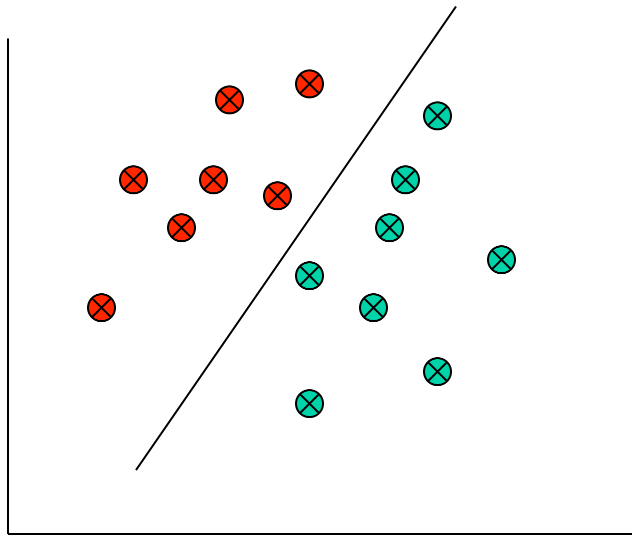
4. Linear Classification

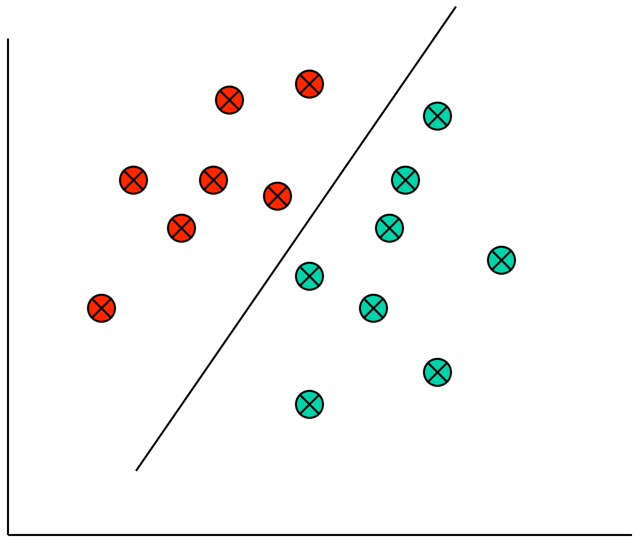
Kai Yu

Linear Classifiers



- A simplest classification model
- Help to understand nonlinear models
- Arguably the most useful classification method!

Linear Classifiers

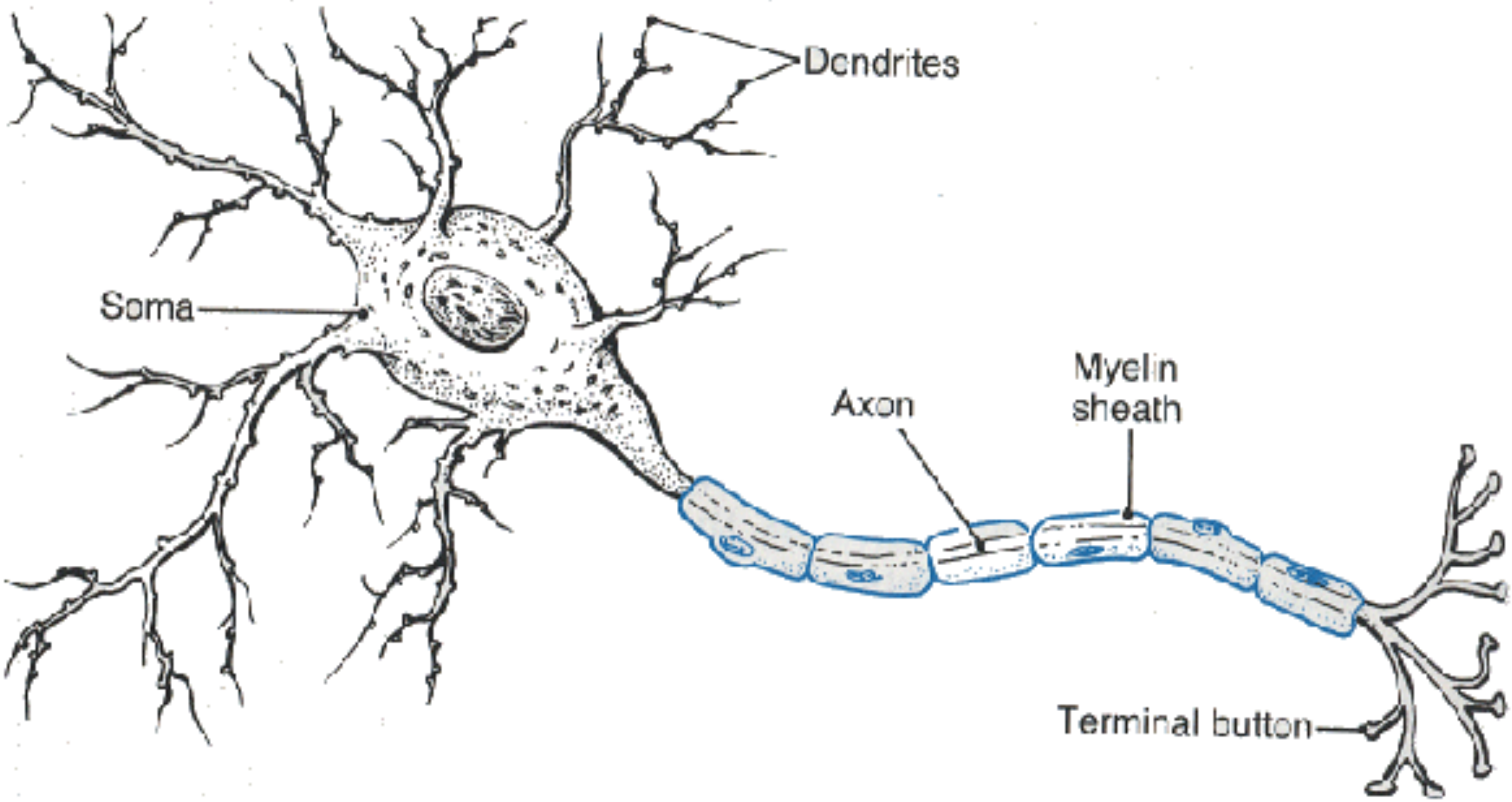


- A simplest classification model
- Help to understand nonlinear models
- Arguably the most useful classification method!

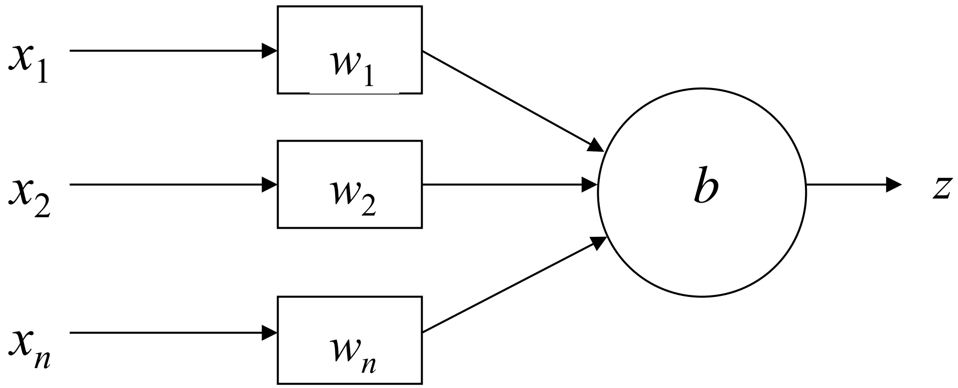
Outline

- Perceptron Algorithm
- Support Vector Machines
- Logistic Regression
- Summary

Basic Neuron

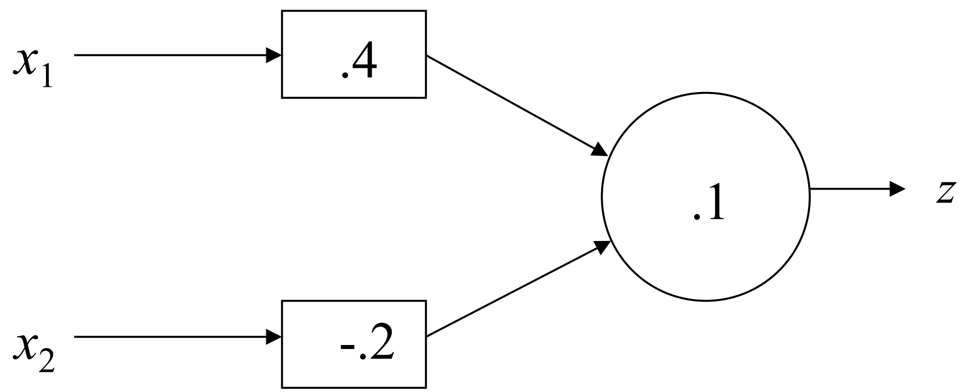


Perceptron Node – Threshold Logic Unit



$$z = \begin{cases} 1 & \text{if } \sum_{i=1}^{n} x_i w_i \geq b \\ 0 & \text{if } \sum_{i=1}^{n} x_i w_i < b \end{cases}$$

Perceptron Learning Algorithm



x_1	x_2	t
.8	.3	1
.4	.1	0

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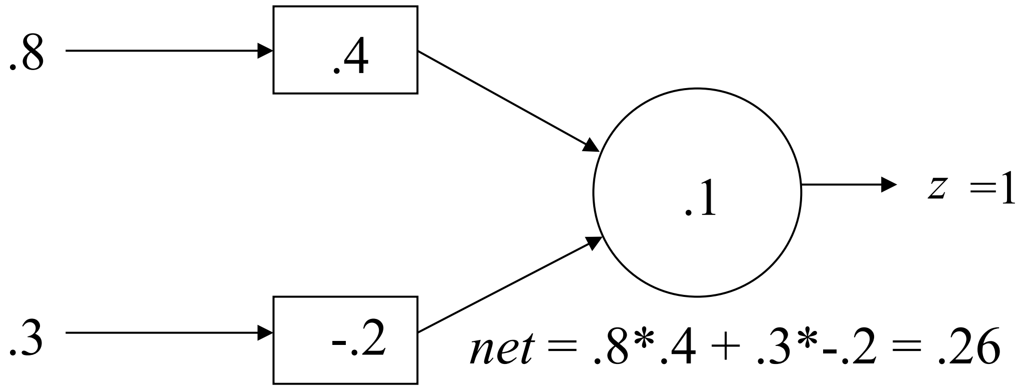
First Training Instance



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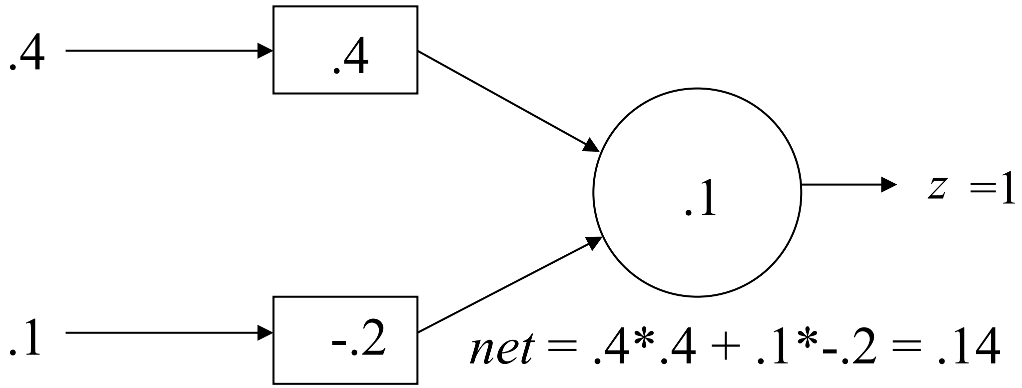
Second Training Instance



$net = .4*.4 + .1*-.2 = .14$

x_1	x_2	t
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$$\Delta w_i = (t - z) * c * x_i$$

The Perceptron Learning Rule

$$\Delta w_{ij} = c(t_j - z_j)\, x_i$$

- Least perturbation principle
  - Only change weights if there is an error (learning from mistakes)
  - The change amounts to x_i *scaled by a small c*
- Iteratively apply an example from the training set
- Each iteration through the training set is an *epoch*
- Continue training until total training error is less than epsilon
- Perceptron Convergence Theorem: Guaranteed to find a solution in finite time if a solution exists

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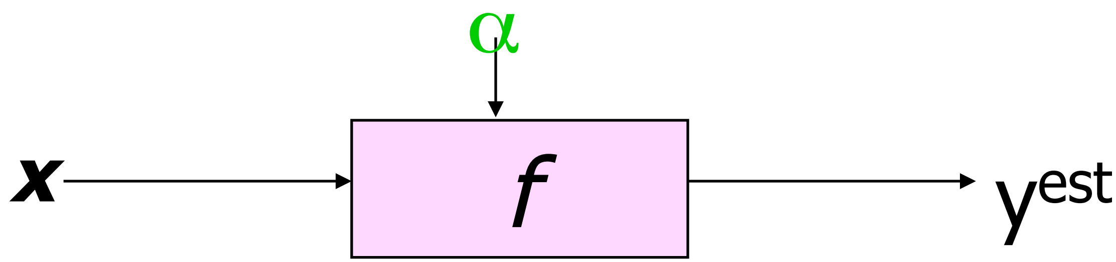
Support Vector Machines: Overview

- A powerful method for 2-class classification
  - Original idea: Vapnik, 1965 for linear classifiers
  - SVM, Corte and Vapnik, 1995
  - Becomes very hot since late 90's

- Better generalization (less overfitting)

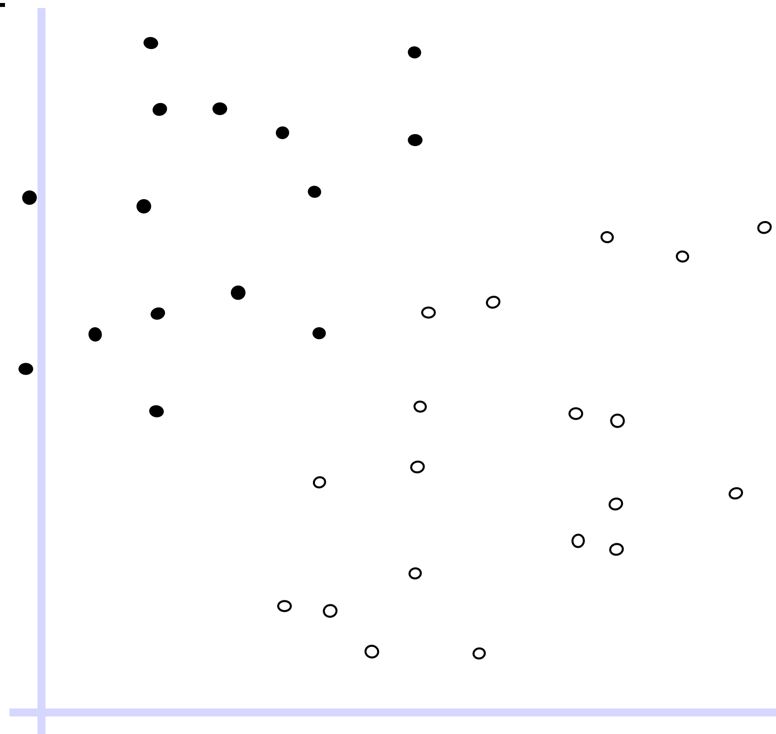
- Key ideas
  - Use kernel function to transform low dimensional training samples to higher dim (for linear separability problem)
  - Use quadratic programming (QP) to find the best classifier boundary hyperplane (for global optima and)

Linear Classifiers



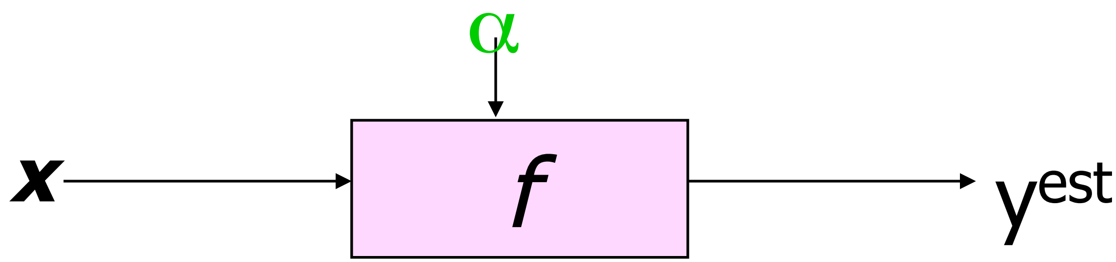
$$f(\mathbf{x},\mathbf{w},b) = \mathrm{sign}(\mathbf{w}.\,\mathbf{x} - b)$$

- • denotes +1
- ° denotes -1



How would you classify this data?

Linear Classifiers



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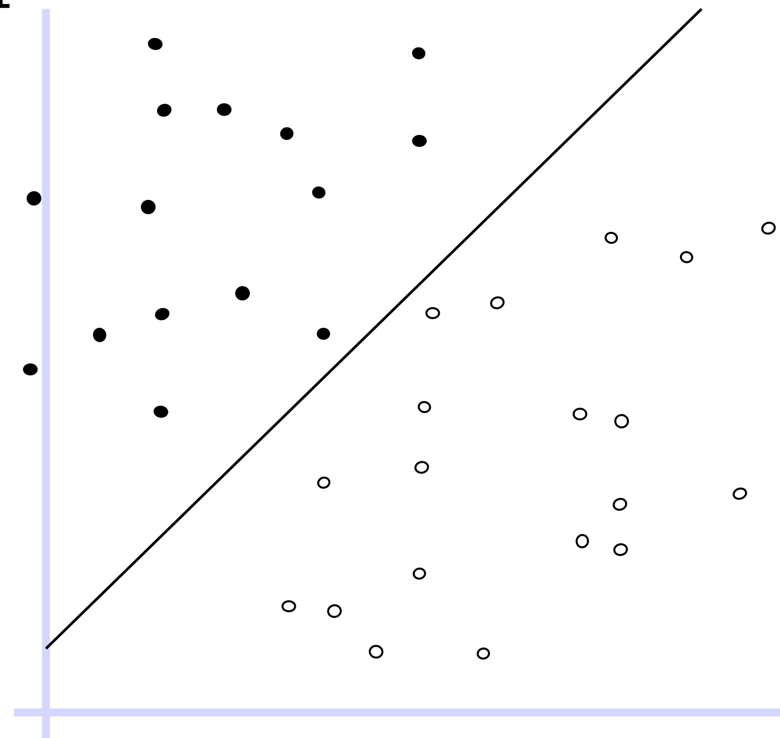

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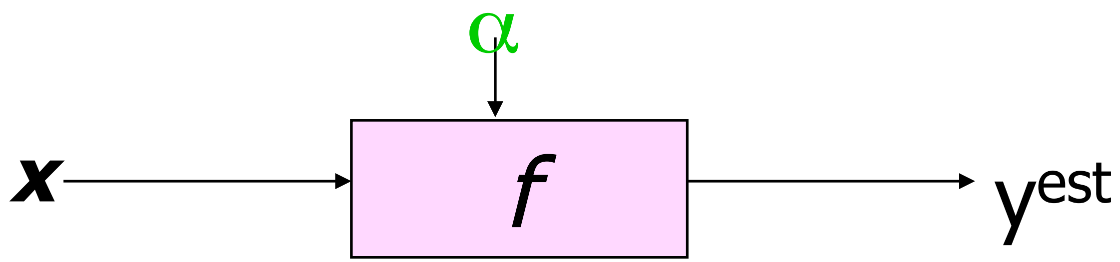

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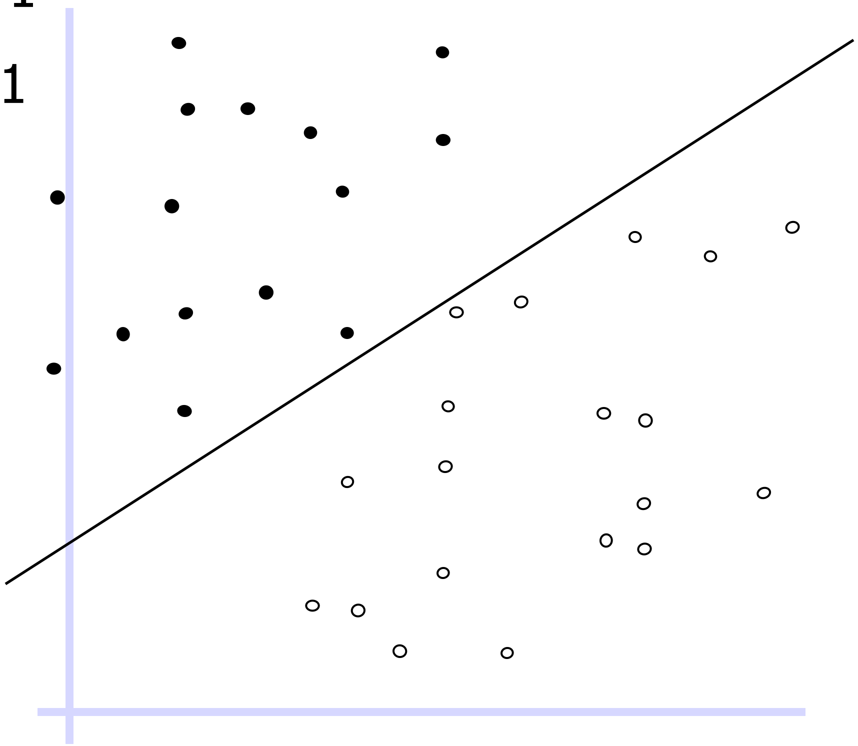

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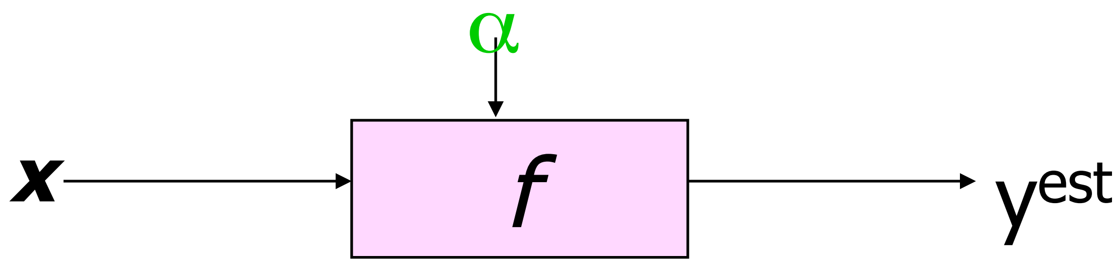

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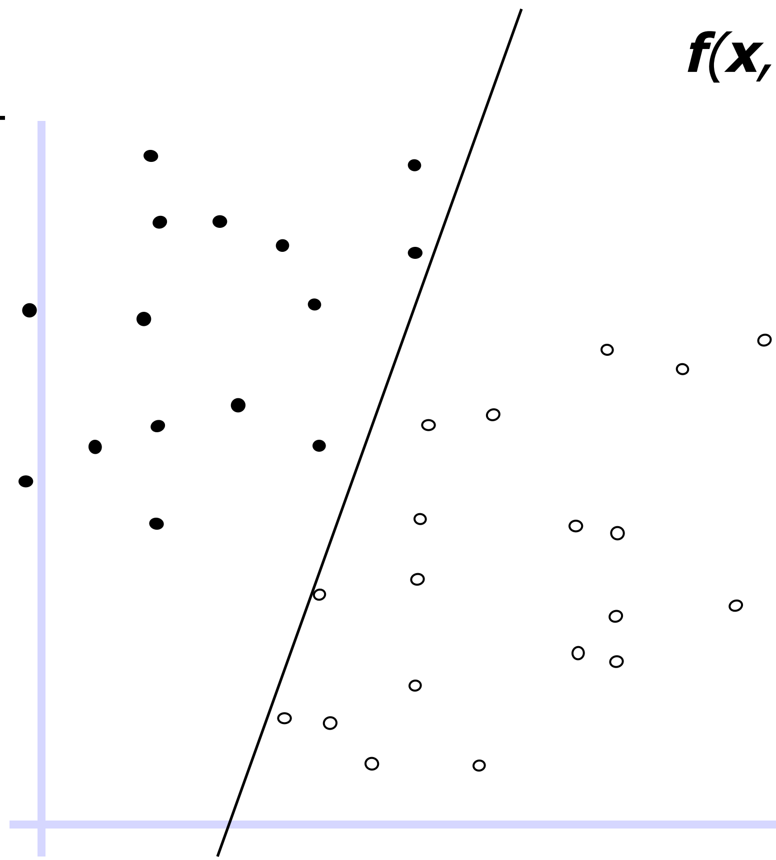

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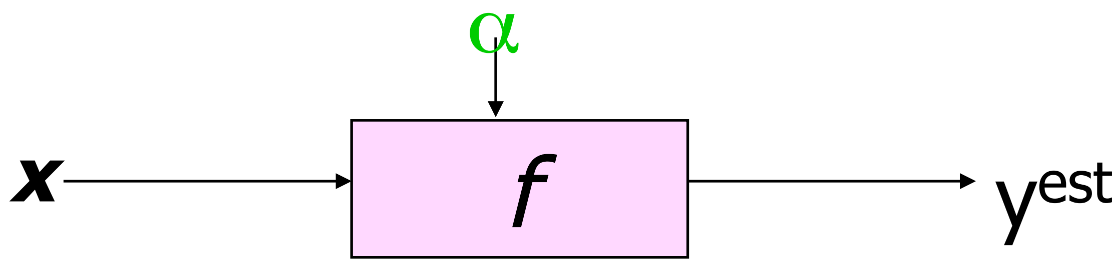

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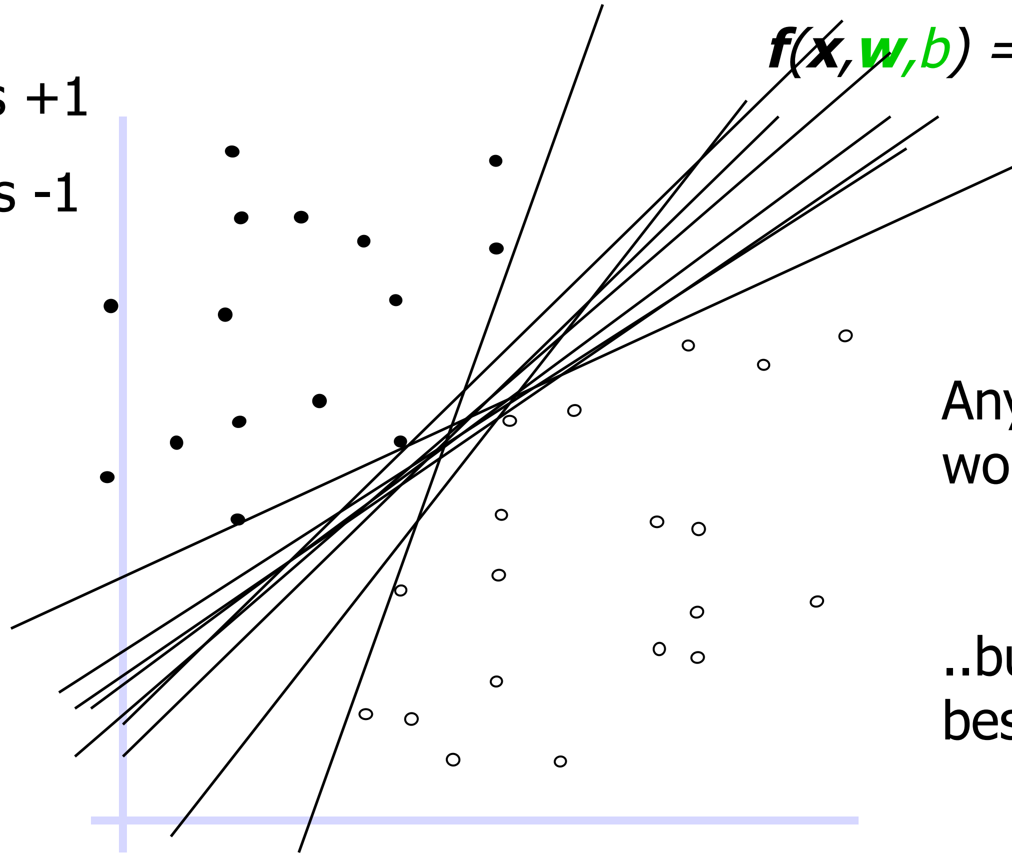
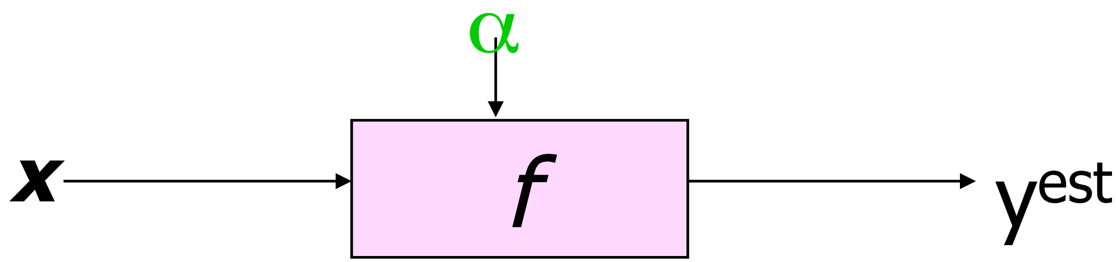


Any of these would be fine..

..but which is best?

Classifier Margin



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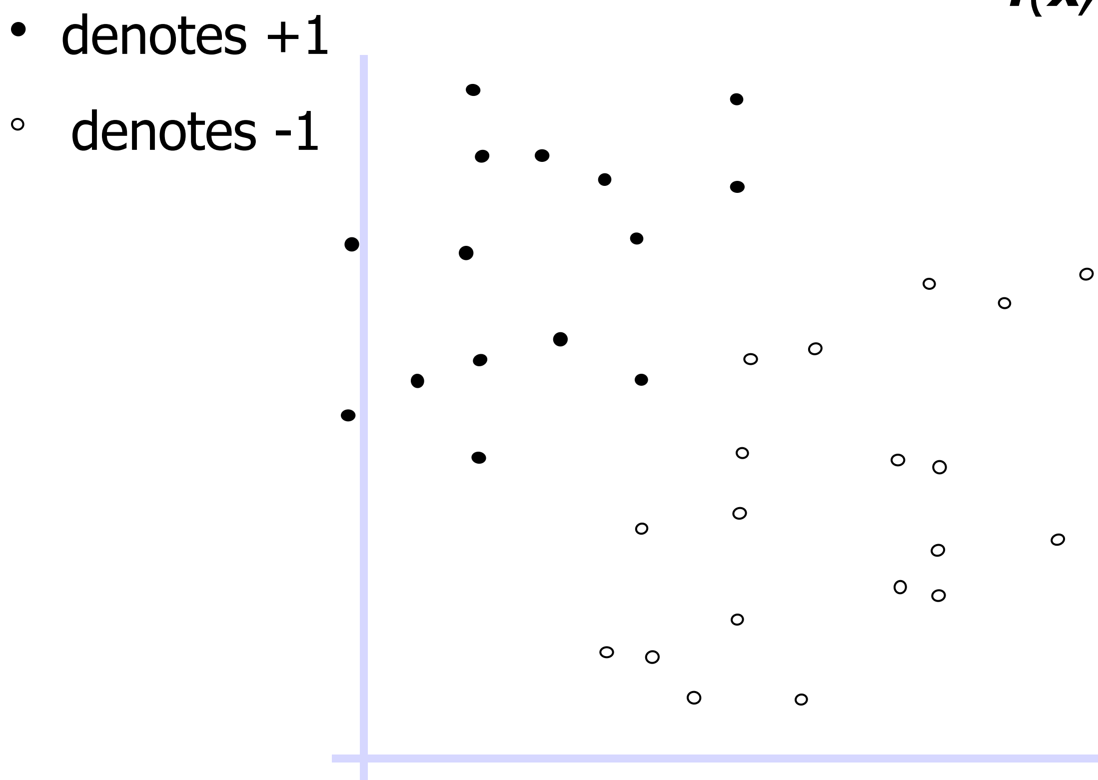
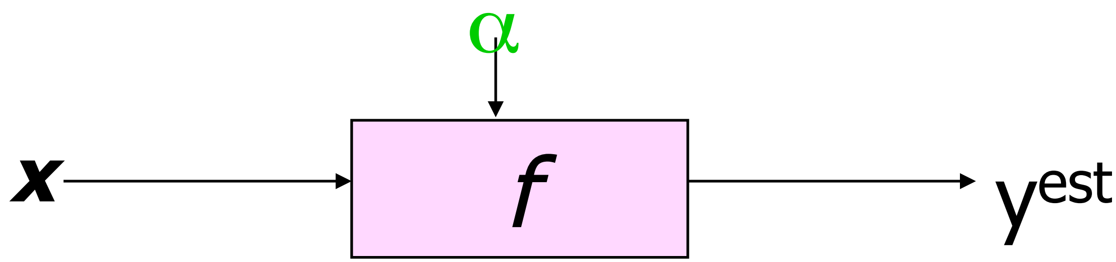


Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Maximum Margin



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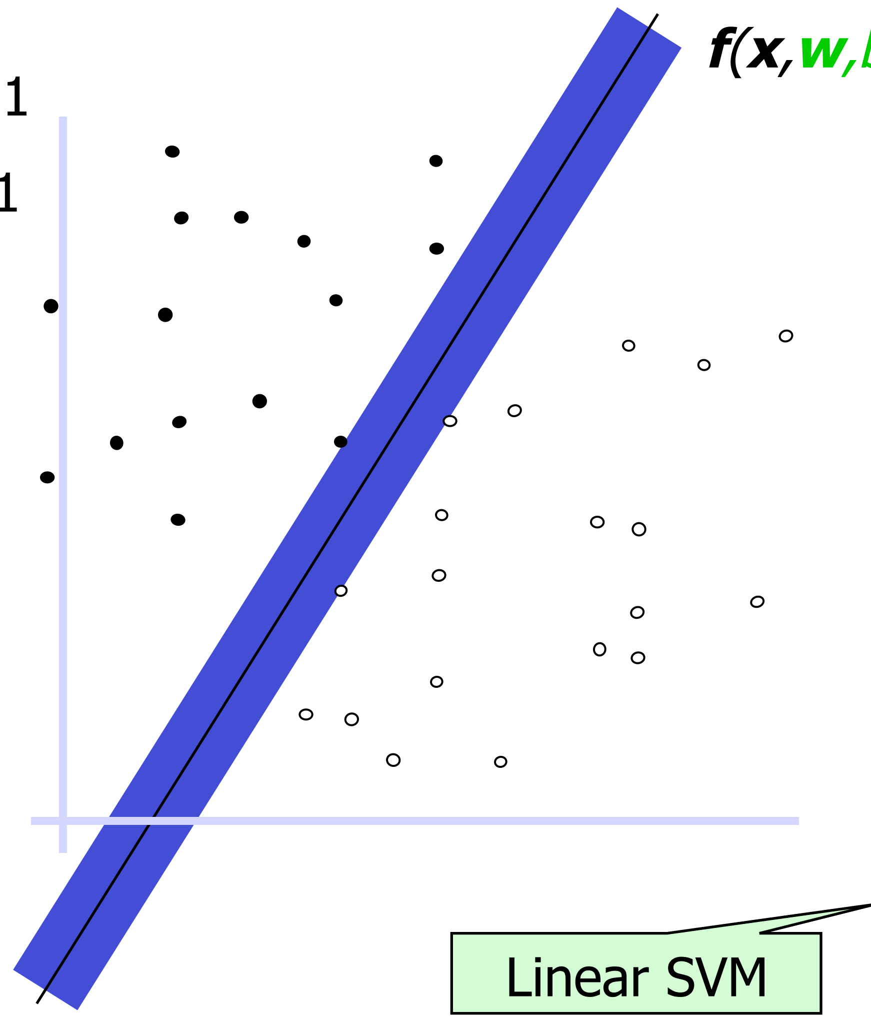
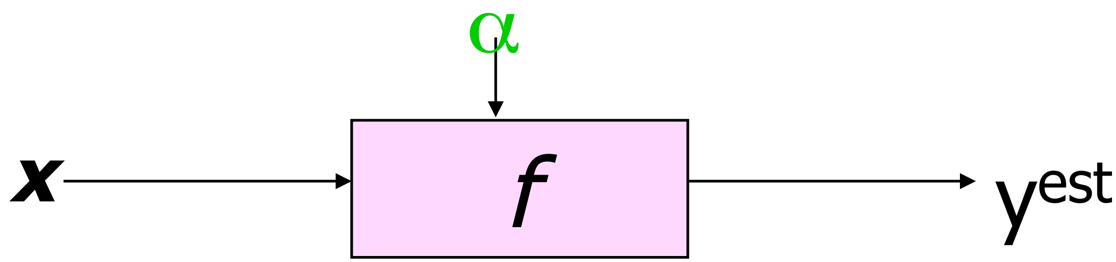


The maximum margin linear classifier is the linear classifier with maximum margin.

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

Maximum Margin



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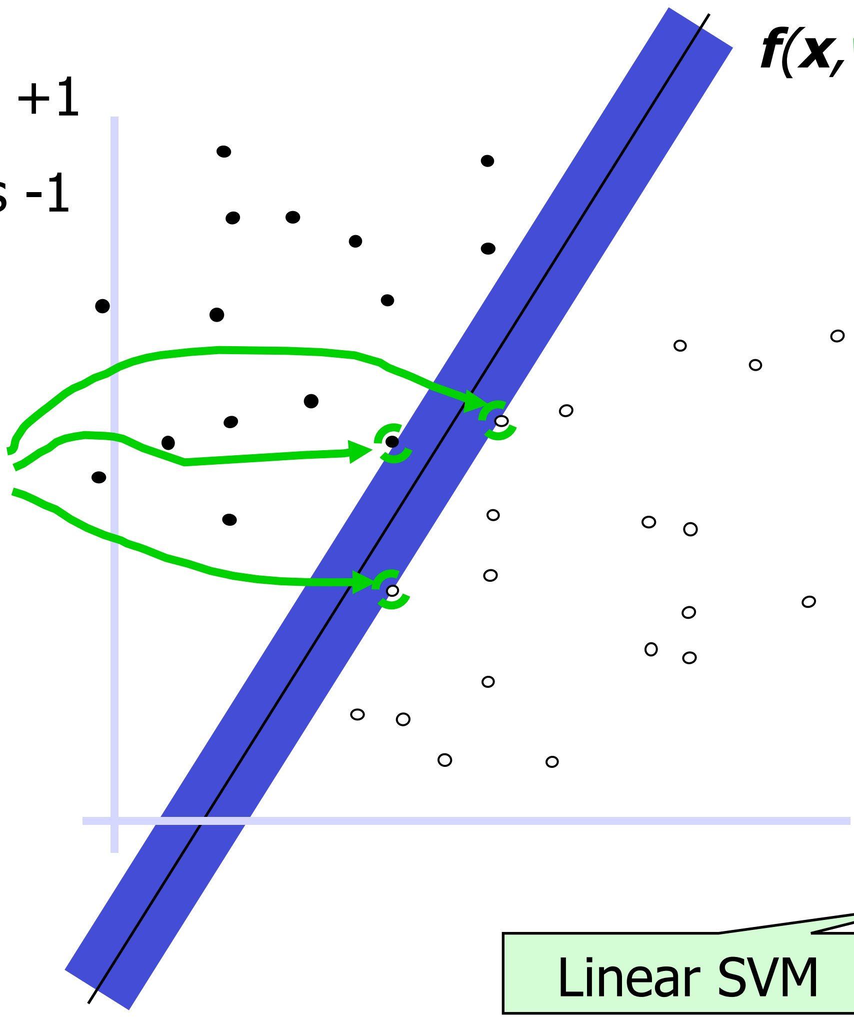

Support Vectors are those datapoints that the margin pushes up against

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

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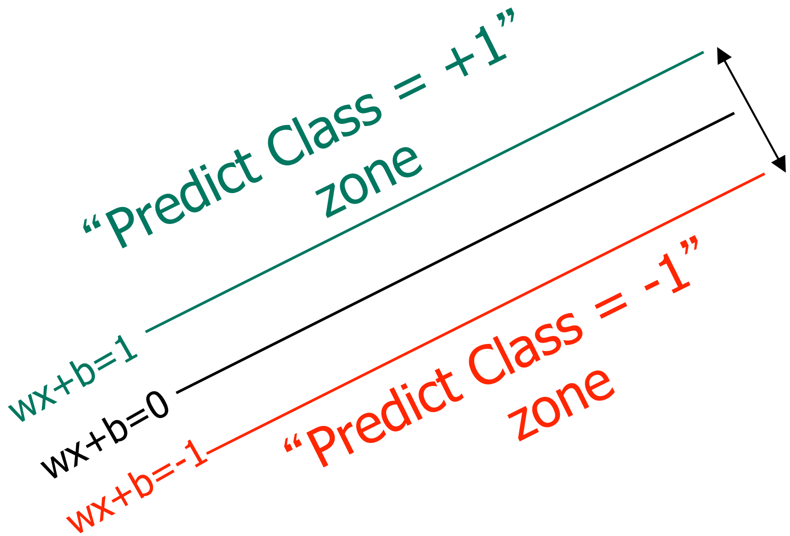
Linear SVM

Computing the margin width



M = Margin Width

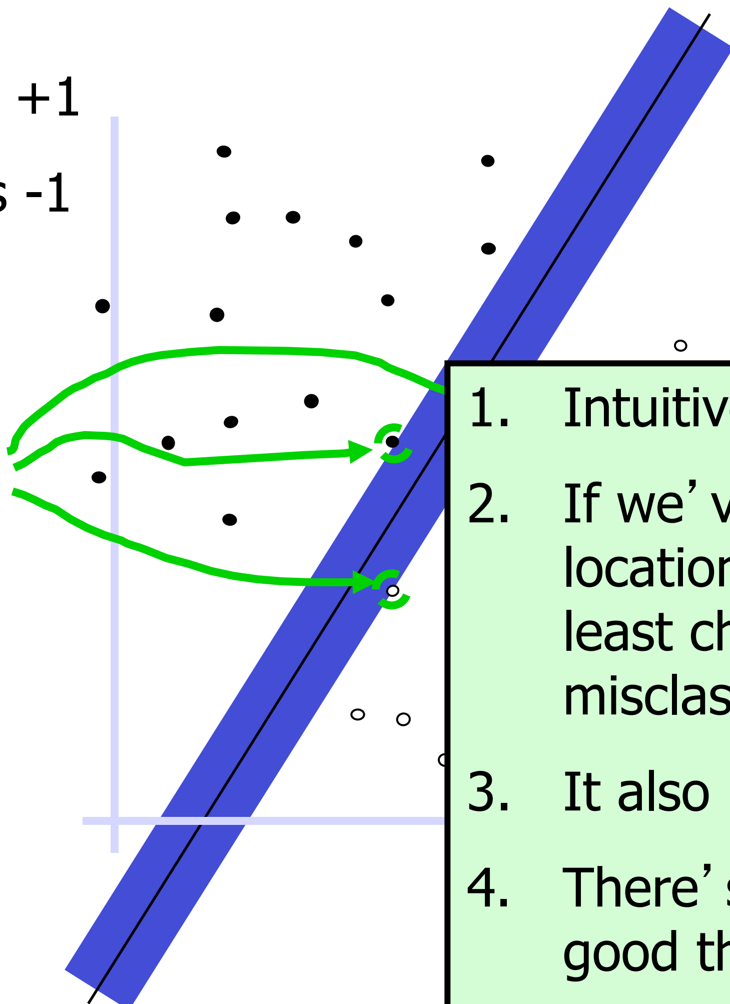
How do we compute M in terms of $\mathbf{w}$ and b?

- Plus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = +1 \}$
- Minus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = -1 \}$
- Margin M= $\dfrac{2}{\sqrt{\mathbf{w}.\mathbf{w}}}$

Why Maximum Margin?

• denotes +1

° denotes -1



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

The maximum margin linear classifier is the

Support Vectors are those datapoints that the margin pushes up against

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. It also helps generalization
4. There's some theory that this is a good thing.
5. Empirically it works very very well.

Another way to understand max margin

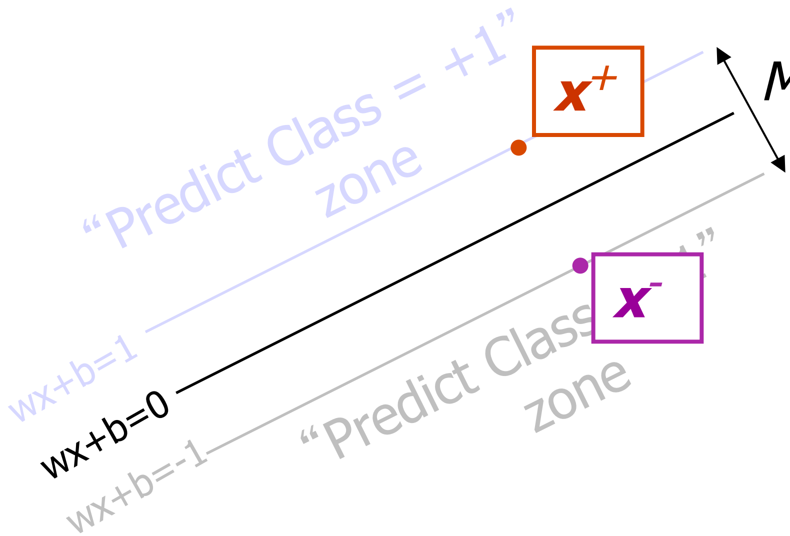
- For f(x)=w.x+b, one way to characterize the smoothness of f(x) is

$$\left|\frac{\partial f(x)}{\partial x}\right| = |w|$$

- Therefore, margin measures the smoothness of f(x).

- As a rule of thumb, machine learning prefers smooth functions: similar x's should have similar y's.

Learning the Maximum Margin Classifier



$$M = \text{Margin Width} = \frac{2}{\sqrt{\mathbf{w}.\mathbf{w}}}$$

Given a guess of ***w*** and *b* we can

- Compute whether all data points in the correct half-planes
- Compute the width of the margin

So now we just need to write a program to search the space of **w**' s and *b*' s to find the widest margin that matches all the data points. *How?*

Learning via Quadratic Programming

- QP is a well-studied class of optimization algorithms to maximize a quadratic function of some real-valued variables subject to linear constraints.

- Minimize both $w \cdot w$ (to maximize M) and misclassification error

Quadratic Programming

Find $\arg\max_{\mathbf{u}} \quad c + \mathbf{d}^T\mathbf{u} + \dfrac{\mathbf{u}^T R\mathbf{u}}{2}$ Quadratic criterion

Subject to

$$\left.\begin{aligned} a_{11}u_1 + a_{12}u_2 + \ldots + a_{1m}u_m &\le b_1 \\ a_{21}u_1 + a_{22}u_2 + \ldots + a_{2m}u_m &\le b_2 \\ &\vdots \\ a_{n1}u_1 + a_{n2}u_2 + \ldots + a_{nm}u_m &\le b_n \end{aligned}\right\}$$

n additional linear inequality constraints

And subject to

$$\left.\begin{aligned} a_{(n+1)1}u_1 + a_{(n+1)2}u_2 + \ldots + a_{(n+1)m}u_m &= b_{(n+1)} \\ a_{(n+2)1}u_1 + a_{(n+2)2}u_2 + \ldots + a_{(n+2)m}u_m &= b_{(n+2)} \\ &\vdots \\ a_{(n+e)1}u_1 + a_{(n+e)2}u_2 + \ldots + a_{(n+e)m}u_m &= b_{(n+e)} \end{aligned}\right\}$$

e additional linear equality constraints

Learning without Noise

What should our quadratic optimization criterion be?

Minimize $$\frac{1}{2}\mathbf{w}.\mathbf{w}$$

What constraints should be?

$$\boldsymbol{w} \,.\, \boldsymbol{x}_k + b >= 1 \text{ if } y_k = 1$$
$$\boldsymbol{w} \,.\, \boldsymbol{x}_k + b <= -1 \text{ if } y_k = -1$$

Solving the Optimization Problem

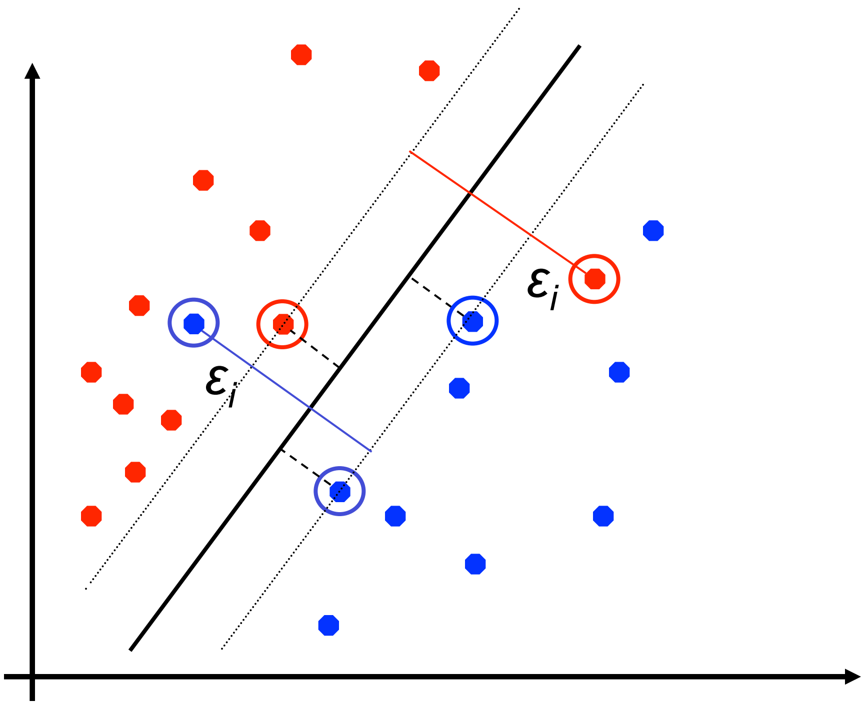
Find **w** and b such that
$\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ is minimized
and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i (\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

- Need to optimize a *quadratic* function subject to *linear* constraints.
- Quadratic optimization problems are a well-known class of mathematical programming problems for which several (non-trivial) algorithms exist.
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every inequality constraint in the primal (original) problem:

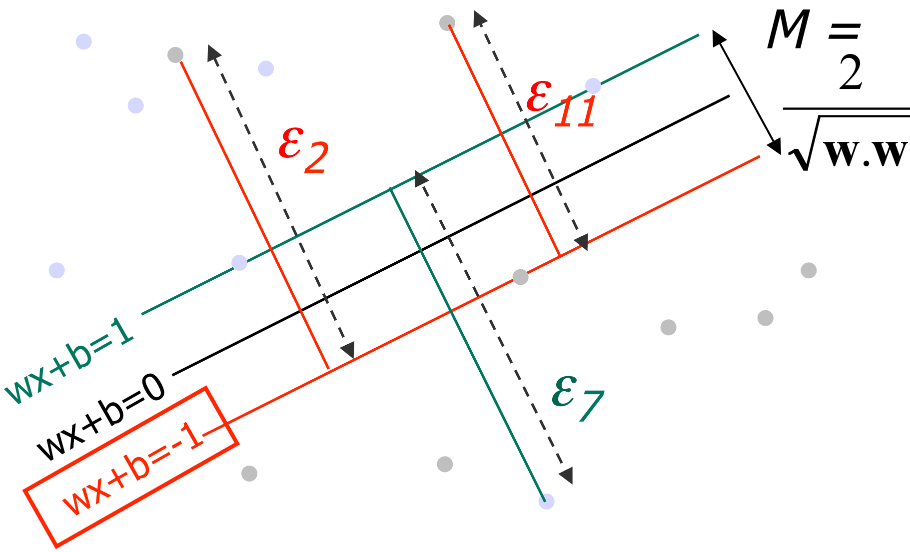
Find $\alpha_1 \dots \alpha_n$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

Soft Margin Classification

- What if the training set is not linearly separable?
- *Slack variables* ε_i can be added to allow misclassification of difficult or noisy examples, resulting so-called *soft margin*.



Learning Maximum Margin with Noise



Given guess of $\boldsymbol{w}$, b we can

- Compute sum of distances of points to their correct zones
- Compute the margin width

Assume R data points, each $(\boldsymbol{x}_k, y_k)$ where y_k = +/- 1

What should our quadratic optimization criterion be?

Minimize $$\frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$$

ε_k = distance of error points to their correct place

How many constraints will we have? *R*

What should they be?

$\boldsymbol{w} \cdot \boldsymbol{x}_k + b >= 1-\varepsilon_k$ if $y_k = 1$

$\boldsymbol{w} \cdot \boldsymbol{x}_k + b <= -1+\varepsilon_k$ if $y_k = -1$

$\varepsilon_k >= 0$ for all k

Soft Margin Classification Mathematically

- The old formulation:

> Find $\mathbf{w}$ and b such that
> $\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ is minimized
> and for all $(\mathbf{x}_i, y_i)$, i=1..n : $\quad y_i (\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

- Modified formulation incorporates slack variables:

> Find $\mathbf{w}$ and b such that
> $\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^T\mathbf{w} + C\Sigma\xi_i$ is minimized
> and for all $(\mathbf{x}_i, y_i)$, i=1..n : $\quad y_i (\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$

- Parameter C can be viewed as a way to control overfitting: it "trades off" the relative importance of maximizing the margin and fitting the training data.

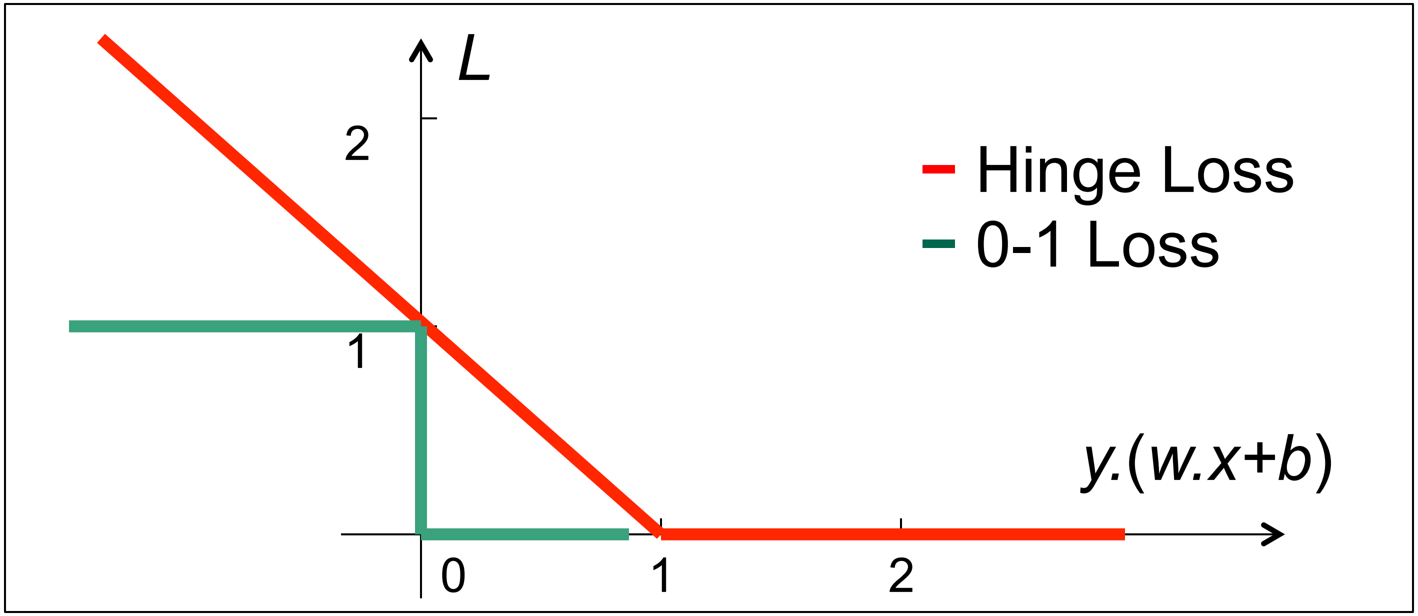
Hinge loss

- The soft margin SVM is equivalent to applying a hinge loss

$$L(w,b) := \sum_{i=1}^{n} \max(1 - y_i(w^T x_i + b), 0)$$

- Equivalent unconstrained optimization formulation

$$\min_{\{\mathbf{w},b\}} L(\mathbf{w},b)+\lambda||\mathbf{w}||^2 \qquad \lambda=0.5/C$$



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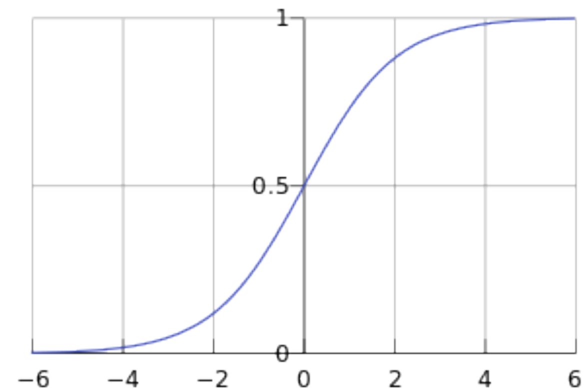
Logistic Regression

- Binary response: Y ={+1, -1}

$$Y_i | X_i \sim \text{Bernoulli}(p_i)$$

where p_i is the probability of Y_i=1

$$p_i = \frac{1}{1 + \exp(-W^T X_i)}$$



- Likelihood

$$\prod_{i=1}^{n} P(Y_i | X_i) = \prod_{i=1}^{n} \Big(\frac{1}{1 + \exp(-Y_i X_i^T W)} \Big)$$

Logistic regression

- Maximum likelihood estimator (MLE) becomes logistic regression

$$\min_W \sum_{i=1}^{n} - \ln p(Y_i|X_i) = \sum_{i=1}^{n} \ln(1 + \exp(Y_i X_i^T W))$$

- Convex optimization problem in terms of W

- MAP is regularized logistic regression

$$\min_W \sum_{i=1}^{n} \ln(1 + \exp(Y_i X_i^T W)) + \lambda \|W\|^2$$

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General formulation of linear classifiers

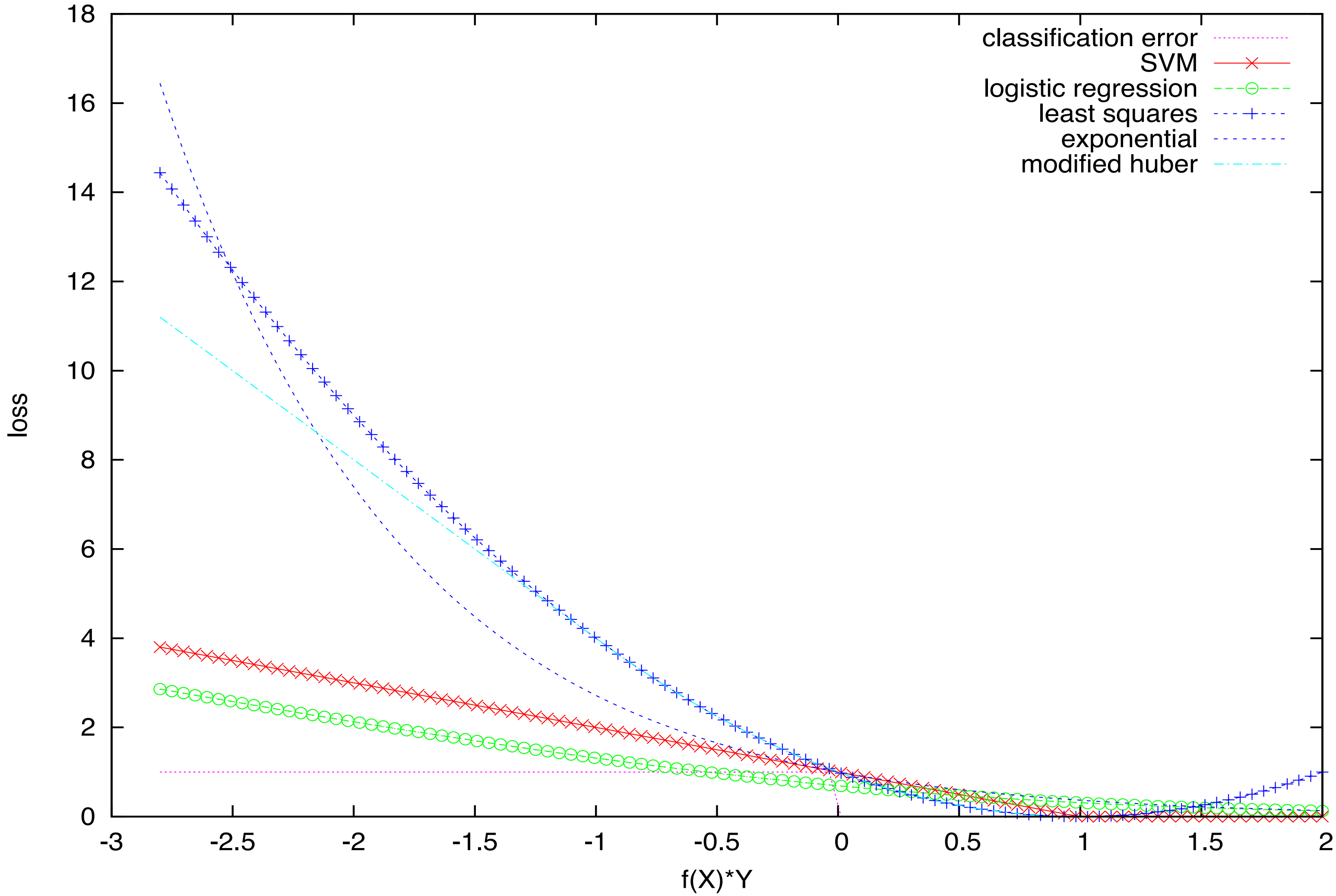
$$\min_{\{\mathbf{w},b\}} L(\mathbf{w},b)+\lambda||\mathbf{w}||^2$$

- The objective: empirical loss + regularization

- The regularization term is usually *L2* norm, but also often *L1* norm for sparse models

- The empirical loss can be hinge loss, logistic loss, smooth hinge loss, … or your own invention

Different loss functions



Comments on linear classifiers

- Choosing logistic regression or SVM?
  – Not that big different!
  – Logistic regression outputs probabilities.
- Smooth loss functions, e.g. logistic
  – Easier to optimize (LBFGS …)
  – Hinge → Differentiable hinge, then you can easily have your own implementation of SVMs
- Try different loss functions and regularization terms
  – Depend on data, e.g., many outliers? Irrelevant features? structure in output?

Linear classifiers in practice and research

- Linear classifiers are simple and scalable
  - Training complexity is linear or sub-linear w.r.t. data size
  - Classification is simple to implement
  - State-of-the-art for texts, images, …

- Their success depends on quality of features
  - A useful practice: use a lot of features, learn sparse w

- Hot topic: large-scale linear classification
  - Many data, many features, many classes
  - Stochastic optimization
  - Parallel implementation