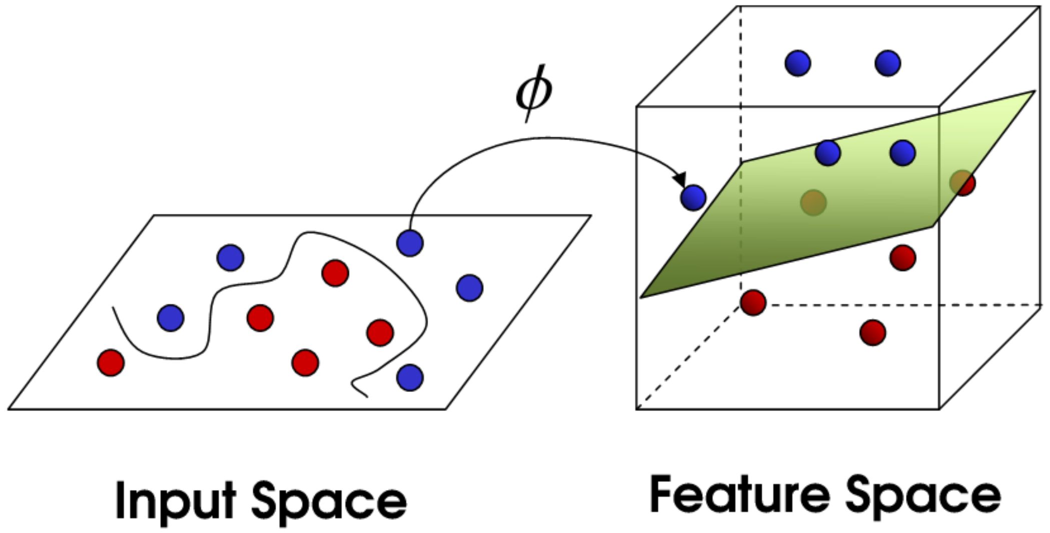
CS109 – Data Science
SVM, Performance evaluation

Joe Blitzstein, Hanspeter Pfister, Verena Kaynig-Fittkau



http://i.stack.imgur.com/1gvce.png

Announcements

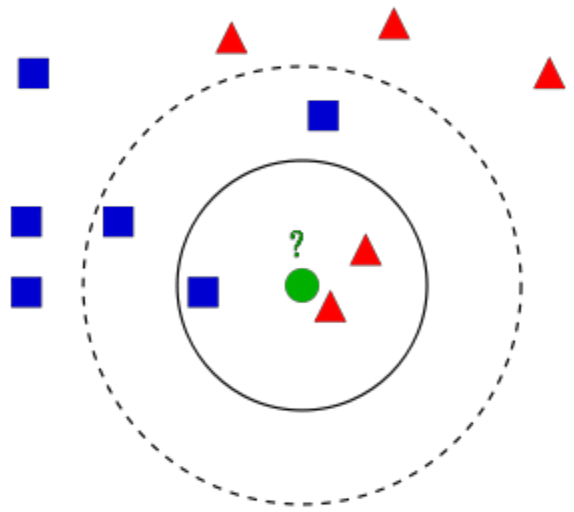
- HW1 grades went out yesterday
- They are looking really good, well done everyone!

- HW2 is due this Thursday!

- You should submit an executed notebook
- But please without pages of test output

Recap K-NN

- Keeps all training data
- Training is fast
- Prediction is slow

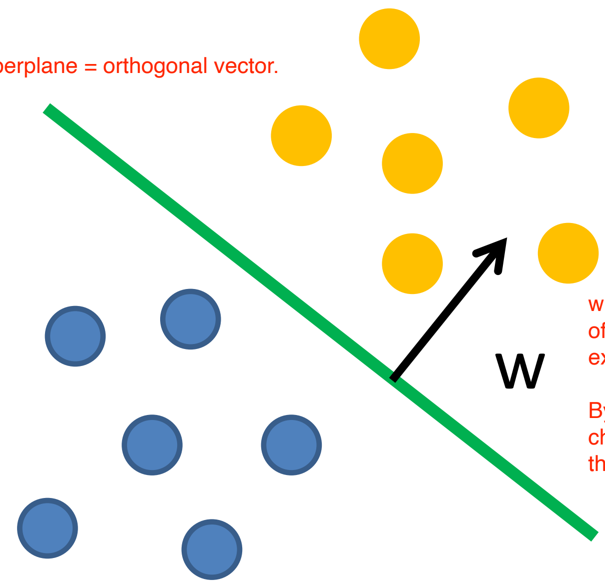


Separating Hyperplane

the goal is to estimate w

- x: data point
- y: label $\in \{-1, +1\}$
- w: weight vector

perpendicular to the hyperplane = orthogonal vector.



w defines the orientation of the hyperplane, in this example.

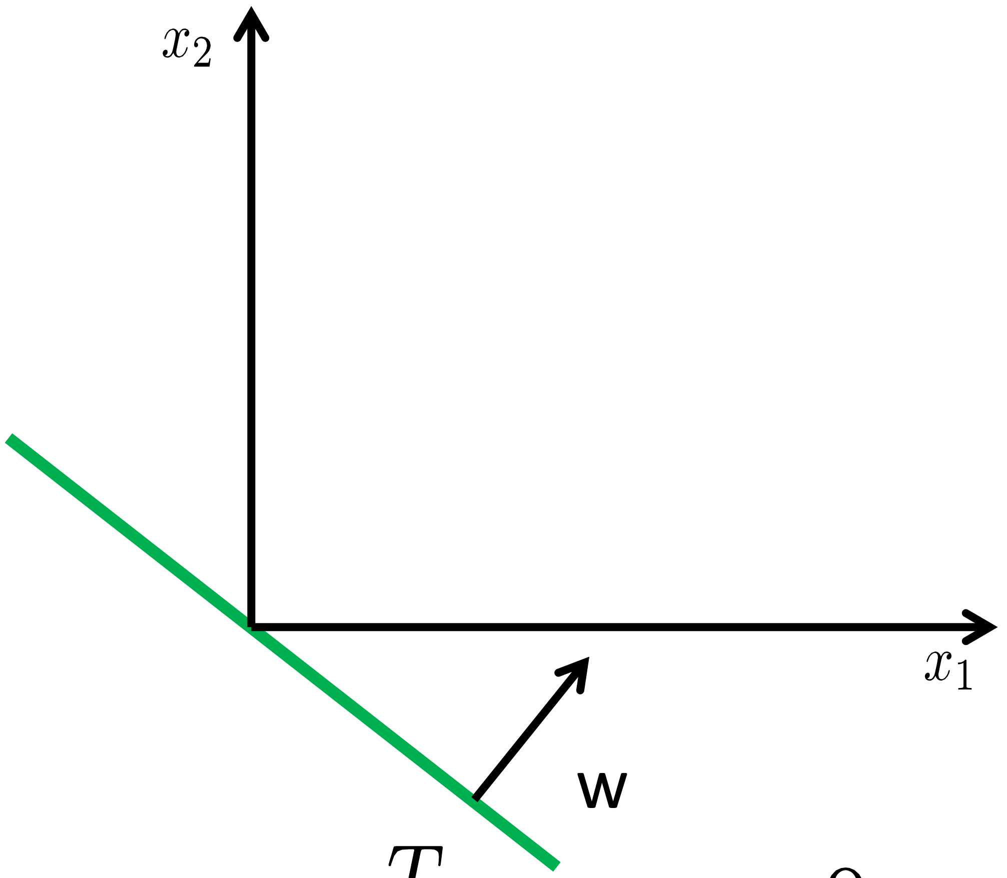
By changing w, you change the orientation of the hyperplane.

Here, the yellow colors are considered to have a label of +1, while blue has the label of -1.

$$w^T x \qquad = 0$$

Separating Hyperplane

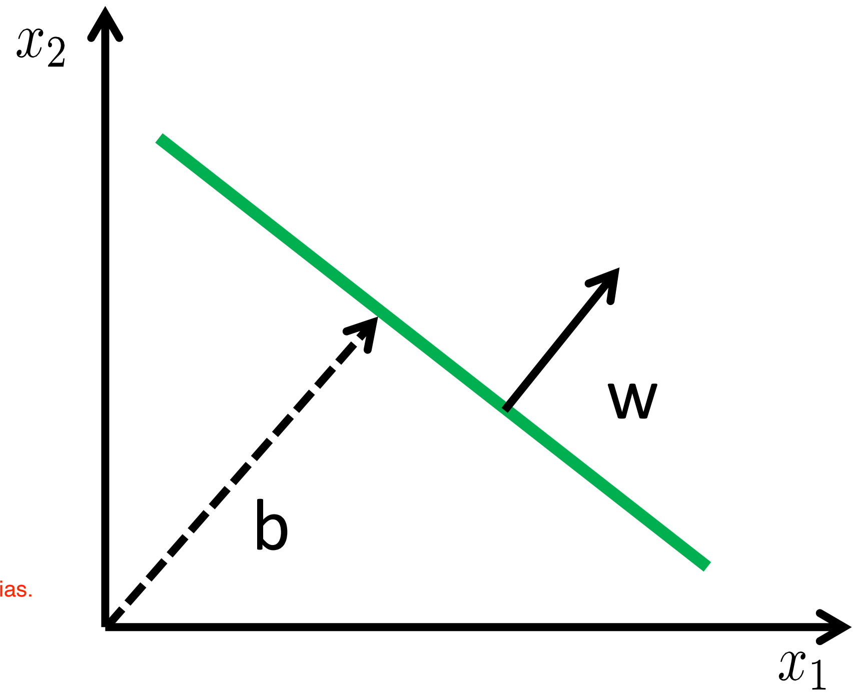
- x: data point
- y: label $\in \{-1, +1\}$
- w: weight vector



$$w^T x \quad = 0$$

Separating Hyperplane

- x: data point
- y: label $\in \{-1, +1\}$
- w: weight vector
- b: bias



Two things needed to know the separating hyperplane: weight & bias.

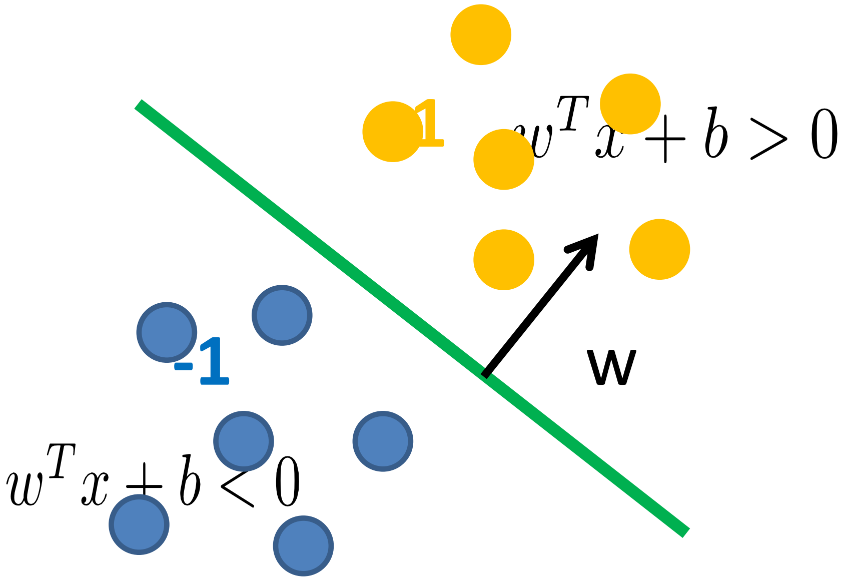
weight, to change orientation
bias to change the height of separating hyperplane.

You can then optimize them randomly and have the hyperplane 'wiggle' in between the two classes/labels.

$$w^T x + b = 0$$

Separating Hyperplane

- x: data point
- y: label $\in \{-1, +1\}$
- w: weight vector
- b: bias



Once you have w & b, prediction becomes much easier.

Here, you take your data point x and you evaluate this equation: w*x+b

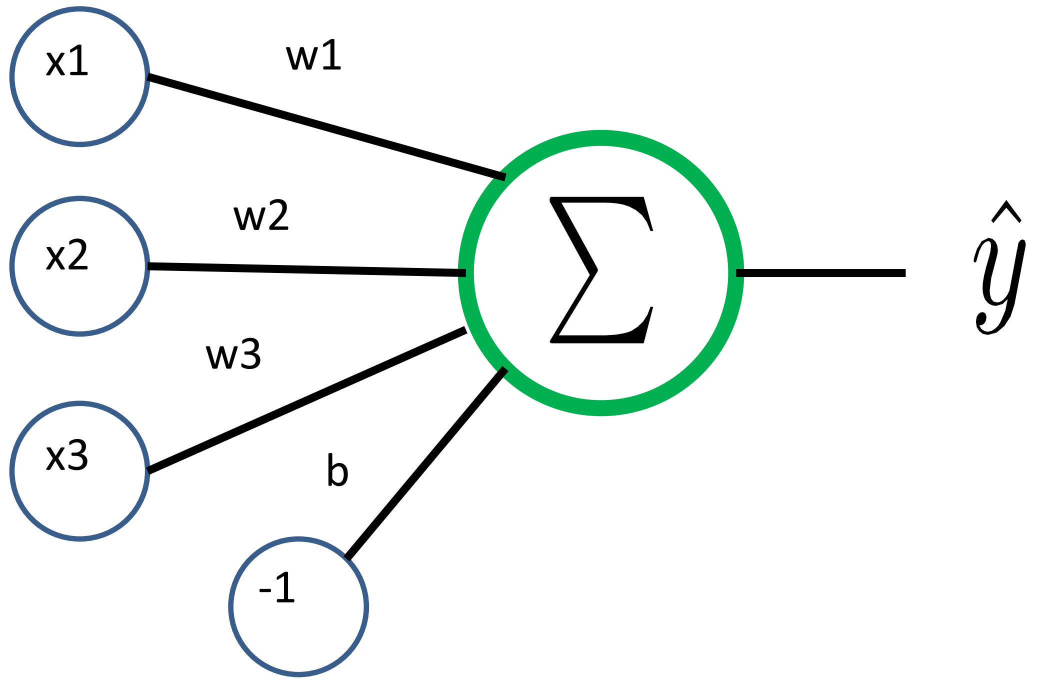
You look at the sine of that result. If it's greater than 0, then it's on the right side of the hyperplane, and if it's less than 0, it's on the other side of the hyperplane.

All you'd need to store, rather than the training data like in KNN, are the above parameters.

However, the tradeoff is that you're now restricted to a line, while KNN can be more tailored to the data points.

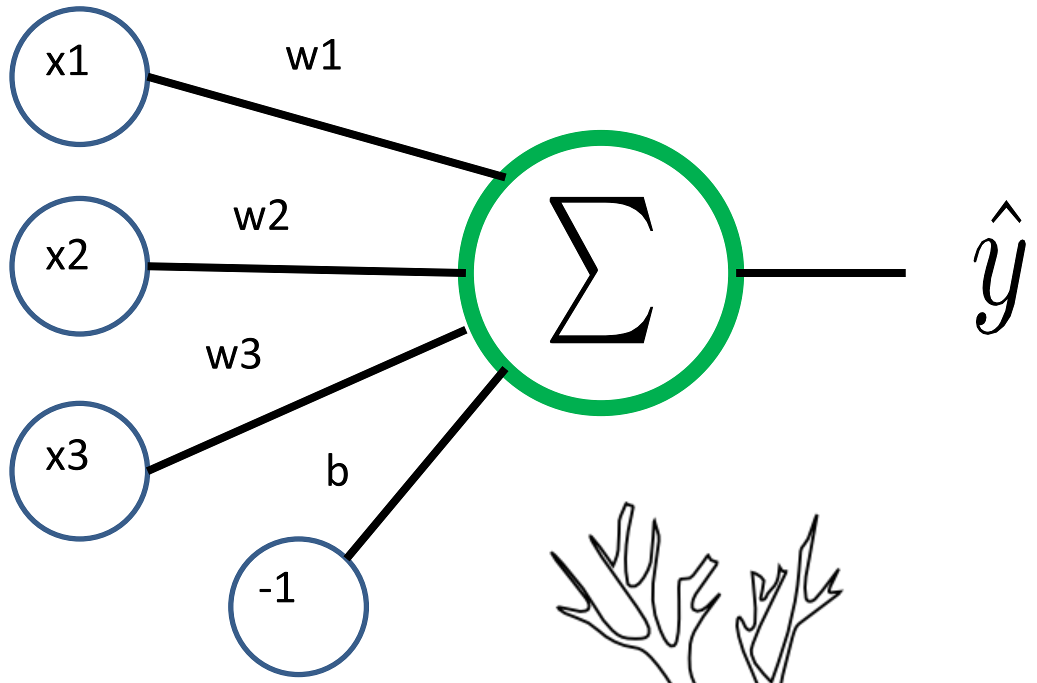
The goal is to keep all the positive things about this without the negative costs of KNN.

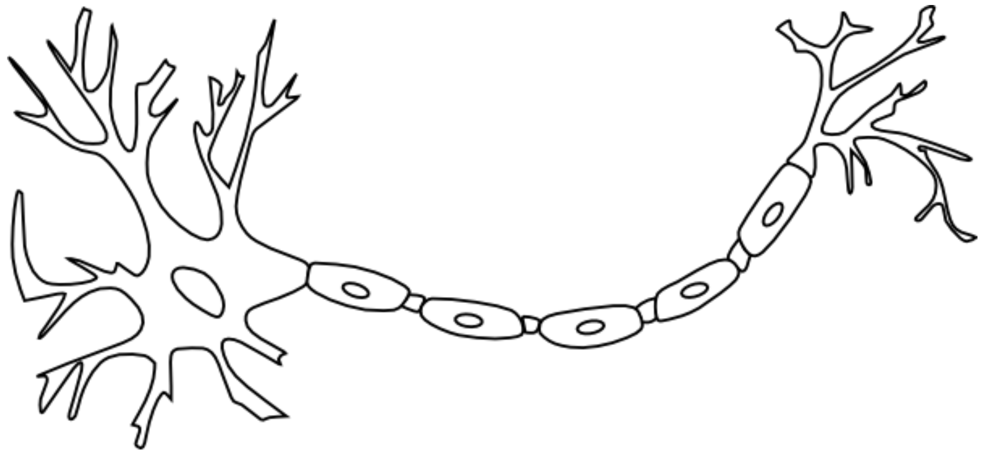
Perceptron



$$w^T x + b = 0$$

Perceptron





Perceptron History

- invented 1957
- by Frank Rosenblatt

- the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence. (NYT 1958)

  (http://en.wikipedia.org/wiki/Perceptron

These perceptron machines were the basic components of what would become Deep Learning.

This was the theory behind the neural network, that it looked like a neuron and therefore how a human brain lerns.

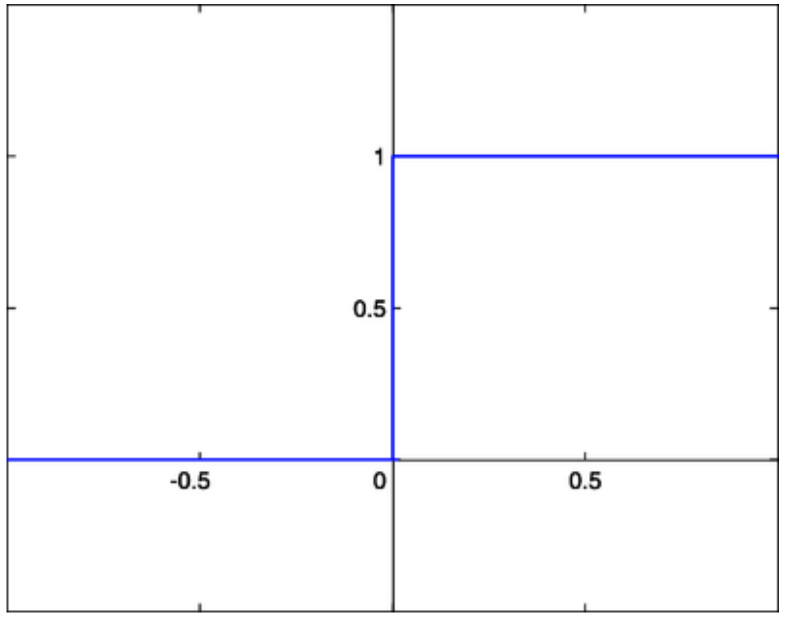
Perceptron.mp4

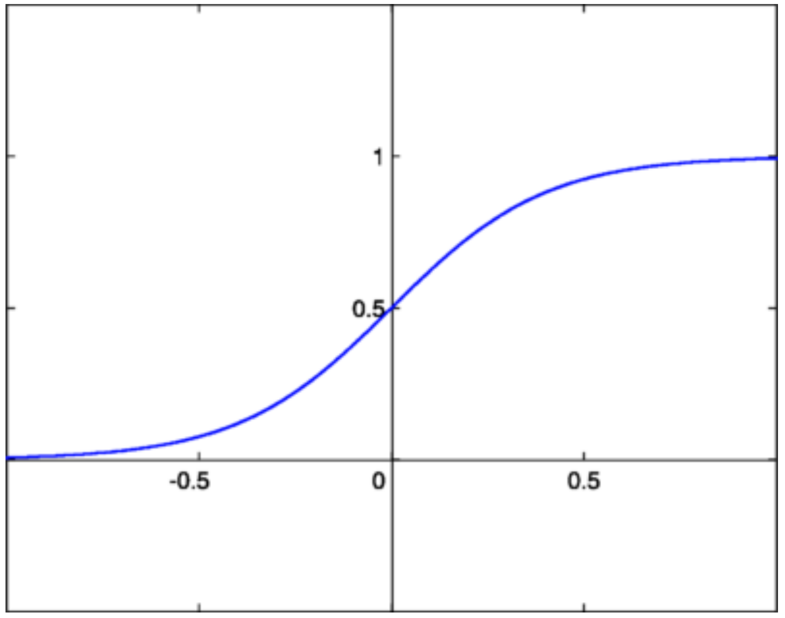
https://www.youtube.com/watch?v=cNxadbrN_aI&list=PLdVOMWcqwwIlaygvb9ZteZ1r4Br6kRuBO

Side Note: Step vs Sigmoid Activation

A sigmoid function is a continuous approximation of the step function.

This is actually a representation of a logistic regression.





$$s(x) = \frac{1}{1 + e^{-cx}}$$

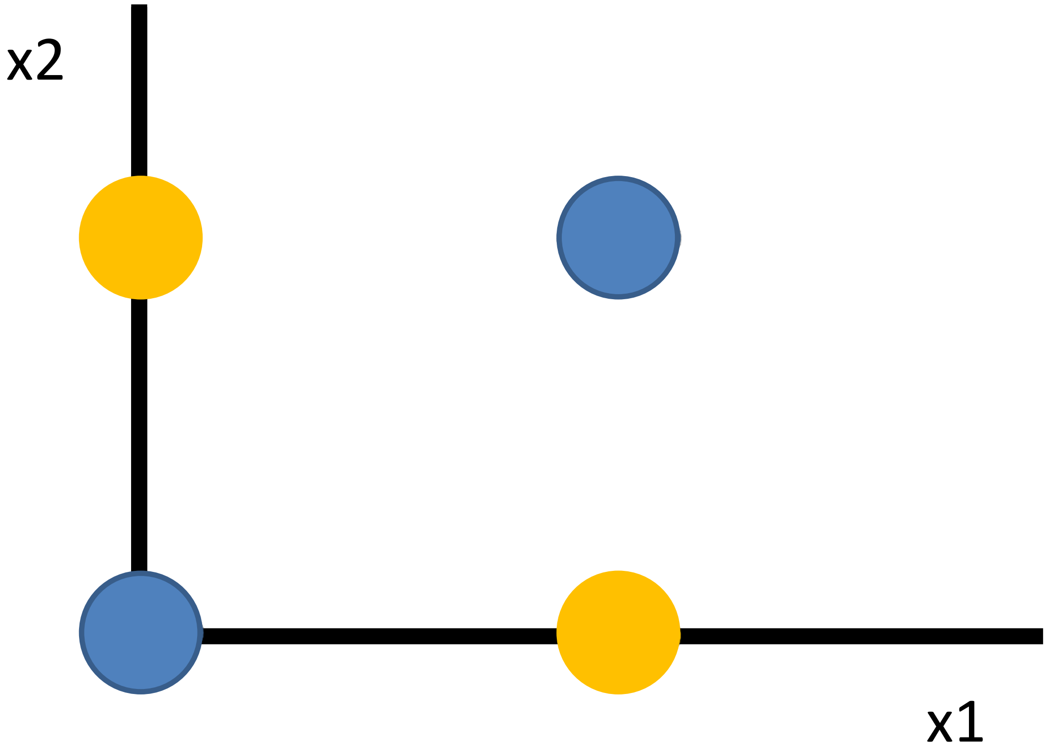
The Critics

- 1969: Minsky and Papert publish their book "Perceptrons"
- Very controversial book, some blame the book for causing the whole research area to stagnate.

https://en.wikipedia.org/wiki/Perceptrons_(book)

The XOR Problem

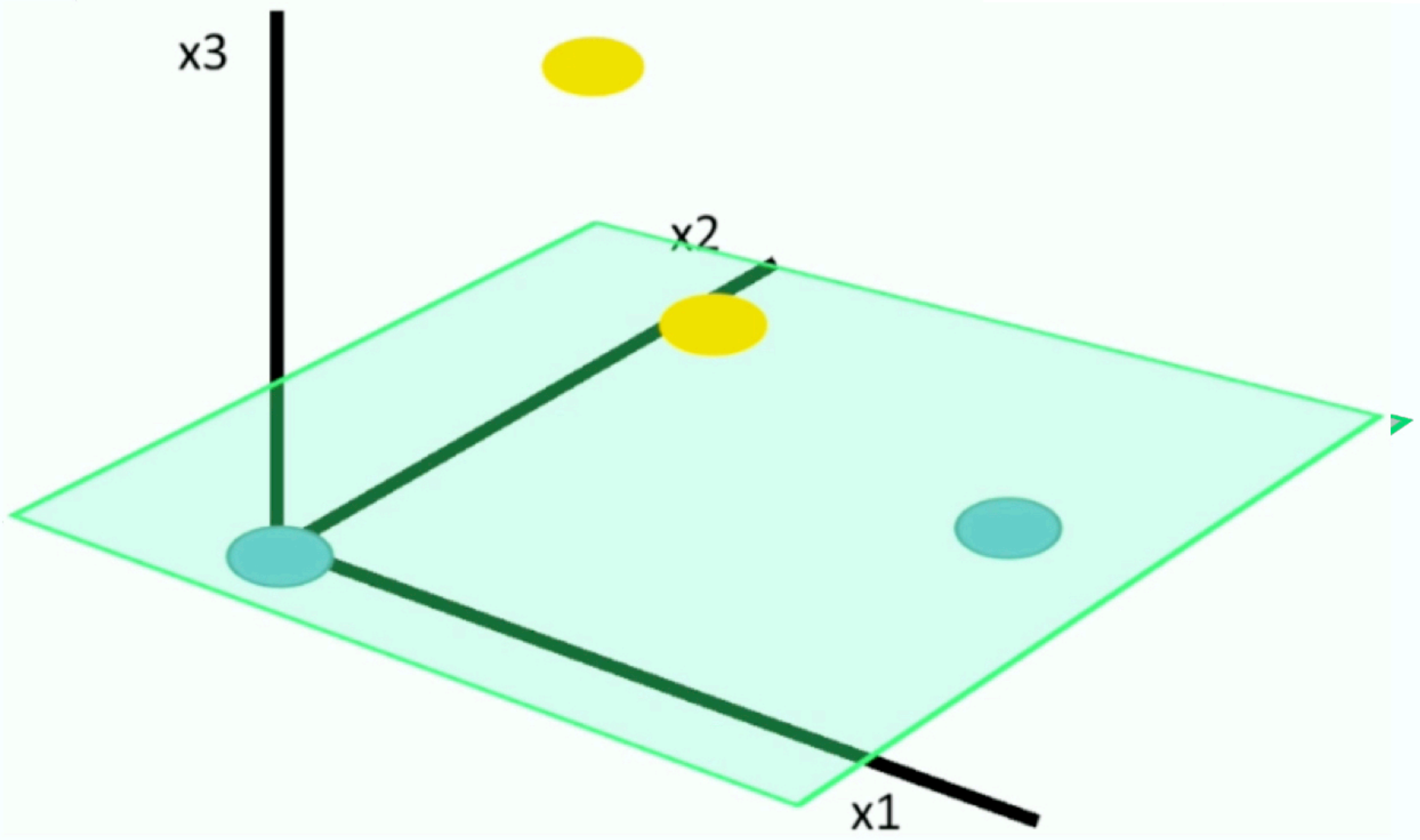
There isn't a single line here that can separate the two classes, cleanly.



The XOR Problem

The solution is to add a third dimension and do a trick right, in order to create that decision boundary.

You can elevate the yellow data points/observations to a third dimension and allow for classification.

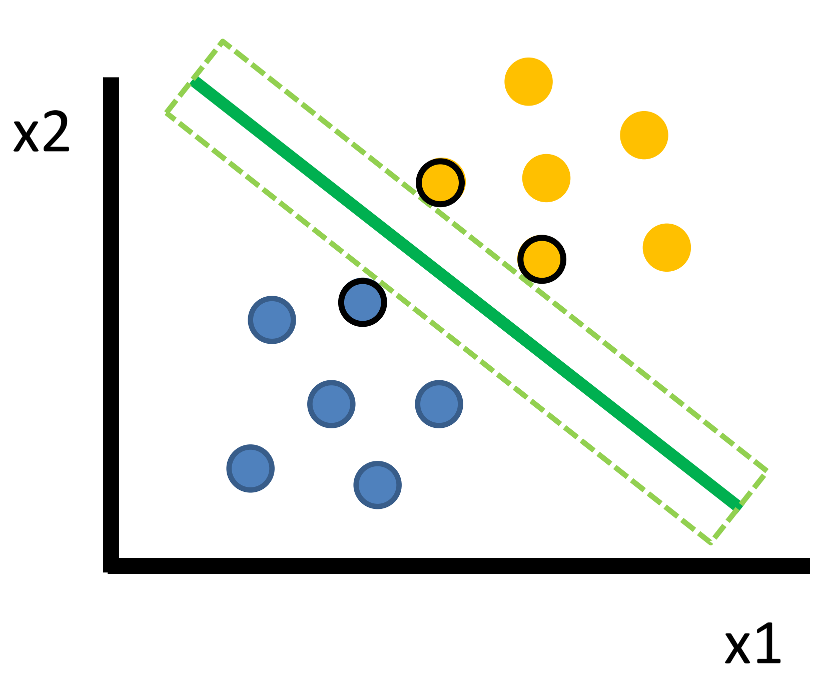


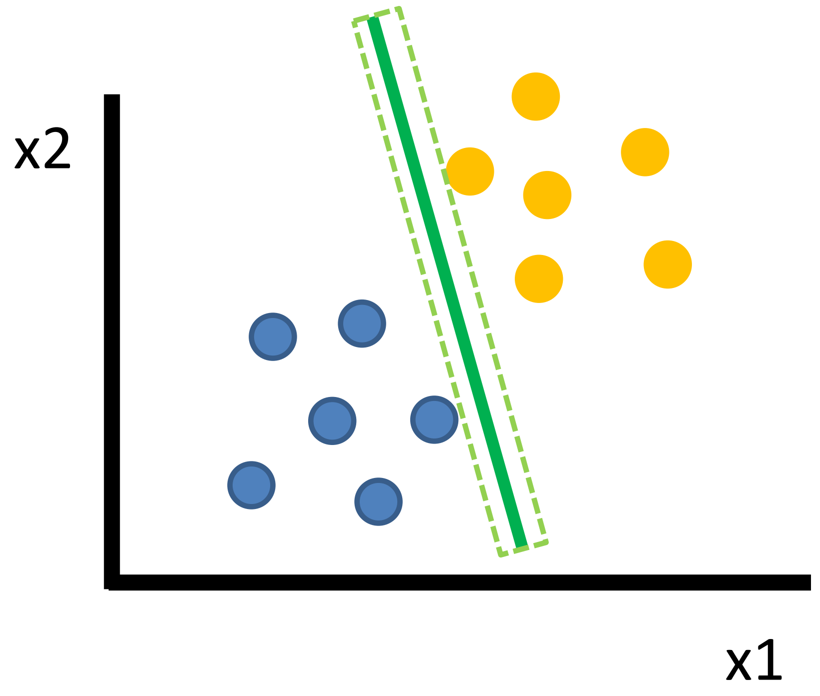
Support Vector Machine

- Widely used for all sorts of classification problems

- Some people say it is the best of the shelf classifier out there

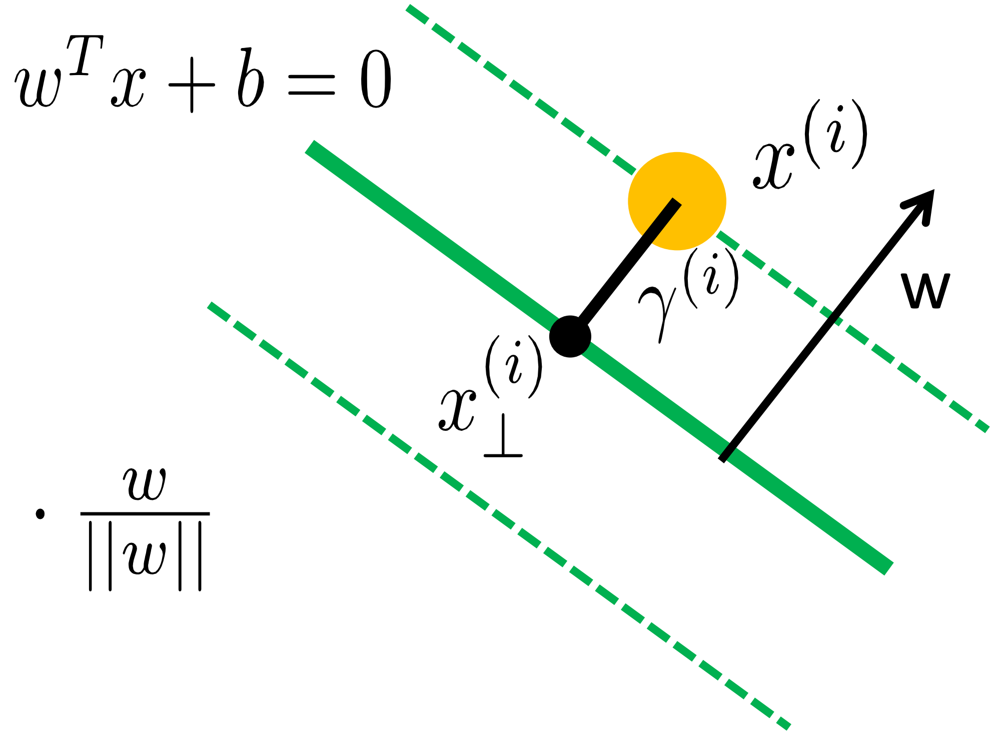
Maximum Margin Classification





Solution depends only on the support vectors!

Maximum Margin Classification



margin:

$$x_\perp^{(i)} = x^{(i)} - \gamma^{(i)} \cdot \frac{w}{||w||}$$

$$w^T x_\perp^{(i)} + b = 0$$

$$\Rightarrow \quad \gamma^{(i)} = \quad \left(\frac{w^T x^{(i)} + b}{||w||}\right)$$

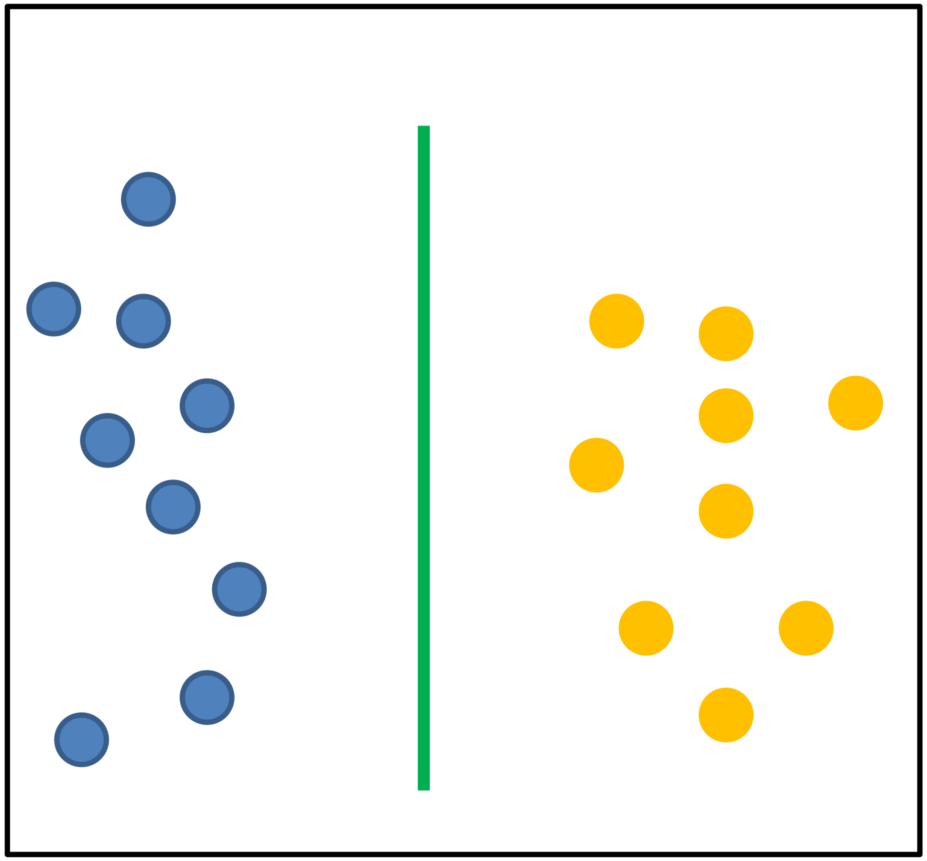
Maximum Margin Classification

$$\gamma^{(i)} = y^{(i)}(w^T x + b)$$

$$\begin{aligned} \max_{\gamma,w,b} \quad & \gamma \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq \gamma, \quad i = 1, \ldots, m \\ & ||w|| = 1. \end{aligned}$$

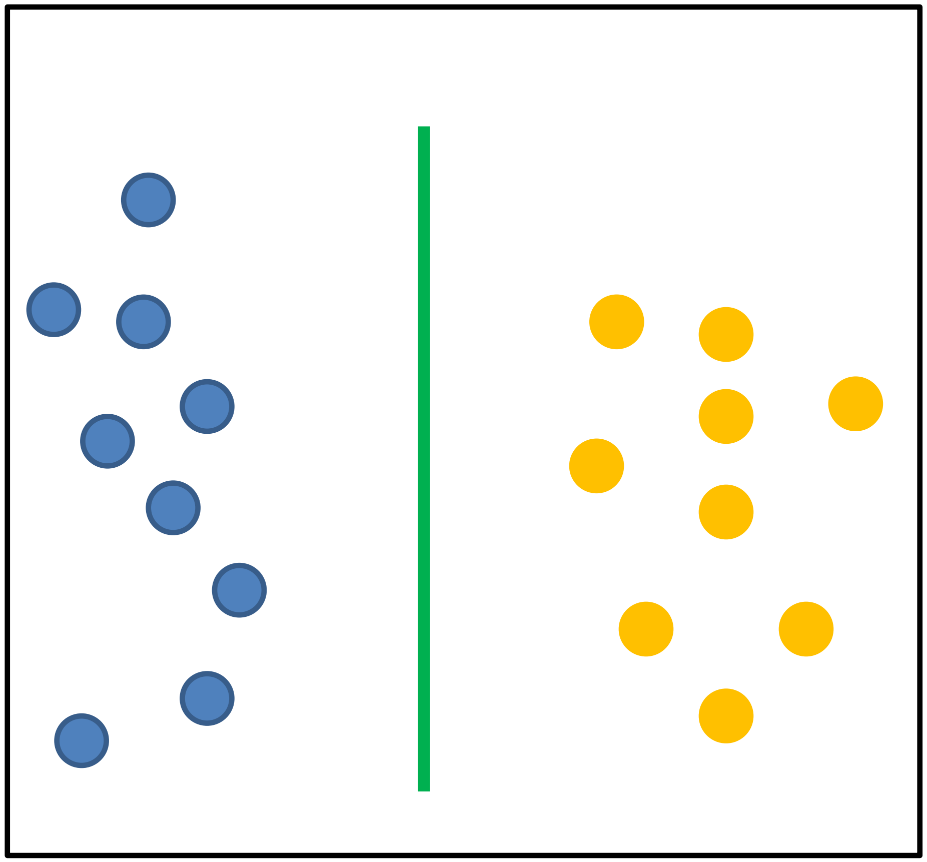
non-convex

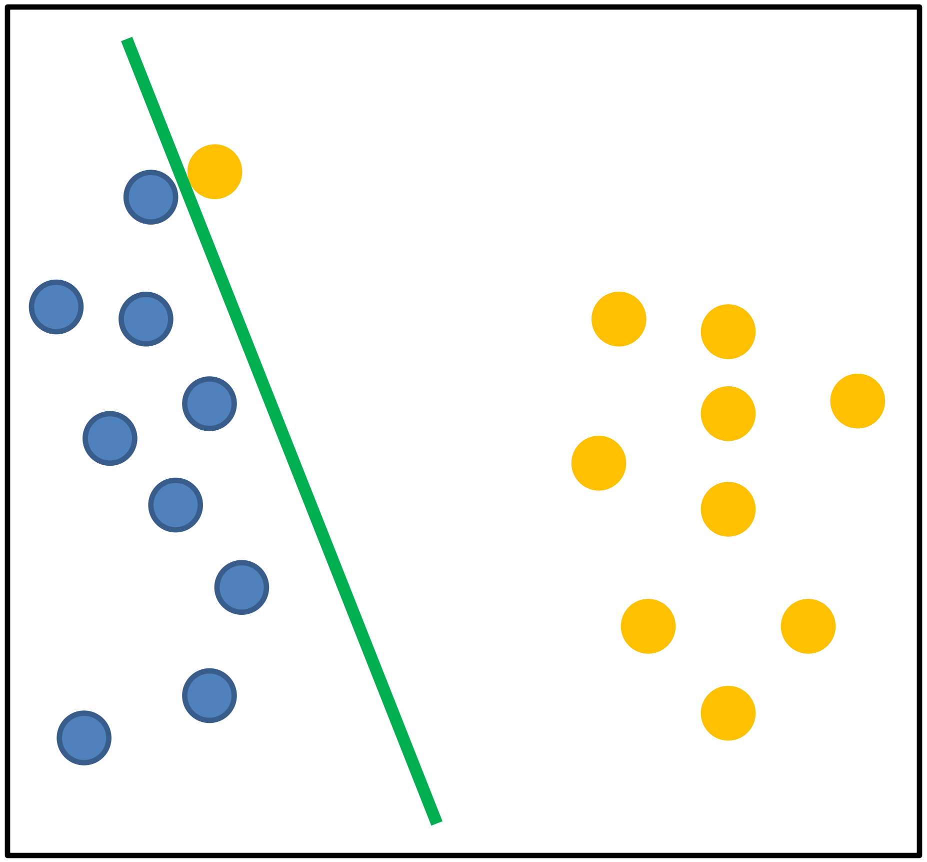
This Is Kind of Odd



- Which data points do we care the most about?
- What would those samples look like?

Two Very Similar Problems





What about outliers?

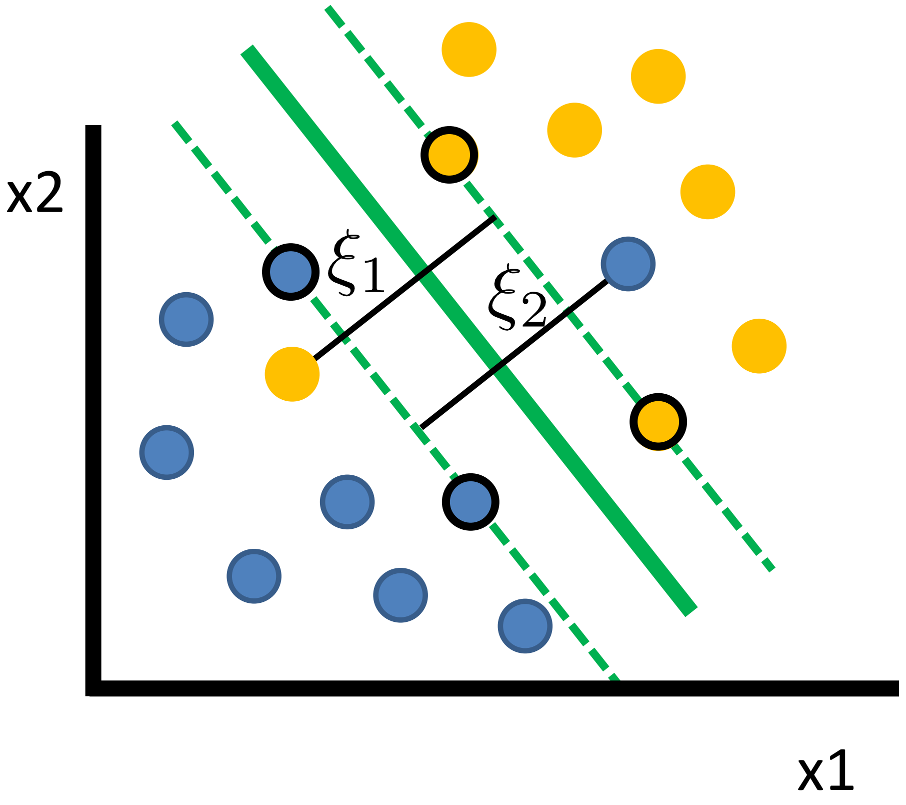
ξ_i: slack variables

$$\min_{w,b,\xi} \frac{1}{2}||w||^2$$

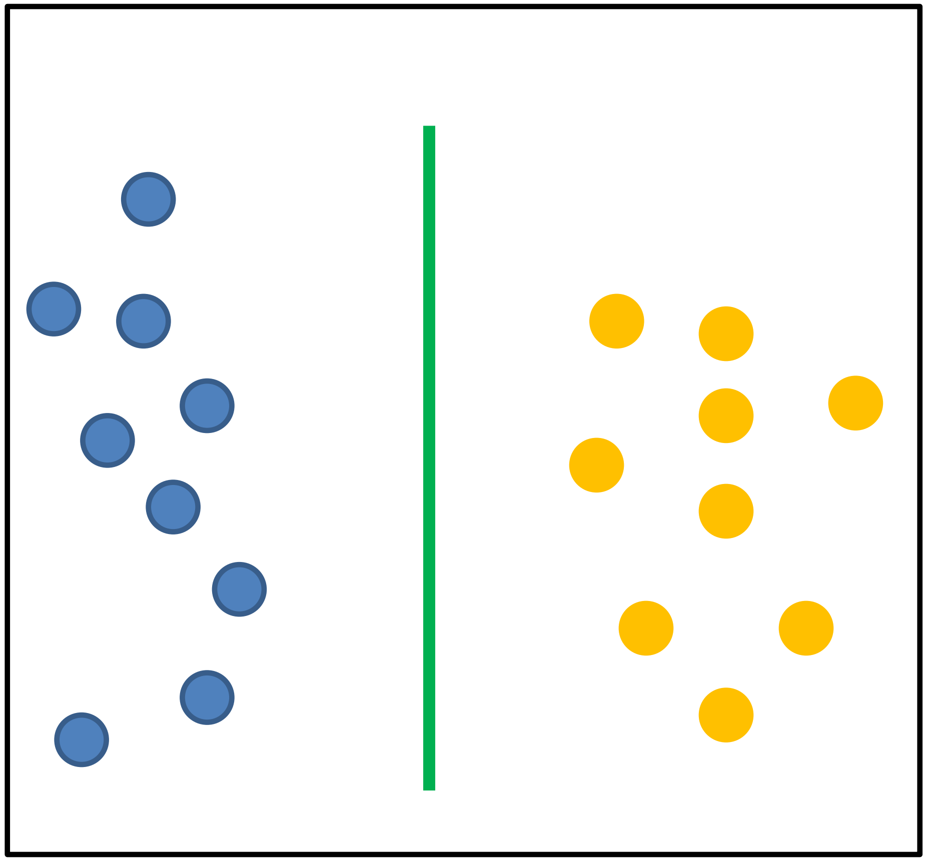
subject to:

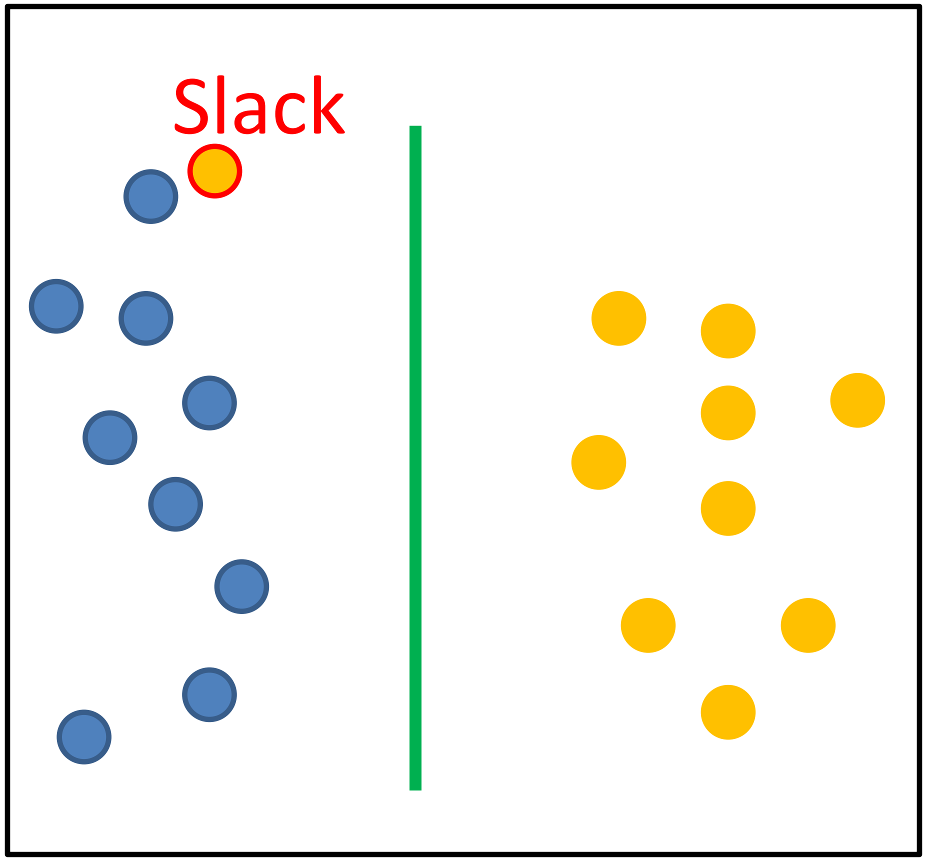
$$y^{(i)}(w^T x^{(i)} + b) \geq 1$$

$$(i = 1, \ldots, n)$$

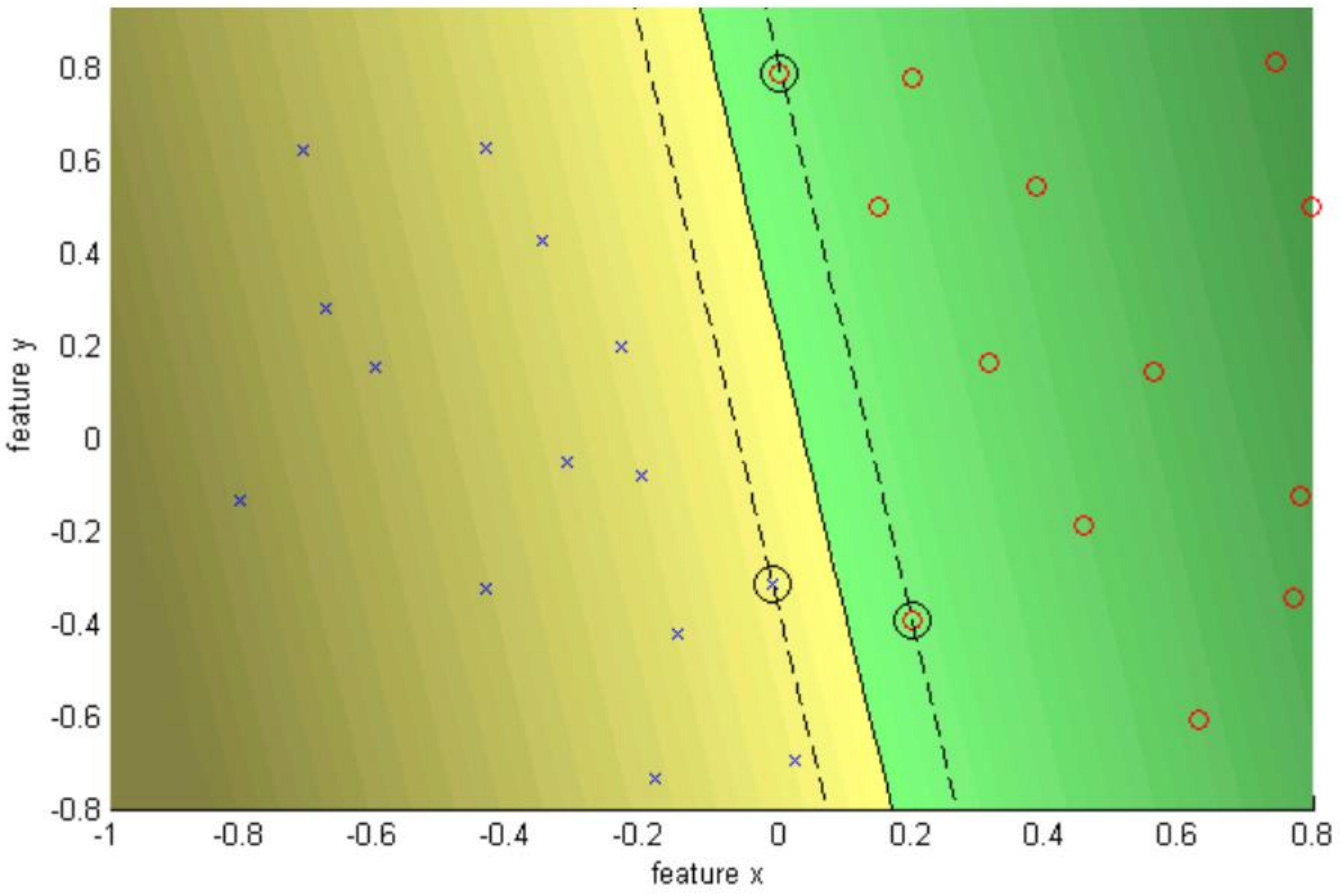


Two Very Similar Problems



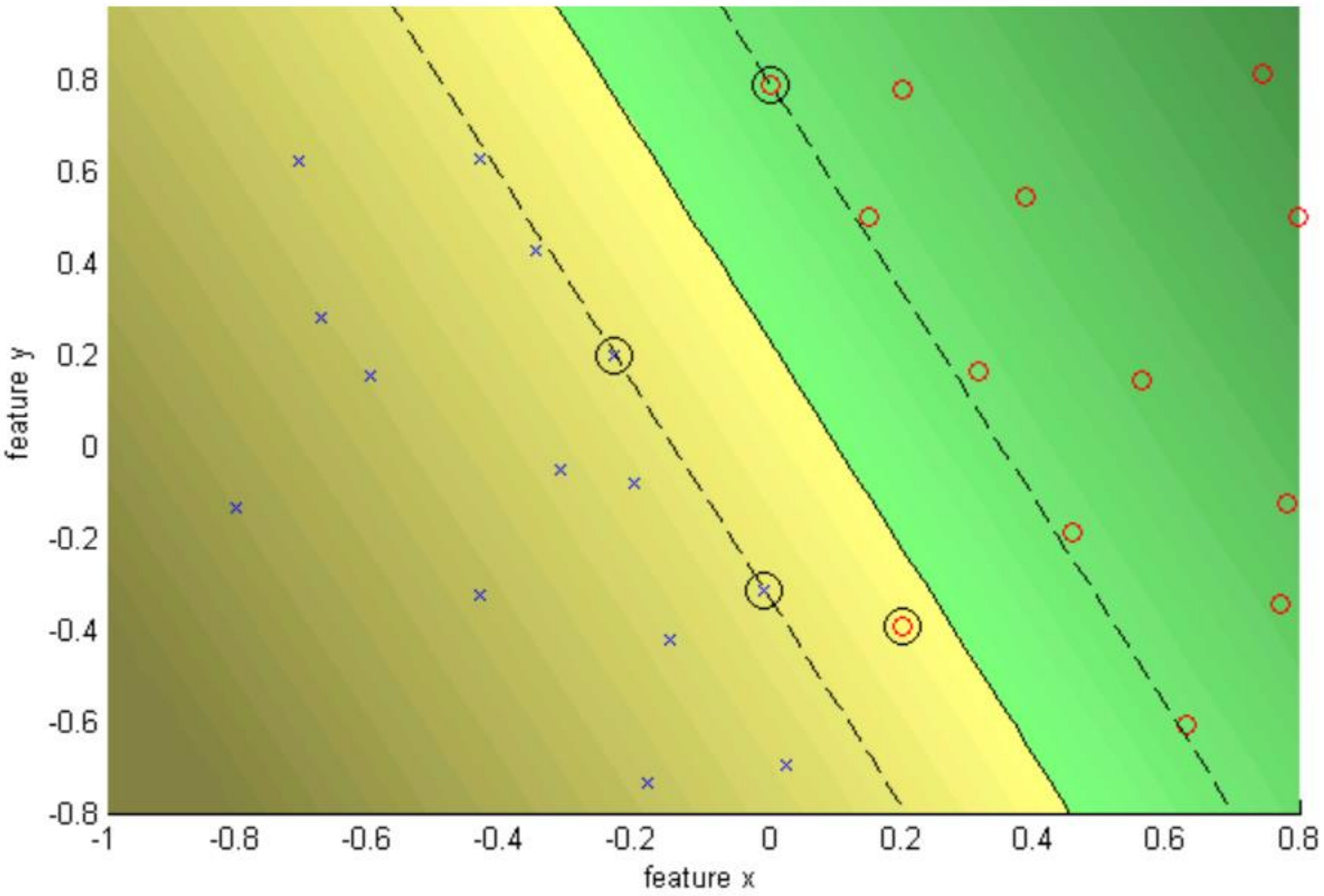


Hard Margin (C = Infinity)



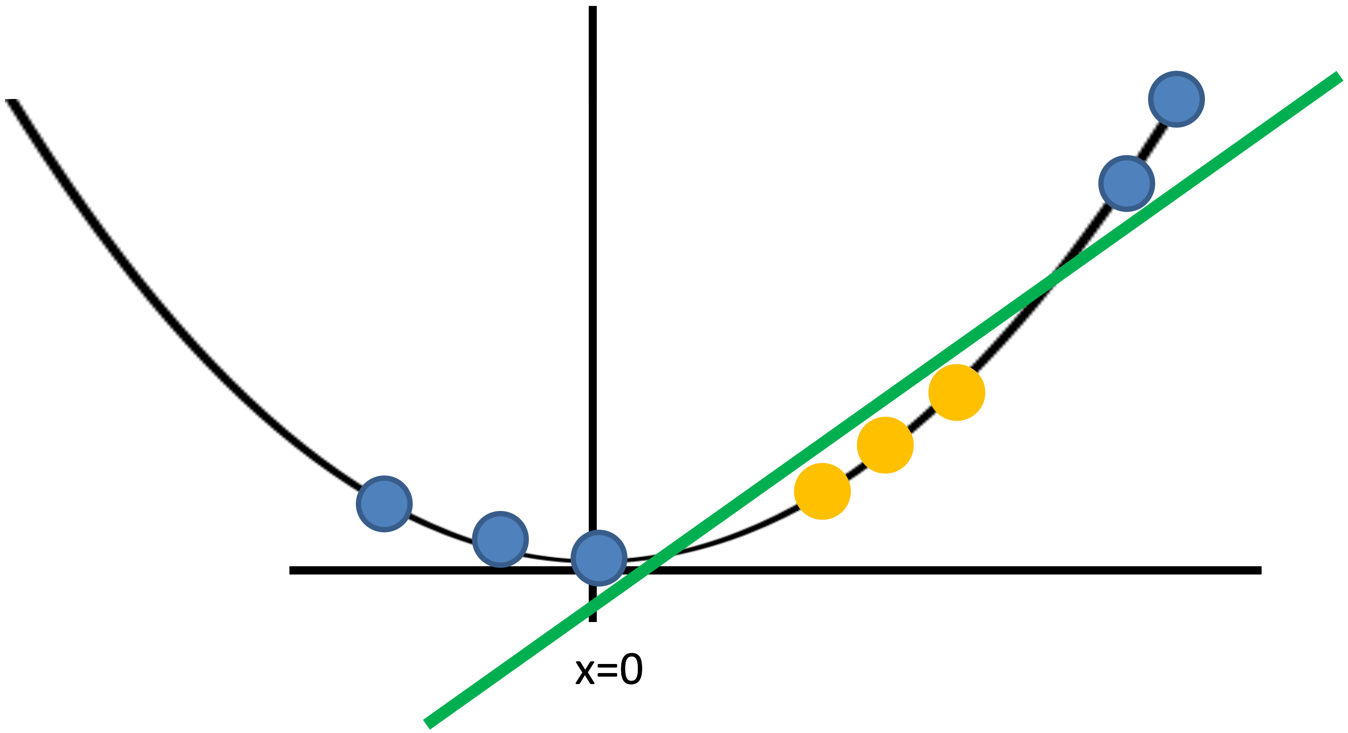
http://www.robots.ox.ac.uk/~az/lectures/ml/lect2.pdf

Soft Margin (C = 10)



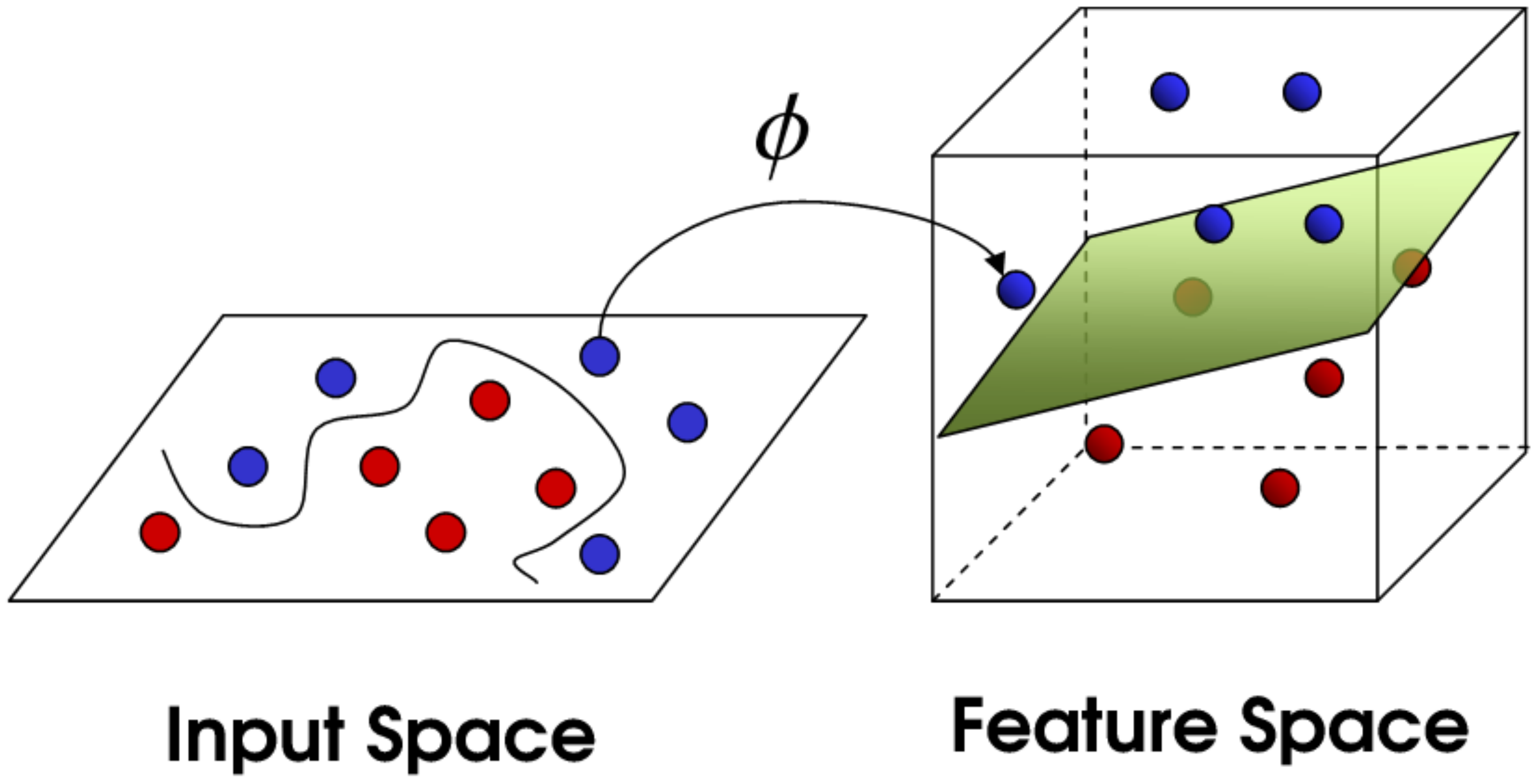
http://www.robots.ox.ac.uk/~az/lectures/ml/lect2.pdf

XOR problem revised



Did we add information to make the problem seperable?

Non-Linear Decision Boundary



SVM with a polynomial Kernel visualization

Created by:
Udi Aharoni

Quadratic Kernel

$$x = (x_1, x_2)$$

$$\Phi(x) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

$$\Phi(x) \cdot \Phi(z) = 1 + 2\sum_{i=1}^{d} x_i z_i$$

$$+ \sum_{i=1}^{d} x_i^2 z_i^2 + 2\sum_{i=1}^{d}\sum_{j=i+1}^{d} x_i x_j z_i z_j$$

$$\boxed{= (1 + x \cdot z)^2}$$

Kernel Functions

$$K(x,z) = \Phi(x) \cdot \Phi(z)$$

- Polynomial:

$$K(x,z) = (1 + x \cdot z)^s$$

- Radial basis function (RBF):

$$K(x,z) = \exp(-\gamma(x-z)^2)$$

So what is the excitement?

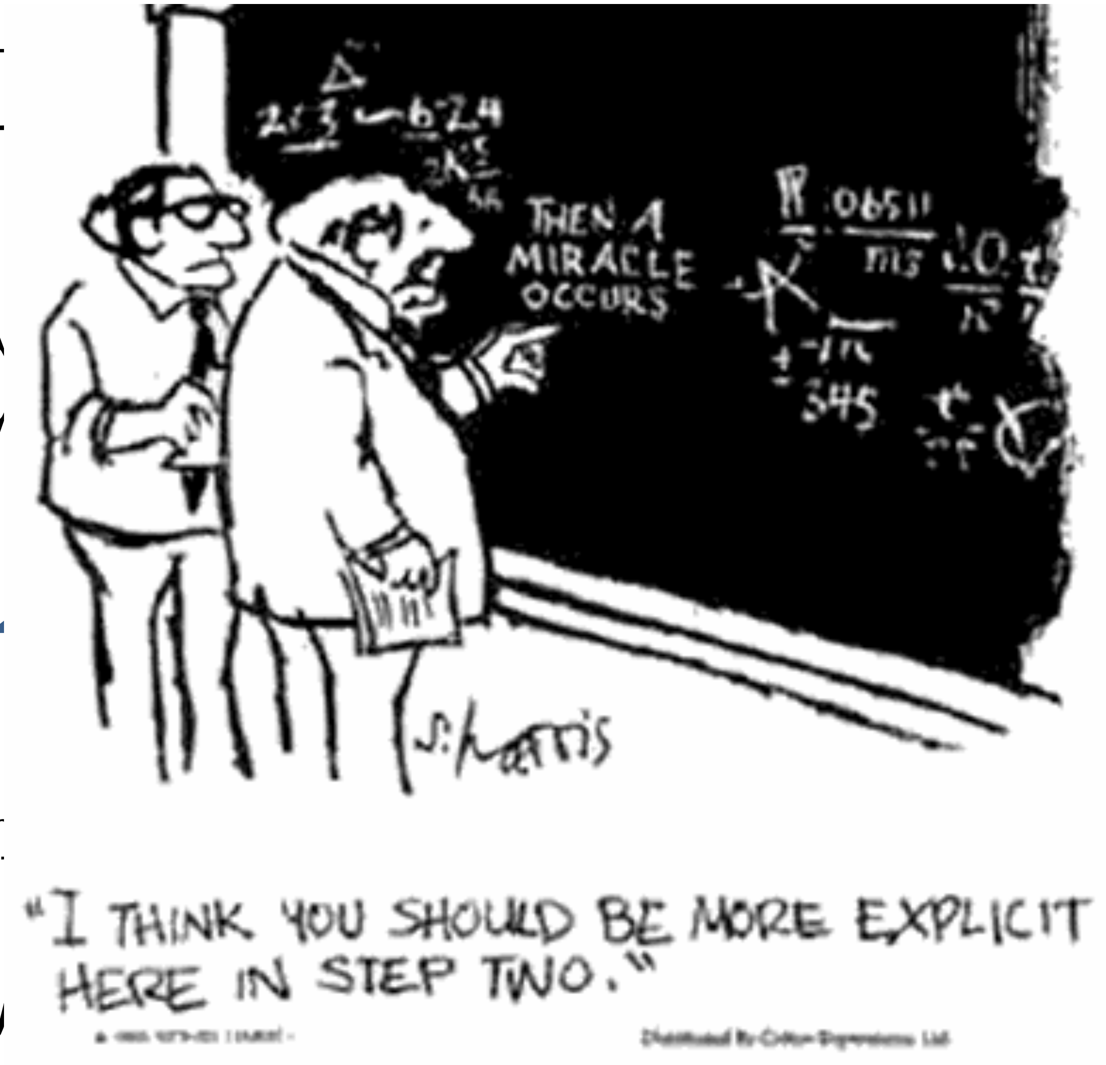
$\max_\alpha \sum$ $\quad {}^{(i)^T} x^{(j)}$

s.t. α_i

$\sum$

arg r

s.t. y



So what is the excitement?

$$\max_\alpha \sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i,j=1}^m y^{(i)}y^{(j)}\alpha_i\alpha_j \boxed{{x^{(i)}}^T x^{(j)}}$$

$$\text{s.t. } \alpha_i \geq 0,\ i = 1, \ldots, m$$

$$\sum_{i=1}^m \alpha_i y^{(i)} = 0$$

$$\boxed{K(x^{(i)}, x^{(j)})}$$

$$\arg\min_{w,b} \frac{1}{2}||w||^2$$

$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq 1$$

Prediction

$$w^T x + b = \sum_{i=1}^{m} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b.$$

- Again we can use the kernel trick!
- Prediction speed depends on number of support vectors

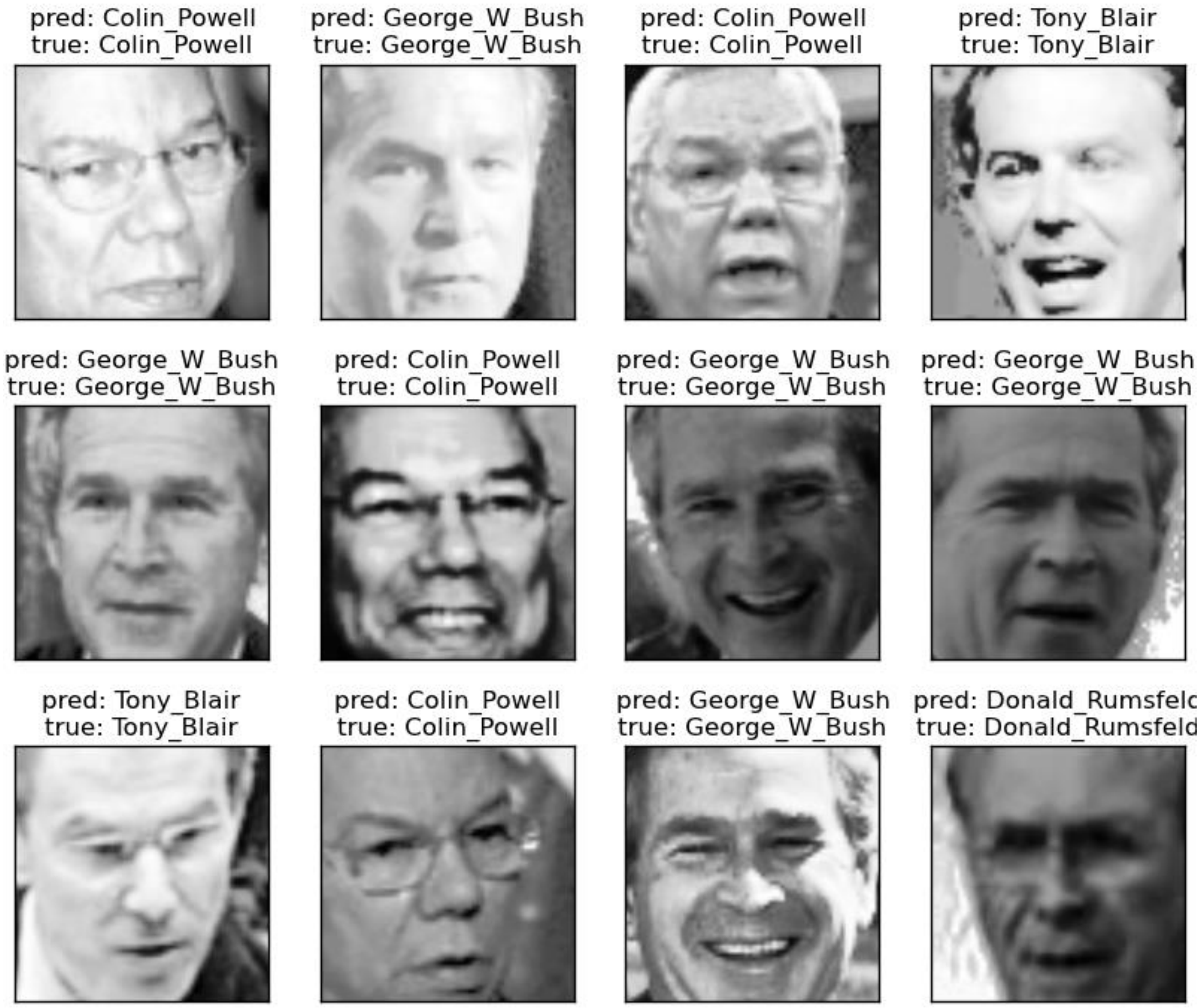
The Miracle Explained

- Andrew Ng does this really well
- http://cs229.stanford.edu/notes/cs229-notes3.pdf
- Course is also on Youtube, ItunesU, etc.

Kernel Trick for SVMs

- Arbitrary many dimensions
- Little computational cost
- Maximal margin helps with curse of dimensionality

Face Recognition



Face Recognition

- Load image data
- Put your test data aside
- Extract Eigenfaces
- Train SVM
- Evaluate performance

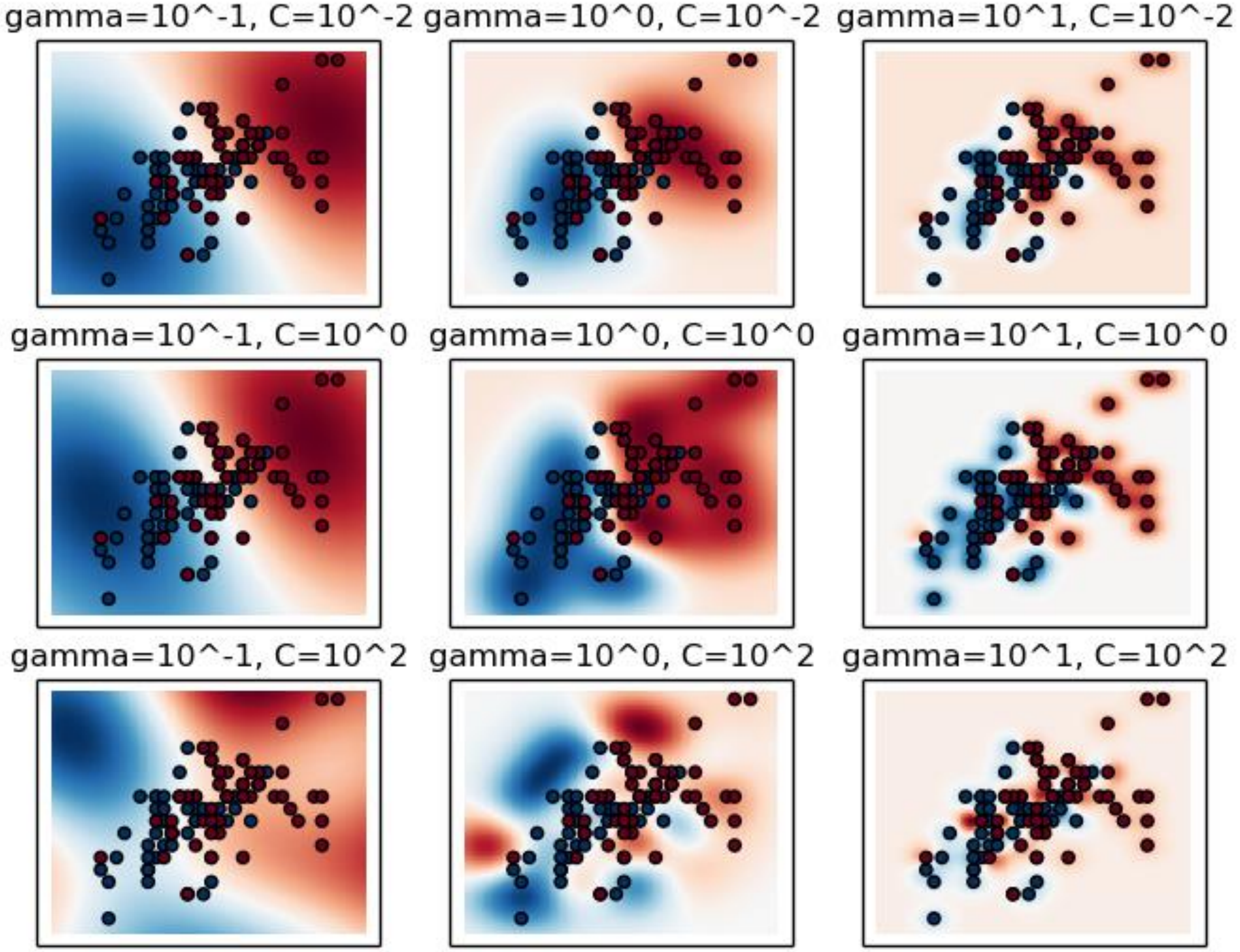
- Red are cross validation steps

http://scikit-learn.org/stable/auto_examples/applications/face_recognition.html#example-applications-face-recognition-py

SVM_sign_language.mp4

Jhon Gonzalez

https://www.youtube.com/watch?v=cxHMgl2_5zg



http://scikit-learn.org/stable/auto_examples/svm/plot_rbf_parameters.html

Tips and Tricks

- SVMs are not scale invariant
- Check if your library normalizes by default
- Normalize your data
  - mean: 0 , std: 1
  - map to [0,1] or [-1,1]
- Normalize test set in same way!

Tips and Tricks

- RBF kernel is a good default
- For parameters try exponential sequences
- Read:

  Chih-Wei Hsu et al., "A Practical Guide to Support Vector Classification", Bioinformatics (2010)

SVM vs KNN

- What are the main key differences?

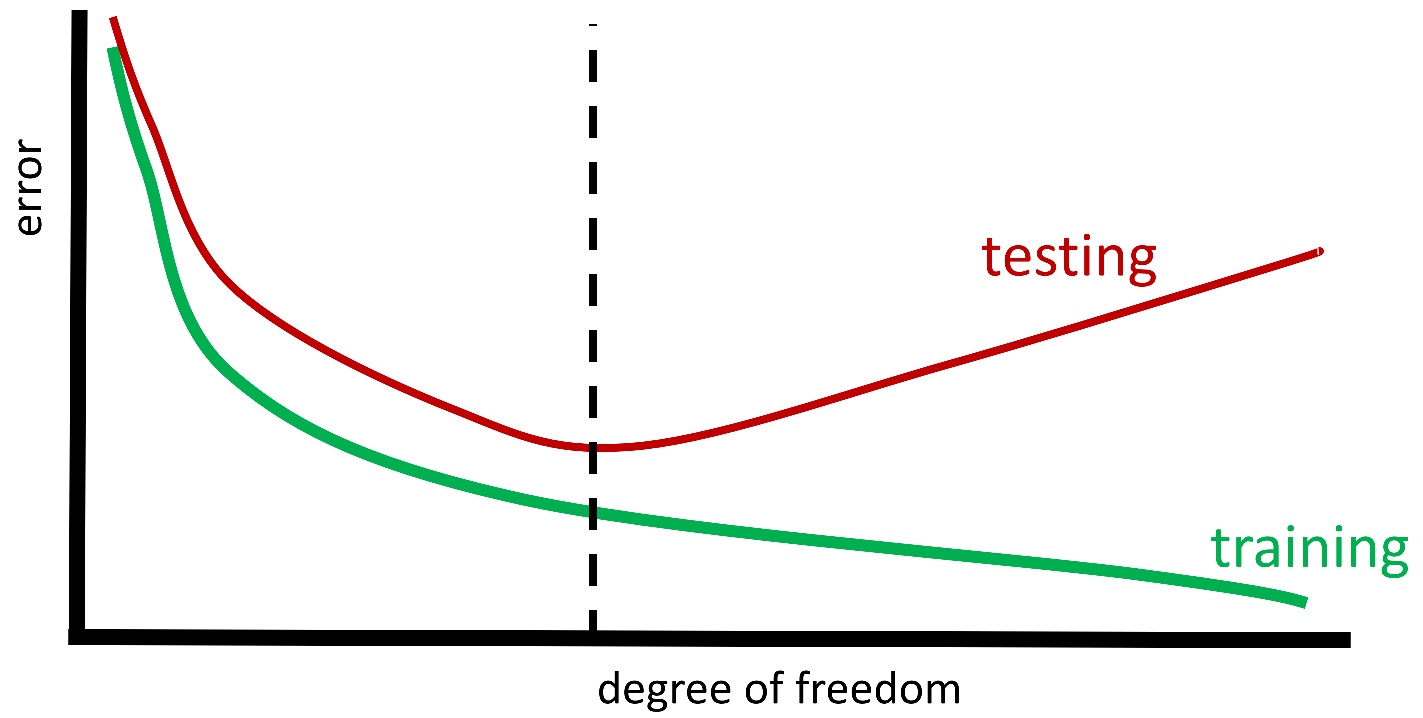
Parameter Tuning

- Given a classification task

- Which kernel ?
- Which kernel parameter values?
- Which value for C?

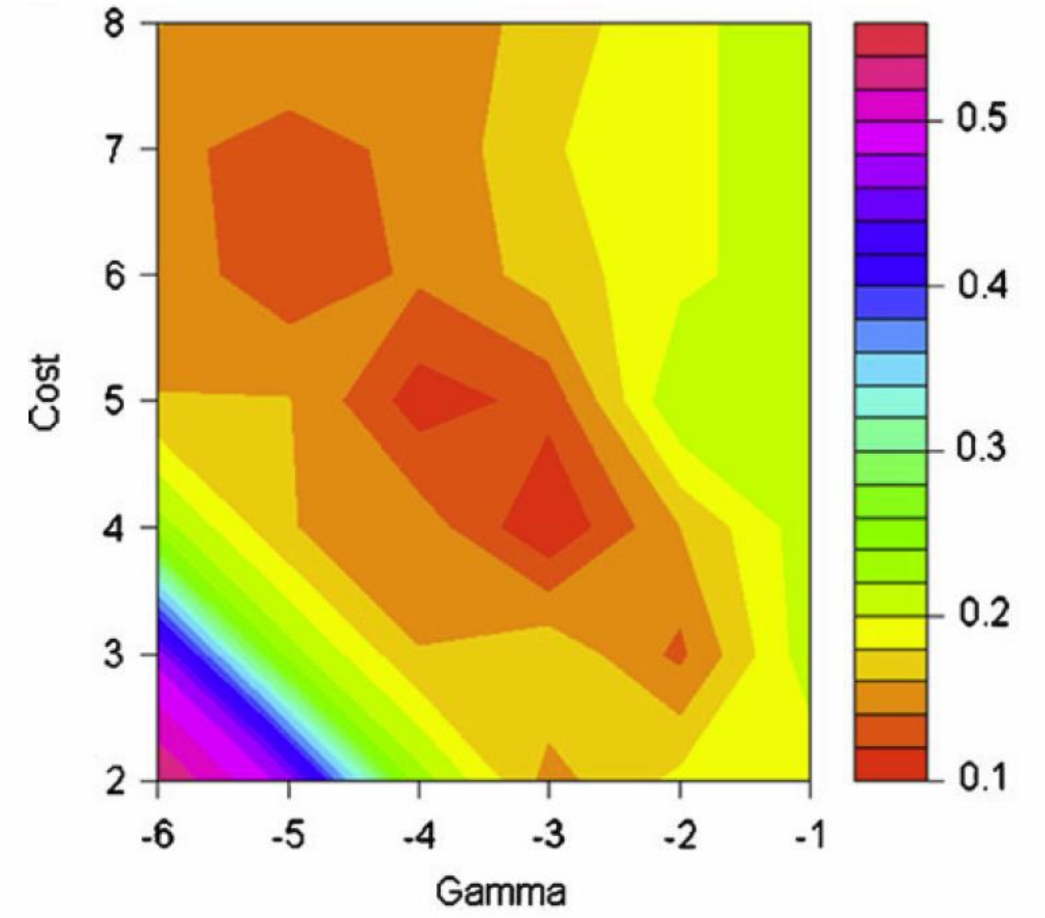
$\Rightarrow$ Try different combinations and take the best.

Train vs. Test Error



Where is KNN on this graph for K=1, or for K=Inf?

Grid Search



Zang et al., “Identification of heparin samples that contain impurities or contaminants by chemometric pattern recognition analysis of proton NMR spectral data”, Anal Bioanal Chem (2011)

Error Measures

- True positive (tp)
- True negative (tn)
- False positive (fp)
- False negative (fn)

		predicted	
		1	-1
true	1	tp	fn
	-1	fp	tn

TPR and FPR

- True Positive Rate:

$$\frac{tp}{tp+fn}$$

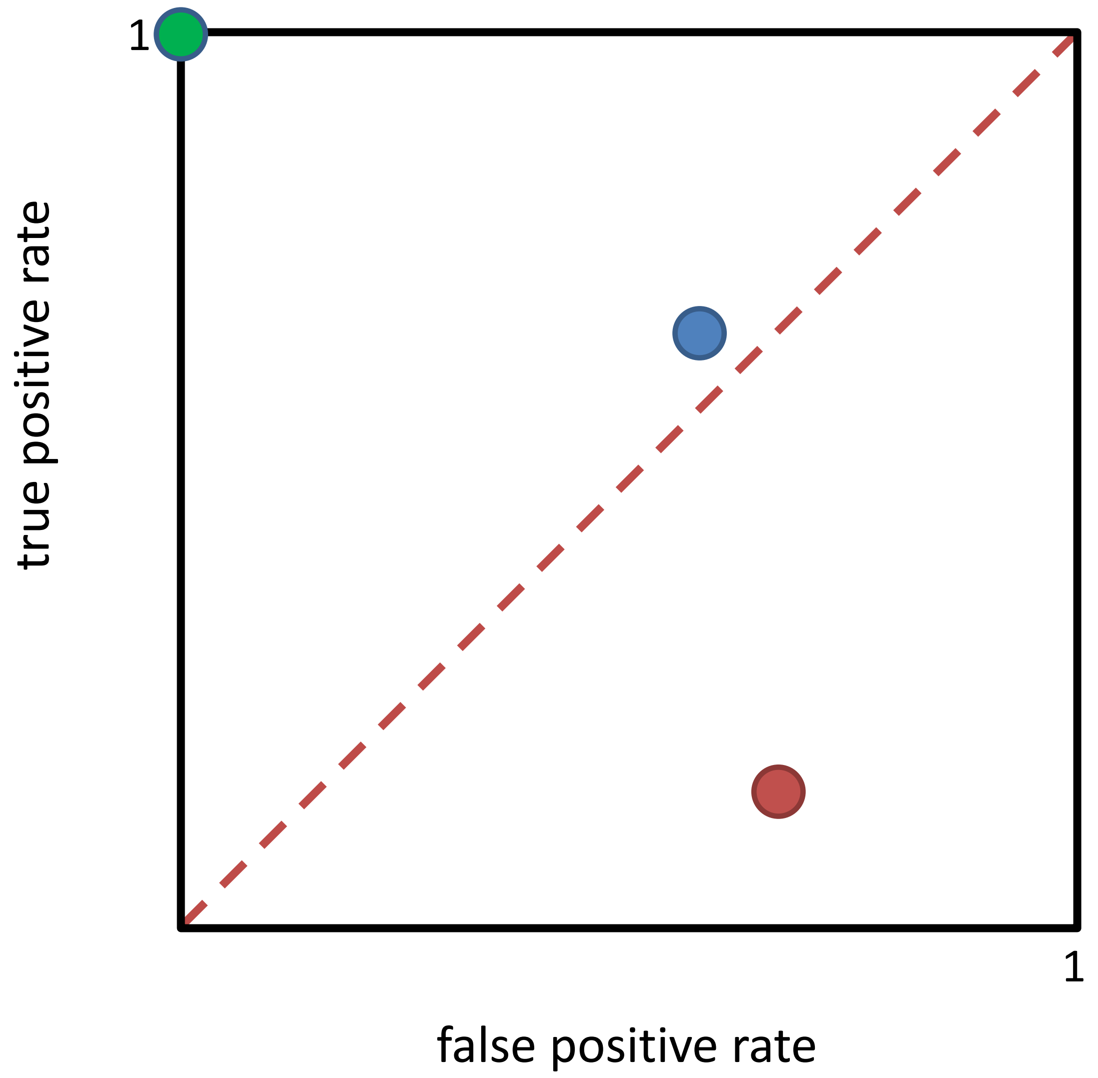
- False Positive Rate:

$$\frac{fp}{fp+tn}$$

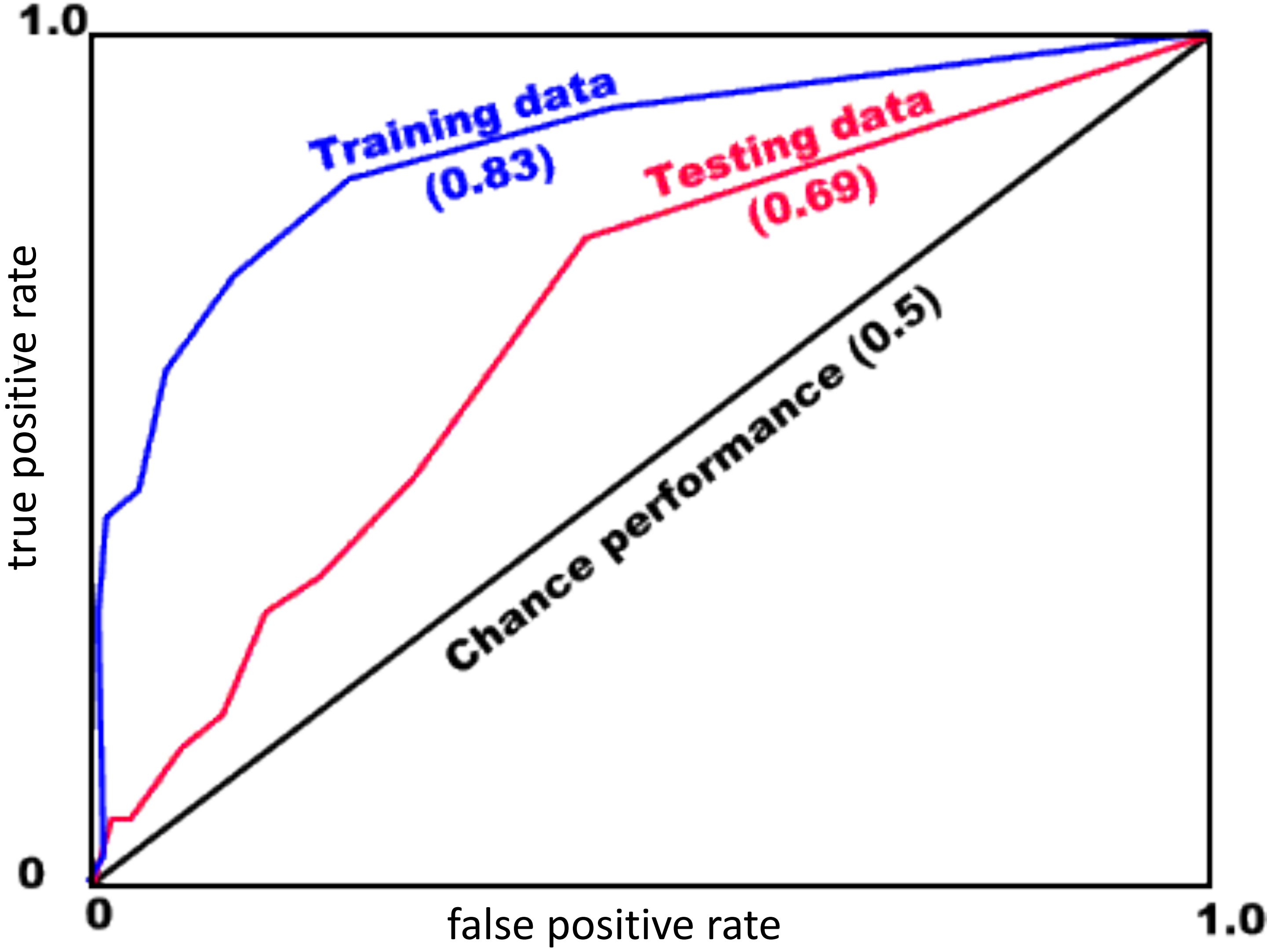
predicted

true	1	-1
1	tp	fn
-1	fp	tn

Reciever Operating Characteristic



ROC Example



https://inclass.kaggle.com/c/ca-2015/details/evaluation

Precision Recall

- Recall: $\frac{tp}{tp+fn}$

- Precision: $\frac{tp}{tp+fp}$

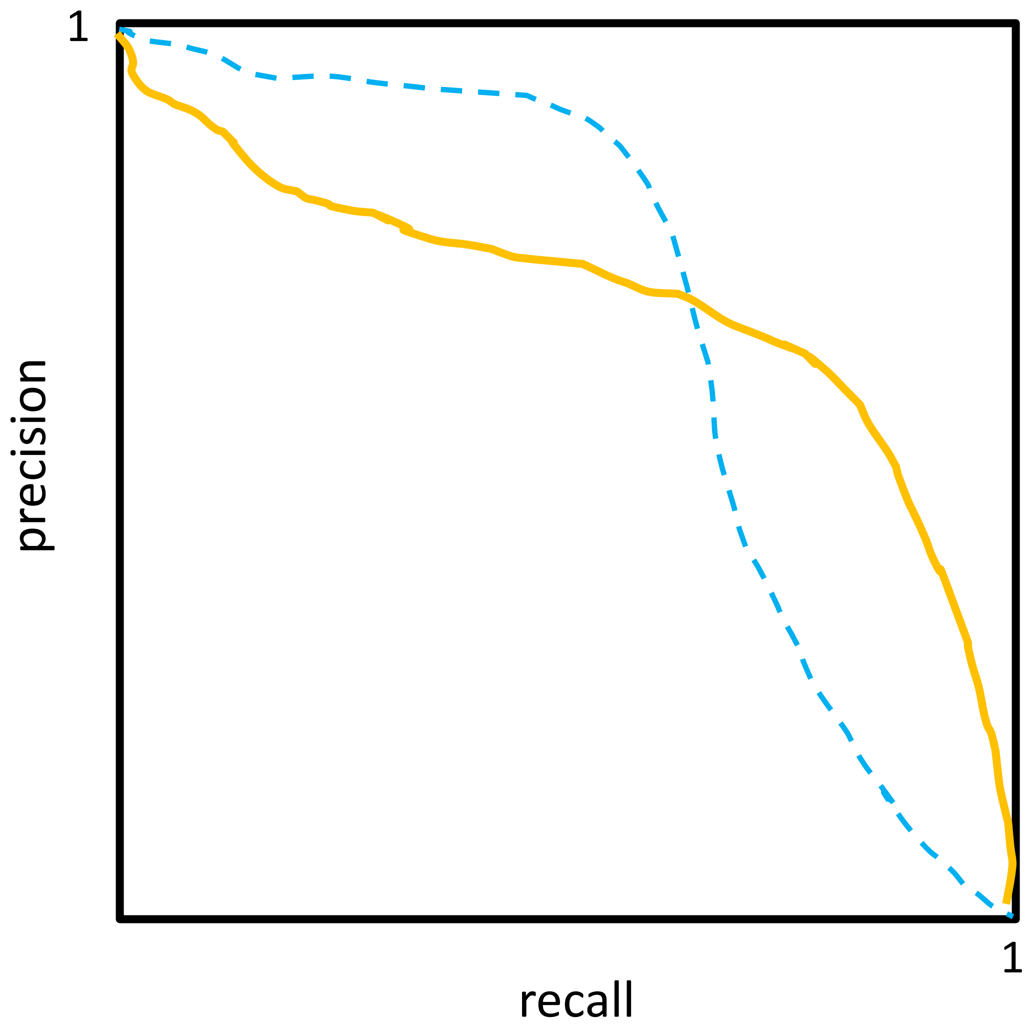
		predicted	
		1	-1
true	1	tp	fn
	-1	fp	tn

Precision Recall

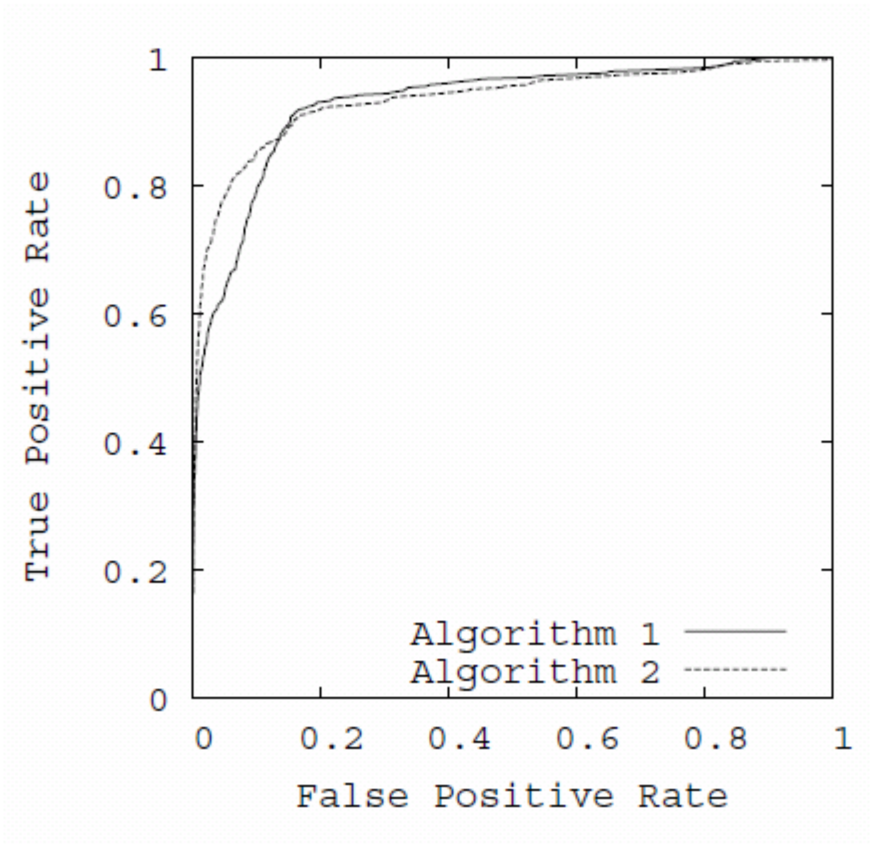
- **Recall**: If I pick a random positive example, what is the probability of making the right prediction?

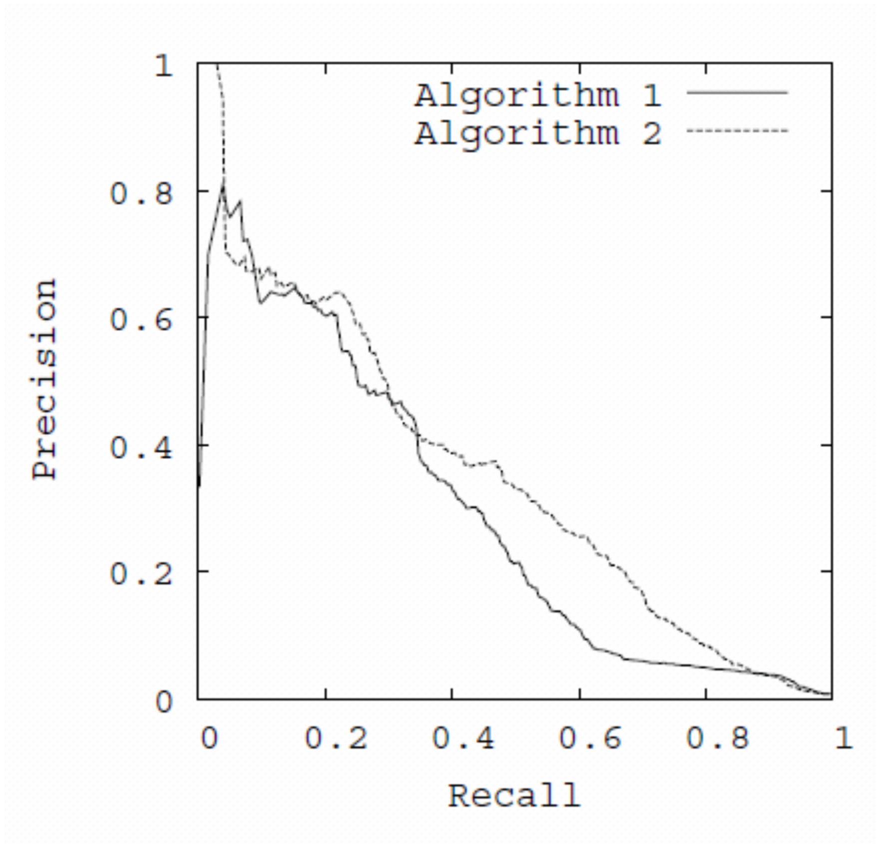
- **Precision**: If I take a positive prediction example, what is the probability that it is indeed a positive example?

Precision Recall Curve



Comparison





J. Davis & M. Goadrich,
“The Relationship Between Precision-Recall and ROC Curves.”,
ICML (2006)

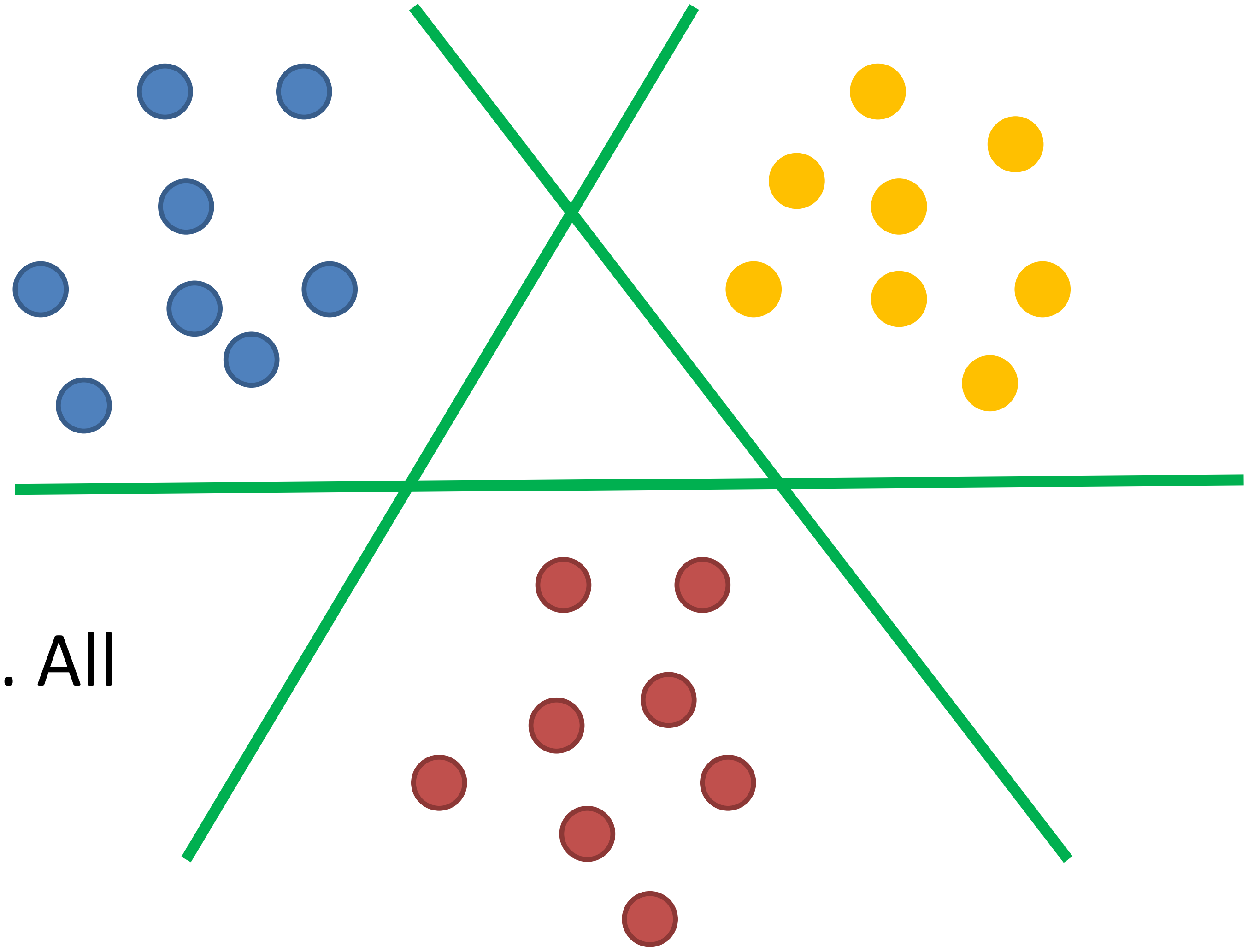
F-measure

- Weighted average of precision and recall

$$F_\beta = \frac{(\beta^2+1)\cdot P\cdot R}{\beta^2\cdot P+R}$$

- Usual case: $\beta = 1$
- Increasing β allocates weight to recall

Multi Class

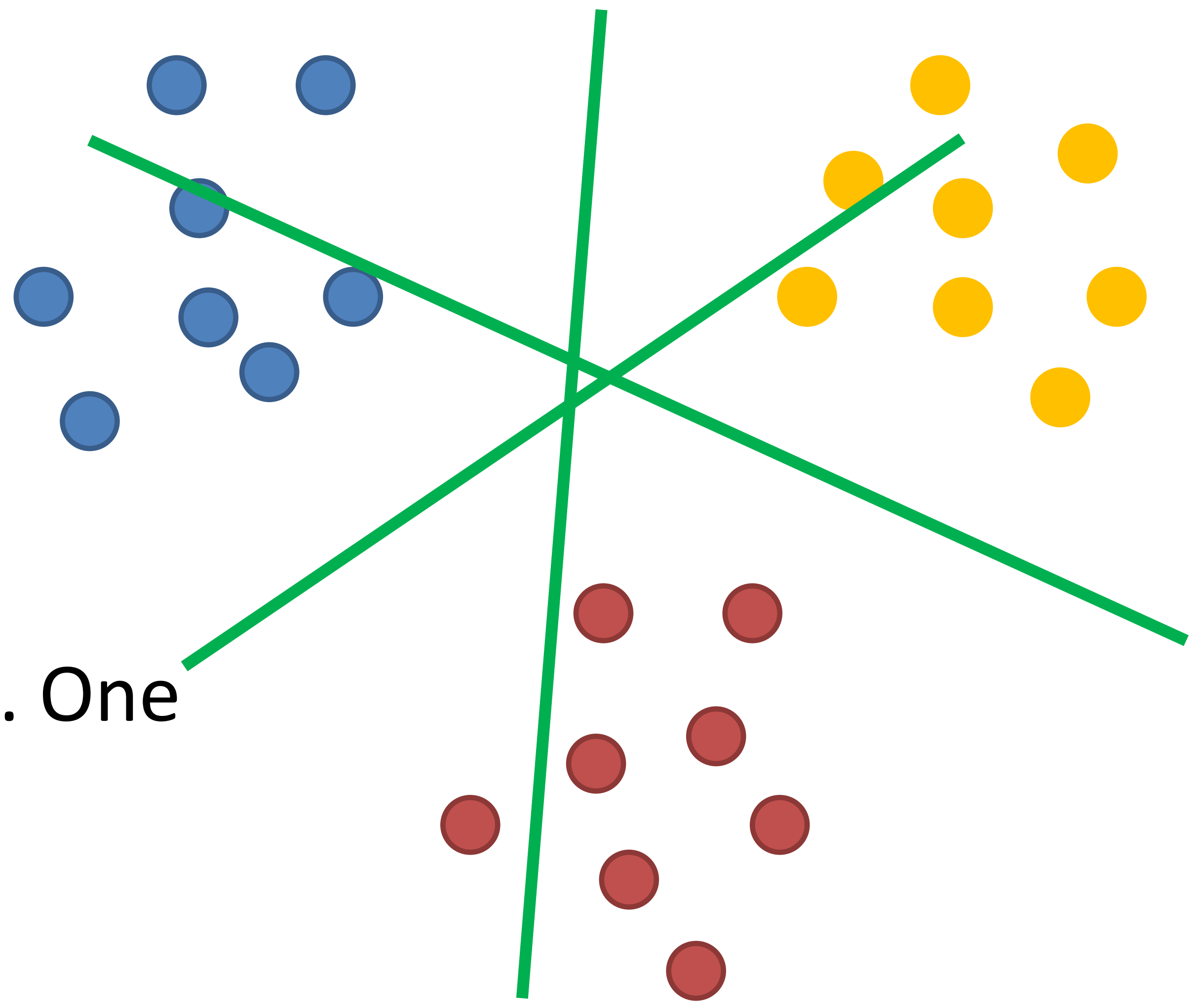


One vs. All

One vs All

- Train n classifier for n classes
- Take classification with greatest margin
- Slow training

Multi Class

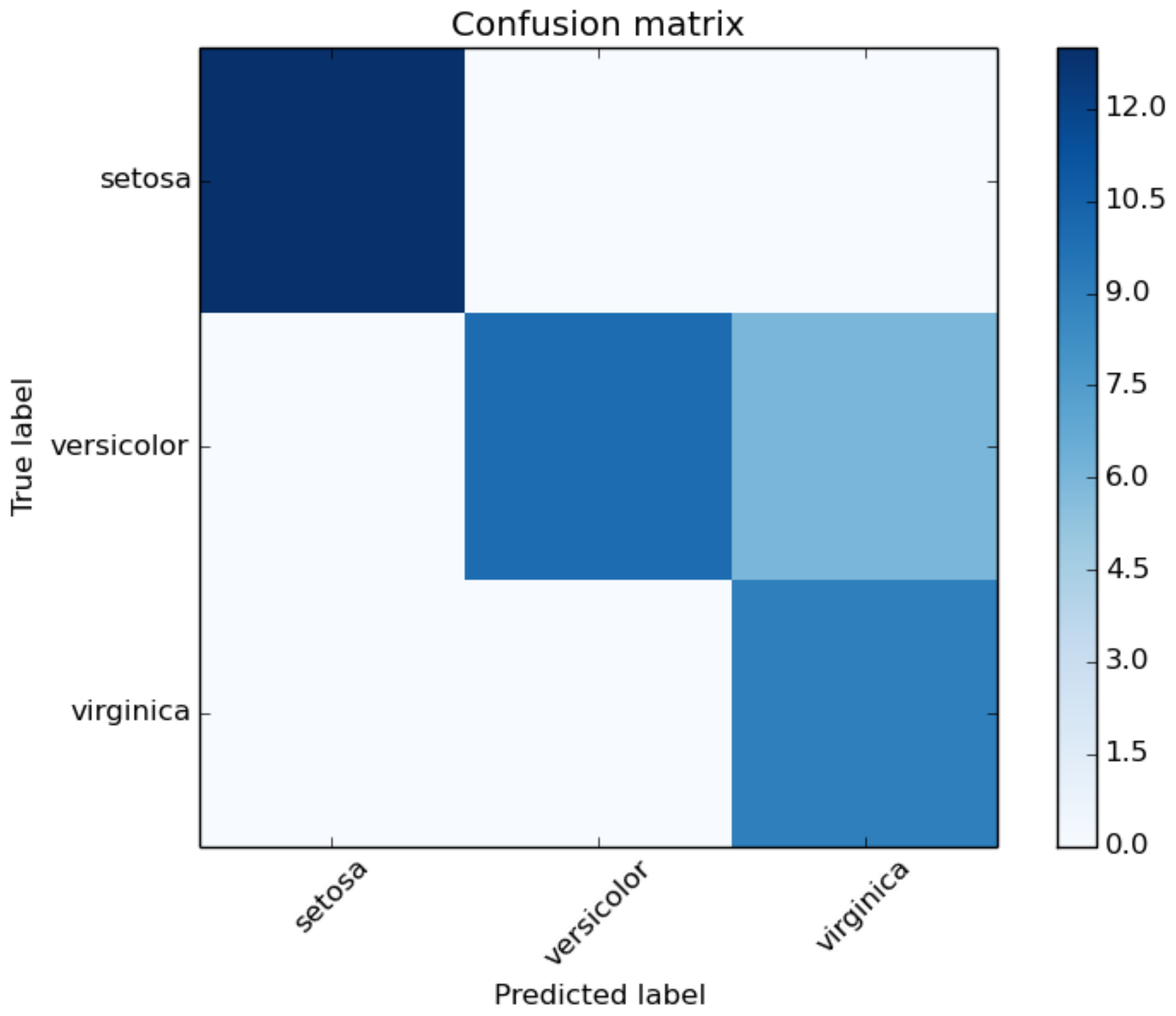


One vs. One

One vs One

- Train n(n-1)/2 classifiers
- Take majority vote
- Fast training

Confusion Matrix



http://scikit-learn.org/stable/auto_examples/model_selection/plot_confusion_matrix.html

Recap

- Perceptrons are great
- But really just a separating hyperplane
- So is SVM
- Kernels are neat
- Evaluation metrics are important