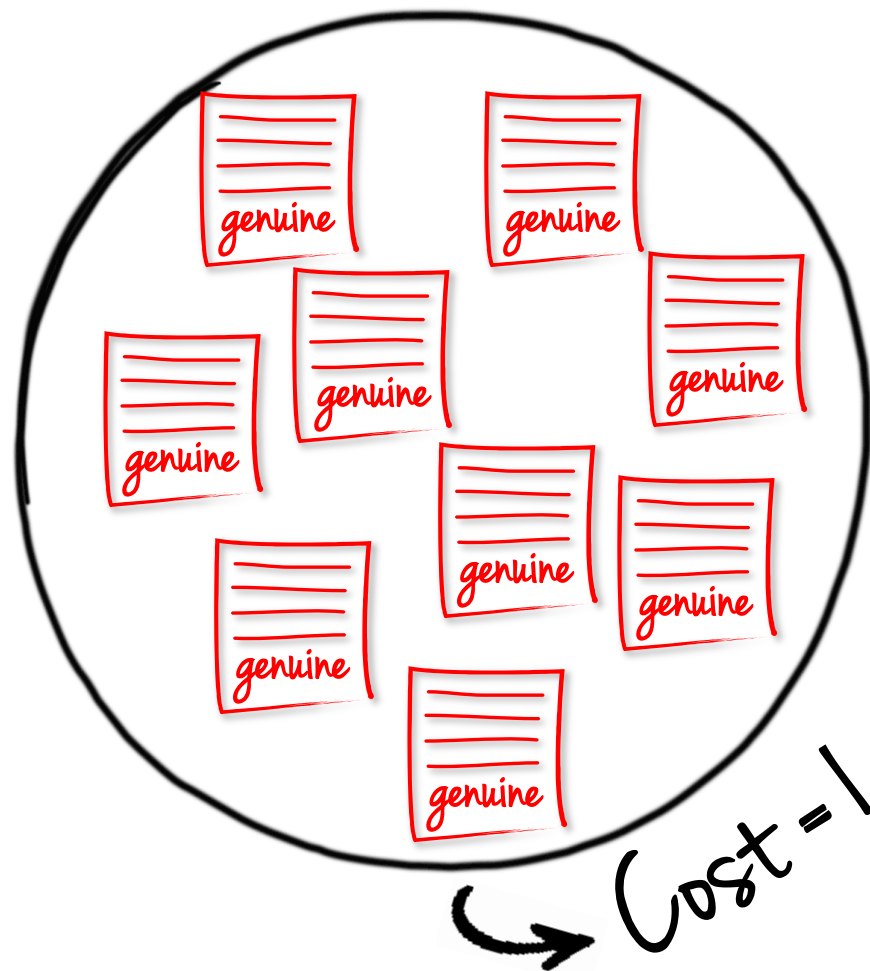
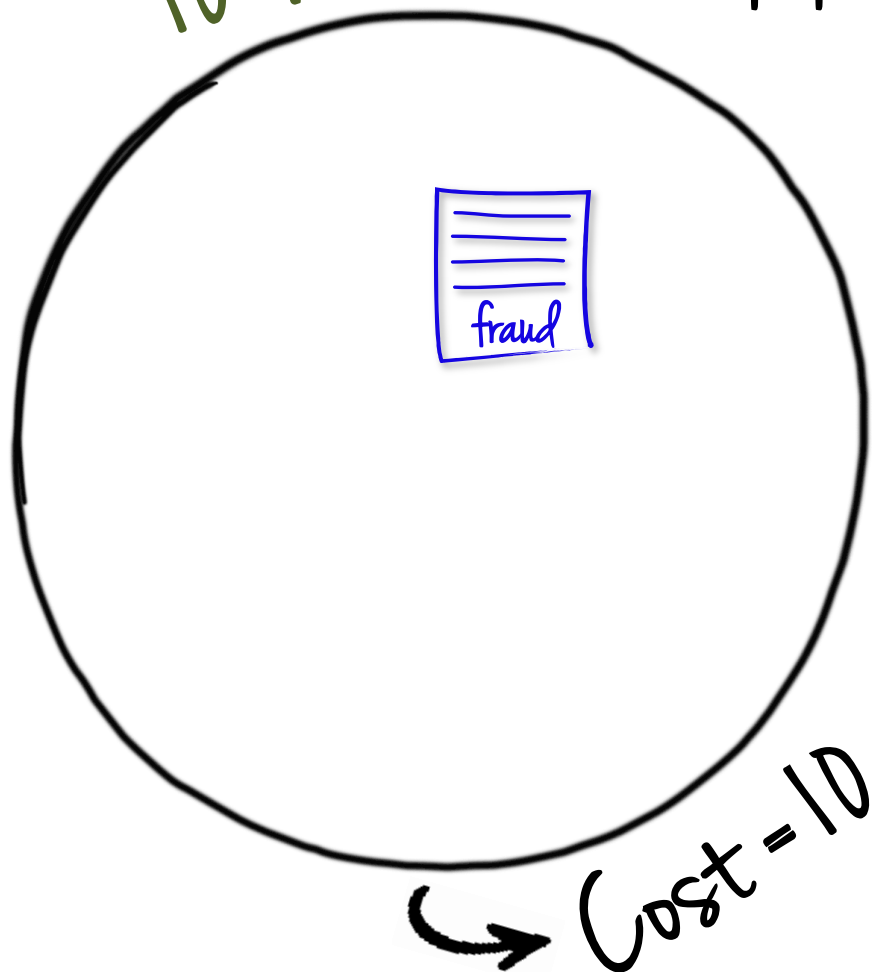


10% 'fraud'



10% fraud

# Approach 1



10% fraud

# Approach 1

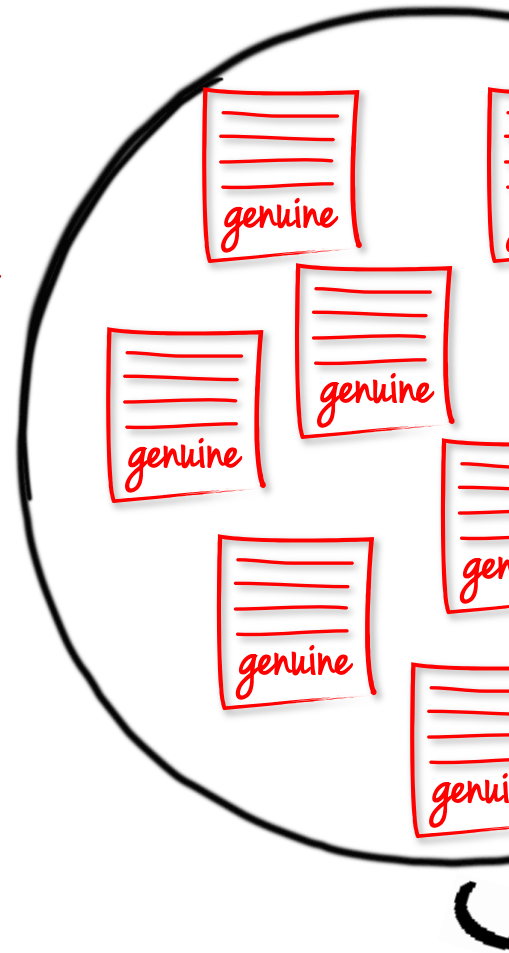
Balanced Logistic Regression

Balanced SVM

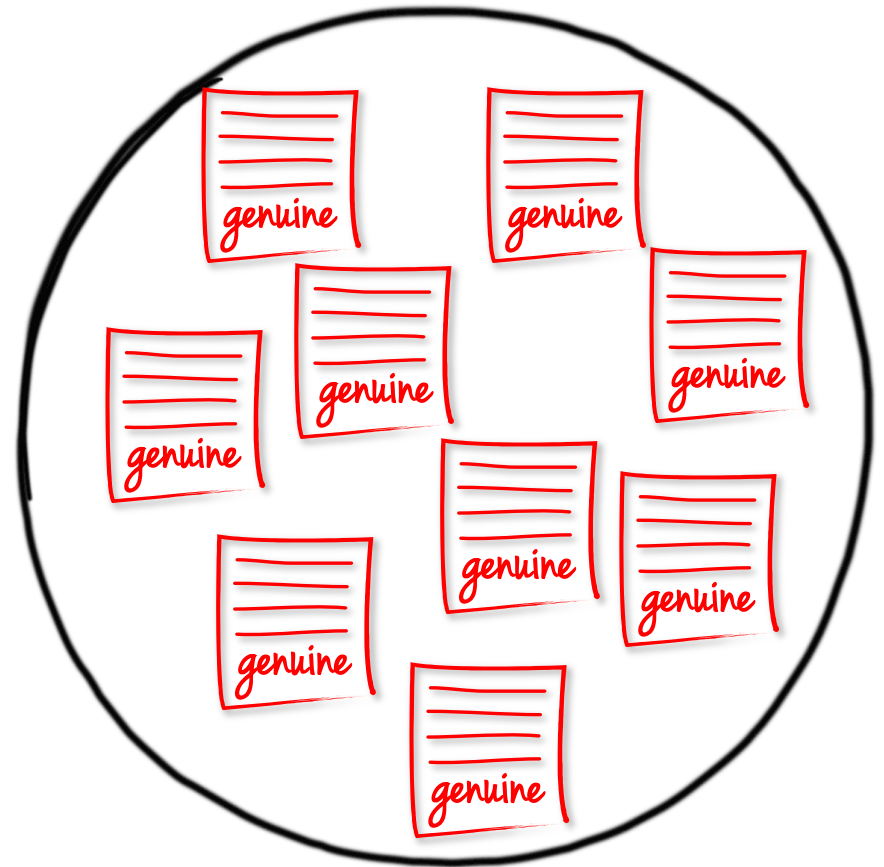
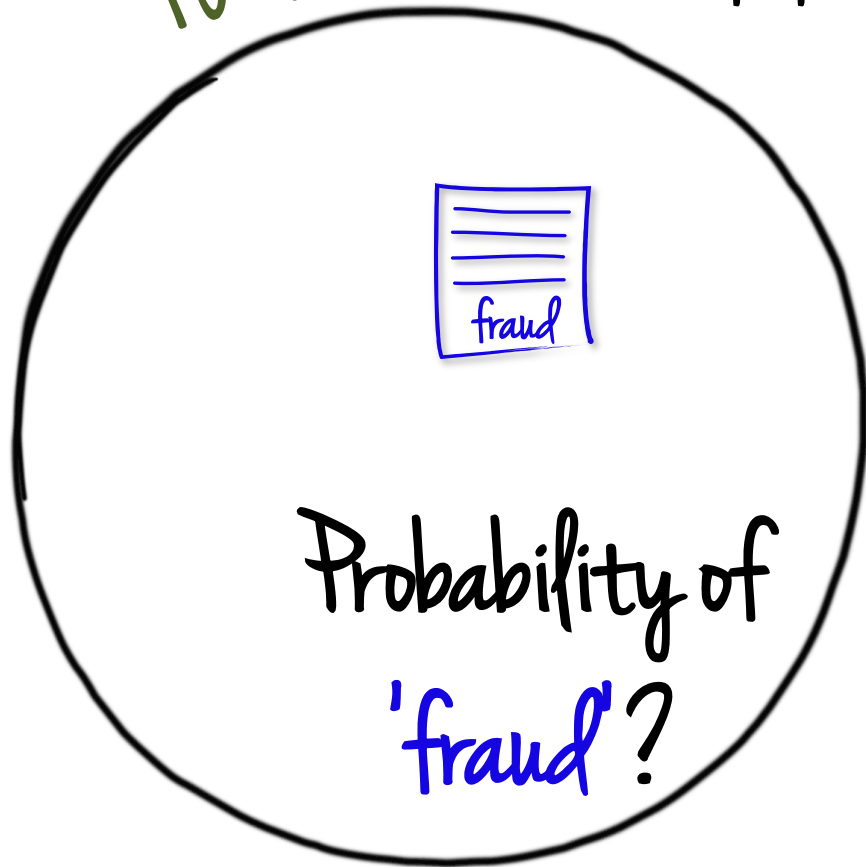
Balanced AdaBoost

Balanced Decision Trees

...



10% 'fraud' Approach II



10% fraud

# Approach II



Probability of  
'fraud'?



# Experiments

AM-measure

$$\frac{\text{True Positive Rate} + \text{True Negative Rate}}{2}$$

# Experiments

## Thyroid Diagnosis

2% positive

|                 | AM-measure |
|-----------------|------------|
| Standard Method | 84.91      |
| Approach 1      | 97.66      |
| Approach 2      | 96.69      |

# Experiments

## Drug Discovery

~2% positive

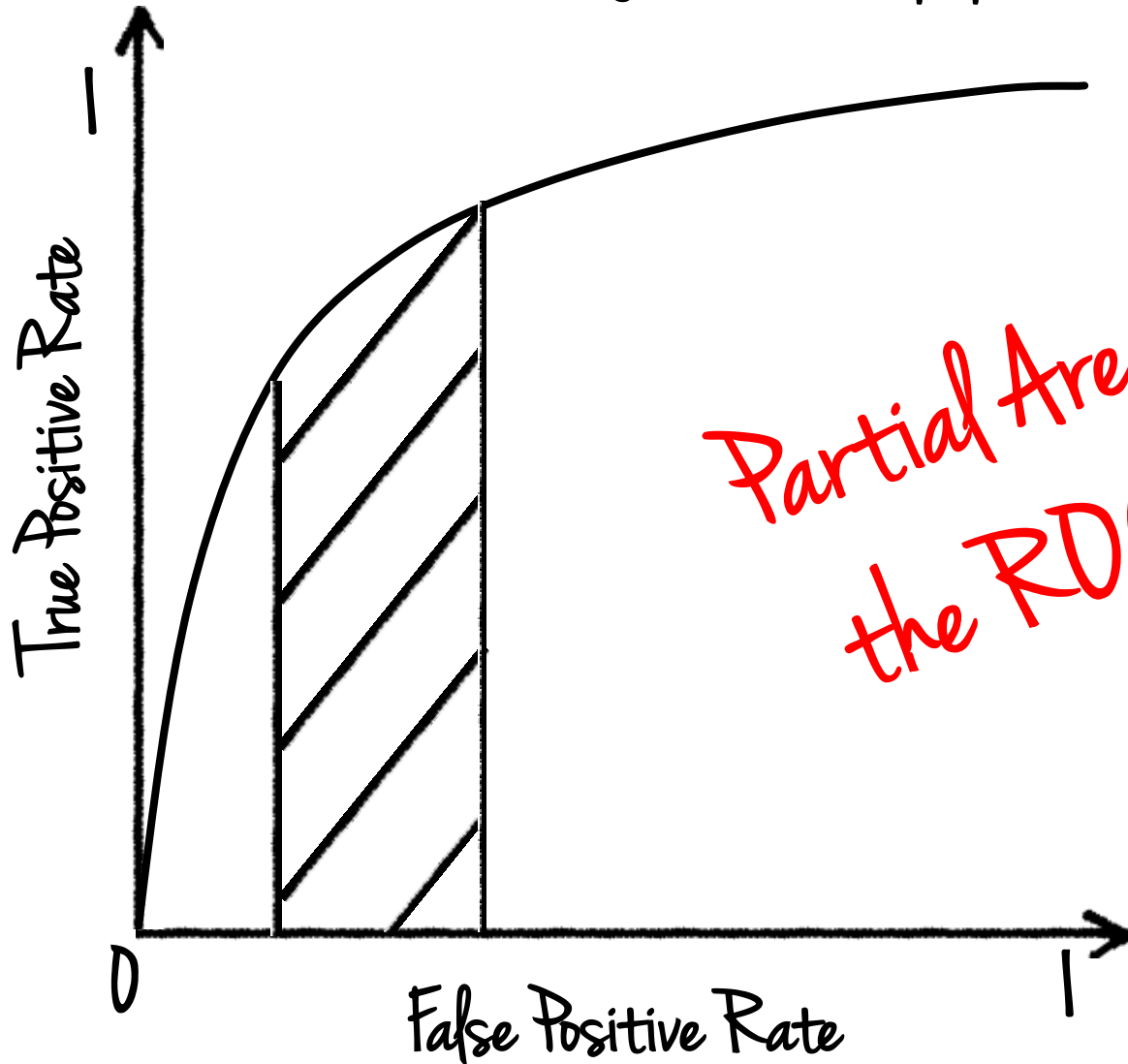
|                 | AM-measure   |
|-----------------|--------------|
| Standard Method | 82.74        |
| Approach 1      | 89.87        |
| Approach 2      | <b>91.55</b> |

# Algorithms

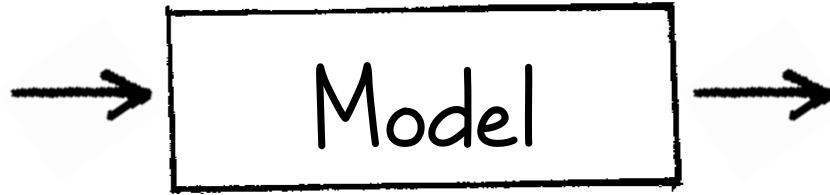


*A Case Study  
for Approach 1*

# A Case Study for Approach II



Partial Area Under  
the ROC Curve

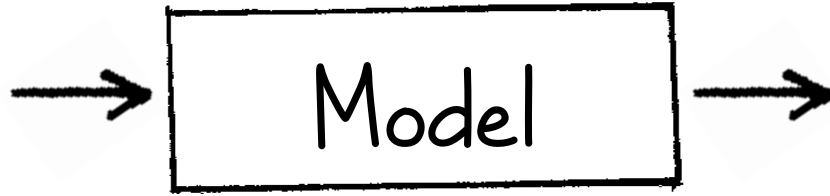


Positive



Positive  
(Fraud)

|  |  |
|--|--|
|  |  |
|  |  |

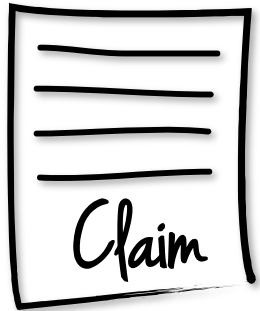
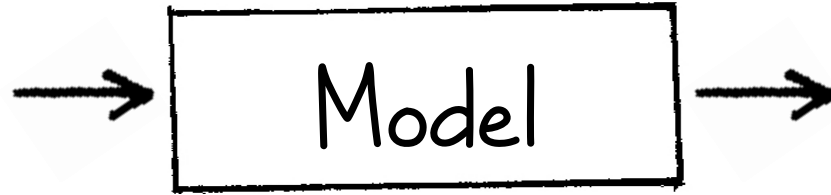


Positive

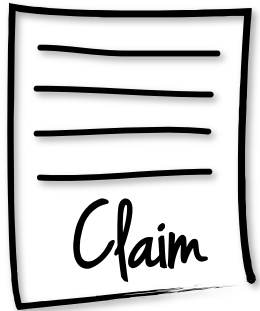
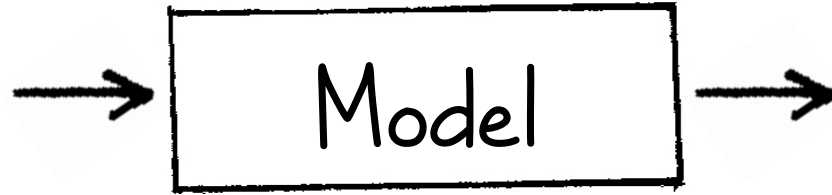


Positive  
(Fraud)

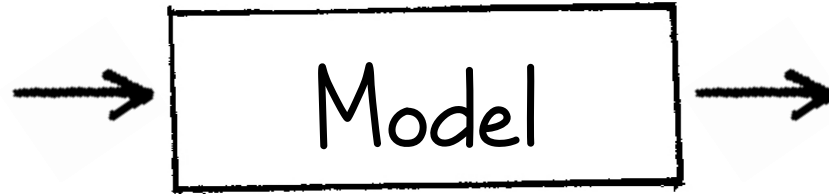
| Positive      |  |
|---------------|--|
| True Positive |  |
|               |  |



|                    | Positive      | Negative      |
|--------------------|---------------|---------------|
| Positive (Fraud)   | True Positive |               |
| Negative (Genuine) |               | True Negative |



|                    | Positive       | Negative       |
|--------------------|----------------|----------------|
| Positive (Fraud)   | True Positive  | False Negative |
| Negative (Genuine) | False Positive | True Negative  |



Positive  
(Fraud)

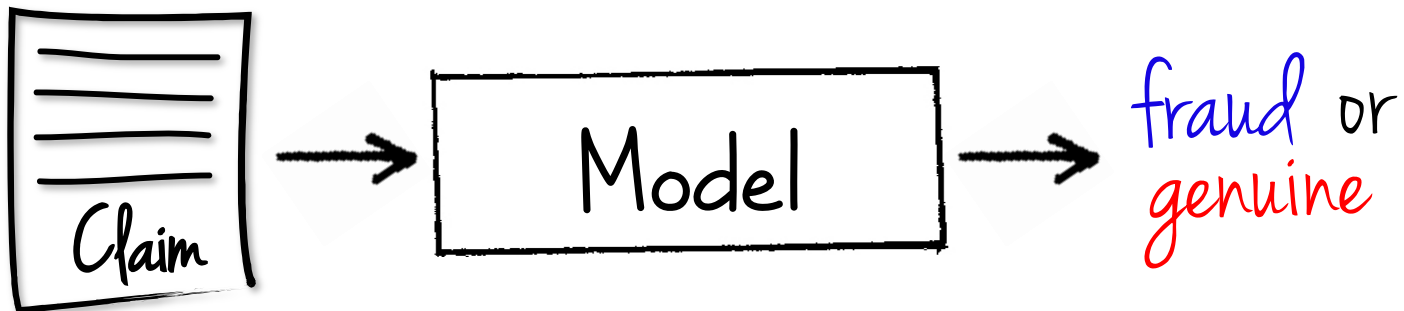
Negative  
(Genuine)

Positive

Negative

|                   |                   |
|-------------------|-------------------|
| True<br>Positive  | False<br>Negative |
| False<br>Positive | True<br>Negative  |

# Fraud Detection



# Fraud Detection

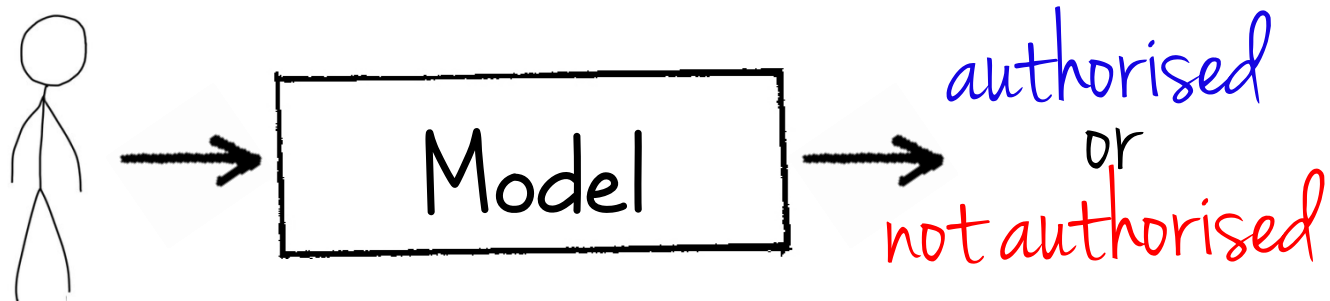


high true  
positive rate  
desirable



fraud or  
genuine

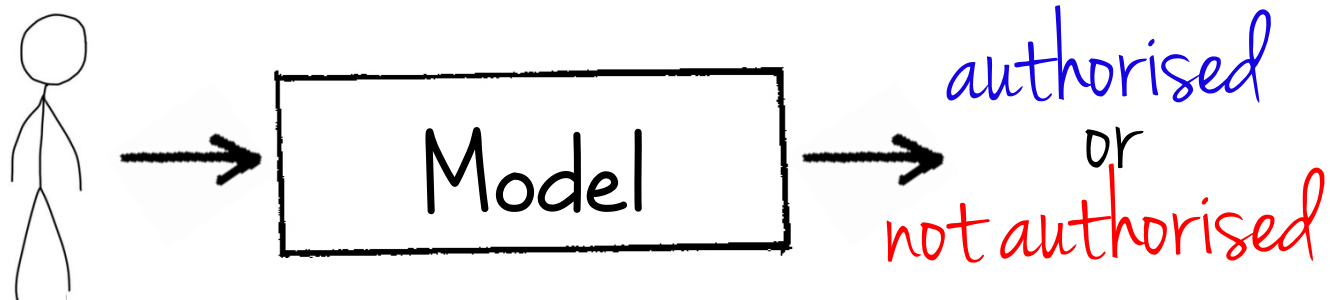
# Biometric Screening



# Biometric Screening



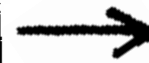
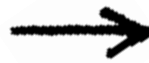
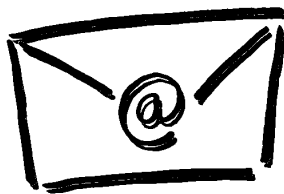
*low false  
positive rate  
desirable*



# Spam Filtering

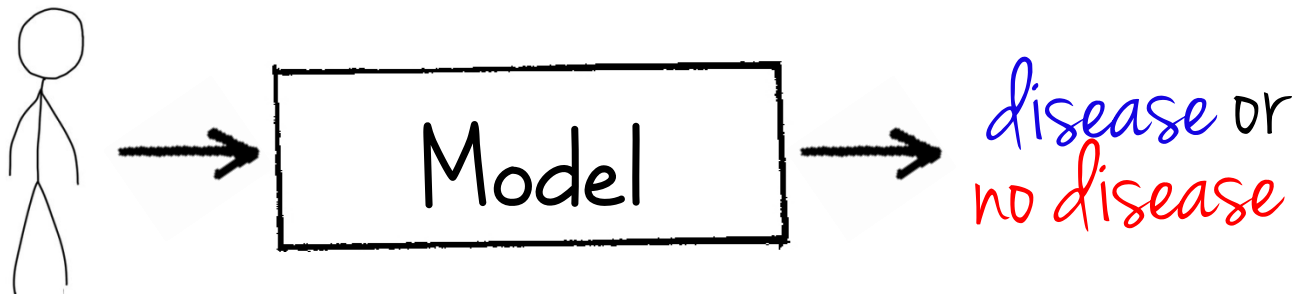


*low false  
positive rate  
desirable*



*spam or  
non-spam*

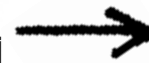
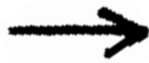
# Medical Diagnosis



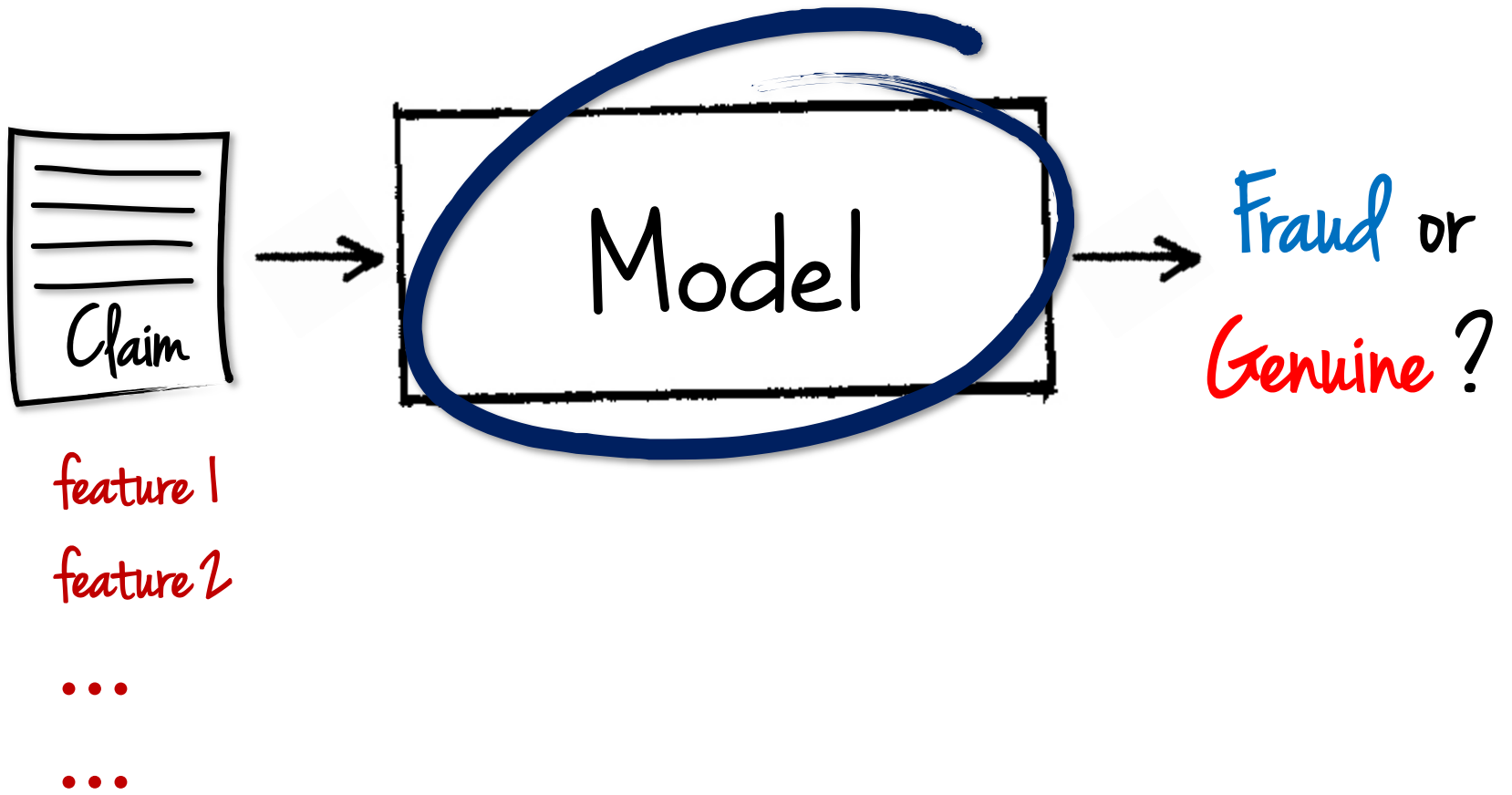
# Medical Diagnosis

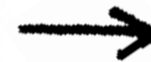
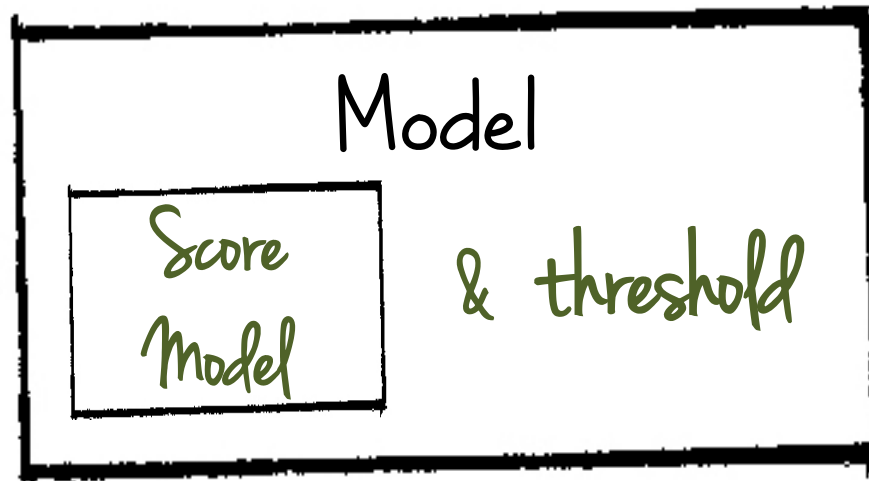
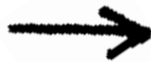


false positives  
within a range

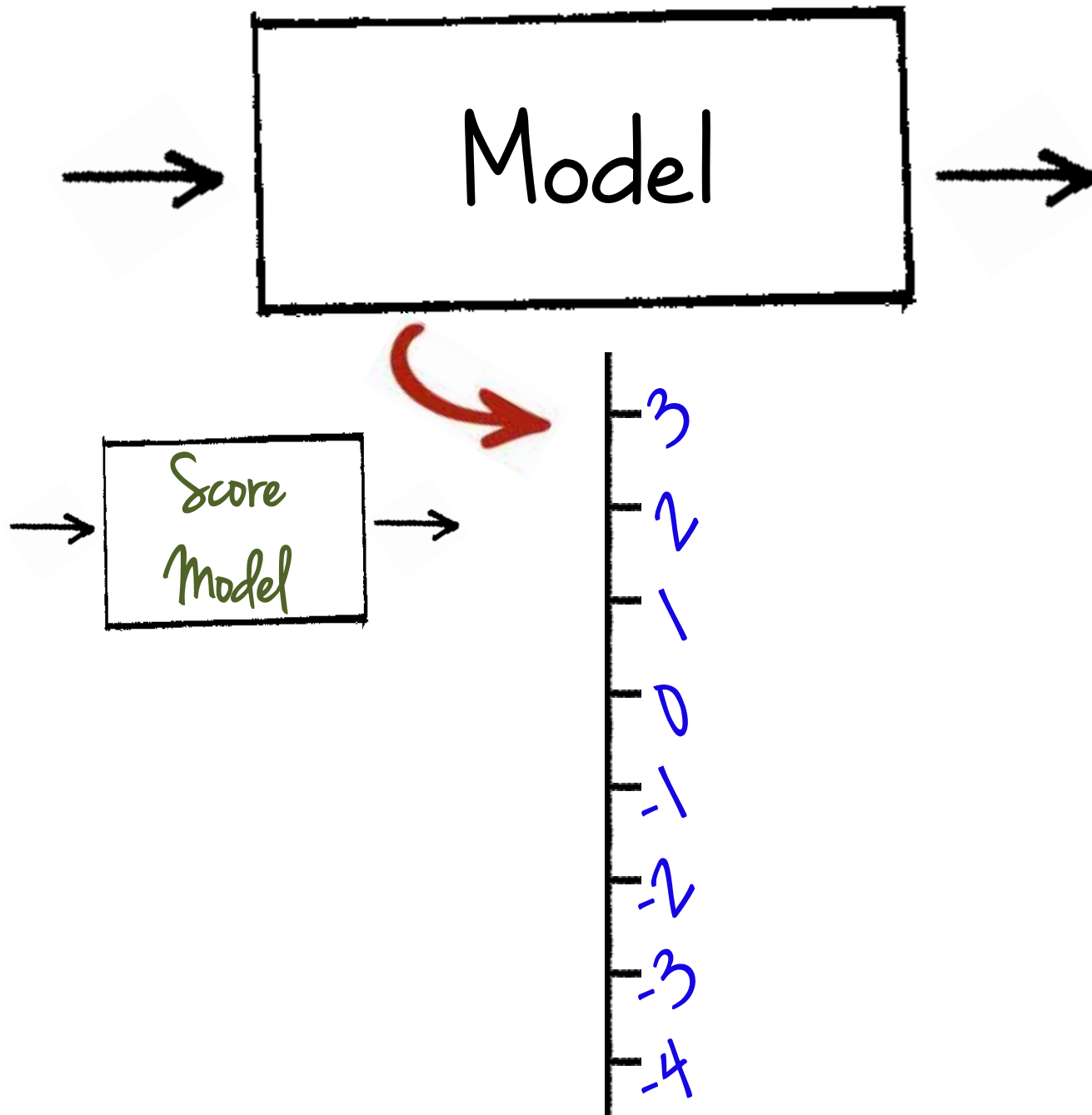


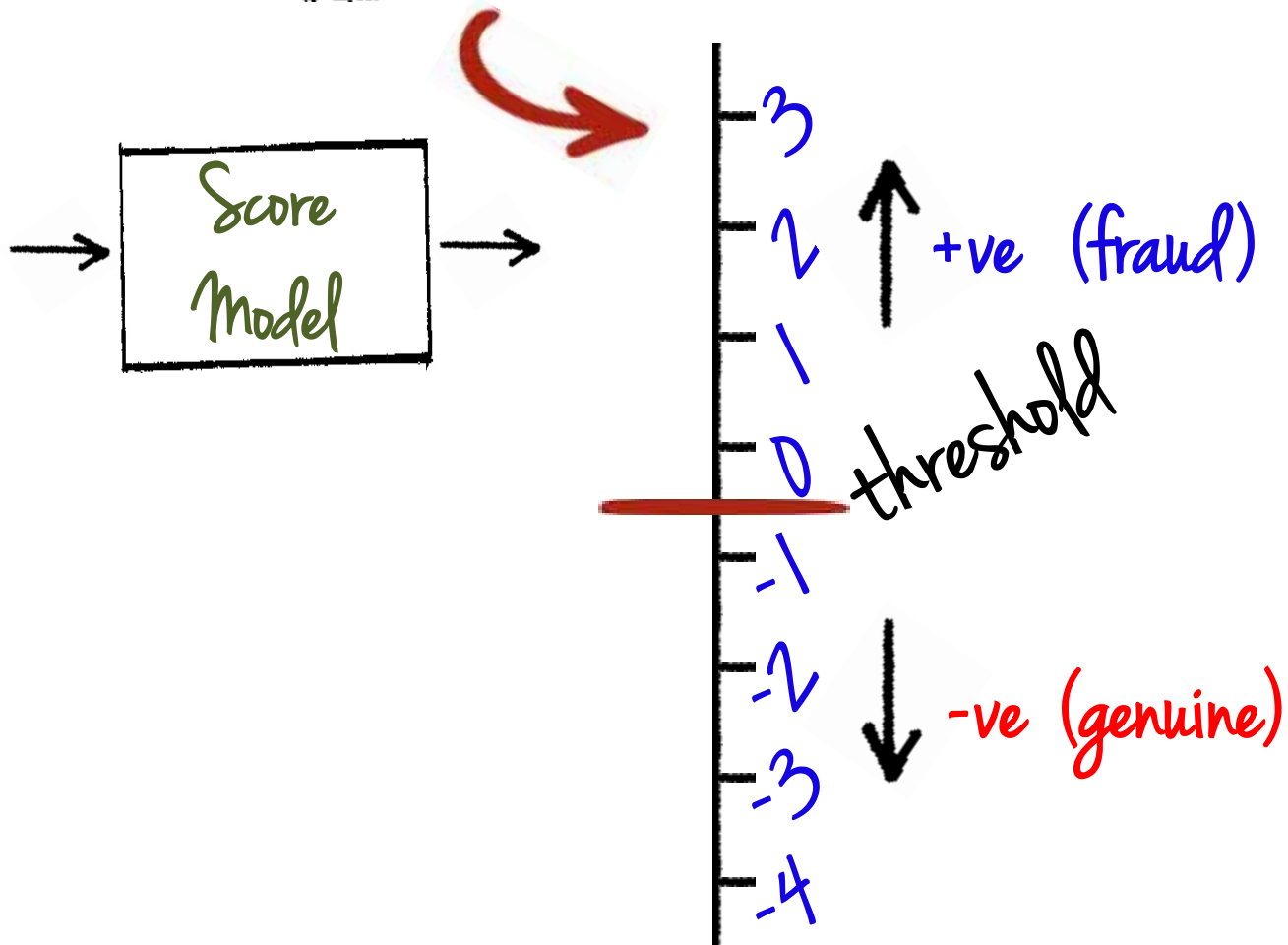
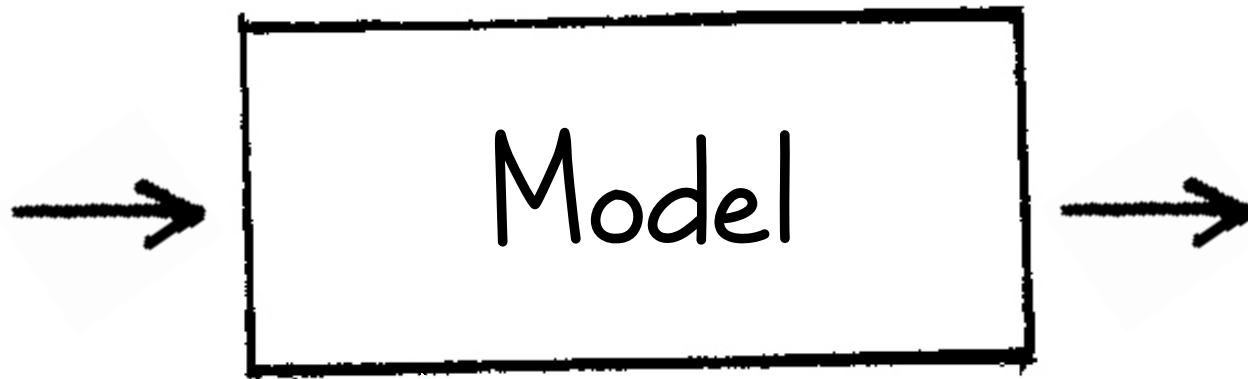
disease or  
no disease

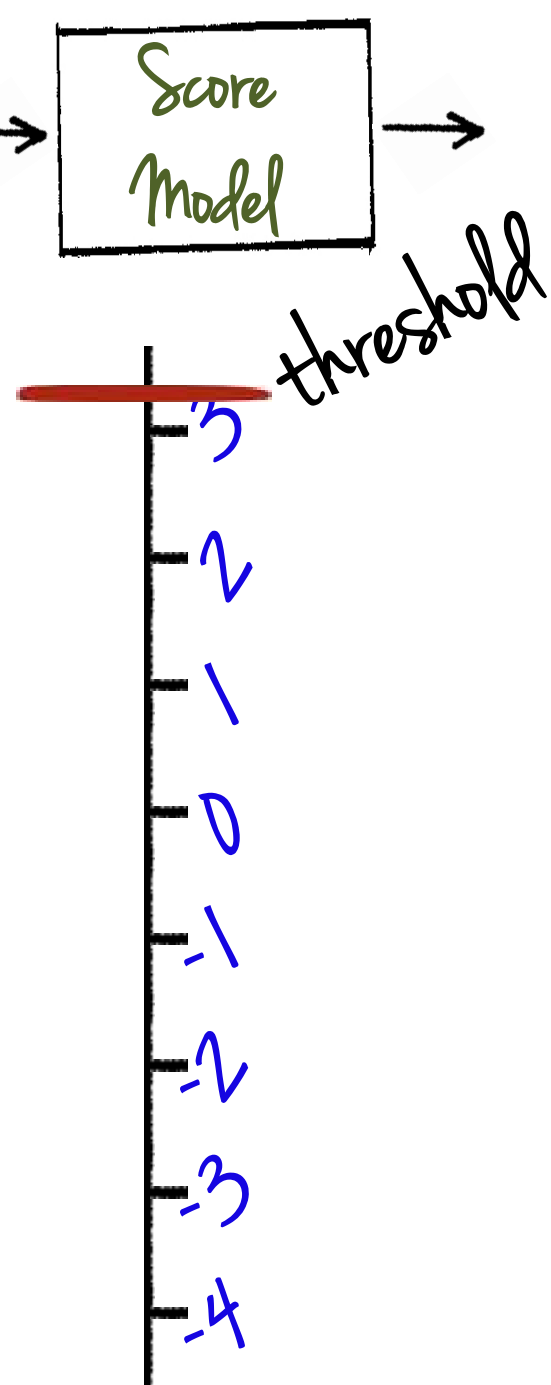


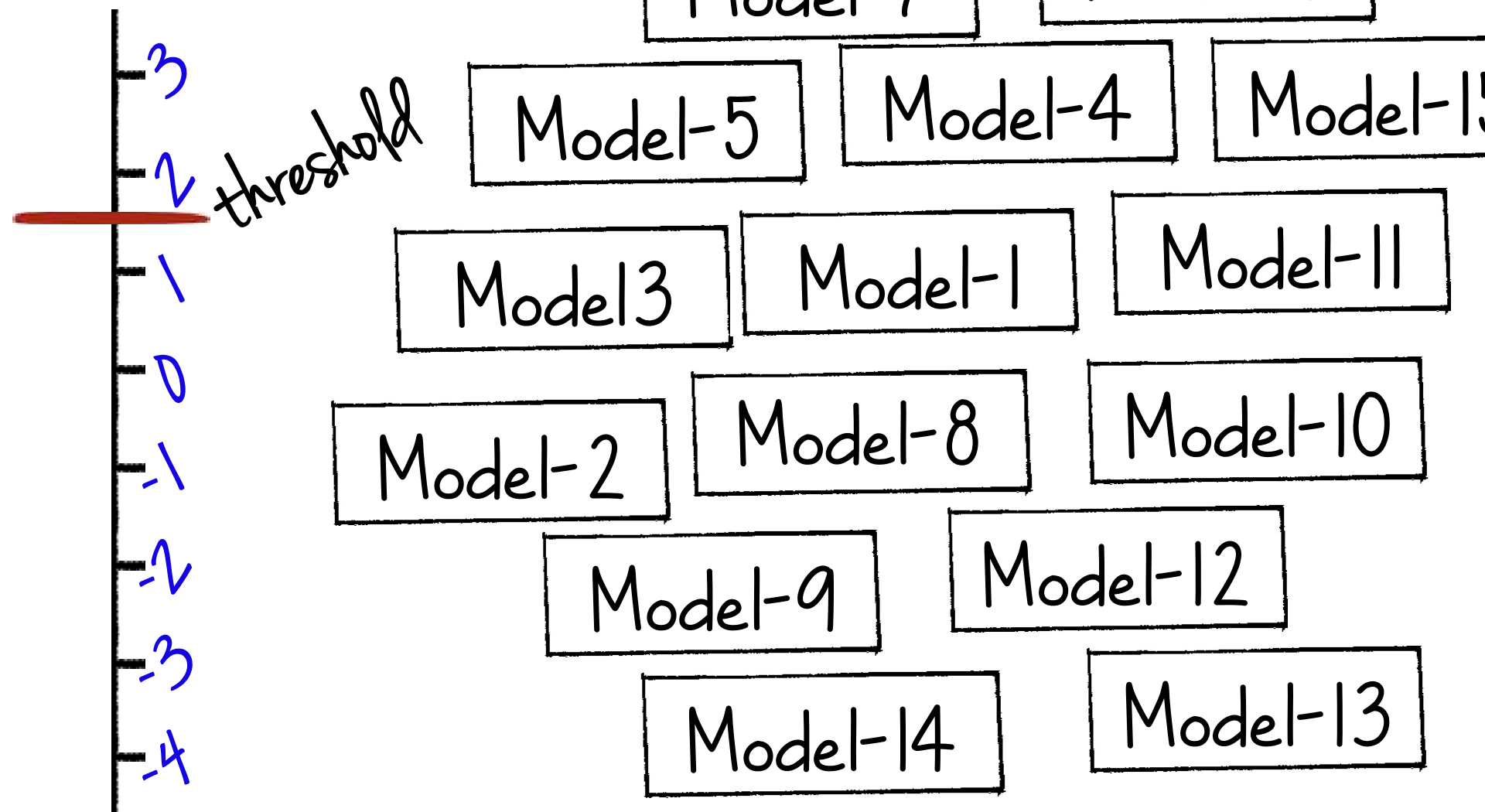


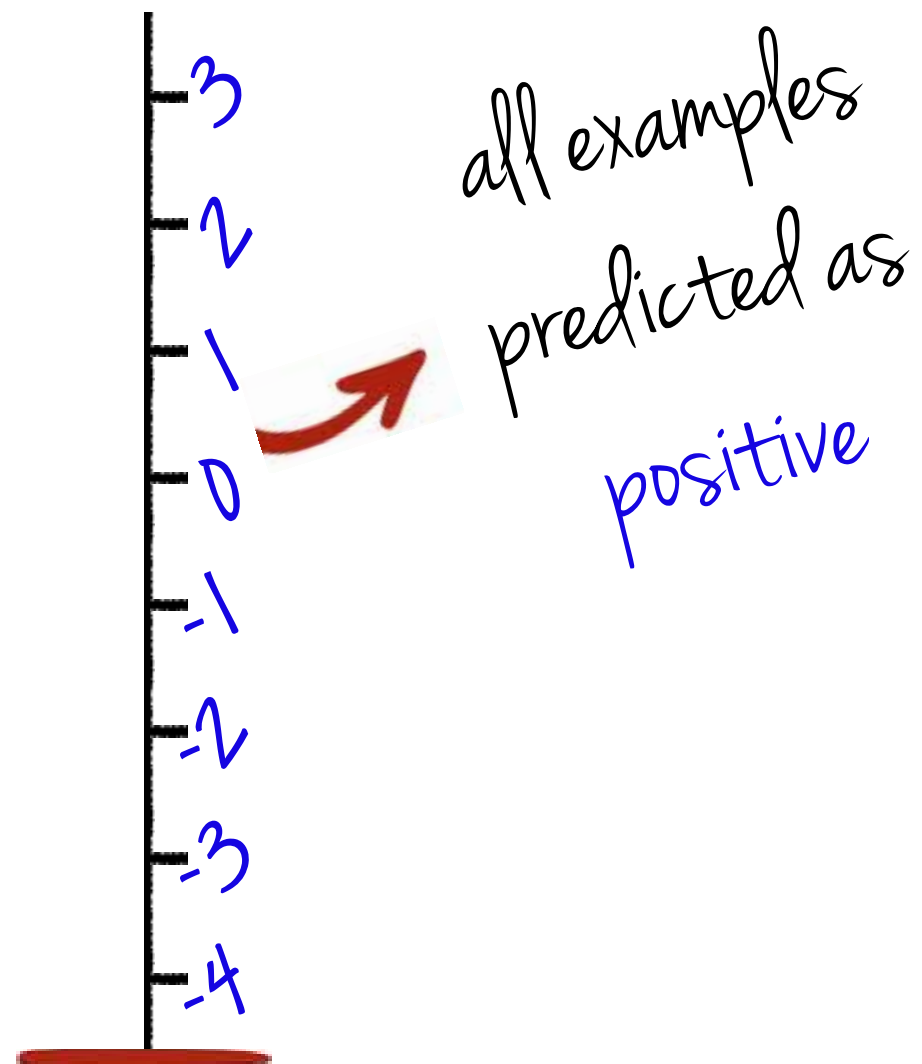
Fraud or  
Genuine?

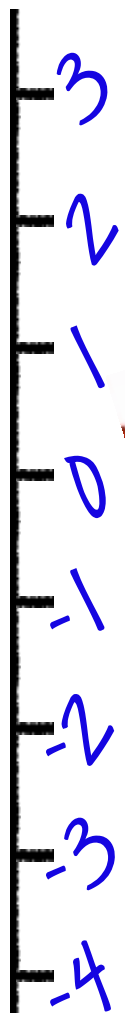












all examples  
predicted as

positive

Positive  
(Fraud)

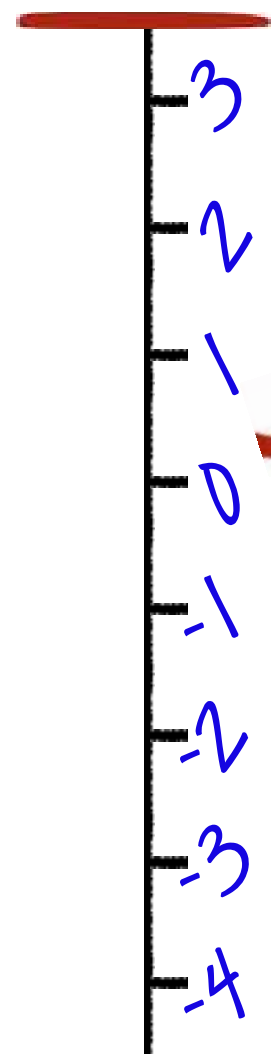
Negative  
(Genuine)

Positive

Negative

Maximum  
True Positive  
Rate

Maximum  
False Positive  
Rate



all examples  
predicted as

negative

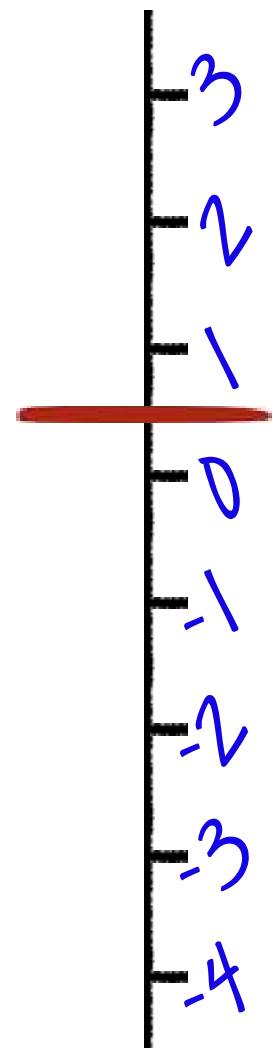
Positive  
(Fraud)

Negative  
(Genuine)

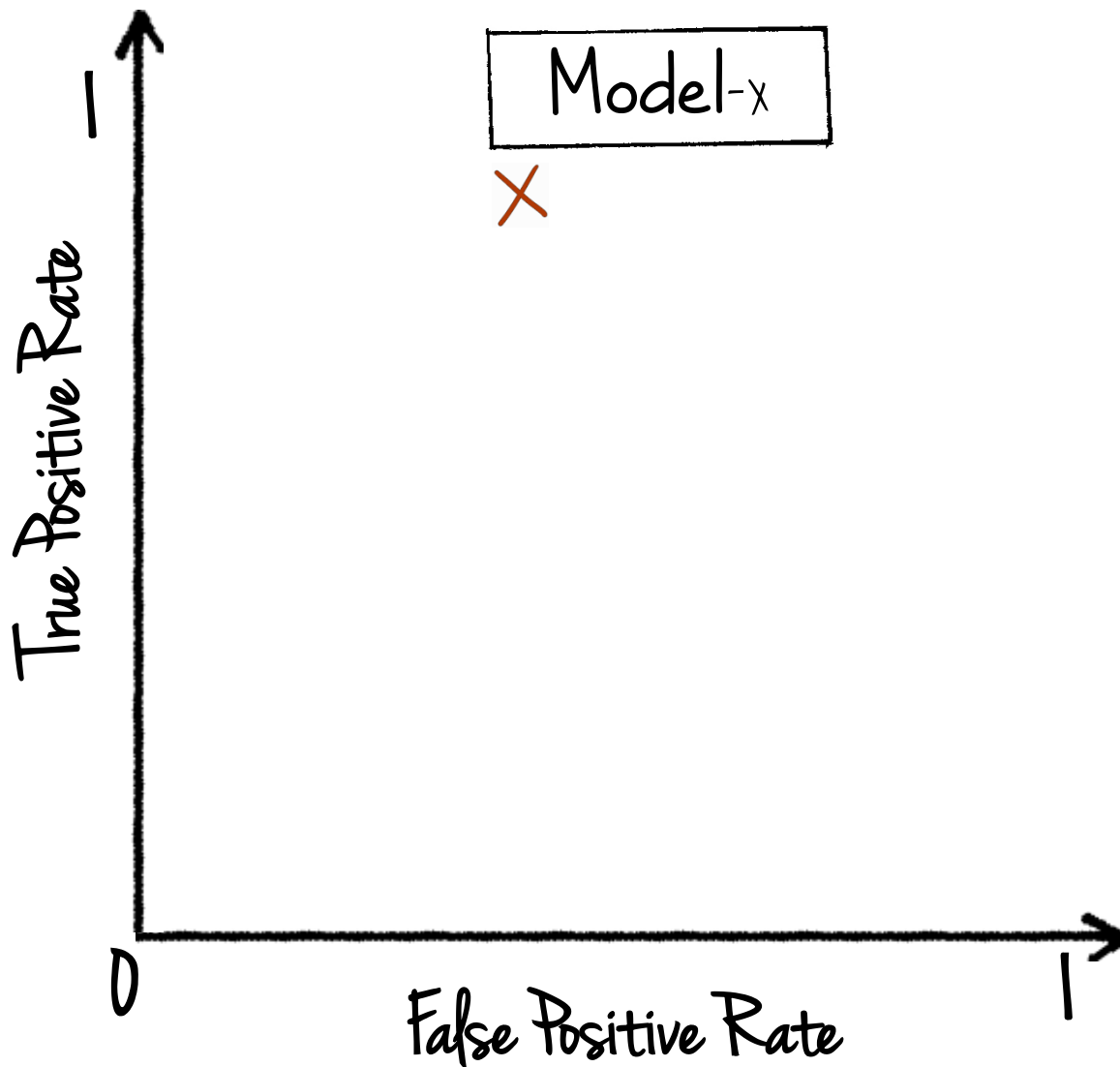
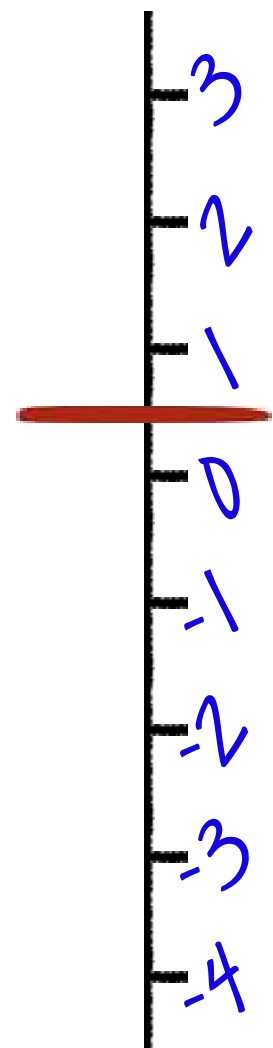
Positive

Negative

| Positive                       | Negative |
|--------------------------------|----------|
| Zero<br>True Positive<br>Rate  |          |
| Zero<br>False Positive<br>Rate |          |



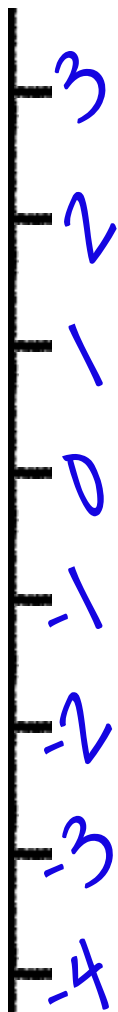
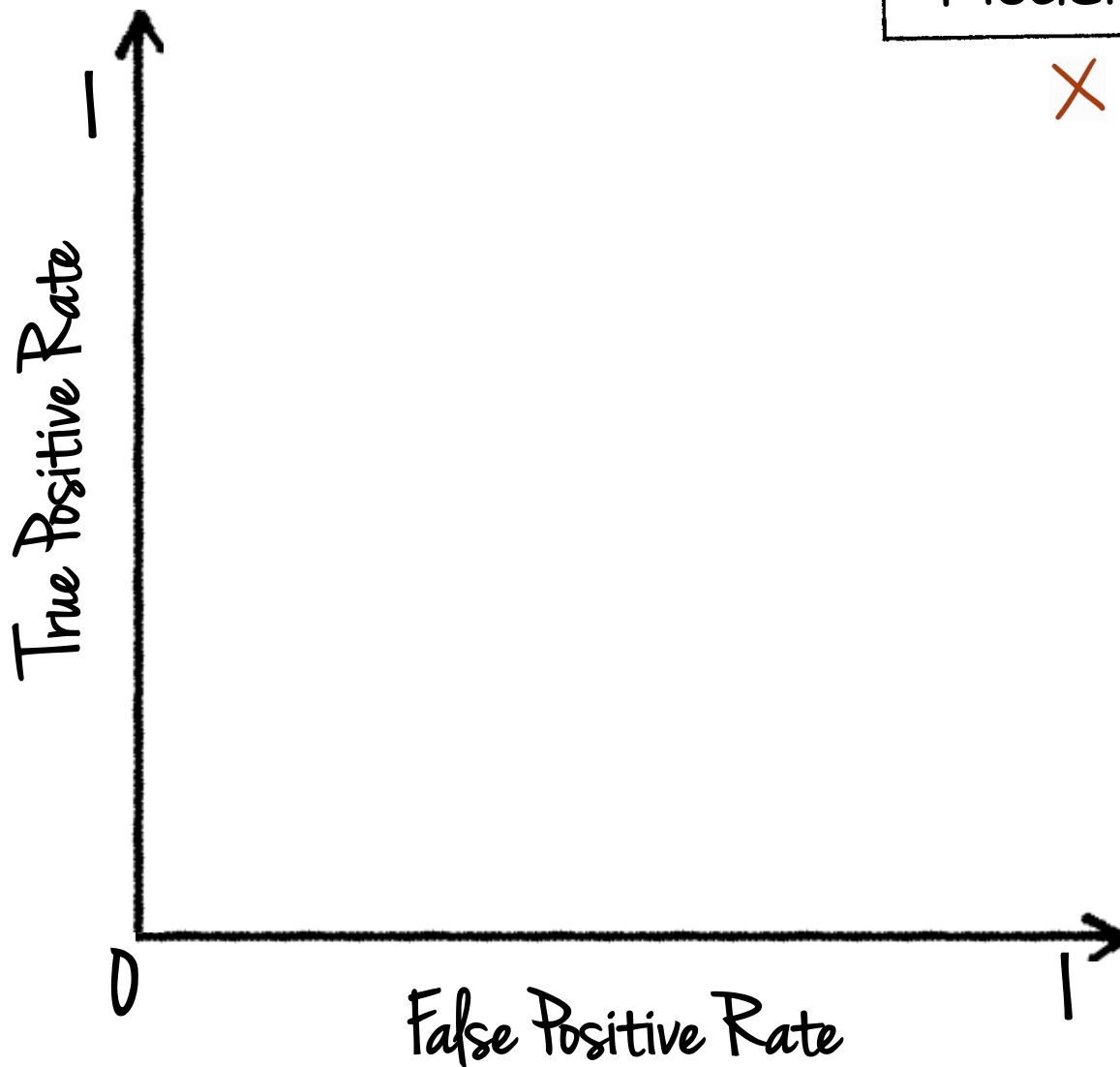
|                    | Positive | Negative |
|--------------------|----------|----------|
| Positive (Fraud)   | ?        |          |
| Negative (Genuine) | ?        |          |

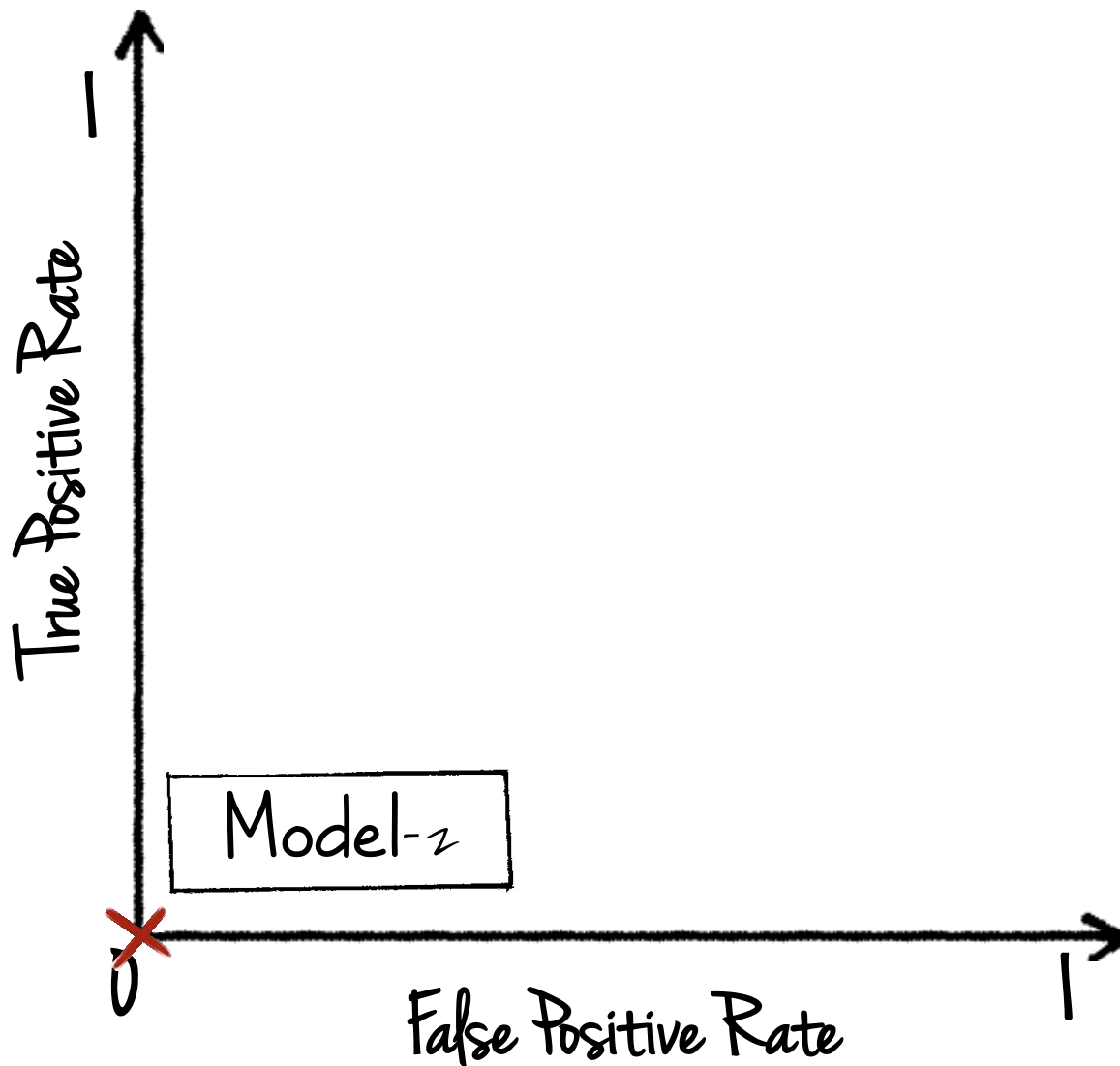
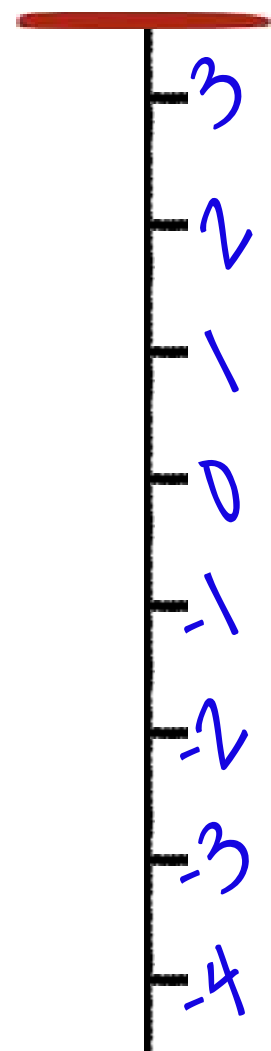


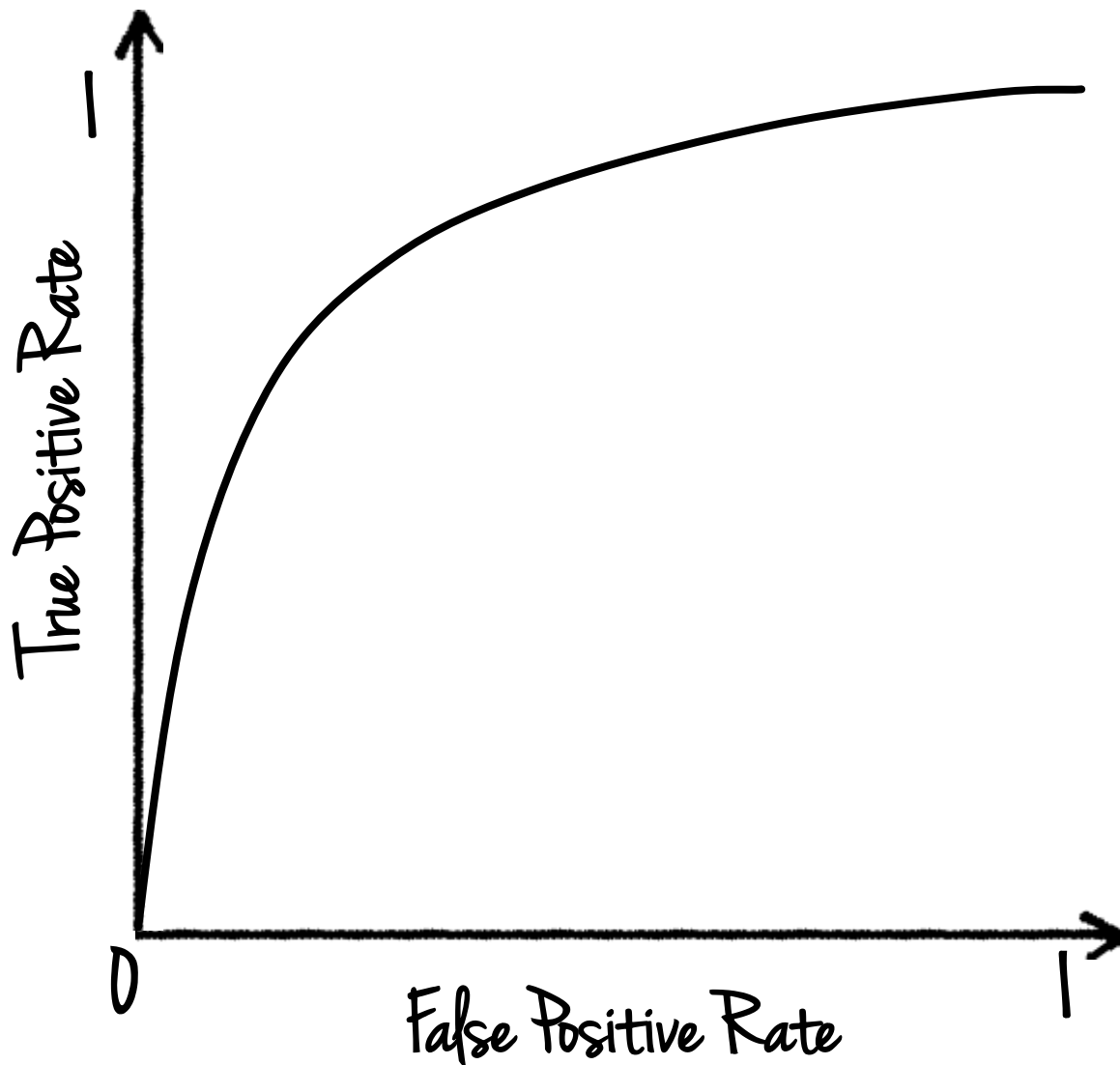
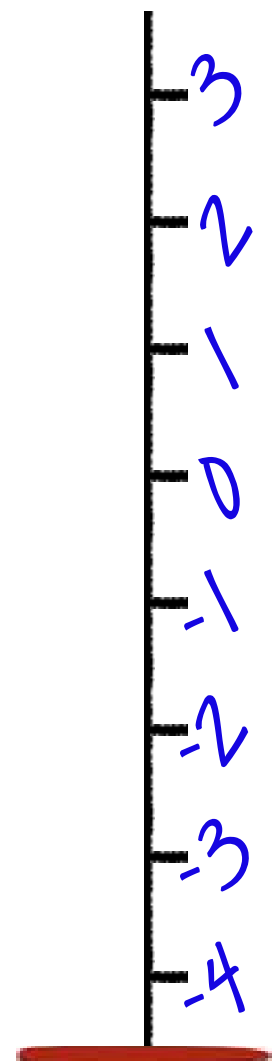


Model-y

X

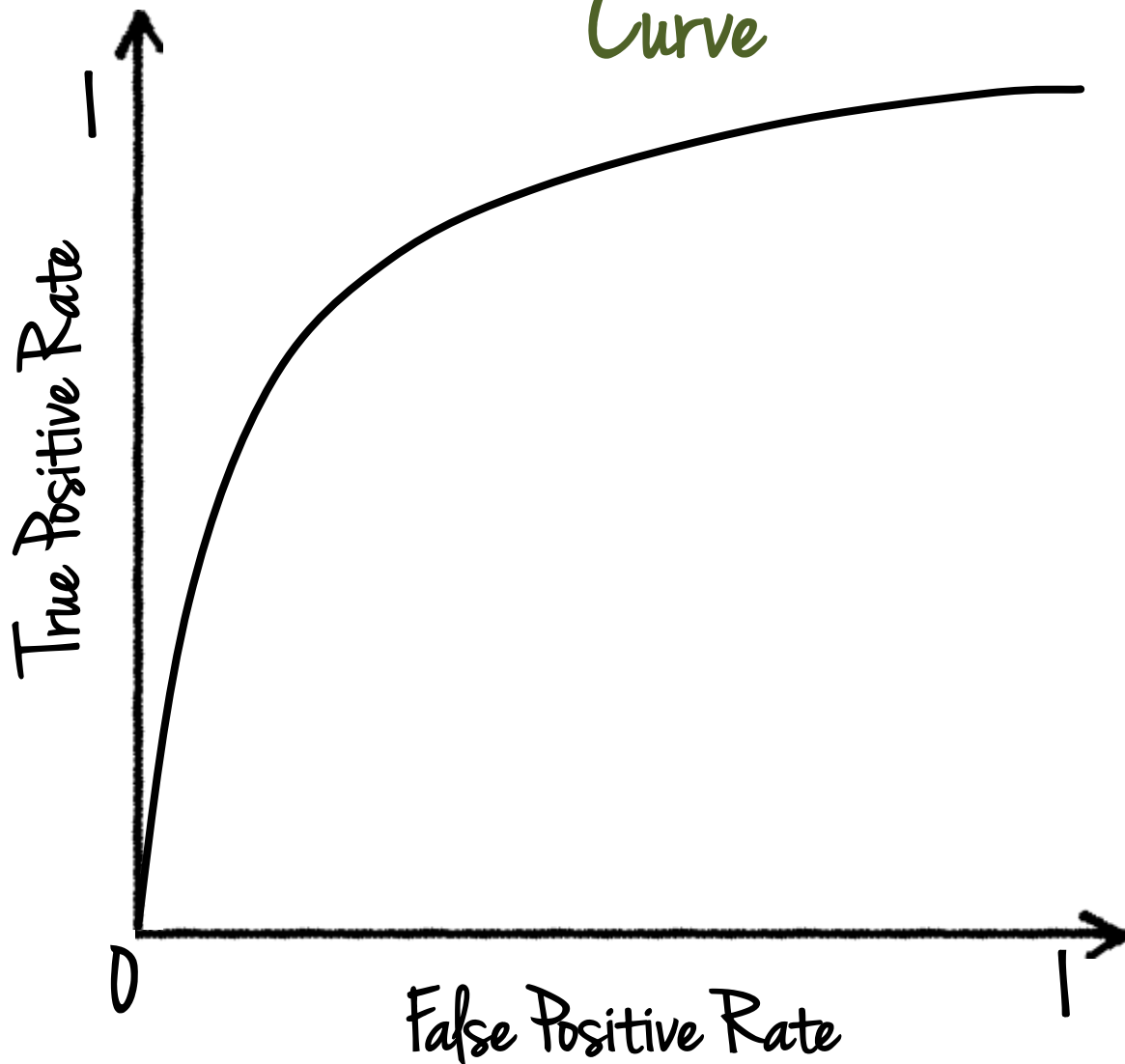








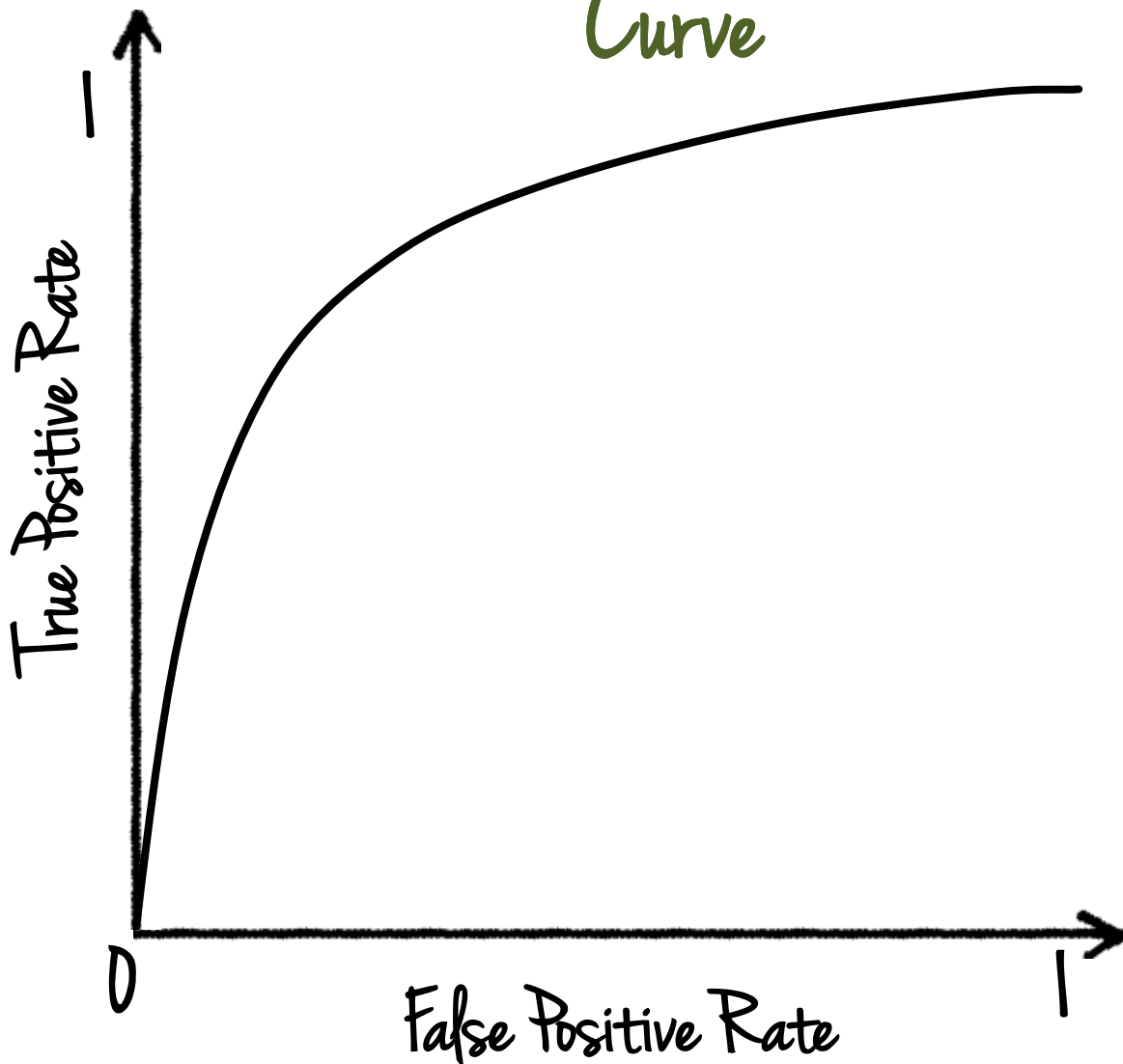
# Receiver Operating Characteristic Curve



3  
2  
1  
0  
-1  
-2  
-3  
-4



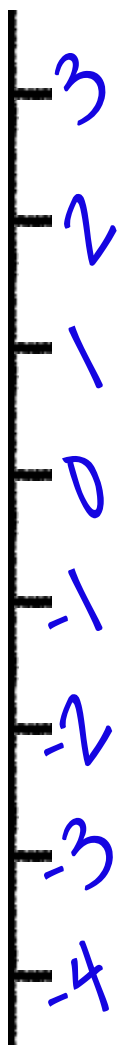
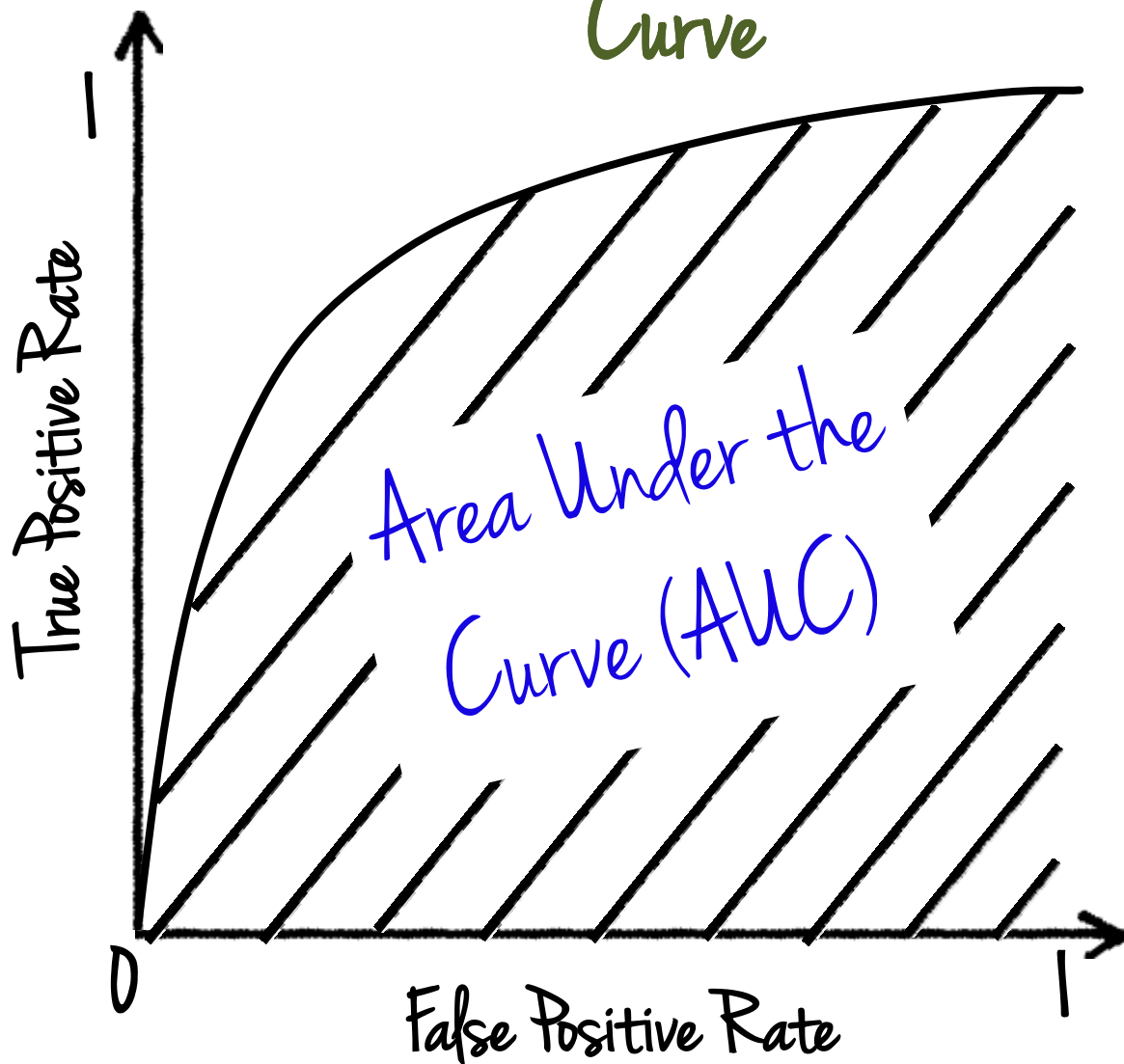
# Receiver Operating Characteristic Curve



3  
2  
1  
0  
-1  
-2  
-3  
-4

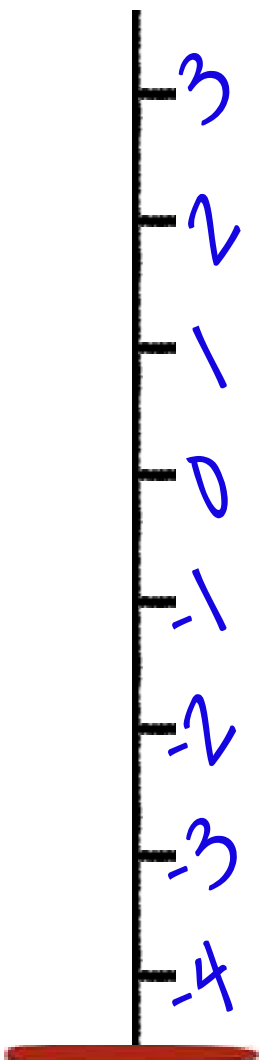
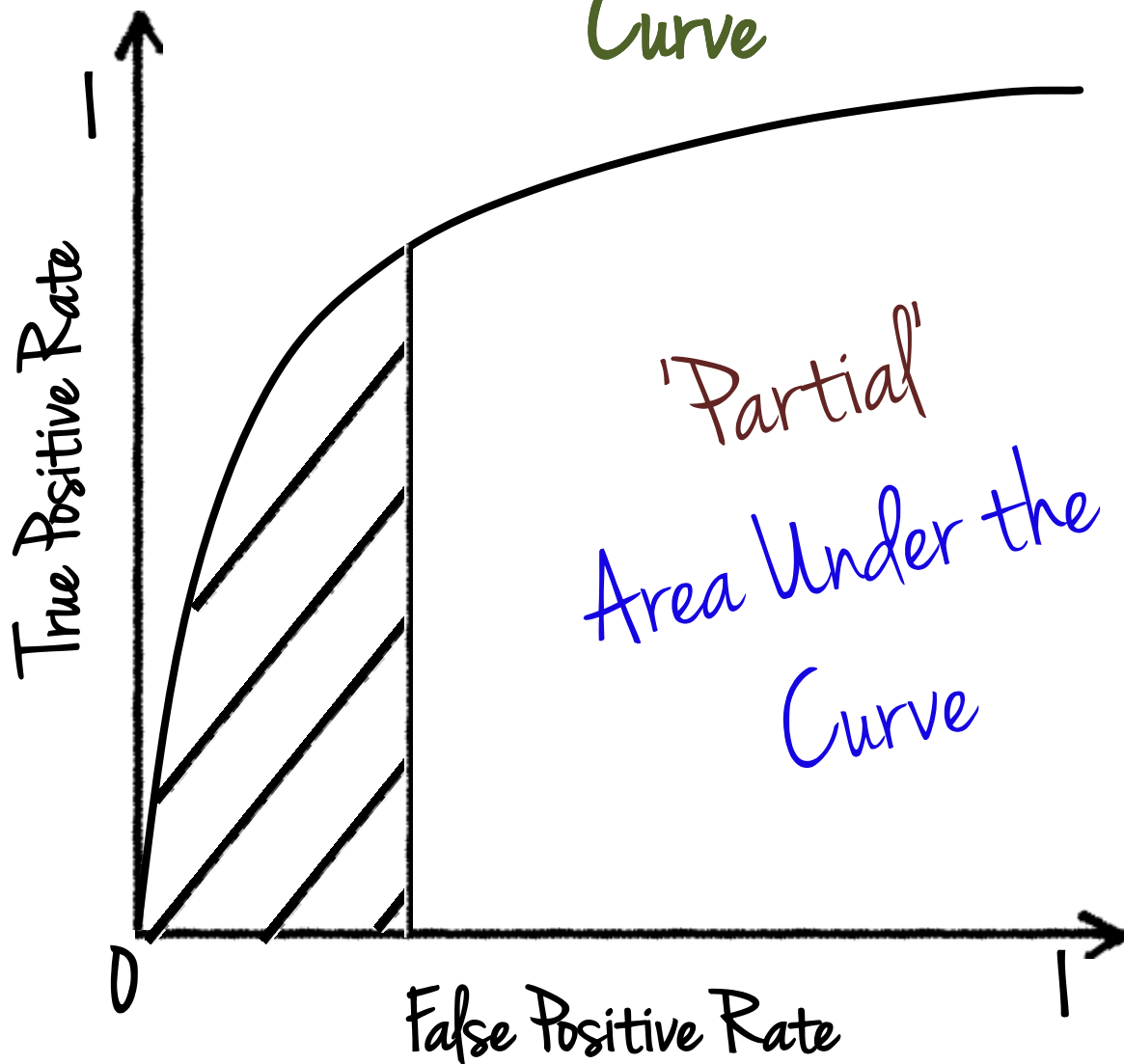


# Receiver Operating Characteristic Curve



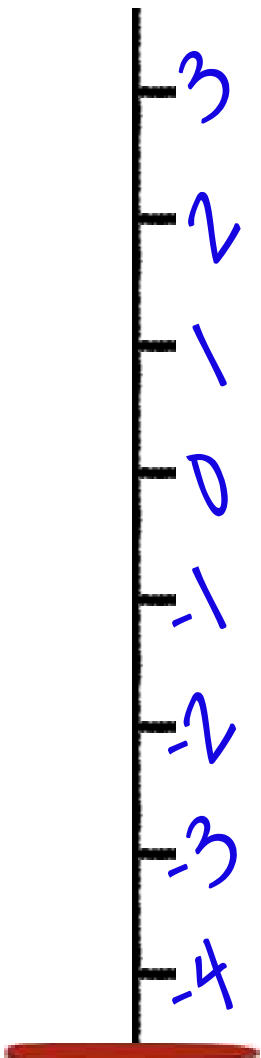
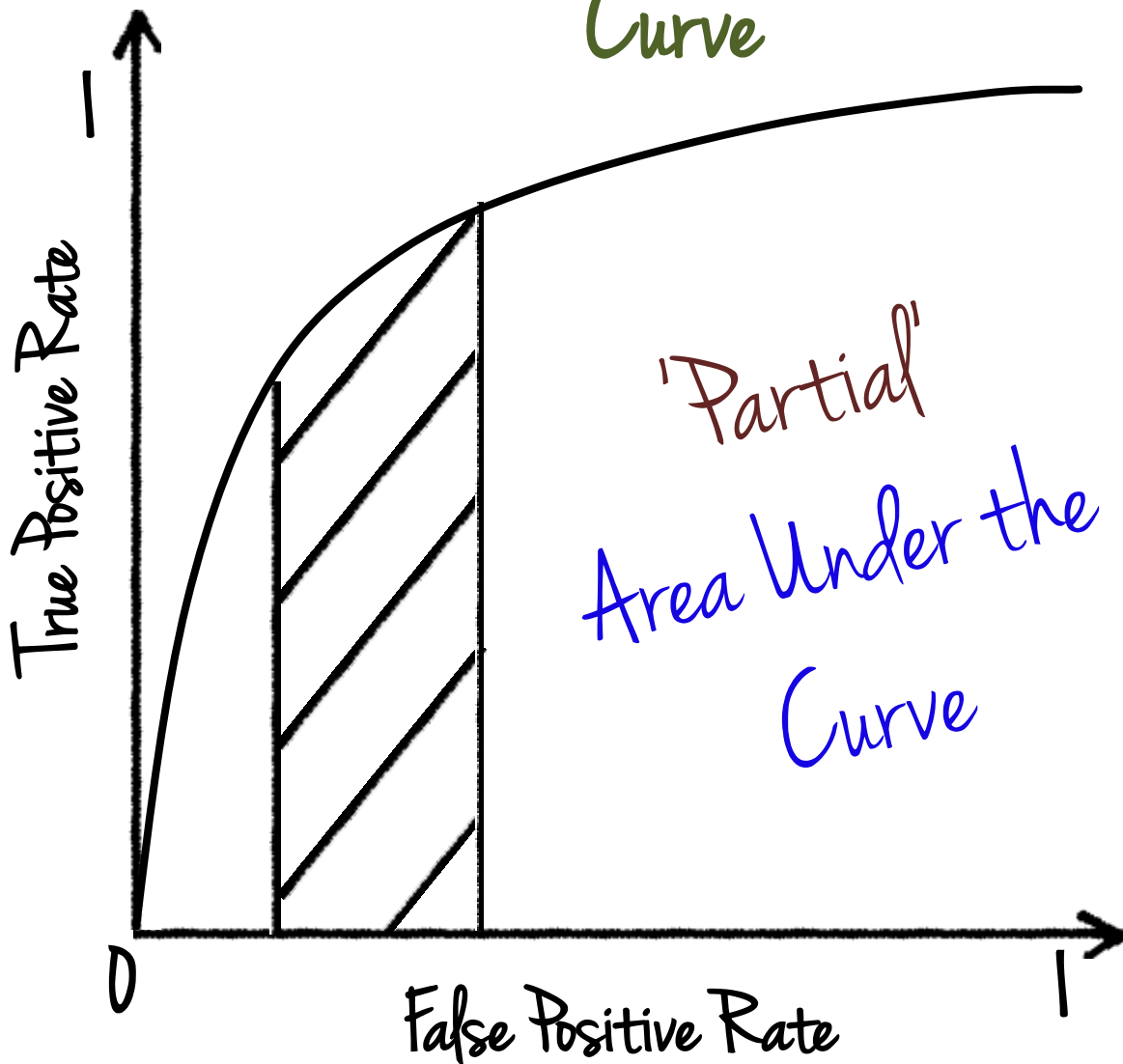


# Receiver Operating Characteristic Curve

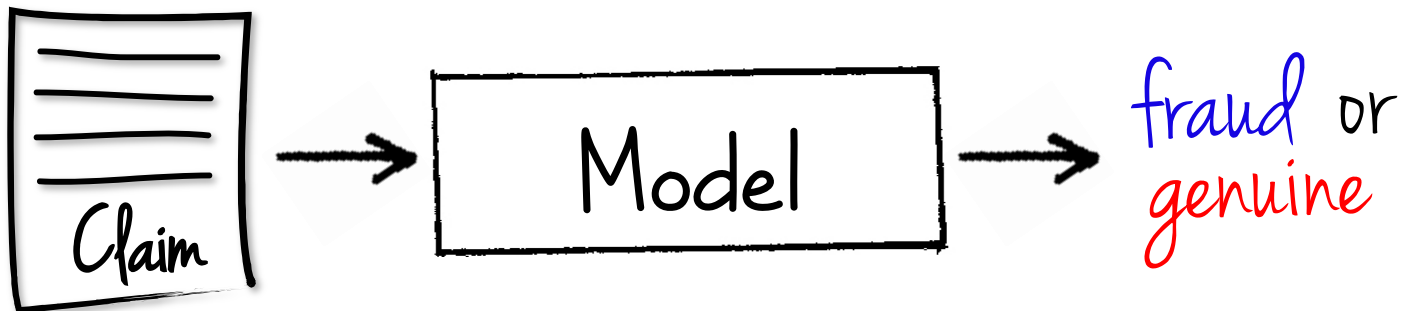




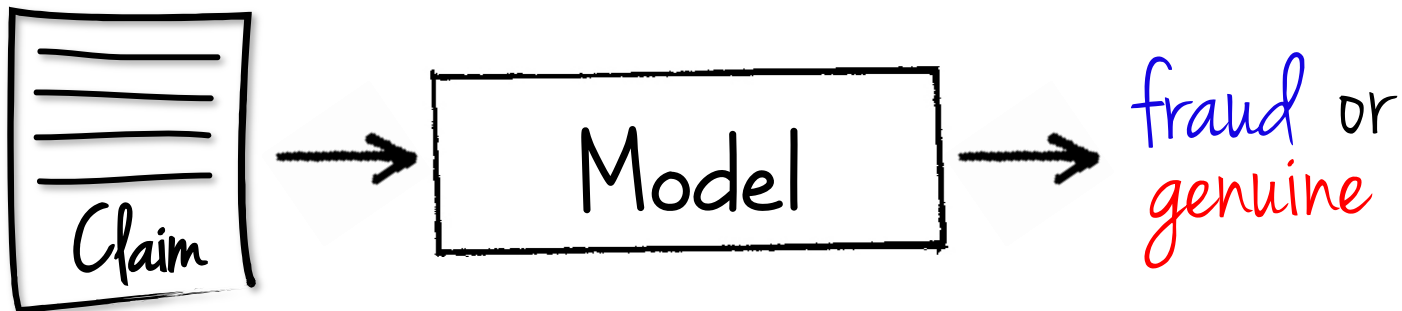
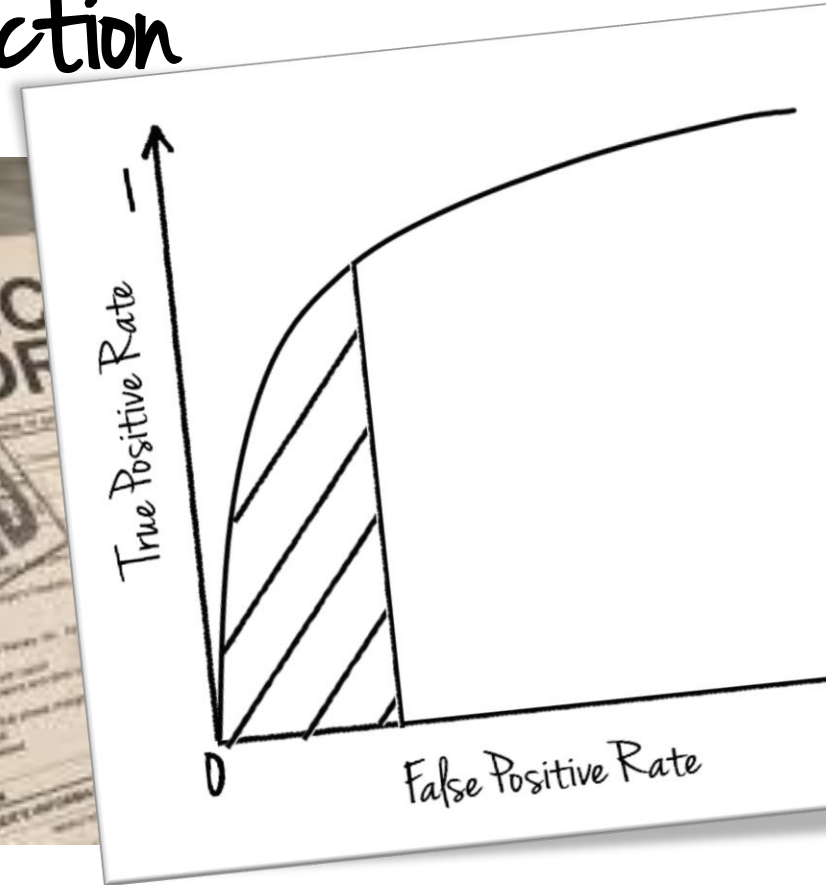
# Receiver Operating Characteristic Curve



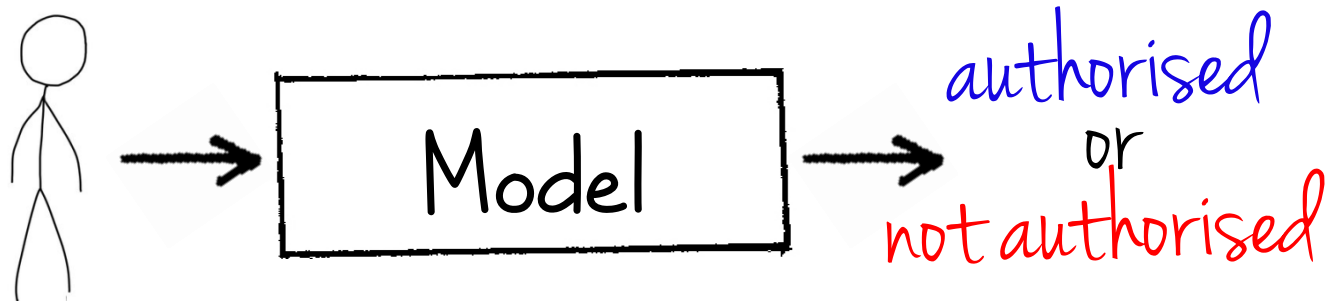
# Fraud Detection



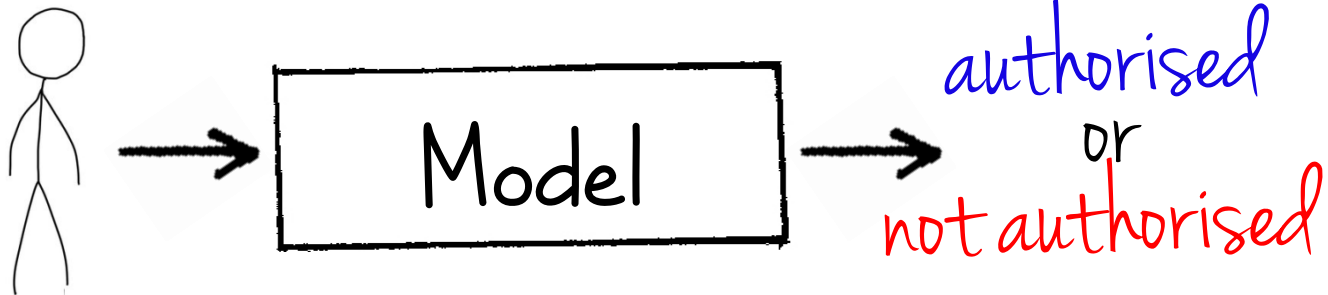
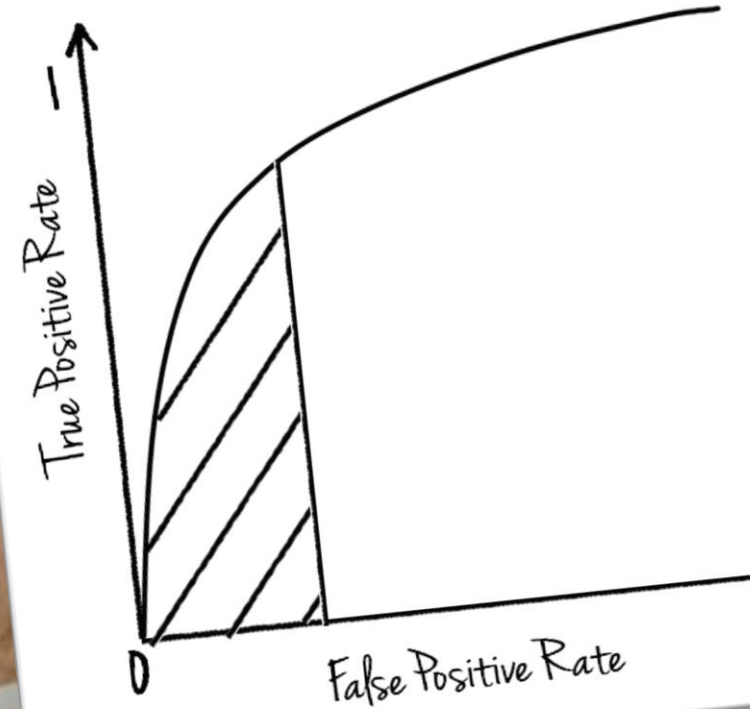
# Fraud Detection



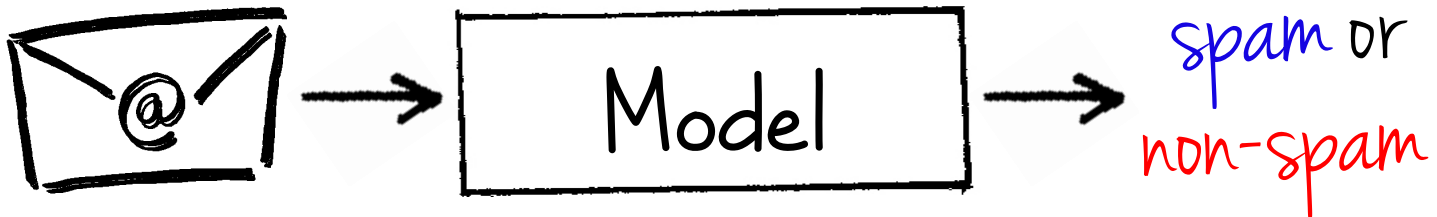
# Biometric Screening



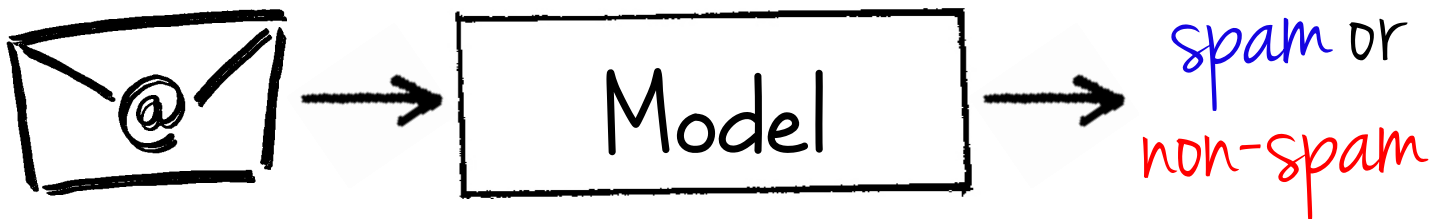
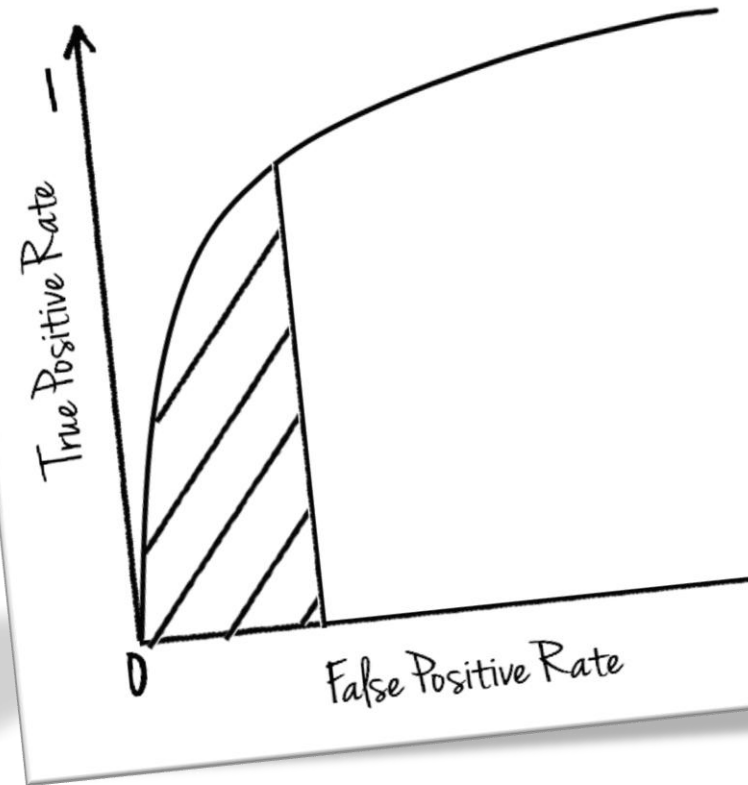
# Biometric Screening



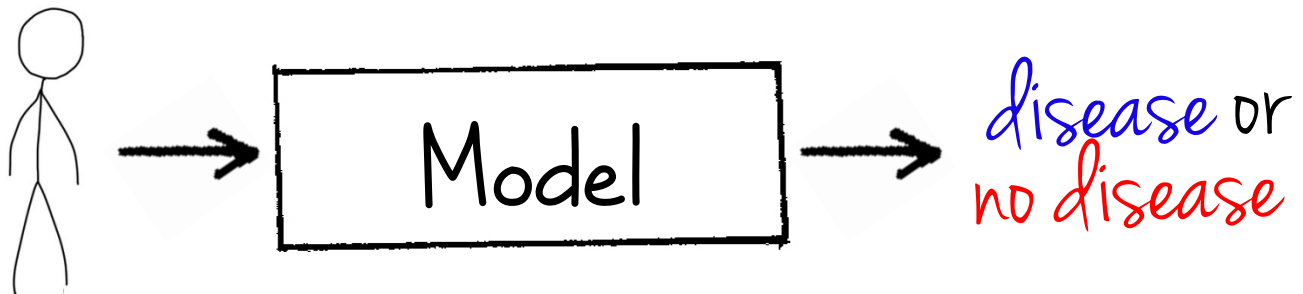
# Spam Filtering



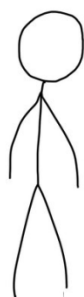
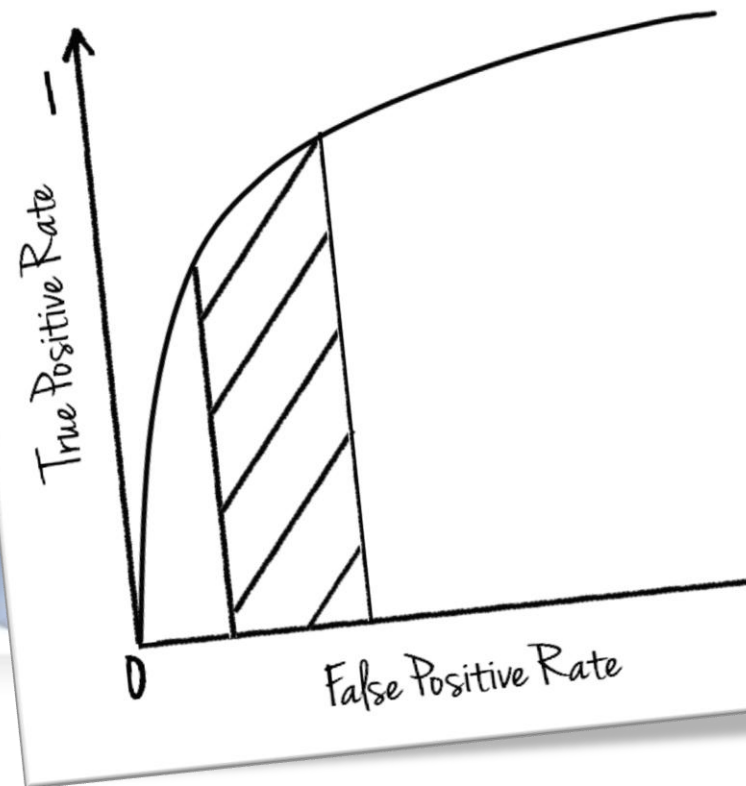
# Spam Filtering



# Medical Diagnosis

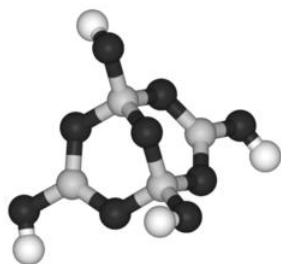
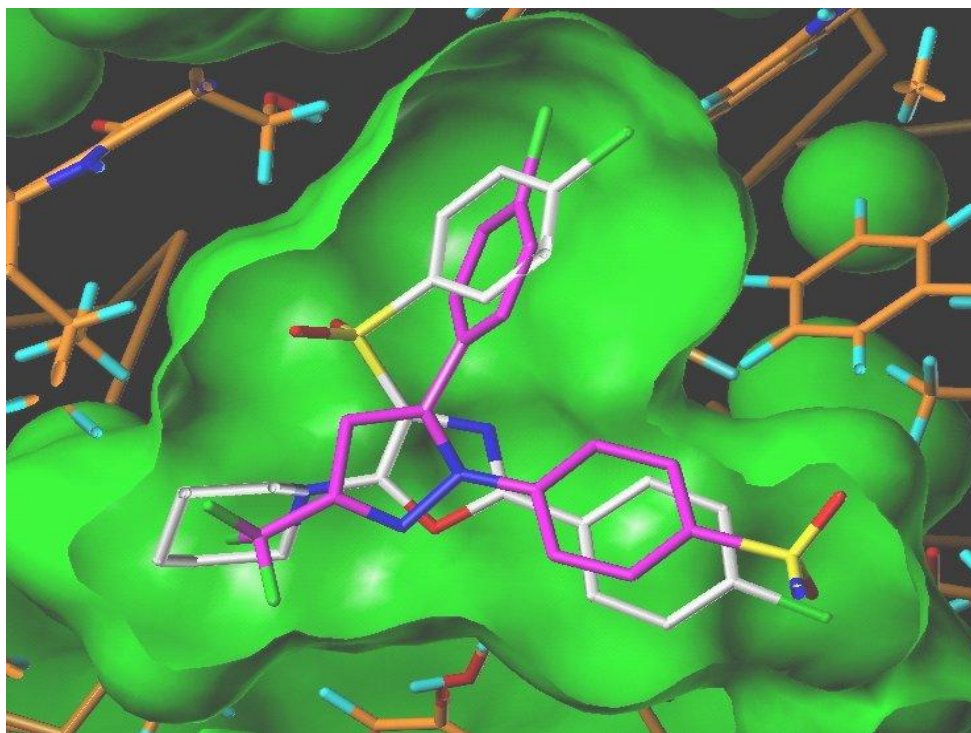


# Medical Diagnosis



disease or  
no disease

# Drug Discovery

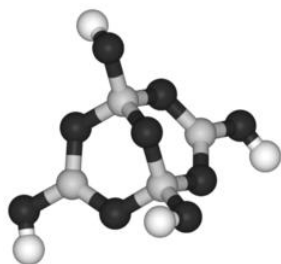
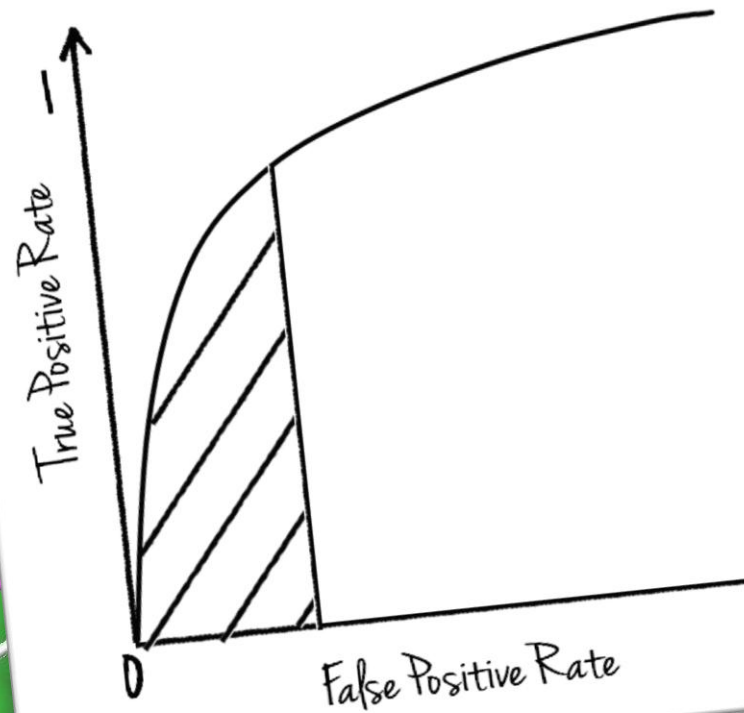
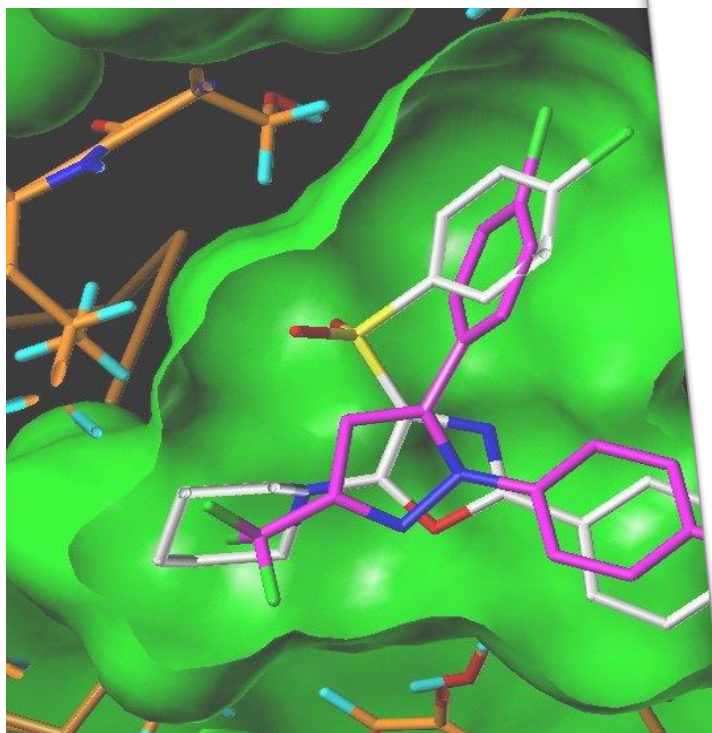


Model



active or  
inactive

# Drug Discovery



Model



active or  
inactive

# Training Set

Claim 1

Genuine

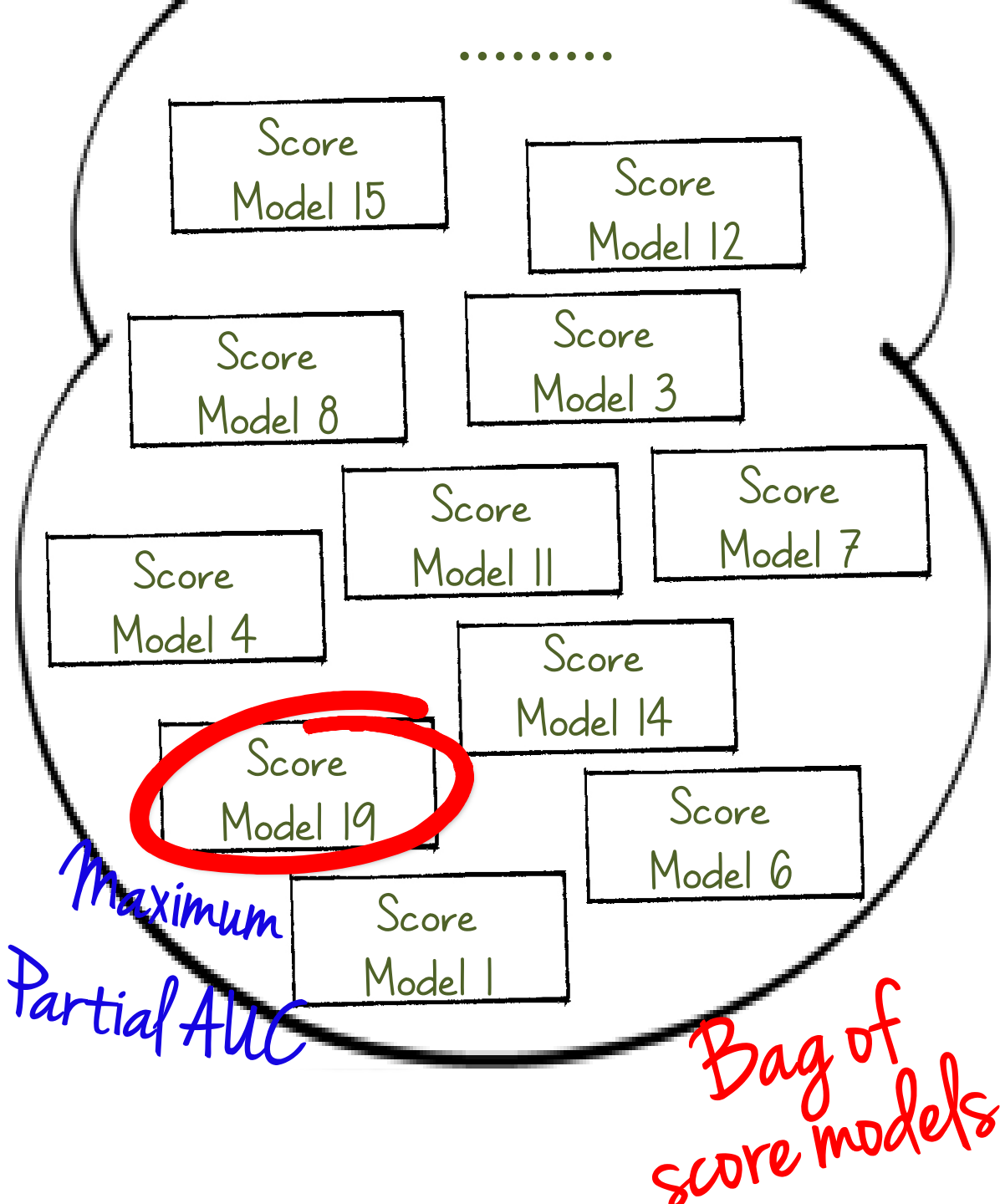
Claim 2

Fraud

.....

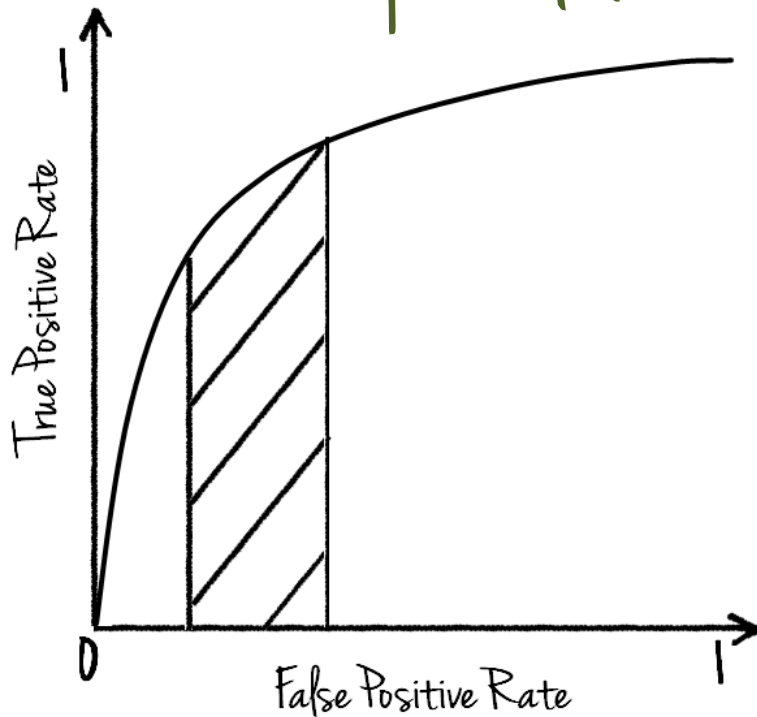
Claim N

Genuine



# Optimization Problem

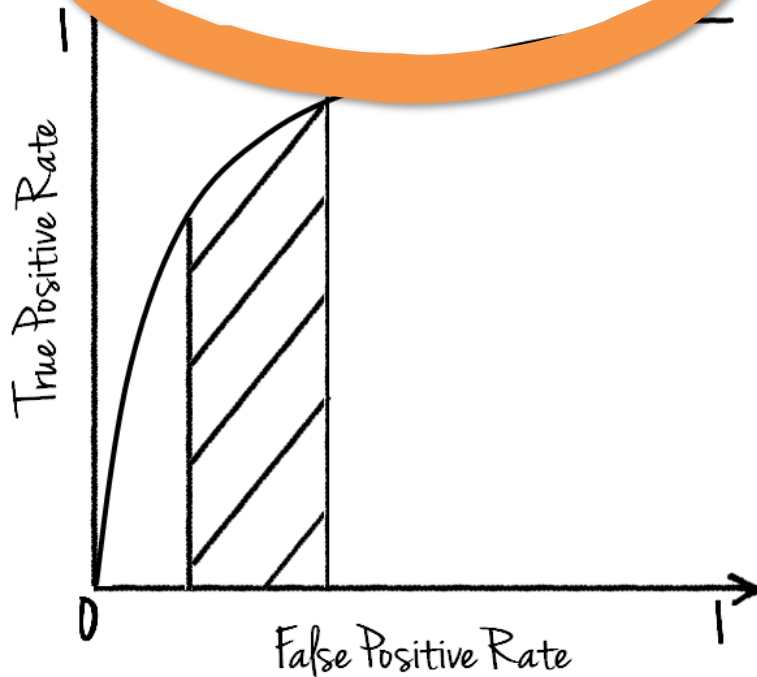
find score model with  
maximum 'partial AUC'



# Optimization Problem

find score model with  
maximum 'partial AUC'

Intractable /  
Hard



Proxy  
Optimization  
Problem

(using structural SVMs)

# Proxy Optimization Problem

(using structural SVMs)

maximize { 'partial AUC' }

# Proxy Optimization Problem

(using structural SVMs)

~~maximize { 'partial AUC' }~~

maximize { an approximation of 'partial AUC' }

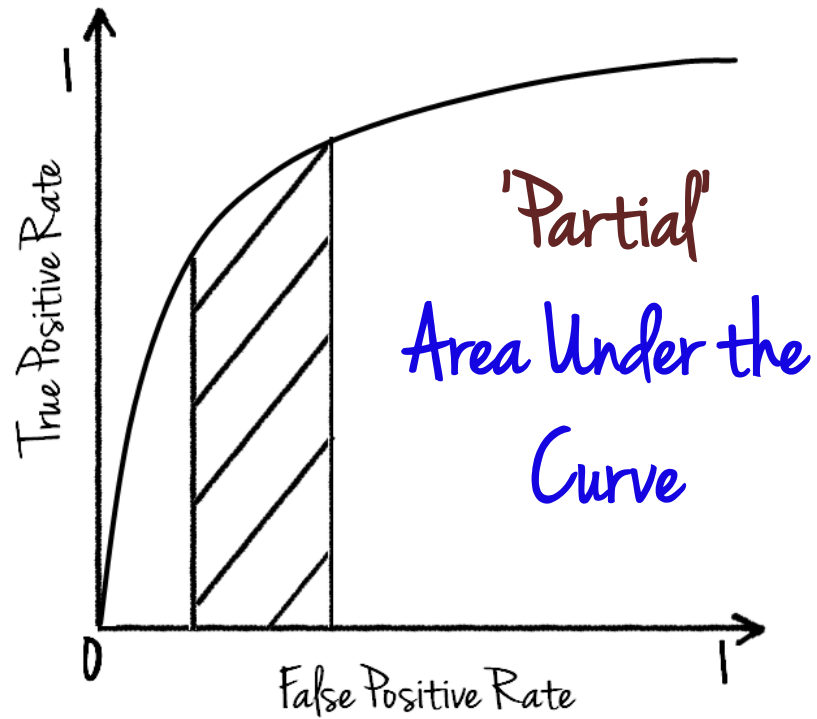
SVM<sub>p</sub>AUC-struct (ICML 2013)

SVM<sub>p</sub>AUC-tight (KDD 2013)

Narasimhan, H. and Agarwal, S. "A structural SVM based approach for optimizing partial AUC", ICML 2013.

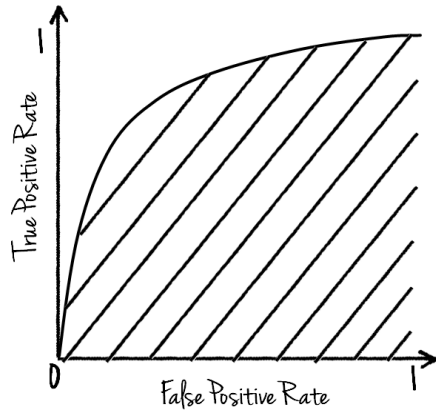
Narasimhan, H. and Agarwal, S. "SVM<sub>p</sub>AUC<sup>tight</sup>: A new support vector method for optimizing partial AUC based on a tight convex upper bound", KDD 2013.

# Experiments

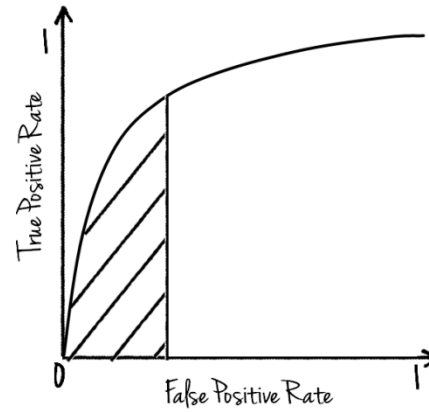


# Experimental Results

- Baseline Methods:
  - Method for 'Full AUC' (Joachims, 2005)

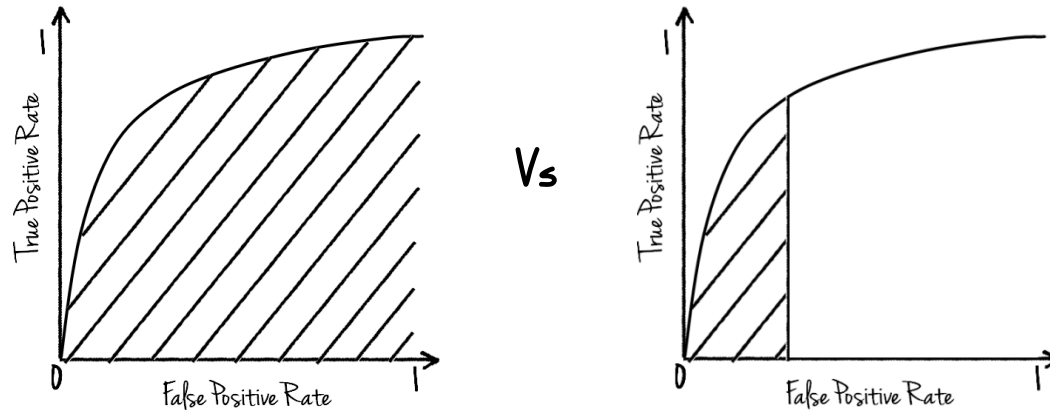


Vs



# Experimental Results

- Baseline Methods:
  - Method for 'Full AUC' (Joachims, 2005)

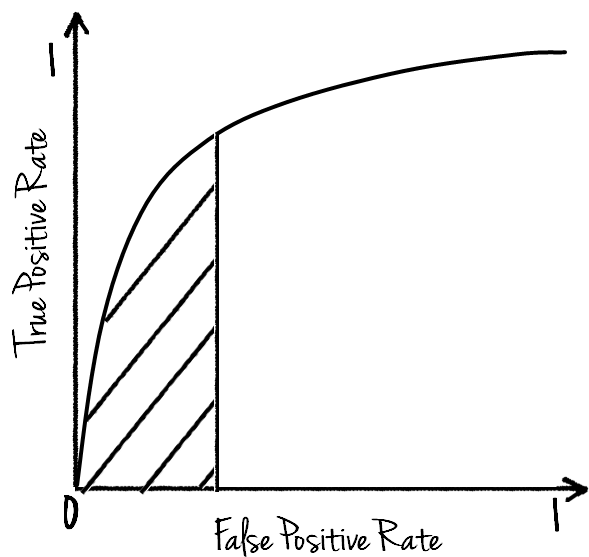


- Baseline 1 (Wu et al., 2008)
- Baseline 2 (Komori & Eguchi, 2010)
- Baseline 3 (Ricamato & Tortorella, 2011)

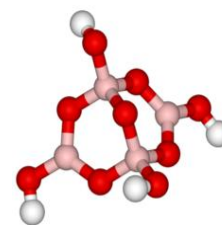
# Experimental Results

## Drug Discovery

50 active compounds / 2092 inactive compounds



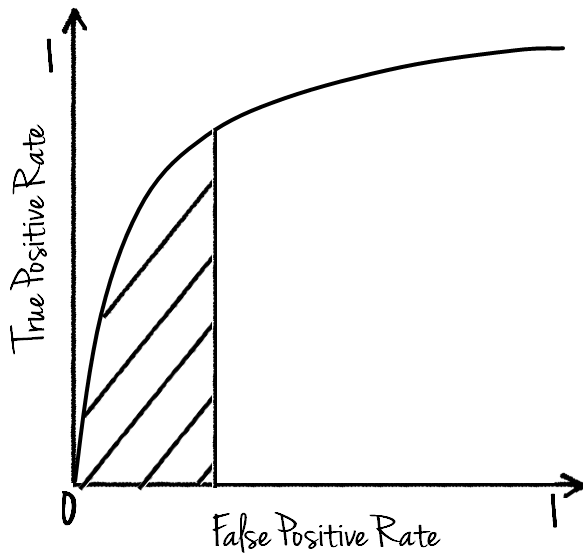
|                    | Partial AUC<br>in [0, 0.1] |
|--------------------|----------------------------|
| Partial AUC Method | <b>65.25</b>               |
| Full AUC Method    | 62.64                      |
| Baseline 1         | 63.80                      |
| Baseline 2         | 43.89                      |
| Baseline 3         | 8.33                       |



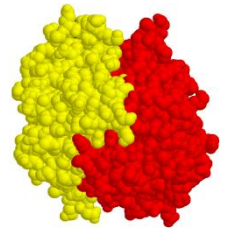
# Experimental Results

## Protein-Protein Interaction Prediction

$\sim 3 \times 10^3$  interacting pairs /  $\sim 2 \times 10^5$  non-interacting pairs



|                    | Partial AUC<br>in [0, 0.1] |
|--------------------|----------------------------|
| Partial AUC Method | <b>51.79</b>               |
| Full AUC Method    | 39.72                      |
| Baseline 1         | 44.51                      |
| Baseline 2         | 48.65                      |
| Baseline 3         | 47.33                      |

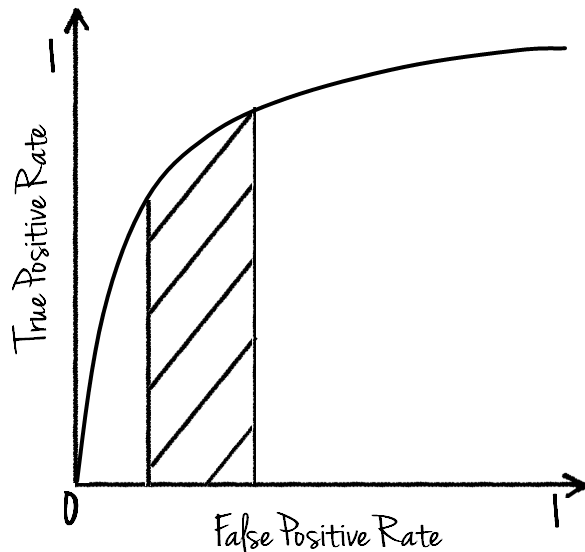


# Experimental Results

KDD Cup 2008

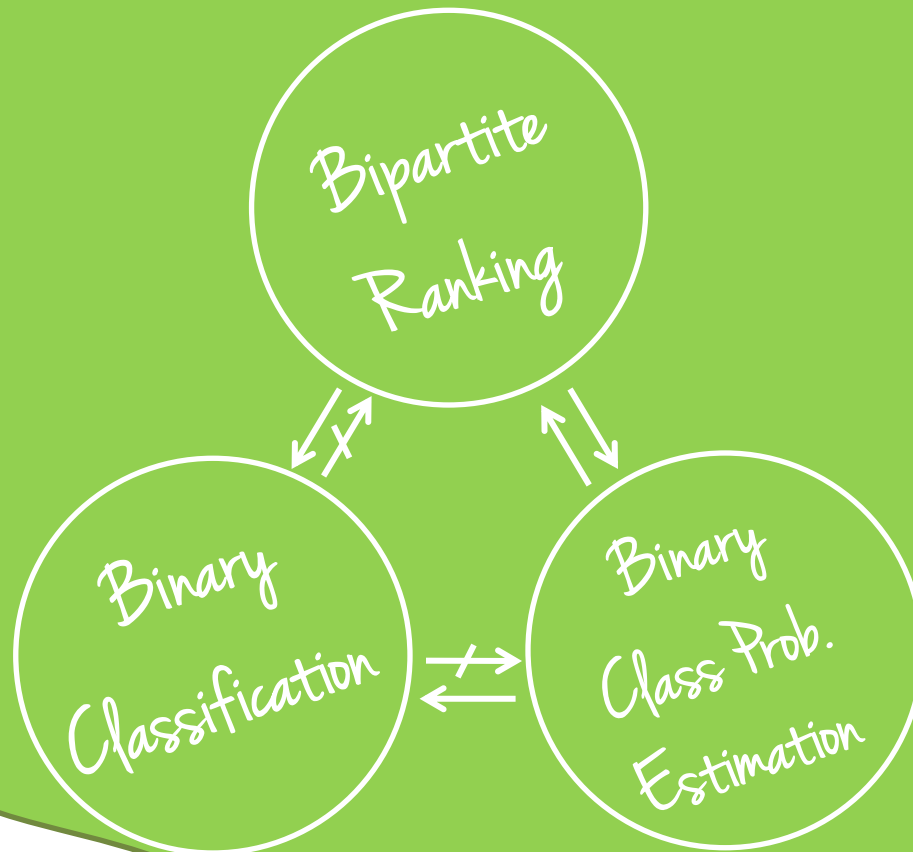
Breast Cancer Detection

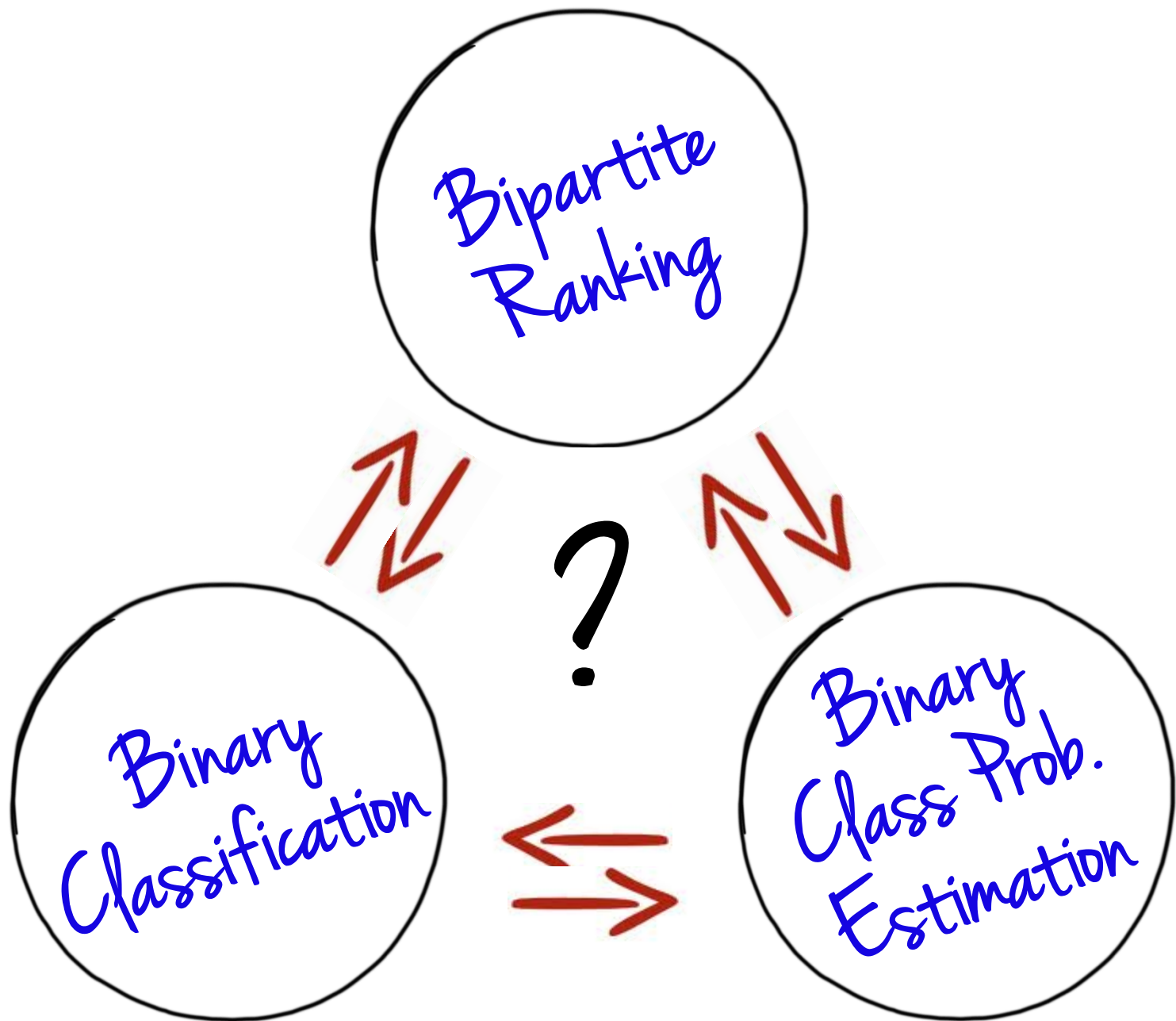
$\sim 600$  malignant ROIs /  $\sim 10^5$  benign ROIs

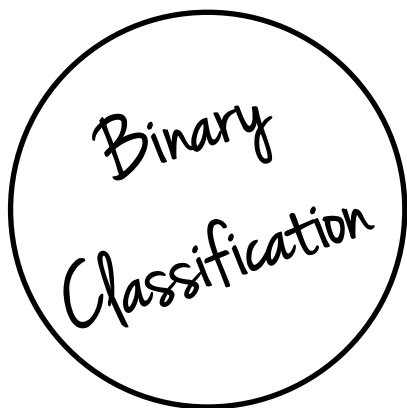


|                    | Partial AUC in<br>[0.2s, 0.3s] |
|--------------------|--------------------------------|
| Partial AUC Method | 51.44                          |
| Full AUC Method    | 50.50                          |
| Baseline 1         | 48.06                          |
| Baseline 2         | 46.99                          |

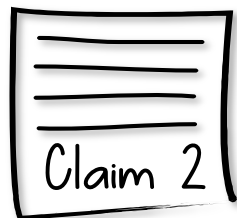
# Algorithms







Genuine



Fraud

.....



Genuine

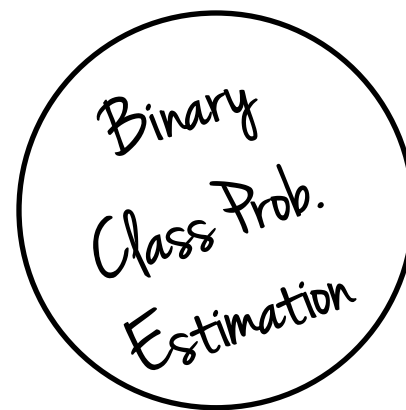


>



>

.....



0.4

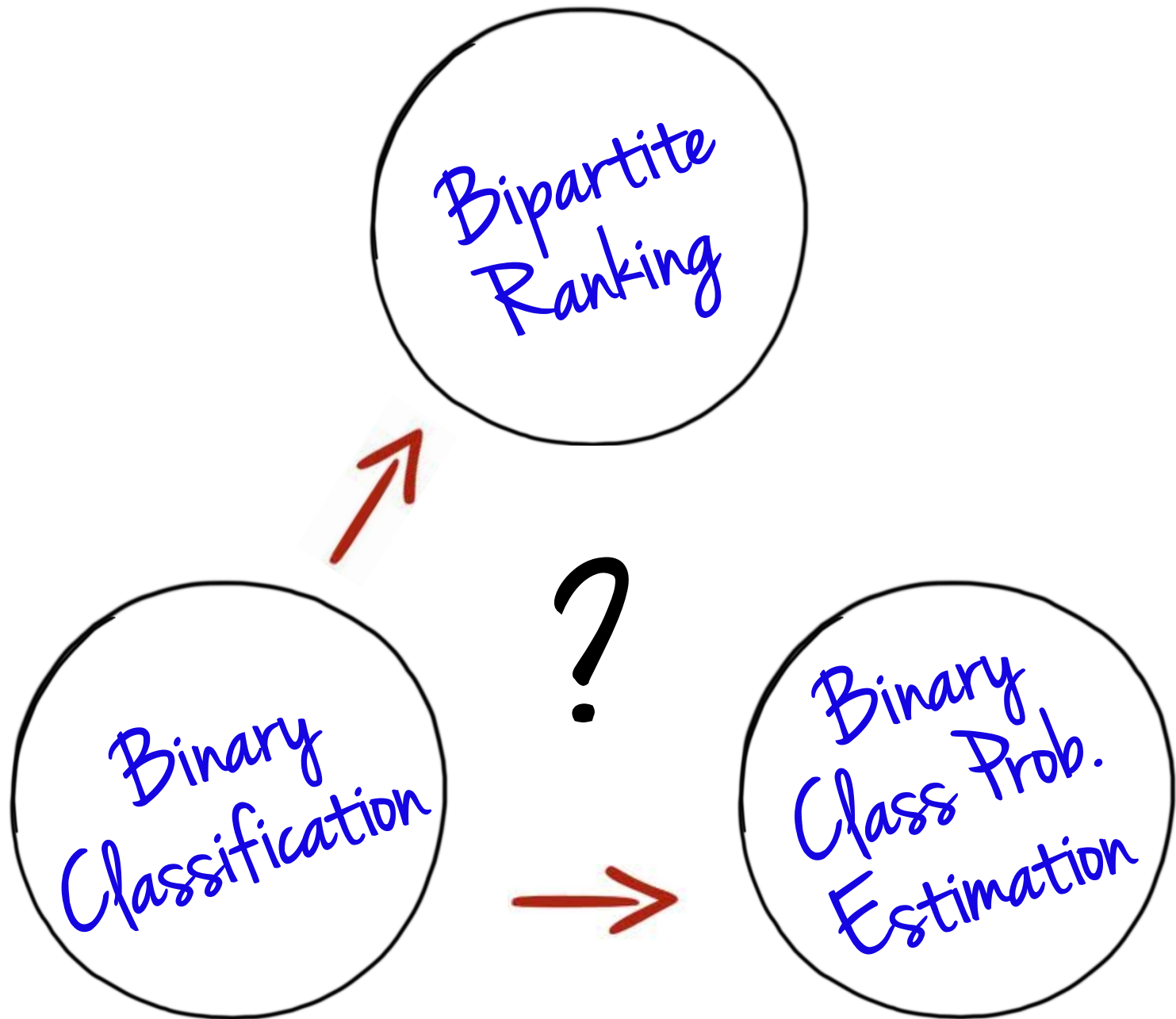


0.9

.....



0.1



Bipartite  
Ranking



?



Binary  
Classification

Binary  
Class Prob.  
Estimation

Bipartite  
Ranking

?

Binary  
Classification

Binary  
Class Prob.  
Estimation



Binary  
Classification

Binary  
Class Prob.  
Estimation

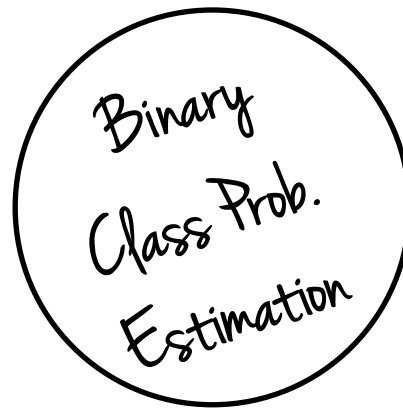
Bipartite  
Ranking

positive  
or  
negative

threshold at  
0.5  
←

1  
0.8  
0.6  
0.4  
0.2  
0

⋮  
6  
4  
2  
0  
-2  
-4  
⋮

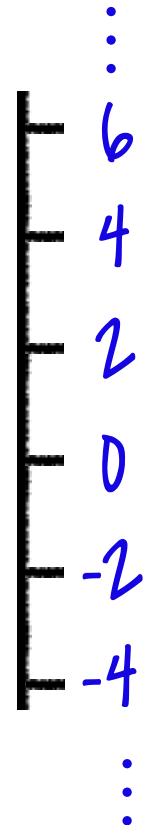


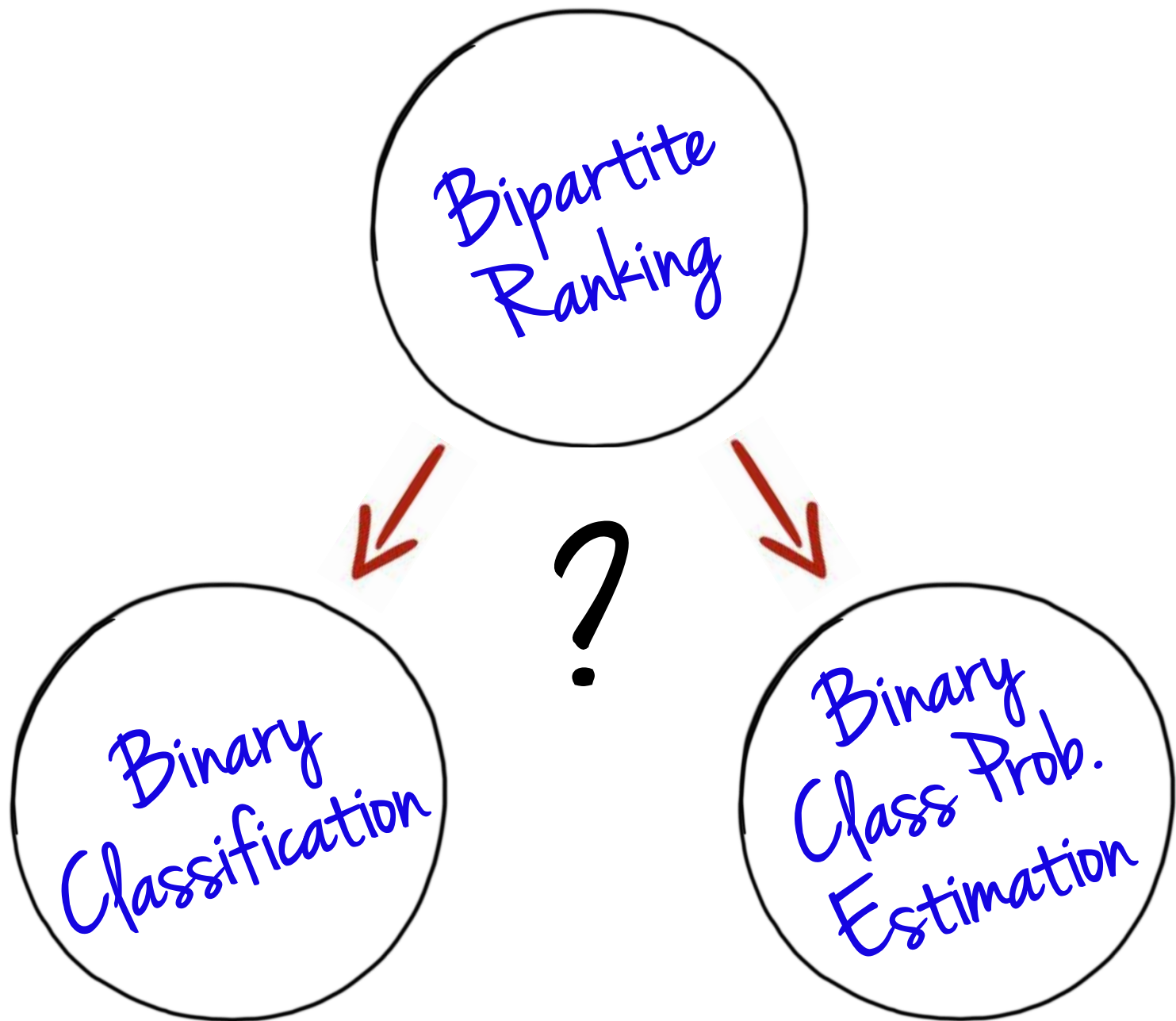
positive  
or  
negative

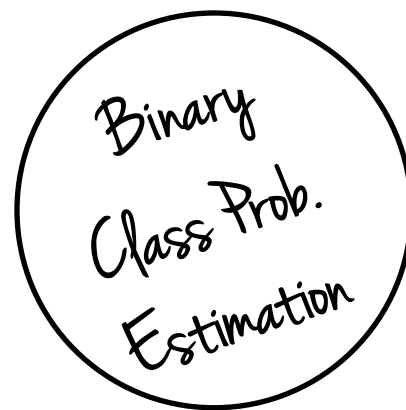
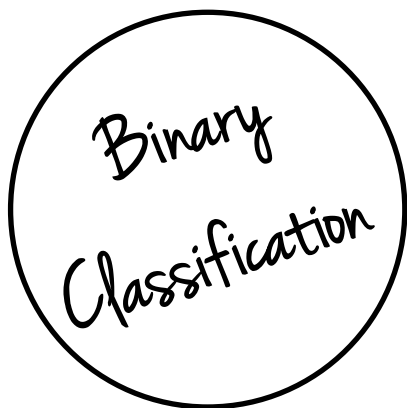
threshold at  
0.5  
←



rank by  
probabilities  
→







positive  
or  
negative

additional  
training data



Binary  
Classification

Bipartite  
Ranking

Binary  
Class Prob.  
Estimation

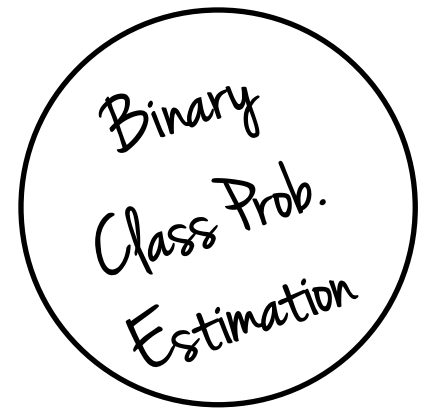
positive  
or  
negative

additional  
training data



Optimal  
threshold





positive  
or  
negative

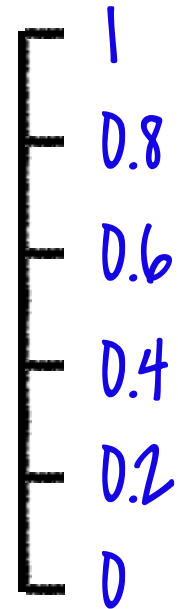
additional  
training data

←  
Optimal  
threshold

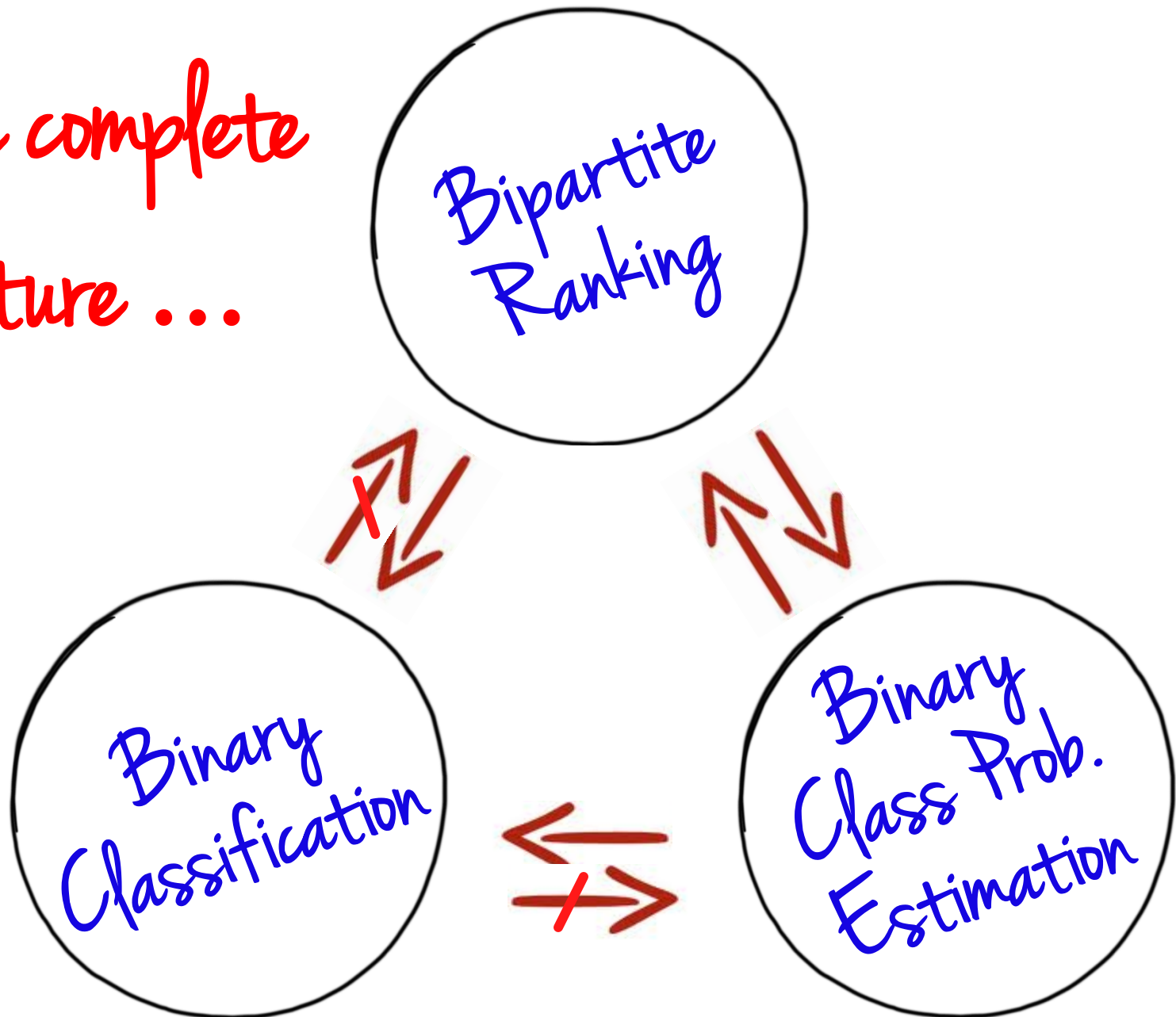


additional  
training data

→  
Calibration

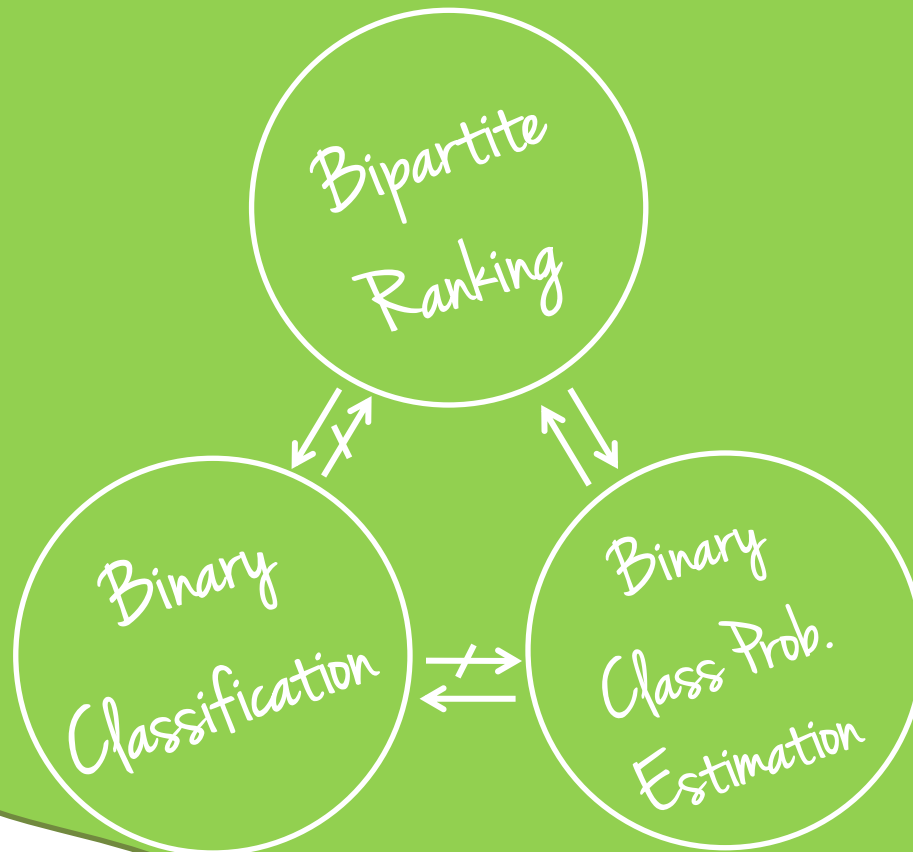


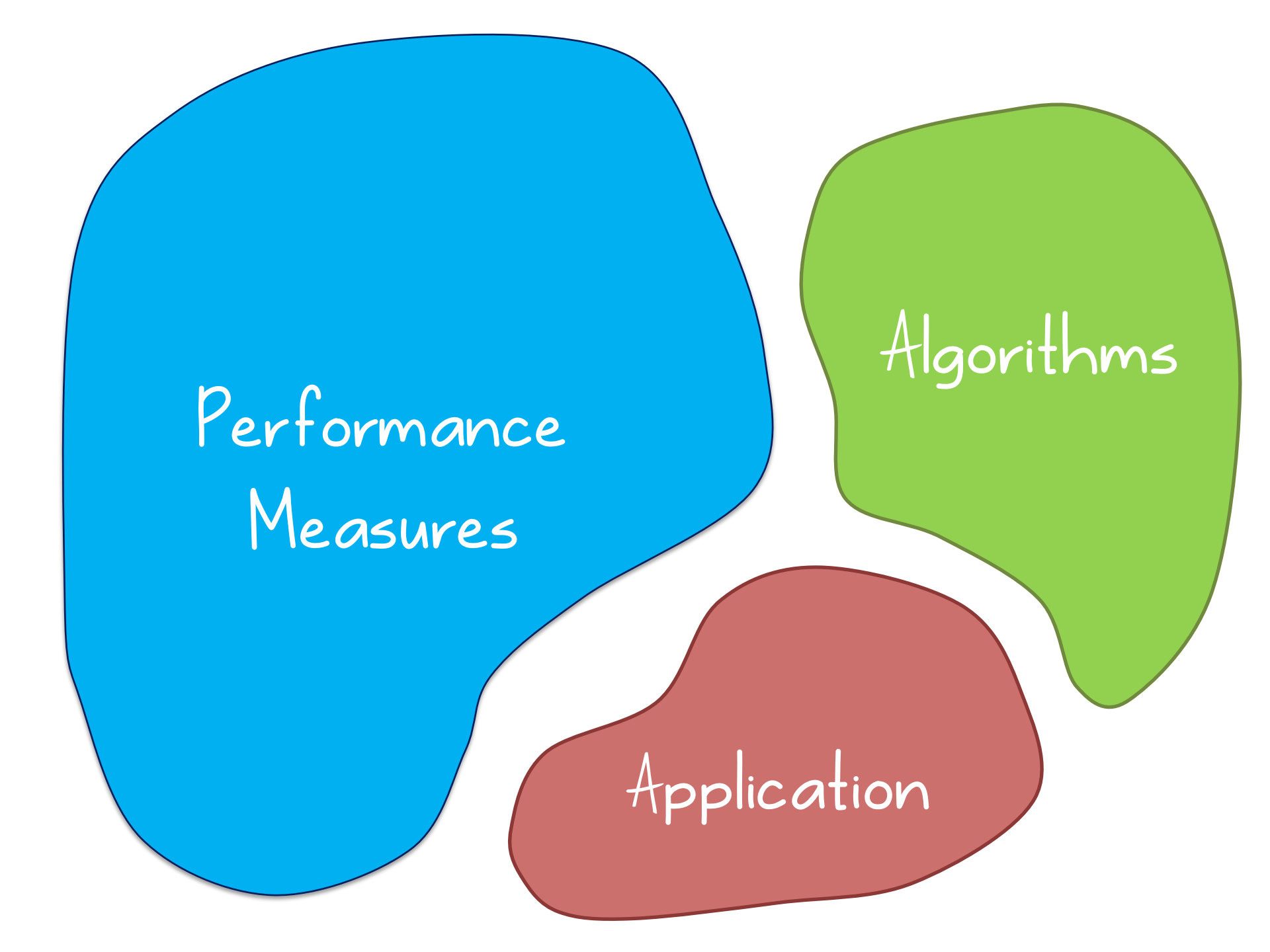
the complete  
picture ...



Narasimhan, H. and Agarwal, S. "On the relationship between binary classification, bipartite ranking, and binary class probability estimation". NIPS 2013.

# Algorithms





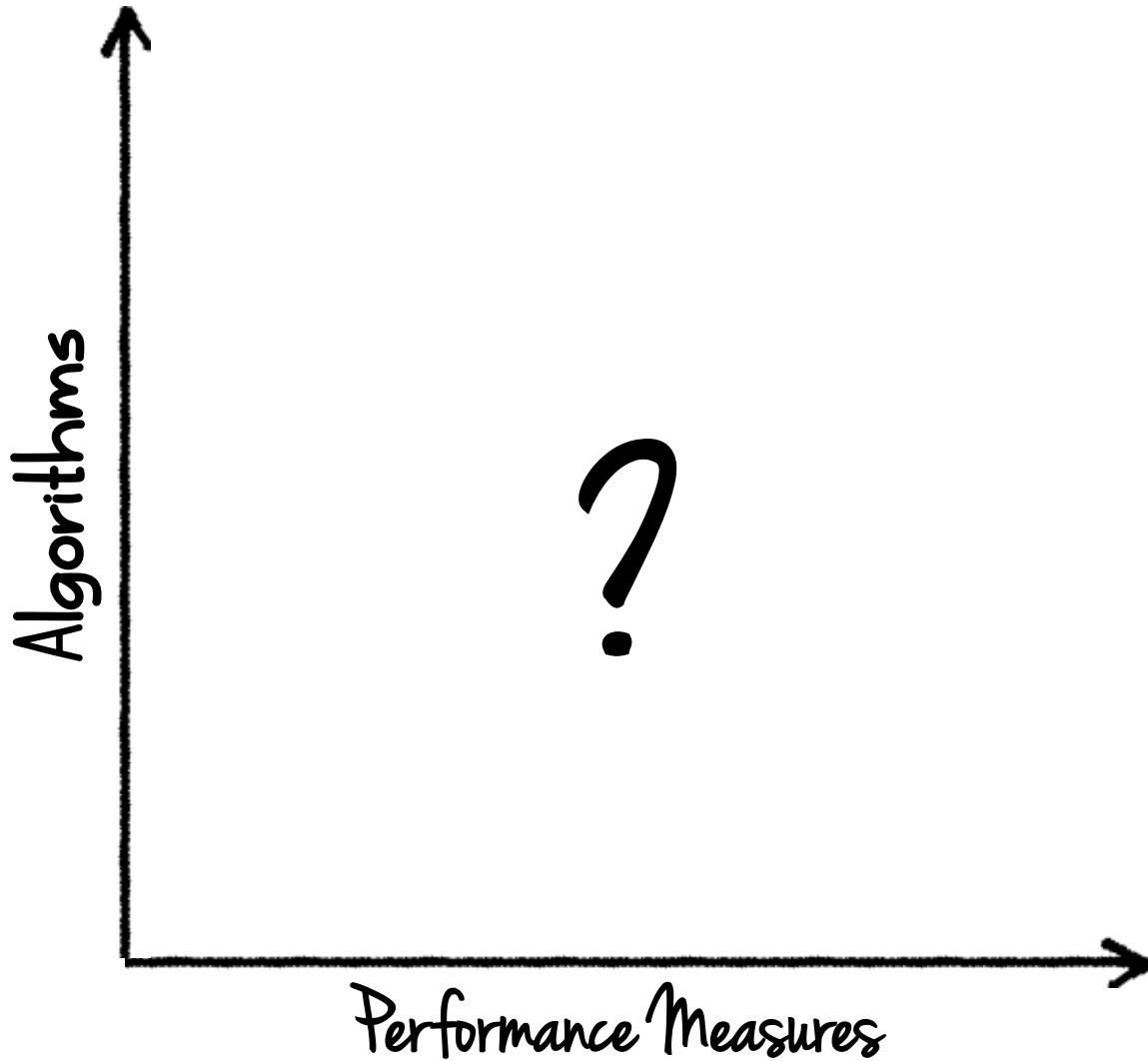
A diagram consisting of three irregular, hand-drawn shapes. The largest shape on the left is blue and contains the text 'Performance Measures'. To its right is a green shape containing the text 'Algorithms'. Below the blue shape is a red shape containing the text 'Application'.

Performance  
Measures

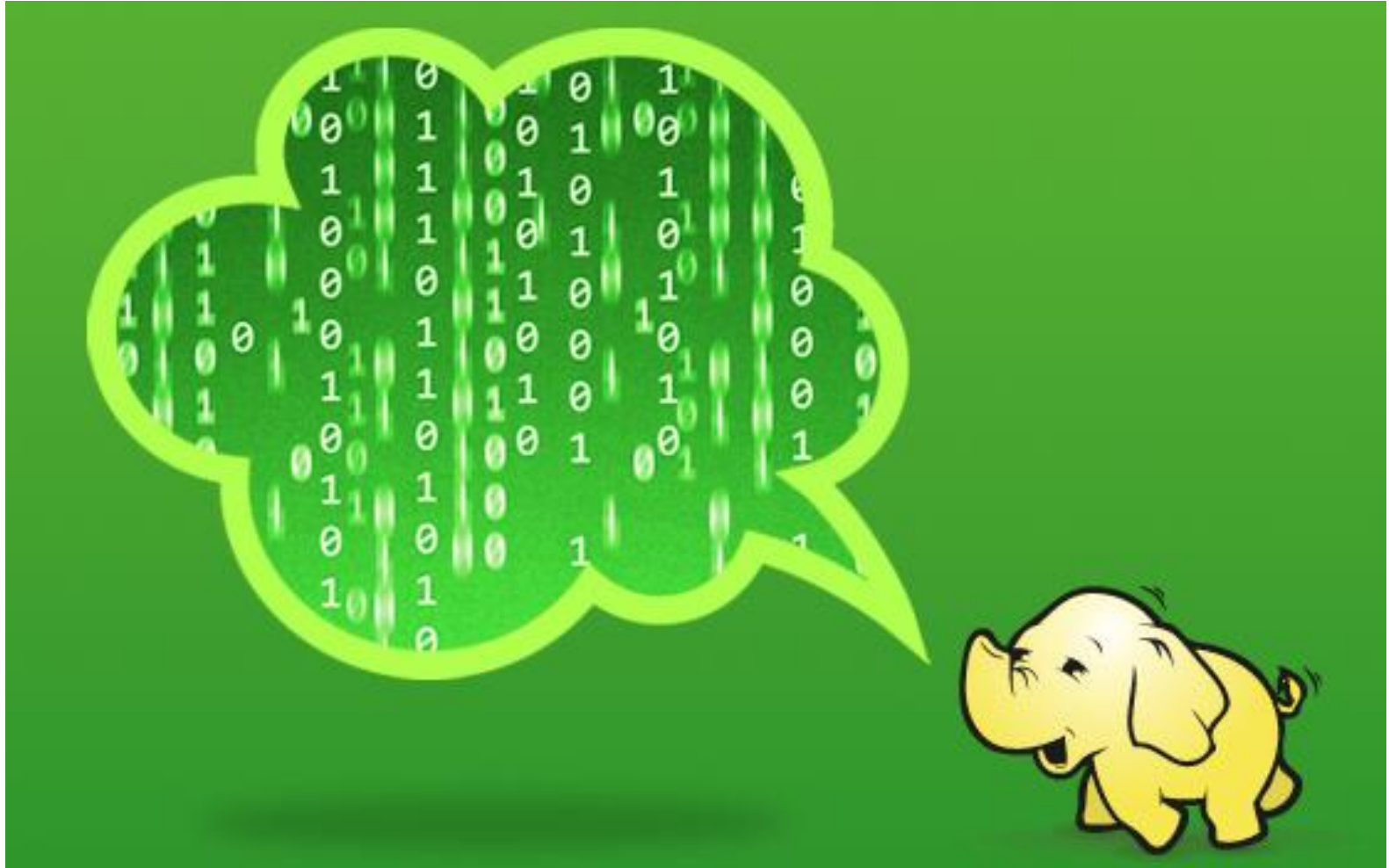
Algorithms

Application

take away message ...



open challenges ...



open challenges ...

Big Data?

| Performance Measure                | Run-time            | References                                                   |
|------------------------------------|---------------------|--------------------------------------------------------------|
| F-measure<br>PBREP<br>Precision@K  | $O(N^2)$            | Joachims (2005);                                             |
| AUC<br>Partial AUC<br>Pos@Top      | $O(N \log N)$       | Joachims (2005, 2006);<br>Narasimhan & Agarwal<br>(2013 a,b) |
| Average Precision                  | $O(N^2)$            | Yue et al. (2007)                                            |
| Discounted Cumulative Gain (DCG) * | $O(Nk)$             | Chakrabarti et al. (2008)                                    |
| Mean Reciprocal Rank (MRR) *       | $O(N \log N + k^2)$ | Chakrabarti et al. (2008)                                    |

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## Machine Learning and Learning Theory Group @ IISc

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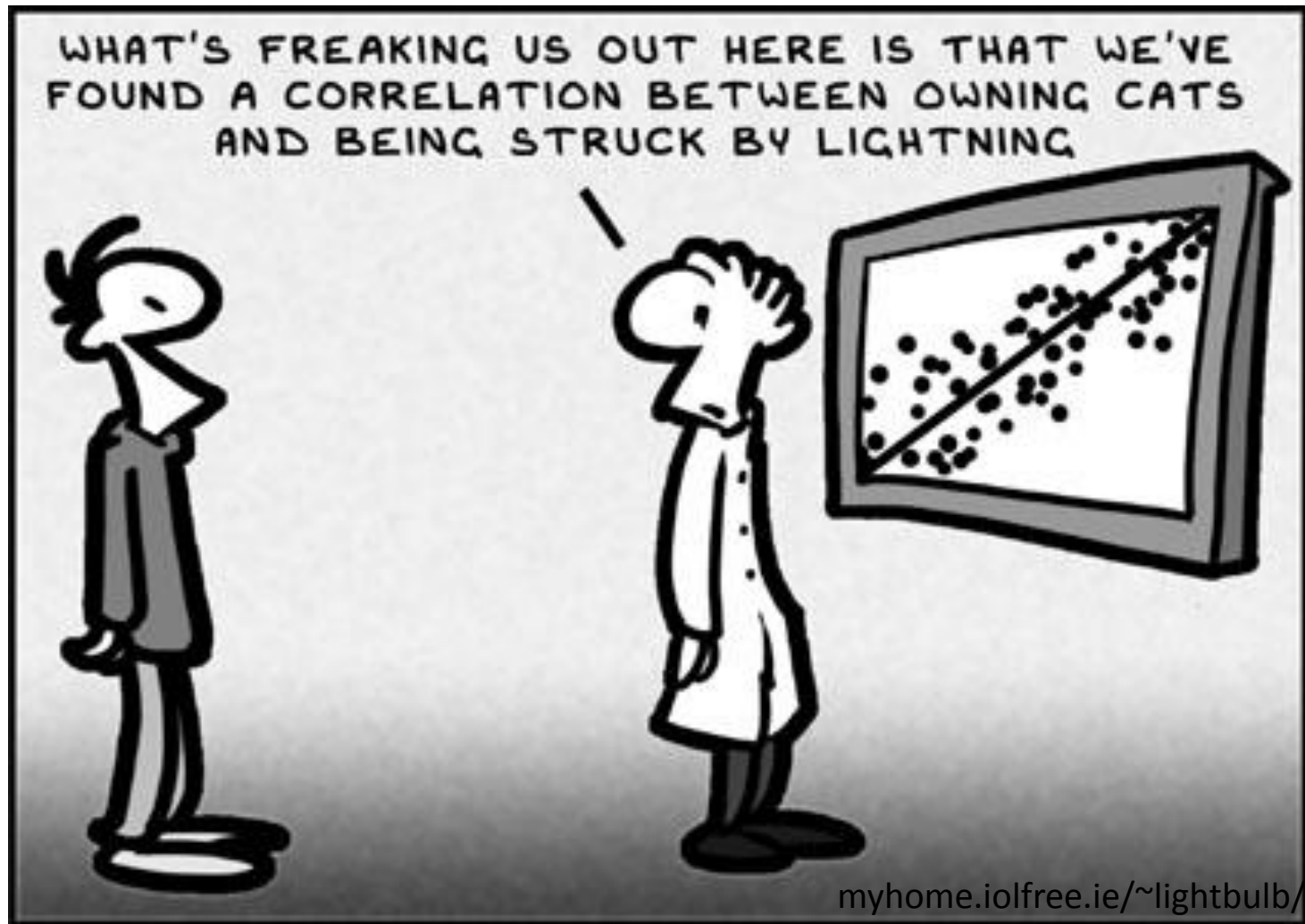
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Questions?

Most images in this presentation were obtained using  
Google image search (<http://www.google.co.in/imghp>)

Some of the hand-drawn shapes & clipart images were obtained from the following  
sites:

<http://www.clker.com/>

<http://www.free-power-point-templates.com/>

<http://neilsforance.wordpress.com/>

<http://yukaihan.deviantart.com/>

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