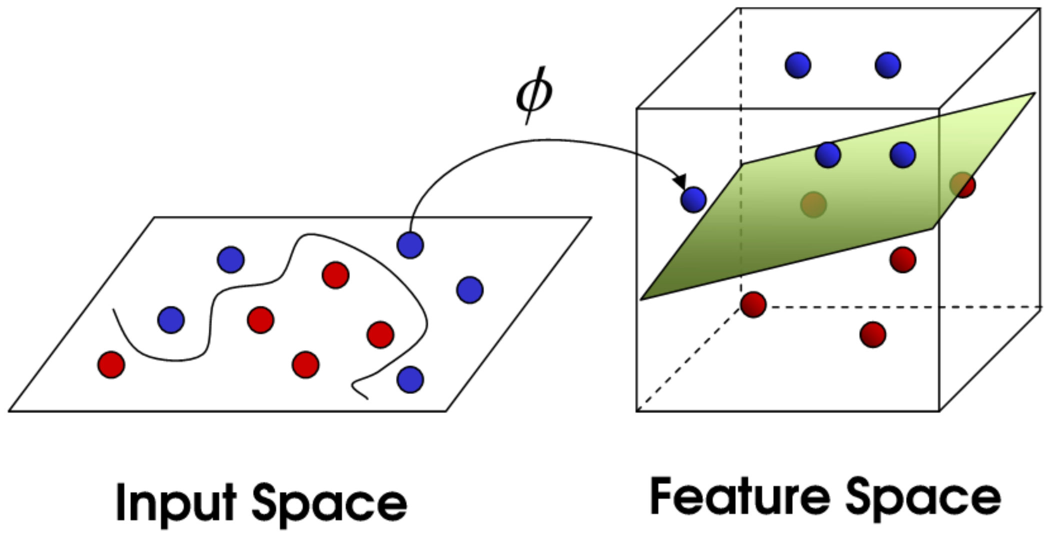
CS109 – Data Science
SVM, Performance evaluation

Joe Blitzstein, Hanspeter Pfister, Verena Kaynig-Fittkau



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

Announcements

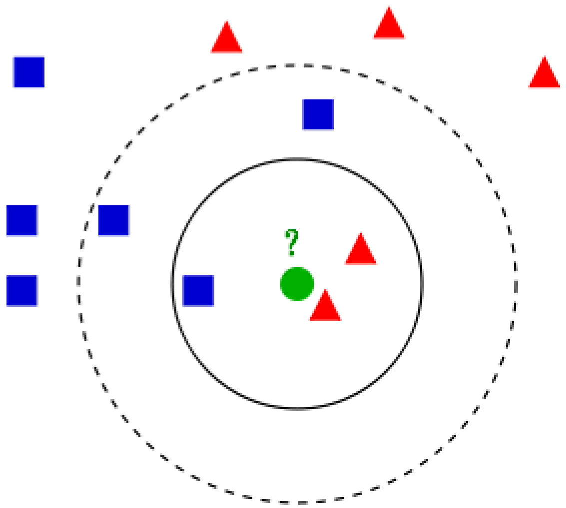
- HW1 grades went out yesterday
- They are looking really good, well done everyone!

- HW2 is due this Thursday!

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

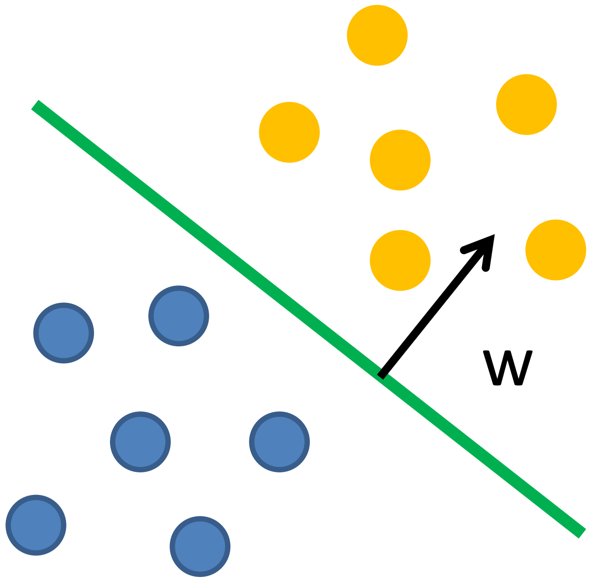
Recap K-NN

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



Separating Hyperplane

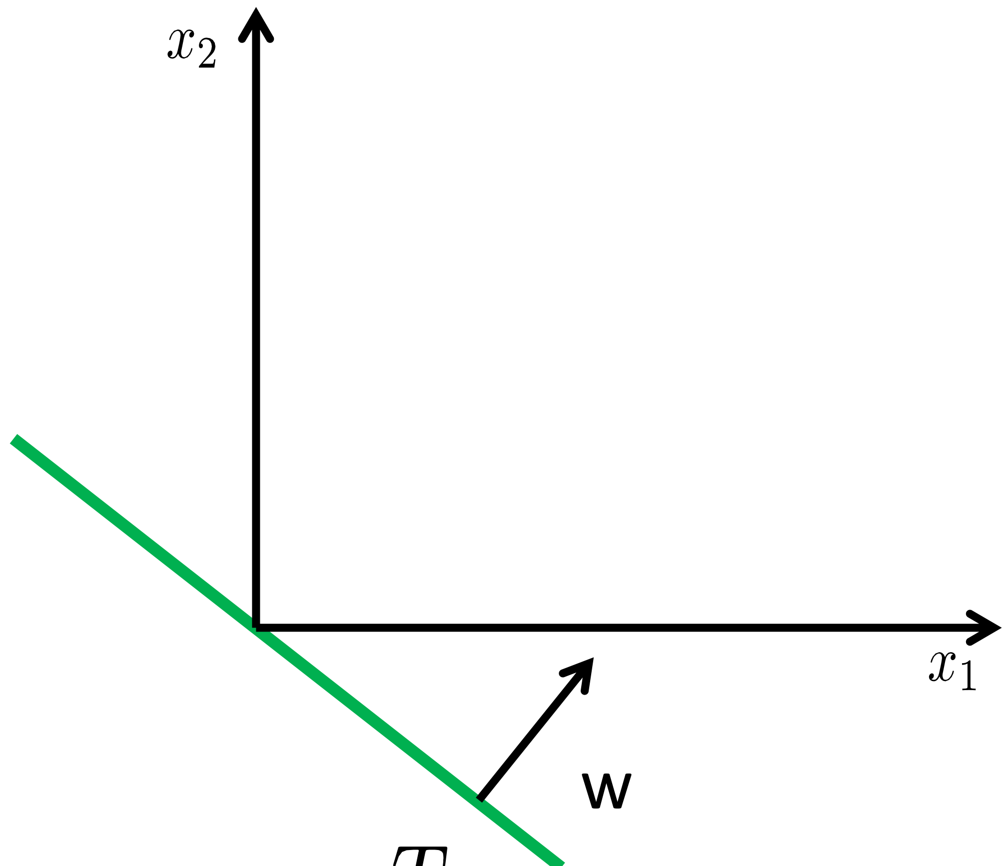
- x: data point
- y: label $\in \{-1, +1\}$
- w: weight vector



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

Separating Hyperplane

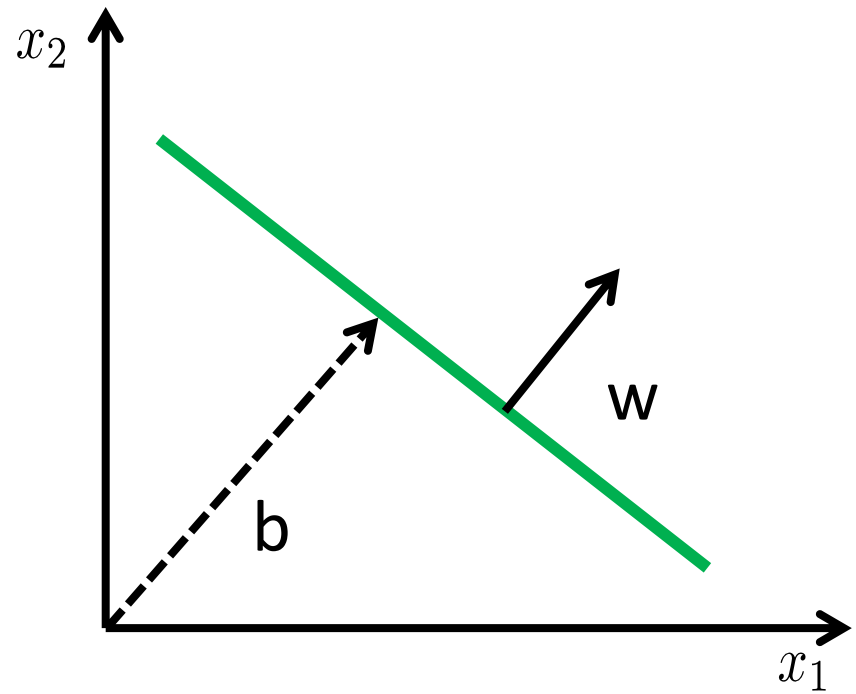
- x: data point
- y: label $\in \{-1, +1\}$
- w: weight vector



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

Separating Hyperplane

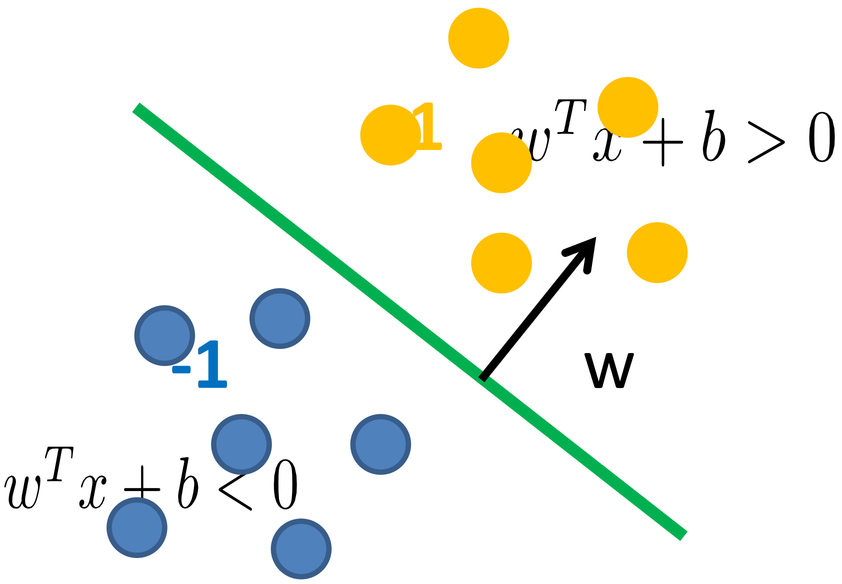
- x: data point
- y: label $\in \{-1, +1\}$
- w: weight vector
- b: bias



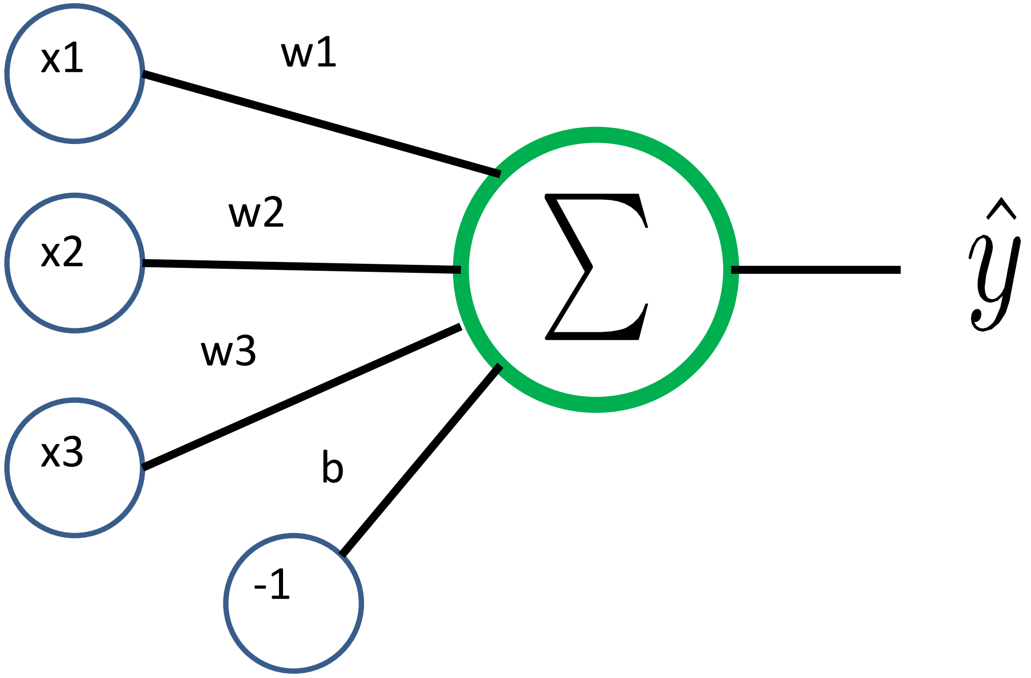
$$w^T x + b = 0$$

Separating Hyperplane

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

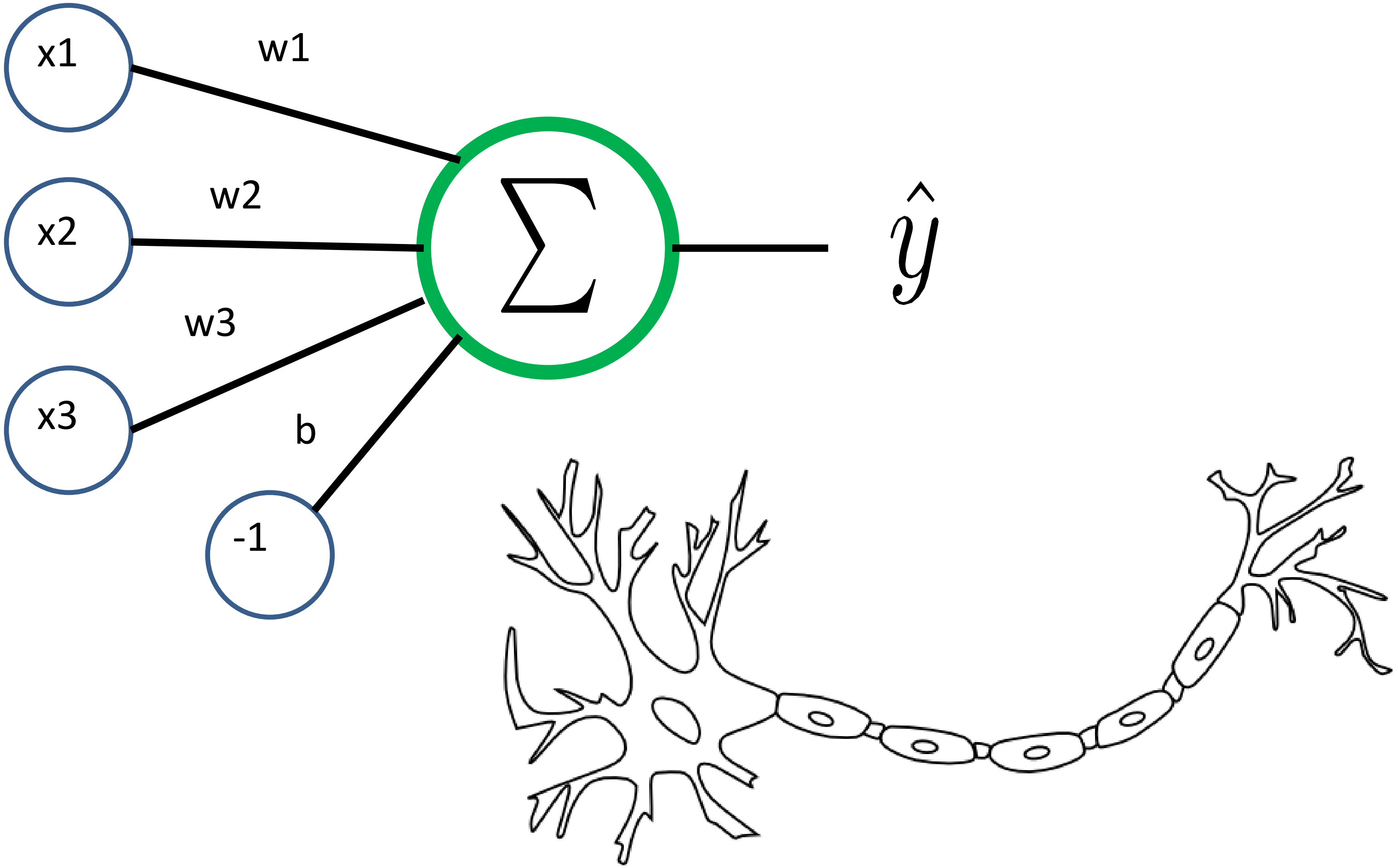


Perceptron



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

Perceptron



Perceptron History

- invented 1957
- by Frank Rosenblatt

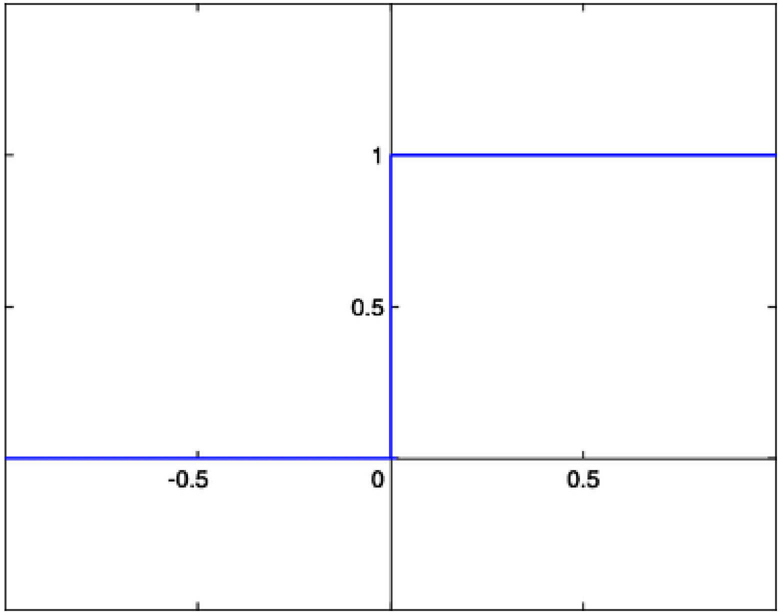
- the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence. (NYT 1958)

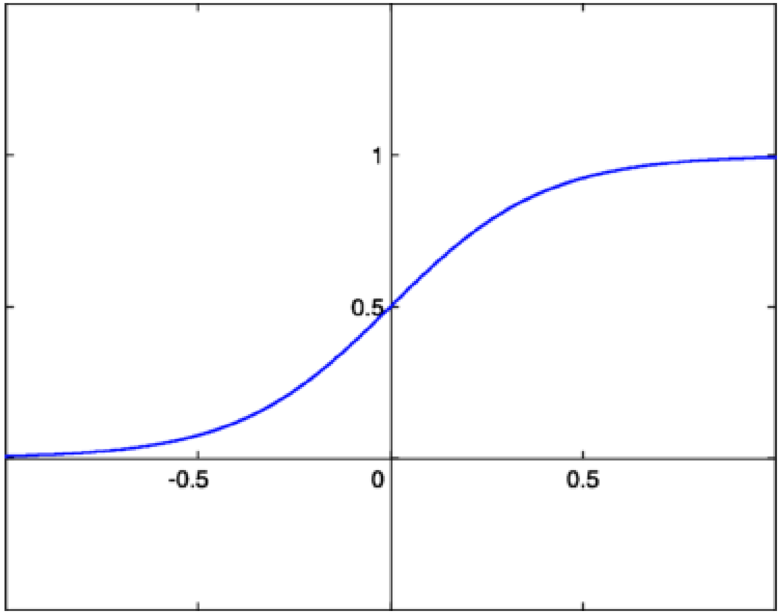
  (http://en.wikipedia.org/wiki/Perceptron

Perceptron.mp4

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

Side Note: Step vs Sigmoid Activation





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

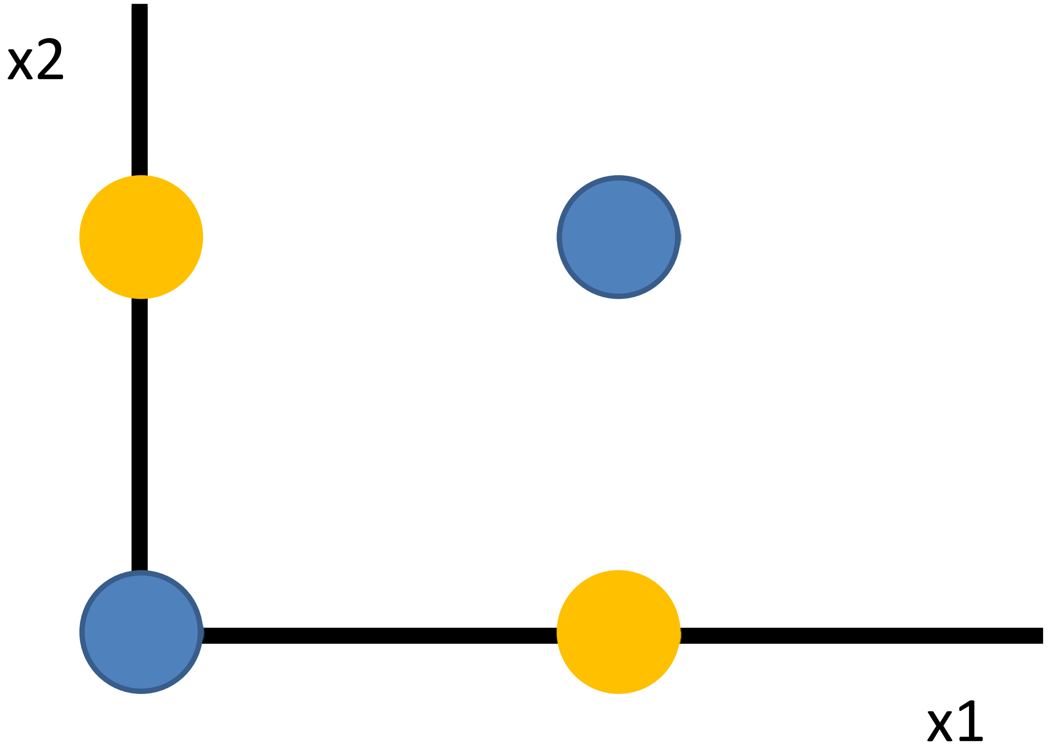
The Critics

- 1969: Minsky and Papert publish their book "Perceptrons"

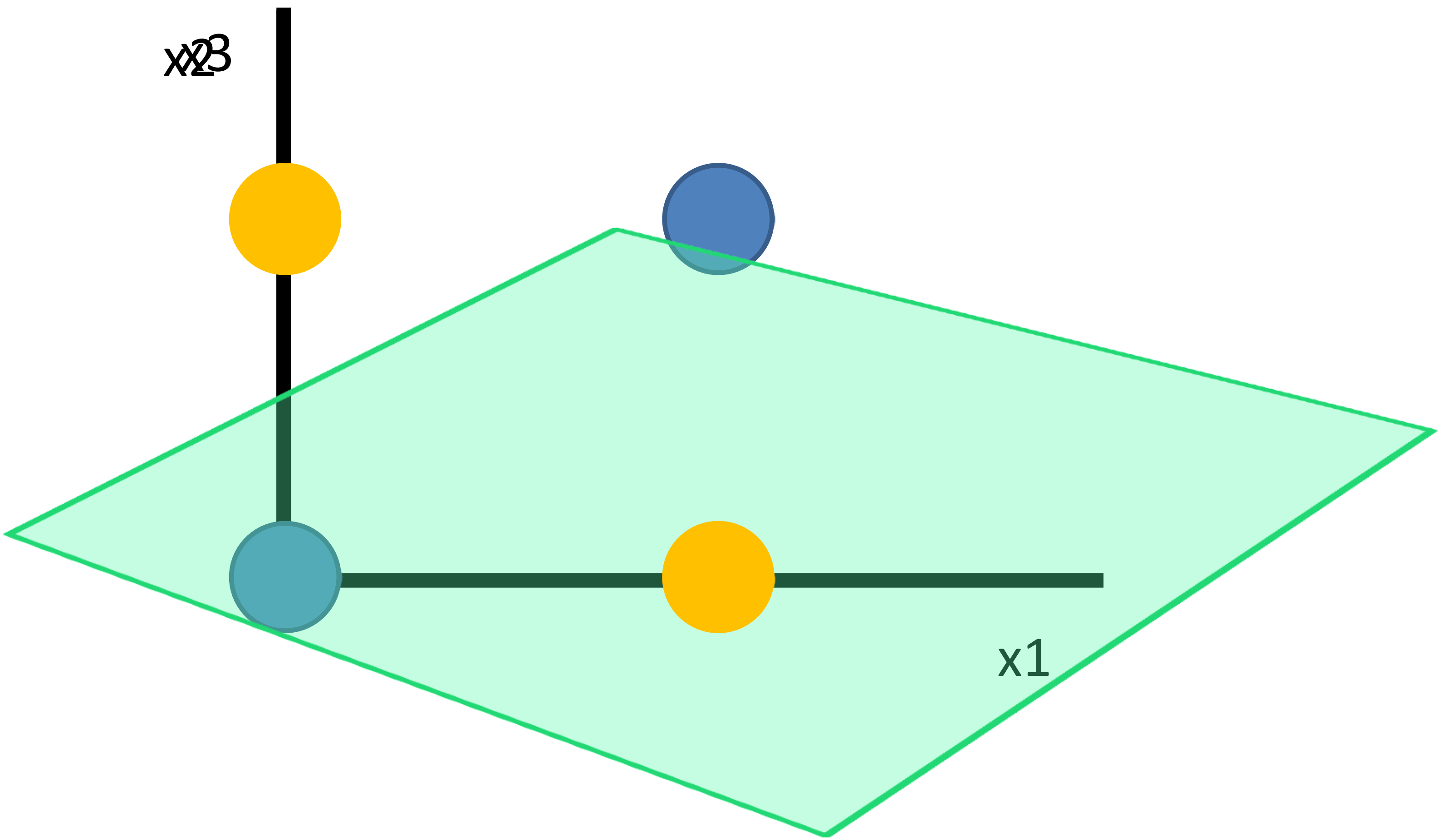
- Very controversial book, some blame the book for causing the whole research area to stagnate.

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

The XOR Problem



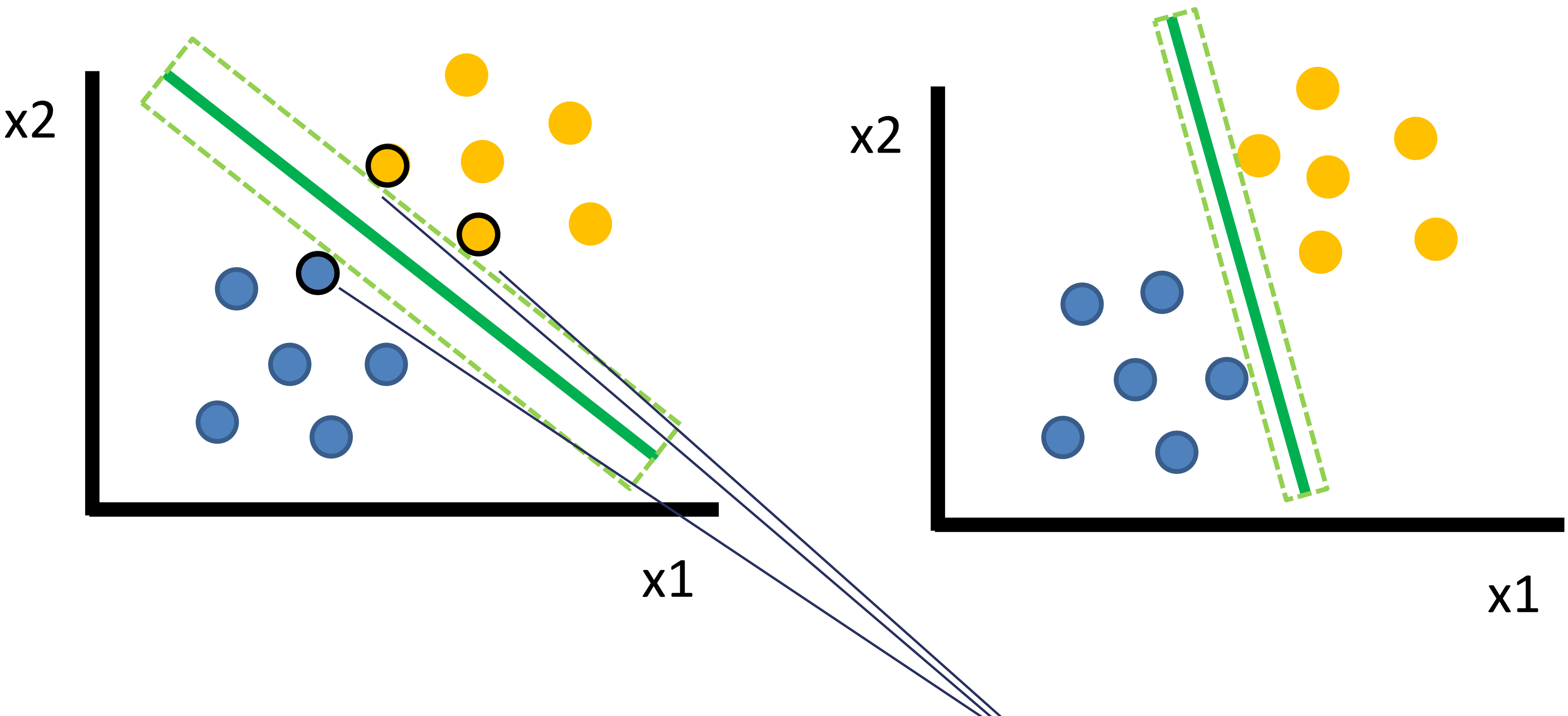
The XOR Problem



Support Vector Machine

- Widely used for all sorts of classification problems
- Some people say it is the best of the shelf classifier out there

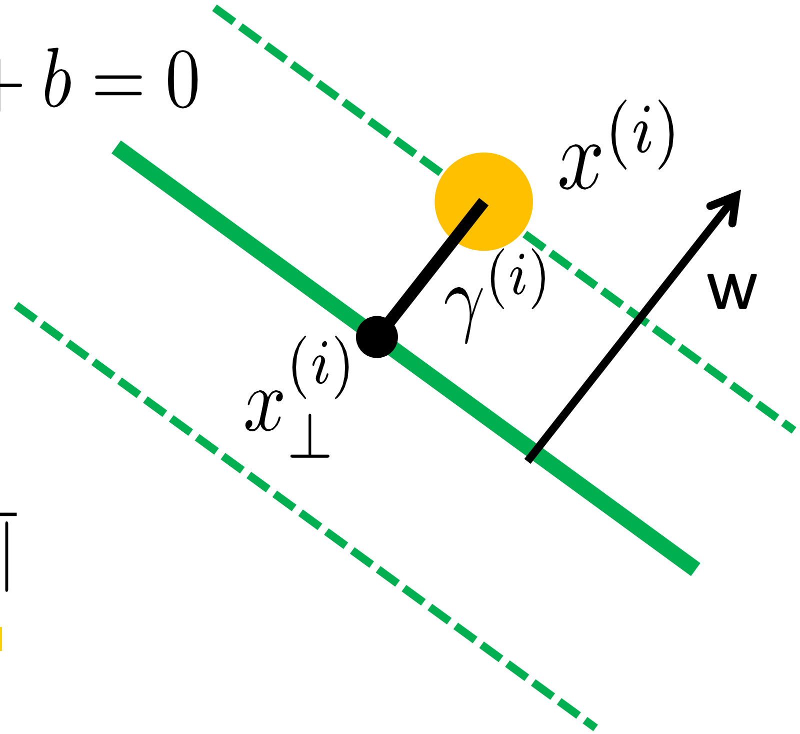
Maximum Margin Classification



Solution depends only on the support vectors!

Maximum Margin Classification

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



margin:

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

normalizing

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

+1 or -1

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

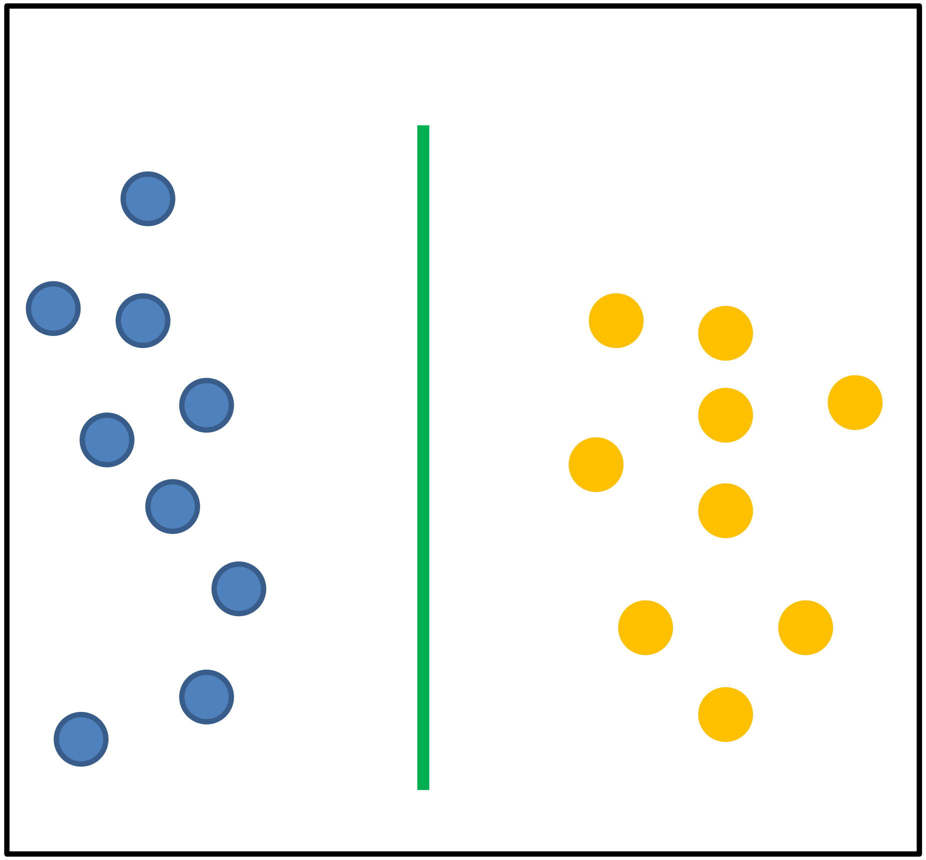
Maximum Margin Classification

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

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

non-convex

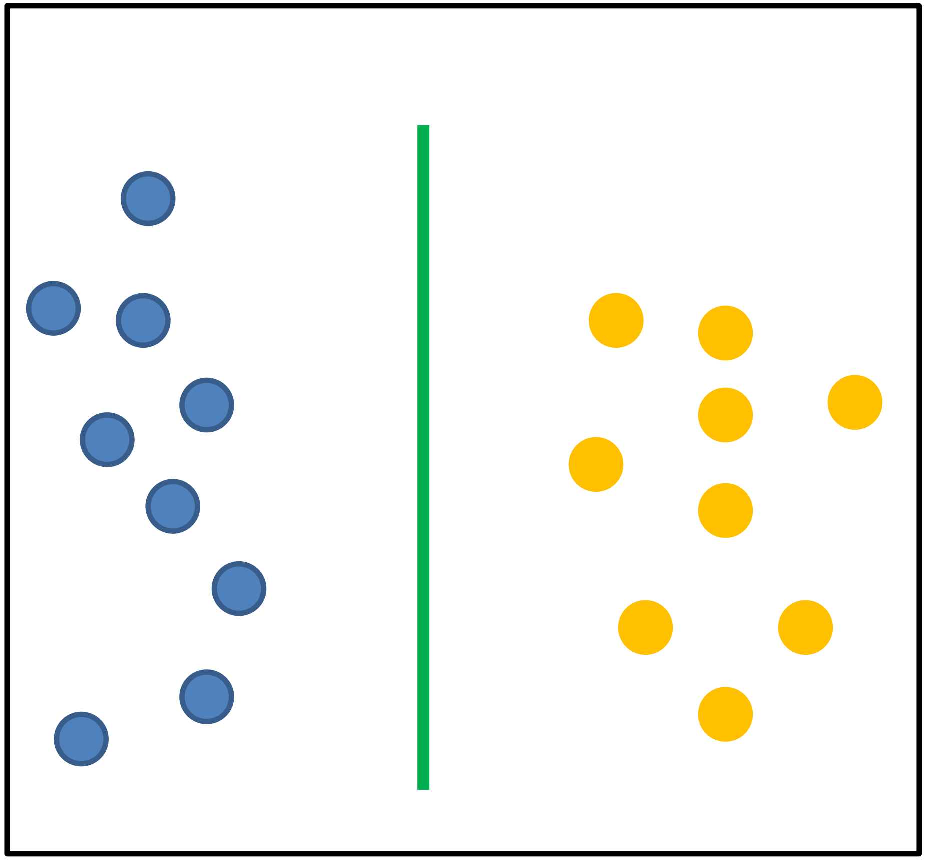
This Is Kind of Odd

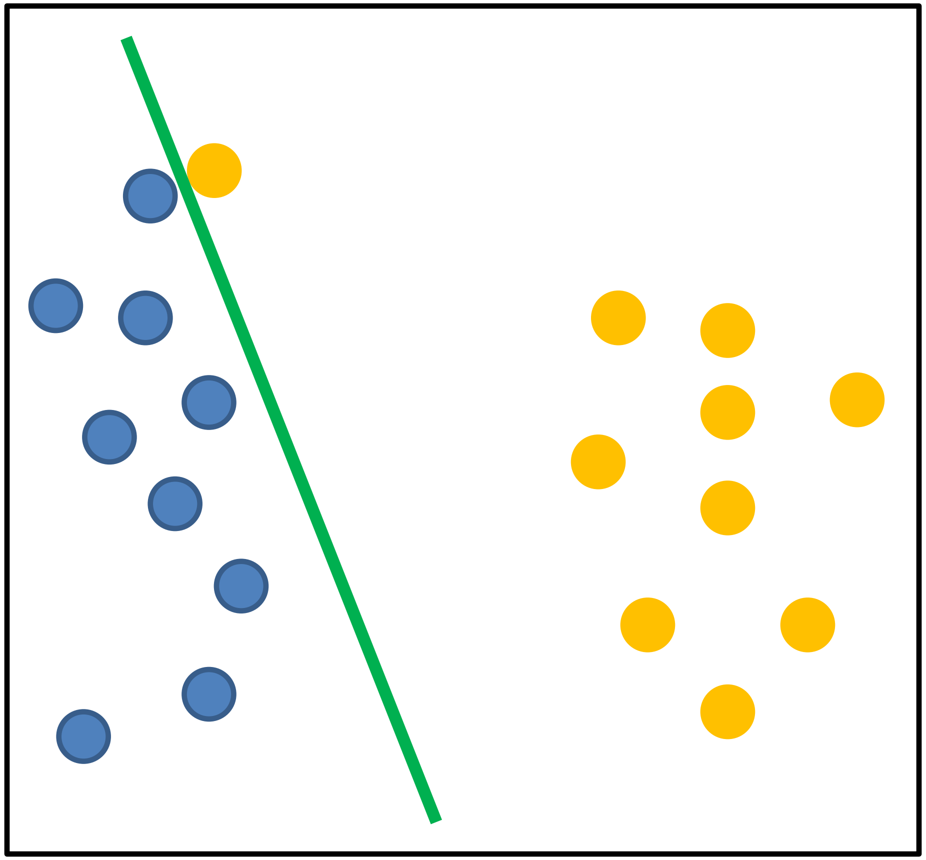


- Which data points do we care the most about?
- What would those samples look like?

those that are the most like the other class

Two Very Similar Problems





What about outliers?

ξ_i: slack variables

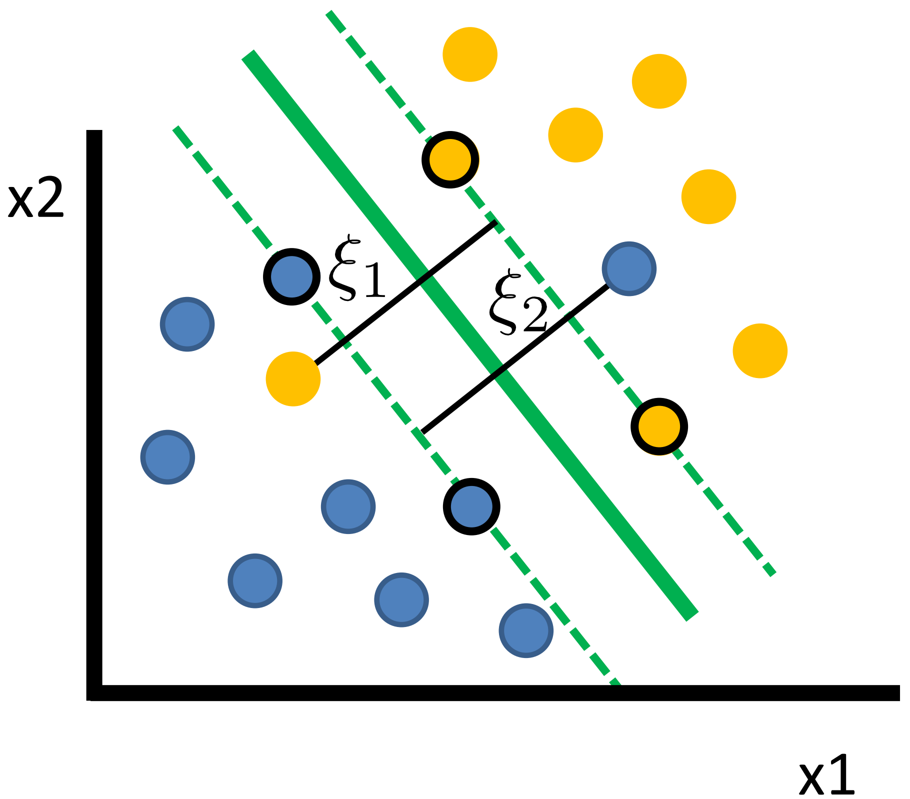
$\min_{w,b,\xi} \frac{1}{2}||w||^2$ + C

the smaller C the more robust to outlier

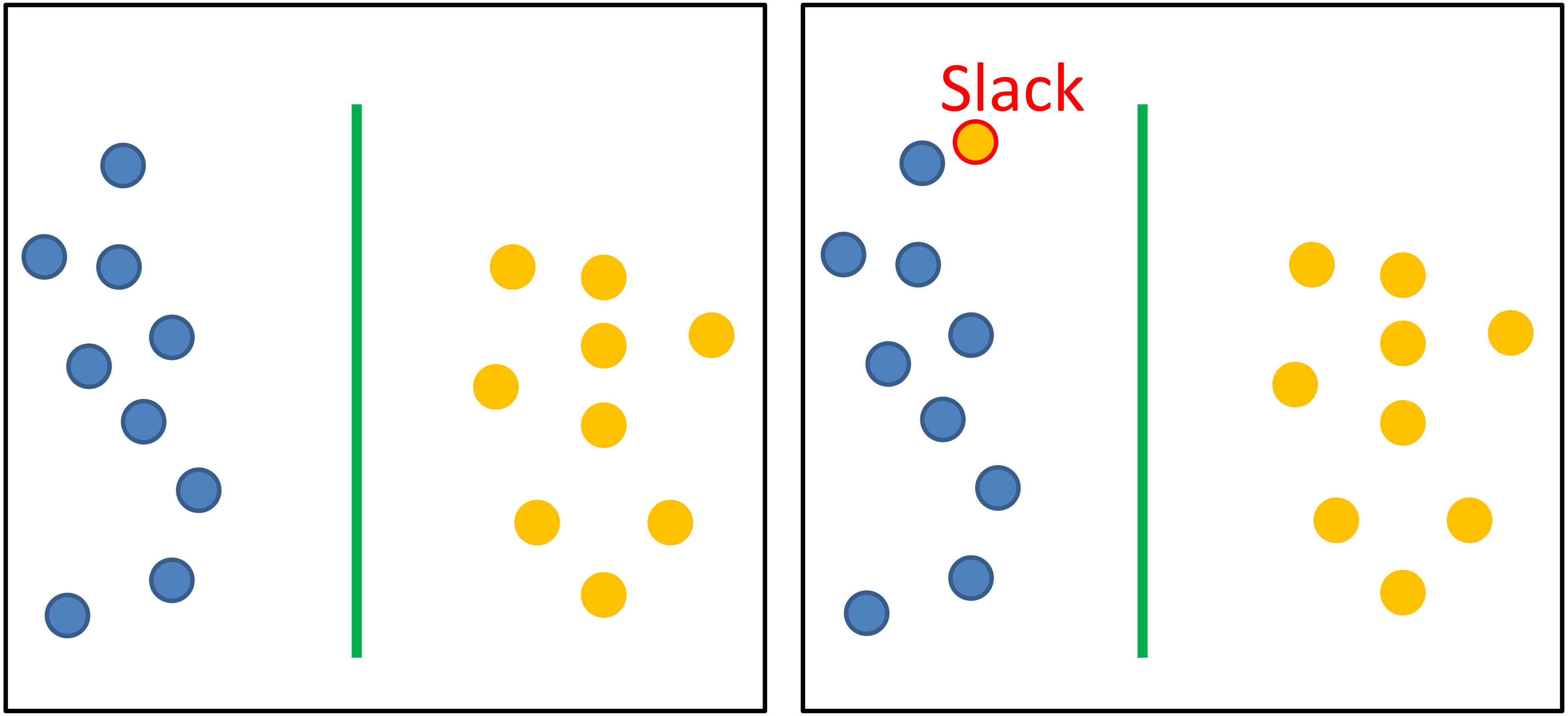
subject to:

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

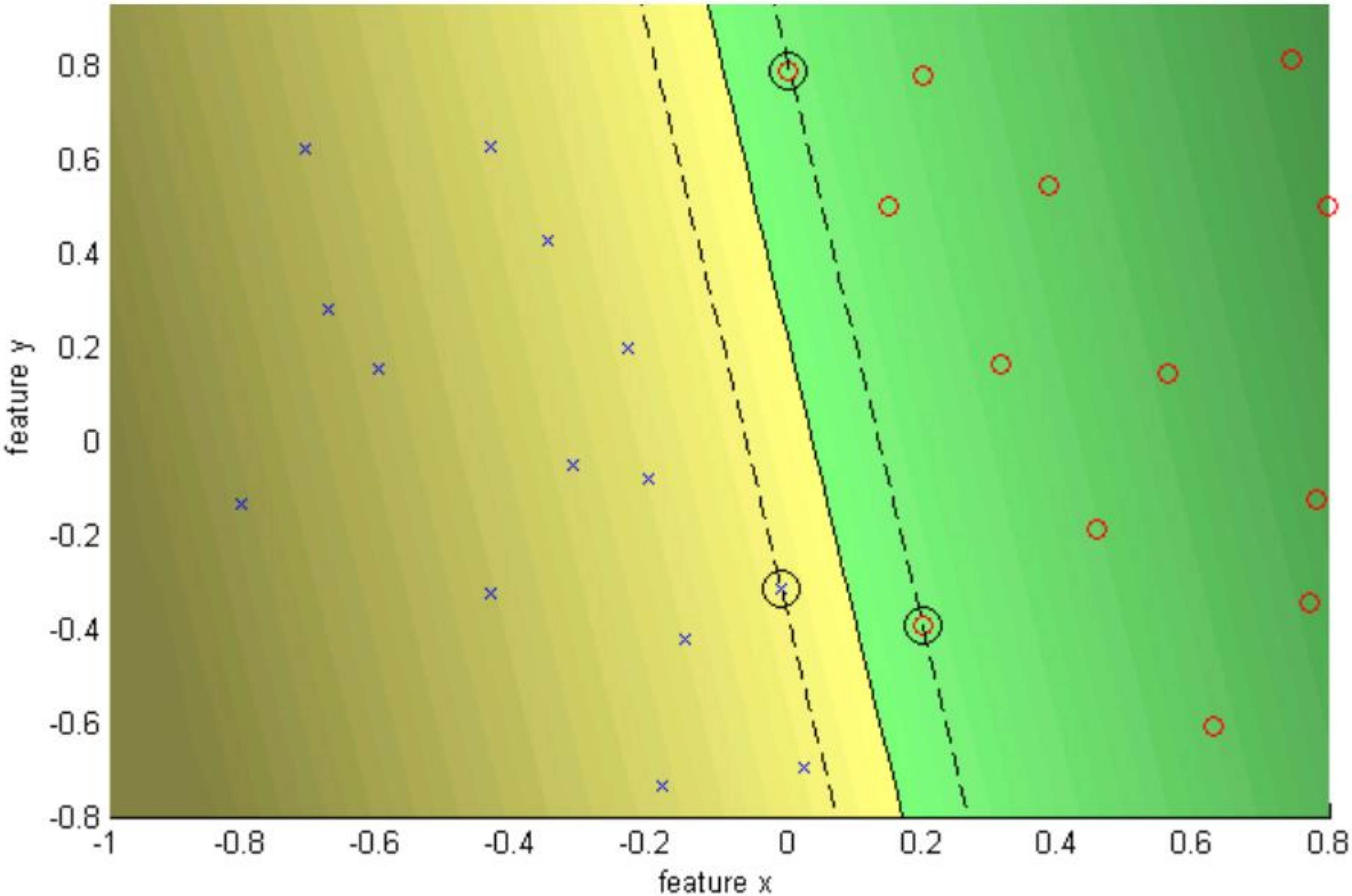
$$(i = 1, \ldots, n)$$



Two Very Similar Problems

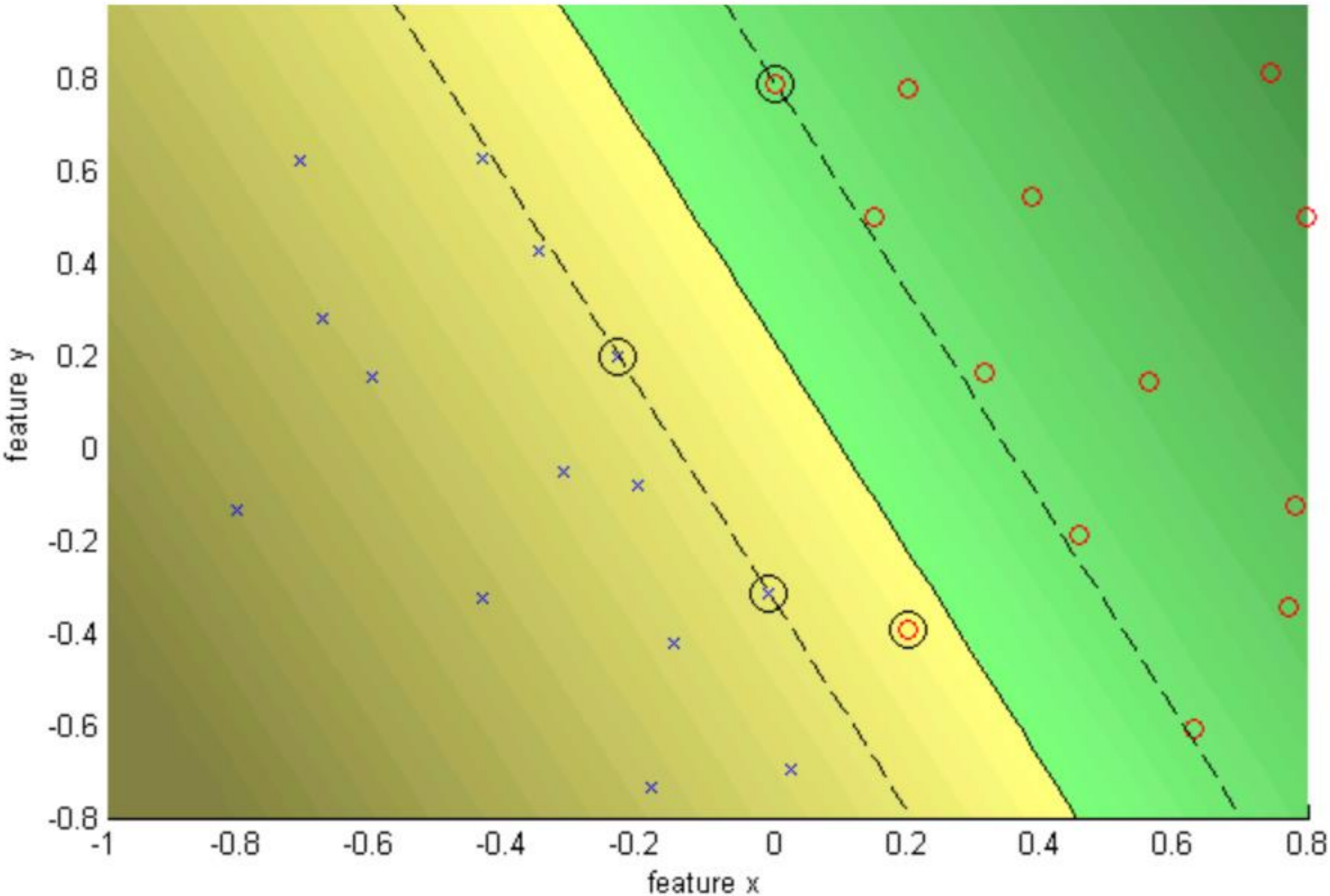


Hard Margin (C = Infinity)



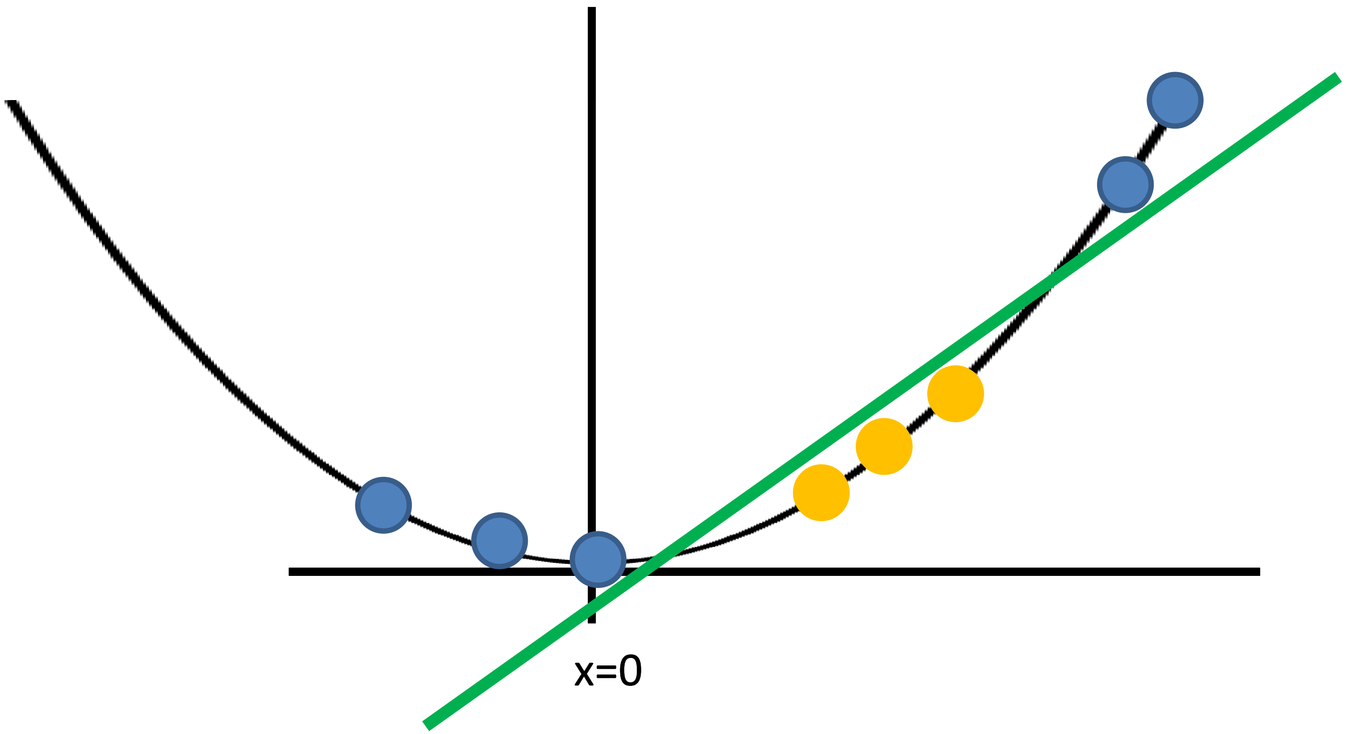
http://www.robots.ox.ac.uk/~az/lectures/ml/lect2.pdf

Soft Margin (C = 10)



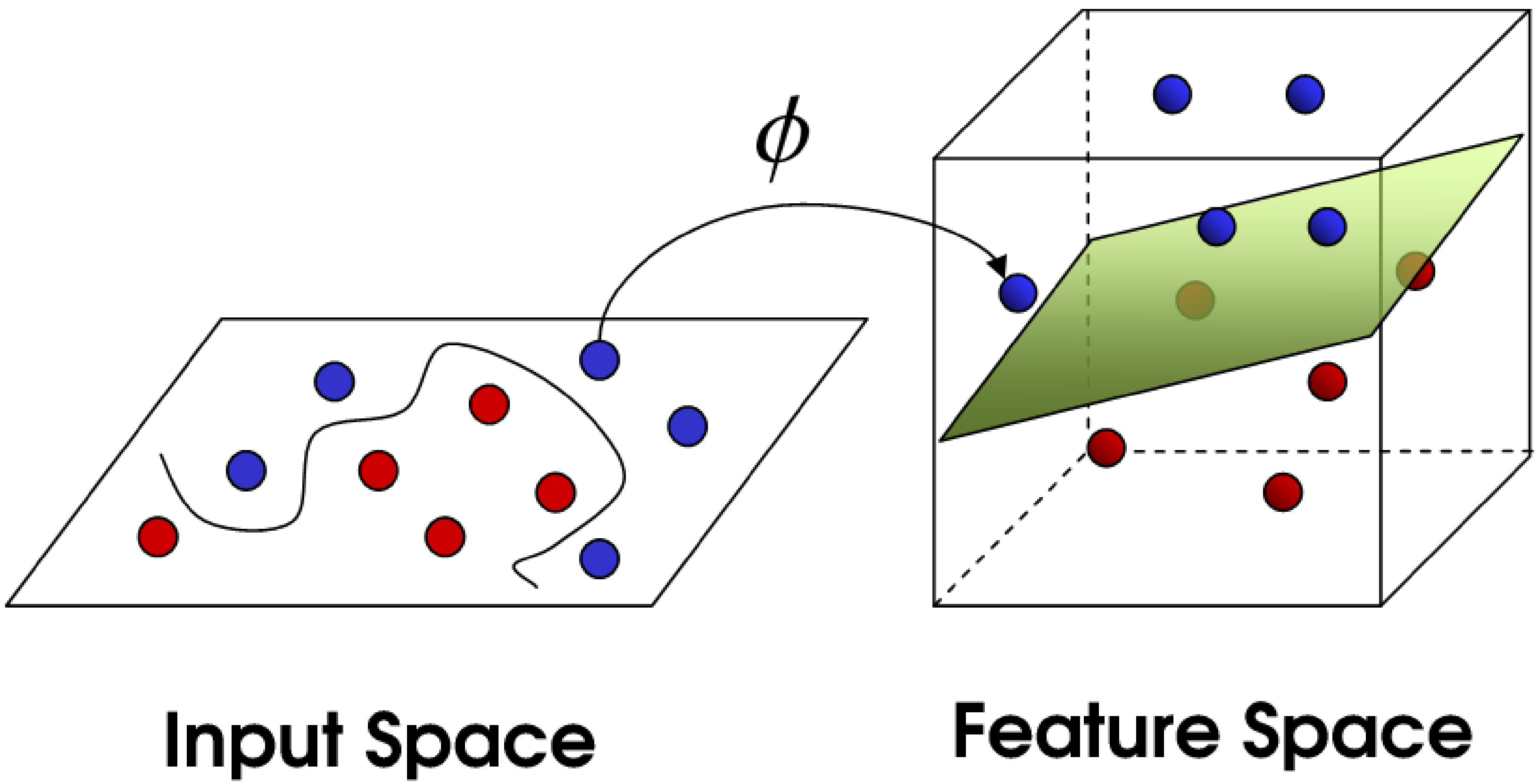
http://www.robots.ox.ac.uk/~az/lectures/ml/lect2.pdf

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

$$x = (x_1, x_2)$$

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

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

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

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

Kernel Functions

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

- Polynomial:

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

- Radial basis function (RBF):

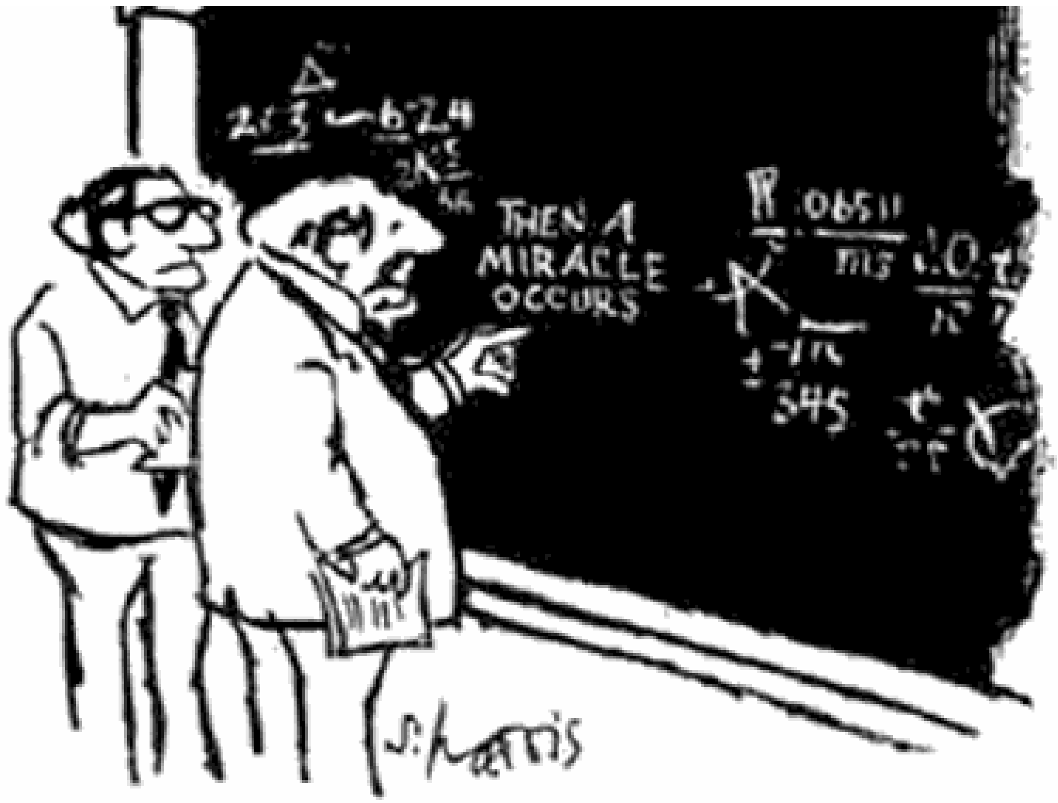
$$K(x,z) = \exp(-\gamma(x-z)^2)$$

So what is the excitement?

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

s.t. α_i

$\sum$



$\arg\mathrm{r}$

"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

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 ie PCA
- Train SVM decide on Kernel
- Evaluate performance

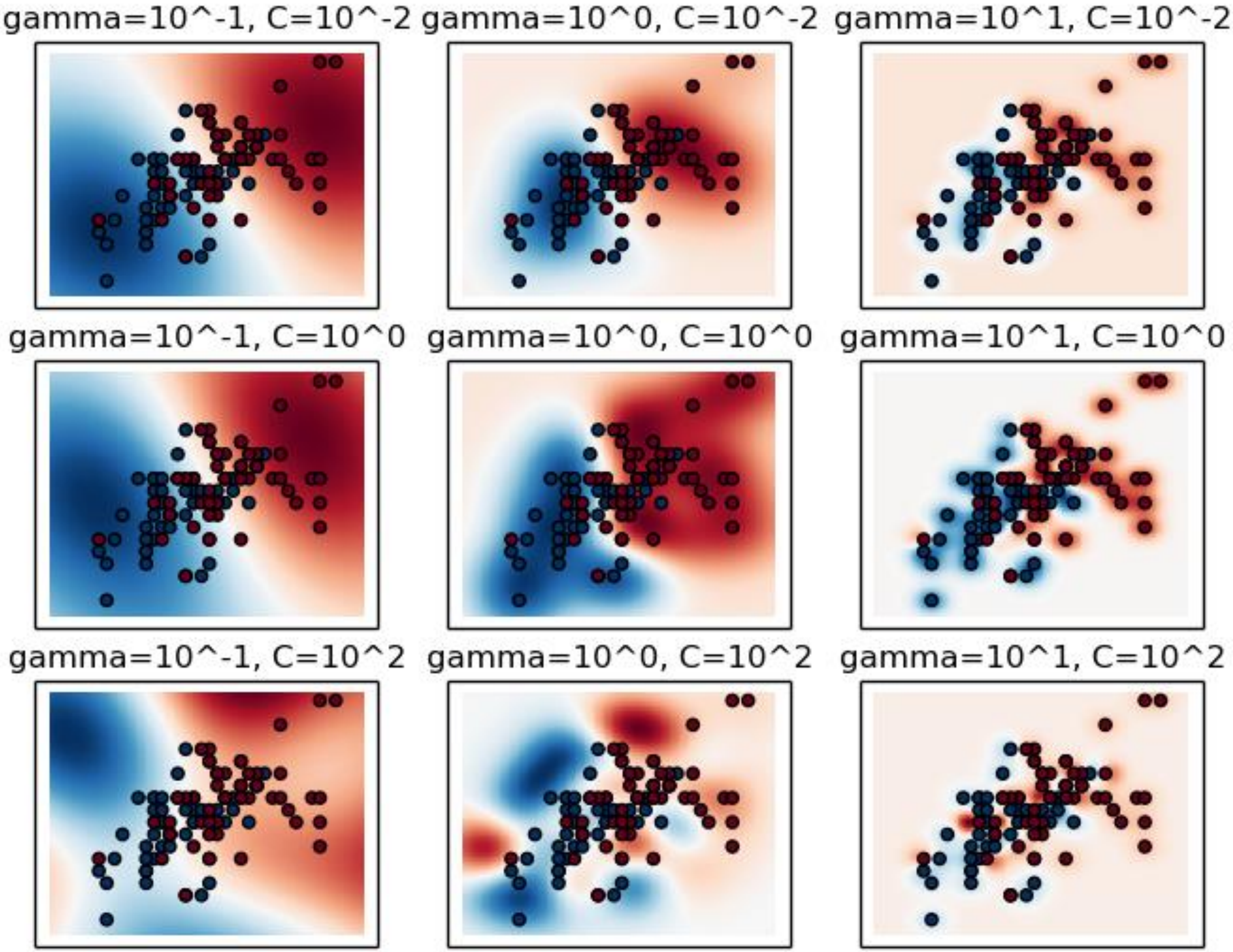
- Red are cross validation steps

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?

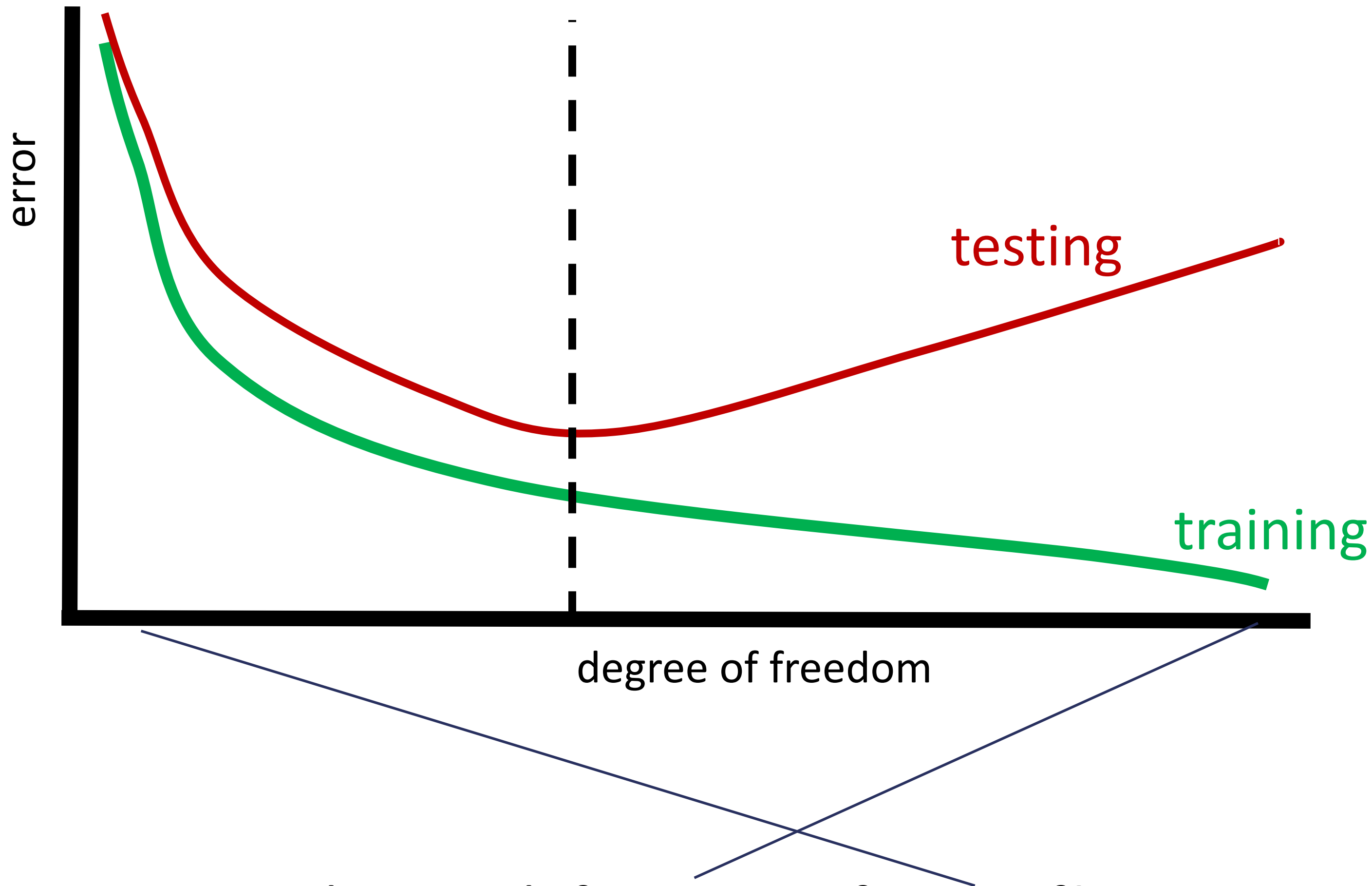
Parameter Tuning

- Given a classification task

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

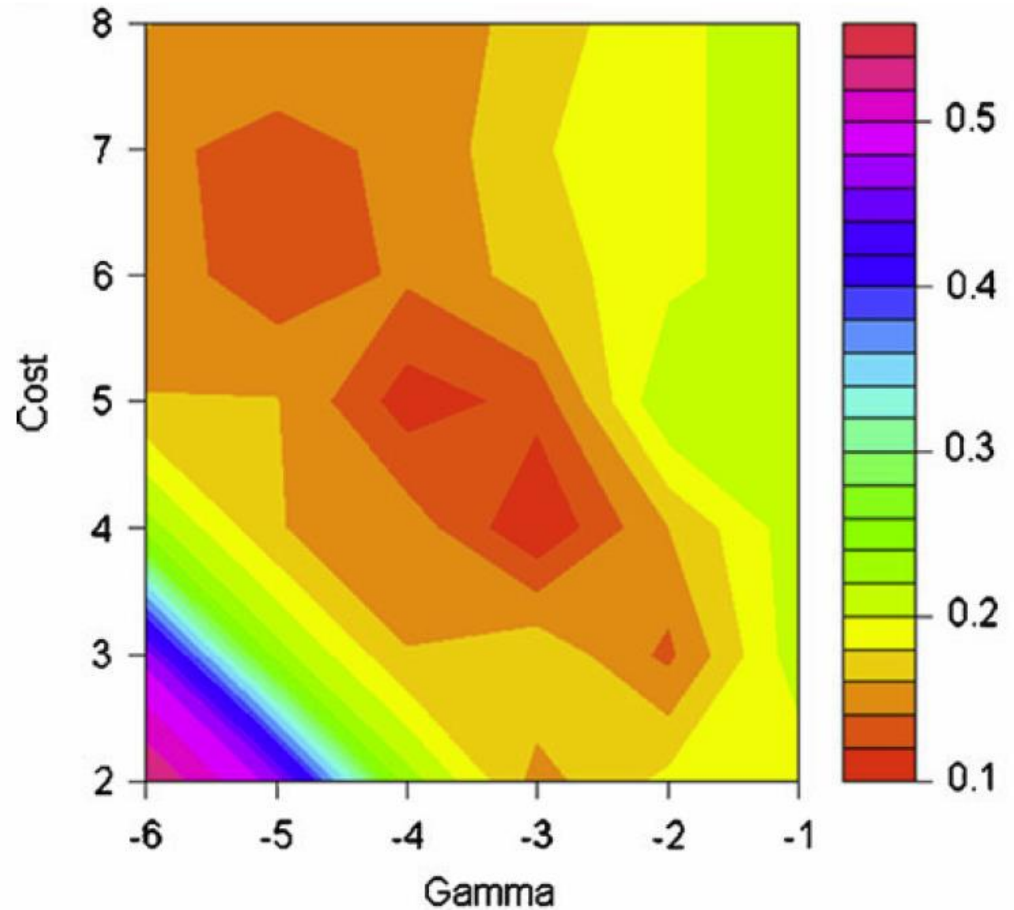
Try different combinations
and take the best.

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:

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

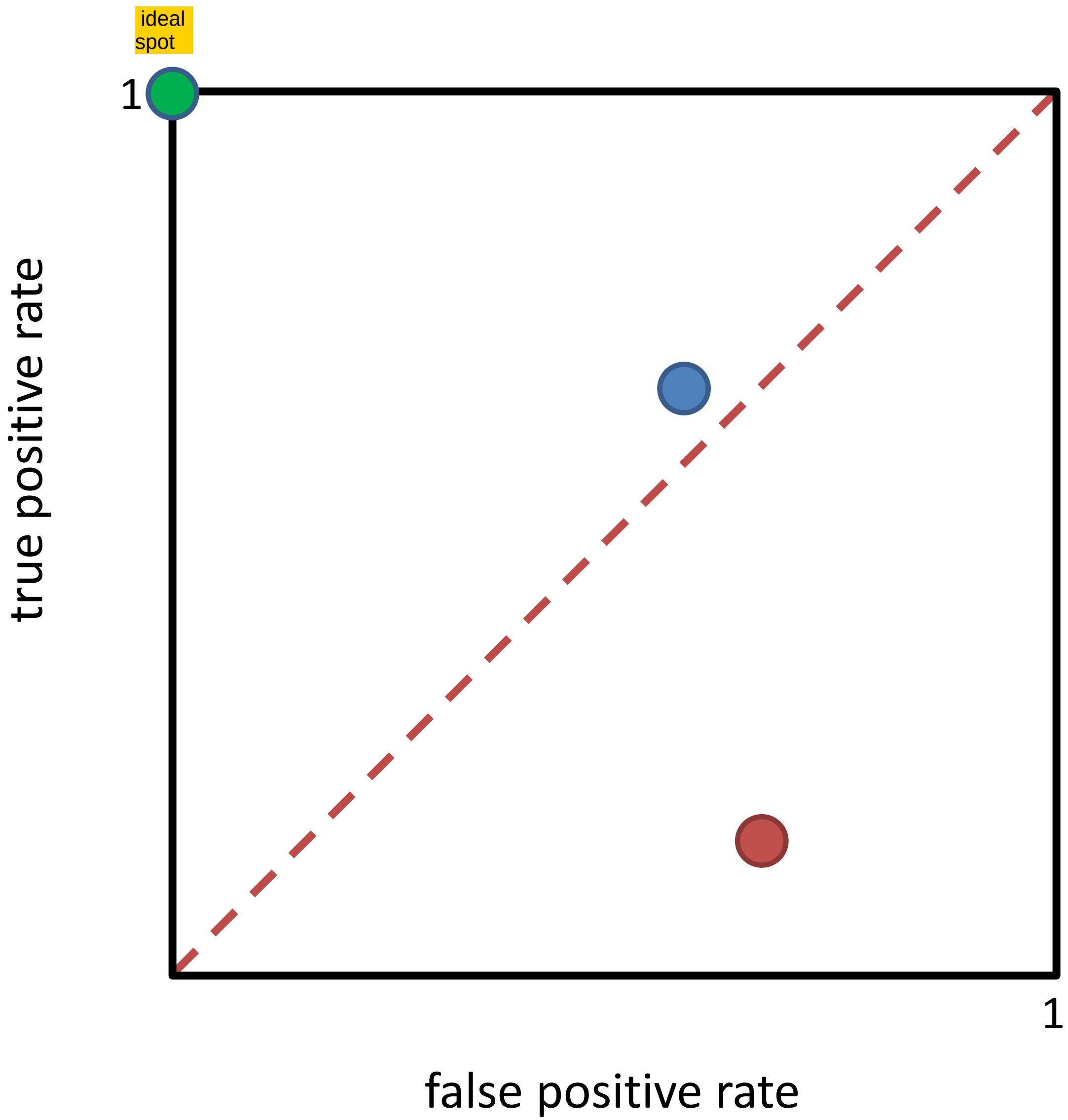
- False Positive Rate:

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

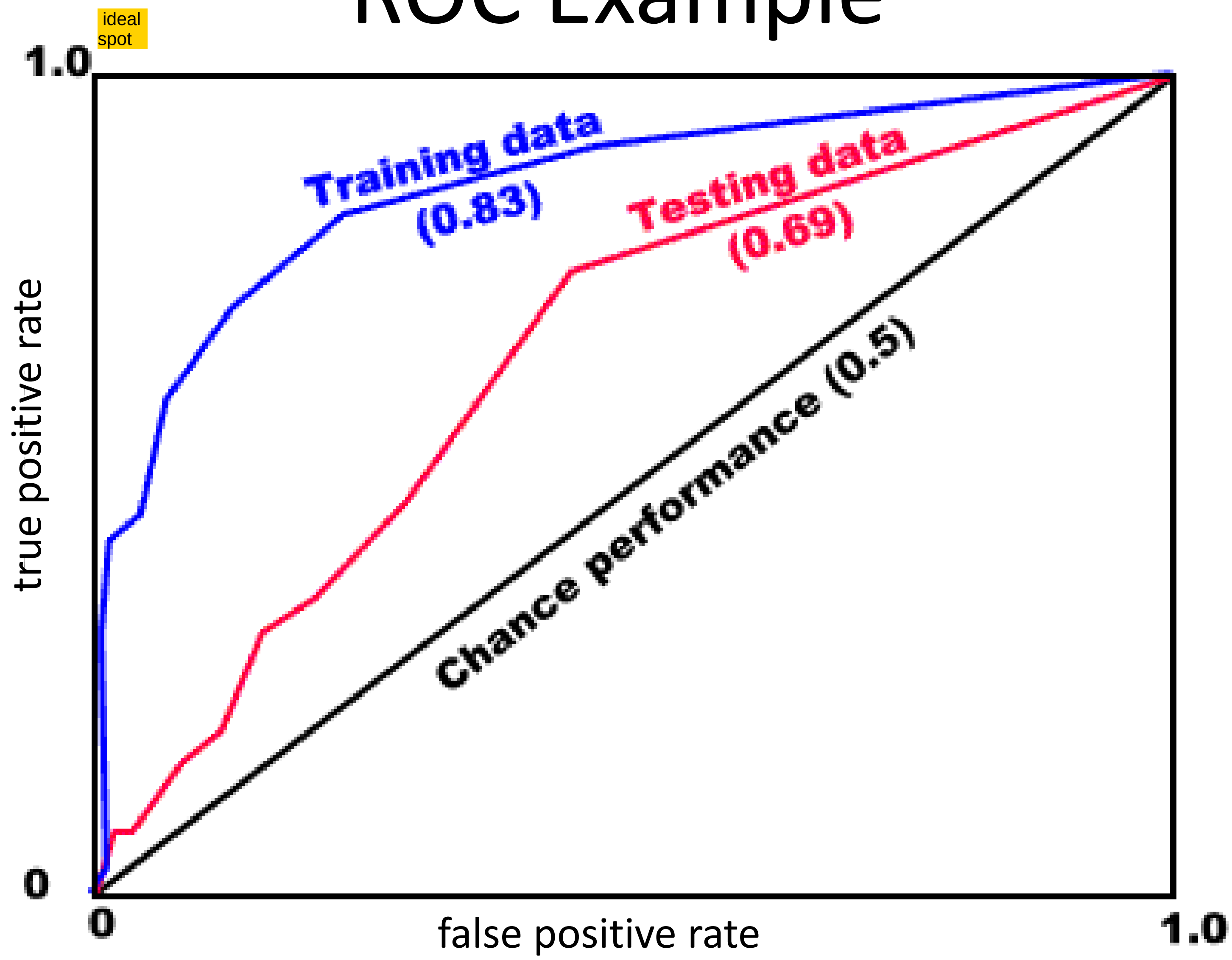
predicted

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: $\dfrac{tp}{tp+fn}$ = true positive rate

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

predicted

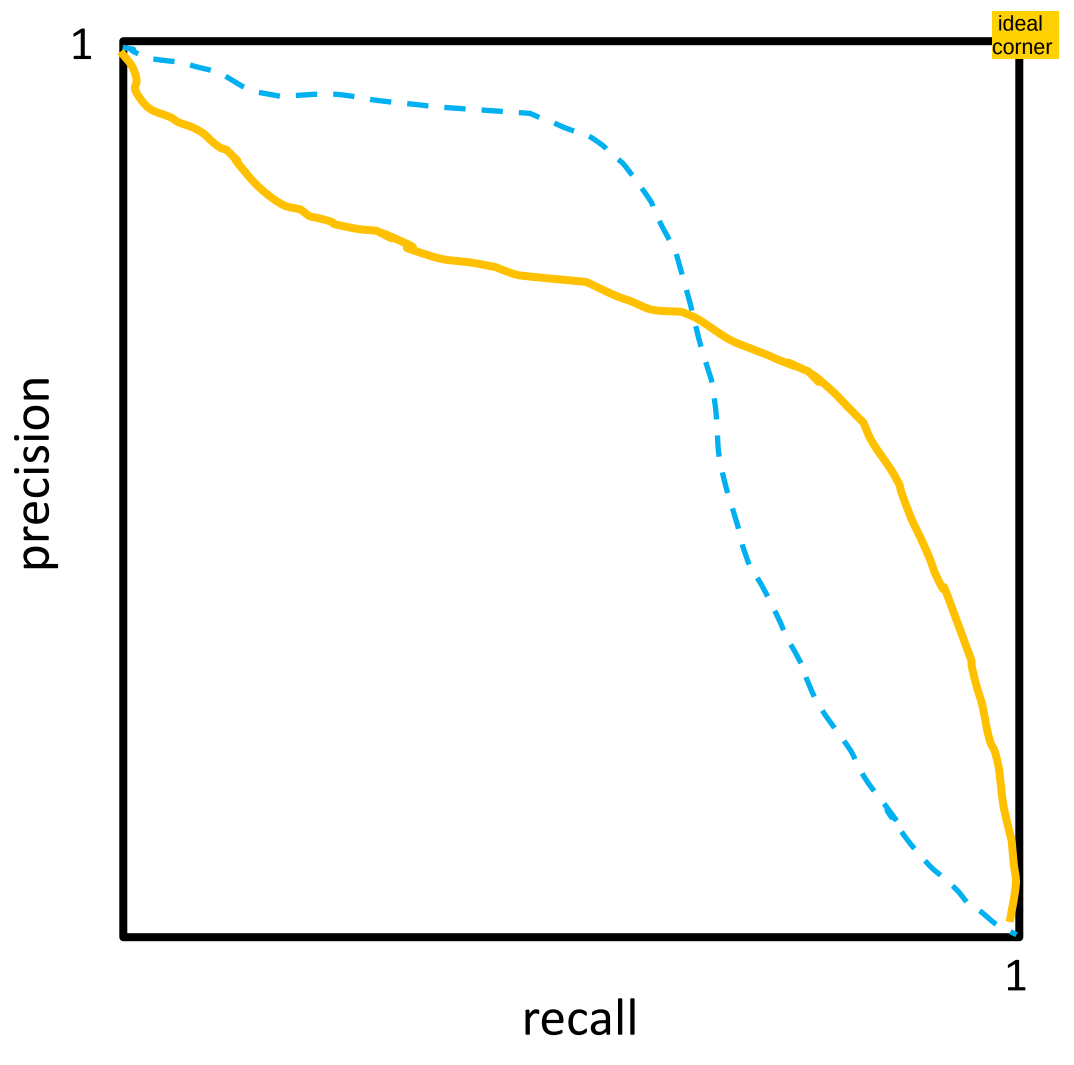
true	1	-1
1	tp	fn
-1	fp	tn

Precision Recall

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

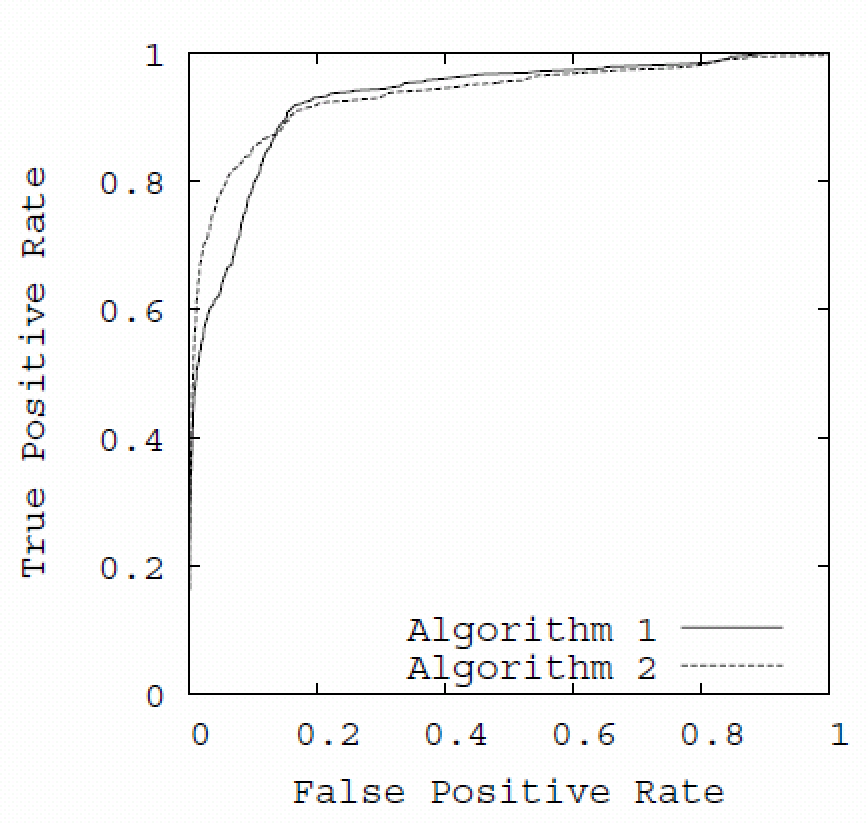
- **Precision**: If I take a positive prediction example, what is the probability that it is indeed a positive example?

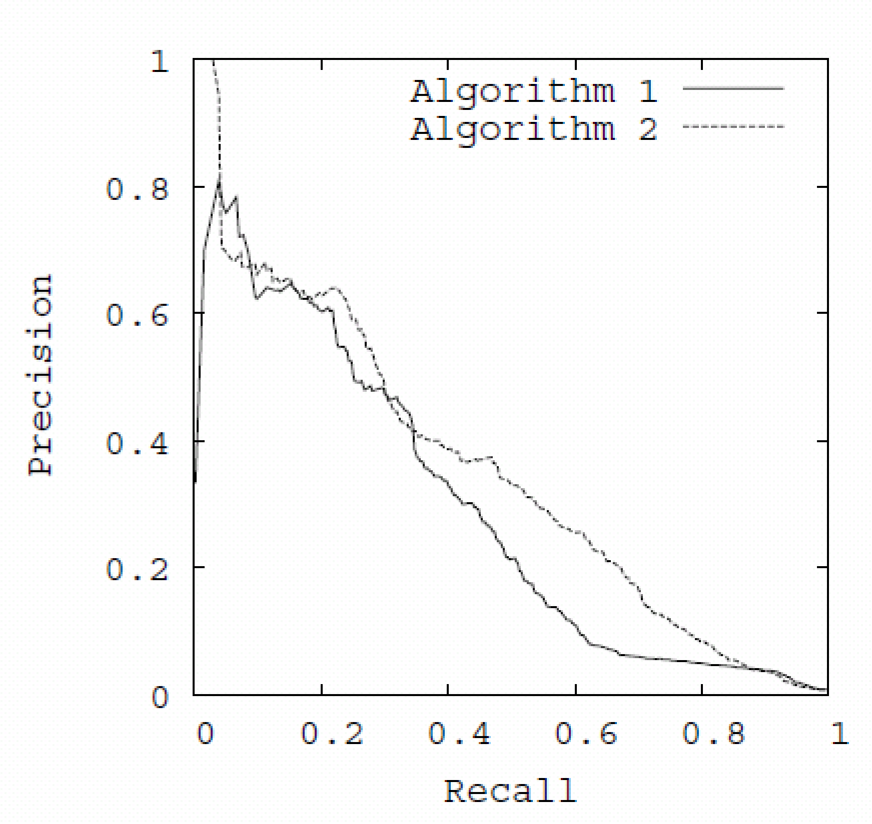
Precision Recall Curve



Comparison

ROC curve & precision recall curve lead to same decision





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

F-measure

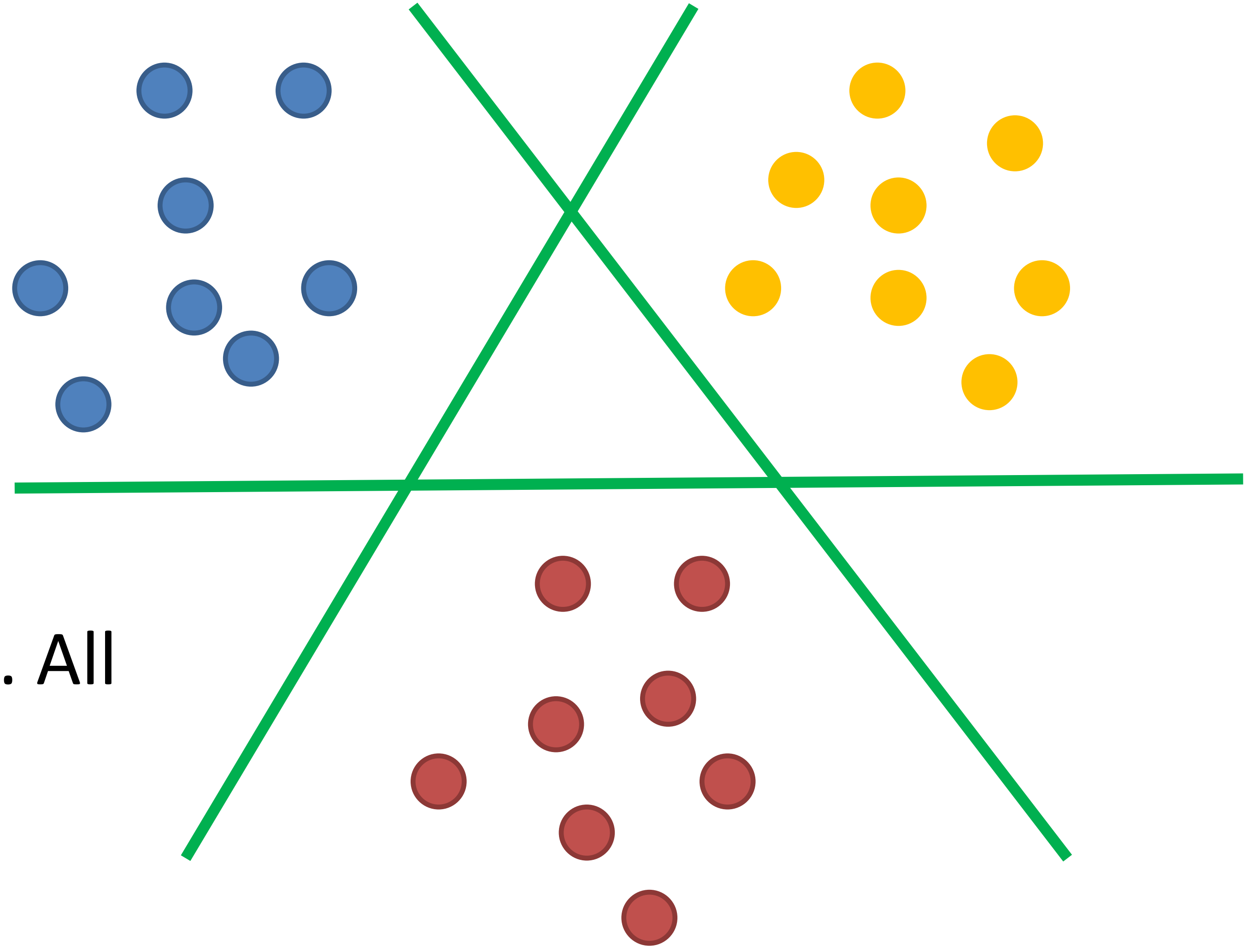
- Weighted average of precision and recall

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

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

Multi Class

yelllow vs background class (= red + blue)
red vs background class (= yellow + blue)



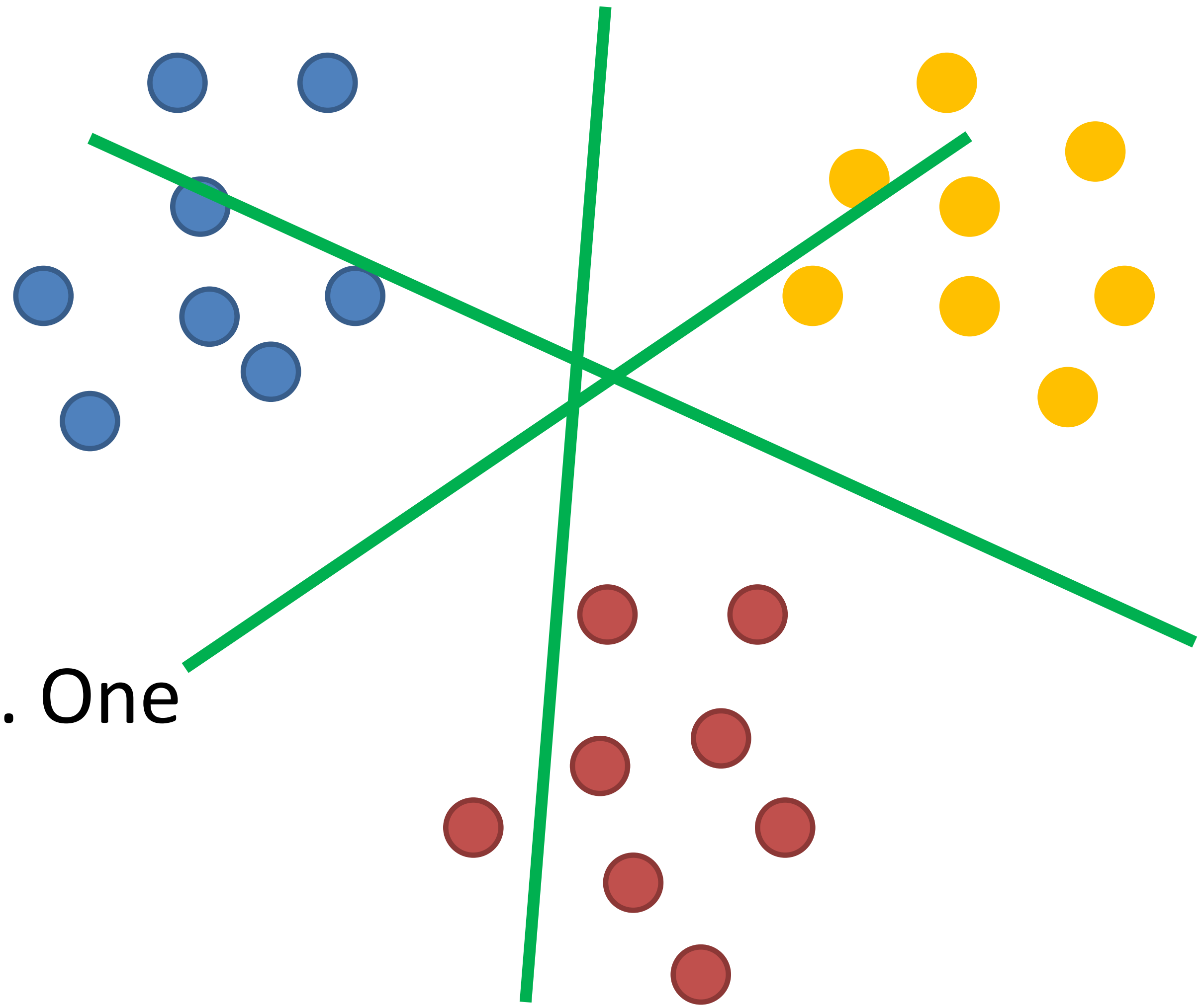
One vs. All

One vs All

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

Multi Class

yellow vs blue, yellow vs red, red vs blue



One vs. One

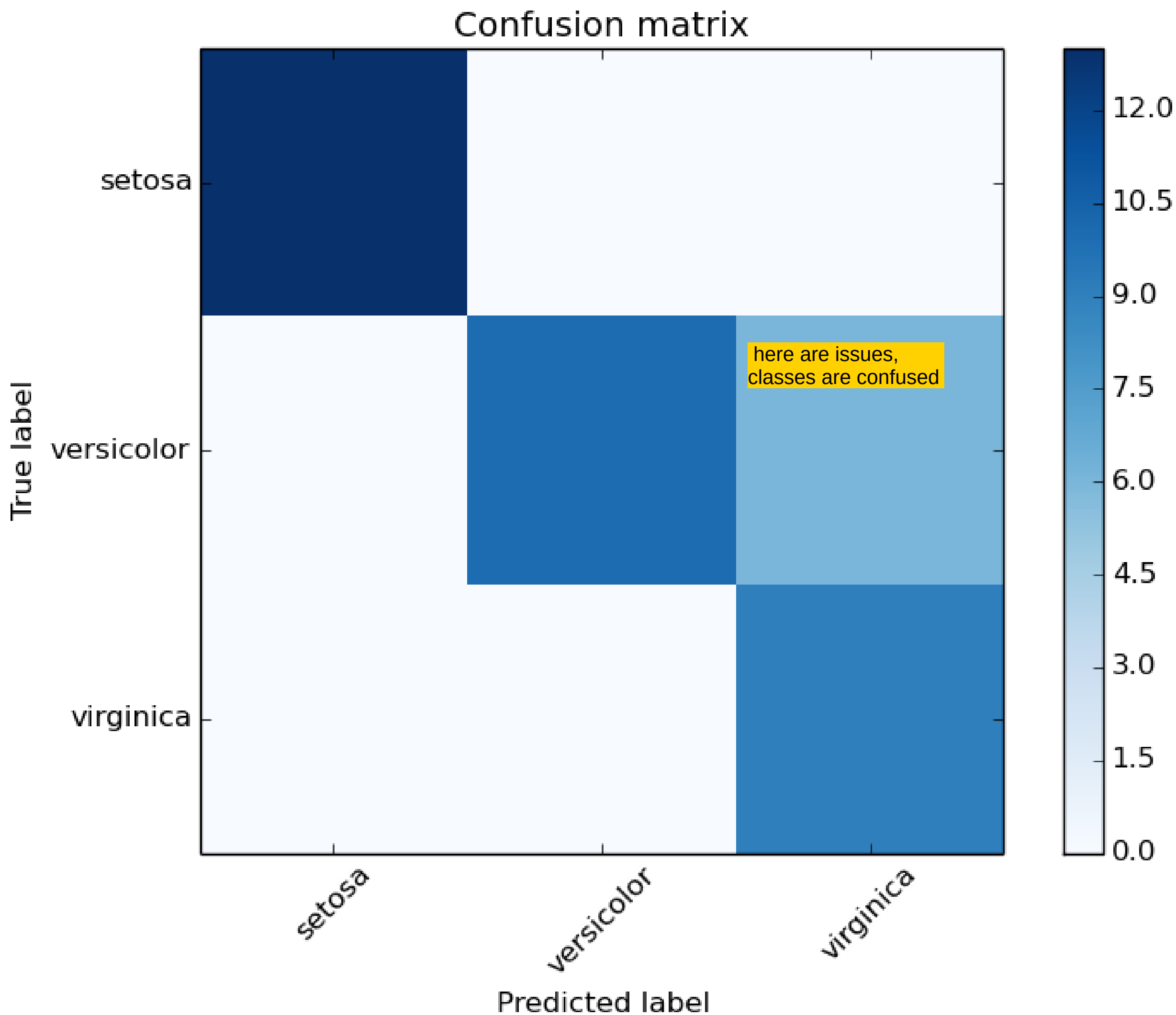
One vs One

- Train n(n-1)/2 classifiers

run all classifier and

- 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