Support Vector Machines

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Support vector machines

Similar to linear regression they aim to find a hyperplane that linearly separates data points belong to different classes

In addition SVMs aim to find the hyperplane that is least likely to over fit the training data

- By design, similar to pruning in Decision Trees, SVMs attempt to regulate the hypothesis space to ensure good performance on validation set…

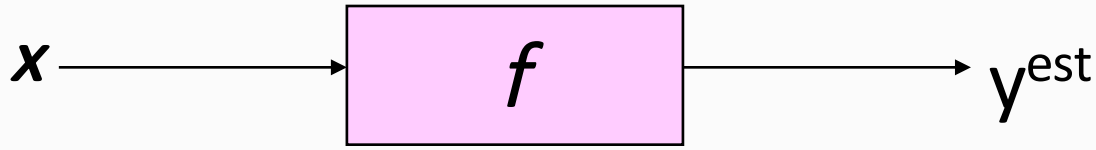
- Fast in the nonlinear case
  - Use a mathematical trick to avoid creating “pseudoattributes”
  - The nonlinear space is created implicitly

SVM, in a nutshell…

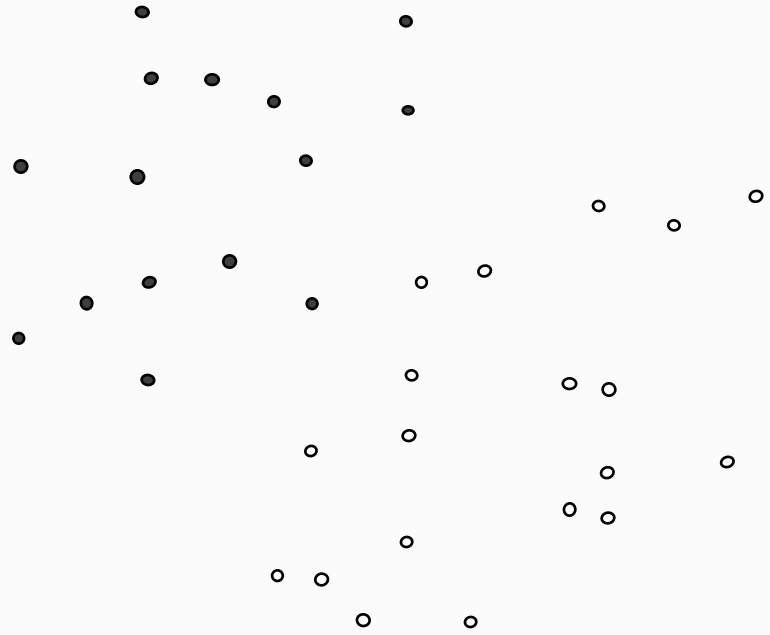
- SVM views the input data as two sets of vectors in an n-dimensional space. It constructs a separating hyperplane in that space, one which maximizes the margin between the two data sets.
- To calculate the margin, two parallel hyperplanes are constructed, one on each side of the separating hyperplane.
- A good separation is achieved by the hyperplane that has the largest distance to the neighboring data points of both classes.
- The vectors (points) that constrain the width of the margin are the support vectors.

Linear Classifiers

Estimation:



- denotes +1
- denotes -1

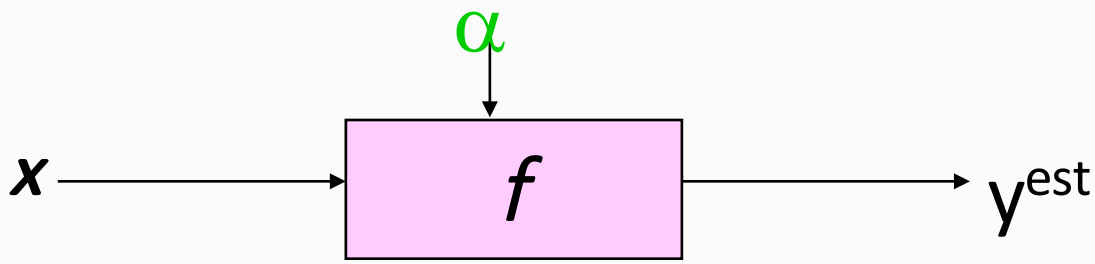


$f(x, w, b) = sign(w \cdot x - b)$

w: weight vector
x: data vector

How would you classify this data?

Linear Classifiers



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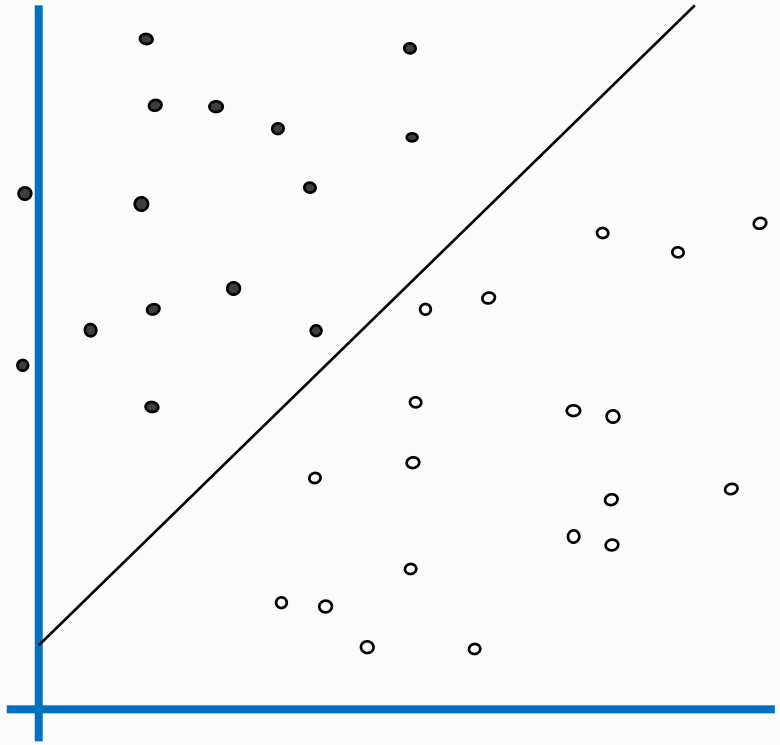

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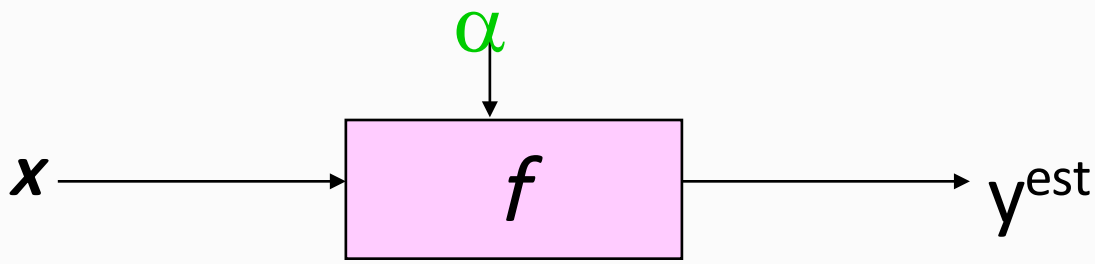

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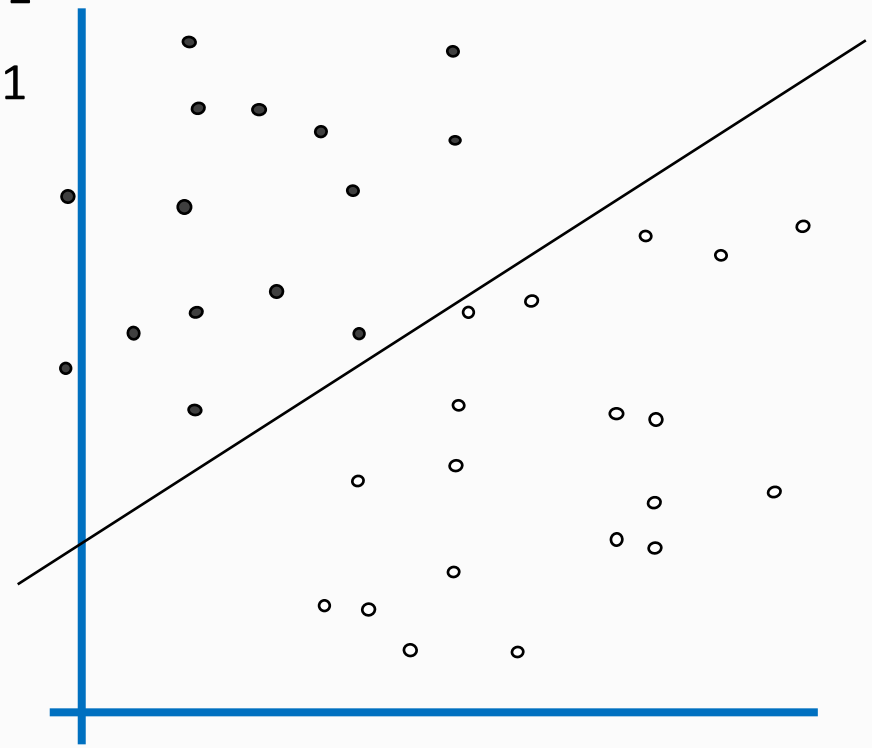

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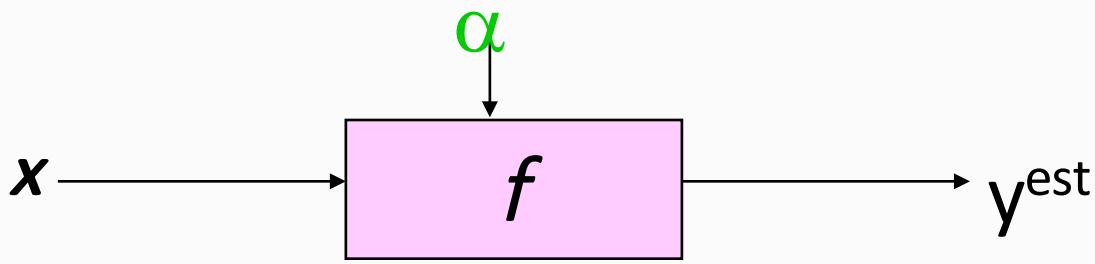
Linear Classifiers



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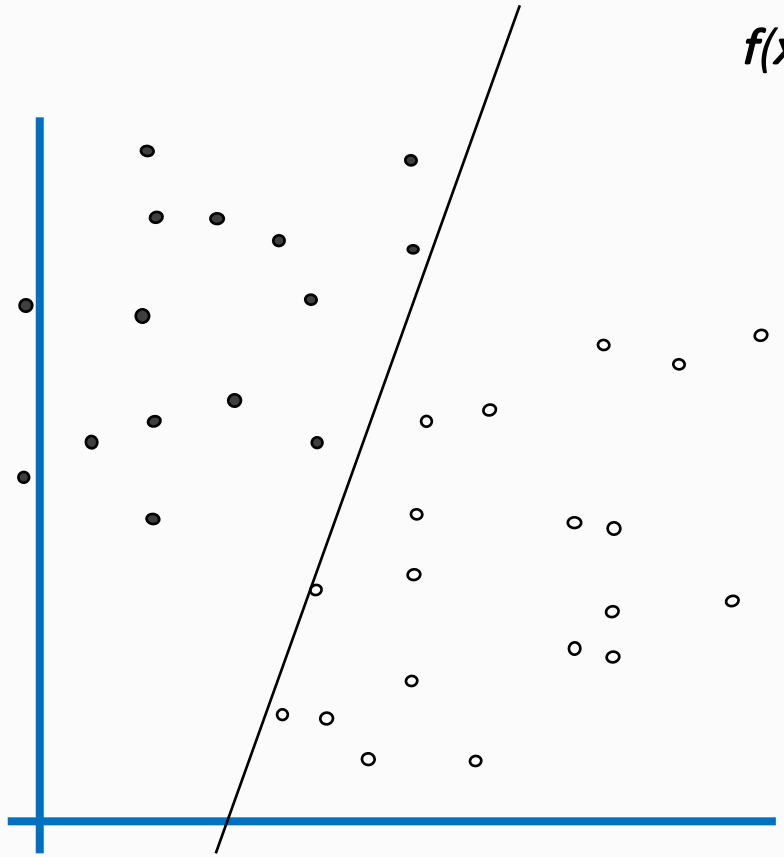

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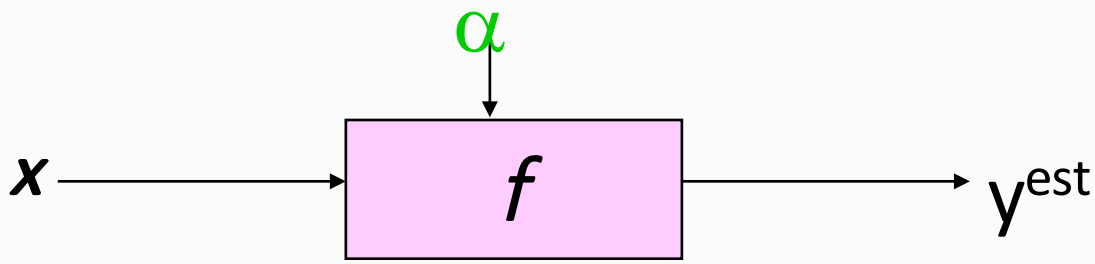
Linear Classifiers



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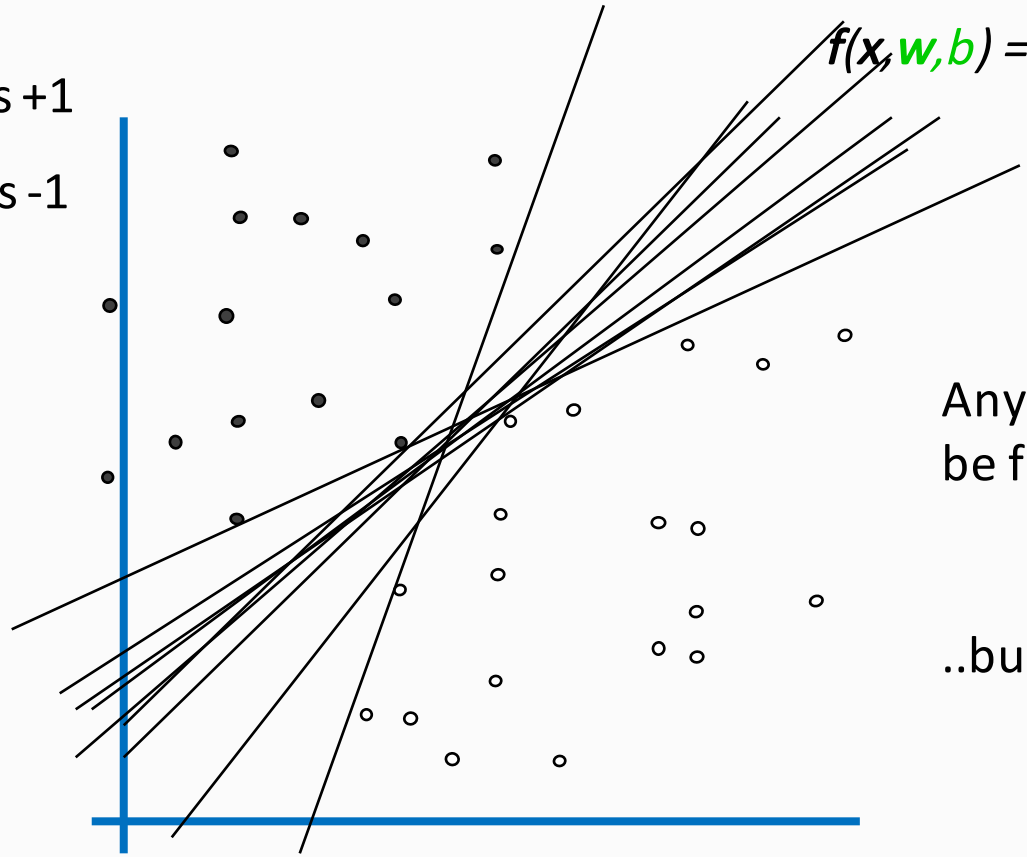
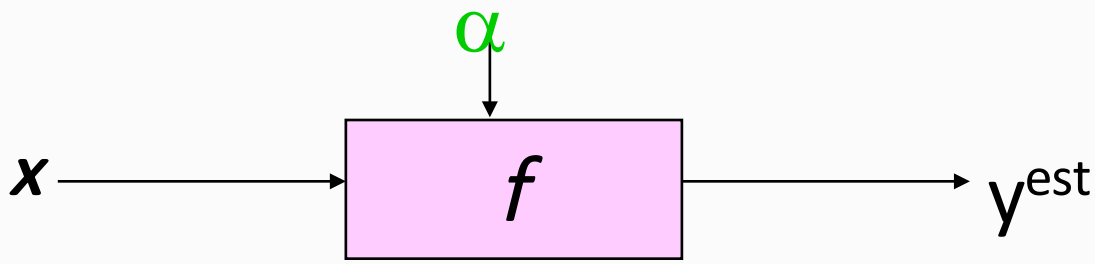
$f(x,w,b) = sign(w.x - b)$



Any of these would be fine..

..but which is best?

Classifier Margin



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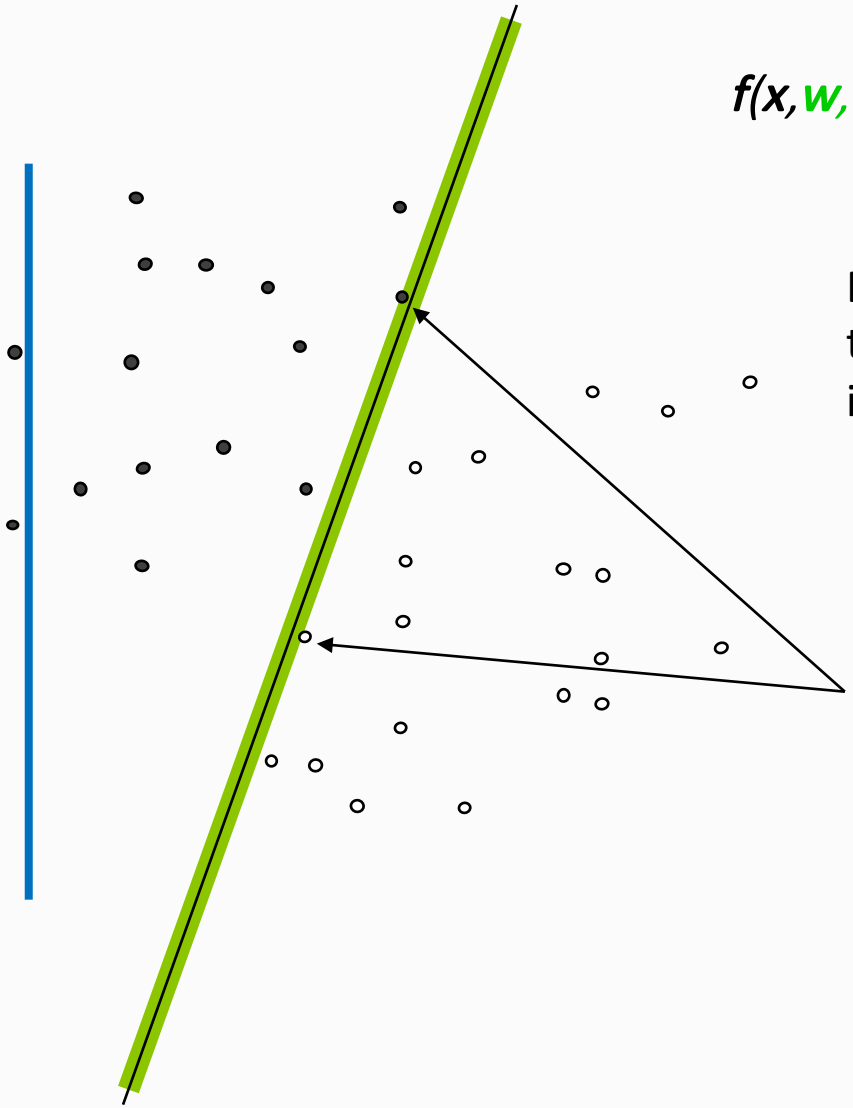
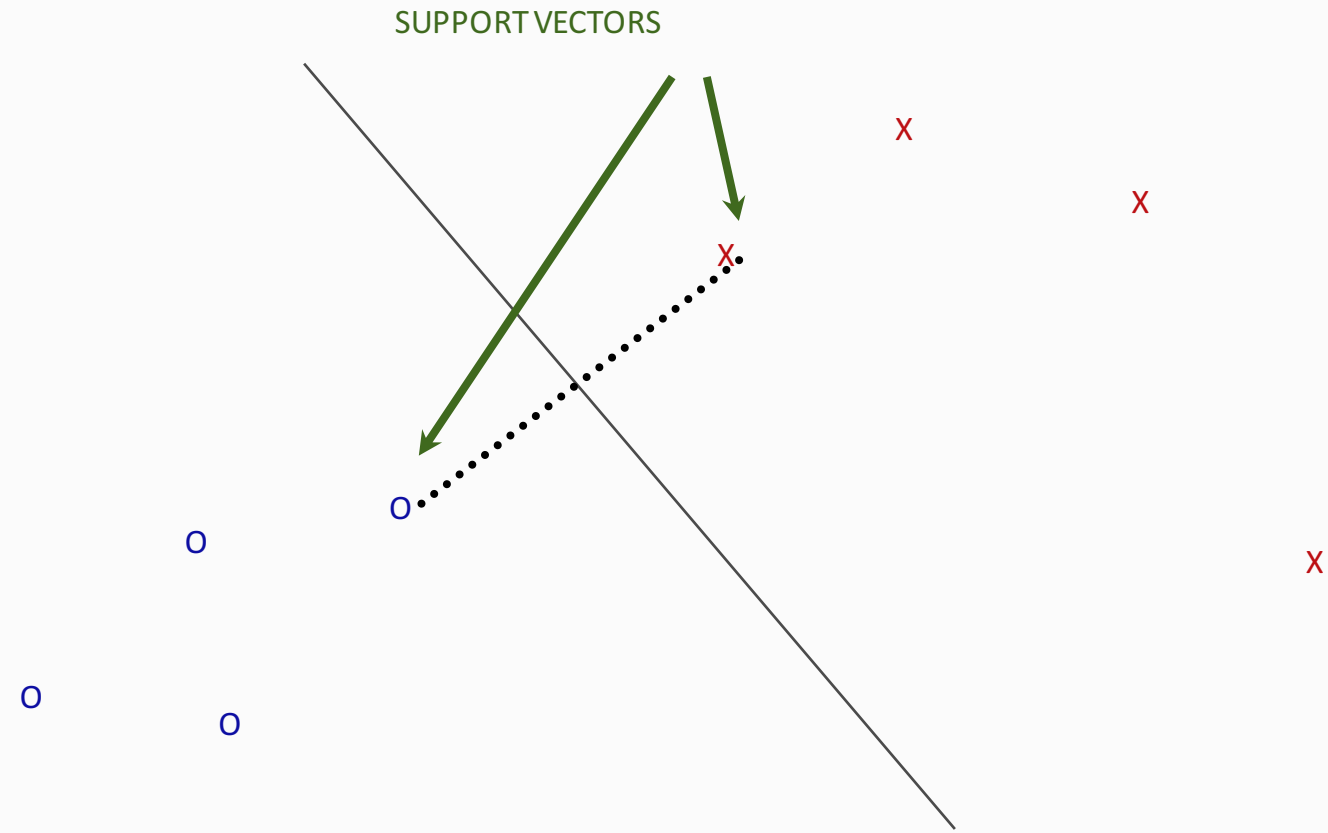


Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Geometric Intuition



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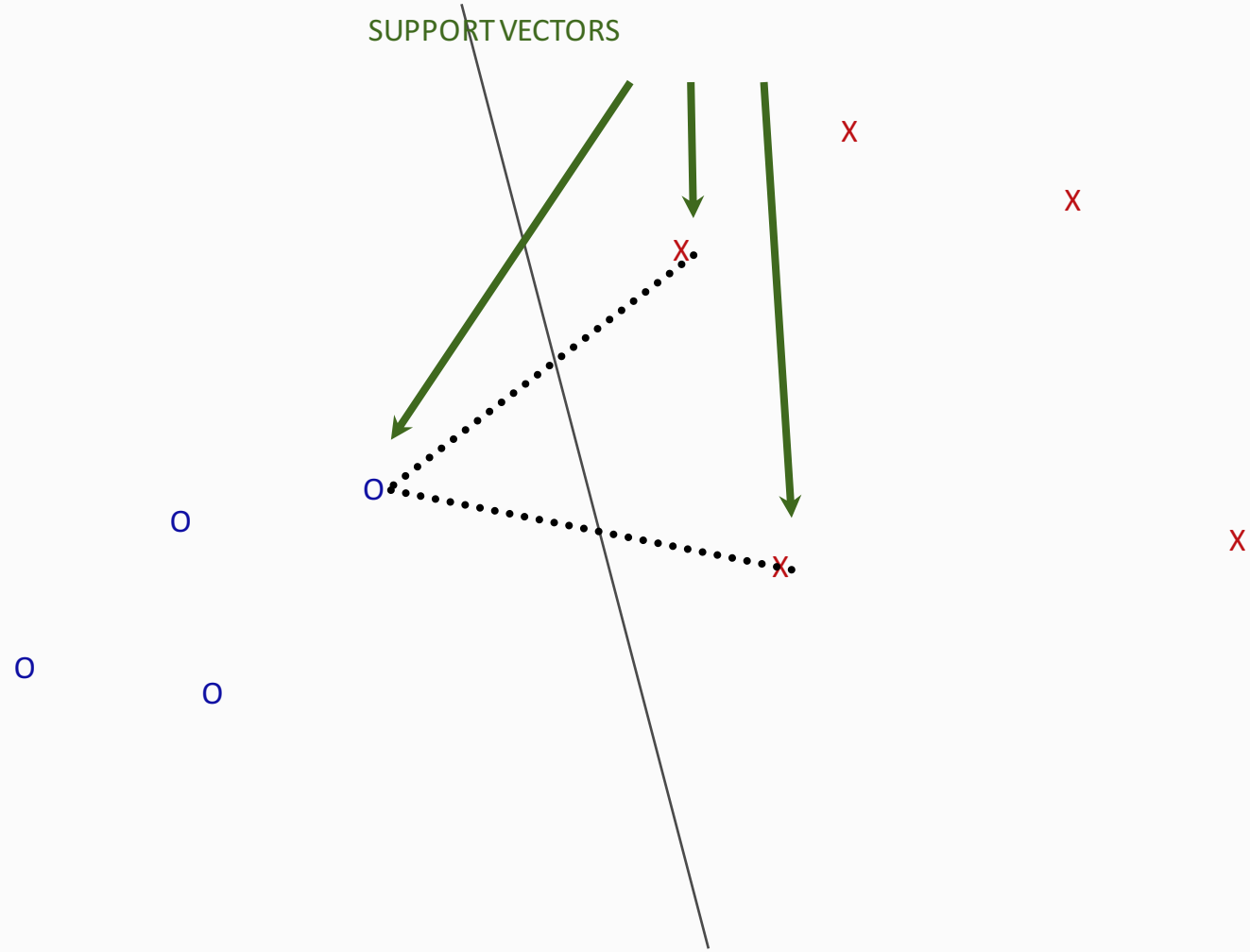
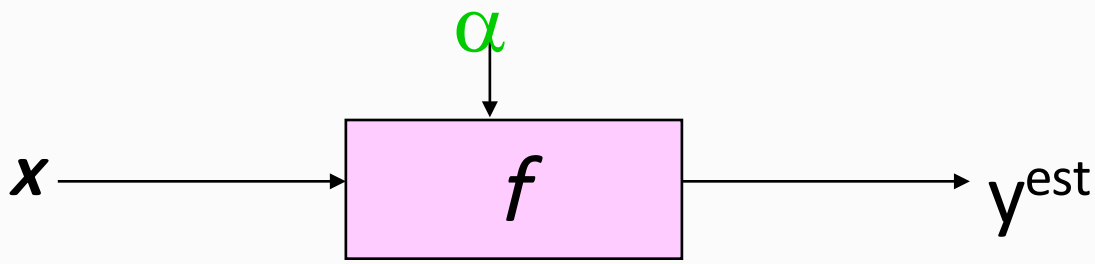


Maximum Margin



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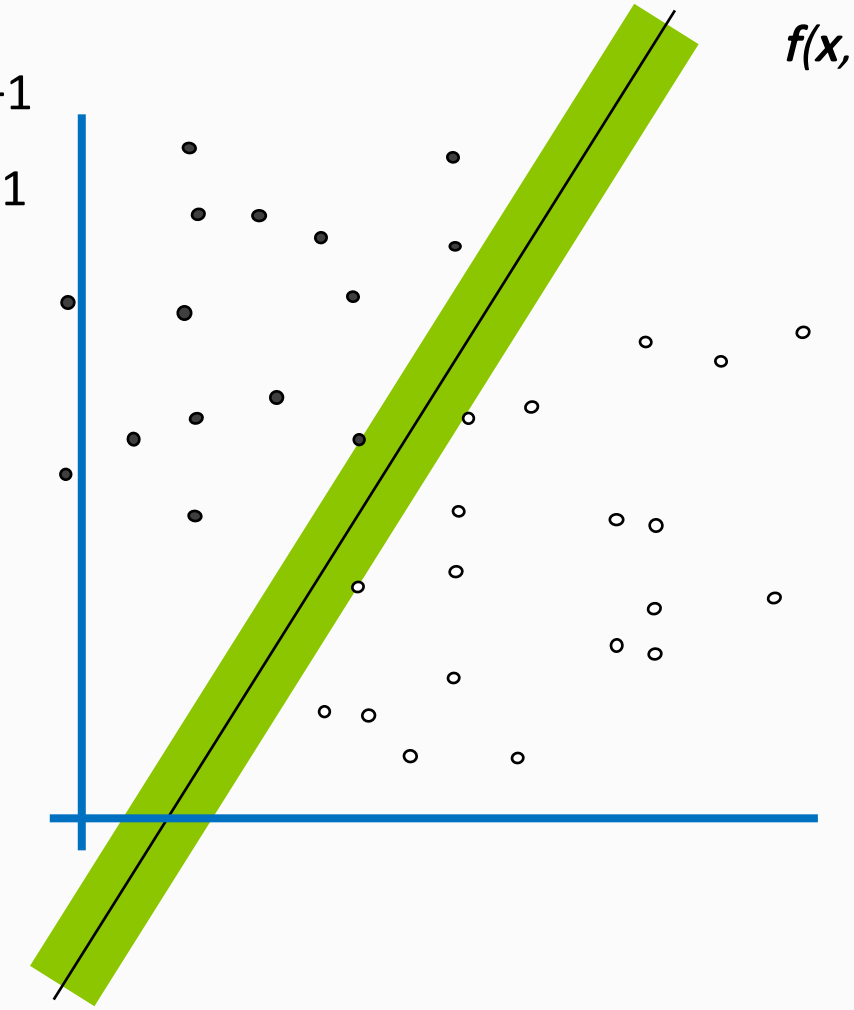


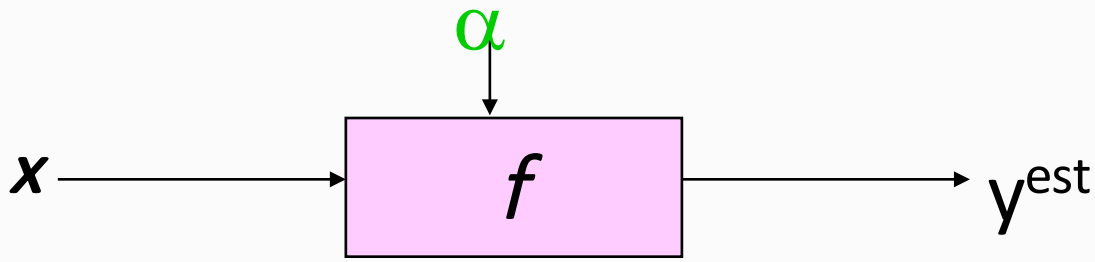
$f(x,w,b) = sign(w.x - b)$

The maximum margin linear classifier is the linear classifier with the, um, maximum margin.

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

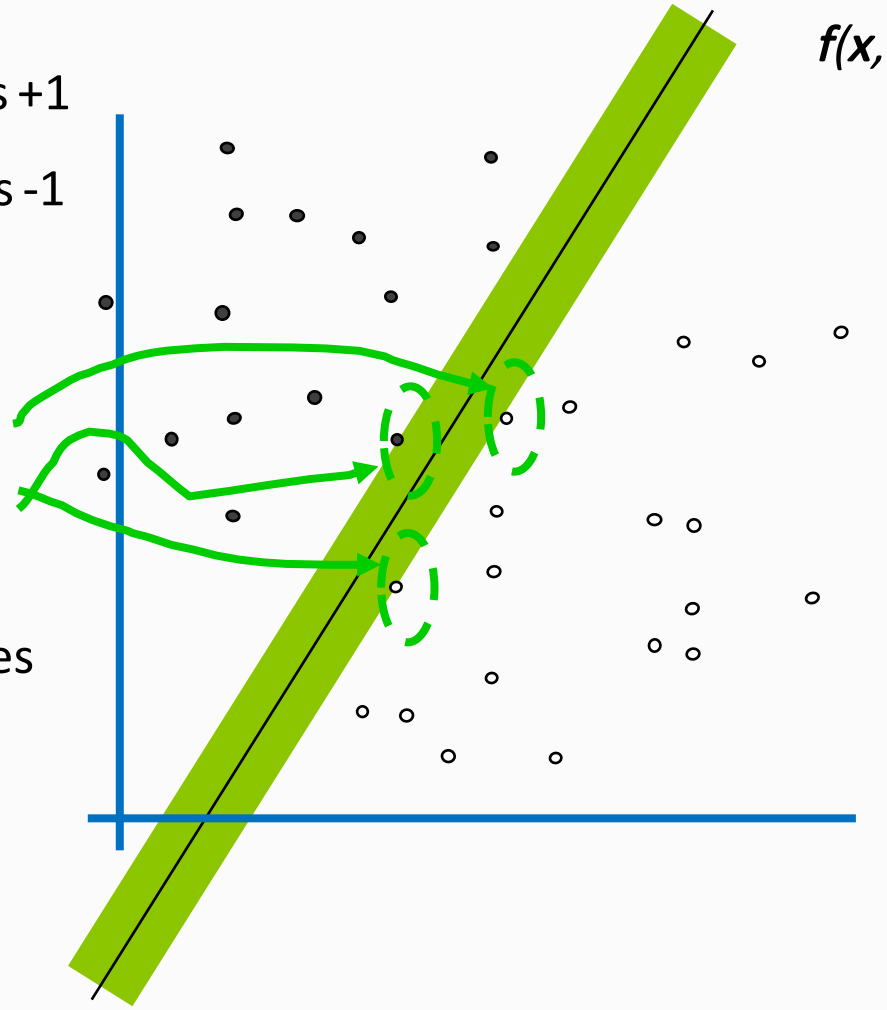
Linear SVM

Maximum Margin



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

- denotes +1
- denotes -1



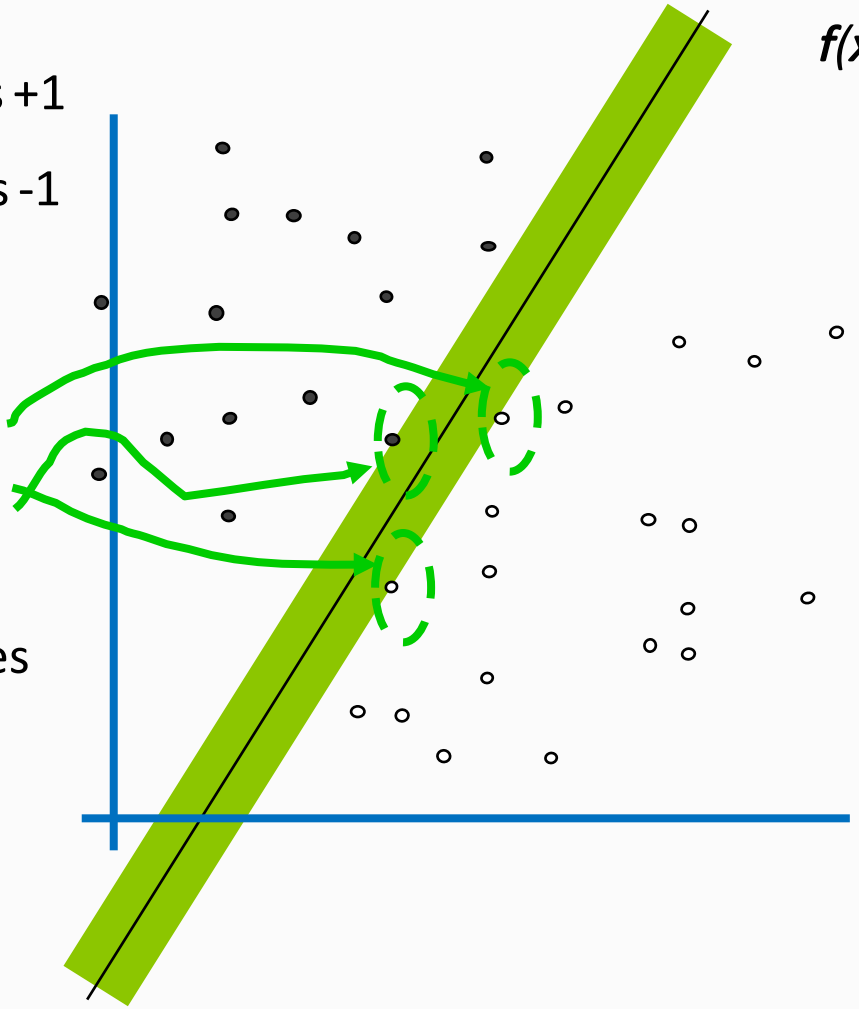
Support Vectors are those datapoints that the margin pushes up against

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

Why Maximum Margin?



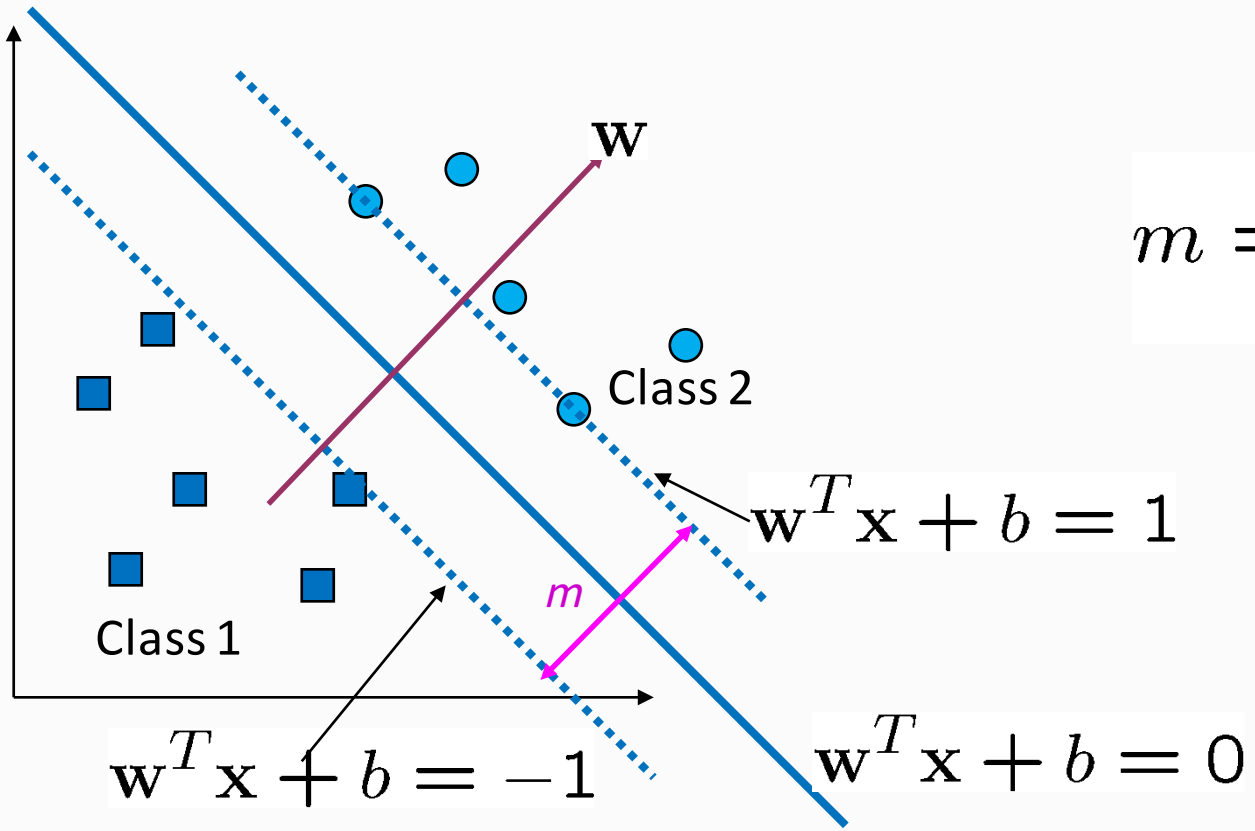
$f(x, w, b) = sign(w.\ x - b)$

1. Intuitively this feels safest.
2. If we've made a small error in the location of the boundary this gives us least chance of causing a misclassification.
3. LOOCV (leave one out cross validation) is easy since the model is immune to removal of any nonsupport-vector data points.
5. Empirically it works **very** well.

Large-Margin Decision Boundary

The decision boundary should be as far away from the data of both classes as possible

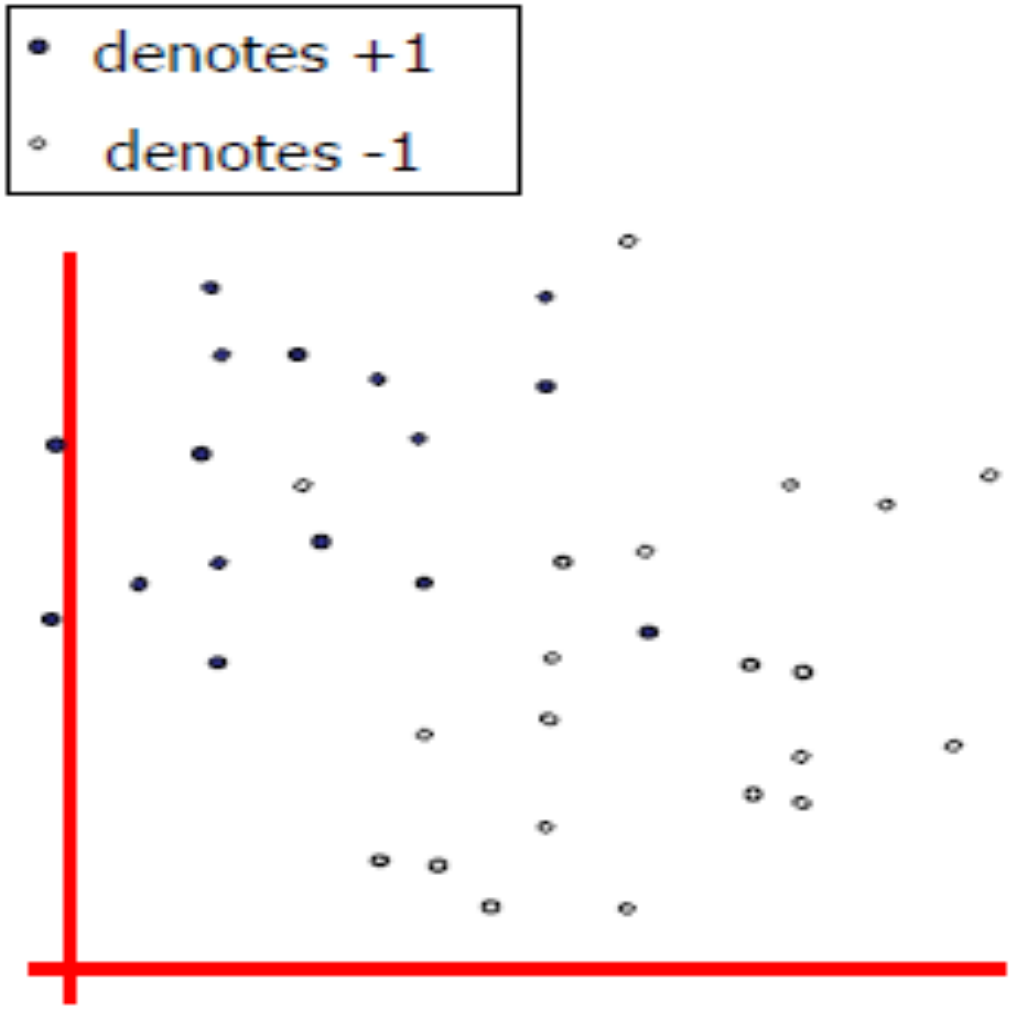
- We should maximize the margin, *m*
- Distance between the origin and the line $w^t x=-b$ is $b/||w||$



$$m = \frac{2}{||\mathbf{w}||}$$

Uh-oh!

This is going to be a problem!



Slack Variables

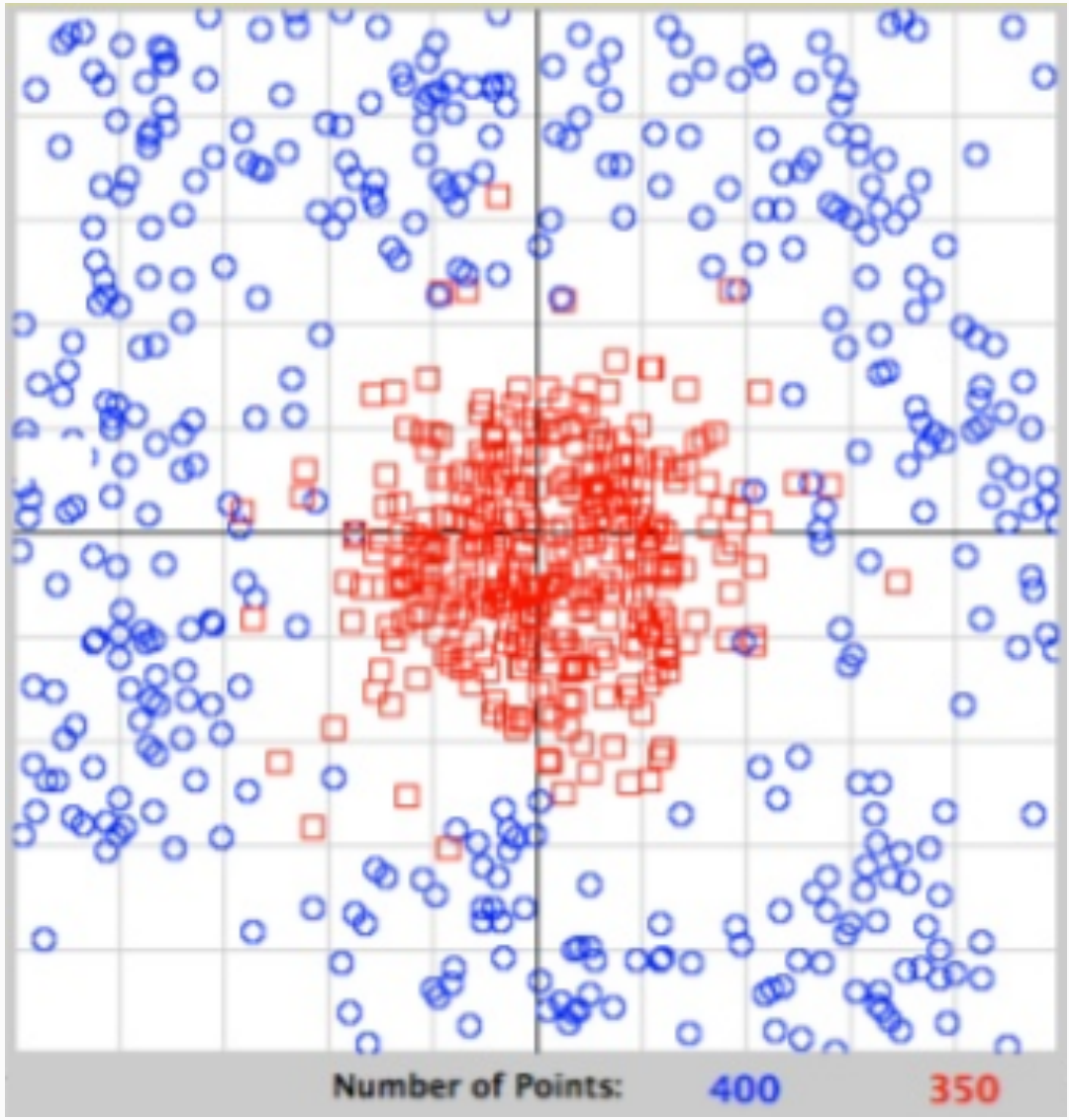
- SVMs are made robust by adding 'slack variables' that allow training error to be non-zero;
- One for each data point. Slack variable == 0 for correctly classified points

Noise

- Have assumed that the data is separable (in original or transformed space)
- Can apply SVMs to noisy data by introducing a “noise” parameter *C*
- C bounds the influence of any one training instance on the decision boundary
- Still a quadratic optimization problem
- Have to determine C by experimentation

The Kernel Trick

What if the data looks like that below?...

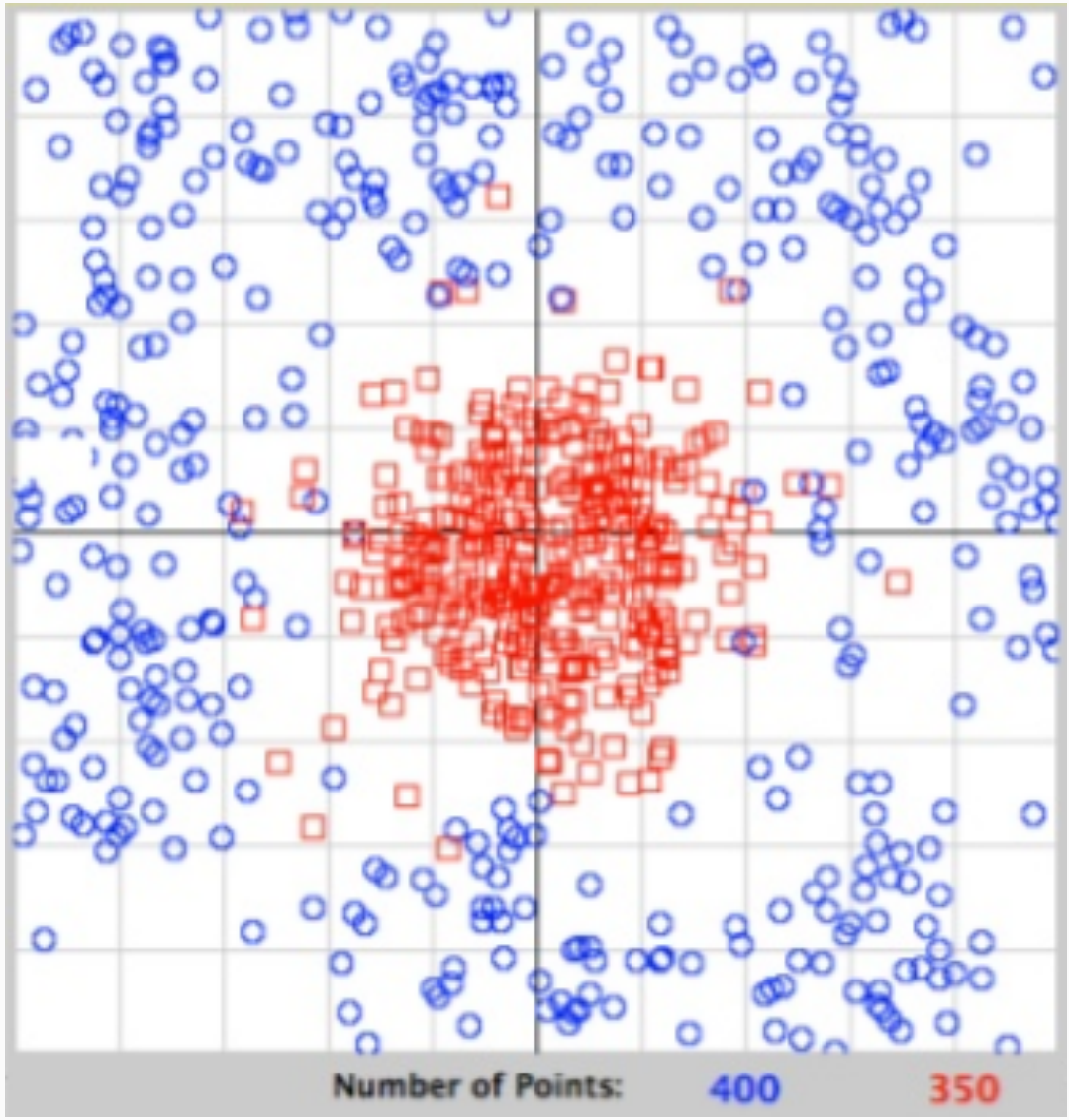


The simplest way to divide two groups is with a straight line, flat plane or an N-dimensional hyperplane. But what if the points are separated by a nonlinear region?

Rather than fitting nonlinear curves to the data, SVM handles this by using a *kernel function* to map the data into a different space where a hyperplane can be used to do the separation.

The Kernel Trick

What if the data looks like that below?...



The kernel trick allows you to use SVMs with non-linear separators

Different kernels

- Polynomial
- Gaussian
- Exponential
- …

The Kernel Trick

Everything you need to know in one slide…

Sometimes it improves your classifier if you map (i.e. transform) your data into a different feature space.

- Example 1: you have nonlinear data but want to use a linear classifier
- Example 2: your original data aren't numbers – for example they could be sequences

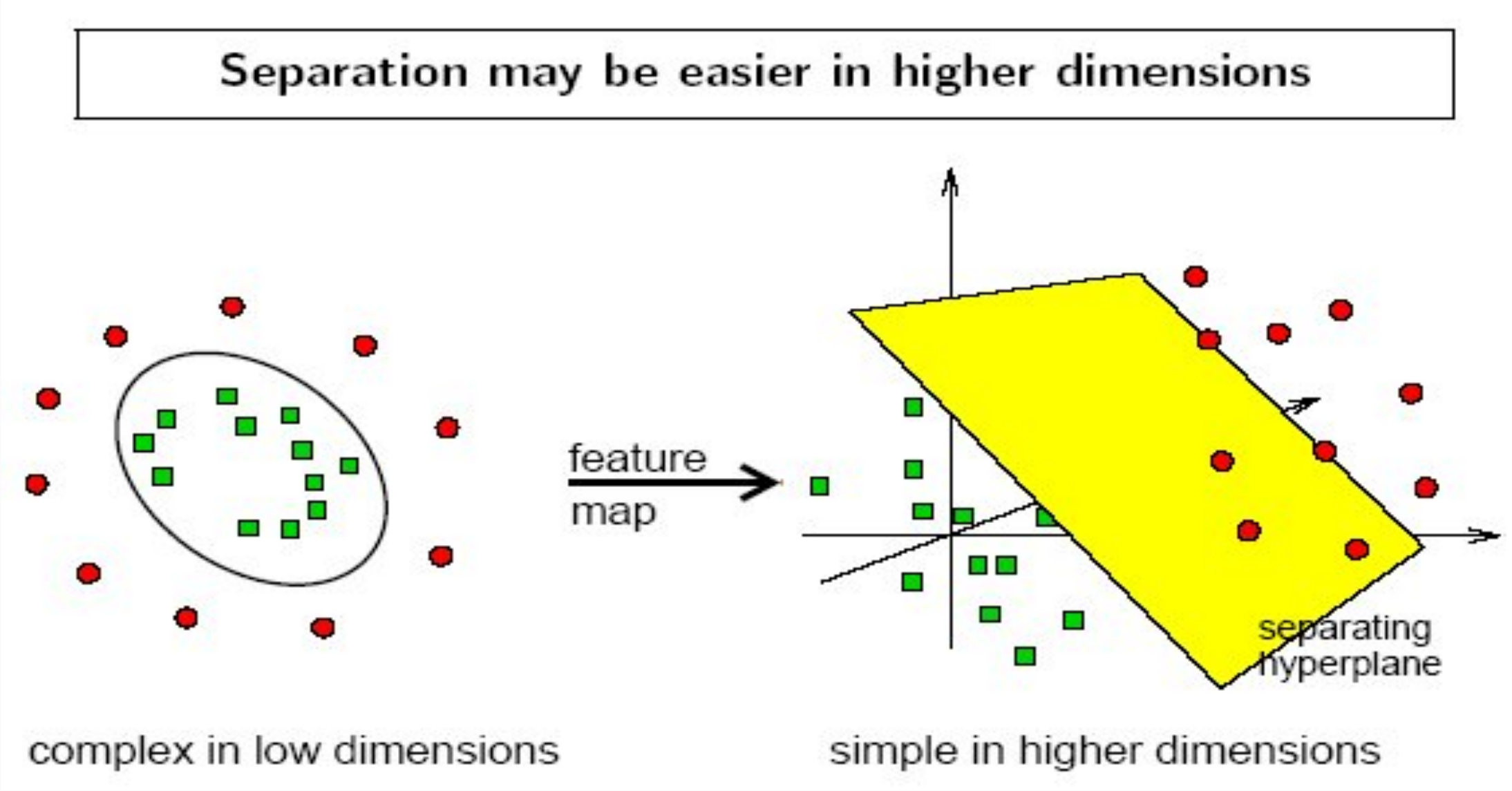
Kernel methods map your original data into a different space so that you can use linear classifiers.

This mapping can often substantially increases the number of features to consider.

- This can be problematic as your number of dimensions grows.

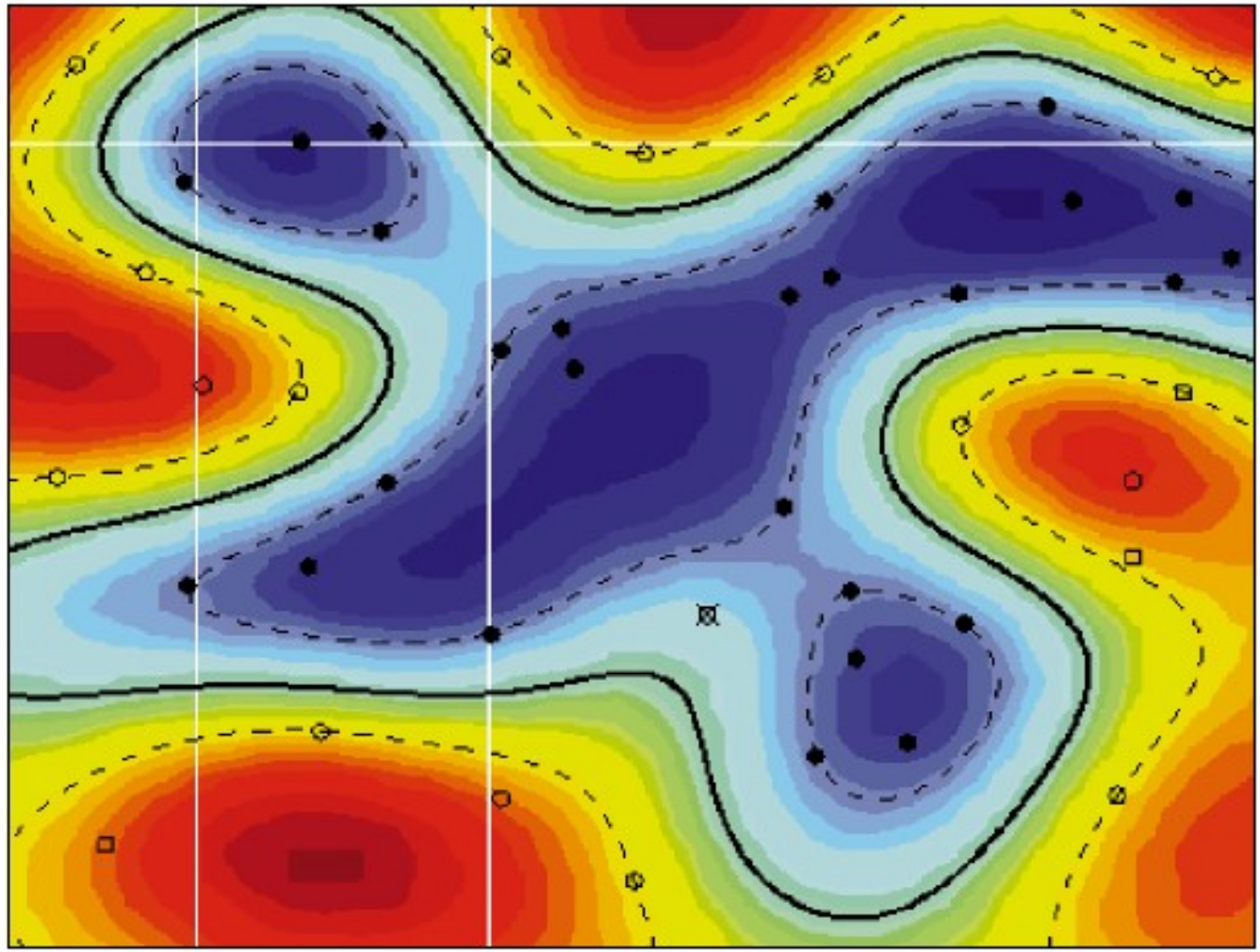
The "Kernel Trick" addresses this by putting a cap on the feature explosion so that the complexity of your classifier increases only linearly with the size of your original data.

Nonlinear Support Vector Machines



Nonlinear Support Vector Machines

The kernel function transforms the data into a higher dimensional space to make it possible to perform the separation.



Choosing the Kernel Function

Probably the most tricky part of using SVM

RBF is a good first option…

Depends on your data—try several.

- *Kernels have even been developed for nonnumeric data like sequences, structures, and trees/graphs.*

May help to use a combination of several kernels.

Don't touch your evaluation data while you're trying out different kernels and parameters.

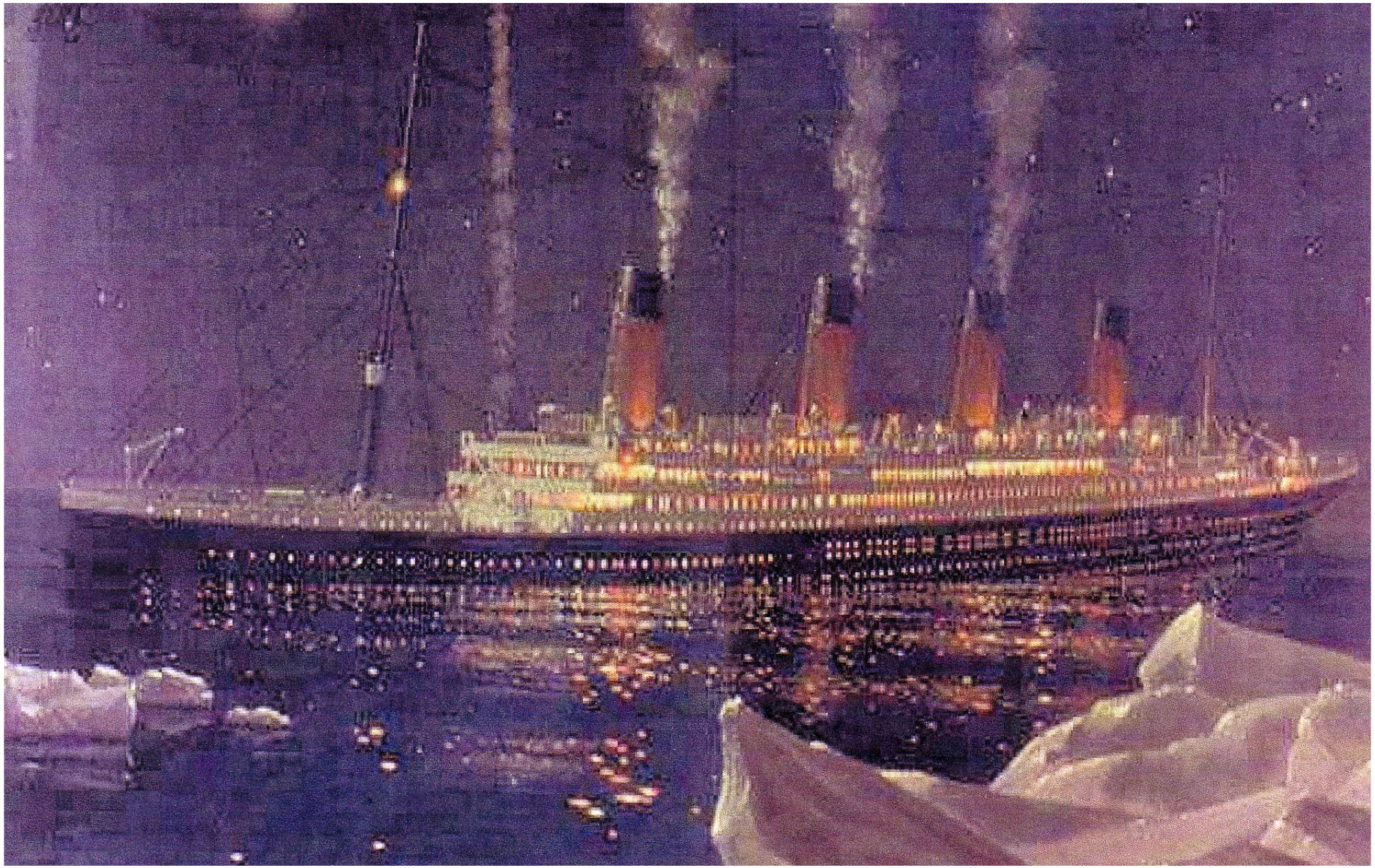
– Use cross-validation for this if you're short on data

Type of Kernel	Inner product kernel $K(\vec{x}, \vec{x}_i),\ i = 1, 2, \ldots, N$	Comments
Polynomial Kernel	$K(\vec{x}, \vec{x}_i) = \left(\vec{x}^T \vec{x}_i + \theta\right)^d$	Power p and threshold θ is specified a priori by the user
Gaussian Kernel	$K(\vec{x}, \vec{x}_i) = e^{-\frac{1}{2\sigma^2}\|\vec{x}-\vec{x}_i\|^2}$	Width σ^2 is specified a priori by the user
Sigmoid Kernel	$K(\vec{x}, \vec{x}_i) = tanh(\eta\, \vec{x}\, \vec{x}_i + \theta)$	Mercer's Theorem is satisfied only for some values of η and θ
Kernels for Sets	$K(\chi, \chi') = \sum_{i=1}^{N_\chi} \sum_{j=1}^{N_{\chi'}} k(x_i, x'_j)$	Where $k(x_i, x'_j)$ is a kernel on elements in the sets χ, χ'
Spectrum Kernel for strings	count number of substrings in common	It is a kernel, since it is a dot product between vectors of indicators of all the substrings.

Table 1: Summary of Inner-Product Kernels [Hay98]

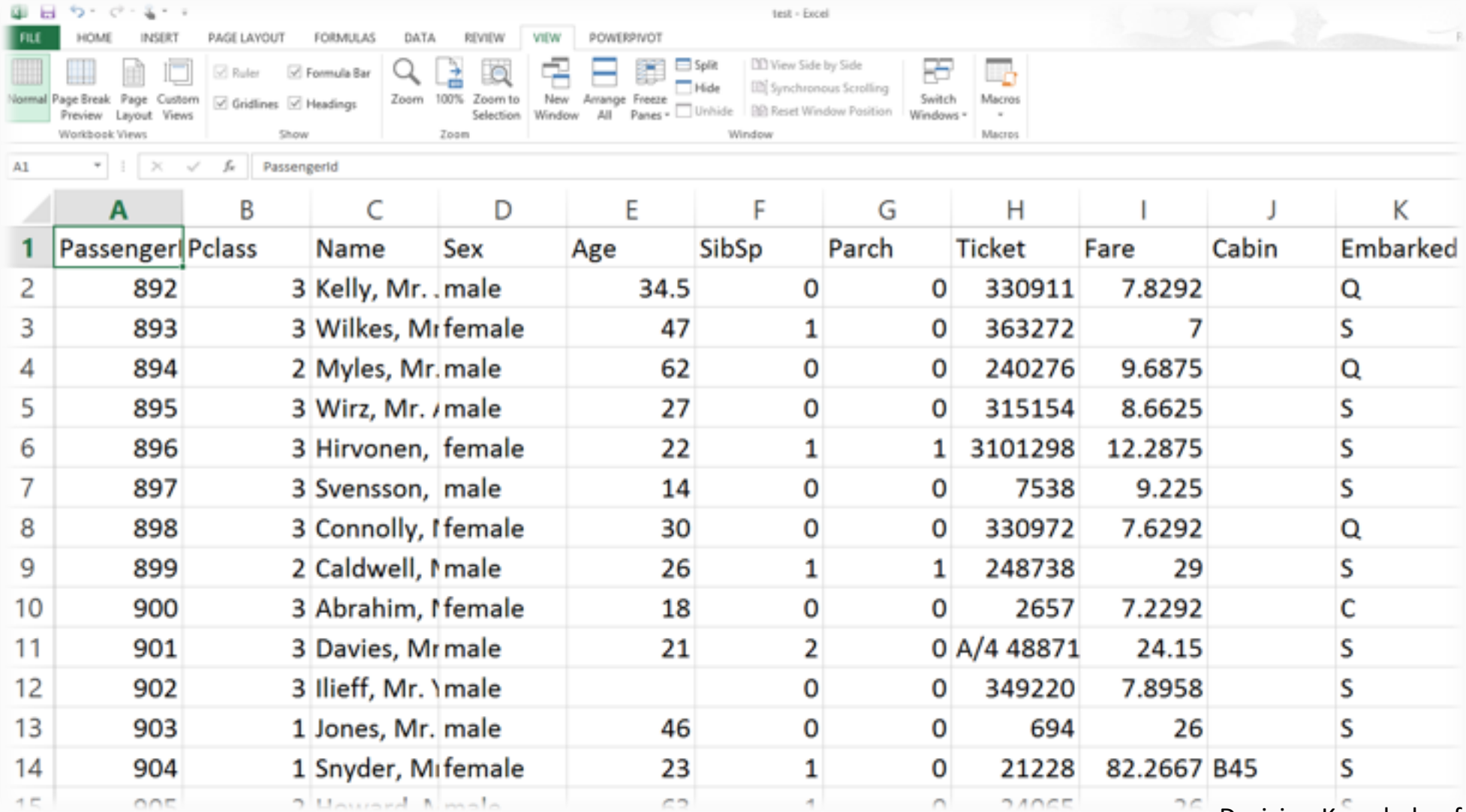
Complexity of the optimization problem remains only dependent on the dimensionality of the input space and not of the feature space!

The Tragedy of the Titanic



First Steps…

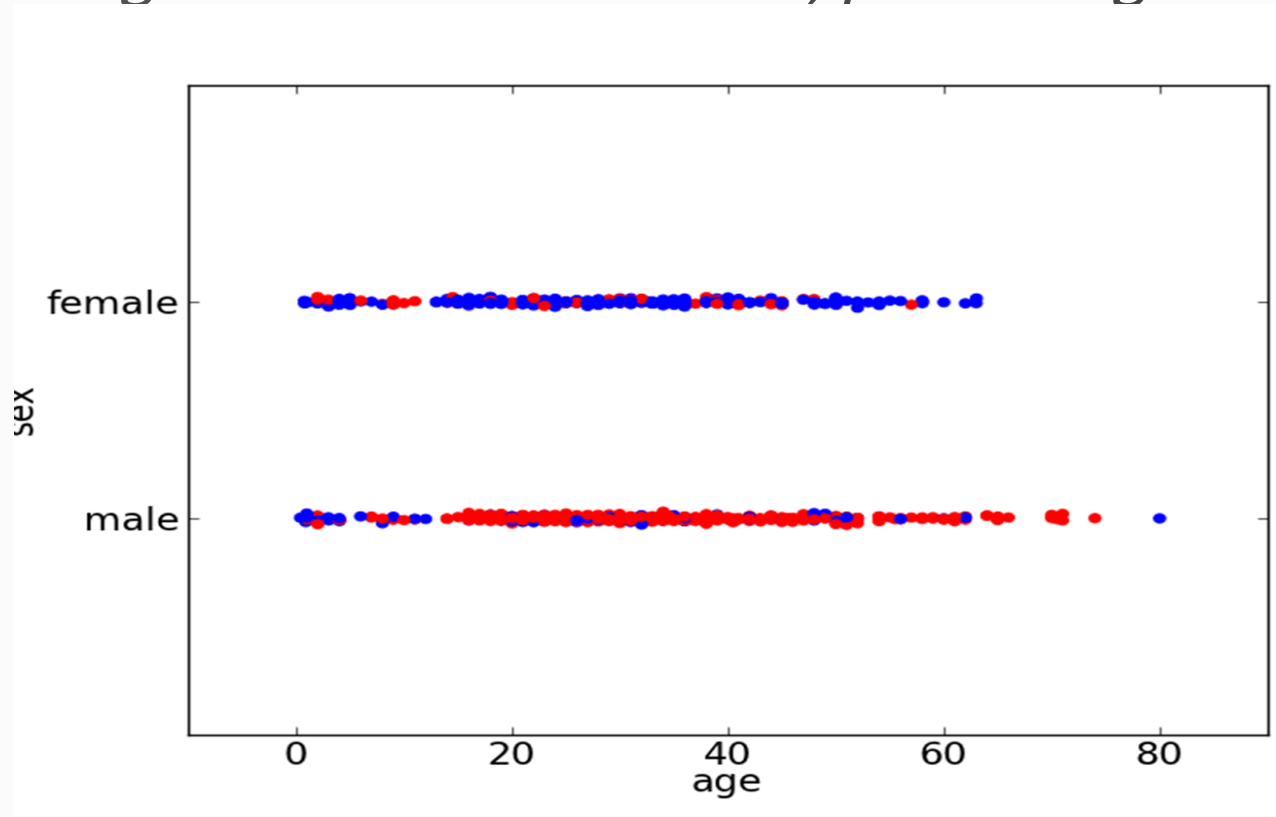
- Look at the data, exploratory data analysis



	A	B	C	D	E	F	G	H	I	J	K
1	PassengerI	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
2	892	3	Kelly, Mr. .	male	34.5	0	0	330911	7.8292		Q
3	893	3	Wilkes, Mr	female	47	1	0	363272	7		S
4	894	2	Myles, Mr.	male	62	0	0	240276	9.6875		Q
5	895	3	Wirz, Mr. /	male	27	0	0	315154	8.6625		S
6	896	3	Hirvonen,	female	22	1	1	3101298	12.2875		S
7	897	3	Svensson,	male	14	0	0	7538	9.225		S
8	898	3	Connolly, I	female	30	0	0	330972	7.6292		Q
9	899	2	Caldwell, I	male	26	1	1	248738	29		S
10	900	3	Abrahim, I	female	18	0	0	2657	7.2292		C
11	901	3	Davies, Mr	male	21	2	0	A/4 48871	24.15		S
12	902	3	Ilieff, Mr. Y	male		0	0	349220	7.8958		S
13	903	1	Jones, Mr.	male	46	0	0	694	26		S
14	904	1	Snyder, Mr	female	23	1	0	21228	82.2667	B45	S

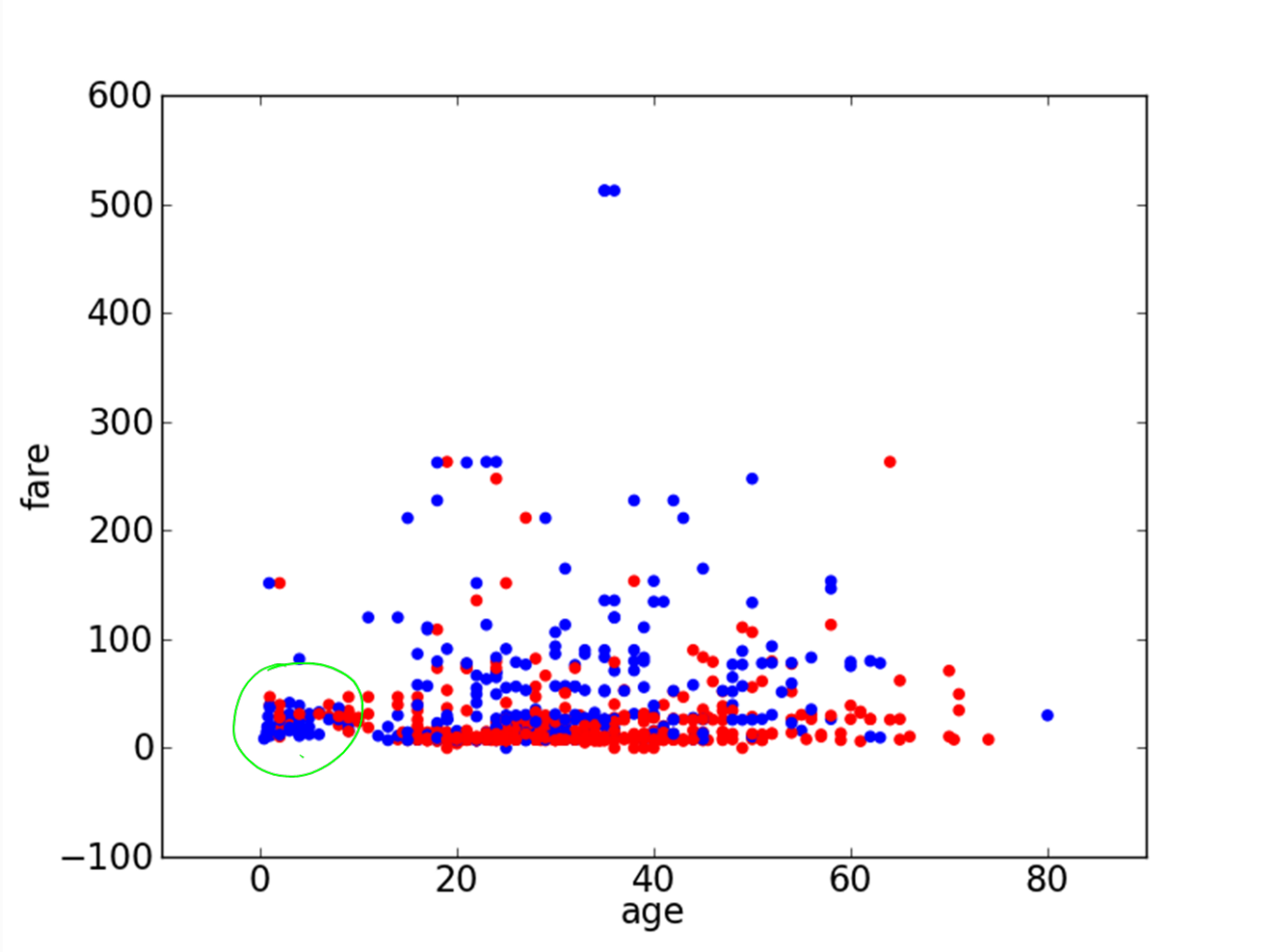
First Steps…

- Look at the data;
- Follow your intuition, *"women and children first…"*
  - *What percentage of Females survived, percentage of males survived?…*



First Steps…

- Other features good predictors?



A very naïve classifier

pclass	sex	age	sibsp	parch	fare	cabin	embarked
1	female	35	1	0	53.1	C123	S

Does the new data point x* ***exactly*** match a previous point x_i?

If so, assign it to the same class as x_i

Otherwise, just guess.

This is the "rote" classifier

A minor improvement

pclass	sex	age	sibsp	parch	fare	cabin	embarked
1	female	35	1	0	53.1	C123	S

Does the new data point x^* match a set of previous points x_i on **some specific attribute**?

If so, take a vote to determine class.

Example: If most females survived, then assume every female survives

But there are lots of possible rules like this.
And an attribute can have more than two values.

If most people under 4 years old survive, then assume everyone under 4 survives
If most people with 1 sibling survive, then assume everyone with 1 sibling survives

How do we choose?

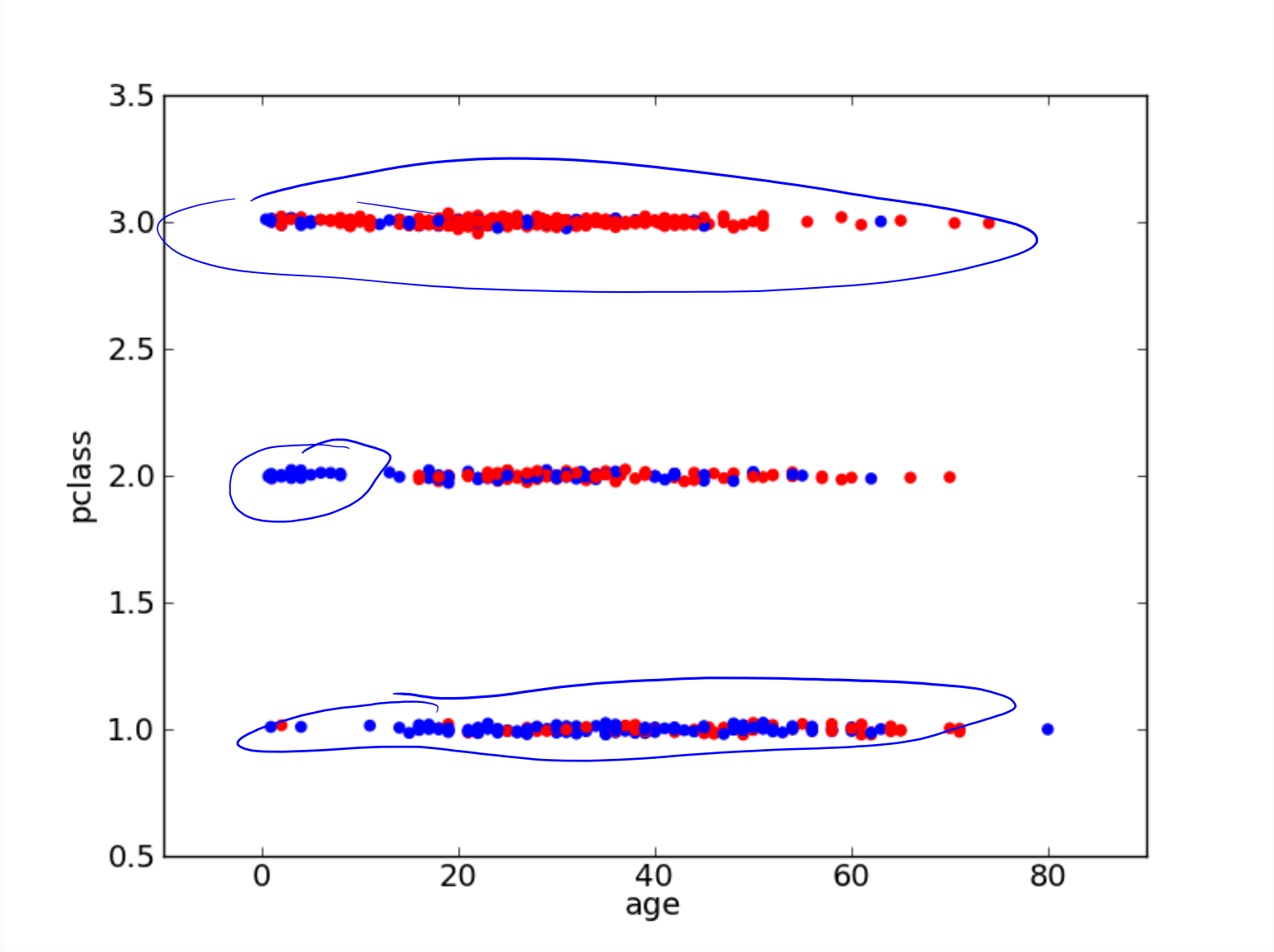
IF sex='female' THEN survive=yes
ELSE IF sex='male' THEN survive = no

```
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!


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

IF pclass='1' THEN survive=yes

ELSE IF pclass='2' THEN survive=yes

ELSE IF pclass='3' THEN survive=no

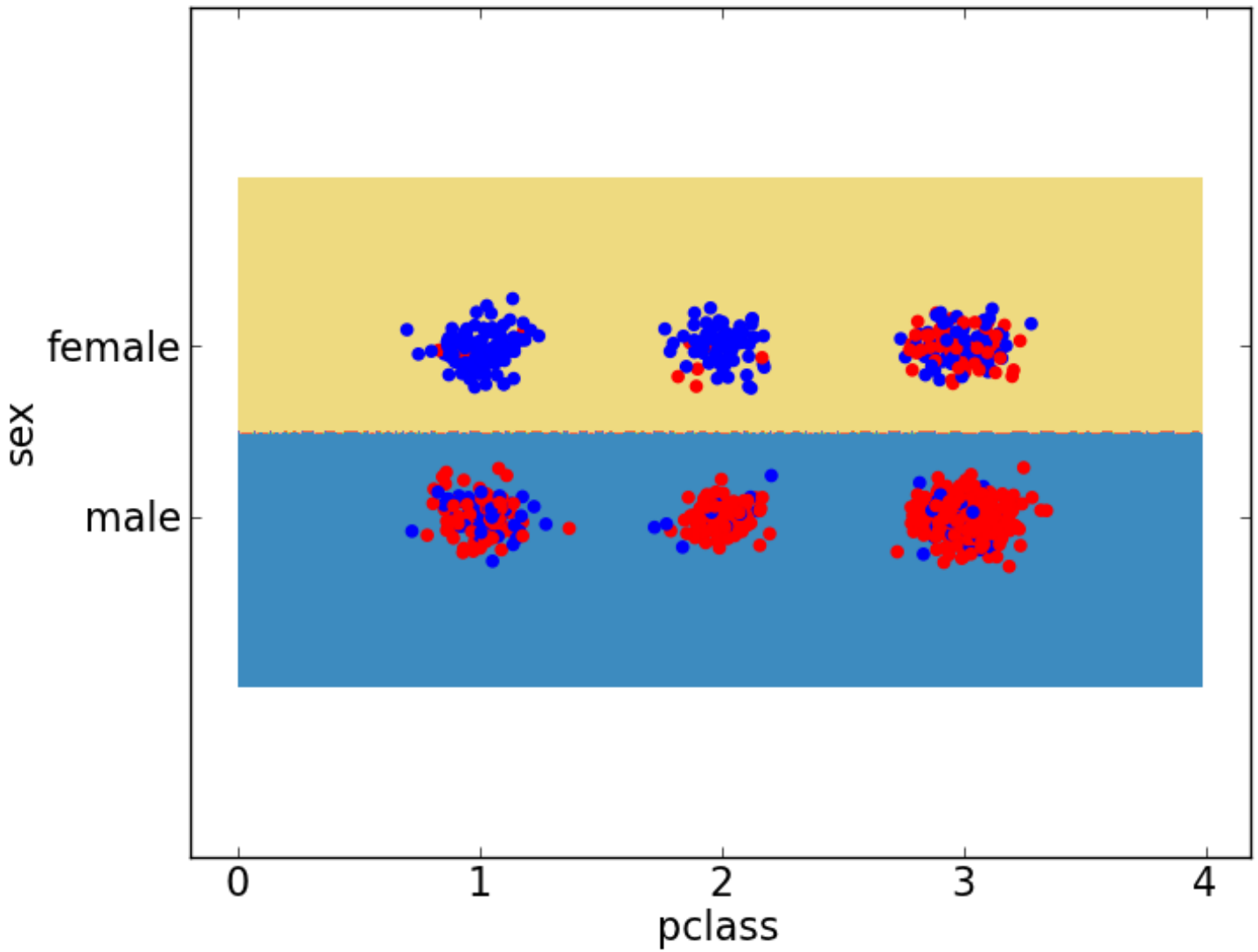
```
confusion matrix

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

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

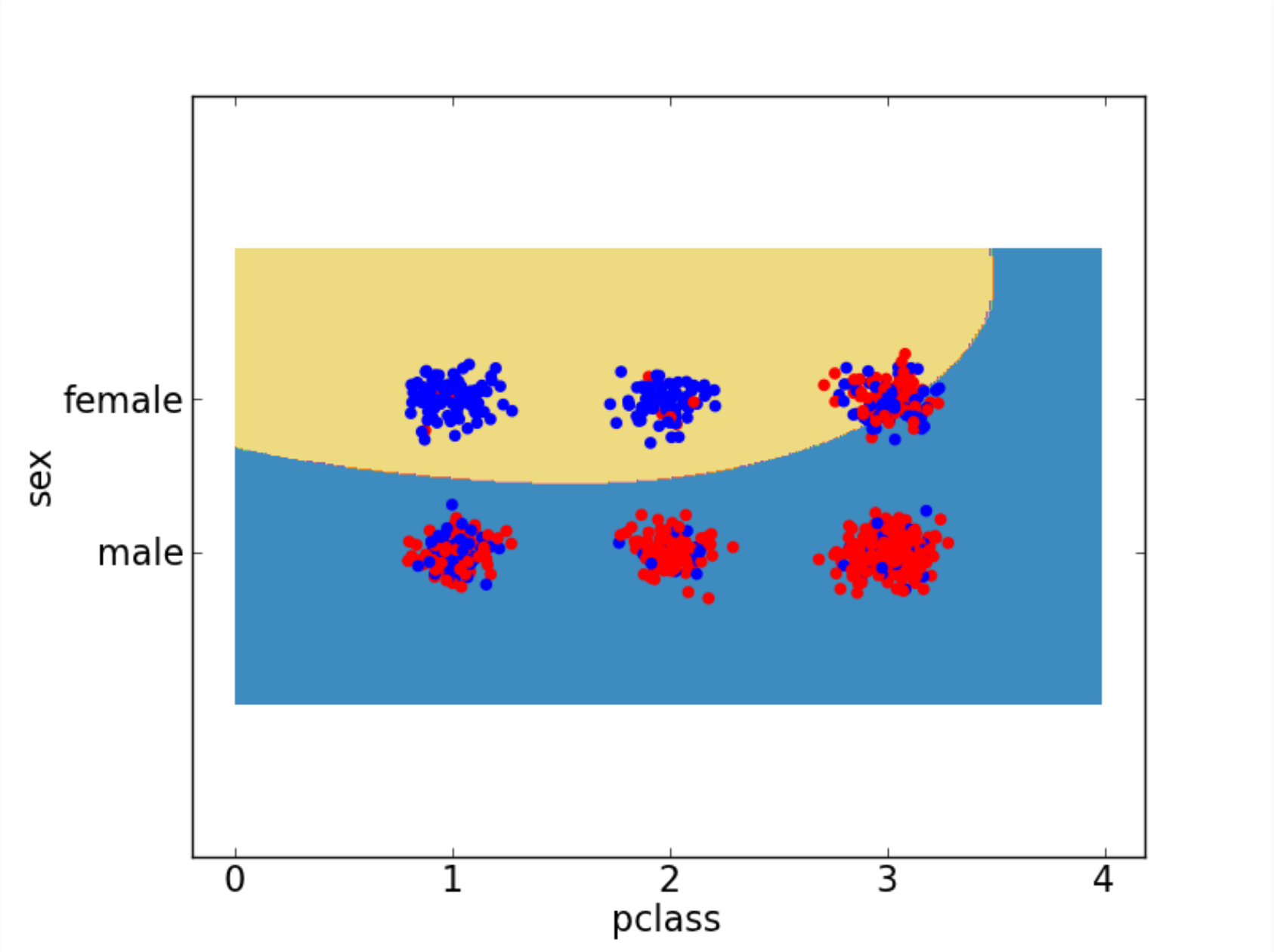
a little worse

Support Vector Machine Model, Titanic Data, Linear Kernel



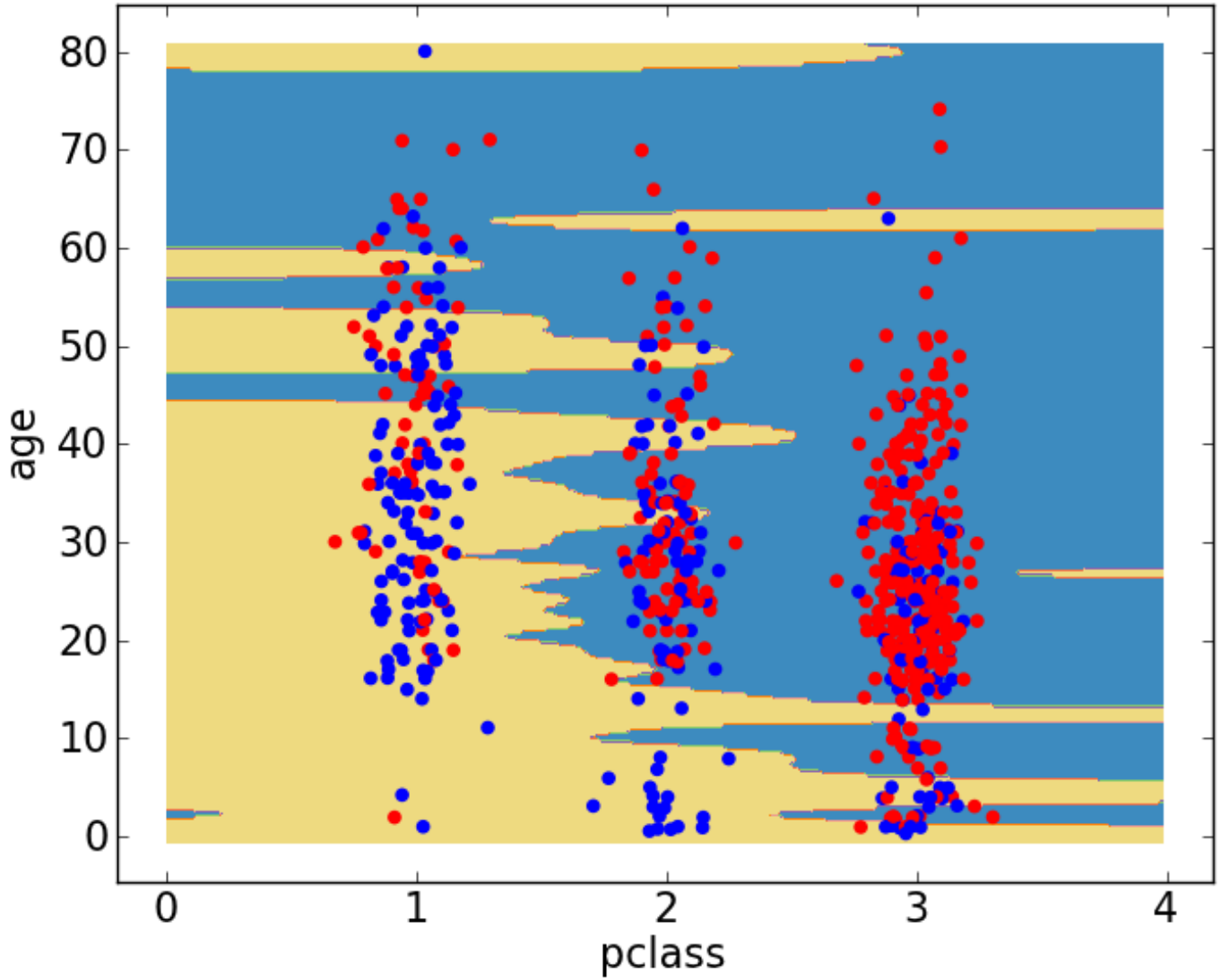
Support Vector Machine Model, RBF Kernel

Titanic Data



Support Vector Machine Model, RBF Kernel

Titanic Data

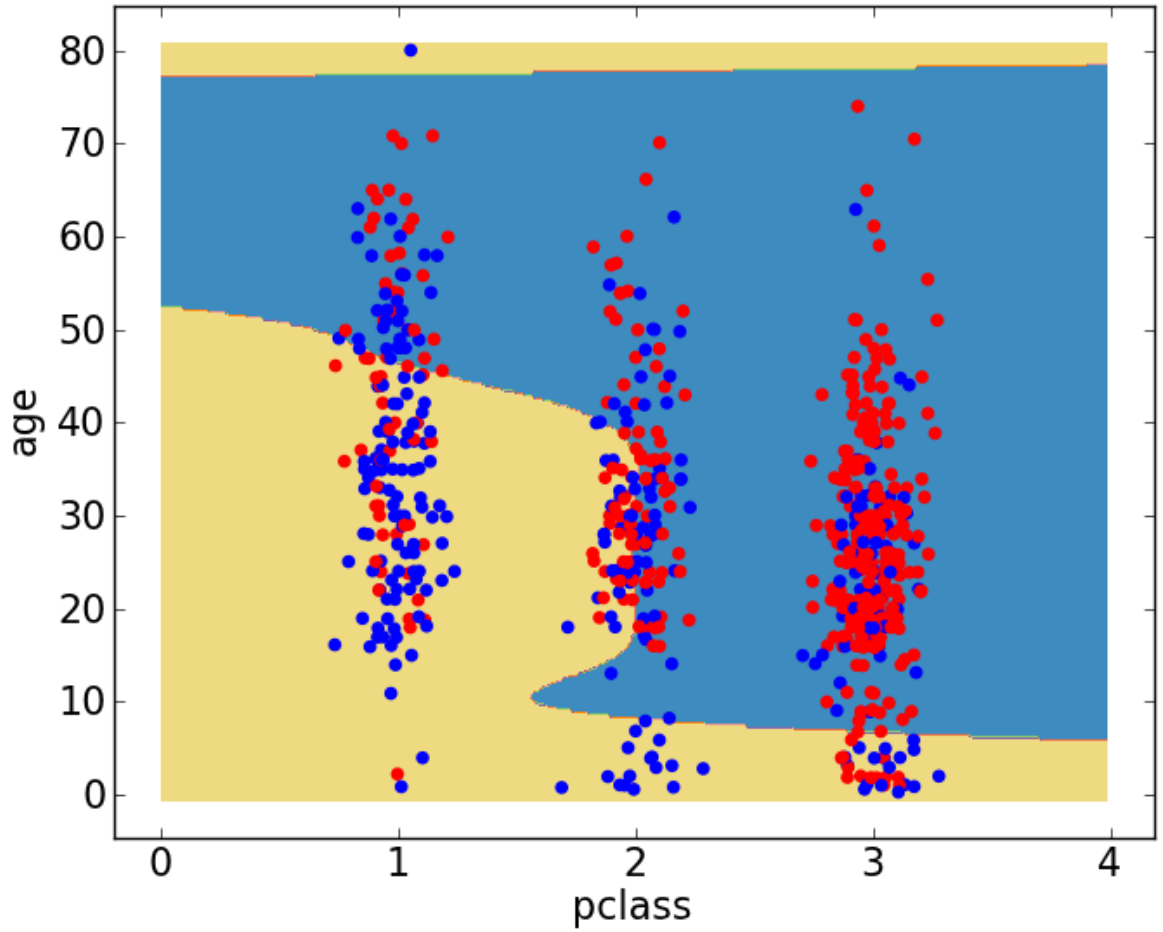


overfitting?

Support Vector Machine Model, RBF Kernel

Titanic Data

A gamma, parameter that controls/balances model complexity against accuracy



Sparse Data

- SVM algorithms speed up dramatically if the data is sparse (i.e. many values are 0)
- Why? Because they compute lots and lots of dot products
- Sparse data compute dot products very efficiently
- Iterate only over nonzero values
- SVMs can process sparse datasets with 10,000s of attributes

Doing multi-class classification

- SVMs can only handle two-class outputs (i.e. a categorical output variable with arity 2).
- What can be done?
- Answer: with output arity N, learn N SVM's
  - SVM 1 learns "Output==1" vs "Output != 1"
  - SVM 2 learns "Output==2" vs "Output != 2"

    ….
  - SVM N learns "Output==N" vs "Output != N"
- Then to predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region.

What you need to know…

- First, try logistic regression. Easy, fast, stable. No 'tuning' parameters.
- Equivalently, you can first try linear SVMs, but you need to tune 'C'
- If results are "good enough", stop
- Else, try SVMs with Gaussian kernels (RBF)

Need to tune bandwidth, C – by using validation data…

Summary: Steps for Classification

- SVMs require vector of real numbers
  - Categorical variables → numeric data {R,G,B} → {0,0,1},…{1,0,0}
  - Scaling to the range [-1, +1] or [0,1]
- Select the kernel function to use
  - RBF is a reasonable first choice, two parameters C and γ
  - Grid search to identify best values for parameters
  - Use v-fold cross validation to ensure good performance on test data
- Unseen data can be classified using support vectors

Conclusion

- SVMs balance between correctness and generalization
  - Decision boundaries
  - Margins
  - Support vector
- Two key concepts of SVM: maximize the margin and the kernel trick
- Many SVM implementations are available on the web for you to try on your data set!

Software

- A list of SVM implementation can be found at http://www.kernel-machines.org/software.html
- Some implementation (such as LIBSVM) can handle multi-class classification
- SVMLight is among one of the earliest implementation of SVM
- Several Matlab toolboxes for SVM are also available

Data Science

Deriving Knowledge from Data at Scale

That's all for tonight….