Programming with Data Bootcamp: Lecture 5

http://dsg.csail.mit.edu/6.S079/

Slides courtesy of Sam Madden / Tim Kraska (6.S079)

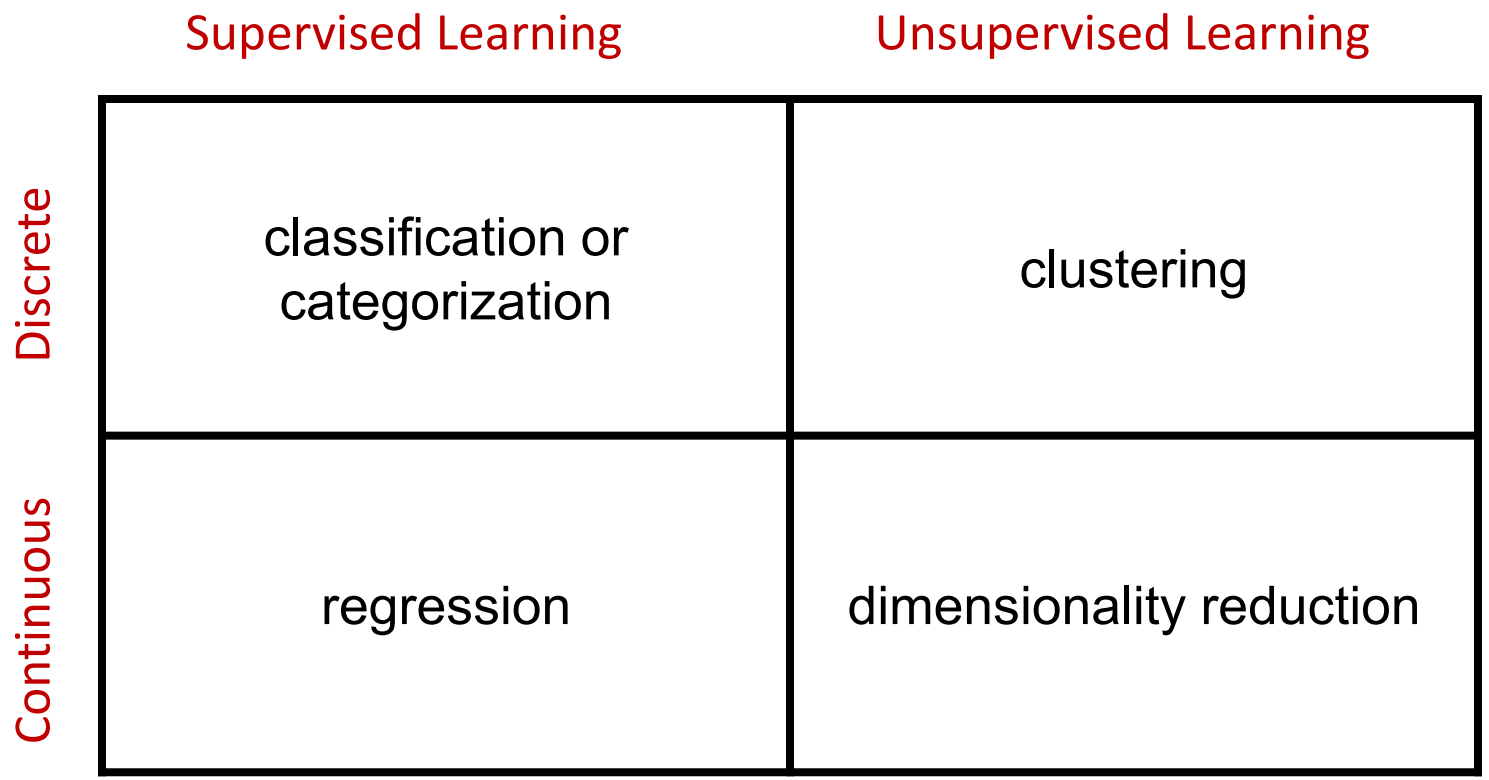
Key ideas:
Traditional ML

- Clustering
- Dim. Reduction
- Classification
- Regression

MACHINE LEARNING PROBLEMS

(Boosted-) Decision Trees

K-Means
Agglomerative clustering
DBScan



(Boosted-) Decision Trees

PCA

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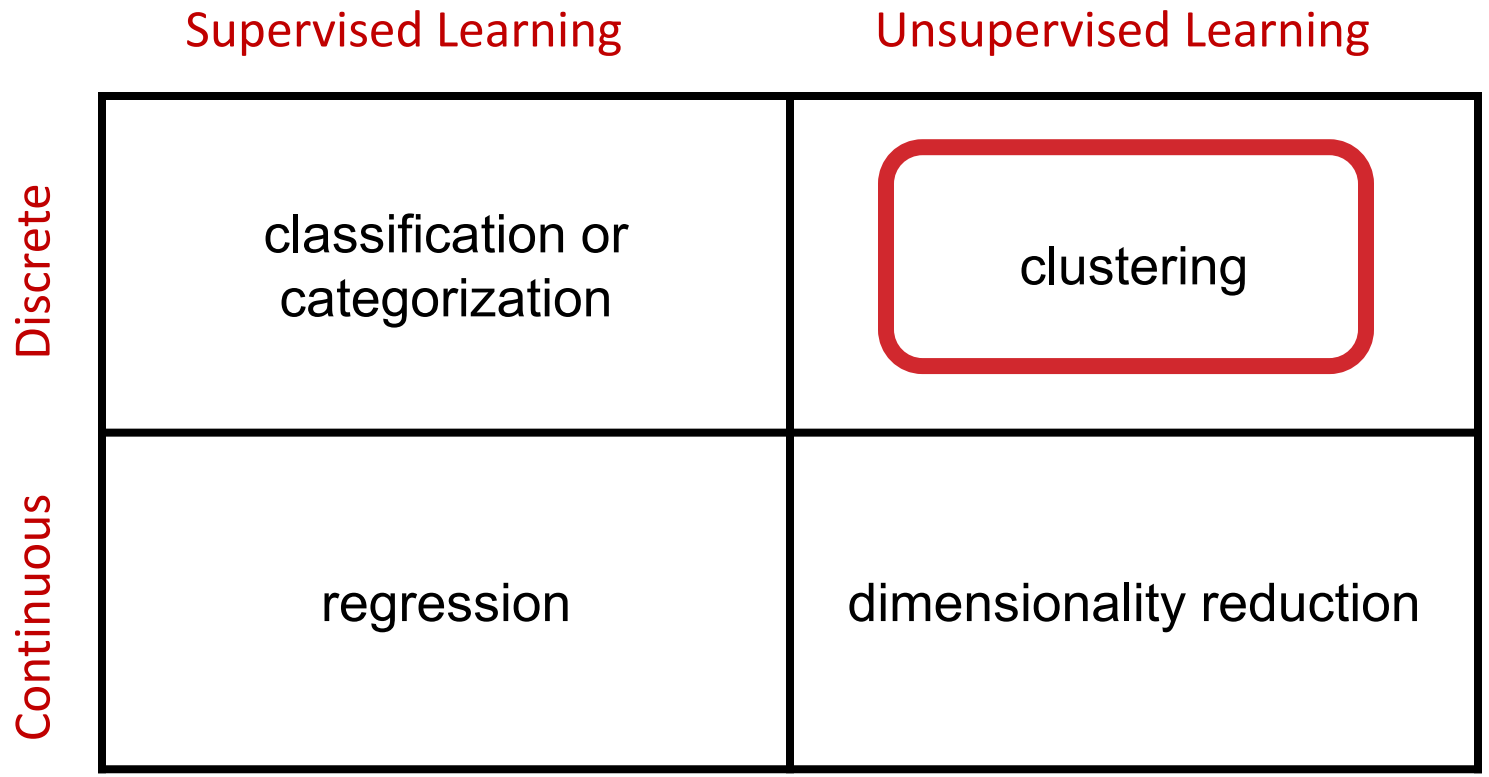

(Boosted-) Decision Trees

PCA

CLUSTERING STRATEGIES

K-means

- Iteratively re-assign points to the nearest cluster center

Agglomerative clustering

- Start with each point as its own cluster and iteratively merge the closest clusters

Mean-shift clustering

- Estimate modes of PDF (i.e., the value x at which its probability mass function takes its maximum value)

Spectral clustering

- Split the nodes in a graph based on assigned links with similarity weights

DBSCAN (Density-based spatial clustering of applications with noise)

As we go down this chart, the clustering strategies have more tendency to transitively group points even if they are not nearby in feature space

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K-MEANS ALGORITHM

Select K random data points $\{s_1, s_2, \ldots s_K\}$ as centroids c_j.

Until clustering converges or other stopping criterion {

  For each data point x_i:

    Assign x_i to the closes centroid such that

      $dist(x_i, c_j)$ is minimal.

    For each cluster c_j, update the centroids

      $c_j = \mu(c_j)$

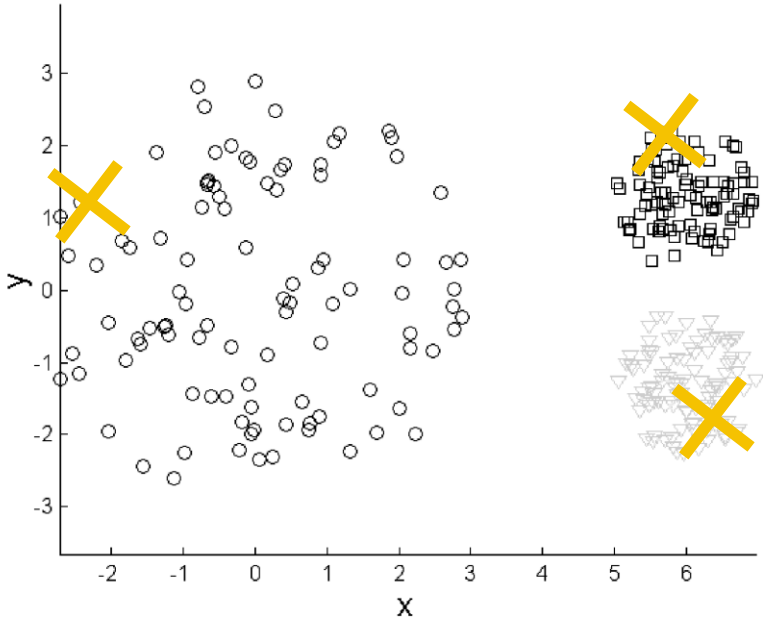
}

TERMINATION CONDITIONS

Several possibilities, e.g.,

- A fixed number of iterations.
- Partition unchanged.
- Centroid positions don't change.

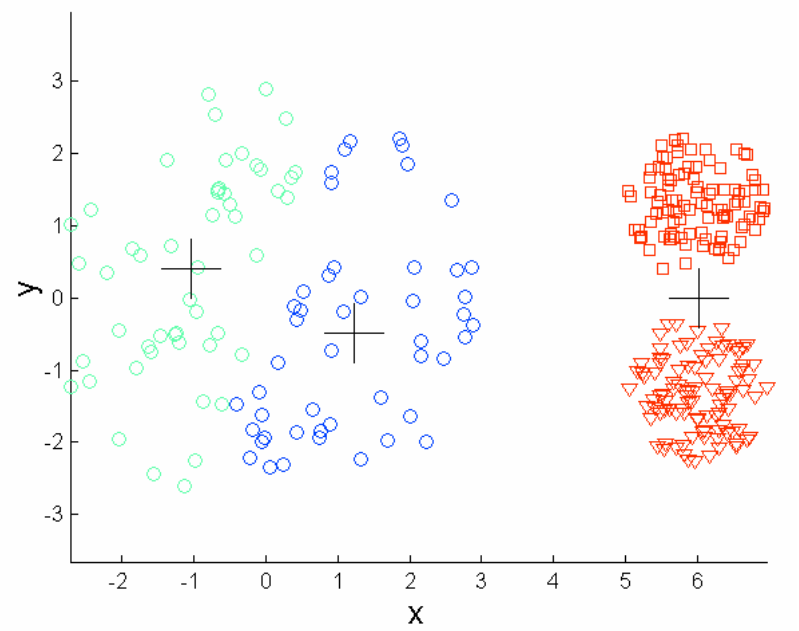
CLASS TASK



Original Points

What cluster will you get with the yellow centroids?

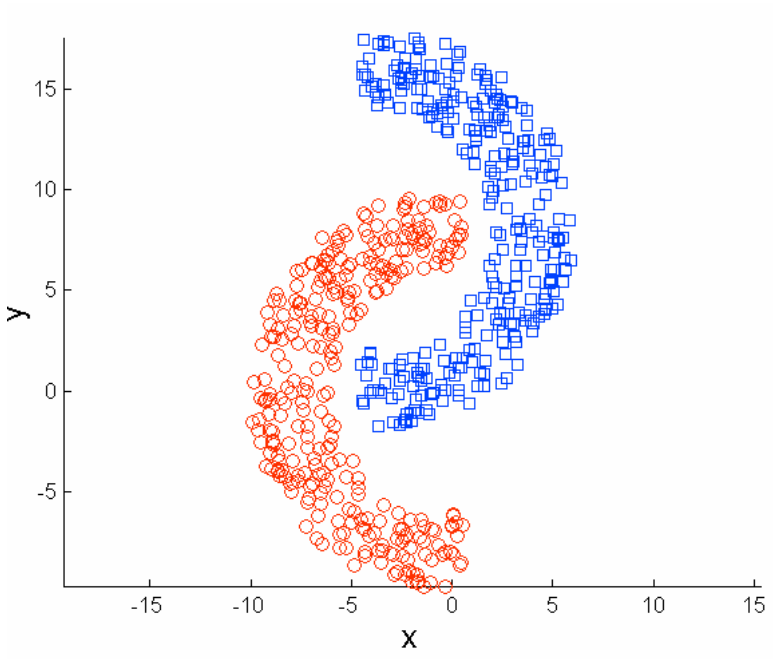
CLASS TASK



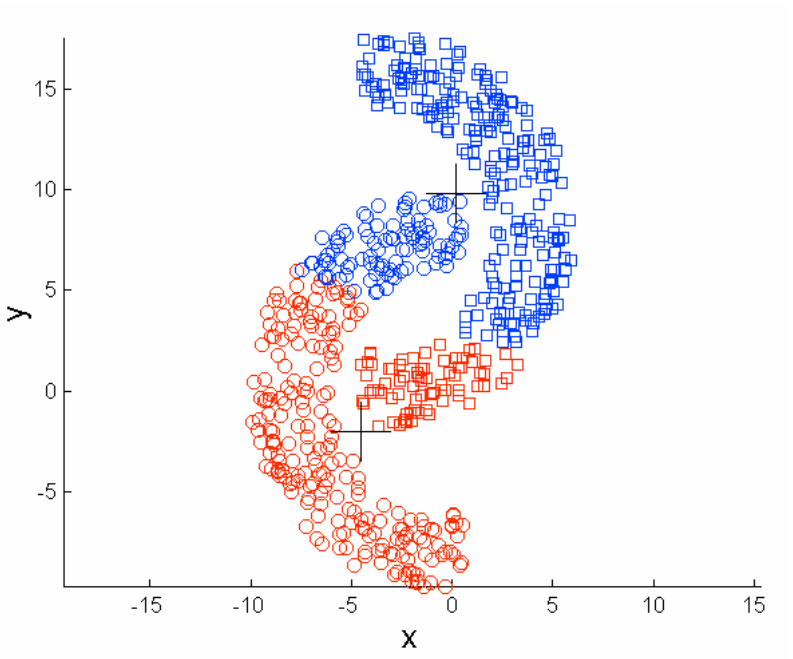
K-means (3 Clusters)

LIMITATIONS OF K-MEANS

Non-globular Shapes

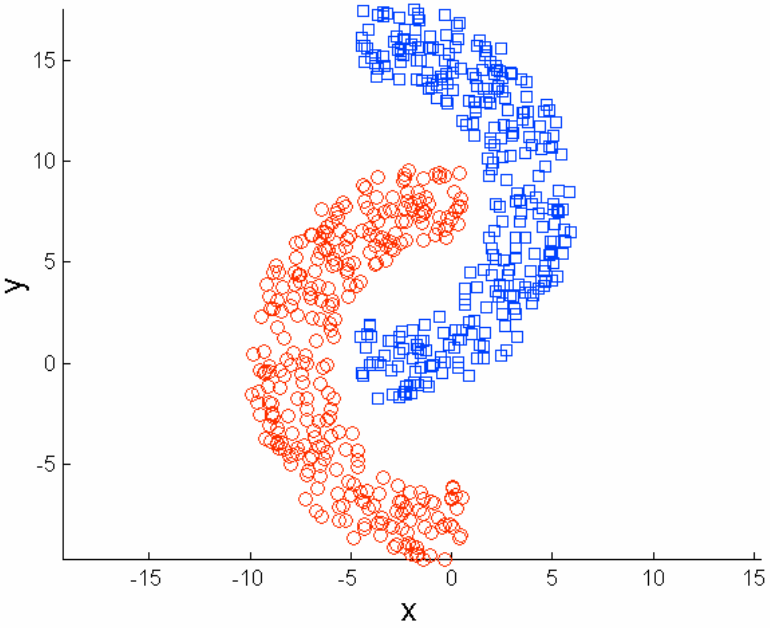


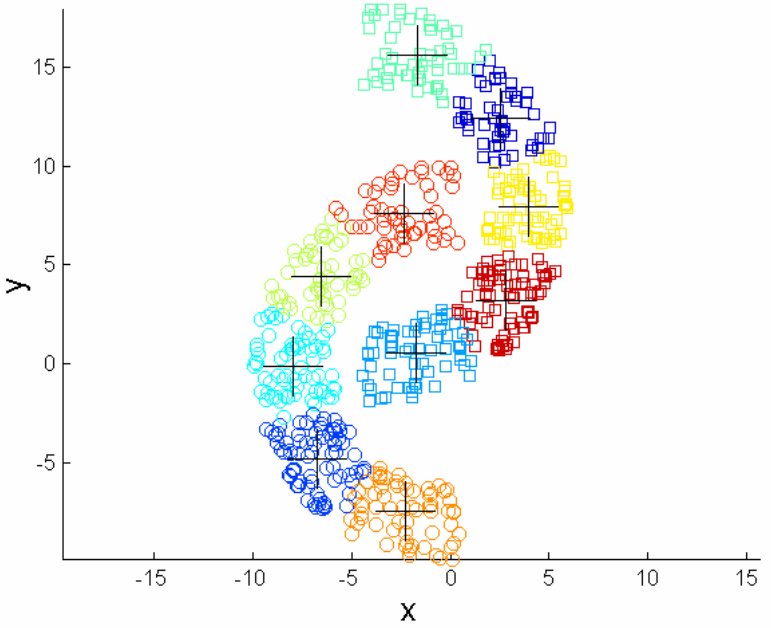
Original Points



K-means (2 Clusters)

OVERCOMING K-MEANS LIMITATIONS



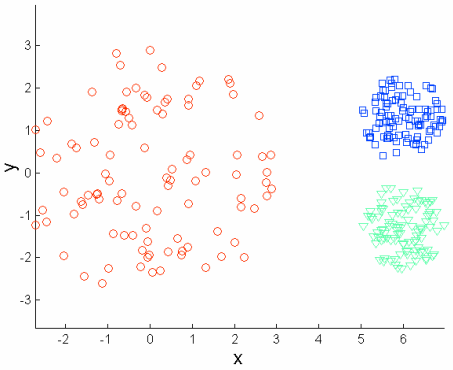


Original Points

K-means Clusters

Can you think of other ways to overcome the limitations?

How do I know how good the clustering is?



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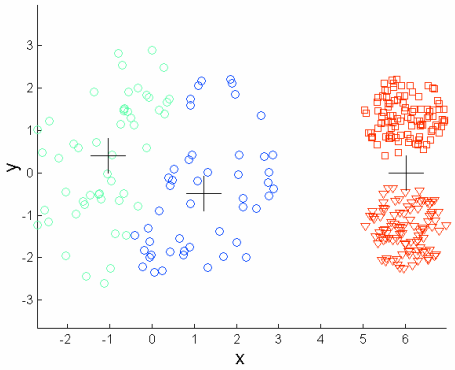
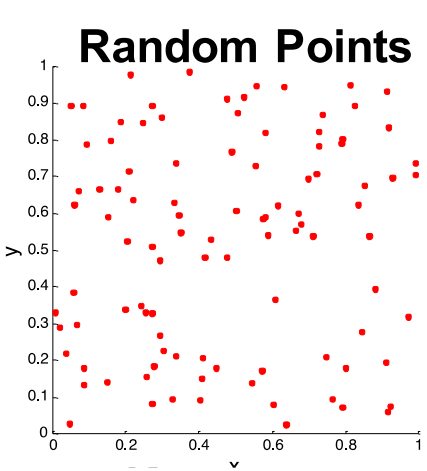
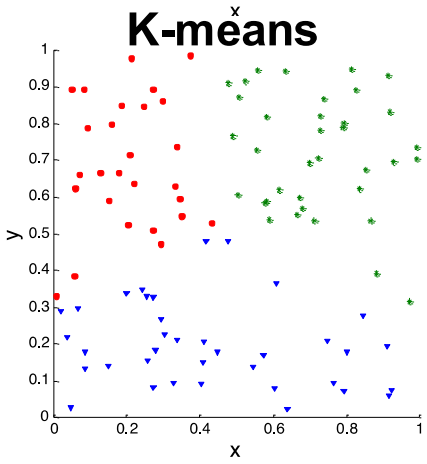


K-means (3 Clusters)

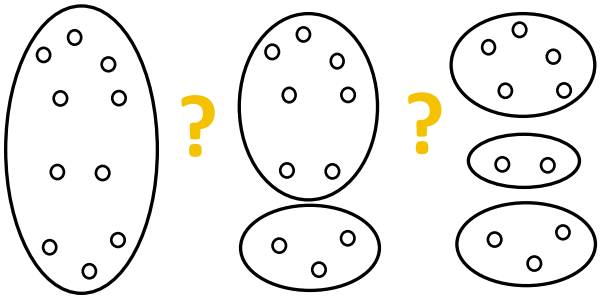




Measuring clustering validity

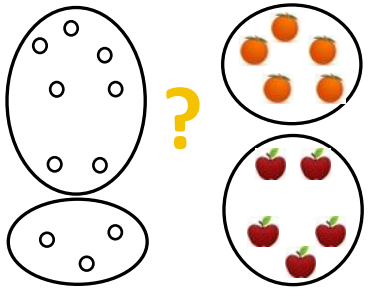
Internal Index:

- Validate *without* external info
- With different number of clusters |



External Index

Validate against ground truth



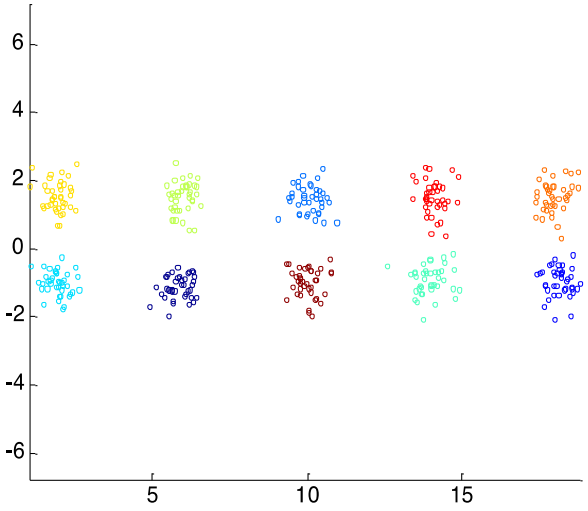
INTERNAL INDEXES

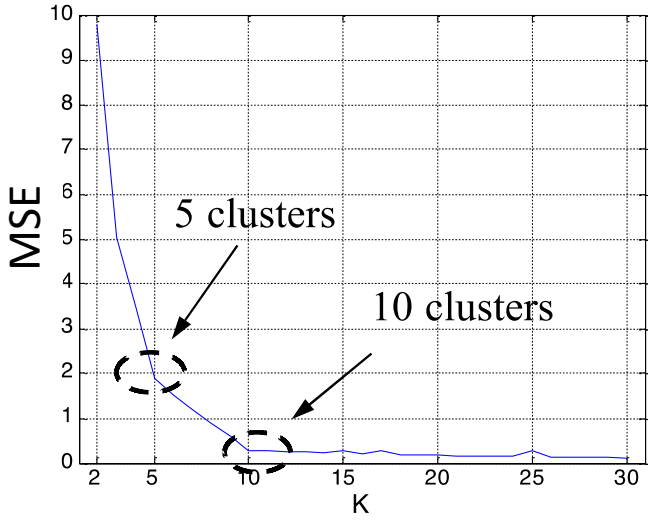
Ground truth is rarely available but unsupervised validation must be done.

Minimizes (or maximizes) internal index:

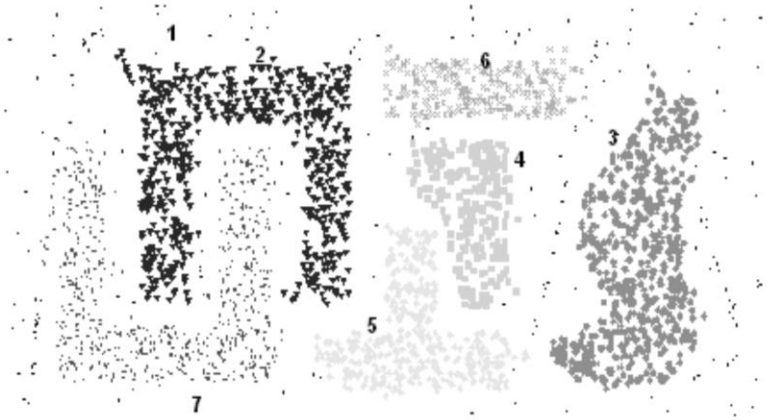
- Variances of within cluster and between clusters
- Rate-distortion method
- F-ratio
- Davies-Bouldin index (DBI)
- Bayesian Information Criterion (BIC)
- Silhouette Coefficient
- Minimum description principle (MDL)
- Stochastic complexity (SC)

MEAN SQUARE ERROR (MSE)



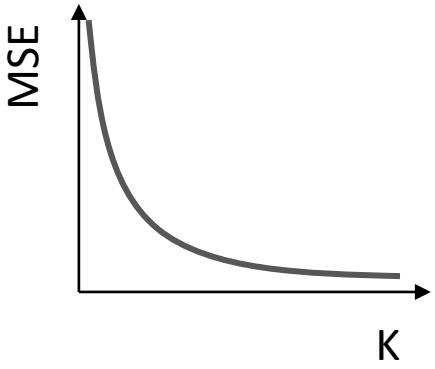


CLICKER - HTTPS://CLICKER.CSAIL.MIT.EDU/6.S079/

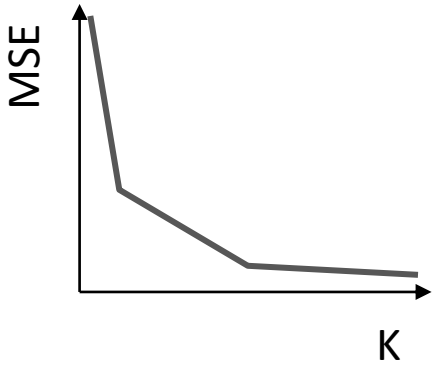


What MSE curve to you expect for this data?

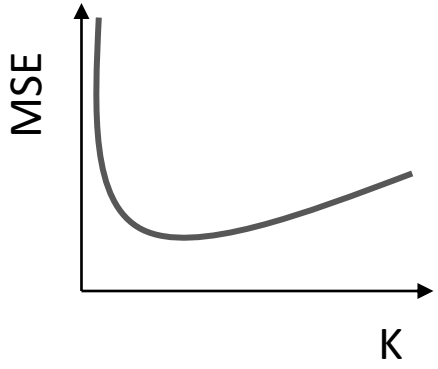
A



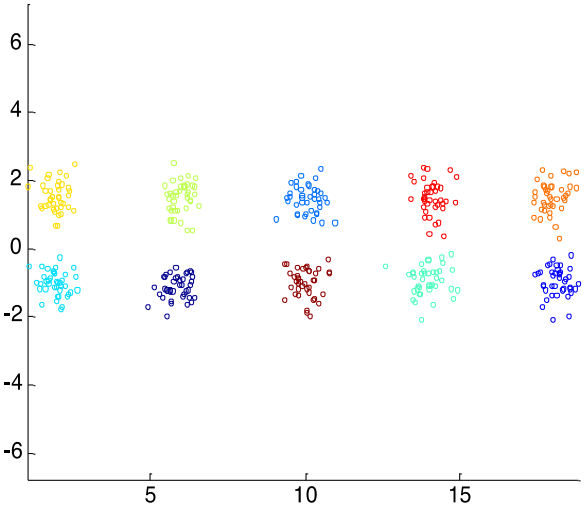
B

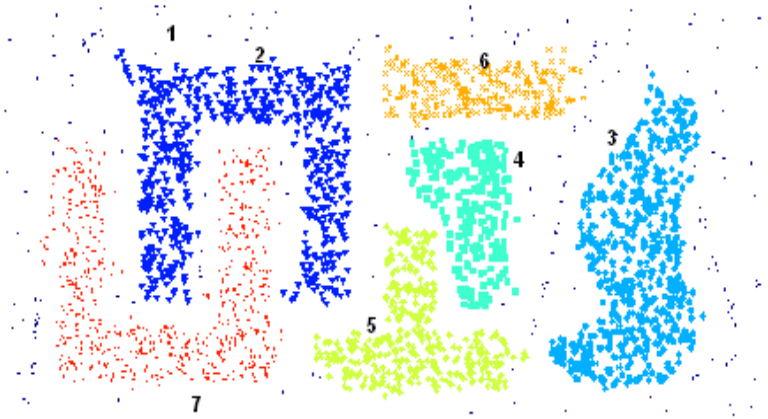


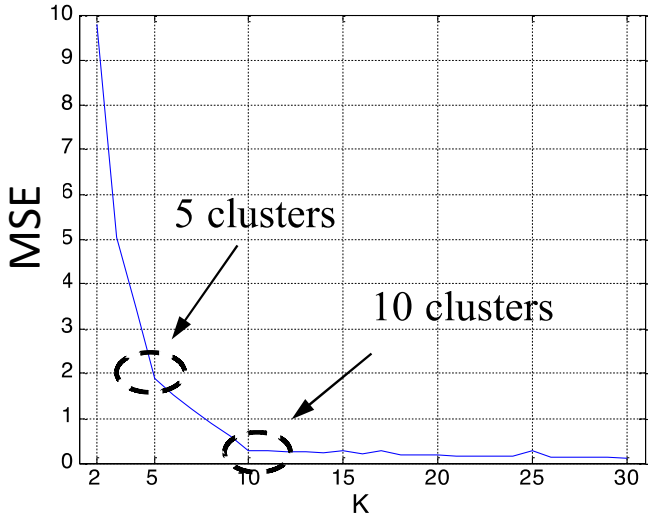
C

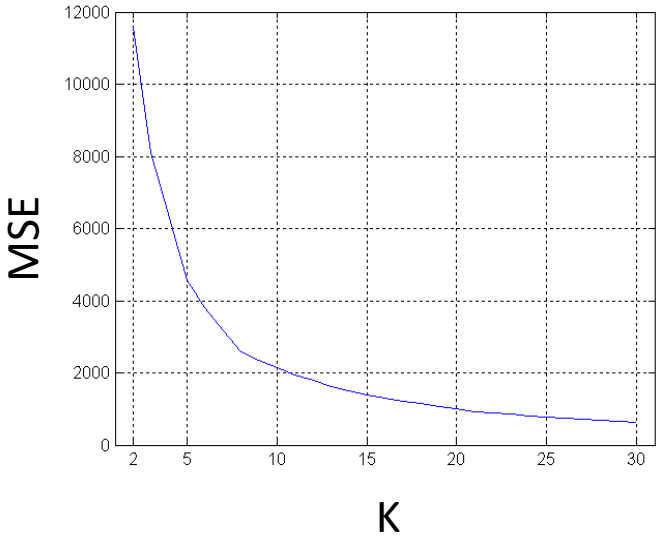


MEAN SQUARE ERROR (MSE)



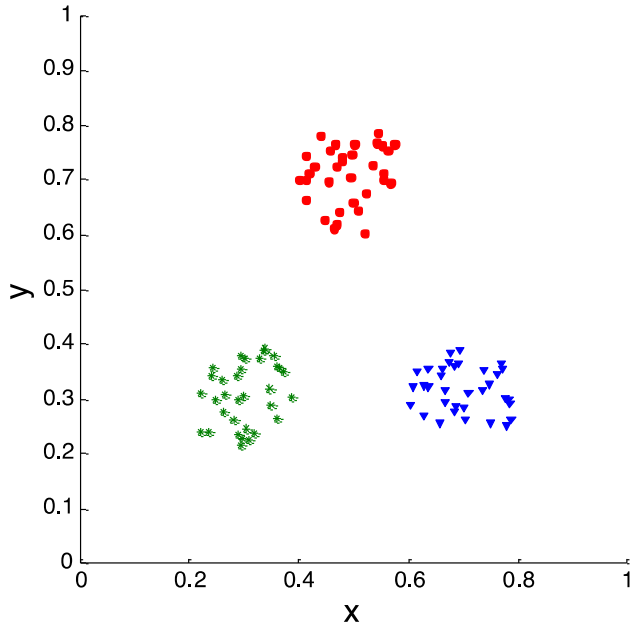


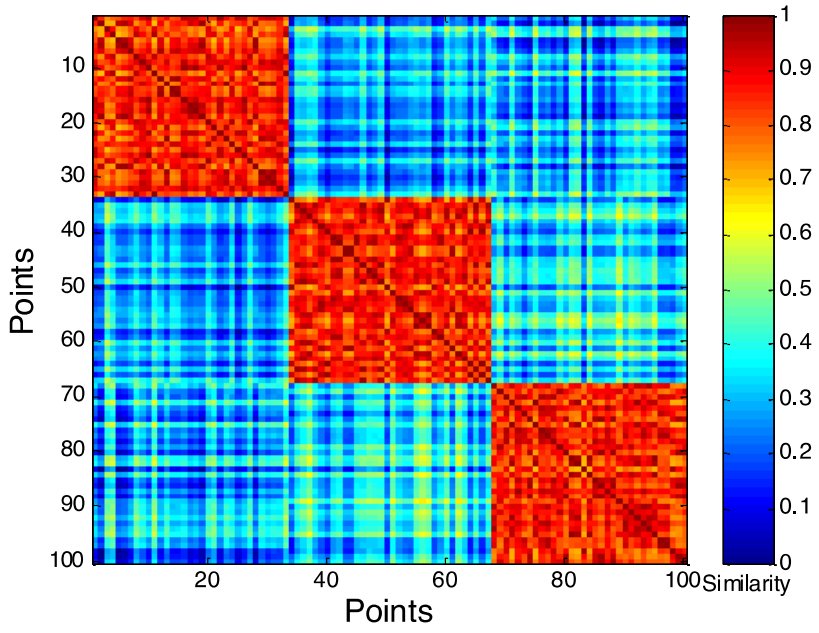




USING SIMILARITY MATRIX FOR CLUSTER VALIDATION

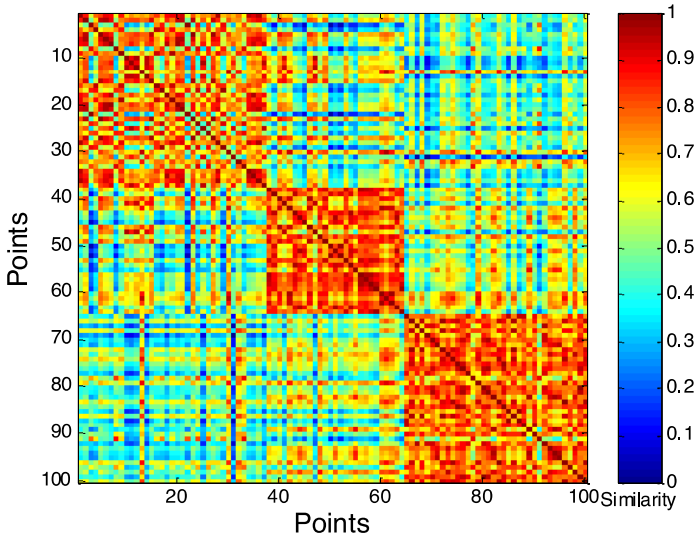
Order the similarity matrix with respect to cluster labels and inspect visually.

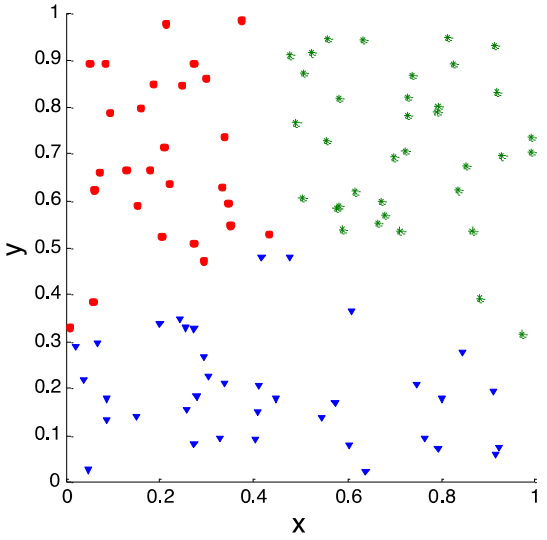




USING SIMILARITY MATRIX FOR CLUSTER VALIDATION

Clusters in random data are not so crisp





K-means

CLUSTERING STRATEGIES

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DBSCAN (Density-based spatial clustering of applications with noise)

As we go down this chart, the clustering strategies have more tendency to transitively group points even if they are not nearby in feature space

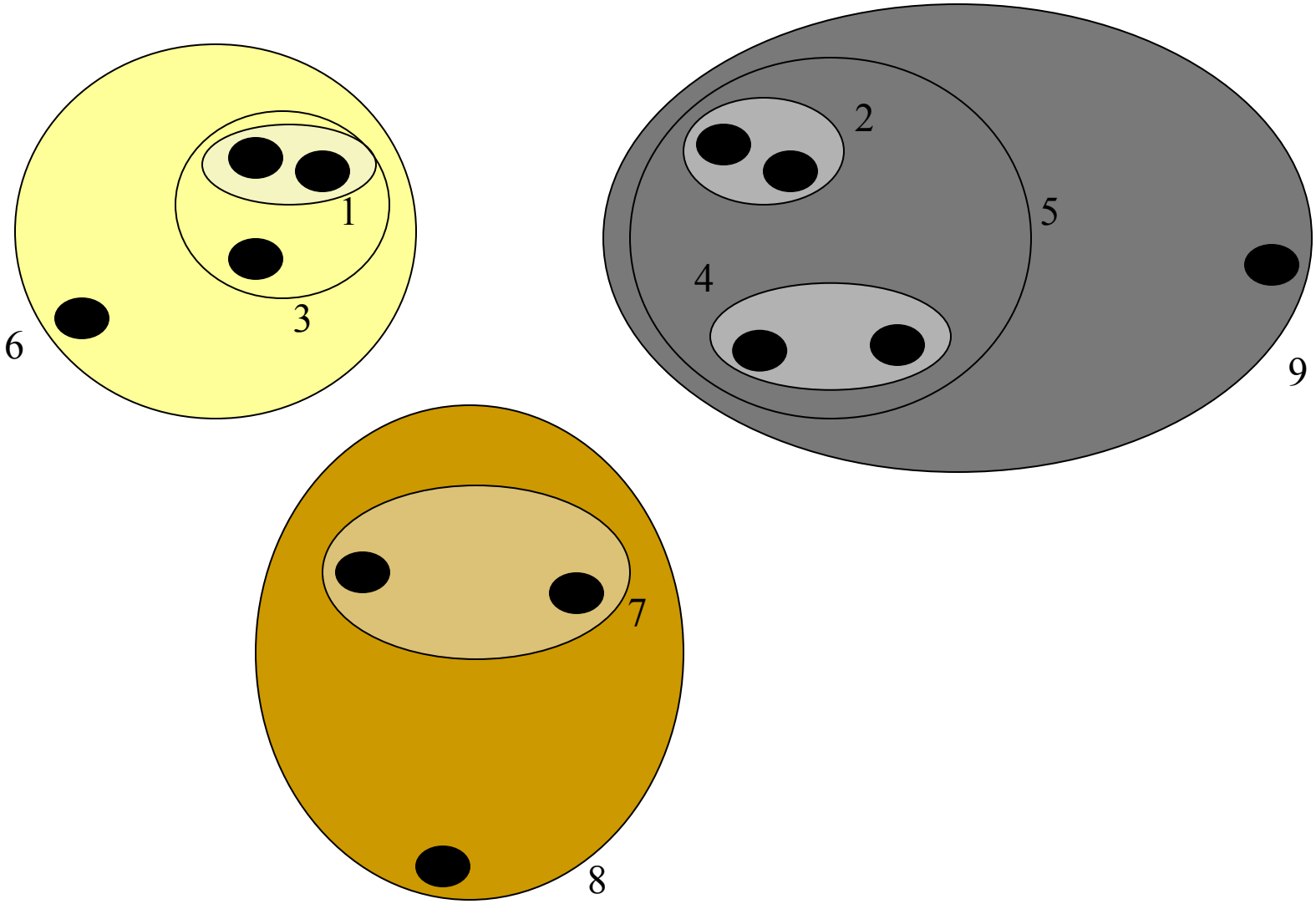
HIERARCHICAL AGGLOMERATIVE CLUSTERING METHODS

Generic Agglomerative Procedure (Salton '89):

- result in nested clusters via iterations

1. Compute all pairwise document-document similarity coefficients
2. Place each of *n* documents into a class of its own
3. Merge the two most similar clusters into one;
   - replace the two clusters by the new cluster
   - recompute intercluster similarity scores w.r.t. the new cluster
4. Repeat the above step until there are only k clusters left (note k could = 1).

Group Agglomerative Clustering



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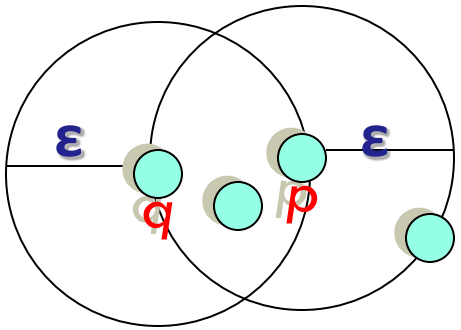
ε-NEIGHBORHOOD

ε-Neighborhood – Objects within a radius of ε from an object.

$$N_{\varepsilon}(p) : \{q \mid d(p,q) \leq \varepsilon\}$$

"High density" - ε-Neighborhood of an object contains at least *MinPts* of objects.



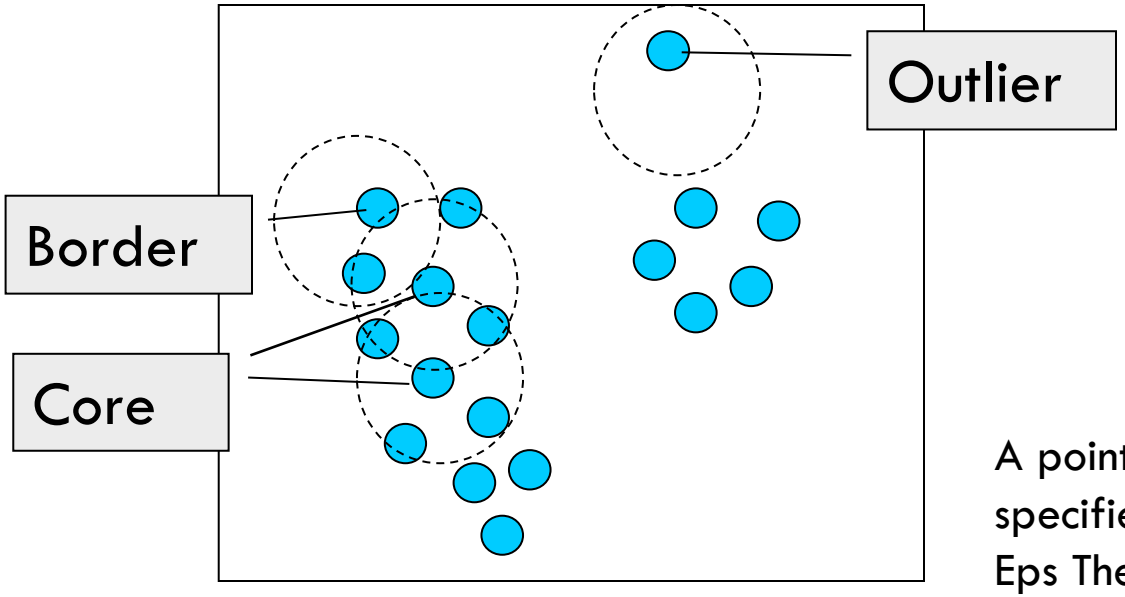
ε-Neighborhood of *p*

ε-Neighborhood of *q*

Density of p is "high" (MinPts = 4)

Density of q is "low" (MinPts = 4)

CORE, BORDER & OUTLIER



$\varepsilon = 1$unit, MinPts $= 5$

Given ε and *MinPts*, categorize the objects into three exclusive groups.

A point is a core point if it has more than a specified number of points (MinPts) within Eps These are points that are at the interior of a cluster.

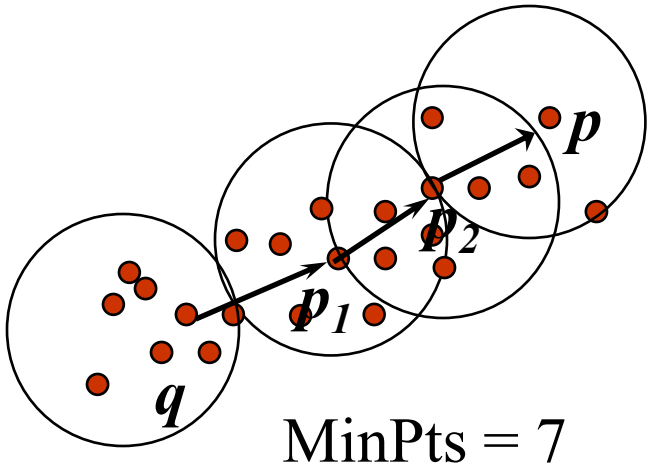
A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point..

A noise point (outlier) is any point that is not a core point nor a border point.

DENSITY-REACHABILITY

Density-Reachable (directly and indirectly):

- A point p is directly density-reachable from p2;
- p2 is directly density-reachable from p1;
- p1 is directly density-reachable from q;
- p←p2←p1←q form a chain.



p is (indirectly) density-reachable from q

q is not density- reachable from p?

DBSCAN ALGORITHM

Input: The data set D

Parameter: ε, MinPts

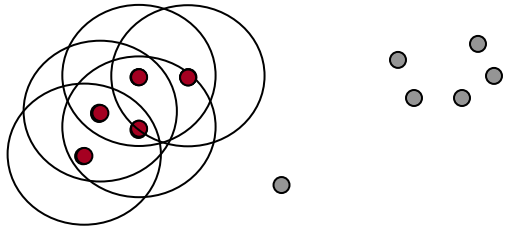
For each object p in D
    if p is a core object and not processed then
        C = retrieve all objects density-reachable from p
        mark all objects in C as processed
        report C as a cluster
    else mark p as outlier
    end if

End For

DBSCAN ALGORITHM: EXAMPLE

Parameter

- $\varepsilon = 2$ cm
- *MinPts* = 3



```
for each o ∈ D do
    if o is not yet classified then
        if o is a core-object then
            collect all objects density-reachable from o
            and assign them to a new cluster.
        else
            assign o to NOISE
```

DBSCAN ALGORITHM: EXAMPLE

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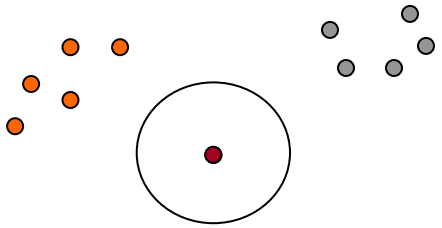

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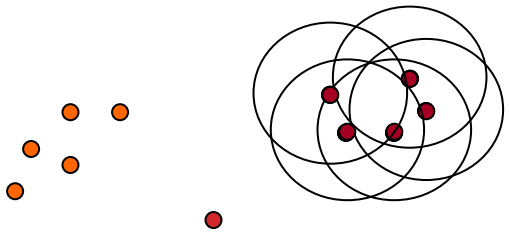

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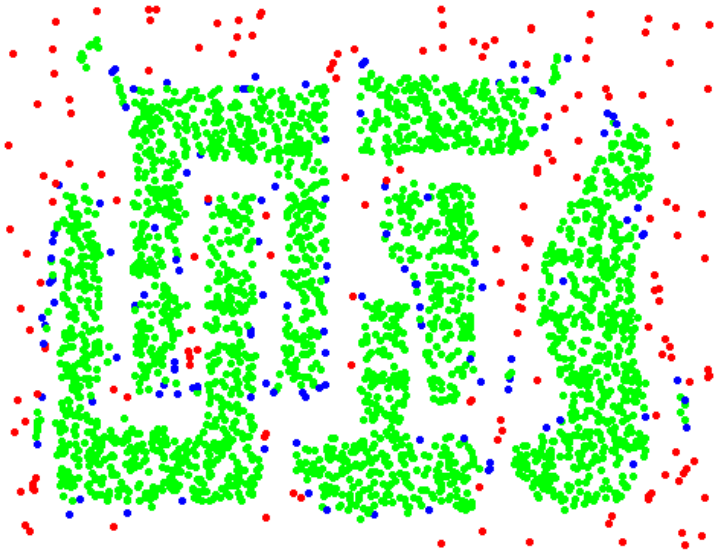
EXAMPLE

Original Points

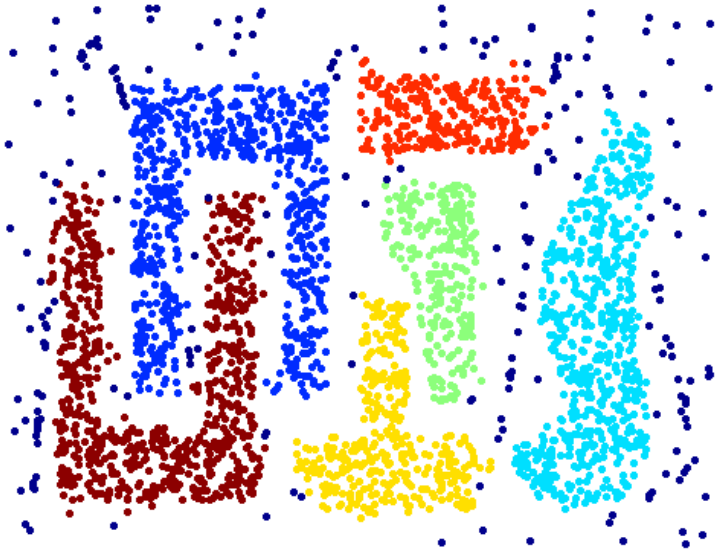


Point types: core, border and outliers

$\varepsilon = 10$, MinPts = 4

WHEN DBSCAN WORKS WELL

Original Points

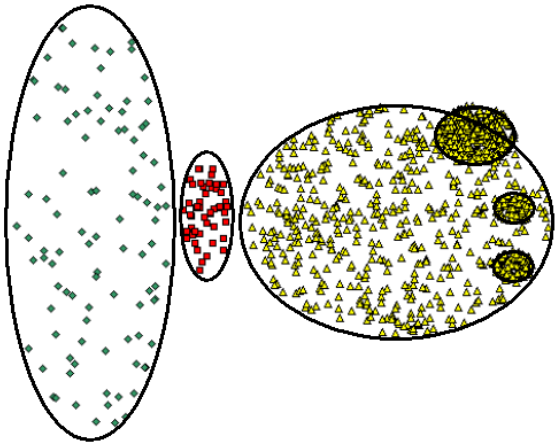


Clusters

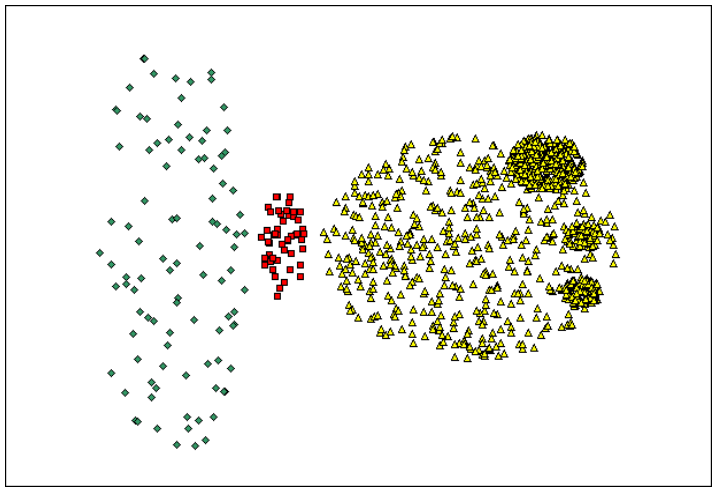
- Resistant to Noise
- Can handle clusters of different shapes and sizes

CAN YOU CREATE AN EXAMPLE FOR WHICH DBSCAN WILL NOT WORK WELL

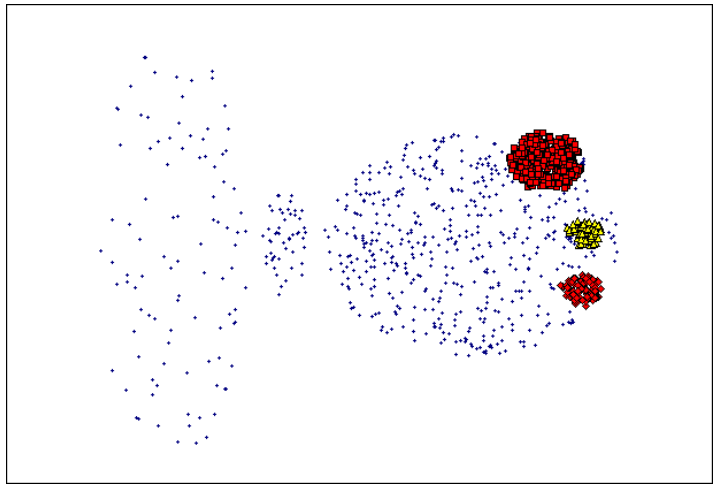
WHEN DBSCAN DOES NOT WORK WELL



Original Points



(MinPts=4, Eps=9.92).

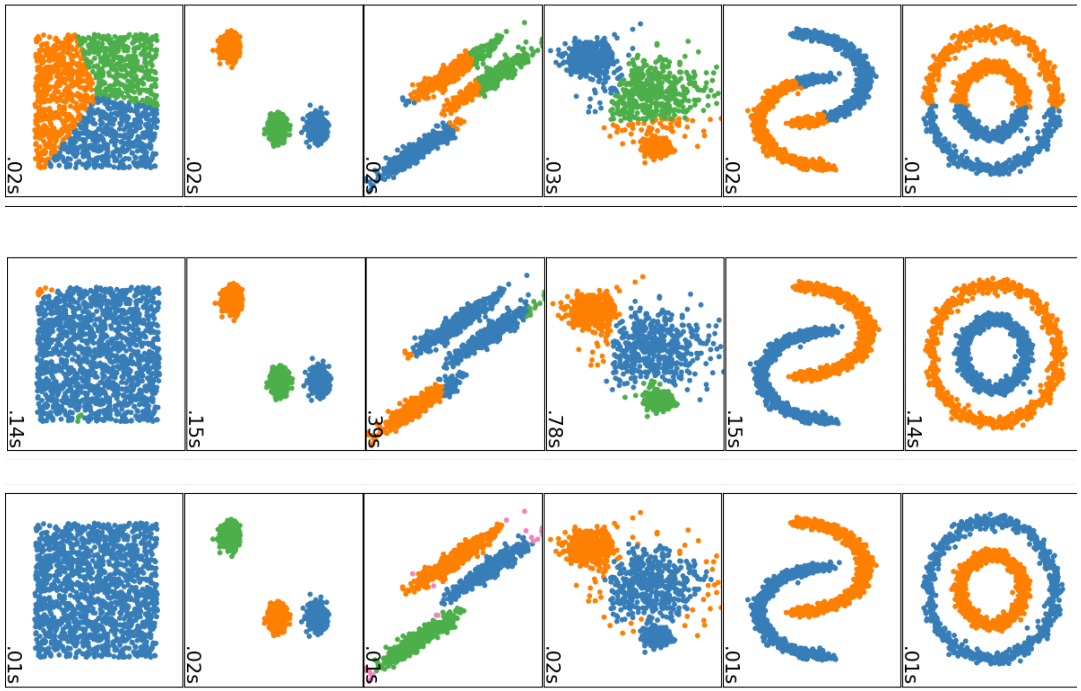


(MinPts=4, Eps=9.75)

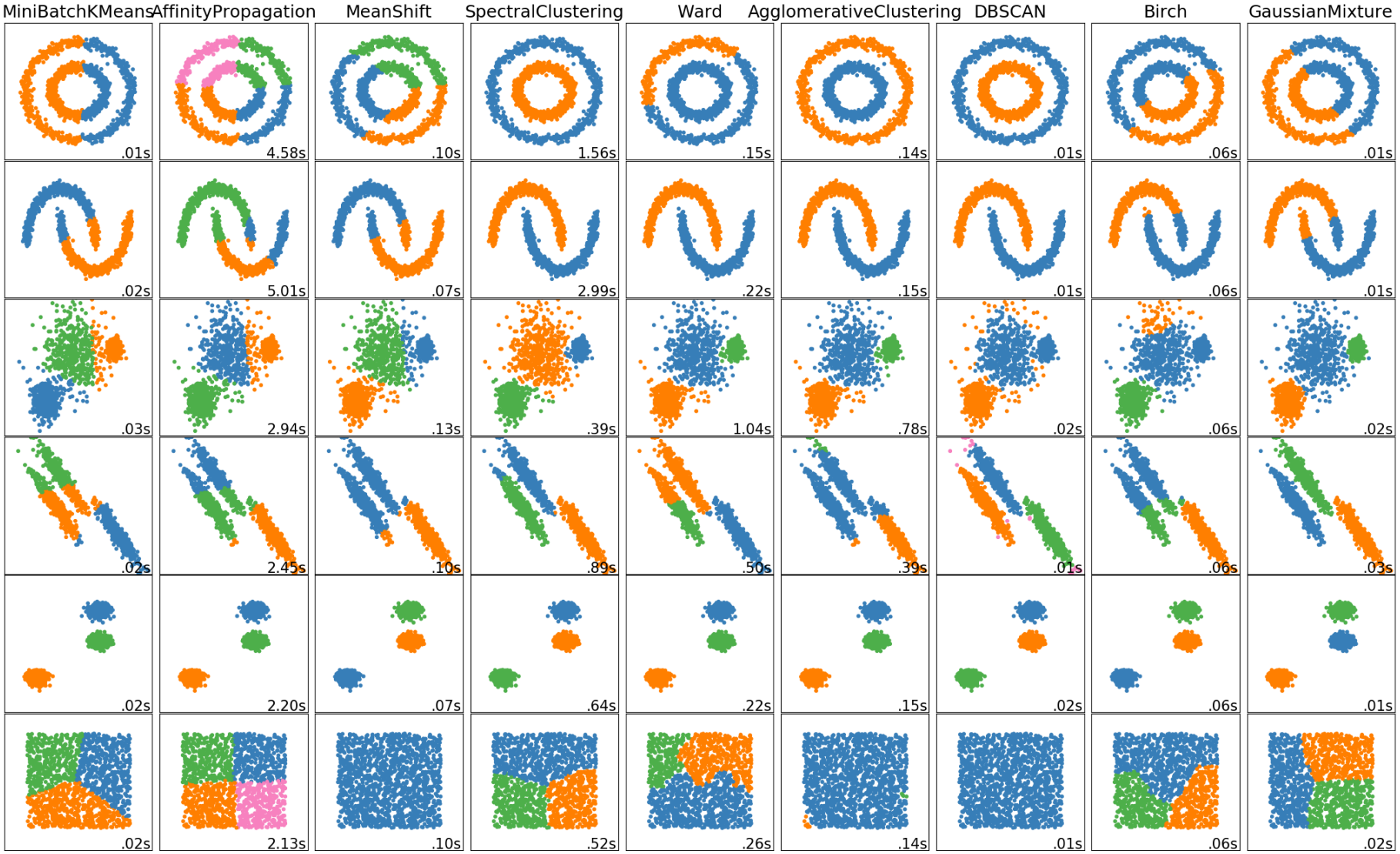
- Cannot handle Varying densities
- Sensitive to parameters

CLICKER - HTTPS://CLICKER.CSAIL.MIT.EDU/6.S079/

A	B	C
KMeans	Aggl. clustering	KMeans
DBScan	KMeans	Aggl. clustering
Aggl. clustering	DBScan	DBScan



CLUSTERING


MiniBatchKMeans
AffinityPropagation
MeanShift
SpectralClustering
Ward
AgglomerativeClustering
DBSCAN
Birch
GaussianMixture
.01s
4.58s
.10s
1.56s
.15s
.14s
.01s
.06s
.01s
.02s
5.01s
.07s
2.99s
.22s
.15s
.01s
.06s
.01s
.03s
2.94s
.13s
.39s
1.04s
.78s
.02s
.06s
.02s
.02s
2.45s
.10s
.89s
.50s
.39s
.01s
.06s
.03s
.02s
2.20s
.07s
.64s
.22s
.15s
.02s
.06s
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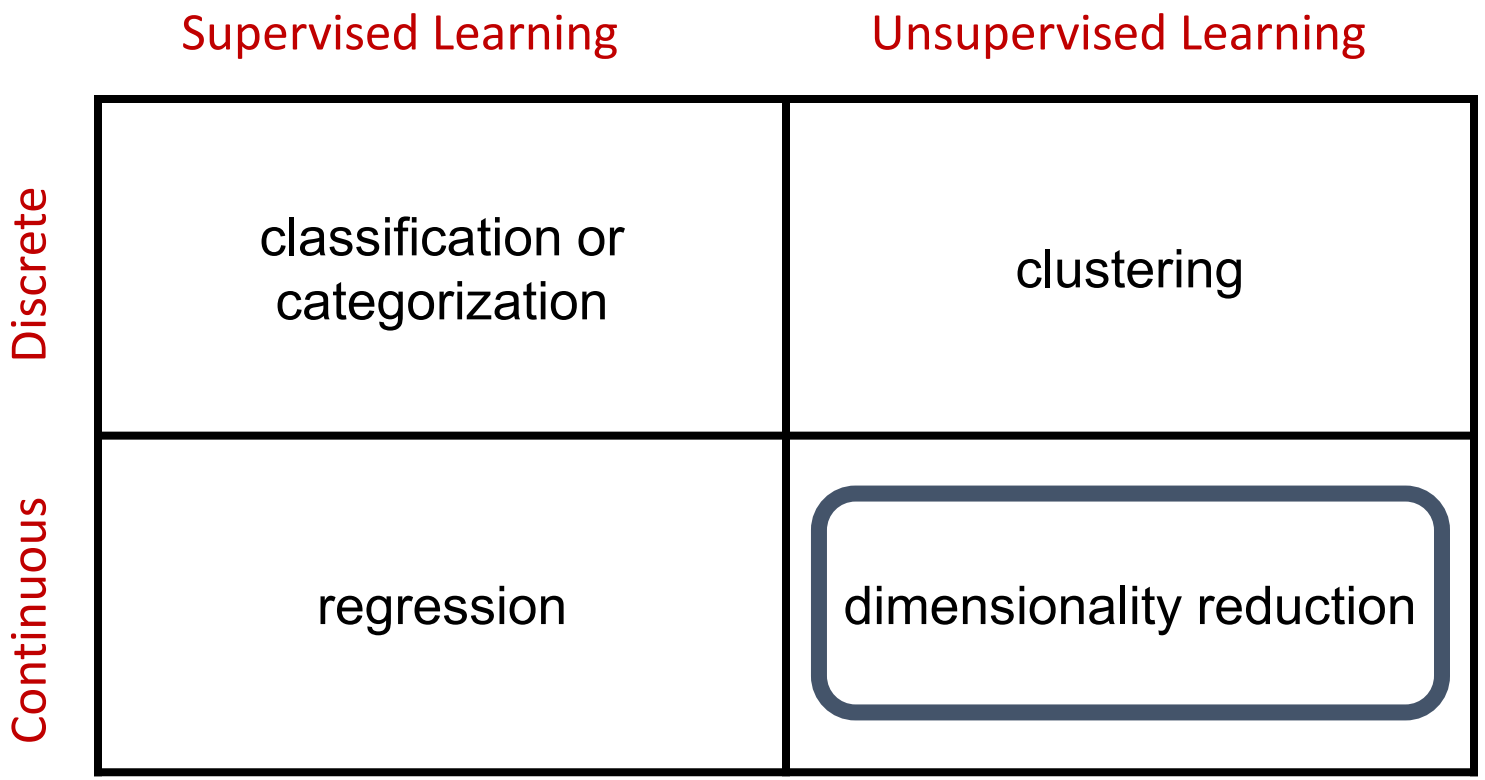
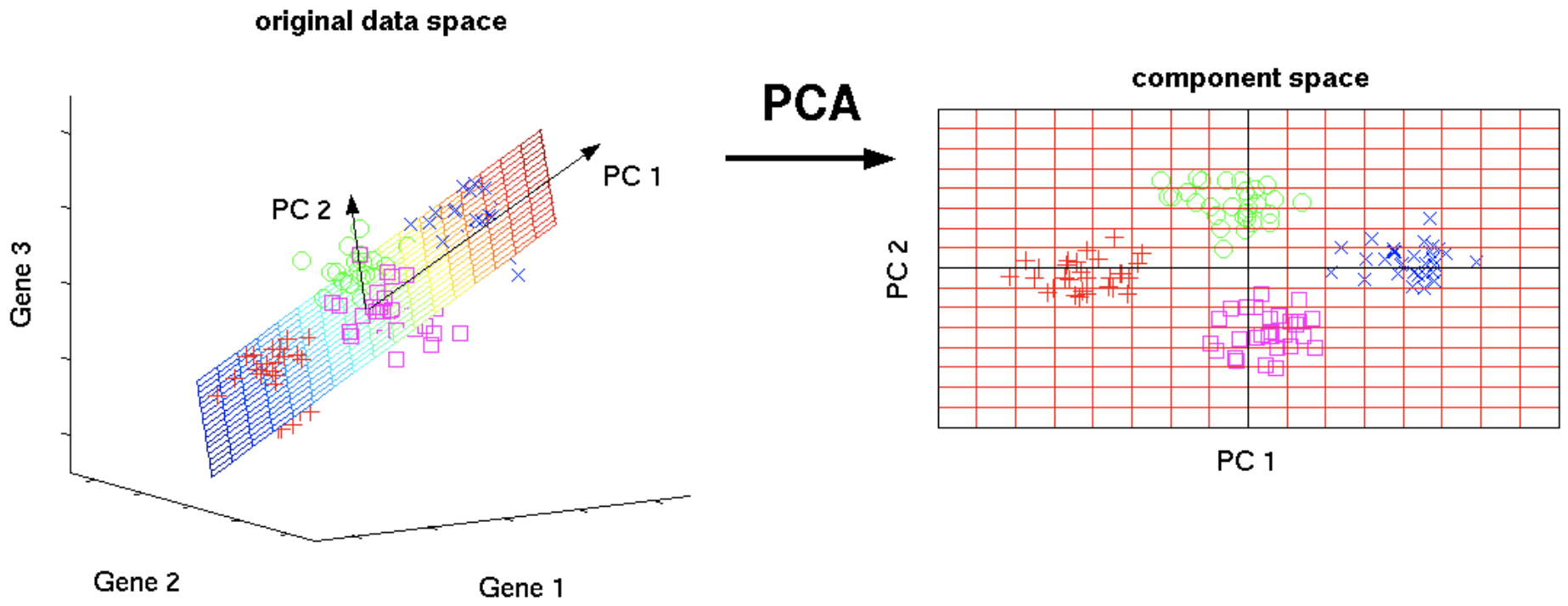
2.13s
.10s
.52s
.26s
.14s
.01s
.06s
.02s

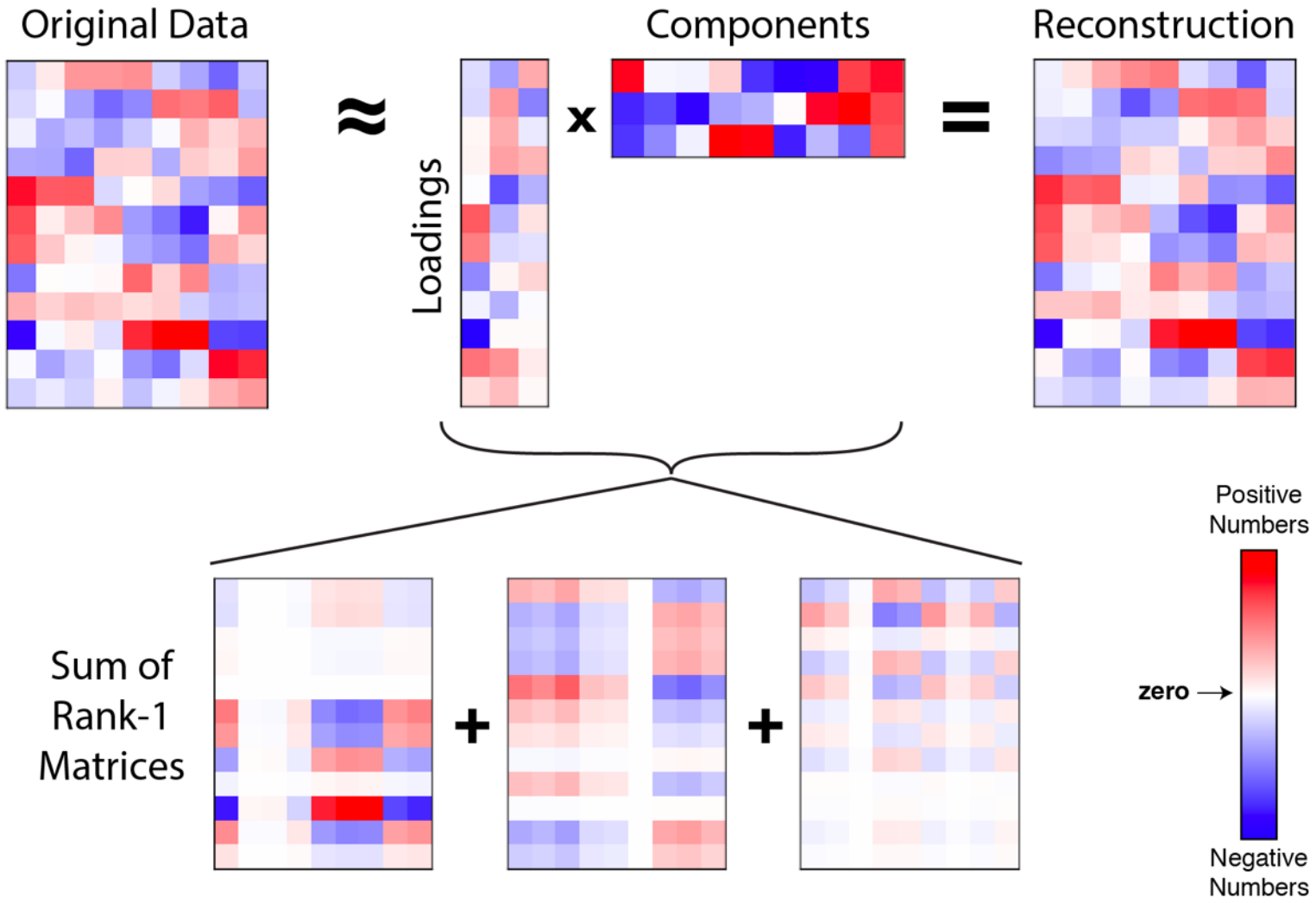
Machine Learning Problems

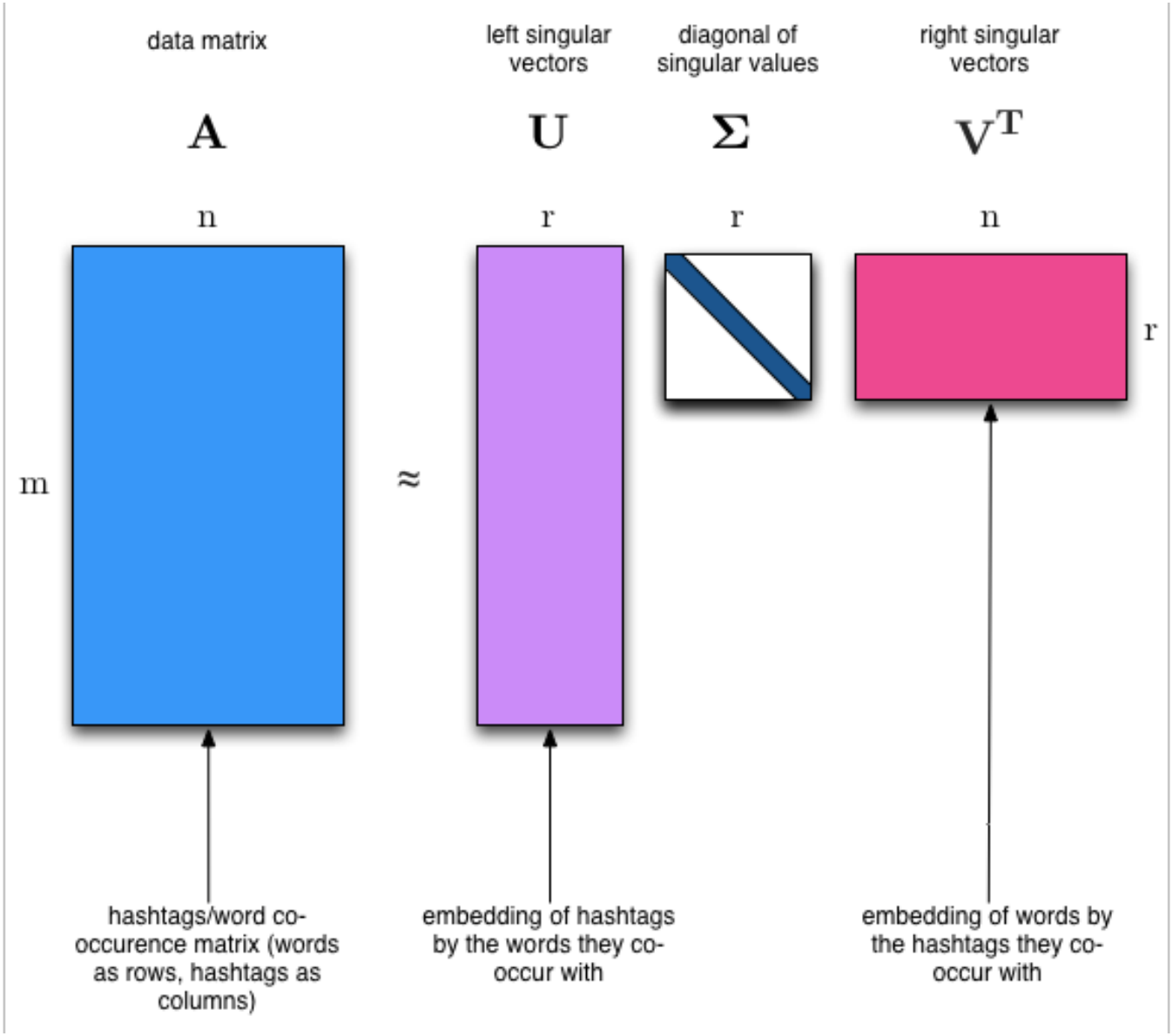


PCA

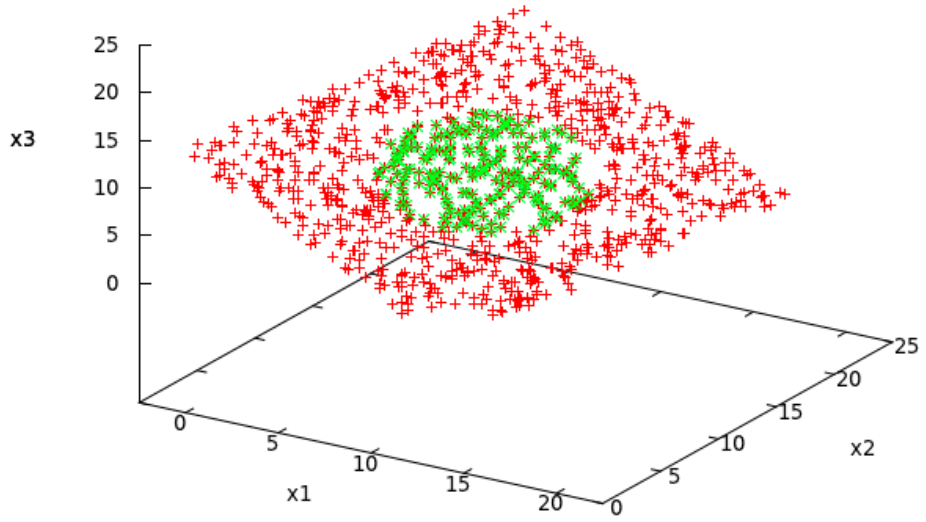

original data space
PC 1
PC 2
Gene 3
Gene 2
Gene 1
PCA
component space
PC 2
PC 1

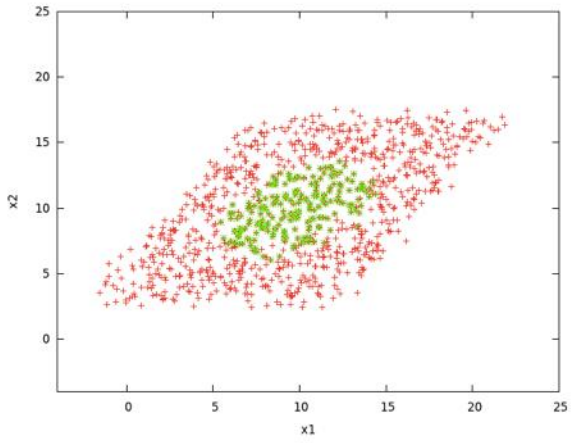
PCA Intuition

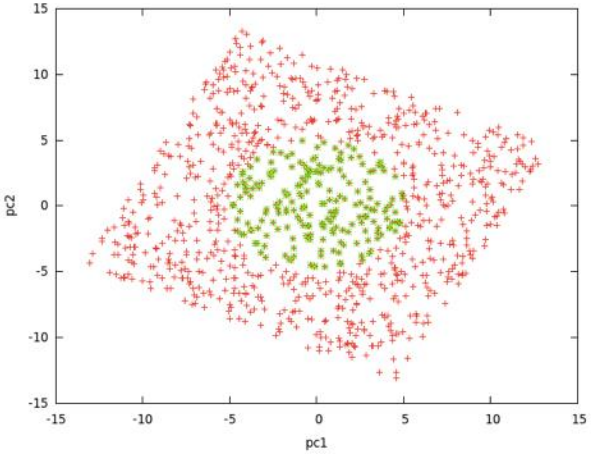



data matrix
left singular vectors
diagonal of singular values
right singular vectors
A
U
Σ
V^T
n
r
r
n
m
≈
r
hashtags/word co-occurence matrix (words as rows, hashtags as columns)
embedding of hashtags by the words they co-occur with
embedding of words by the hashtags they co-occur with

PRINCIPAL COMPONENT ANALYSIS (PCA)



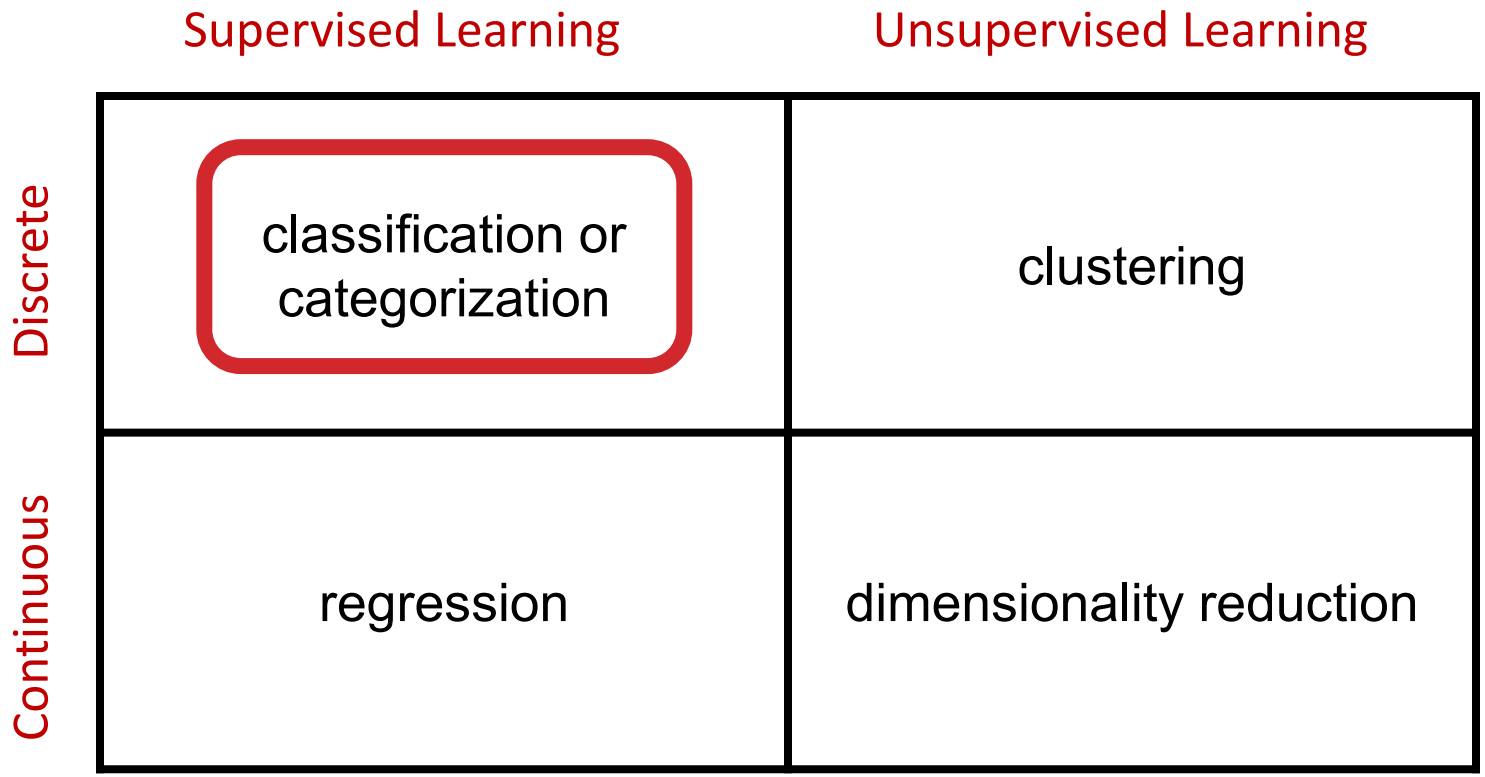




MACHINE LEARNING PROBLEMS

(Boosted-) Decision Trees

K-Means
Agglomerative clustering
DBScan



(Boosted-) Decision Trees

PCA

WHAT IS A CLASSIFIER

Apply a prediction function to a feature representation of an image/data-set to get the desired output:

f() = “apple”

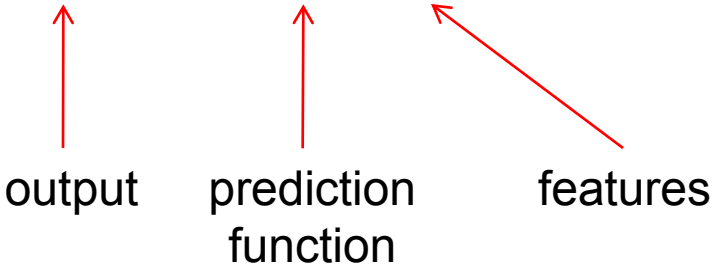
f() = “tomato”

f() = “cow”

Slide credit: L. Lazebnik

THE MACHINE LEARNING FRAMEWORK

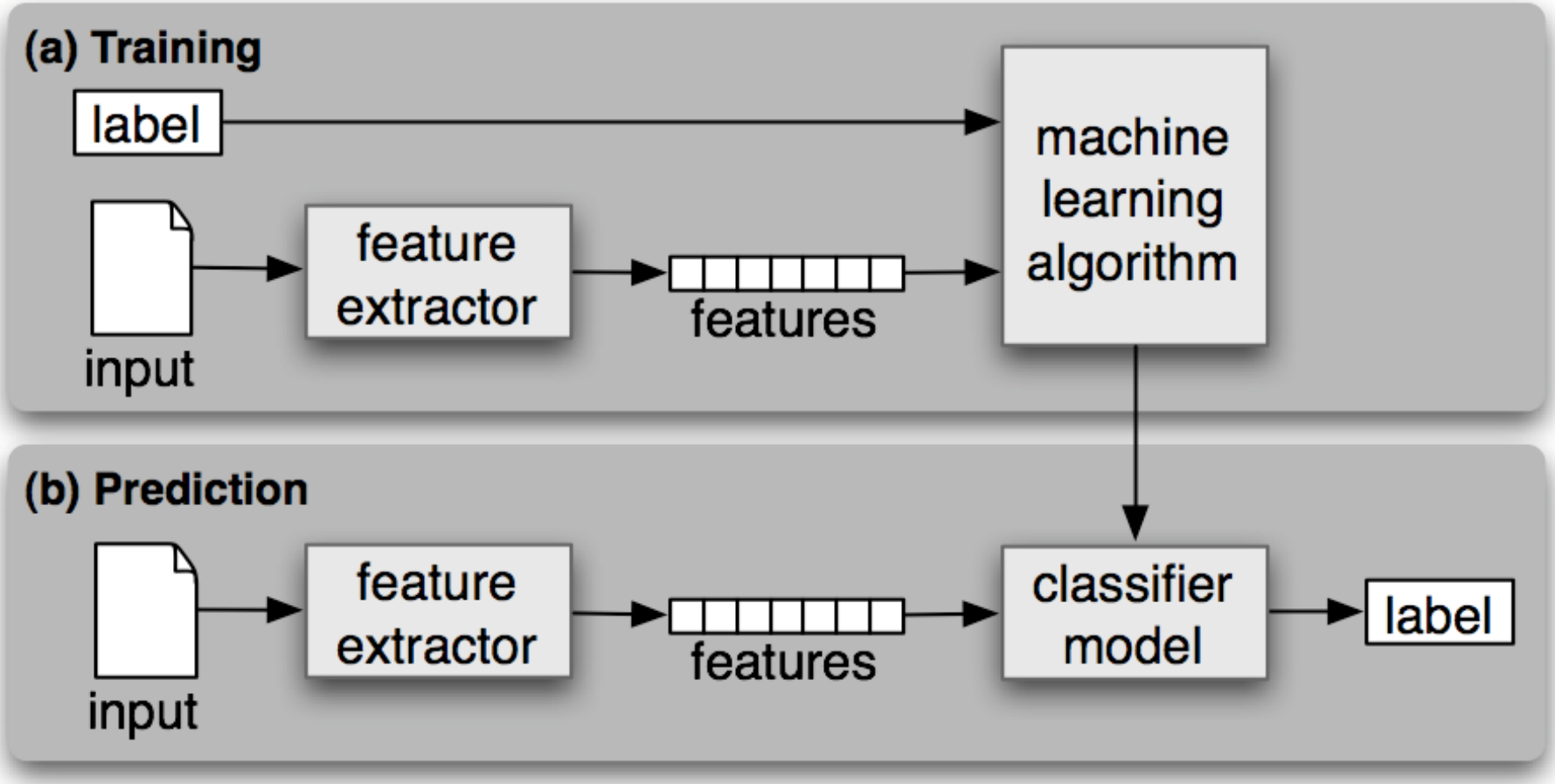
$$y = f(x)$$



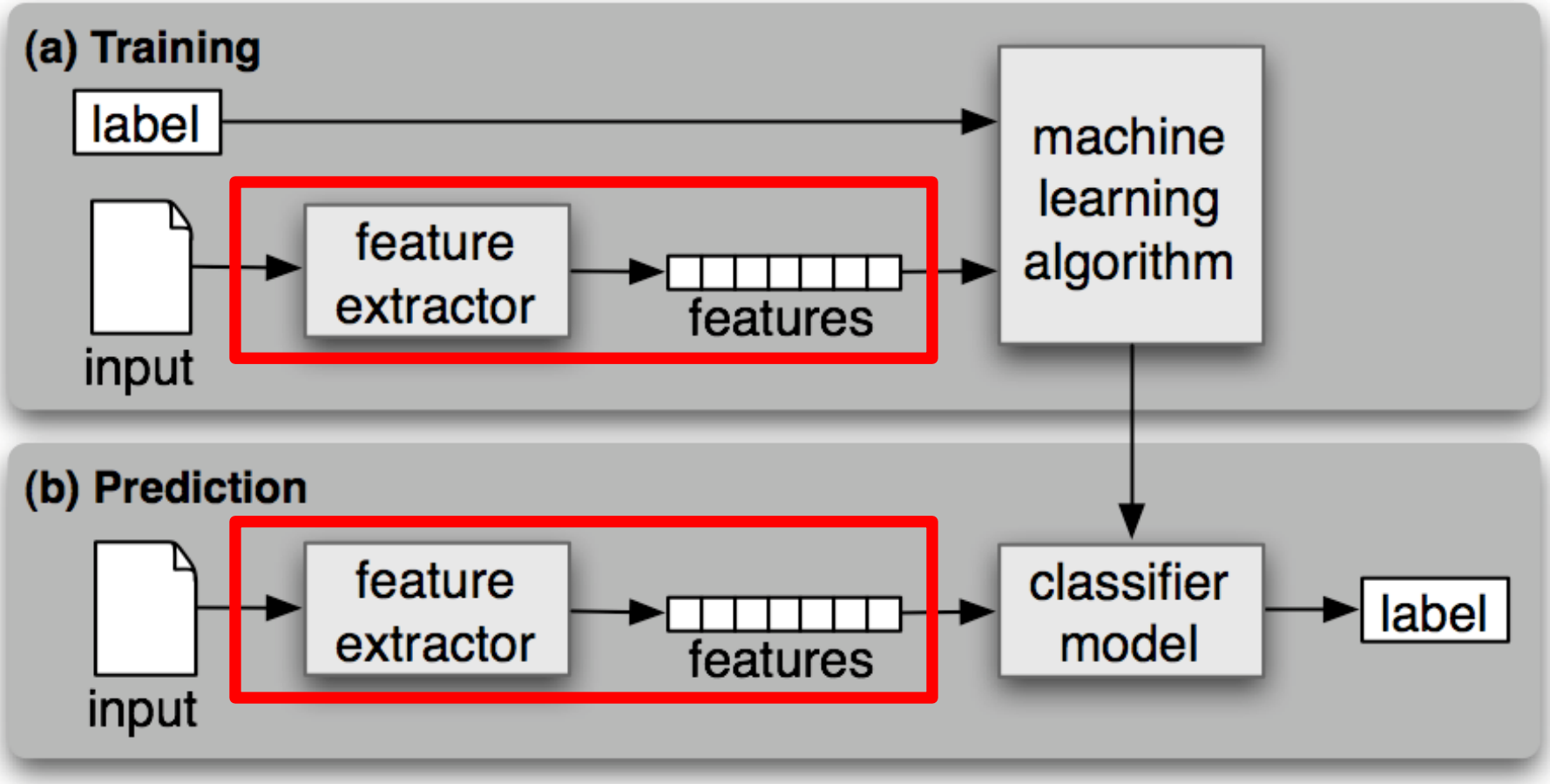
Training: given a *training set* of labeled examples $\{(x_1,y_1), \ldots, (x_N,y_N)\}$, estimate the prediction function f by minimizing the prediction error on the training set

Testing: apply f to a never before seen *test example* x and output the predicted value $y = f(x)$

ML PIPELINE (SUPERVISED)



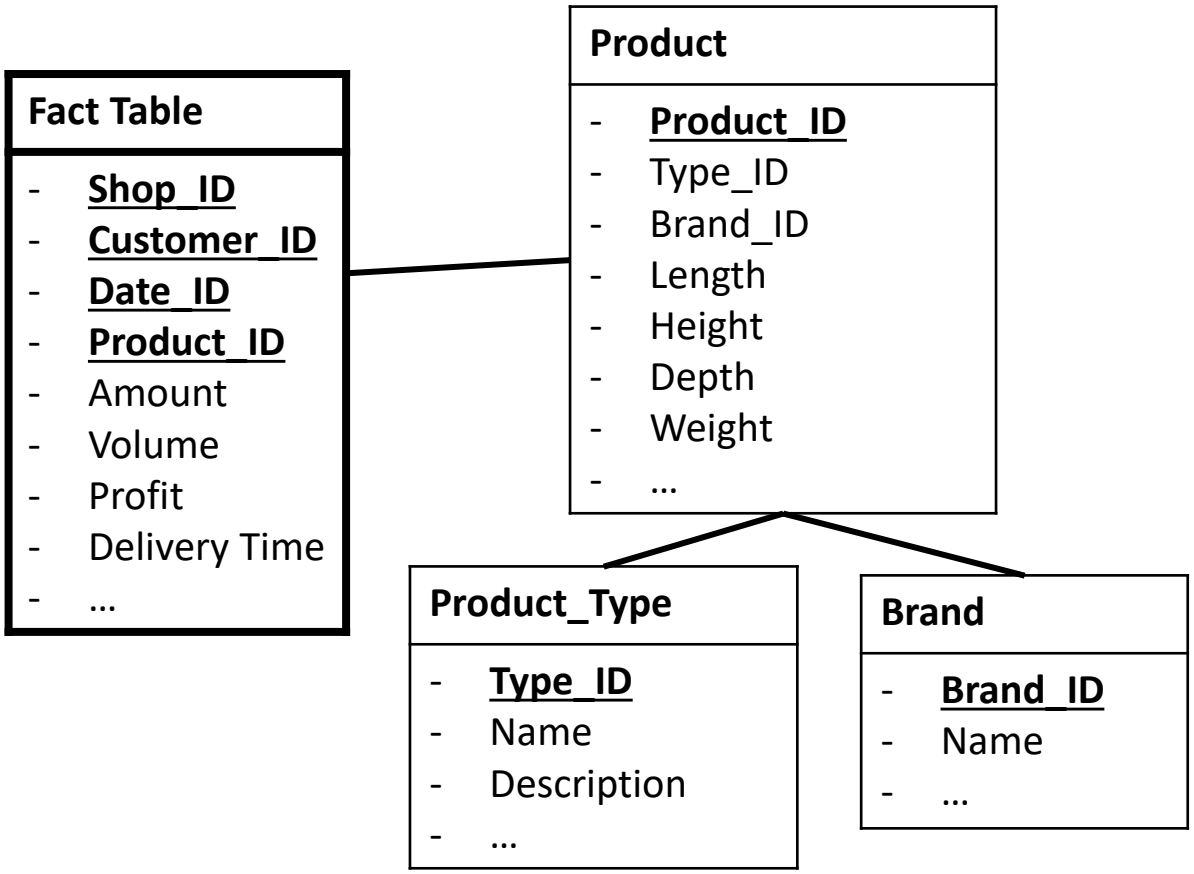
ML PIPELINE (SUPERVISED)



FEATURES

Fact Table

- **Shop_ID**
- **Customer_ID**
- **Date_ID**
- **Product_ID**
- Amount
- Volume
- Profit
- …

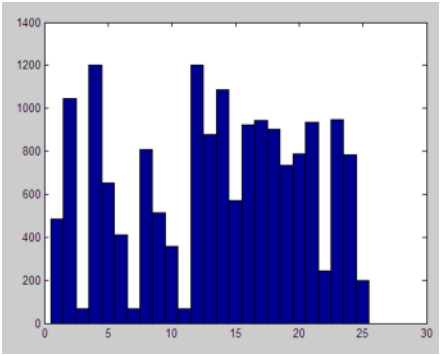


Custermer State	Product Type	Product Weight	Volume (L*H*D)	Month	Delivery Time

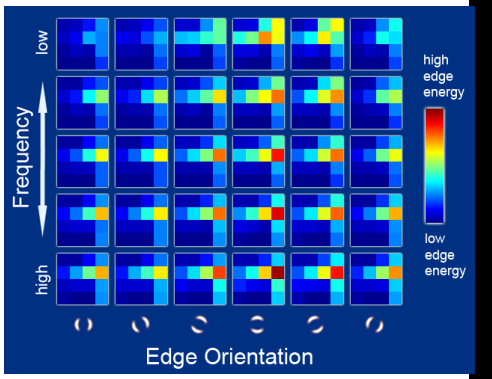
IMAGE FEATURES

Raw pixels

Histograms



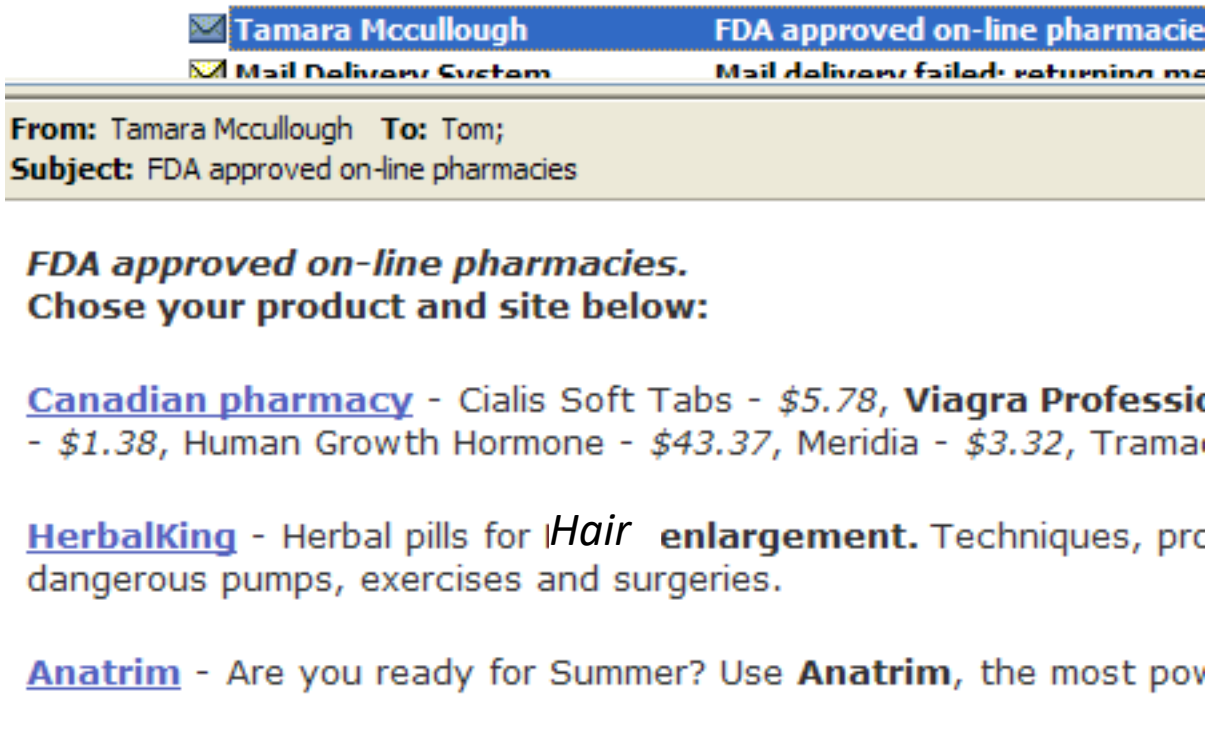
GIST descriptors

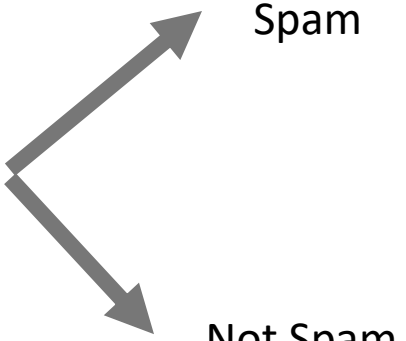


…

Slide credit: L. Lazebnik

TEXT FEATURES





Bag of Words

$$\begin{pmatrix} Viagra: 1 \\ Soft: 1 \\ Herbel: 2 \\ Pills: 2 \\ Are: 1 \\ \dots \end{pmatrix}$$

N-Grams

$$\begin{pmatrix} herbel\ pills: 1 \\ pills\ for: 1 \\ for\ Hair: 2 \\ Hair\ enlargement: 1 \\ surgeries: 2 \\ \dots \end{pmatrix}$$

ONE-HOT ENCODING

Bag of Words

$$\begin{pmatrix} Viagra \\ Soft \\ Herbel \\ Pills \\ Are \\ \dots \end{pmatrix}$$

ID	Viagra	Soft	Herbel	Pills	Are	….
Mail1	0	1	1	0	1	…
Mail2	1	0	0	1	1	…
…	…	…	…	…	…	…

PREDICTOR FOR GRAD-SCHOOL APPLICATIONS

Name	ZipCode	Age	Sex	Area	Avg Grade	Statement	Early admit	Accepted
Mike	02474	23	M	DB	B-	Since I was born, I knew I wanted to code. My first program I wrote in binary code literally in the sandbox, though I am not sure it was correct…	No	NO
Sam	02456	21	M	Sensor	A	Celine Dion's song "A New Day Has Come" taught me that CS is the best subject in the world. I never felt…	Yes	Yes
Amadou	15106	22	M	DB	A+	I want to get out of Pittsburgh.	No	Yes
Anna	02319	22	F	ML	A-	I already wrote 10 papers and I think I am ready to graduate now.	Yes	Yes
…	…	..	…	…	…	…	…	…

HOW WOULD YOU ENCODE THE TABLE?

PREDICTOR FOR GR[illegible]OOL APPLIC[illegible]

Encode as numbers (0-1)

Encode as numbers (0-1)

Bag of words 1-Hot Encoding

Remove (information leakage)

Name	ZipCode	Age	Sex	Area	Avg Grade	Statement	Early admit	Accepted
Mike	02474	23	M	DB	B-	Since I was born, I knew I wanted to code. My first program I wrote in binary code literally in the sandbox, though I am not sure it was correct…	No	NO
Sam	02456	21	null	Sensor	A	Celine Dion's song "A New Day Has Come" taught me that CS is the best subject in the world. I never felt…	Yes	Yes
Amadou	15106	22	M	DB	A+	I want to get out of Pittsburgh.	No	Yes
Anna	null	22	F	ML	A-	I already wrote 10 papers and I think I am ready to graduate now.	Yes	Yes
…	…	..	…	…	…	…	…	…

Remove identifiers

Encode as (1) Lat/Lon and scale to 0-1, or remove

Scale to 0-1

1-Hot Encode or remove

PREDICTOR FOR GRAD-SCHOOL APPLICATIONS

Name	ZipCode	Age	Sex	Area	Avg Grade	Statement	Early admit	Accepted
Mike	02474	23	M	DB	B-	Since I was born, I knew I wanted to code. My first program I wrote in binary code literally in the sandbox, though I am not sure it was correct…	No	NO
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Amadou	15106	22	M	DB	A+	I want to get out of Pittsburgh.	No	Yes
Anna	null	22	F	ML	A-	I already wrote 10 papers and I think I am ready to graduate now.	Yes	Yes
…	…	..	…	…	…	…	…	…

No zip	Lon	Lat	Age	M	F	Other	ML	DB	Sens	Avg Grade	Born	Celine	Pittsburg	…	Accepted
0	.123	.0222	0.8	1	0	1	0	1	0	0.5	1	0	0	…	NO
0	.123	.0123	0.5	1	0	M	0	0	1	0	0	1	0	…	Yes
0	.031	.0322	0.5	1	0	M	0	1	0	0	0	0	1	…	Yes
1			0.5	0	1	F	1	0	0	0.1	0	0	0	…	Yes
…	…	…	…	…	…	…	…	…	…	…	…	…	…	…	…

MANY CLASSIFIERS TO CHOOSE FROM

K-nearest neighbor

Support Vector Machines

Decision Trees

Random Forrest

(Gradient) Boosted Decision Trees

Logistic Regression

Naïve Bayes

Bayesian network

RBMs

….

Which is the best one?

Slide credit: D. Hoiem

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Naïve Bayes

Bayesian network

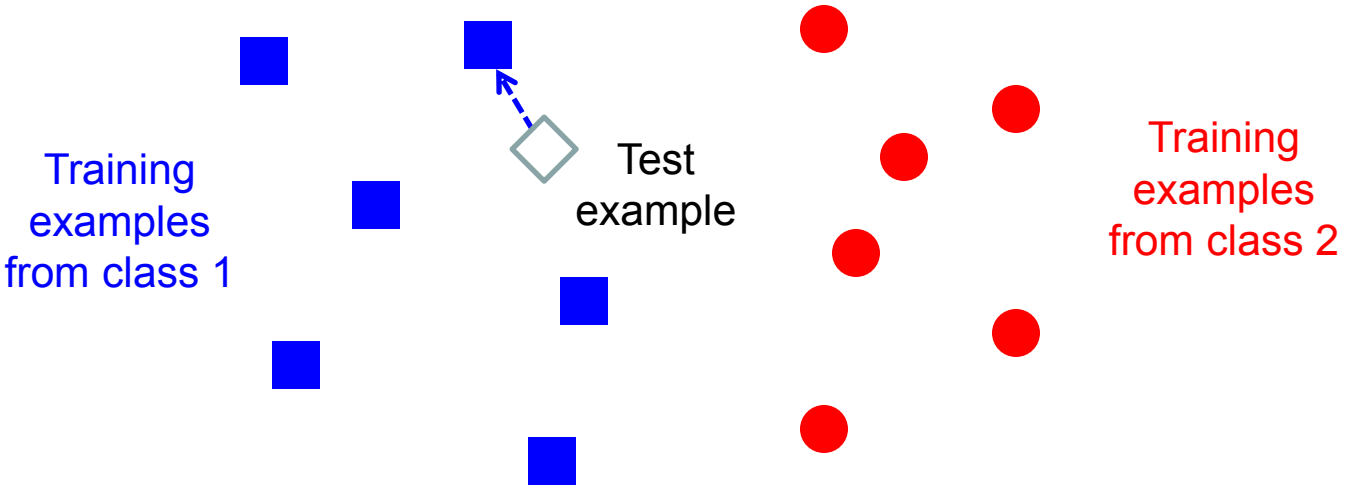
RBMs

….

Which is the best one?

Slide credit: D. Hoiem

CLASSIFIERS: NEAREST NEIGHBOR

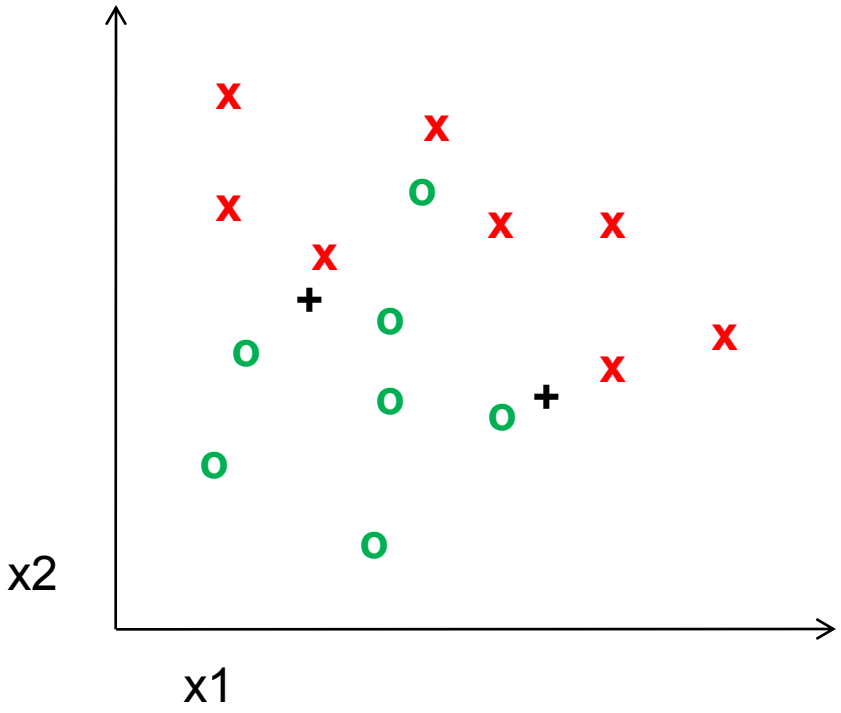


f(**x**) = label of the training example nearest to **x**

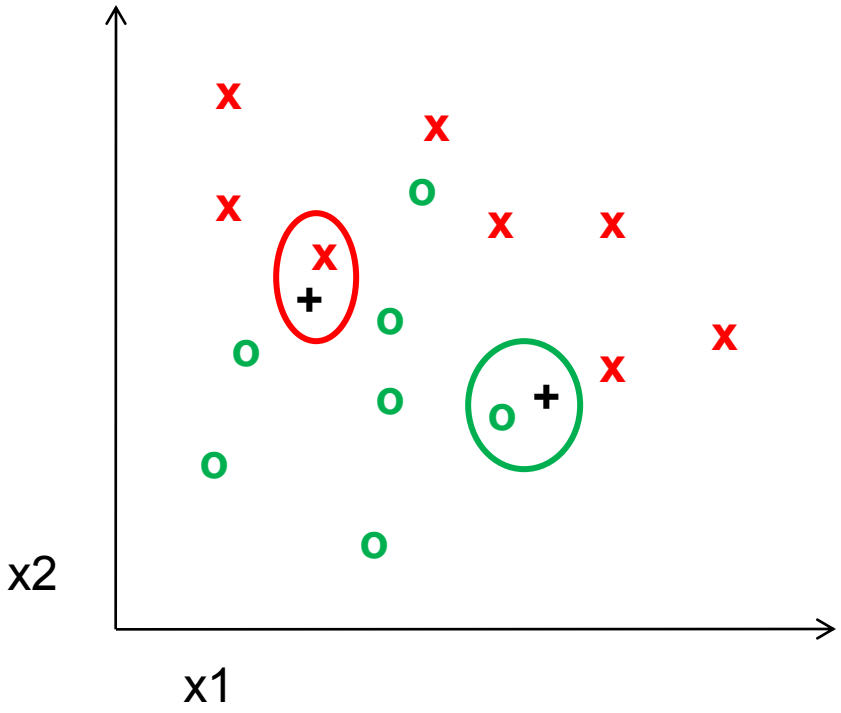
- All we need is a distance function for our inputs
- No training required!

Slide credit: L. Lazebnik

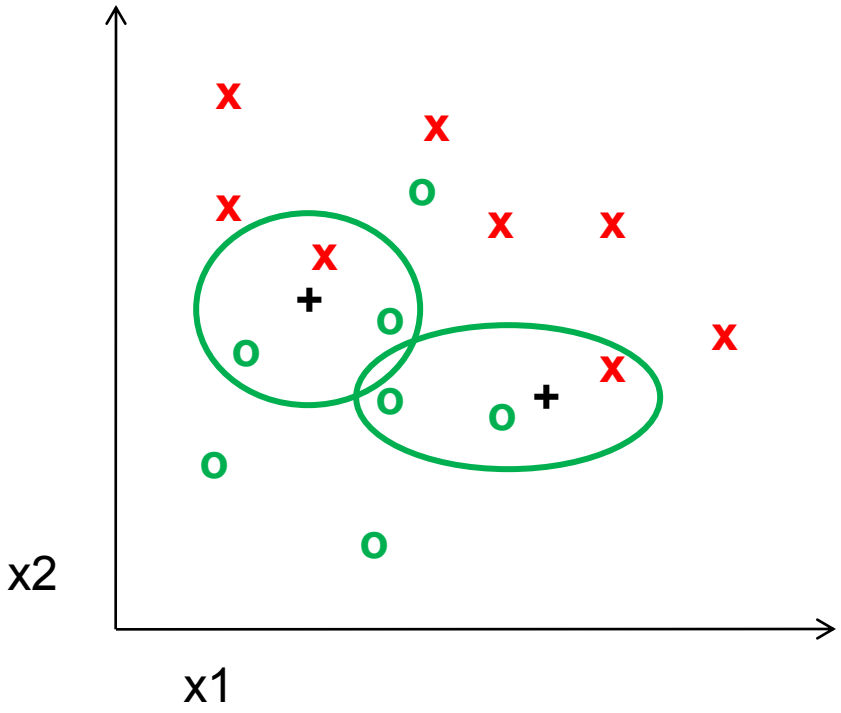
K-NEAREST NEIGHBOR



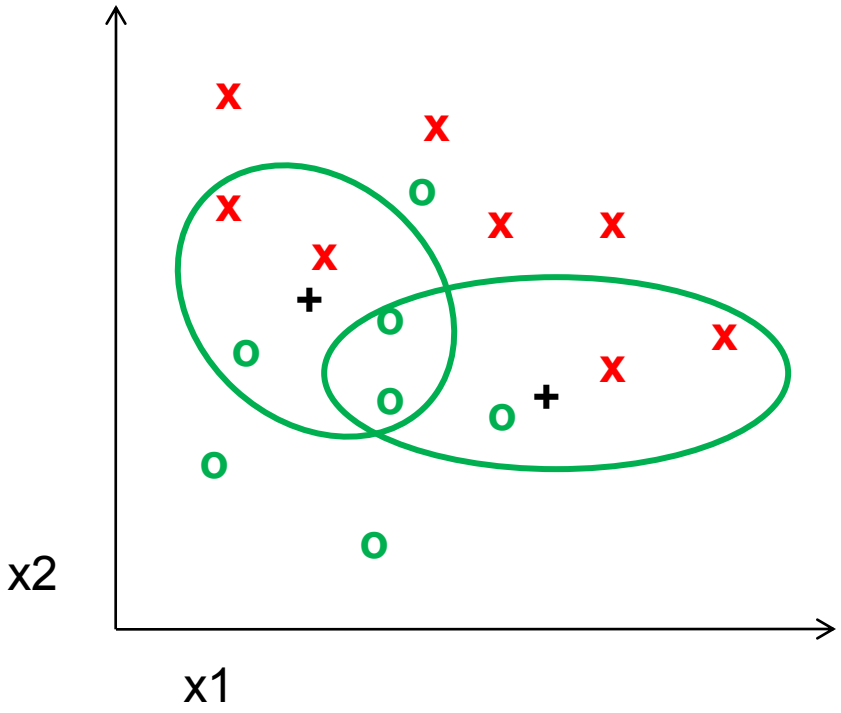
1-NEAREST NEIGHBOR



3-NEAREST NEIGHBOR

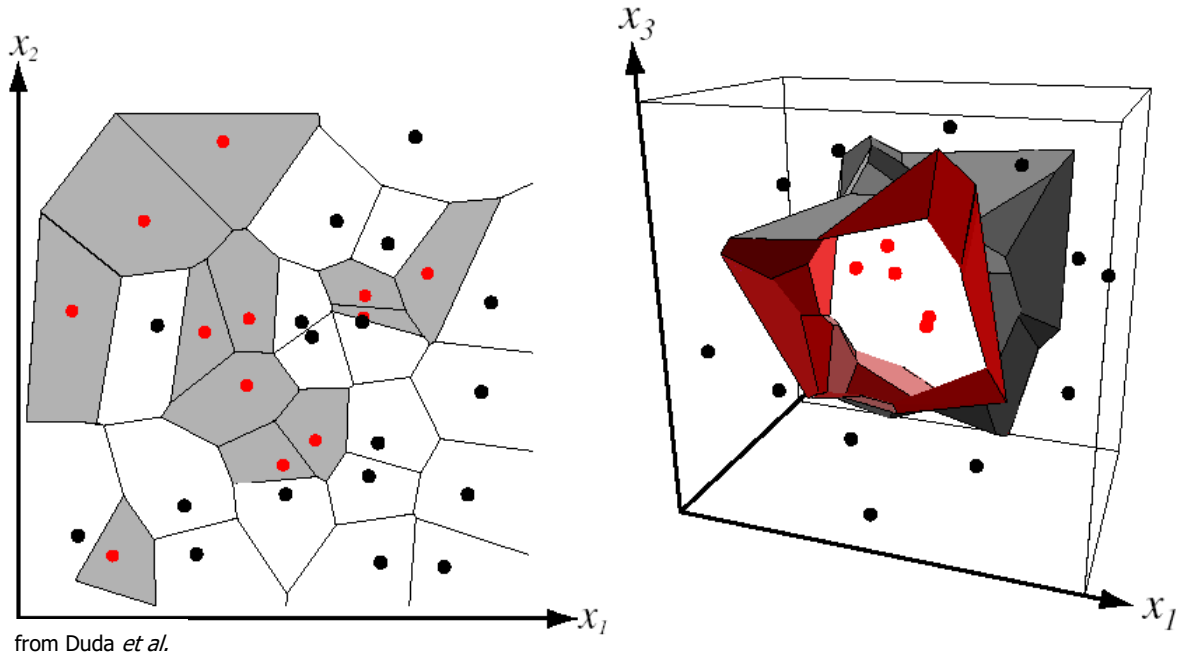


5-NEAREST NEIGHBOR



DECISION BOUNDARIES KNN

Assign label of nearest training data point to each test data point



from Duda *et al.*

Voronoi partitioning of feature space
for two-category 2D and 3D data

Source: D. Lowe

MANY CLASSIFIERS TO CHOOSE FROM

K-nearest neighbor

Support Vector Machines

Decision Trees

Random Forrest

(Gradient) Boosted Decision Trees

Logistic Regression

Naïve Bayes

Bayesian network

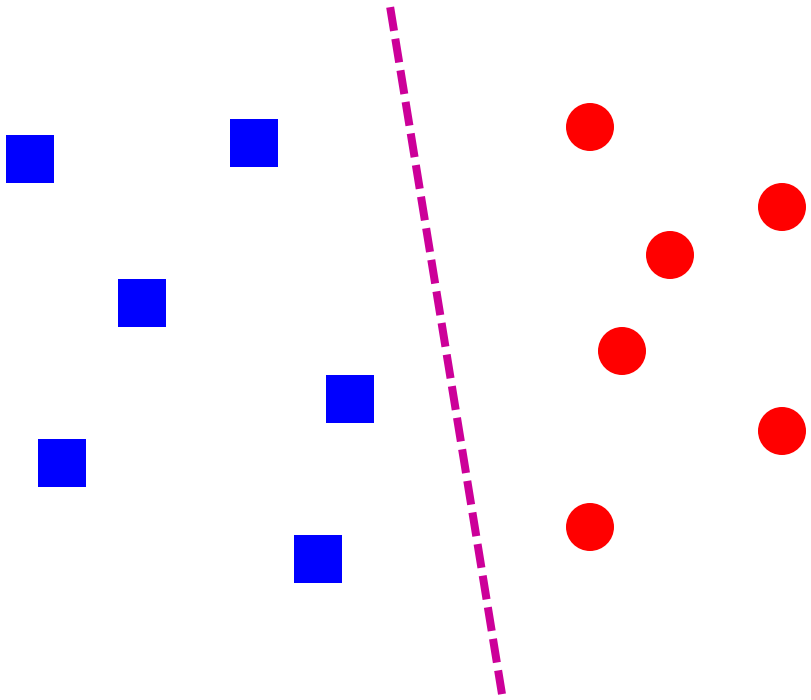
RBMs

….

Which is the best one?

Slide credit: D. Hoiem

CLASSIFIERS: LINEAR

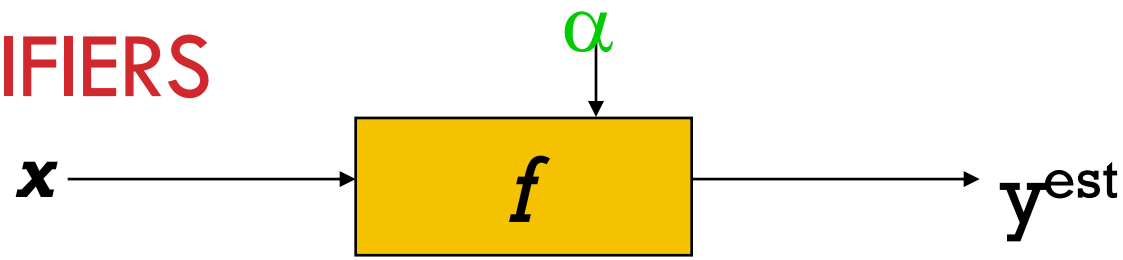


Find a *linear function* to separate the classes:

$$f(x) = \text{sgn}(w \cdot x + b)$$

Slide credit: L. Lazebnik

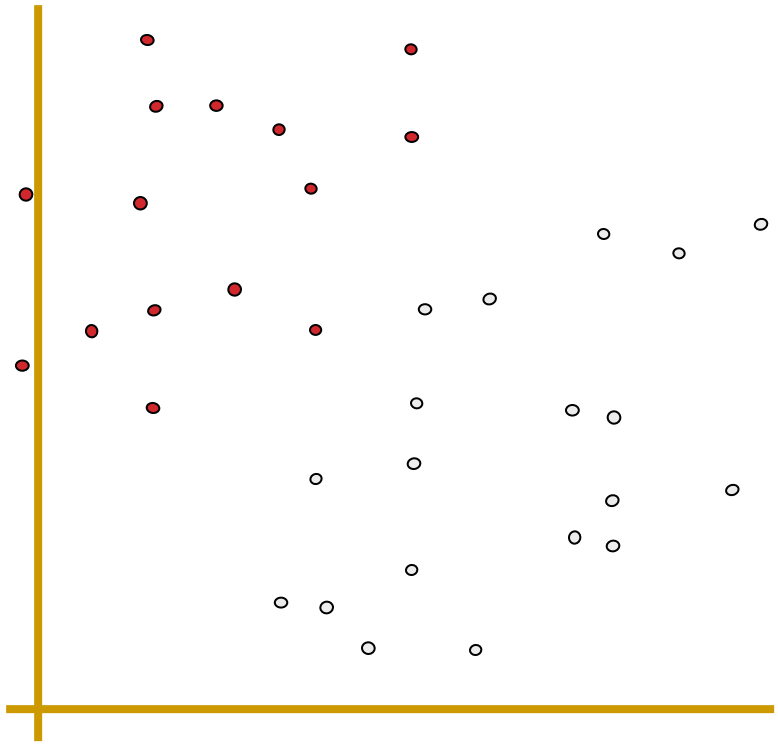
LINEAR CLASSIFIERS



$f(\mathbf{x}, \mathbf{w}, b) = sign(\mathbf{w}.\mathbf{x} - b)$

denotes +1

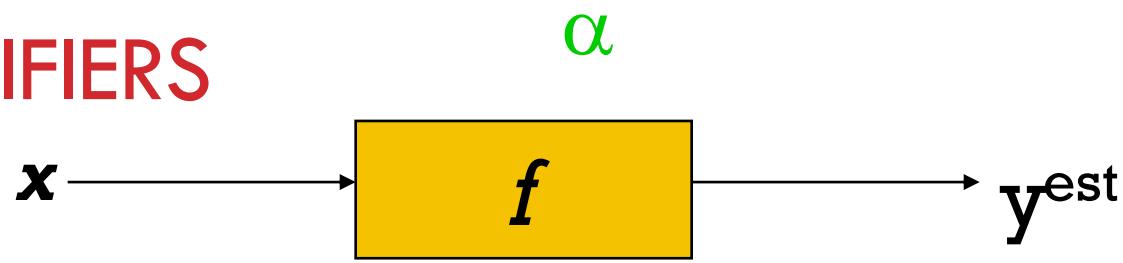
denotes -1



How would you classify this data?

Slides from Andrew W. Moore

LINEAR CLASSIFIERS



$f(x,w,b) = sign(w.x - b)$

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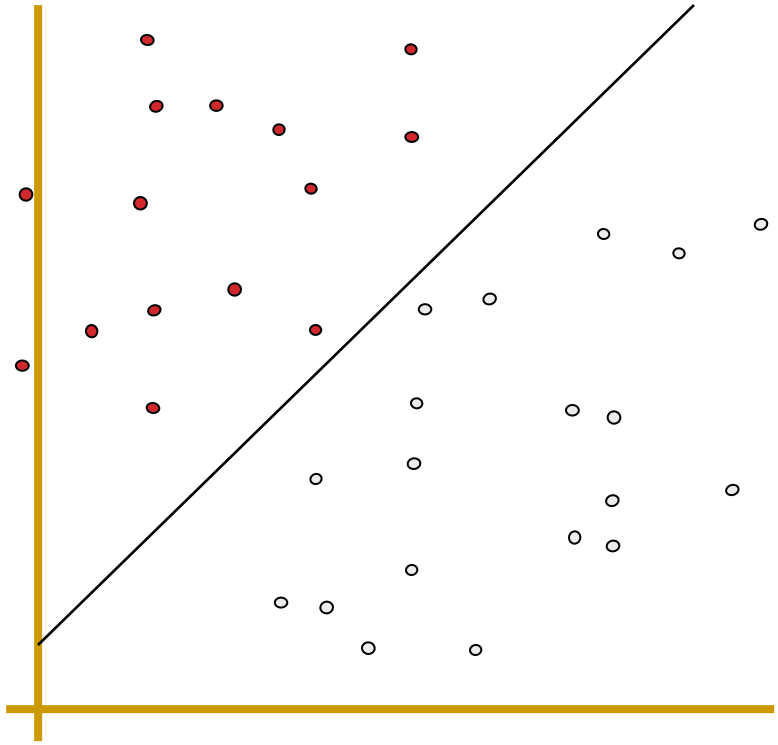

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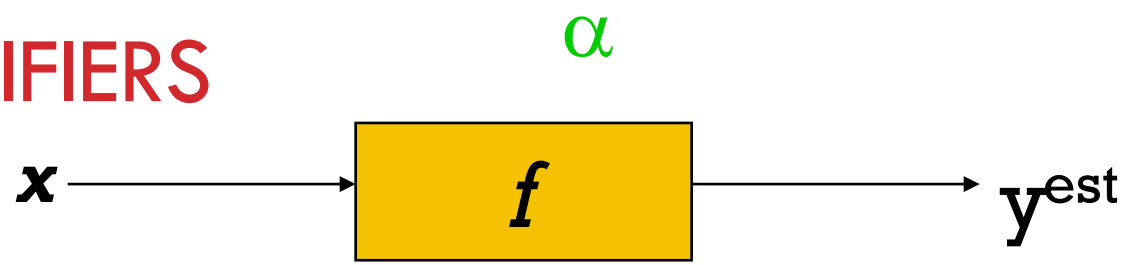
LINEAR CLASSIFIERS



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denotes +1

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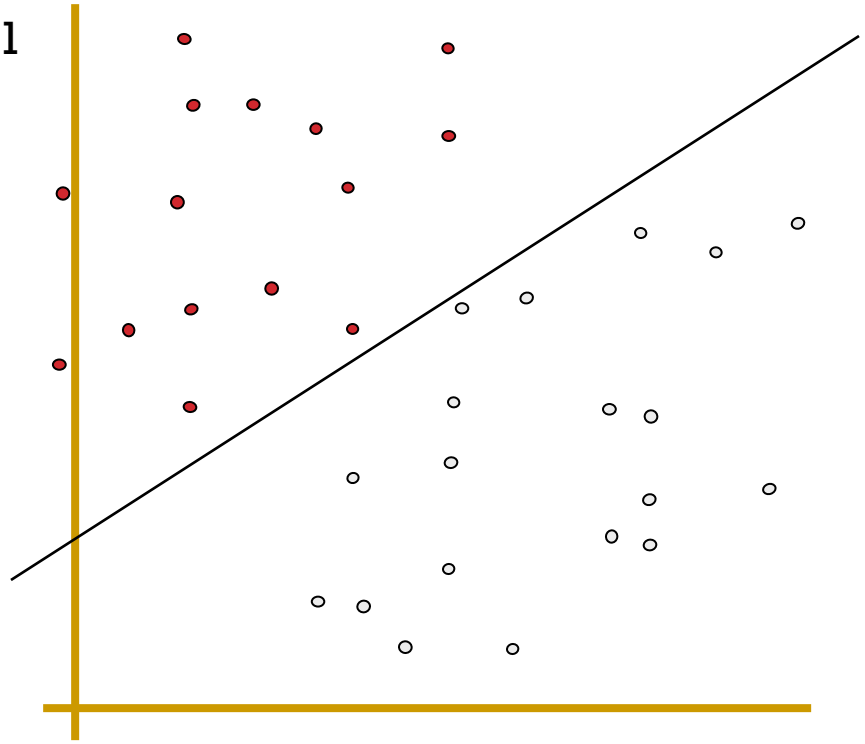

How would you classify this data?

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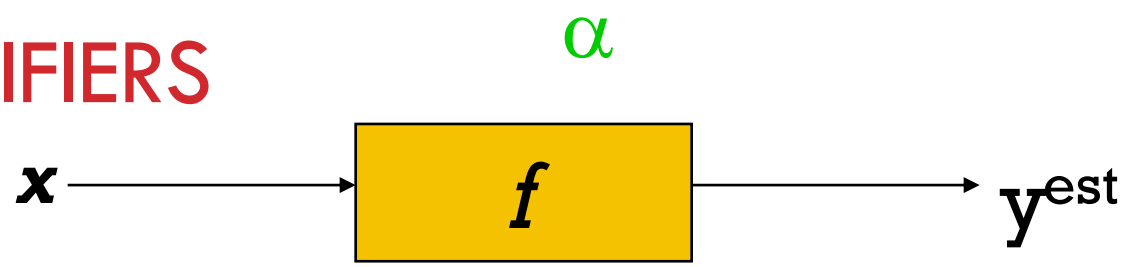
LINEAR CLASSIFIERS



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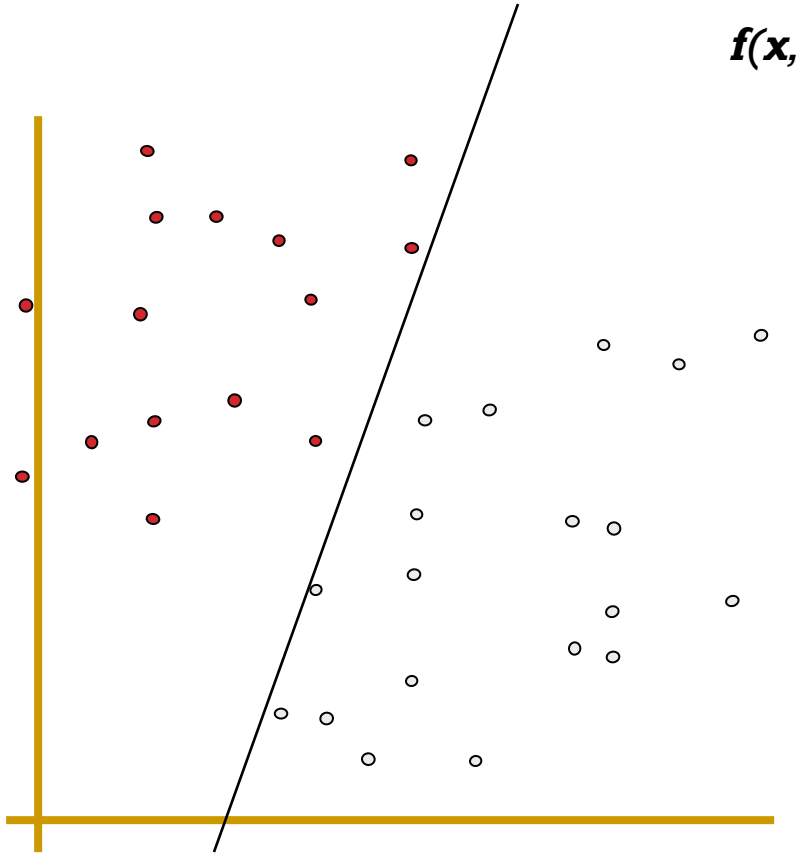
denotes +1

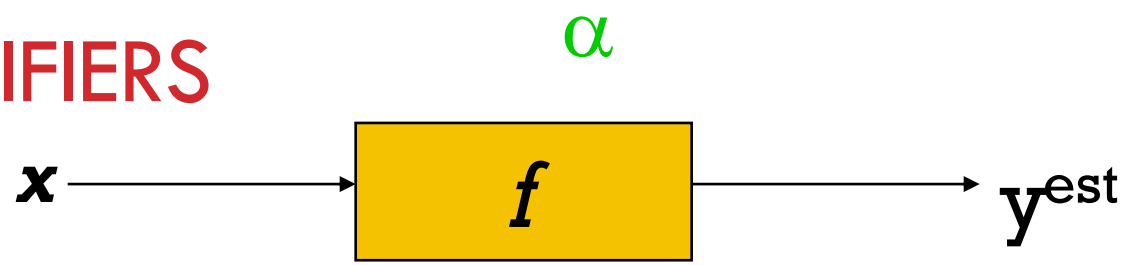
denotes -1

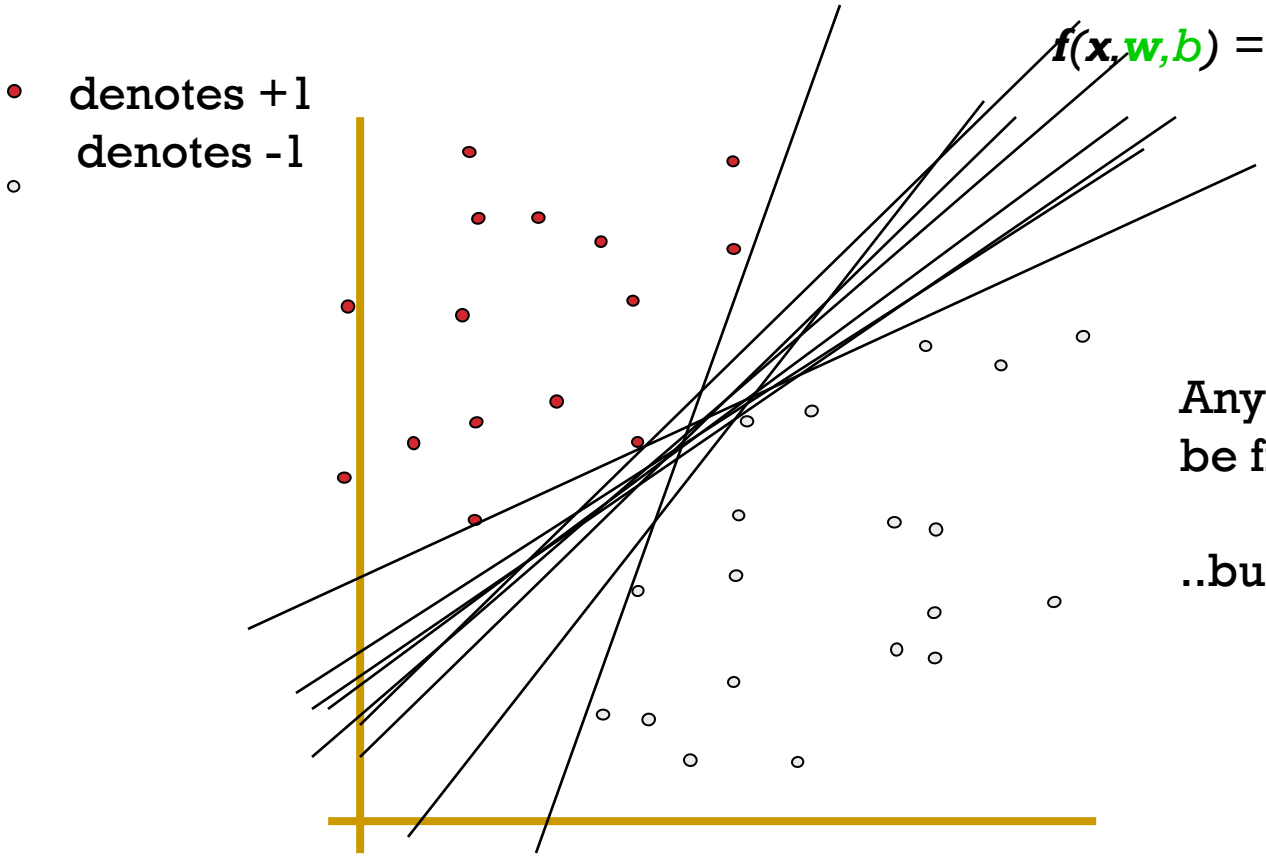


How would you classify this data?

Slides from Andrew W. Moore

LINEAR CLASSIFIERS



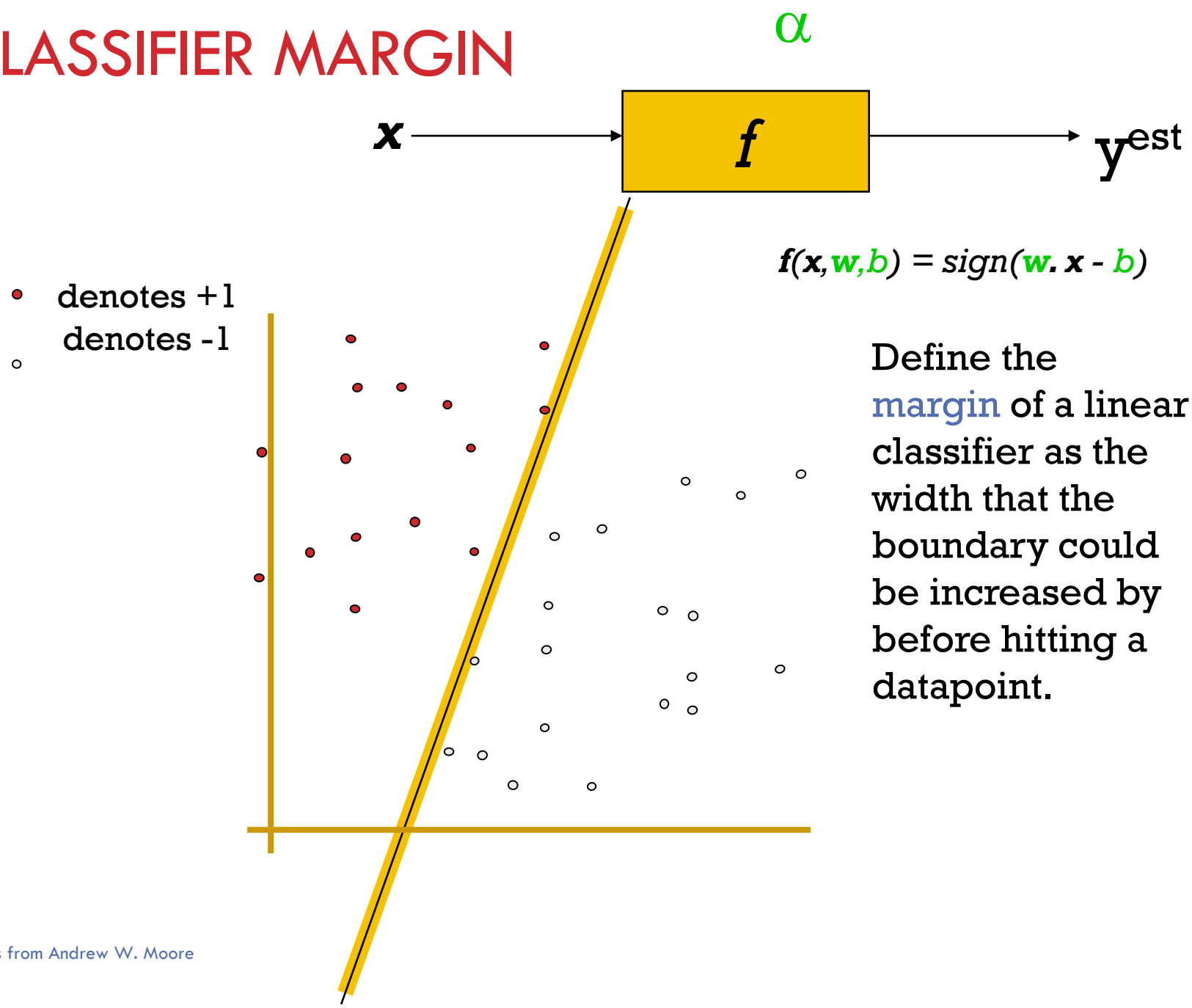


Any of these would be fine..

..but which is best?

Slides from Andrew W. Moore

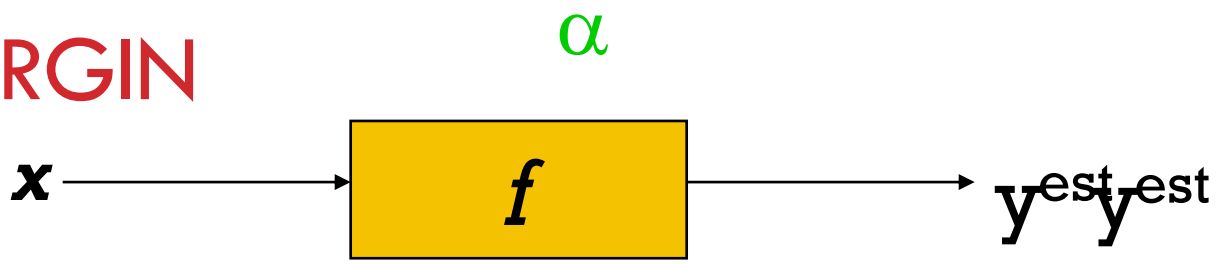
CLASSIFIER MARGIN

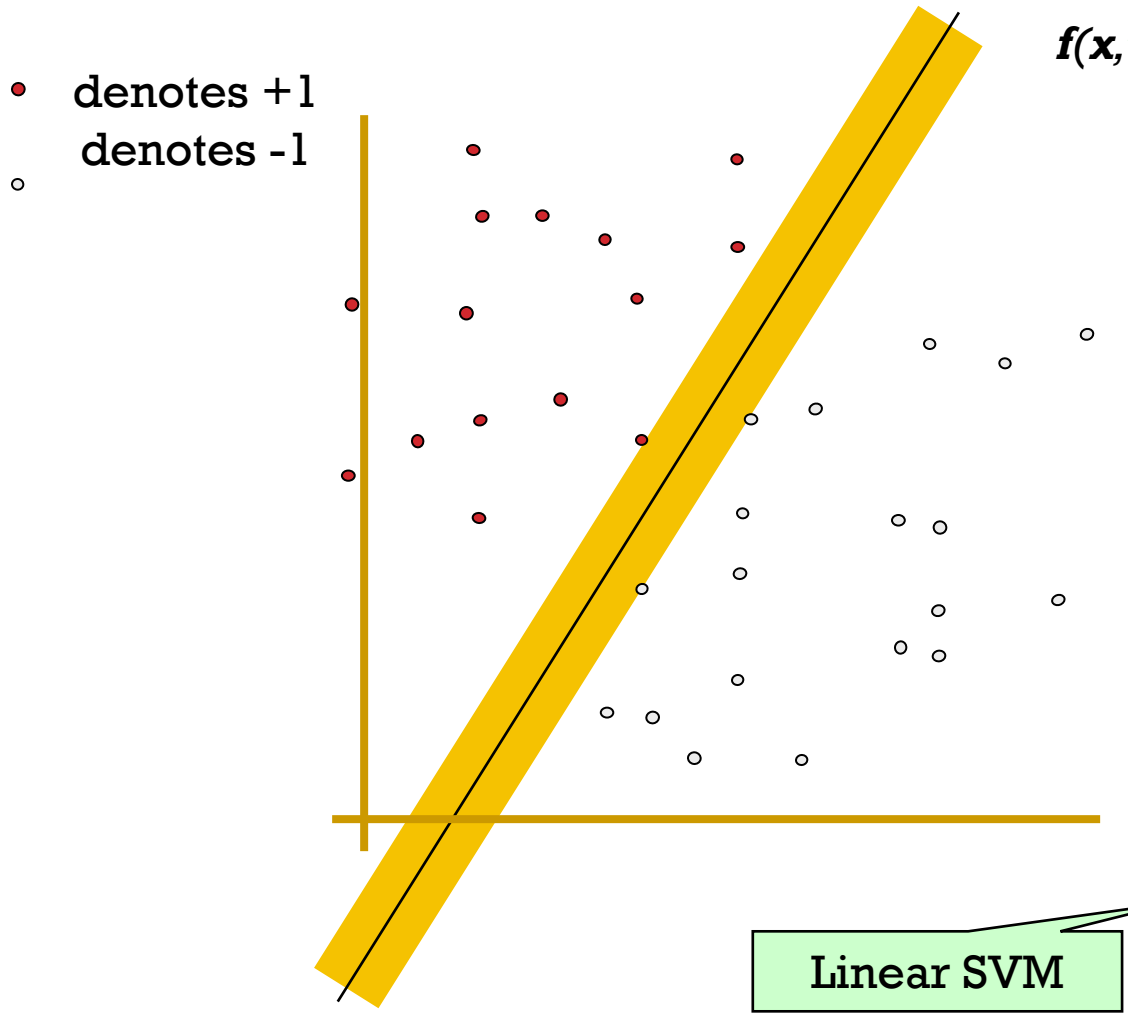


Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Slides from Andrew W. Moore

MAXIMUM MARGIN





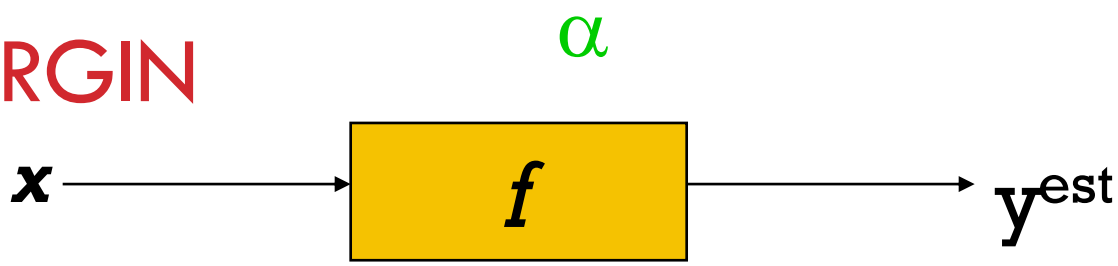
$f(x,w,b) = sign(w.x - b)$

The maximum margin linear classifier is the linear classifier with the, um, maximum margin. This is the simplest kind of SVM (Called an LSVM)

Linear SVM

Slides from Andrew W. Moore

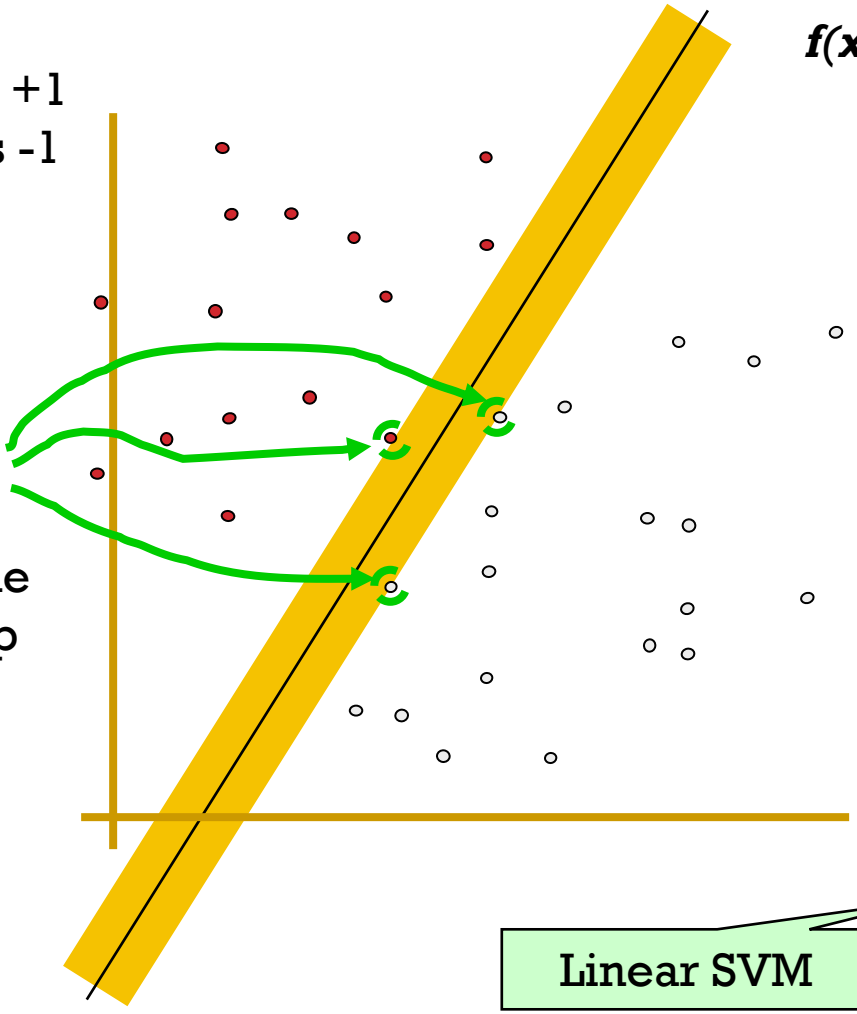
MAXIMUM MARGIN



$f(x,w,b) = sign(w.x - b)$

denotes +1

denotes -1



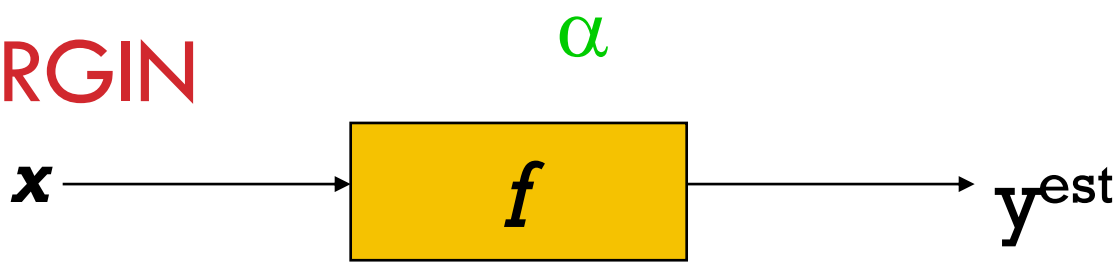
Support Vectors are those datapoints that the margin pushes up against

The maximum margin linear classifier is the linear classifier with the, um, maximum margin. This is the simplest kind of SVM (Called an LSVM)

Linear SVM

Slides from Andrew W. Moore

MAXIMUM MARGIN



$f(x,w,b) = sign(w.x - b)$

denotes +1

denotes -1

The maximum

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the

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n,

margin.

This is the simplest kind of SVM (Called an LSVM)

Linear SVM

Support

are thos

datapoi

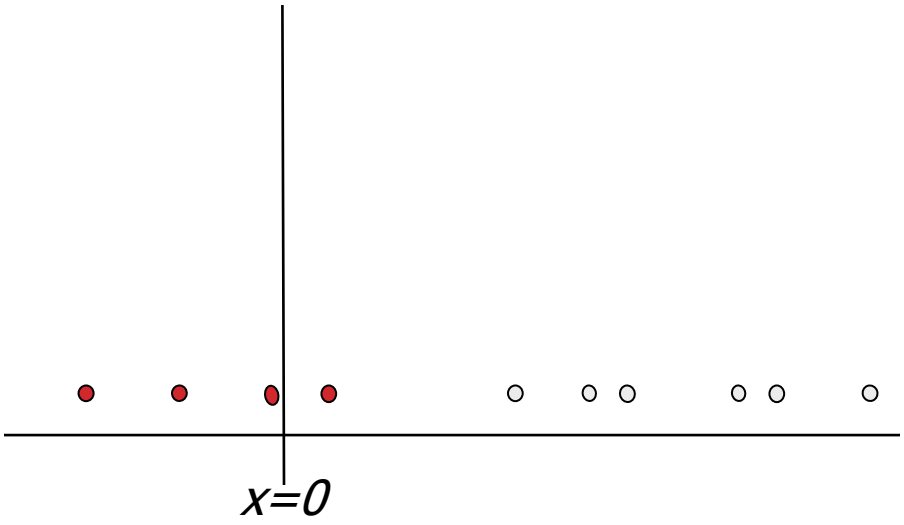
margin pushes up against

`sklearn.linear_model.SGDClassifier`

Default loss: "hinge" → linear SVM.

Slides from Andrew W. Moore

SUPPOSE WE'RE IN 1-DIMENSION

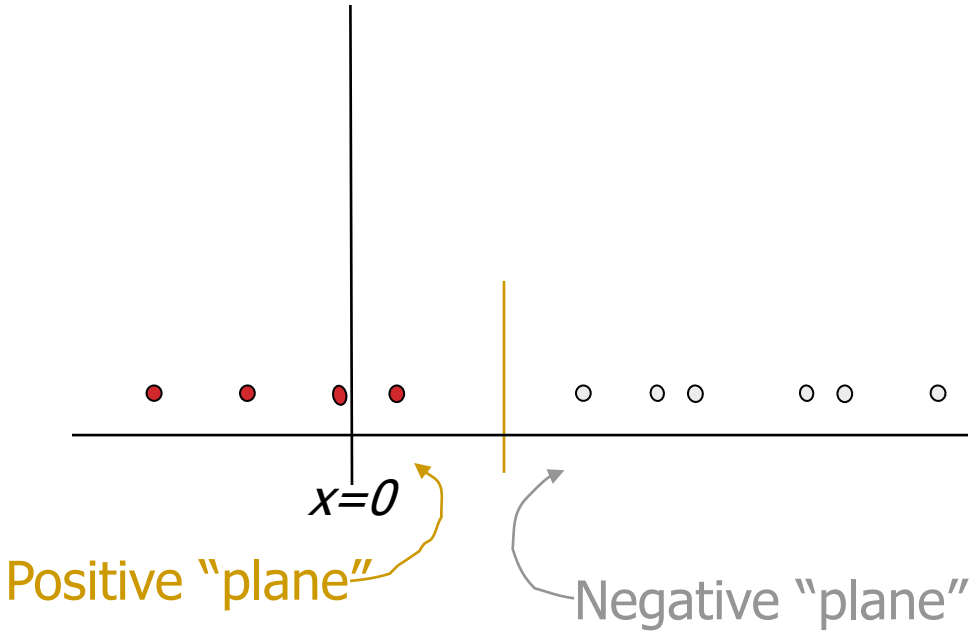


What would SVMs do with this data?

Slides from Andrew W. Moore

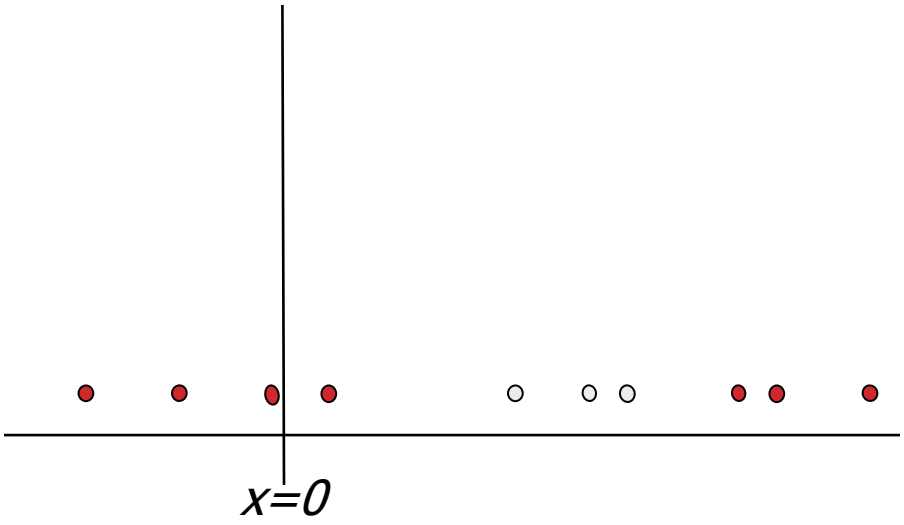
SUPPOSE WE'RE IN 1-DIMENSION

Not a big surprise



Slides from Andrew W. Moore

HARDER 1-DIMENSIONAL DATASET

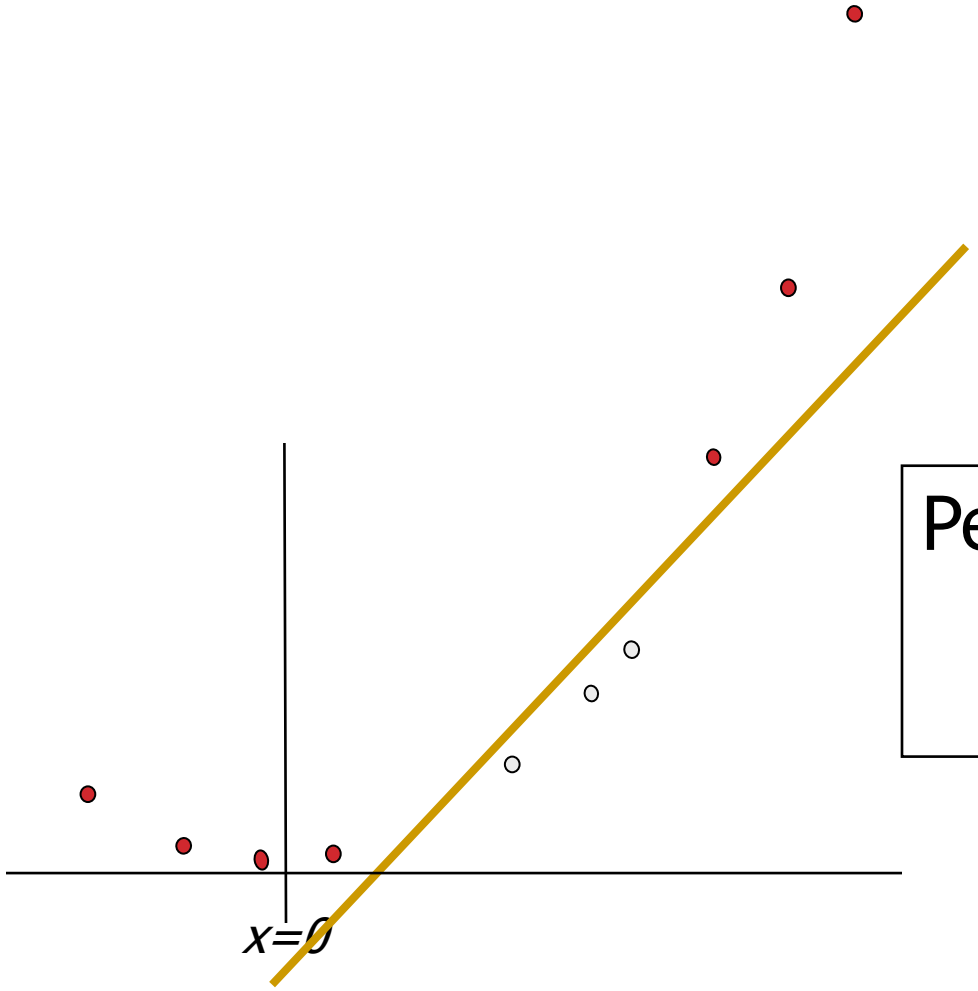


That's wiped the smirk off SVM's face.

What can be done about this?

Slides from Andrew W. Moore

HARDER 1-DIMENSIONAL DATASET

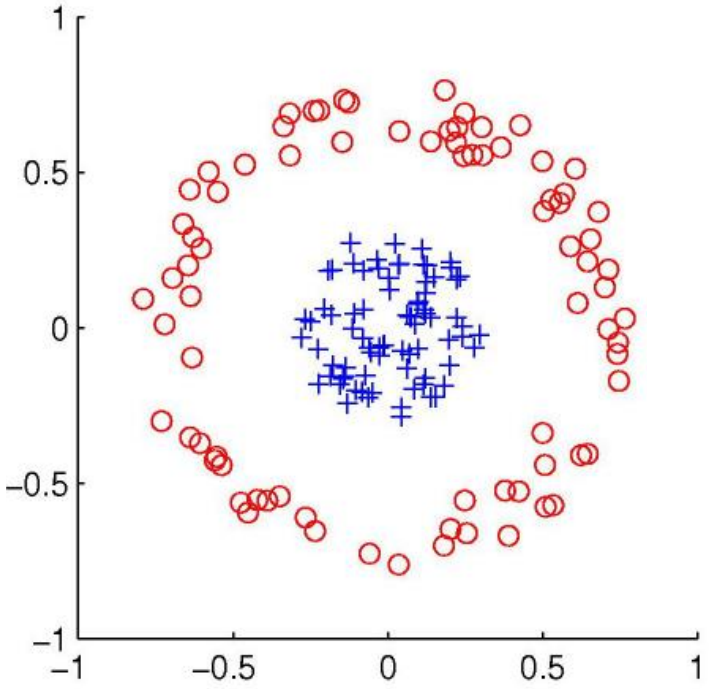


Permitting non-linear basis functions

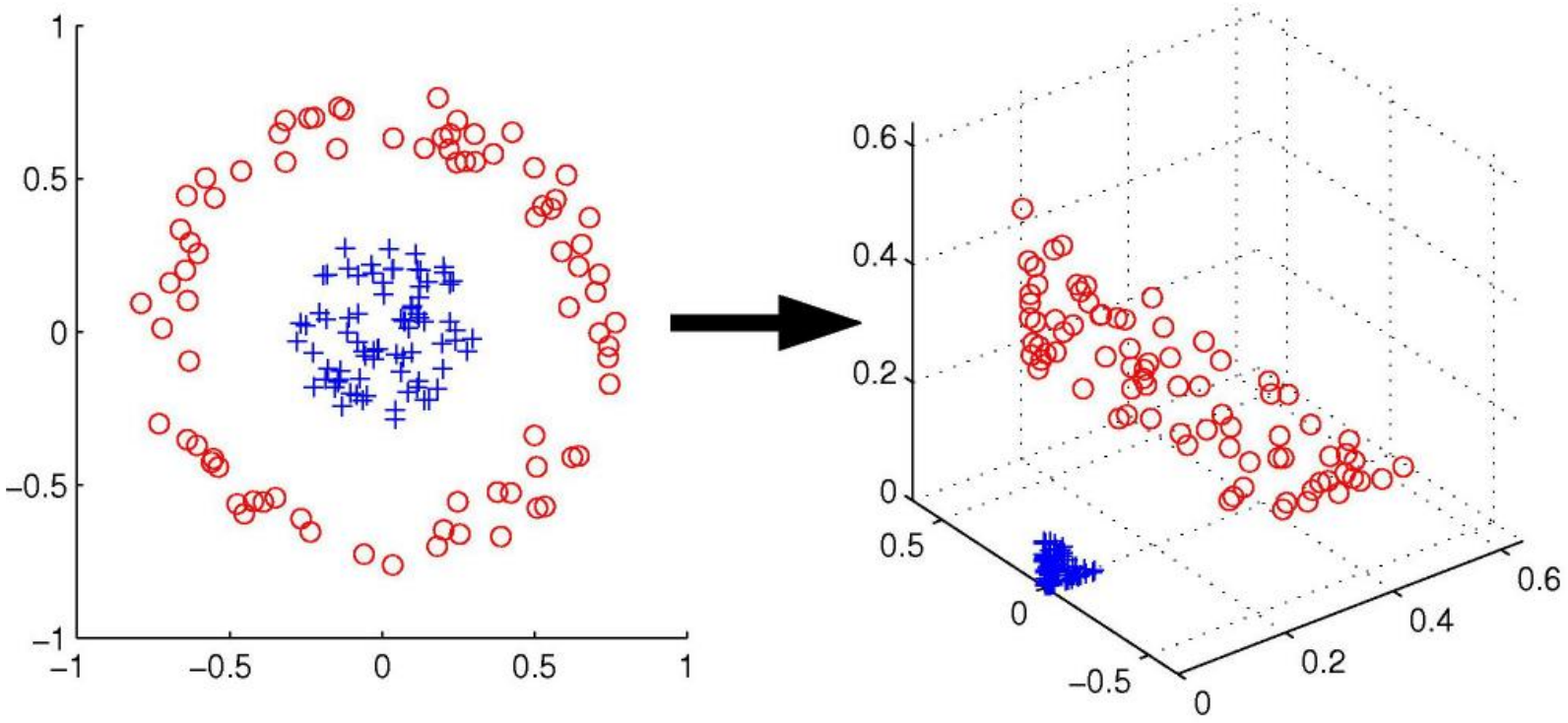
$$\mathbf{z}_k = (x_k, x_k^2)$$

Slides from Andrew W. Moore

THE KERNEL TRICK



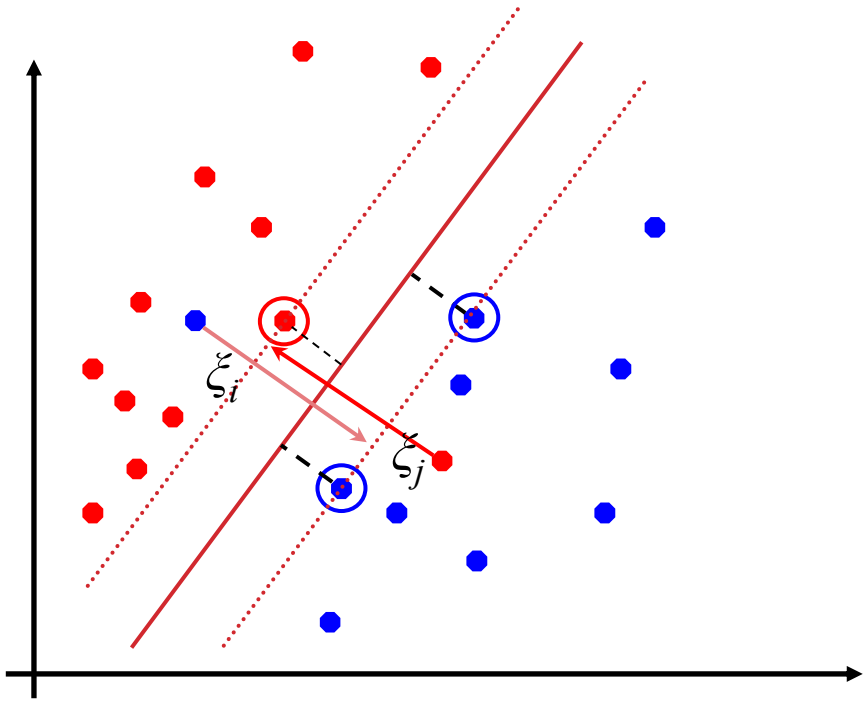
THE KERNEL TRICK



$$\phi: \quad \Re^2 \longrightarrow \Re^3$$
$$(x_1, x_2) \longmapsto (z_1, z_2, z_3) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

[http://www.cs.berkeley.edu/~jordan/courses/281B-spring04/lectures/lec3.pdf]

SOFT MARGIN CLASSIFICATION

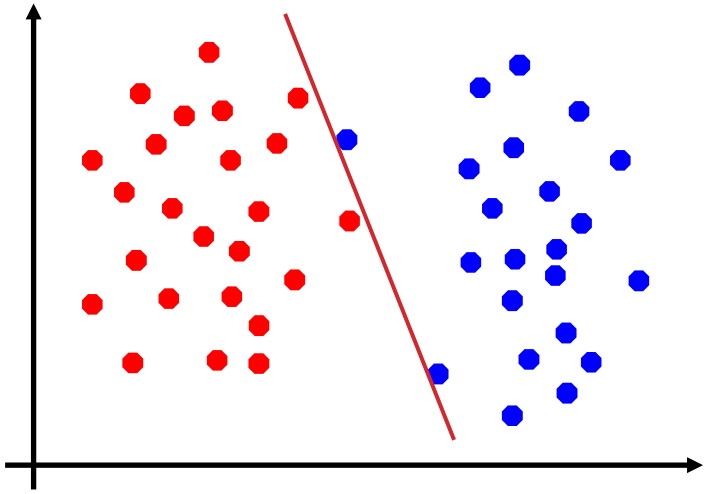


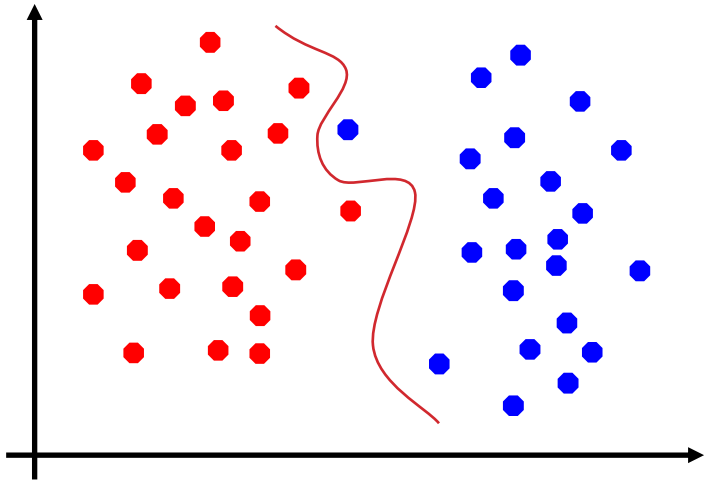
If the training data is not linearly separable, *slack variables* ξ_i (a regularization parameter) can be added to allow misclassification of difficult or noisy examples.

Still, try to minimize training set errors, and to place hyperplane "far" from each class (large margin)

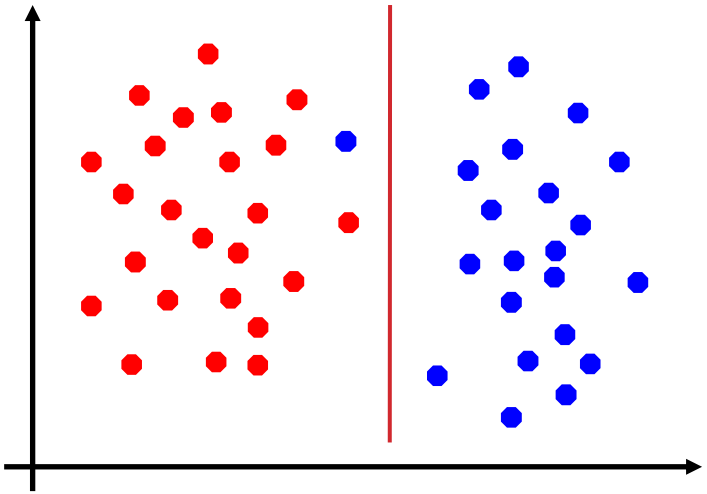
THE IMPACT OF REGULARIZATION

No regularization

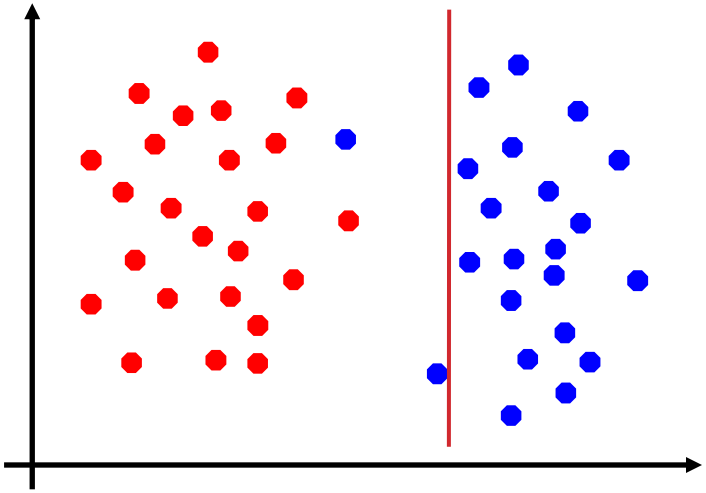




Right amount



Too much



MANY CLASSIFIERS TO CHOOSE FROM

K-nearest neighbor

Support Vector Machines

Decision Trees

Random Forrest

(Gradient) Boosted Decision Trees

Logistic Regression

Naïve Bayes

Bayesian network

RBMs

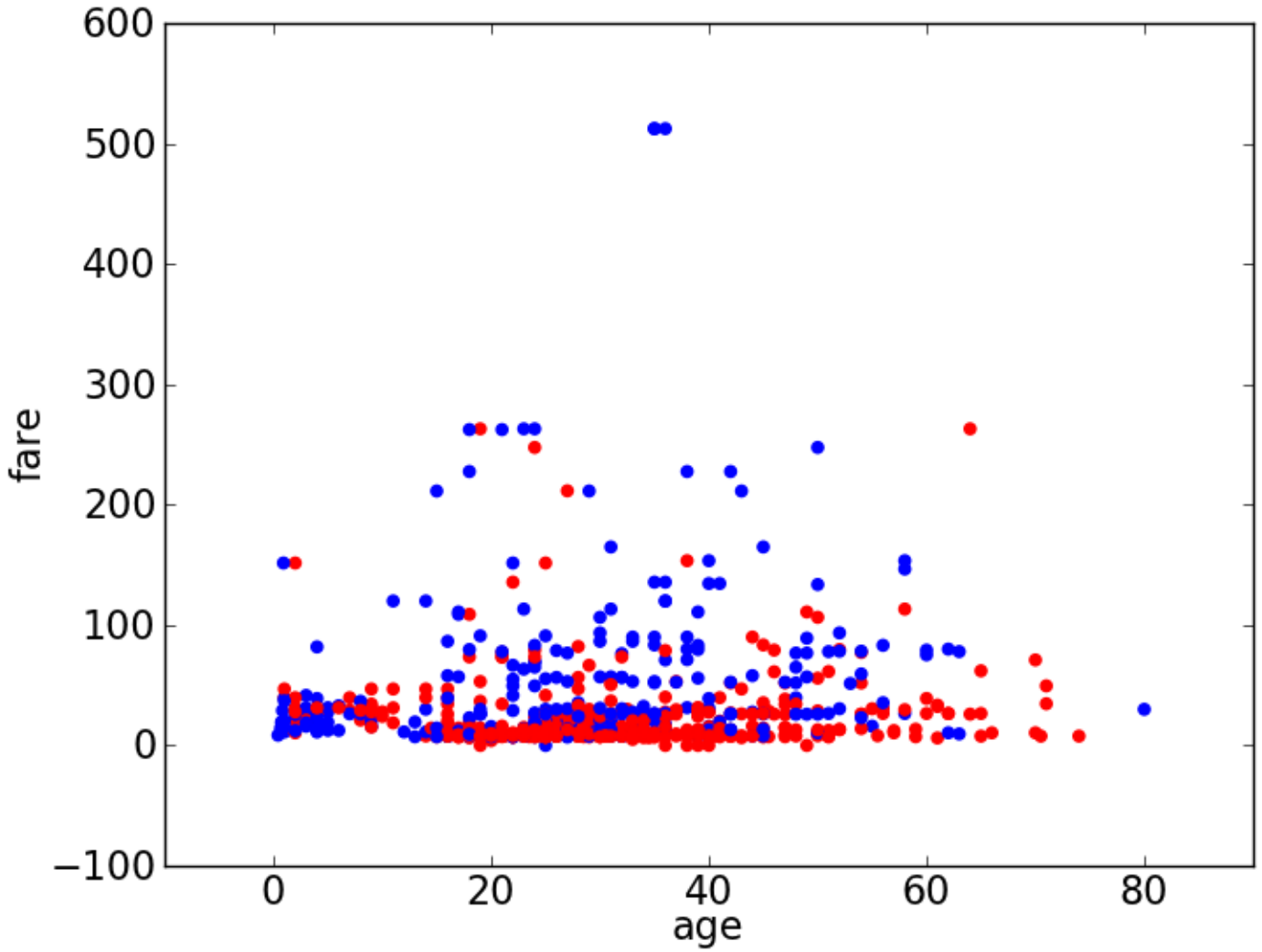
….

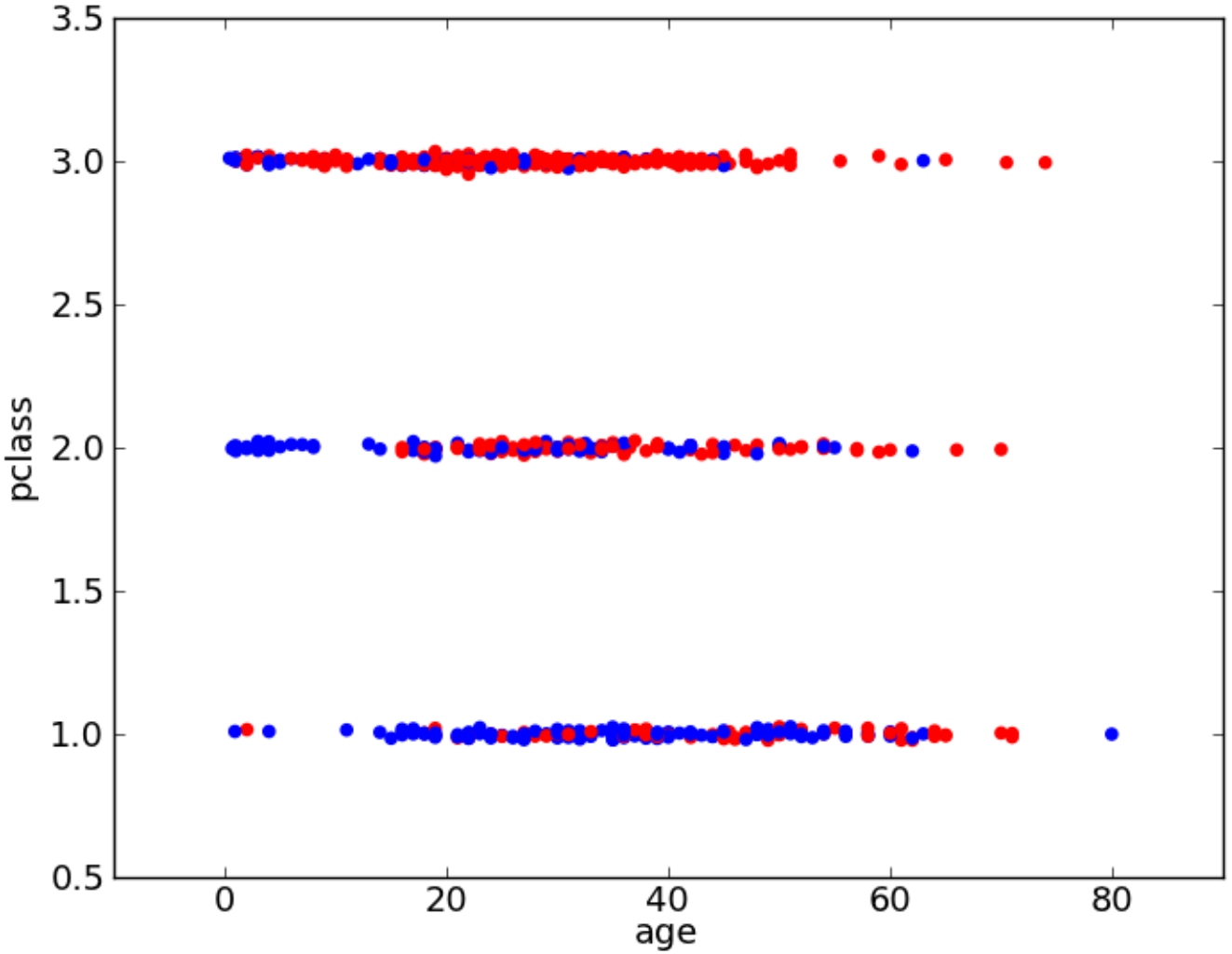
Which is the best one?

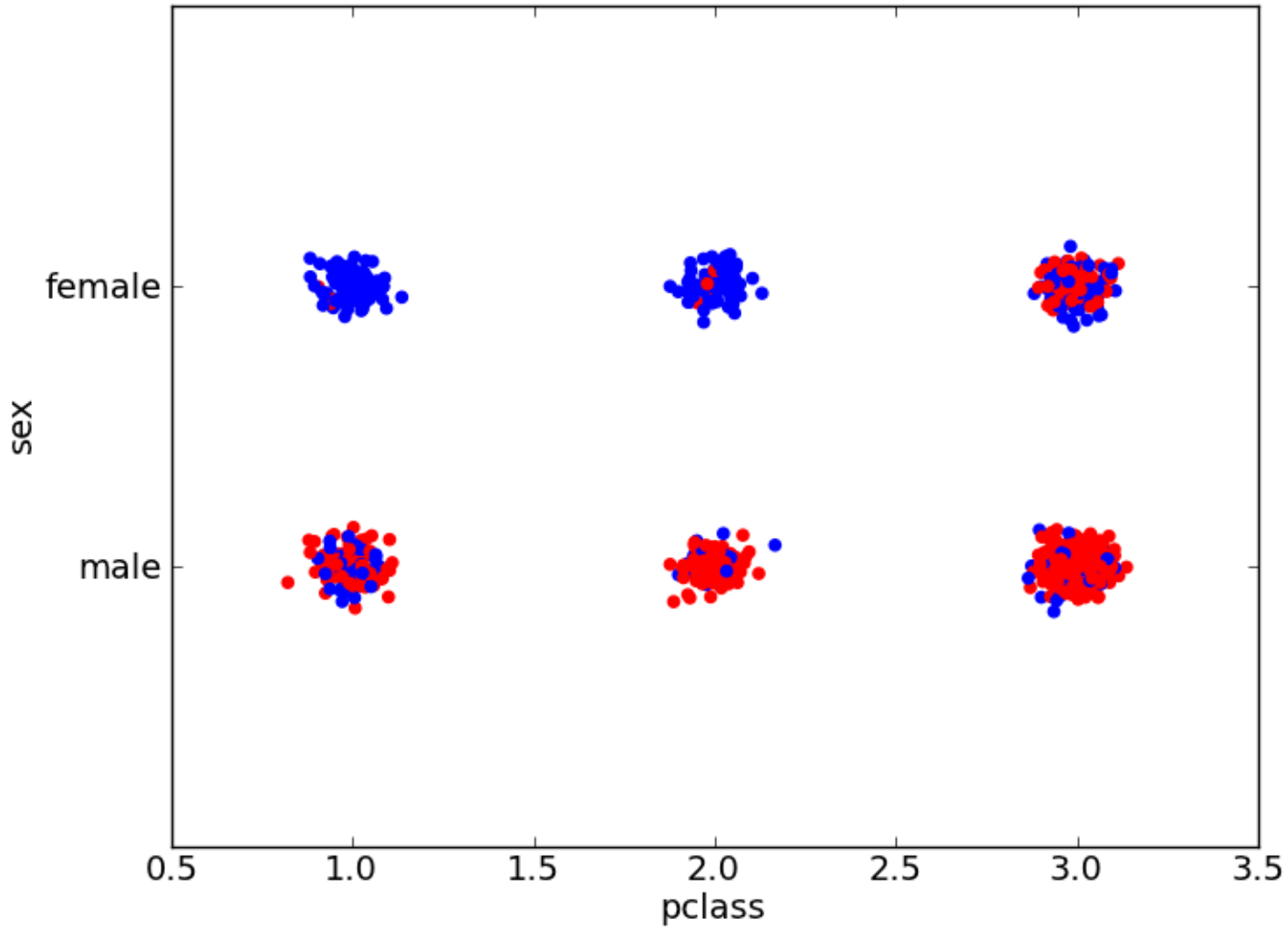
Slide credit: D. Hoiem

TITANIC DATASET

survived	pclass	sex	age	sibsp	parch	fare	cabin	embarked
0	3	male	22	1	0	7.25		S
1	1	female	38	1	0	71.2833	C85	C
1	3	female	26	0	0	7.925		S
1	1	female	35	1	0	53.1	C123	S
0	3	male	35	0	0	8.05		S
0	3	male		0	0	8.4583		Q
0	1	male	54	0	0	51.8625	E46	S
0	3	male	2	3	1	21.075		S
1	3	female	27	0	2	11.1333		S
1	2	female	14	1	0	30.0708		C
1	3	female	4	1	1	16.7	G6	S
1	1	female	58	0	0	26.55	C103	S
0	3	male	20	0	0	8.05		S


600
500
400
300
200
100
0
−100
fare
0
20
40
60
80
age


3.5
3.0
2.5
2.0
1.5
1.0
0.5
pclass
0
20
40
60
80
age


female
male
sex
0.5
1.0
1.5
2.0
2.5
3.0
3.5
pclass

IF sex='female' THEN survive=yes

ELSE IF sex='male' THEN survive = no

```
confusion matrix

no   yes    <-- classified as
468  109  |   no
 81  233  |  yes
```

(468 + 233) / (468+109+81+233) = 79% correct (and 21% incorrect)

Not bad!

IF pclass='1' THEN survive=yes

ELSE IF pclass='2' THEN survive=yes

ELSE IF pclass='3' THEN survive=no

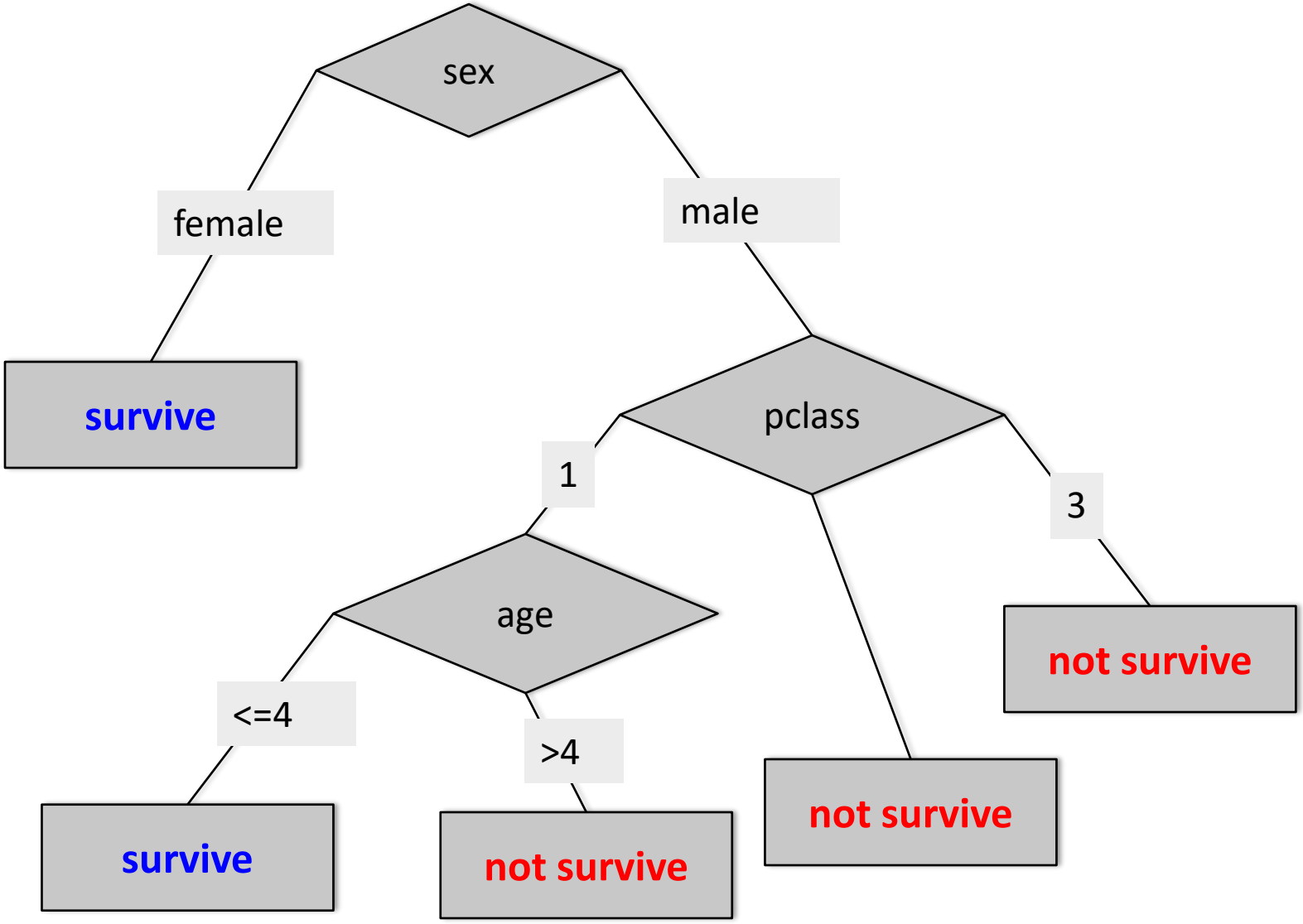
```
confusion matrix

no   yes    <-- classified as
372  119  |   no
177  223  |  yes
```

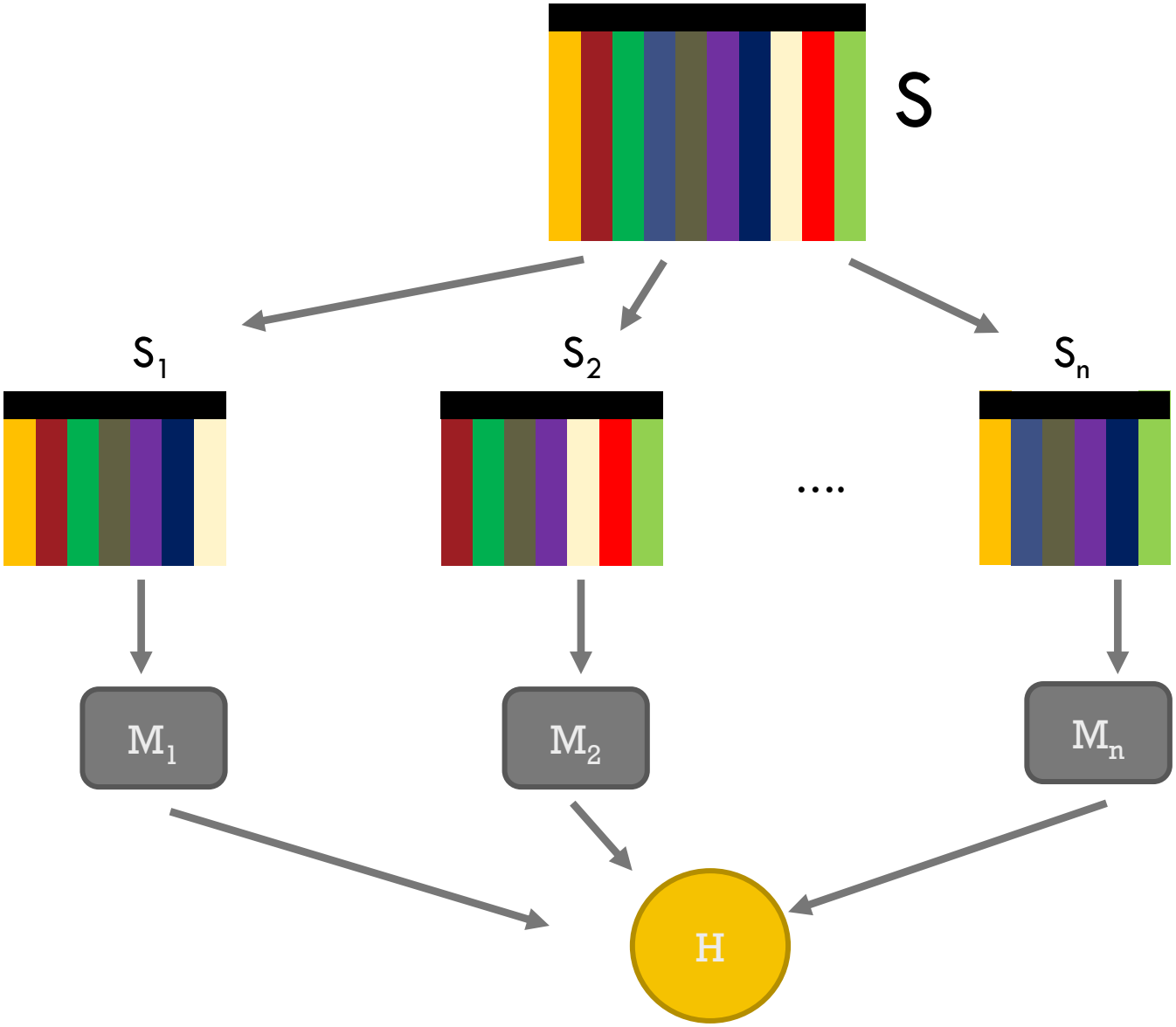
(372 + 223) / (372+119+223+177) = 67% correct (and 33% incorrect)

a little worse

DECISION TREES



RANDOM FORREST



Sample with Replacement & select random subset of features*

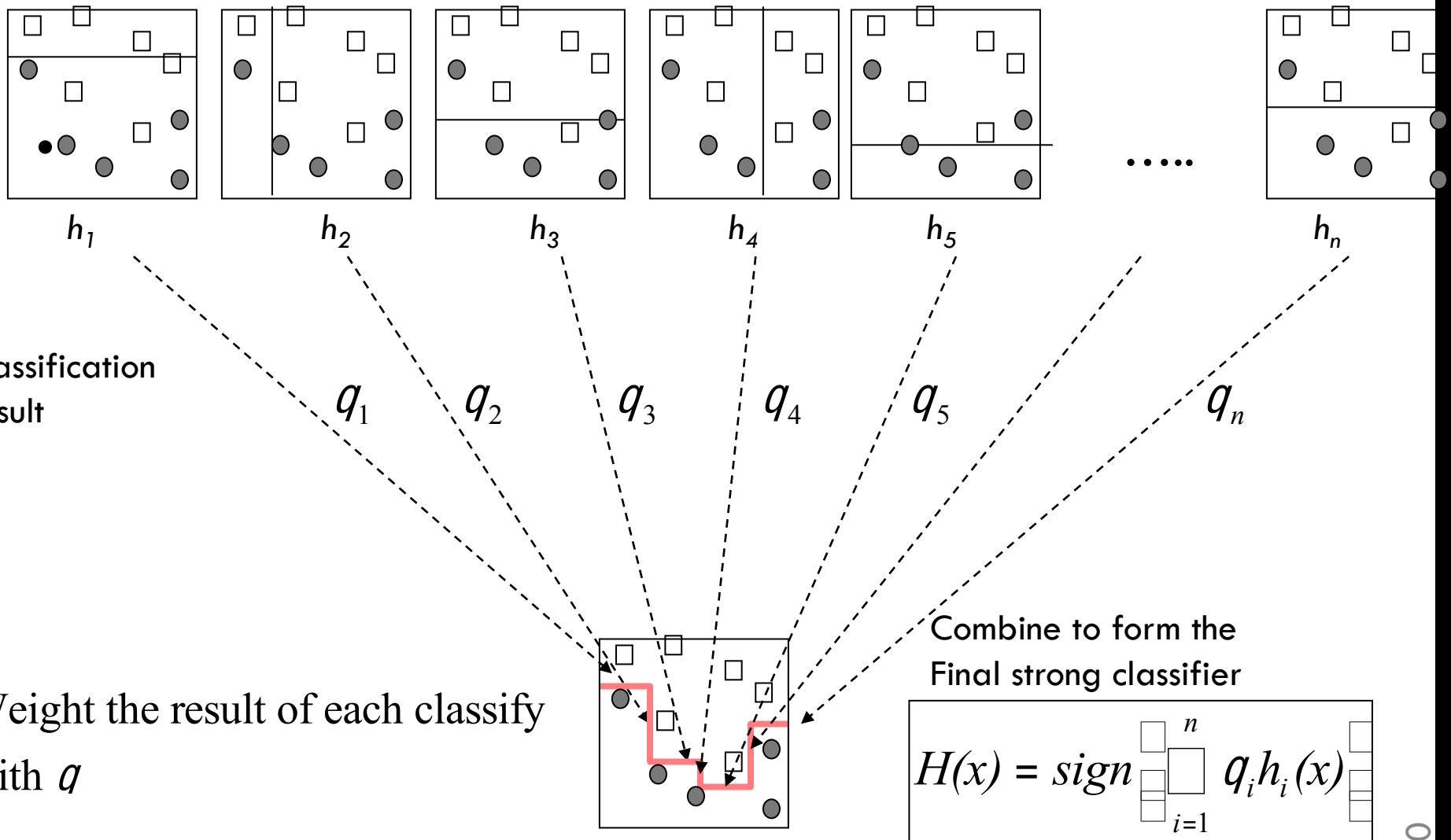
Build classifier over sample

Use majority Vote for classification (or avg. for regression)

* Normally done for each node of the decision tree – not once

ADABOOST - CORE IDEA

Take a set of weak classifiers (normally they should do better than guessing)



ADABOOST - CORE IDEA

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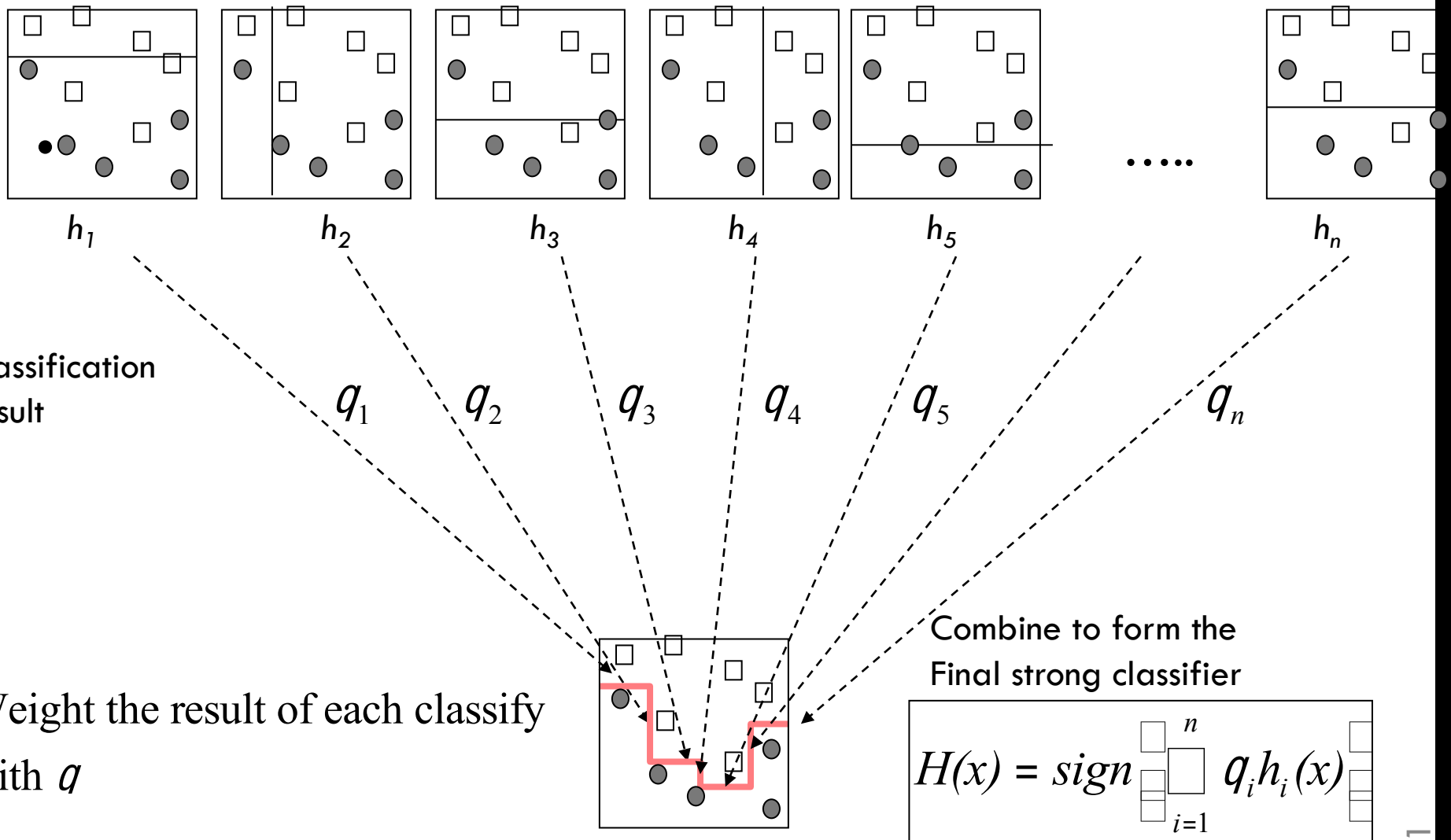

ADABOOST - CORE IDEA

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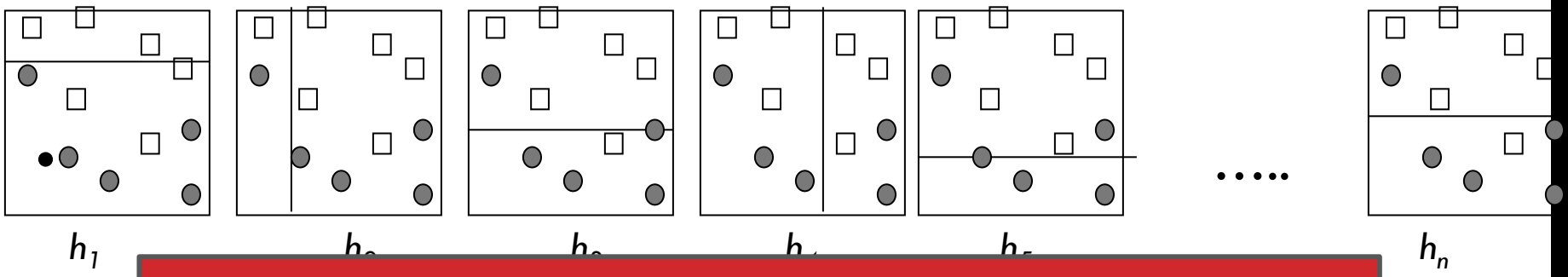
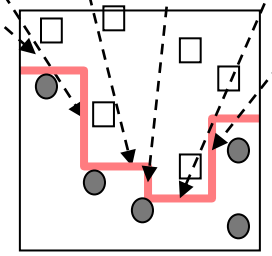


Classificatio
Result

XGBoost follows the same idea



Weight the result of each classify with q

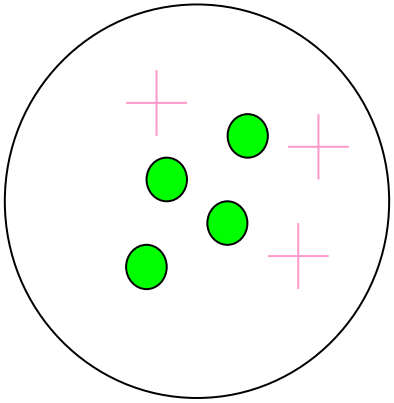
Combine to form the Final strong classifier

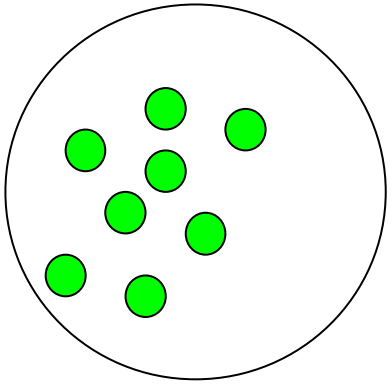
$$H(x) = sign\left[\sum_{i=1}^{n} q_i h_i(x)\right]$$

ASIDE ON ENTROPY

Impurity/Entropy (informal)

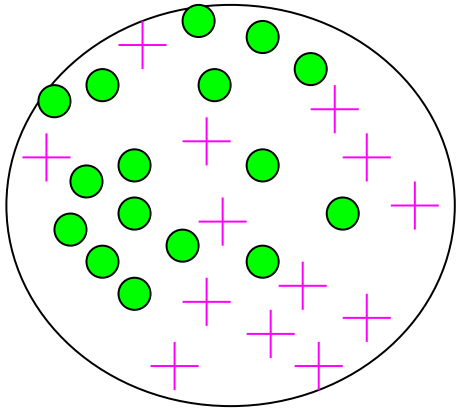
- Measures the level of **impurity** in a group of examples



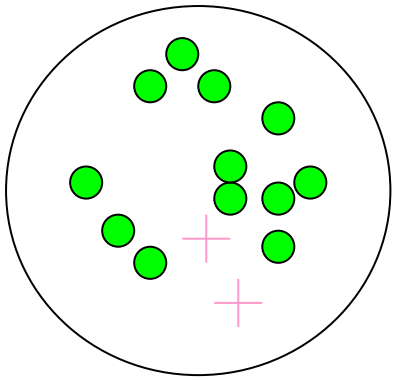


IMPURITY

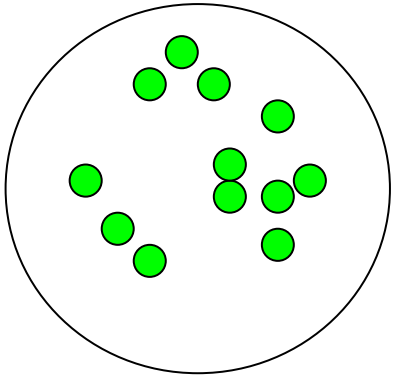
Very impure group



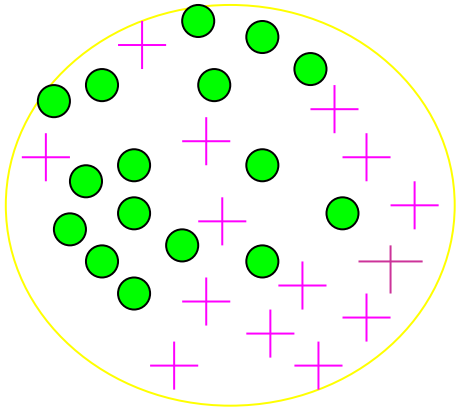
Less impure



Minimum impurity



ENTROPY



- Entropy = $\sum_i p_i \log_2 p_i$

  p_i is the probability of class i

  Compute it as the proportion of class i in the set.

  16/30 are green circles; 14/30 are pink crosses
  $\log_2(16/30) = -.9$; $\log_2(14/30) = -1.1$
  Entropy = -(16/30)(-.9) –(14/30)(-1.1) = .99

- Entropy comes from information theory. The higher the entropy the more the information content.

  What does that mean for learning from examples?

CLICKER

What is the entropy if all examples belong to the same class?

a) 0

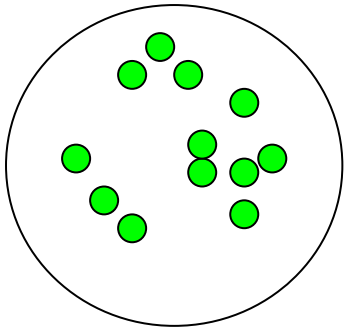
b) 1

c) Infinite

2 CLASS EXAMPLE

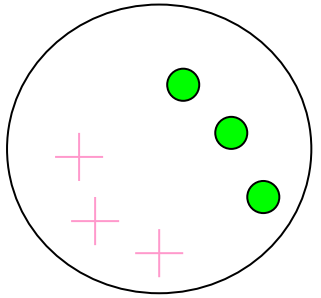
- What is the entropy of a group in which all examples belong to the same class?

Minimum impurity



- What is the entropy of a group with 50% in either class?

Maximum impurity



EXAMPLE: ROLLING A DIE

$$p_1 = \frac{1}{6},\ p_2 = \frac{1}{6},\ p_3 = \frac{1}{6},\ \ldots$$

$$\text{Entropy} = -\sum_i p_i \log_2 p_i$$

$$= -6 \times \left(\frac{1}{6} \log_2 \frac{1}{6} \right)$$

$$\approx 2.58$$

CLICKER

Has an unfair/weighted die a higher or lower entropy?

A) Higher

B) Lower

EXAMPLE: ROLLING A WEIGHTED DIE

$$p_1 = 0.1,\ p_2 = 0.1,\ p_3 = 0.1,\ \ldots\ p_6 = 0.5$$

$$\text{Entropy} = -\sum_i p_x \log_2 p_x$$

$$= -5 \times (0.1 \log_2 0.1) - 0.5 \log_2 0.5$$

$$= 2.16$$

The weighted die is has less uncertainty than a fair die

HOW UNCERTAIN IS YOUR DATA?

342/891 survivors in titanic training set

$$-\left(\frac{342}{891}\log_2\frac{342}{891}+\frac{549}{891}\log_2\frac{549}{891}\right)=0.96$$

Say there were only 50 survivors

$$-\left(\frac{50}{891}\log_2\frac{50}{891}+\frac{841}{891}\log_2\frac{841}{891}\right)=0.31$$

IN CLASS TASK

How can you use Entropy to build a decision tree.

Discuss with your neighbor(s)

Discuss the following ideas

Select the feature based on the highest entropy

Select the feature based on the lowest entropy

Stop splitting if the entropy is 0

Select the feature based on the entropy after the split

What if one group is under-/over represented

BACK TO DECISION TREES

Which attribute do we choose at each level?

The one with the highest information gain

- The one that reduces the uncertainty/impurity the most

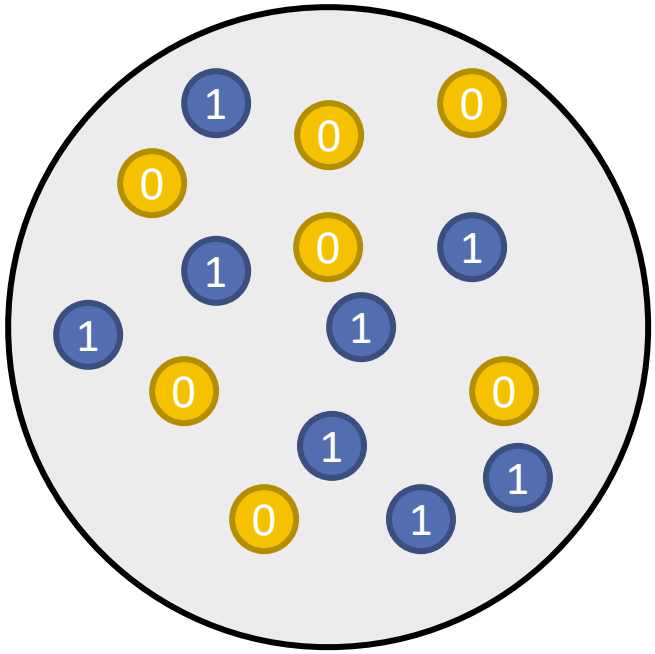
We want to determine which attribute in a given set of training feature vectors is most useful for discriminating between the classes to be learned.

Information gain tells us how important a given attribute of the feature vectors is.

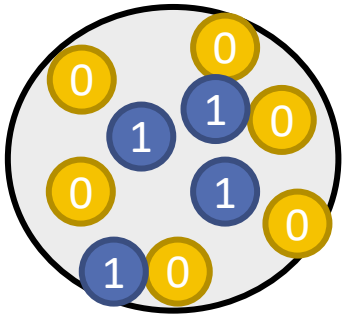
We will use it to decide the ordering of attributes in the nodes of a decision tree.

INFORMATION GAIN

Titanic Entropy = 0.96

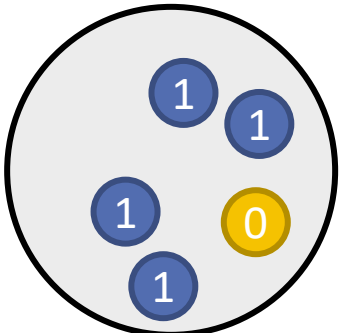


male



Entropy= - 682/843 log(682/843)
- 161/843 log(161/843)
= 0.21

female



Entropy= - 127/466 log(127/466)
- 339/466 log(339/466)
= 0.25

Weighted Entropy: 466/1309 * 0.25 + 843 / 1309 * 0.21 = 0.22
Information Gain for split: 0.96 – 0.22 = 0.74

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **outlook**:

overcast : 4 records, 4 are “yes”

$$-\left(\frac{4}{4}\log_2\frac{4}{4}\right)=0$$

rainy : 5 records, 3 are “yes”

$$-\left(\frac{3}{5}\log_2\frac{3}{5}+\frac{2}{5}\log_2\frac{2}{5}\right)=0.97$$

sunny : 5 records, 2 are “yes”

$$-\left(\frac{2}{5}\log_2\frac{2}{5}+\frac{3}{5}\log_2\frac{3}{5}\right)=0.97$$

Expected new entropy:

$$\frac{4}{14}\times 0.0+\frac{5}{14}\times 0.97+\frac{5}{14}\times 0.97$$

= 0.69

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

Before: 14 records, 9 are "yes"

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

Clicker:

If we choose windy, what is the expected entropy?

a) 0.81

= - (6/8 log(6/8) + 2/8 log(2/8))

b) 0.89

= 6/14 * 1 +
(-8/14* (6/8 log(6/8) + 2/8 log(2/8)))

c) 1

= - (0.5 * log(0.5)+0.5 * log(0.5))

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **windy**:

FALSE: 8 records, 6 are “yes”

0.81 = -(6/8*log(6/8)+2/8*log(2/8))

TRUE: 6 records, 3 are “yes”

1

Expected new entropy:

0.81(8/14) + 1 (6/14)

= 0.89

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

Before: 14 records, 9 are "yes"

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **temperature**:

cool : 4 records, 3 are "yes"

0.81

rainy : 4 records, 2 are "yes"

1.0

sunny : 6 records, 4 are "yes"

0.92

Expected new entropy:

0.81(4/14) + 1.0(4/14) + 0.92(6/14)

= 0.91

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

If we choose **humidity**:

normal : 7 records, 6 are “yes”

0.59

high : 7 records, 2 are “yes”

0.86

Expected new entropy:

0.59(7/14) + 0.86(7/14)

= <u>0.725</u>

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

Before: 14 records, 9 are “yes”

$$-\left(\frac{9}{14}\log_2\frac{9}{14}+\frac{5}{14}\log_2\frac{5}{14}\right)=0.94$$

outlook

0.94 – 0.69 = 0.25 highest gain

temperature

0.94 – 0.91 = 0.03

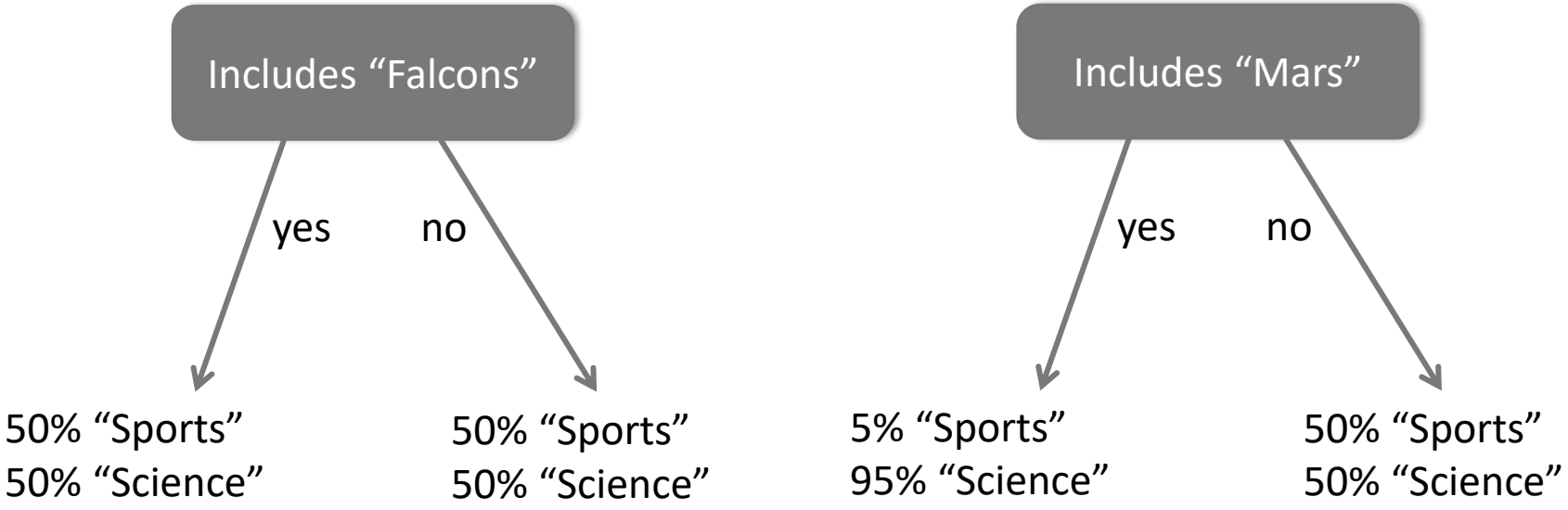
humidity

0.94 – 0.725 = 0.215

windy

0.94 – 0.87 = 0.07

DOCUMENT CLASSIFICATION



Clicker Question (assuming equal size):
a) Falcon’s Information Gain is higher
b) Mars’ Information Gain is higher

BUILDING A DECISION TREE (ID3 ALGORITHM)

Assume attributes are discrete

- Discretize continuous attributes

Choose the attribute with the highest Information Gain

Create branches for each value of attribute

Examples partitioned based on selected attributes

Repeat with remaining attributes

Stopping conditions

- All examples assigned the same label
- No examples left

PROBLEMS

Expensive to train

Prone to overfitting

- Drive to perfection on training data, bad on test data
- Pruning can help: remove or aggregate subtrees that provide little discriminatory power (C45)

C4.5 EXTENSIONS

Continuous Attributes

outlook	temperature	humidity	windy	play
overcast	cool	60	TRUE	yes
overcast	hot	80	FALSE	yes
overcast	hot	63	FALSE	yes
overcast	mild	81	TRUE	yes
rainy	cool	58	TRUE	no
rainy	mild	90	TRUE	no
rainy	cool	54	FALSE	yes
rainy	mild	92	FALSE	yes
rainy	mild	59	FALSE	yes
sunny	hot	90	FALSE	no
sunny	hot	89	TRUE	no
sunny	mild	90	FALSE	no
sunny	cool	60	FALSE	yes
sunny	mild	62	TRUE	yes

Consider every possible binary partition; choose the partition with the highest gain

outlook	temperature	humidity	windy	play
rainy	mild	54	FALSE	yes
overcast	hot	58	FALSE	yes
overcast	cool	59	TRUE	yes
rainy	cool	60	FALSE	yes
overcast	mild	60	TRUE	yes
overcast	hot	62	FALSE	yes
rainy	mild	63	TRUE	no
sunny	cool	80	FALSE	yes
rainy	mild	81	FALSE	yes
sunny	mild	89	TRUE	yes
sunny	hot	90	FALSE	no
rainy	cool	90	TRUE	no
sunny	hot	90	TRUE	no
sunny	mild	92	FALSE	no

E(6/6) = 0.0

E(3/8) + E(5/8) = 0.95

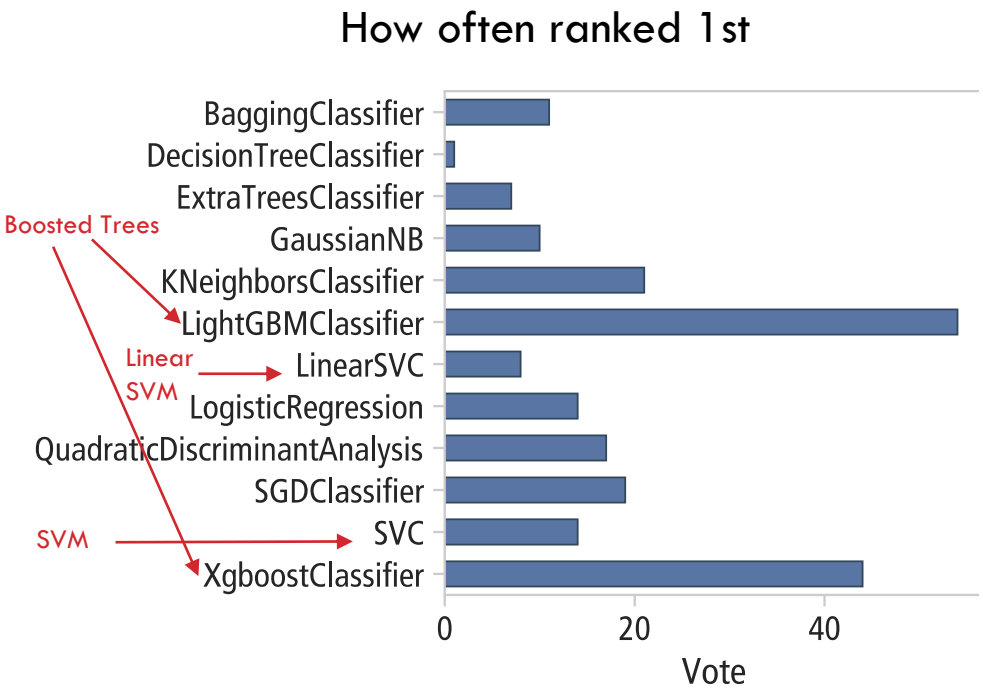
E(9/10)+ E(1/10) = 0.47

E(4/4) = 0.0

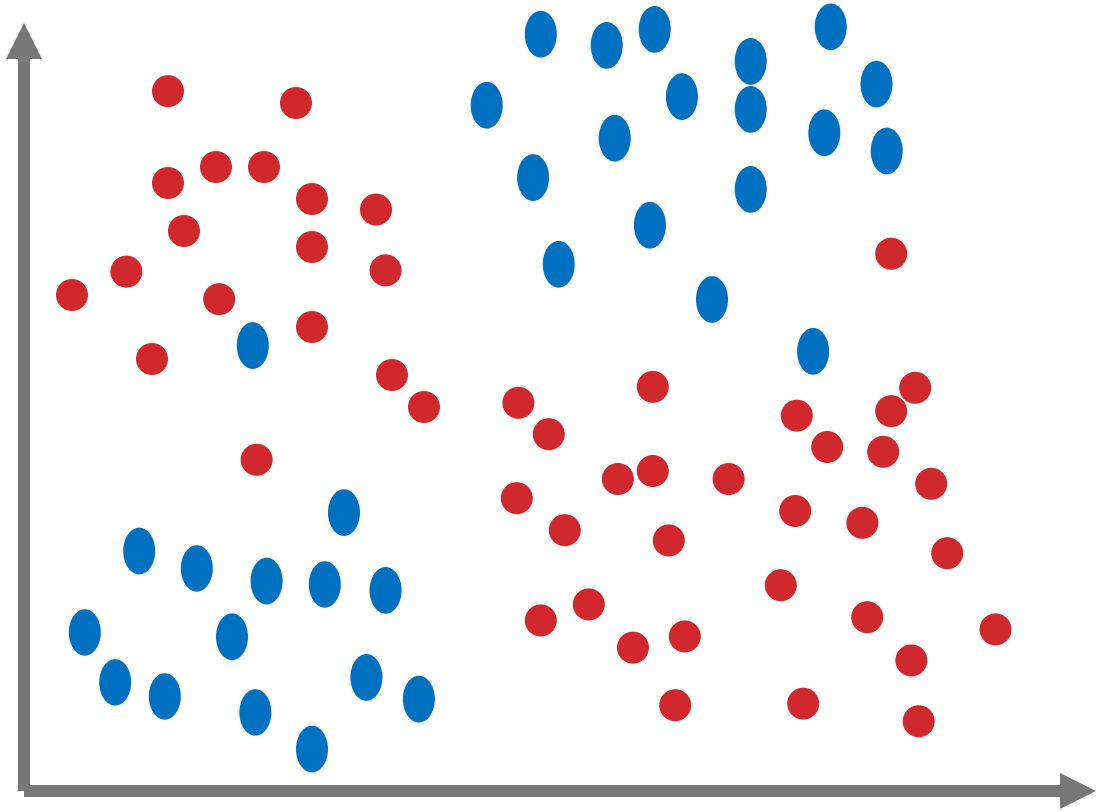
Expect = 8/14*0.95 + 6/14*0 = 0.54

Expect = 10/14*0.47 + 4/14*0 = 0.33

PERFORMANCE OF DIFFERENT ML MODEL FAMILIES



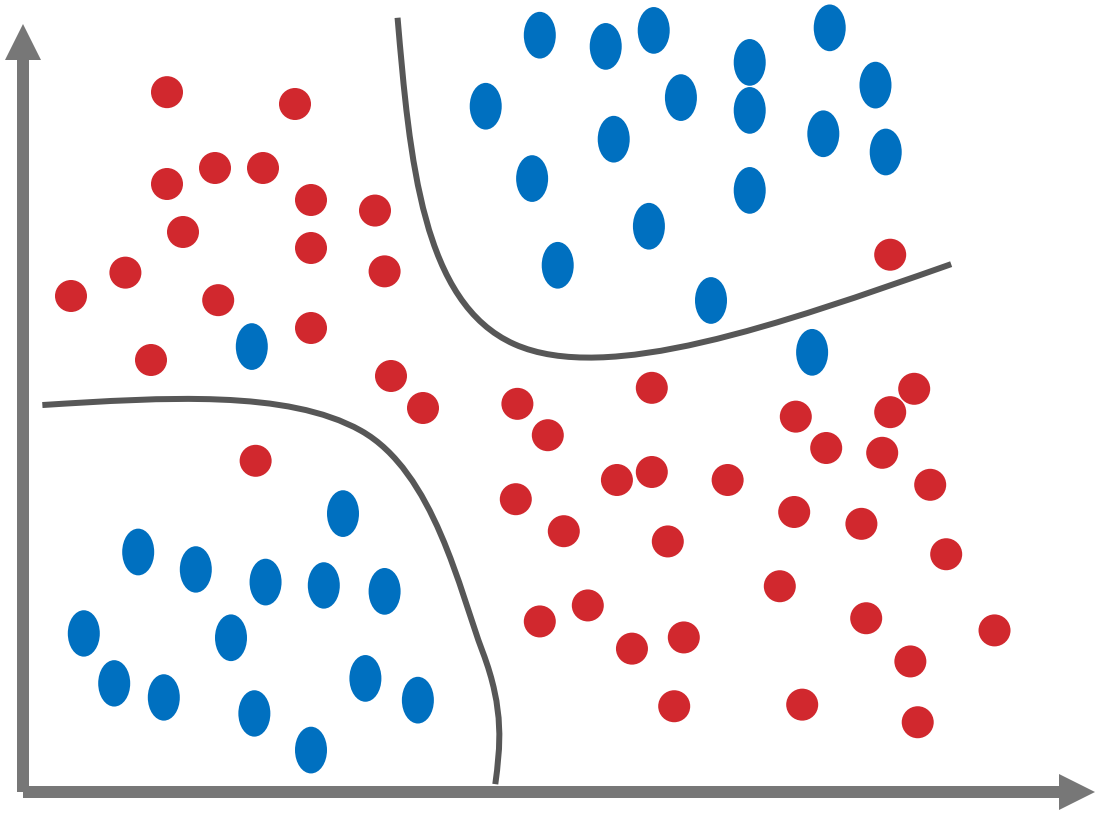
IN-CLASS TASK



How would you draw the expected decision boundary for

- Random Forrest
- SVM w/ kernel and regularization
- 1-KNN

CLICKER



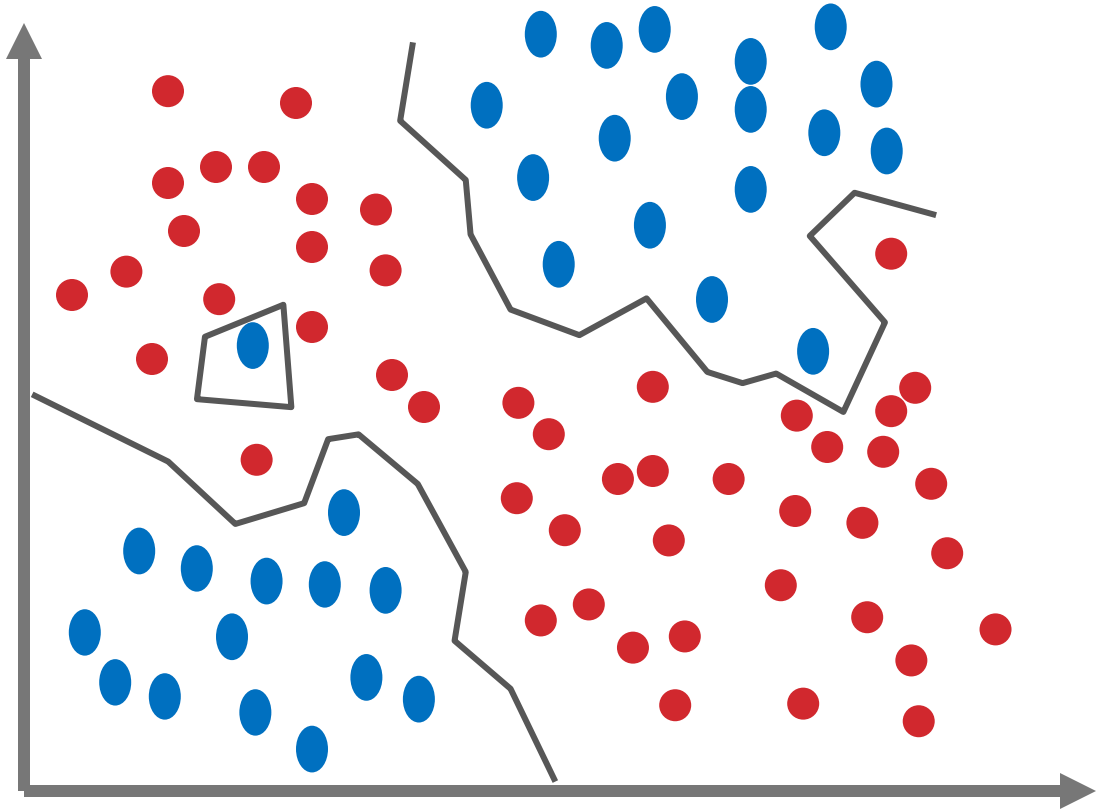
The decision boundary looks like the one of:

a) Random Forrest

b) SVM w/ kernel and regularization

c) 1-KNN

CLICKER



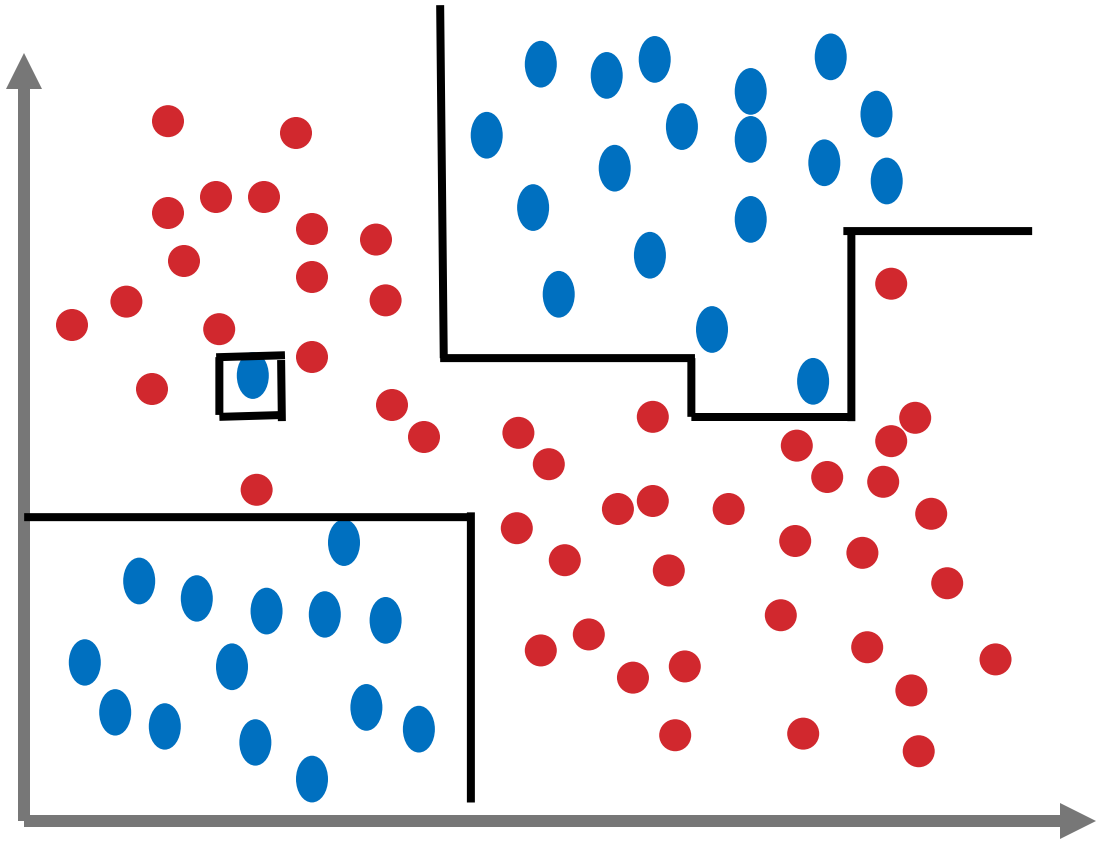
The decision boundary looks like the one of:

a) Random Forrest

b) SVM w/ kernel and regularization

c) 1-KNN

RANDOM FORREST



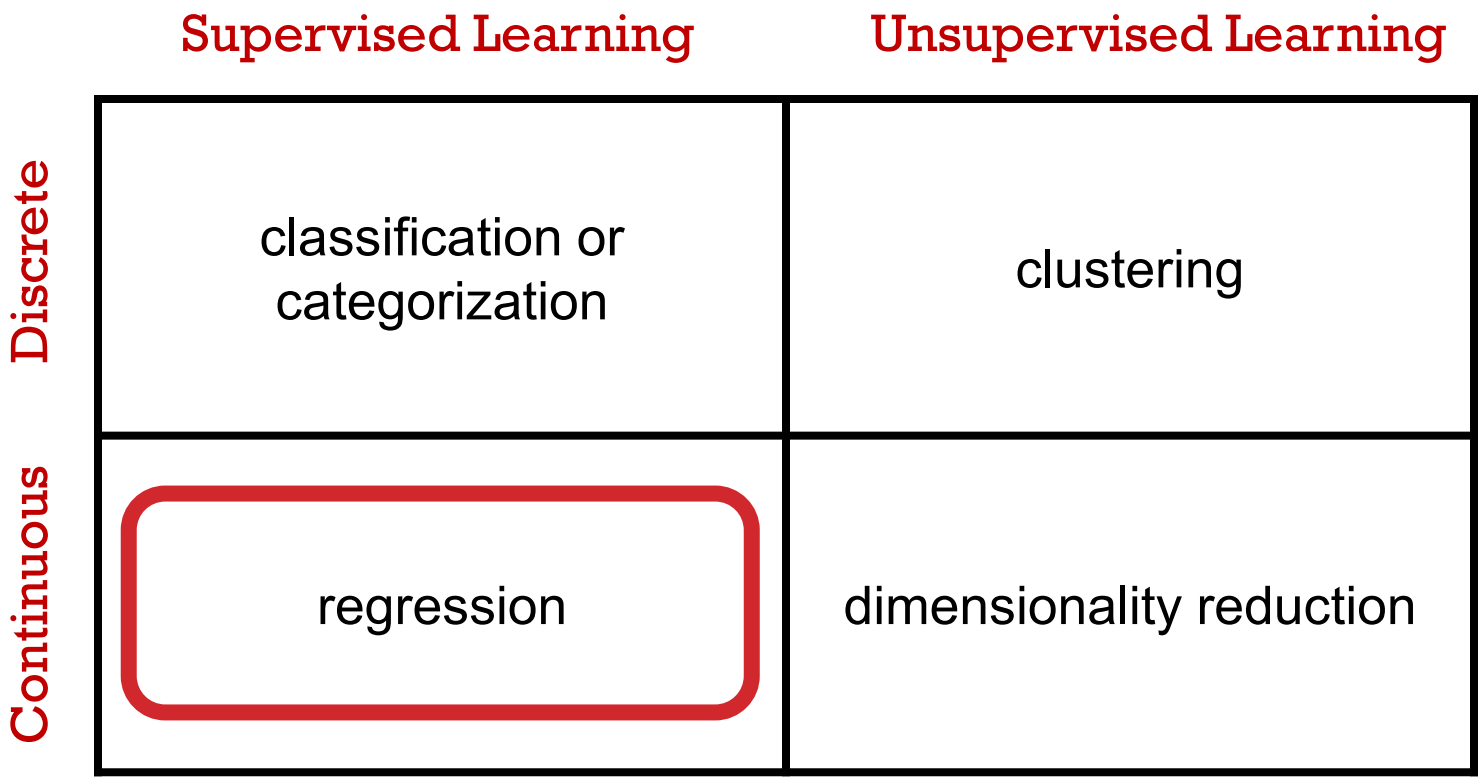
The decision boundary looks like the one of:

a) Random Forrest

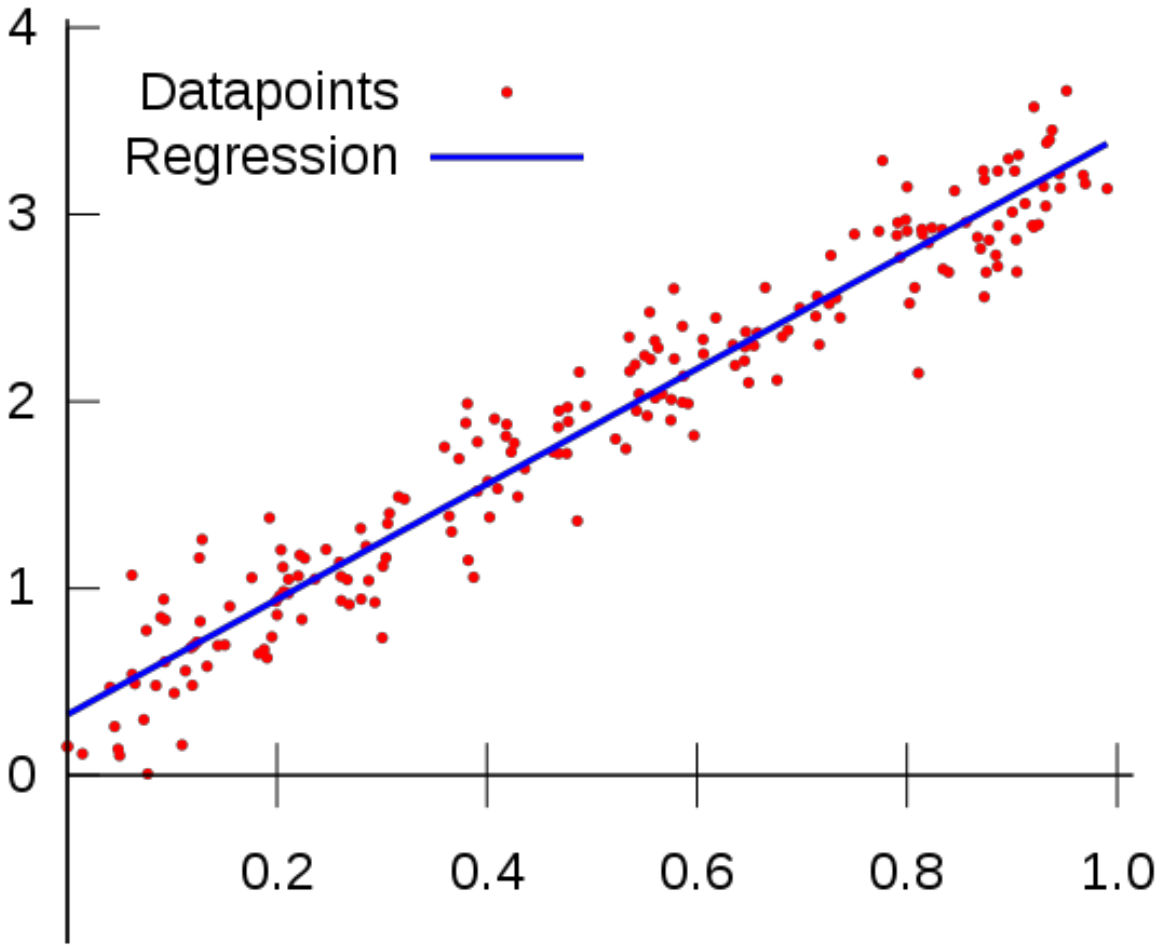
b) SVM w/ kernel and regularization

c) 1-KNN

MACHINE LEARNING PROBLEMS

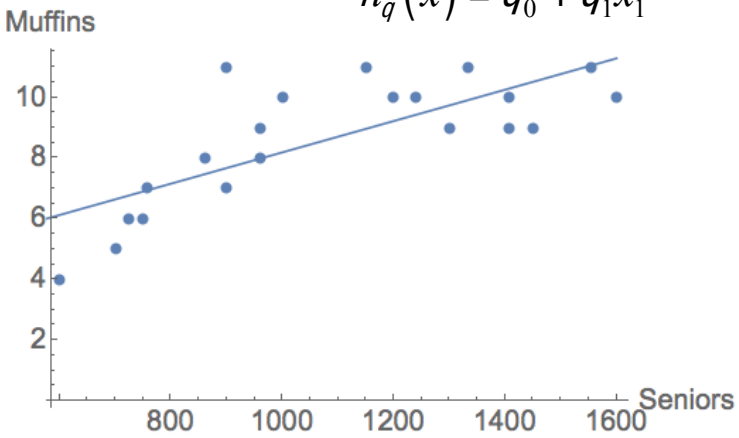


LINEAR REGRESSION

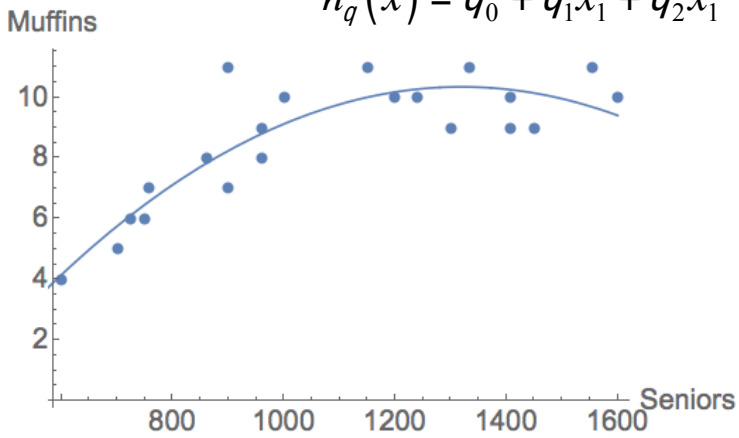


POLYNOMIAL REGRESSION

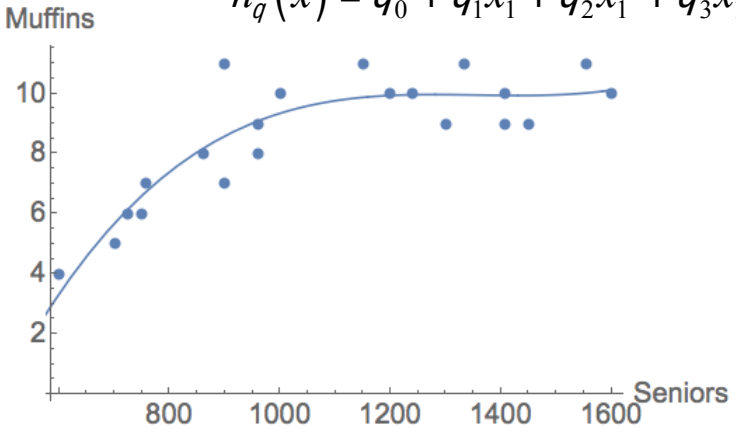
$$h_q(x) = q_0 + q_1 x_1$$



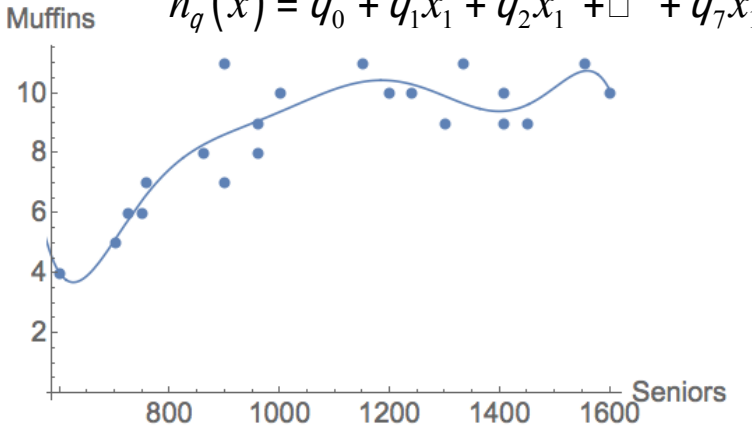
$$h_q(x) = q_0 + q_1 x_1 + q_2 x_1^2$$



$$h_q(x) = q_0 + q_1 x_1 + q_2 x_1^2 + q_3 x_1^3$$

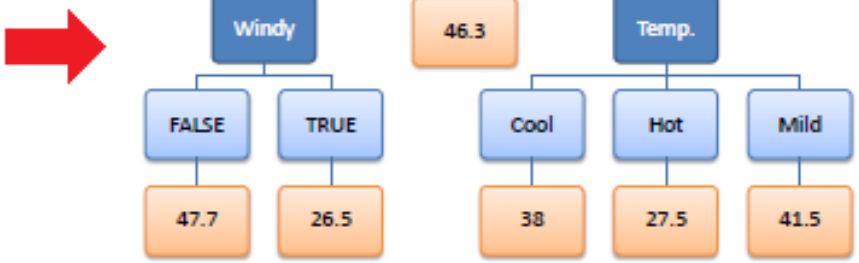


$$h_q(x) = q_0 + q_1 x_1 + q_2 x_1^2 + \square + q_7 x_1^7$$



DECISION TREE - REGRESSION

Predictors				Target
Outlook	Temp.	Humidity	Windy	Hours Played
Rainy	Hot	High	False	25
Rainy	Hot	High	True	30
Overcast	Hot	High	False	48
Sunny	Mild	High	False	46
Sunny	Cool	Normal	False	62
Sunny	Cool	Normal	True	23
Overcast	Cool	Normal	True	43
Rainy	Mild	High	False	36
Rainy	Cool	Normal	False	38
Sunny	Mild	Normal	False	48
Rainy	Mild	Normal	True	48
Overcast	Mild	High	True	62
Overcast	Hot	Normal	False	44
Sunny	Mild	High	True	30



PERFORMANCE