

Support Vector Machine

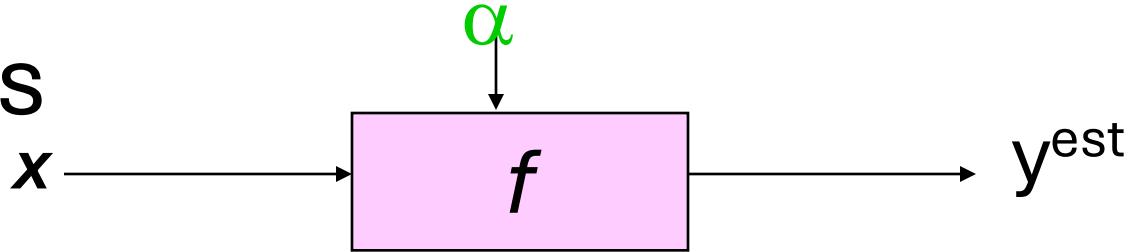
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Department of Computational Mathematics

University of Moratuwa

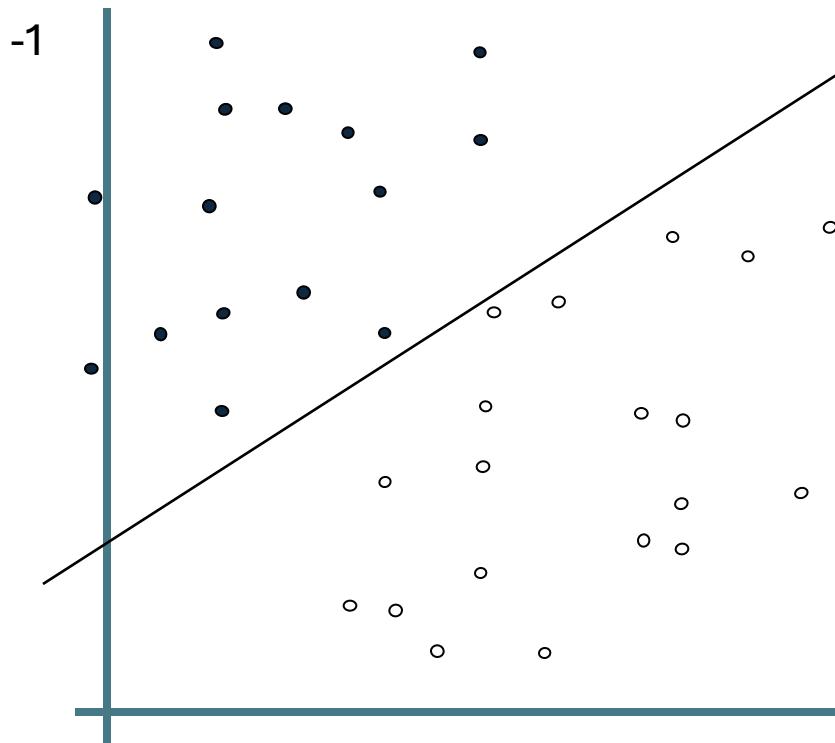
Linear Classifiers



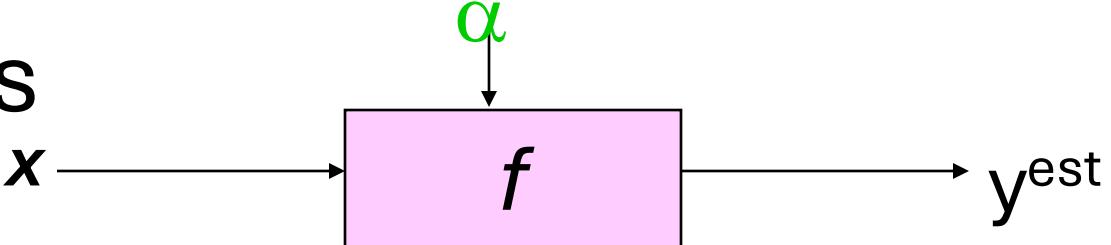
- denotes +1
- denotes -1

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

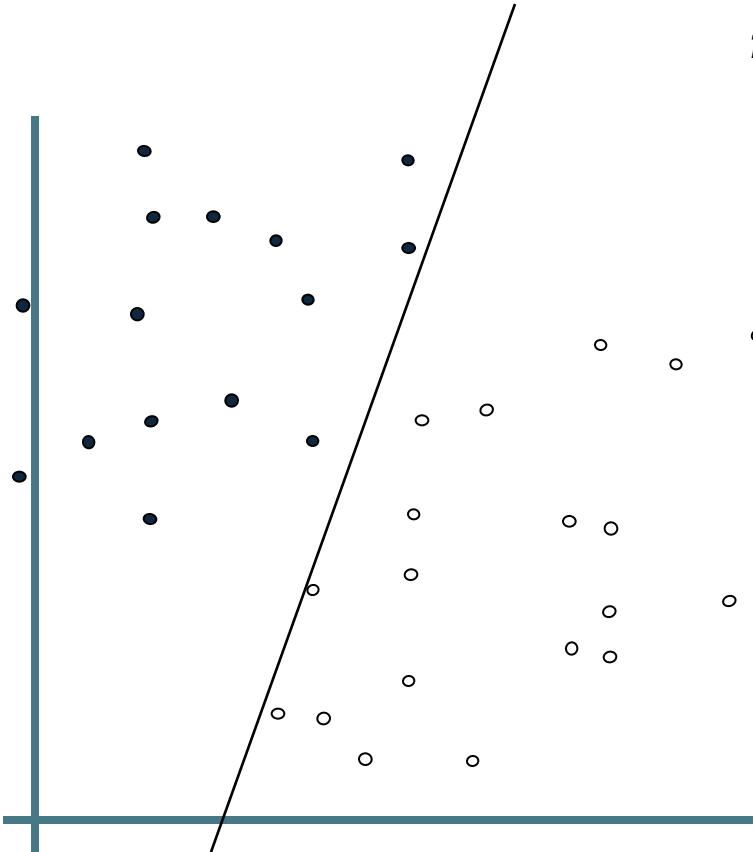
How would you
classify this data?



Linear Classifiers



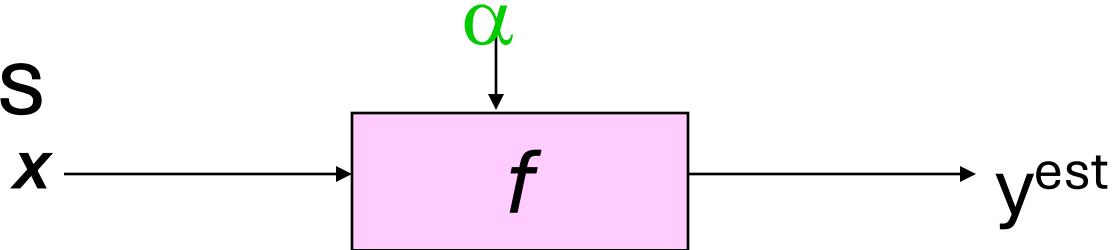
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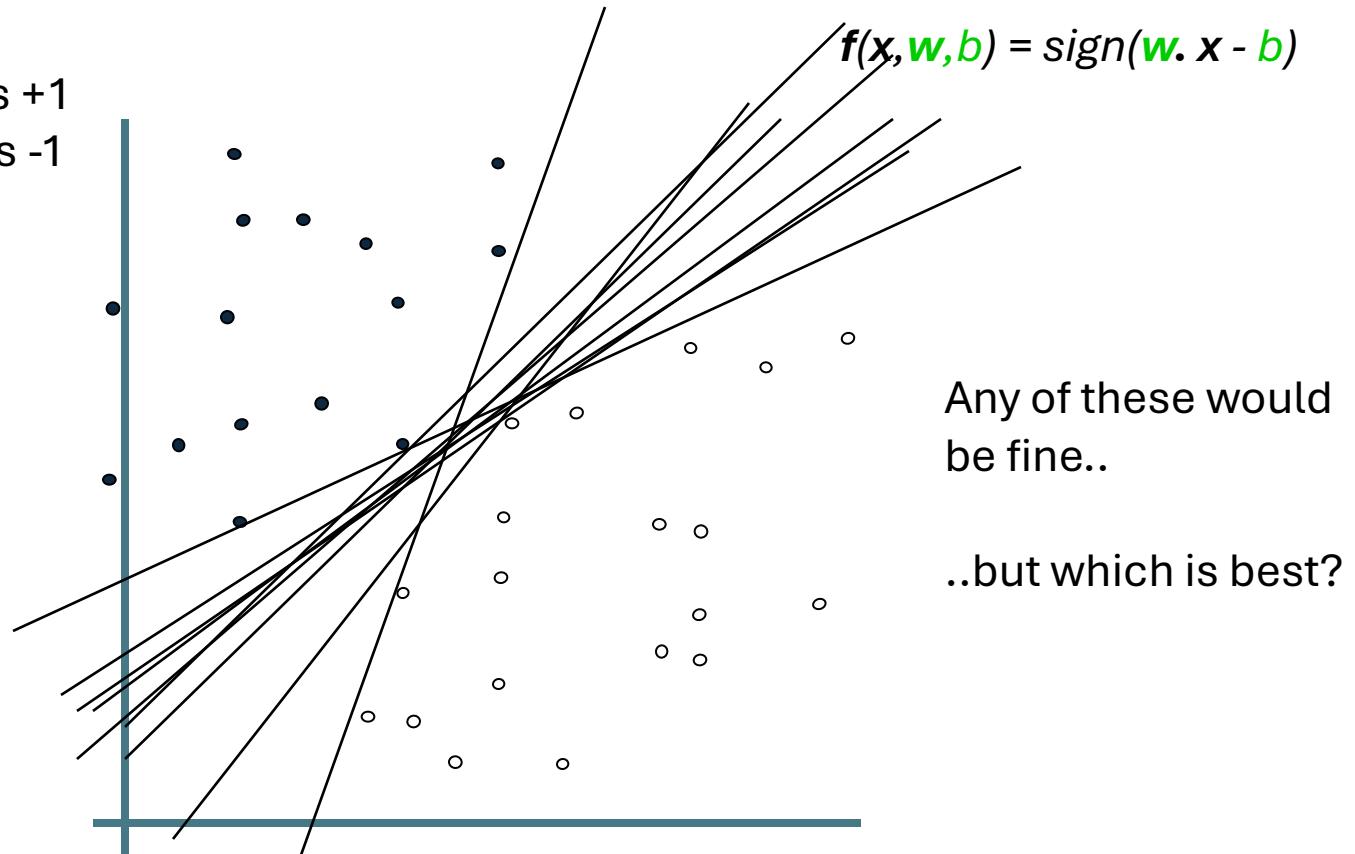
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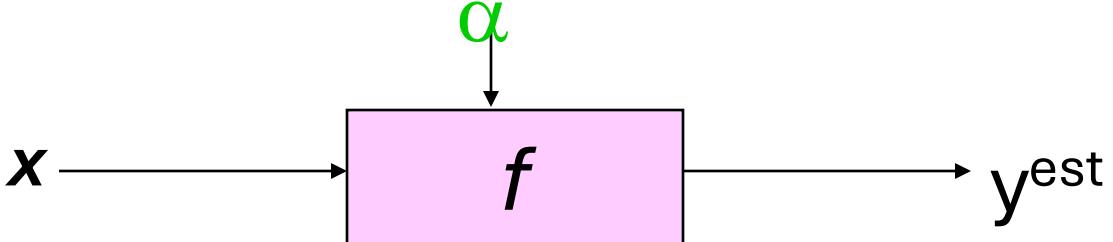
Linear Classifiers



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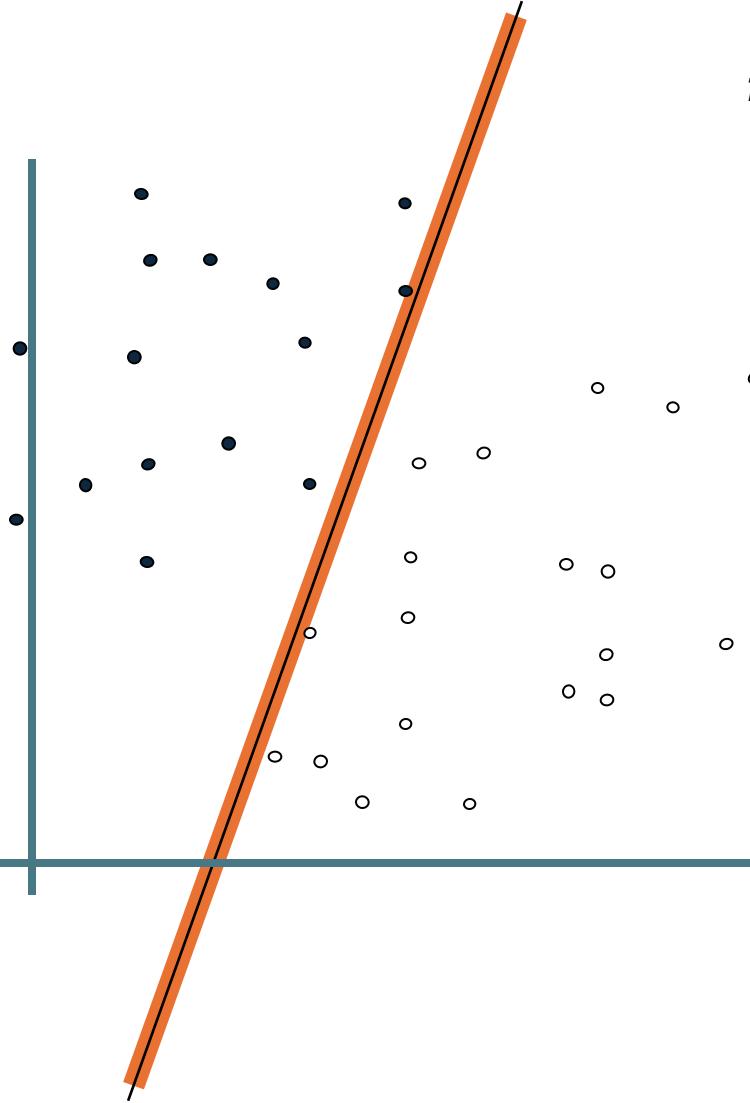


Classifier Margin



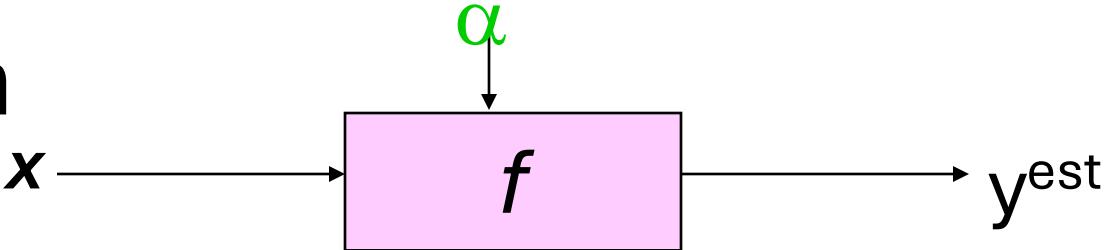
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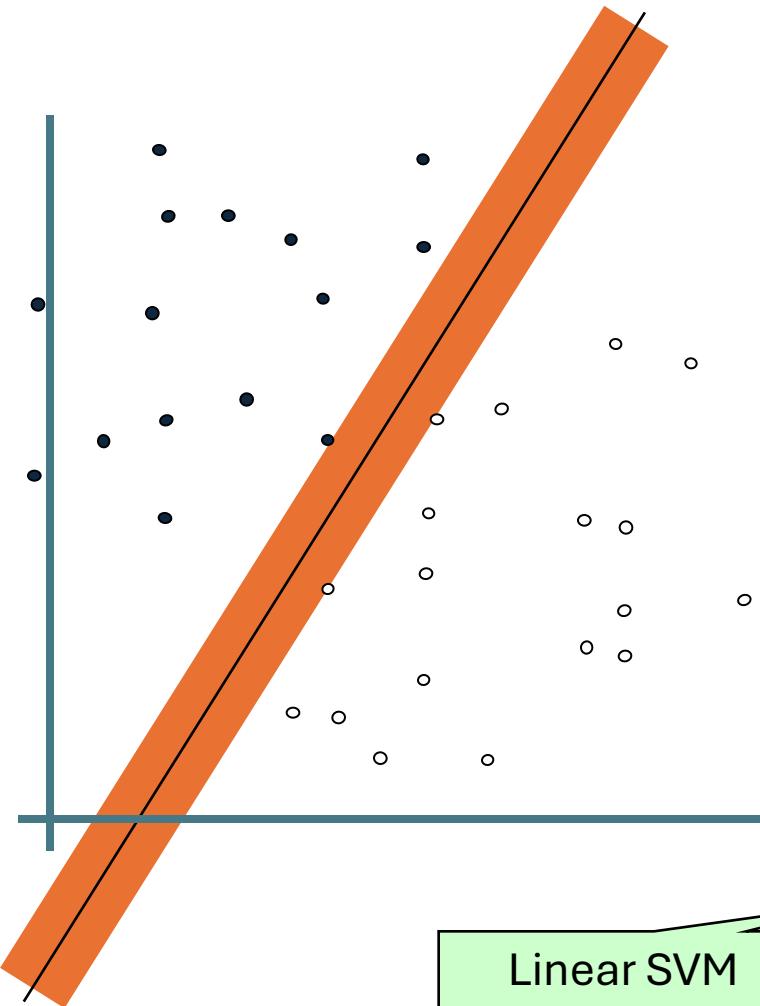


Define the **margin** of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Maximum Margin



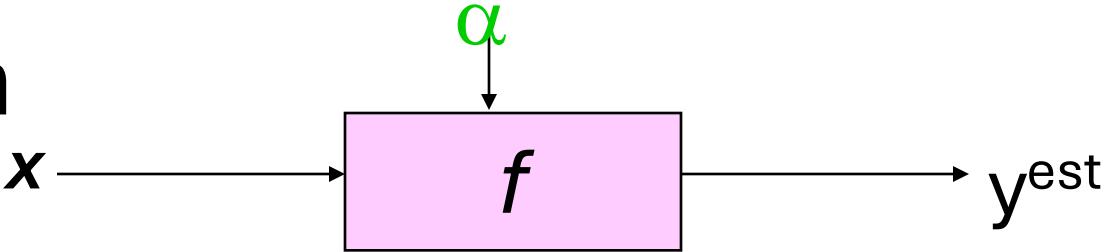
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$$f(x, \mathbf{w}, b) = \text{sign}(\mathbf{w} \cdot \mathbf{x} - b)$$

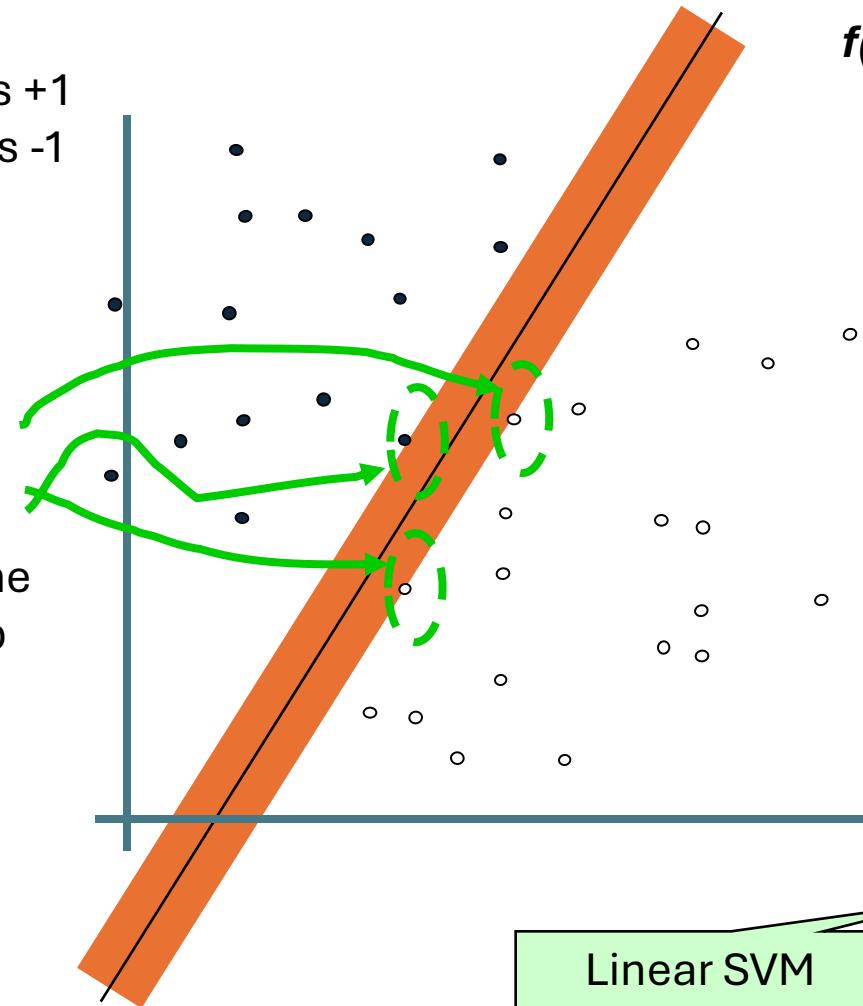
The maximum margin linear classifier is the linear classifier with the, um, maximum margin. This is the simplest kind of SVM (Called an LSVM)

Maximum Margin



- denotes +1
- denotes -1

Support Vectors
are those
datapoints that the
margin pushes up
against



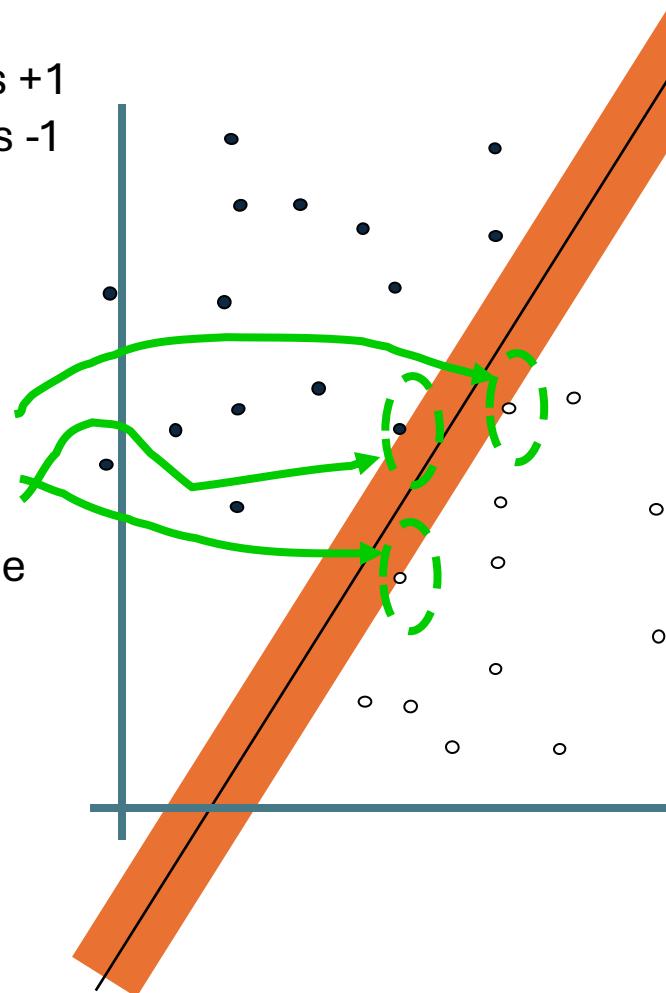
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Why Maximum Margin?

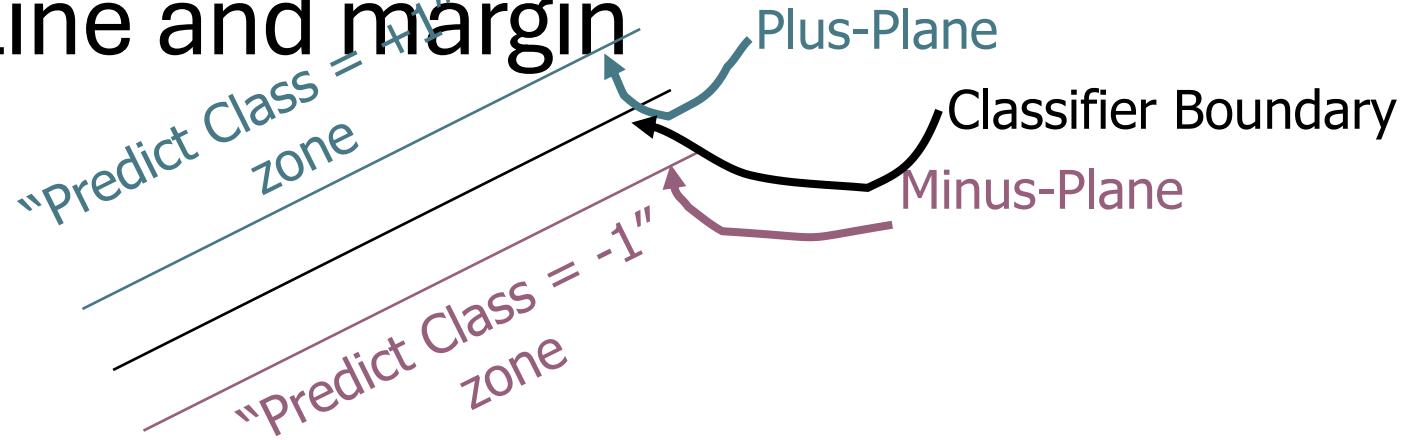
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Support Vectors
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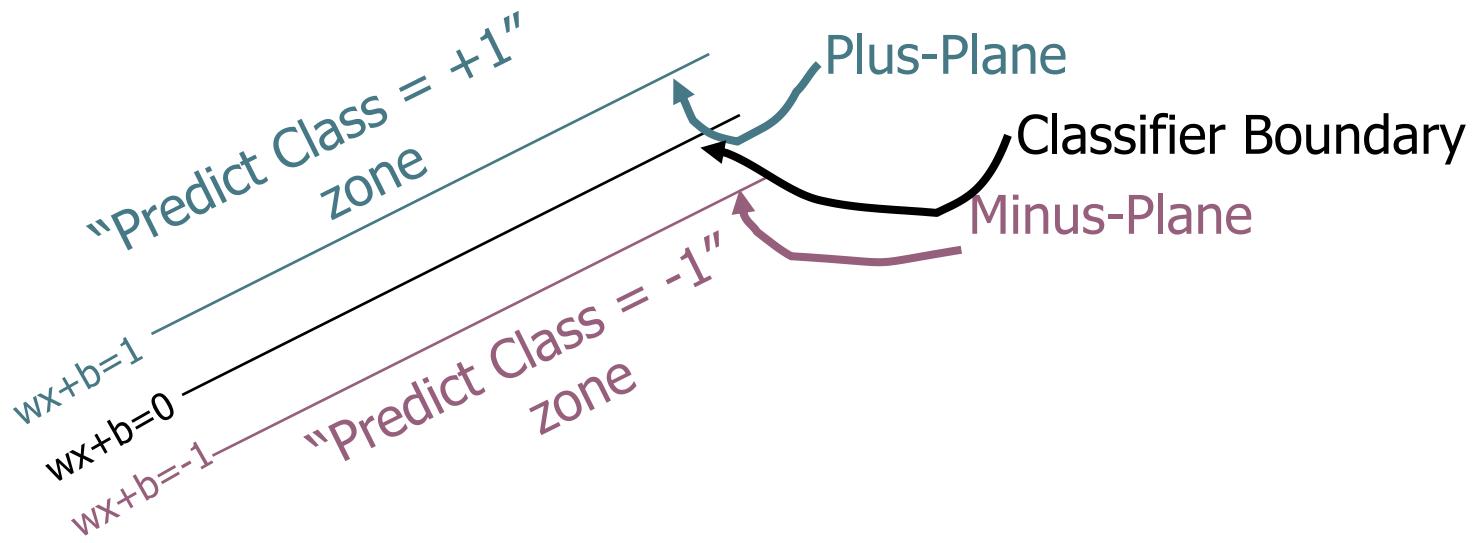
1. Intuitively this feels safest.
2. If we've made a small error in the location of the boundary (it's been jolted in its perpendicular direction) this gives us least chance of causing a misclassification.
3. LOOCV is easy since the model is immune to removal of any non-support-vector datapoints.
4. There's some theory (using VC dimension) that is related to (but not the same as) the proposition that this is a good thing.
5. Empirically it works very very well.

Specifying a line and margin



- How do we represent this mathematically?
- ...in m input dimensions?

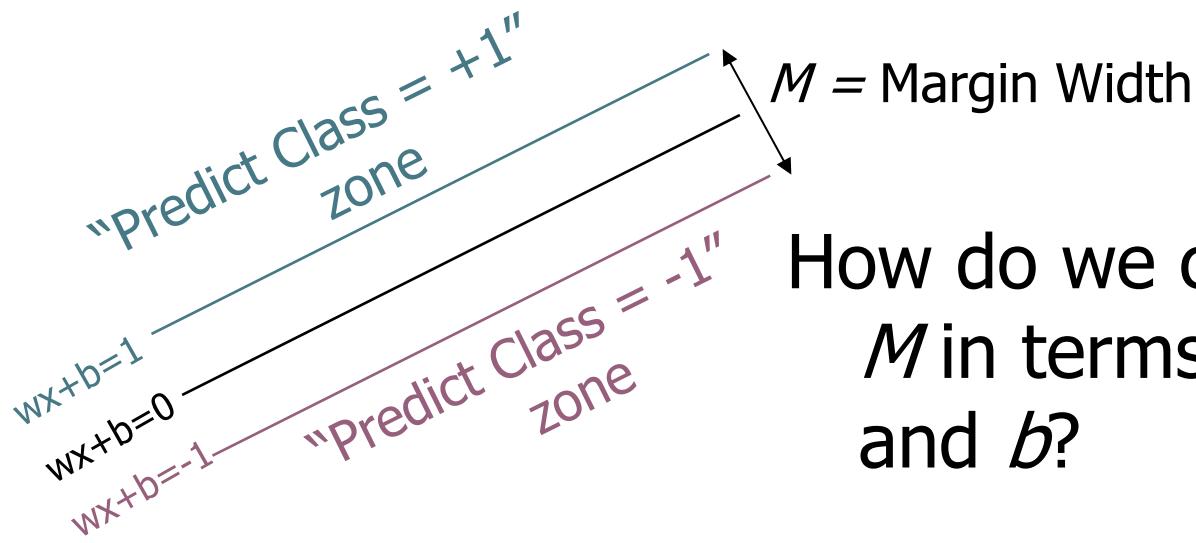
Specifying a line and margin



- Plus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = +1 \}$
- Minus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = -1 \}$

Classify as..	+1	if	$\mathbf{w} \cdot \mathbf{x} + b \geq 1$
	-1	if	$\mathbf{w} \cdot \mathbf{x} + b \leq -1$
	Universe explodes	if	$-1 < \mathbf{w} \cdot \mathbf{x} + b < 1$

Computing the margin width

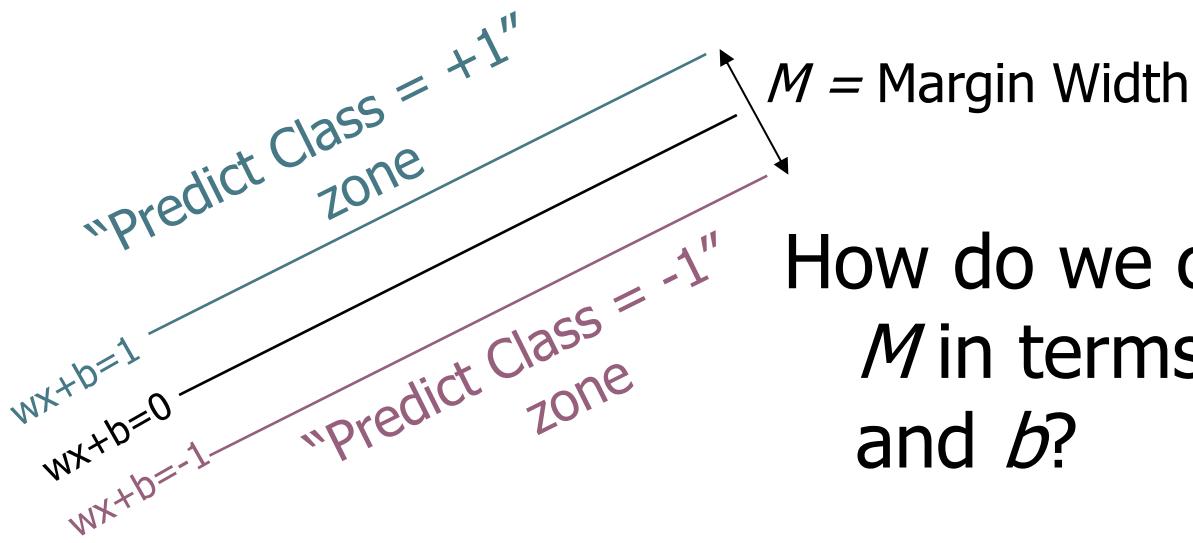


How do we compute
 M in terms of \mathbf{w}
and b ?

- Plus-plane = $\{ \mathbf{x} : \mathbf{w} \cdot \mathbf{x} + b = +1 \}$
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Claim: The vector \mathbf{w} is perpendicular to the Plus Plane. **Why?**

Computing the margin width



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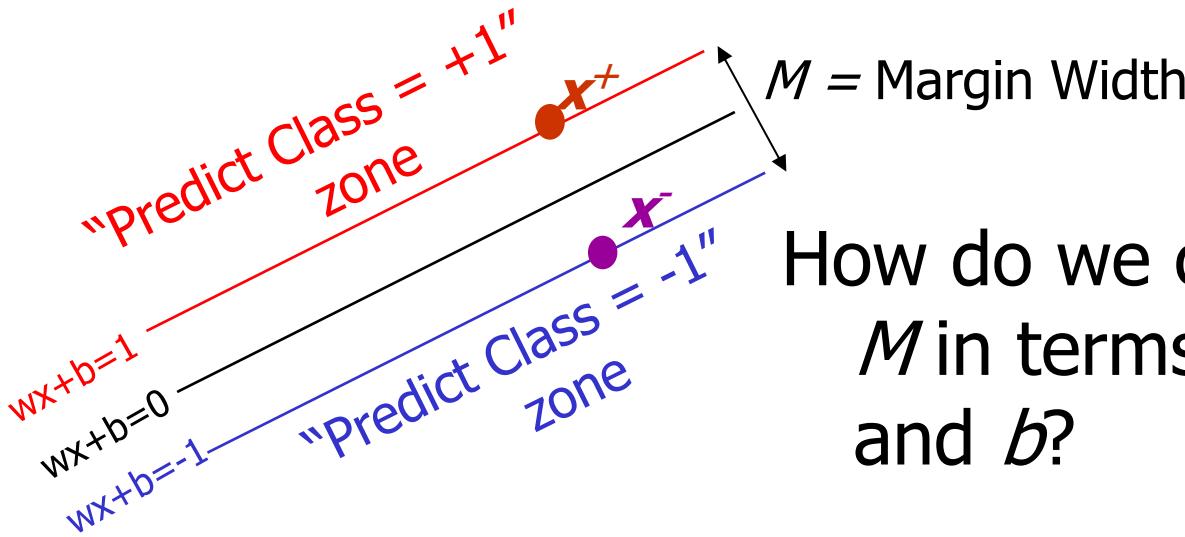
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Claim: The vector \mathbf{w} is perpendicular to the Plus Plane. **Why?**

Let \mathbf{u} and \mathbf{v} be two vectors on the
Plus Plane. What is $\mathbf{w} \cdot (\mathbf{u} - \mathbf{v})$?

And so of course the vector \mathbf{w} is also
perpendicular to the Minus Plane

Computing the margin width

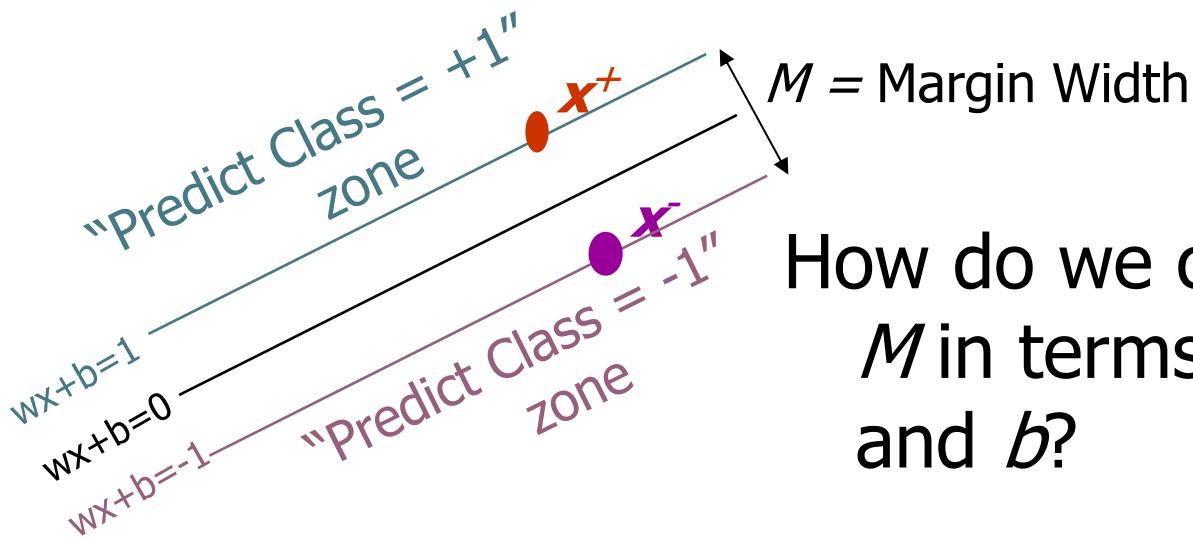


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- The vector \mathbf{w} is perpendicular to the Plus Plane
- Let \mathbf{x}^- be any point on the minus plane
- Let \mathbf{x}^+ be the closest plus-plane-point to \mathbf{x}^- .

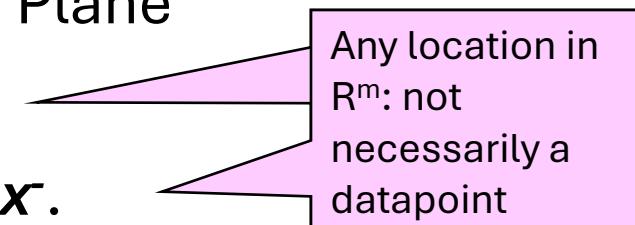
Any location in \mathbb{R}^m : not necessarily a datapoint

Computing the margin width

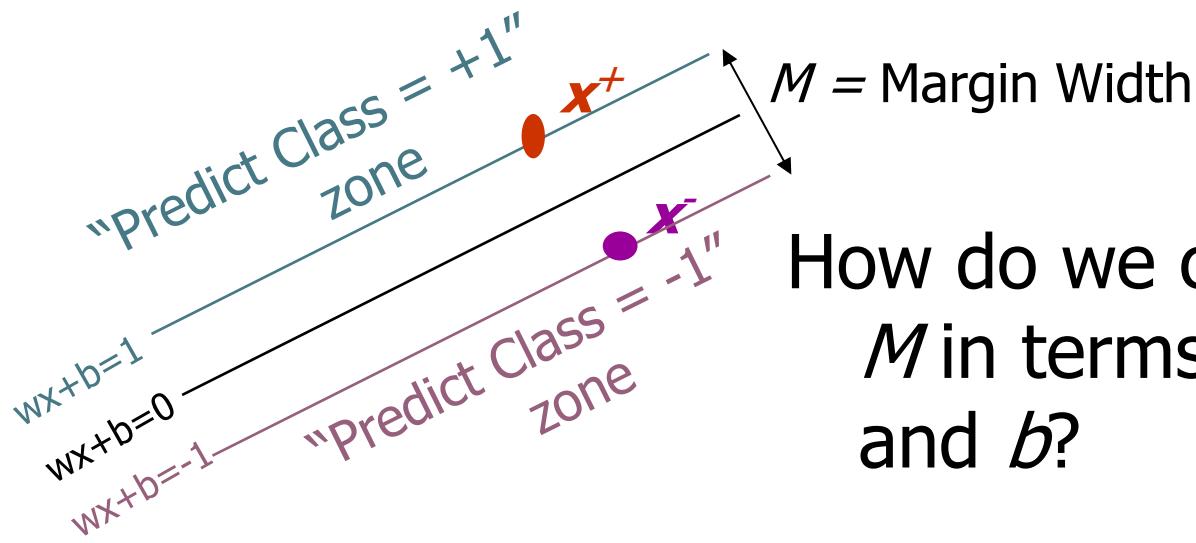


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Computing the margin width



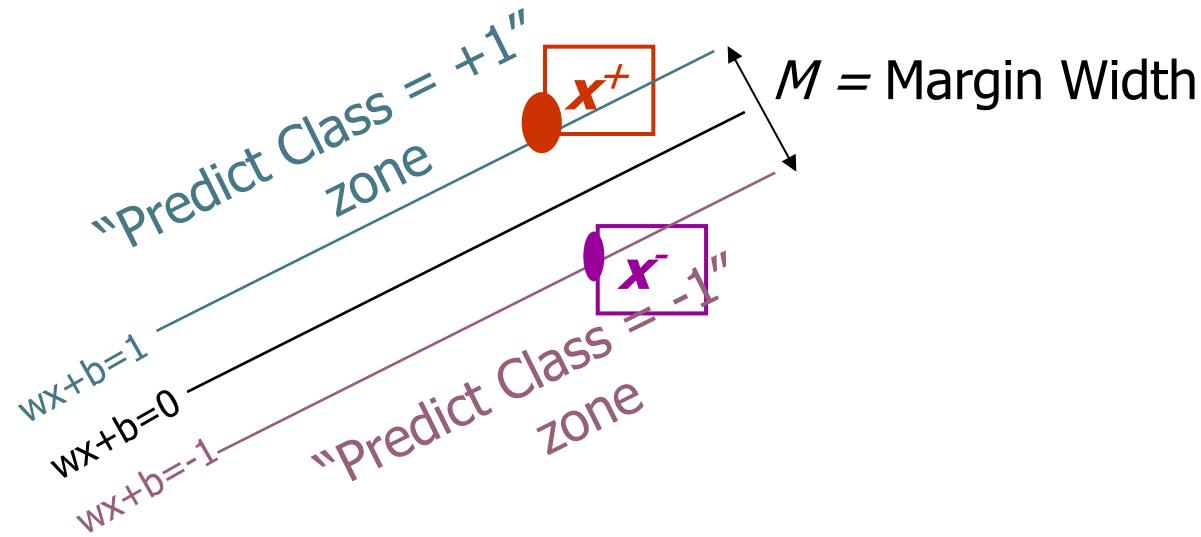
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- **Claim:** $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$ for some value of λ . **Why?**

Computing the margin width

-
- The diagram shows three parallel planes in a 2D space. The top plane is labeled $wx+b=1$, the middle plane is labeled $wx+b=0$, and the bottom plane is labeled $wx+b=-1$. A point x^- is on the bottom plane, and a point x^+ is on the top plane. A red line segment connects x^- and x^+ . This line segment is perpendicular to the planes. The distance between the planes is labeled $M = \text{Margin Width}$.
- Plus-plane = $\{x : \mathbf{w} \cdot \mathbf{x} + b = +1\}$
 - Minus-plane = $\{x : \mathbf{w} \cdot \mathbf{x} + b = -1\}$
 - The vector \mathbf{w} is perpendicular to the Plus Plane
 - Let \mathbf{x}^- be any point on the minus plane
 - Let \mathbf{x}^+ be the closest plus-plane-point to \mathbf{x}^- .
 - **Claim:** $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$ for some value of λ . **Why?**
- The line from \mathbf{x}^- to \mathbf{x}^+ is perpendicular to the planes.
- So to get from \mathbf{x}^- to \mathbf{x}^+ travel some distance in direction \mathbf{w} .

Computing the margin width

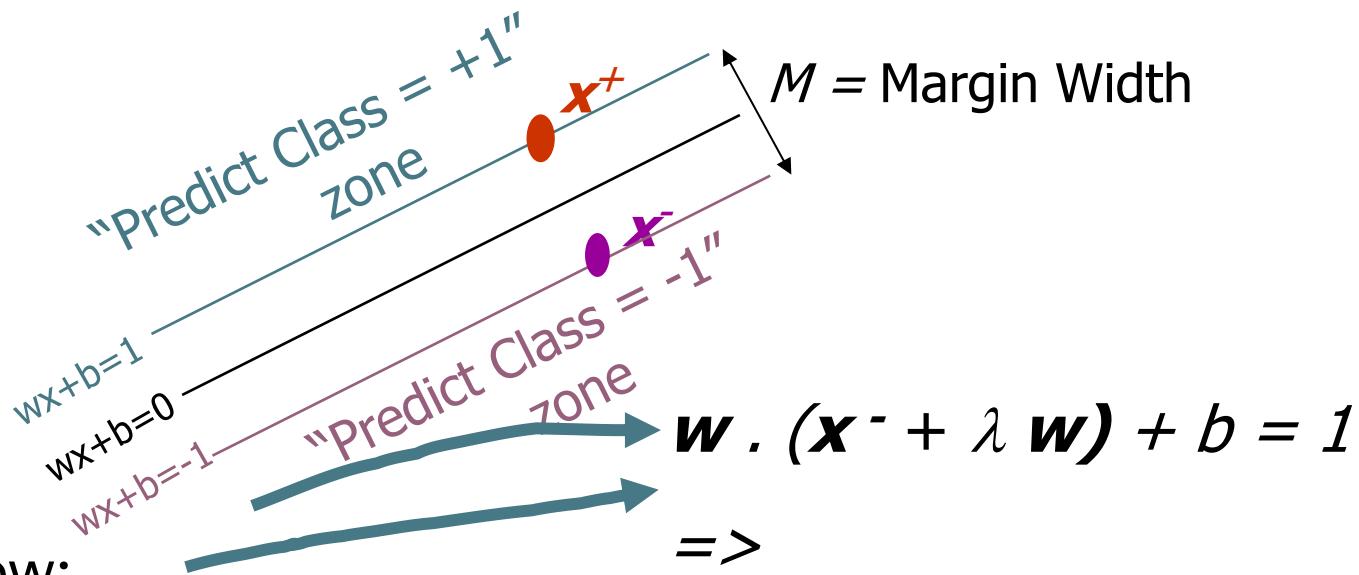


What we know:

- $\mathbf{w} \cdot \mathbf{x}^+ + b = +1$
- $\mathbf{w} \cdot \mathbf{x}^- + b = -1$
- $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$
- $|\mathbf{x}^+ - \mathbf{x}^-| = M$

It's now easy to get M
in terms of \mathbf{w} and b

Computing the margin width



What we know:

$$\bullet \quad w \cdot x^+ + b = +1$$

$$w \cdot x^- + b + \lambda w \cdot w = 1$$

$$\bullet \quad w \cdot x^- + b = -1$$

$$=>$$

$$\bullet \quad x^+ = x^- + \lambda w$$

$$-1 + \lambda w \cdot w = 1$$

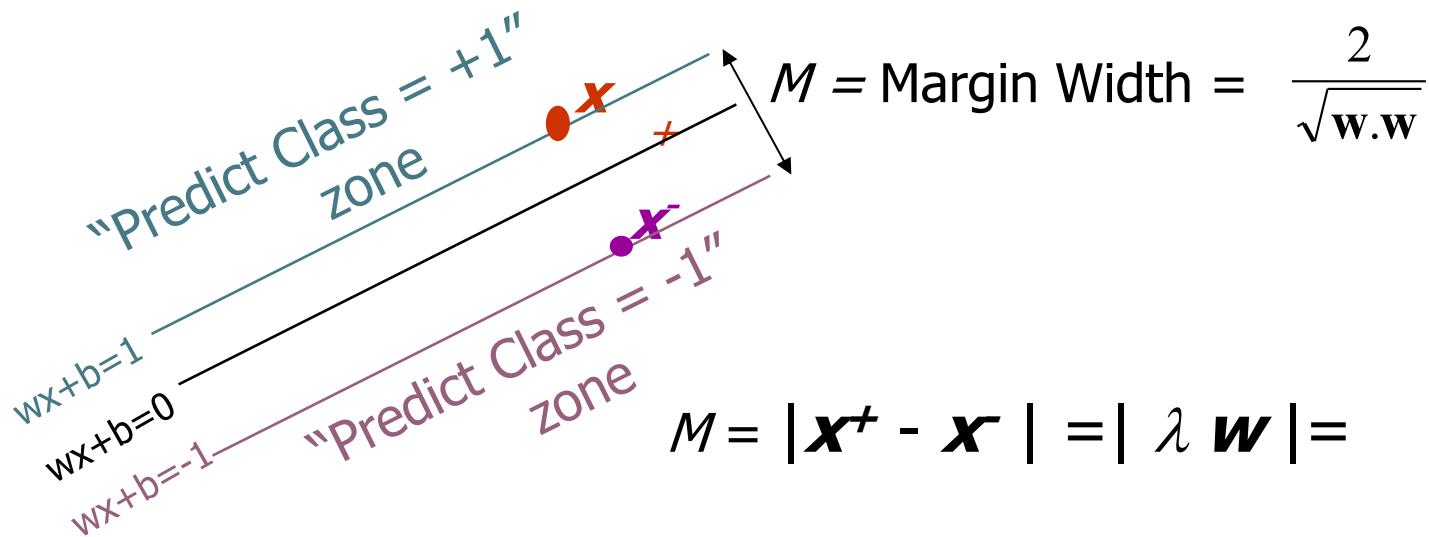
$$\bullet \quad |x^+ - x^-| = M$$

$$=>$$

It's now easy to get M
in terms of w and b

$$\lambda = \frac{2}{w \cdot w}$$

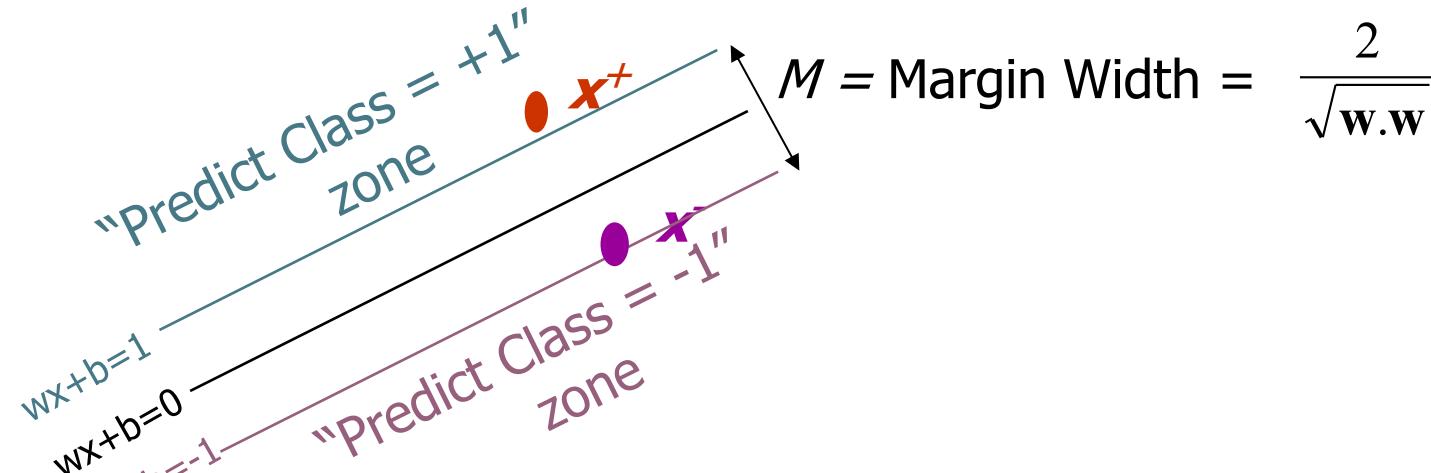
Computing the margin width



What we know:

- $\mathbf{w} \cdot \mathbf{x}^+ + b = +1$
- $\mathbf{w} \cdot \mathbf{x}^- + b = -1$
- $\mathbf{x}^+ = \mathbf{x}^- + \lambda \mathbf{w}$
- $|\mathbf{x}^+ - \mathbf{x}^-| = M$
- $\lambda = \frac{2}{\mathbf{w} \cdot \mathbf{w}}$

Learning the Maximum Margin Classifier



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 datapoints. *How?*

Gradient descent? Simulated Annealing? Matrix Inversion? EM?
Newton's Method?

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.

Quadratic Programming

Find $\arg \max_{\mathbf{u}} c + \mathbf{d}^T \mathbf{u} + \frac{\mathbf{u}^T R \mathbf{u}}{2}$

Quadratic criterion

Subject to

$$a_{11}u_1 + a_{12}u_2 + \dots + a_{1m}u_m \leq b_1$$

$$a_{21}u_1 + a_{22}u_2 + \dots + a_{2m}u_m \leq b_2$$

:

$$a_{n1}u_1 + a_{n2}u_2 + \dots + a_{nm}u_m \leq b_n$$

n additional linear
inequality
constraints

And subject to

$$a_{(n+1)1}u_1 + a_{(n+1)2}u_2 + \dots + a_{(n+1)m}u_m = b_{(n+1)}$$

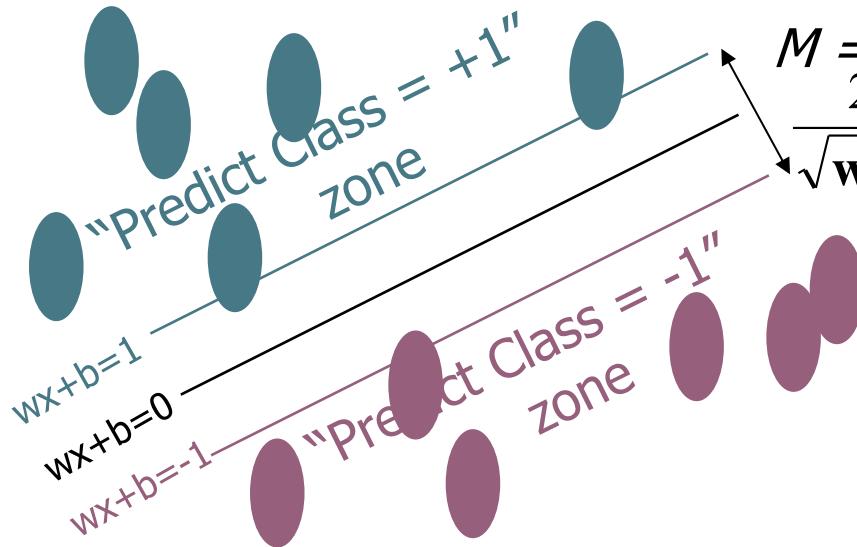
$$a_{(n+2)1}u_1 + a_{(n+2)2}u_2 + \dots + a_{(n+2)m}u_m = b_{(n+2)}$$

:

$$a_{(n+e)1}u_1 + a_{(n+e)2}u_2 + \dots + a_{(n+e)m}u_m = b_{(n+e)}$$

e additional linear
equality
constraints

Learning the Maximum Margin Classifier

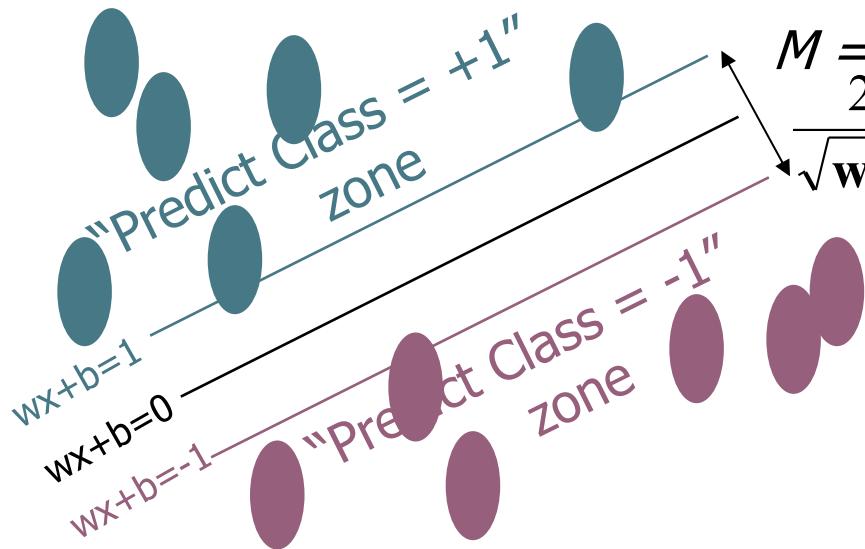


- Given guess of \mathbf{w} , b we can
- Compute whether all data points are in the correct half-planes
 - Compute the margin width
- Assume R datapoints, each (\mathbf{x}_k, y_k) where $y_k = +/- 1$

What should our quadratic optimization criterion be?

How many constraints will we have?
What should they be?

Learning the Maximum Margin Classifier



- Given guess of \mathbf{w} , b we can
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Assume R datapoints, each (\mathbf{x}_k, y_k) where $y_k = +/- 1$

What should our quadratic optimization criterion be?

Minimize $\mathbf{w} \cdot \mathbf{w}$

How many constraints will we have? R

What should they be?

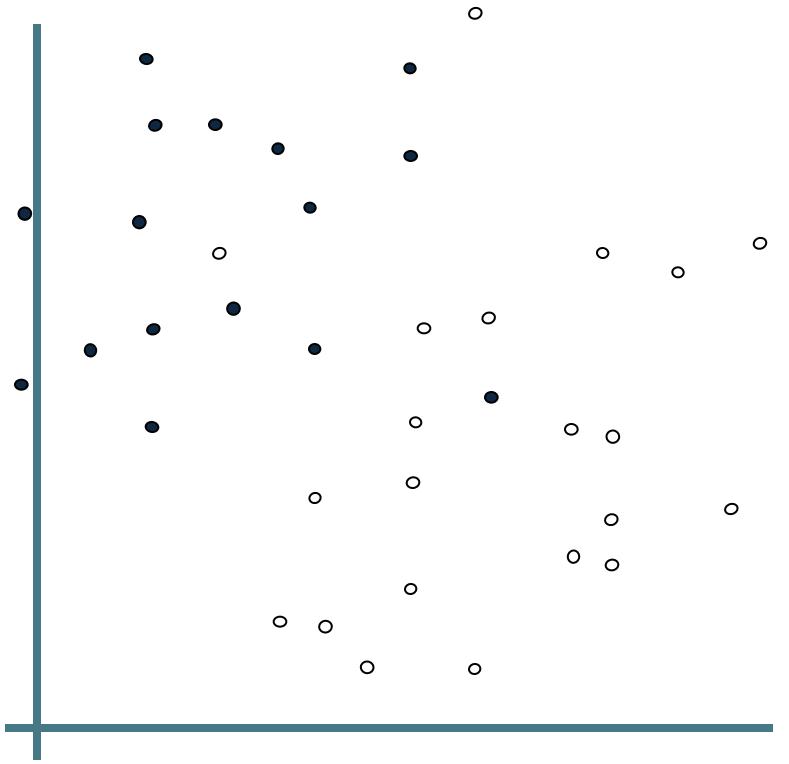
$$\mathbf{w} \cdot \mathbf{x}_k + b \geq 1 \text{ if } y_k = 1$$

$$\mathbf{w} \cdot \mathbf{x}_k + b \leq -1 \text{ if } y_k = -1$$

Uh-oh!

This is going to be a problem!
What should we do?

- denotes +1
- denotes -1



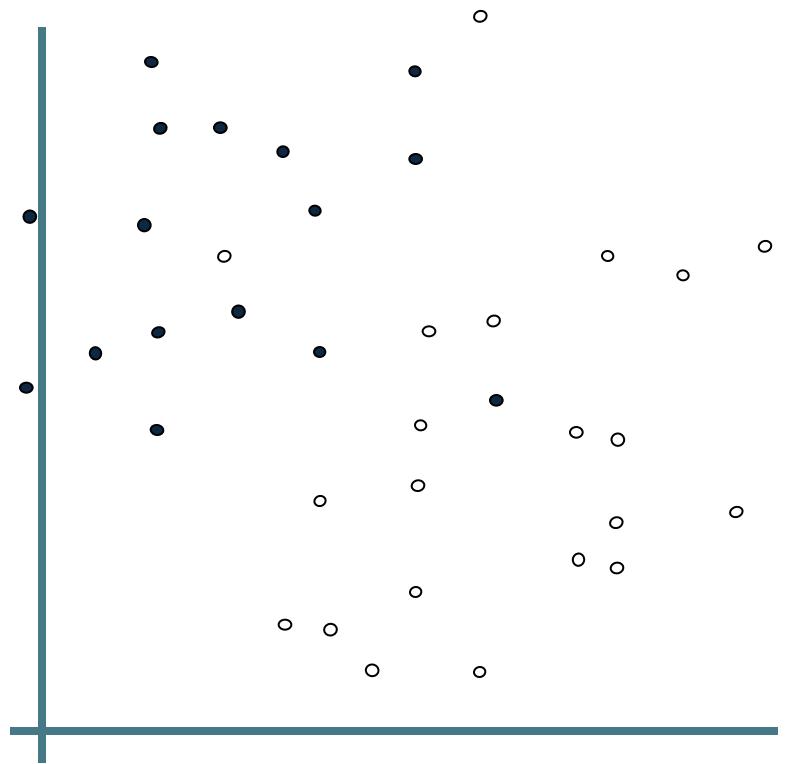
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What should we do?

Idea 1:

Find minimum $\mathbf{w} \cdot \mathbf{w}$, while
minimizing number of
training set errors.

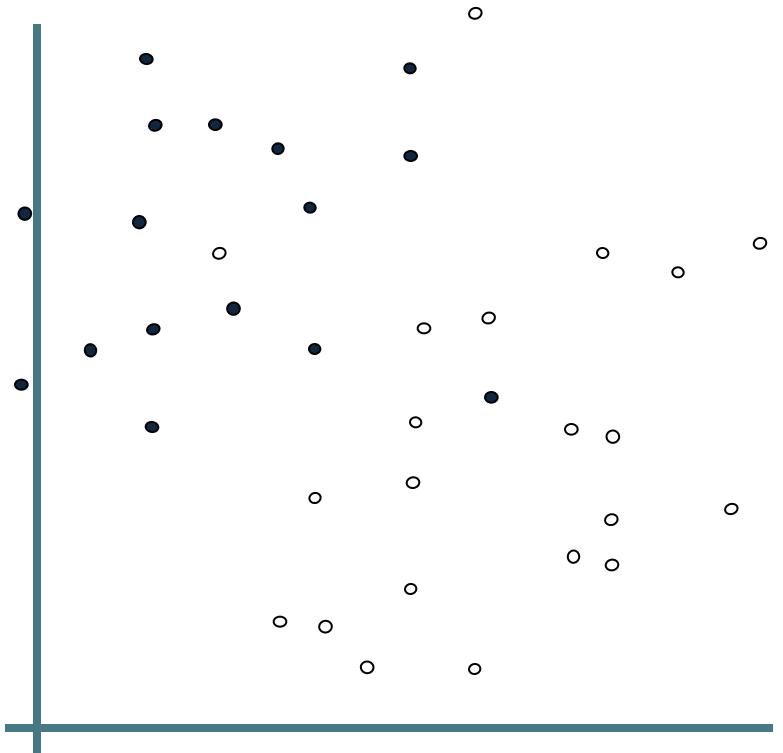
Problemette: Two things
to minimize makes for an
ill-defined optimization



- denotes +1
- denotes -1

Uh-oh!

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This is going to be a problem!
What should we do?

Idea 1.1:

Minimize
 $\mathbf{w} \cdot \mathbf{w} + C (\#\text{train errors})$

Tradeoff parameter

There's a serious practical problem that's about to make us reject this approach. Can you guess what it is?

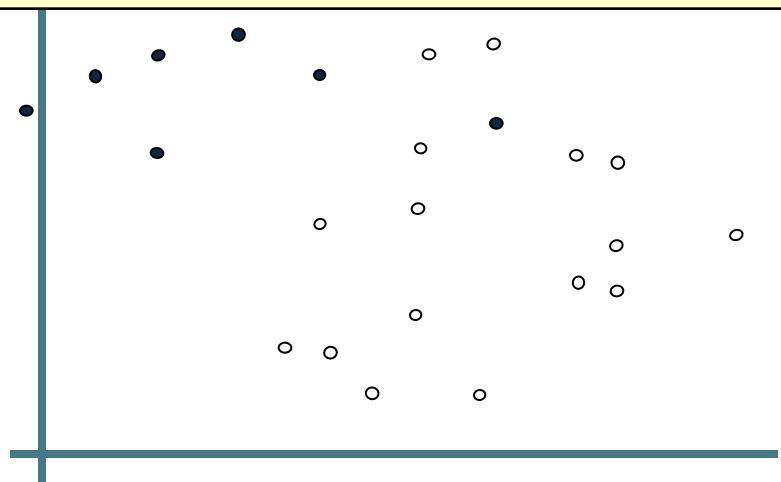
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Can't be expressed as a Quadratic Programming problem.

Solving it may be too slow.

(Also, doesn't distinguish between disastrous errors and near misses)



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Idea 1.1:

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$$\mathbf{w} \cdot \mathbf{w} + C (\#\text{train errors})$$

Tradeoff parameter

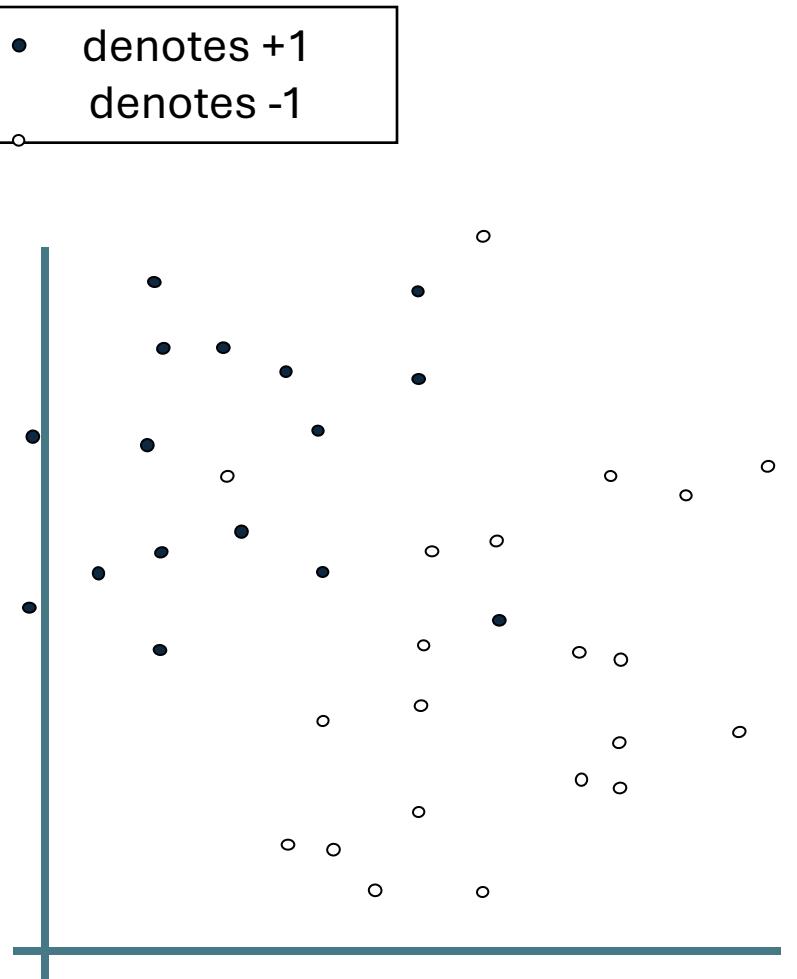
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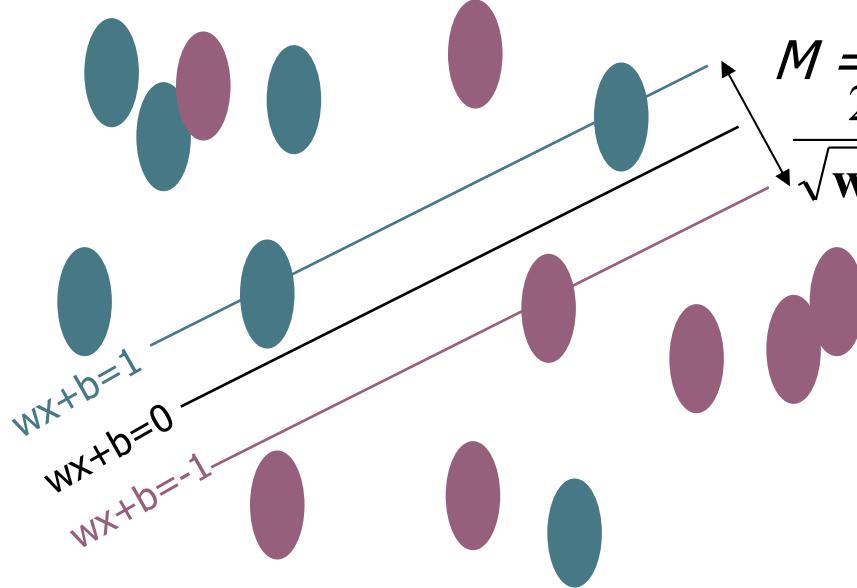
Idea 2.0:

Minimize
 $\mathbf{w} \cdot \mathbf{w} + C$ (*distance of error
points to their
correct place*)



- denotes +1
- denotes -1

Learning Maximum Margin with Noise



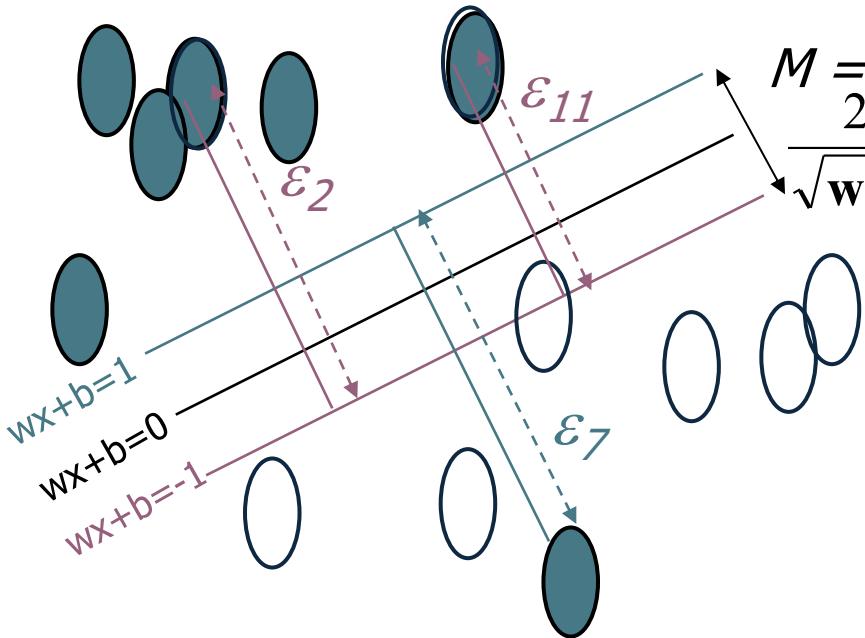
- Given guess of \mathbf{w} , b we can
- Compute sum of distances of points to their correct zones
 - Compute the margin width

Assume R datapoints, each (\mathbf{x}_k, y_k) where $y_k = +/- 1$

What should our quadratic optimization criterion be?

How many constraints will we have?
What should they be?

Learning Maximum Margin with Noise



Given guess of \mathbf{w} , b we can

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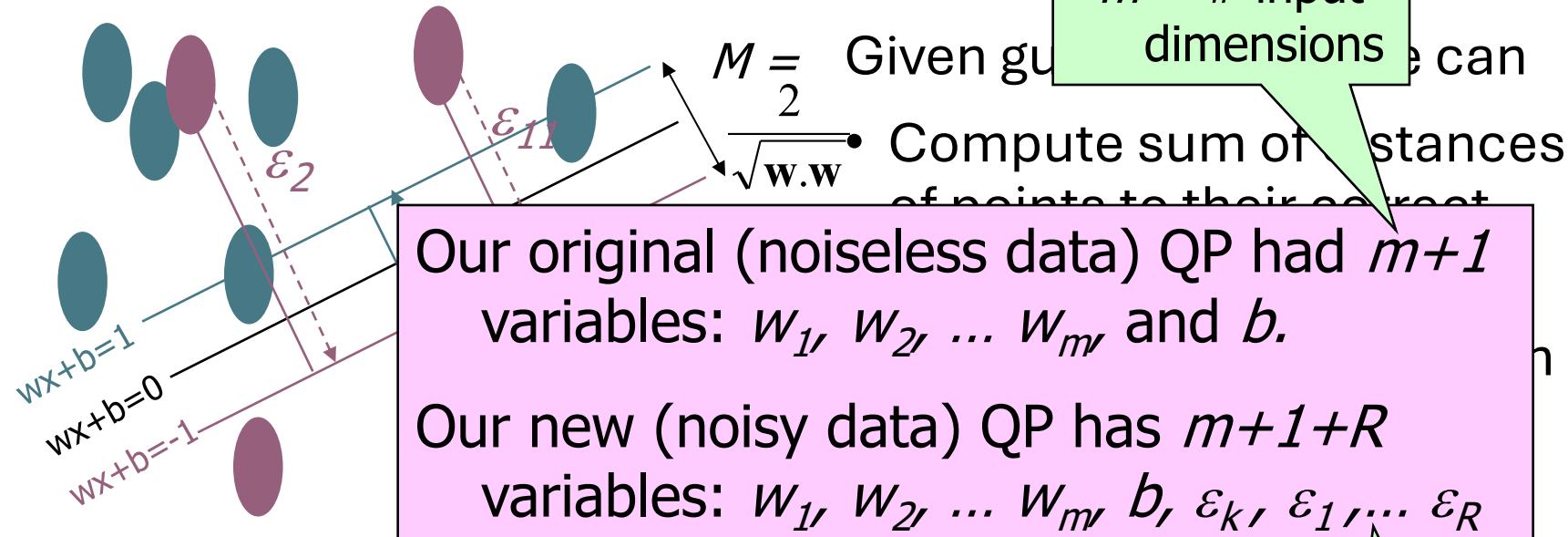
What should our quadratic optimization criterion be?

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

How many constraints will we have? R

What should they be?
 $\mathbf{w} \cdot \mathbf{x}_k + b \geq 1 - \varepsilon_k \text{ if } y_k = 1$
 $\mathbf{w} \cdot \mathbf{x}_k + b \leq -1 + \varepsilon_k \text{ if } y_k = -1$

Learning Maximum Margin with Noise



What should our quadratic optimization criterion be?

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

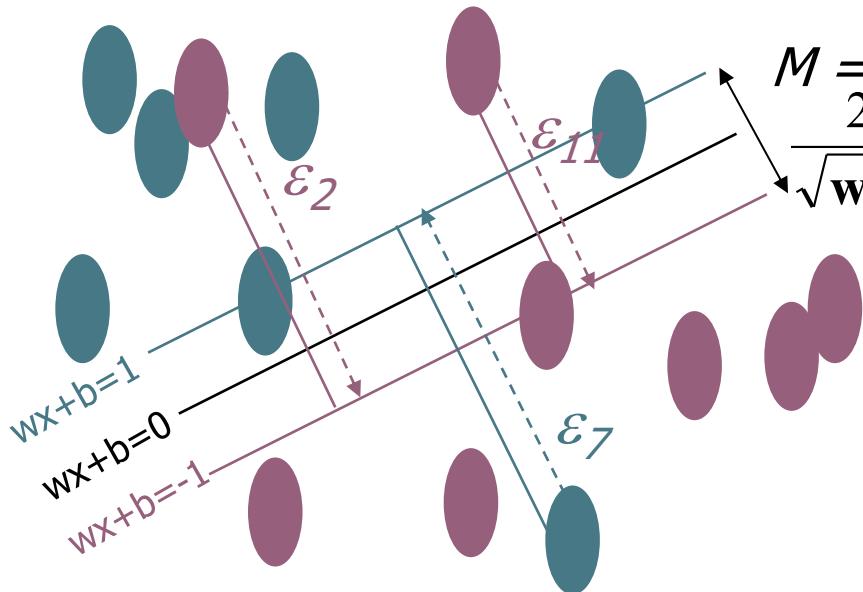
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$R = \# \text{ records}$

Learning Maximum Margin with Noise



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How many constraints will we have? R

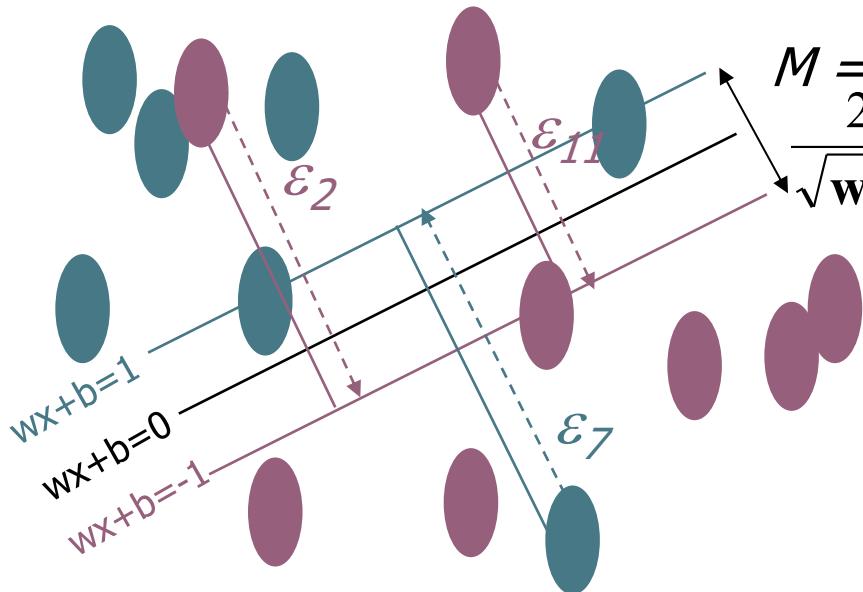
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[There's a bug in this QP. Can you spot it?]

Learning Maximum Margin with Noise



Given guess of \mathbf{w} , b we can

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

Assume R datapoints, each (\mathbf{x}_k, y_k) where $y_k = +/- 1$

What should our quadratic optimization criterion be?

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

How many constraints will we have? $2R$

What should they be?

$$\mathbf{w} \cdot \mathbf{x}_k + b \geq 1 - \varepsilon_k \text{ if } y_k = 1$$

$$\mathbf{w} \cdot \mathbf{x}_k + b \leq -1 + \varepsilon_k \text{ if } y_k = -1$$

$$\varepsilon_k \geq 0 \text{ for all } k$$

QP Problems Nature

$$\max_{\alpha} \quad \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N y_n y_m \alpha_n \alpha_m \mathbf{x}_n^\top \mathbf{x}_m$$

$$\min_{\alpha} \quad \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N y_n y_m \alpha_n \alpha_m \mathbf{x}_n^\top \mathbf{x}_m - \sum_{n=1}^N \alpha_n$$

$$\min_{\alpha} \quad \frac{1}{2} \alpha^\top \underbrace{\begin{bmatrix} y_1 y_1 \mathbf{x}_1^\top \mathbf{x}_1 & y_1 y_2 \mathbf{x}_1^\top \mathbf{x}_2 & \dots & y_1 y_N \mathbf{x}_1^\top \mathbf{x}_N \\ y_2 y_1 \mathbf{x}_2^\top \mathbf{x}_1 & y_2 y_2 \mathbf{x}_2^\top \mathbf{x}_2 & \dots & y_2 y_N \mathbf{x}_2^\top \mathbf{x}_N \\ \dots & \dots & \dots & \dots \\ y_N y_1 \mathbf{x}_N^\top \mathbf{x}_1 & y_N y_2 \mathbf{x}_N^\top \mathbf{x}_2 & \dots & y_N y_N \mathbf{x}_N^\top \mathbf{x}_N \end{bmatrix}}_{\text{quadratic coefficients}} \alpha + \underbrace{(-1^\top) \alpha}_{\text{linear}}$$

subject to

$$\underbrace{\mathbf{y}^\top \alpha = 0}_{\text{linear constraint}}$$

$$\underbrace{0}_{\text{lower bounds}} \leq \alpha \leq \underbrace{\infty}_{\text{upper bounds}}$$

Solving the Optimization Problem

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

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

$$y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1$$

- 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
 $\mathbf{Q}(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and

- (1) $\sum \alpha_i y_i = 0$
- (2) $\alpha_i \geq 0$ for all α_i

The Optimization Problem Solution

- Given a solution $\alpha_1 \dots \alpha_n$ to the dual problem, solution to the primal is:

$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i \quad b = y_k - \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x}_k \quad \text{for any } \alpha_k > 0$$

- Each non-zero α_i indicates that corresponding \mathbf{x}_i is a support vector.
- Then the classifying function is (note that we don't need \mathbf{w} explicitly):

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$

- Notice that it relies on an *inner product* between the test point \mathbf{x} and the support vectors \mathbf{x}_i – we will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x}_i^T \mathbf{x}_j$ between all training points.

Testing

- For testing with a new data z :
- Compute $WZ + b = \sum_{i=1}^{N_1} \alpha_i y_i (X_i \cdot Z) + b$ and classify Z as $y_i = +1$ if the sum is positive , $y_i = -1$ otherwise.
- Note that we do not need to form W explicitly.

- Suppose we are given the following positively labeled data points in \mathbb{R}^2 :

$$\begin{pmatrix} 3 \\ 1 \end{pmatrix}, \begin{pmatrix} 3 \\ -1 \end{pmatrix}, \begin{pmatrix} 6 \\ 1 \end{pmatrix}, \begin{pmatrix} 6 \\ -1 \end{pmatrix}$$

and

- the following negatively labeled data points in \mathbb{R}^2 :

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$

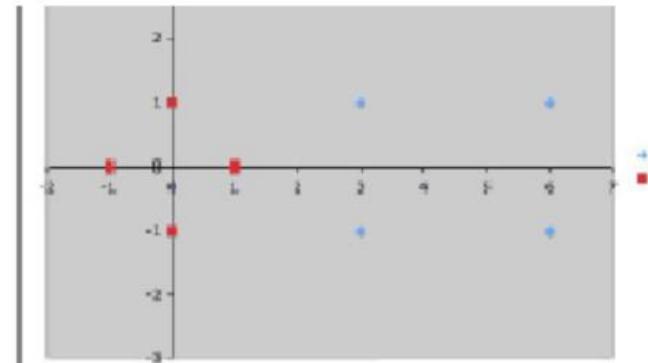


Figure 1: Sample data points in \mathbb{R}^2 . Blue diamonds are positive examples
red squares are negative examples.

Lets define simple SVM that accurately discriminates the two classes. Since the data is linearly separable, we can use a linear SVM. it should be obvious that there are three support vectors:

$$s_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, s_2 = \begin{pmatrix} 3 \\ 1 \end{pmatrix}, s_3 = \begin{pmatrix} 3 \\ -1 \end{pmatrix}$$

- We will use vectors augmented with a 1 as a bias input, and for clarity we will differentiate these with an over-tilde. So, if $s_1 = (10)$, then $\tilde{s}_1 = (101)$.

$$\tilde{s}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \tilde{s}_2 = \begin{pmatrix} 3 \\ 1 \\ 1 \end{pmatrix}, \tilde{s}_3 = \begin{pmatrix} 3 \\ -1 \\ 1 \end{pmatrix}$$

- Our task is to find values for the α_i such that,

$$\begin{aligned} \alpha_1 \tilde{s}_1 \cdot \tilde{s}_1 + \alpha_2 \tilde{s}_2 \cdot \tilde{s}_1 + \alpha_3 \tilde{s}_3 \cdot \tilde{s}_1 &= -1 \\ \alpha_1 \tilde{s}_1 \cdot \tilde{s}_2 + \alpha_2 \tilde{s}_2 \cdot \tilde{s}_2 + \alpha_3 \tilde{s}_3 \cdot \tilde{s}_2 &= +1 \\ \alpha_1 \tilde{s}_1 \cdot \tilde{s}_3 + \alpha_2 \tilde{s}_2 \cdot \tilde{s}_3 + \alpha_3 \tilde{s}_3 \cdot \tilde{s}_3 &= +1 \end{aligned}$$

Example

- Our task is to find values for the α_i such that,

$$\begin{aligned}\alpha_1 \tilde{s}_1 \cdot \tilde{s}_1 + \alpha_2 \tilde{s}_2 \cdot \tilde{s}_1 + \alpha_3 \tilde{s}_3 \cdot \tilde{s}_1 &= -1 \\ \alpha_1 \tilde{s}_1 \cdot \tilde{s}_2 + \alpha_2 \tilde{s}_2 \cdot \tilde{s}_2 + \alpha_3 \tilde{s}_3 \cdot \tilde{s}_2 &= +1 \\ \alpha_1 \tilde{s}_1 \cdot \tilde{s}_3 + \alpha_2 \tilde{s}_2 \cdot \tilde{s}_3 + \alpha_3 \tilde{s}_3 \cdot \tilde{s}_3 &= +1\end{aligned}$$

- Computing the dot product

For example, $\tilde{s}_1 \cdot \tilde{s}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = 1 \times 1 + 0 \times 0 + 1 \times 1 = 2$

$$\begin{aligned}2\alpha_1 + 4\alpha_2 + 4\alpha_3 &= -1 \\ 4\alpha_2 + 11\alpha_2 + 9\alpha_3 &= +1 \\ 4\alpha_1 + 9\alpha_2 + 11\alpha_3 &= +1\end{aligned}$$

$$\alpha_1 = -3.5 \text{ and } \alpha_2 = 0.75 \text{ and } \alpha_3 = 0.75$$

Example

- How to find the hyper-plane that discriminates the positive values?

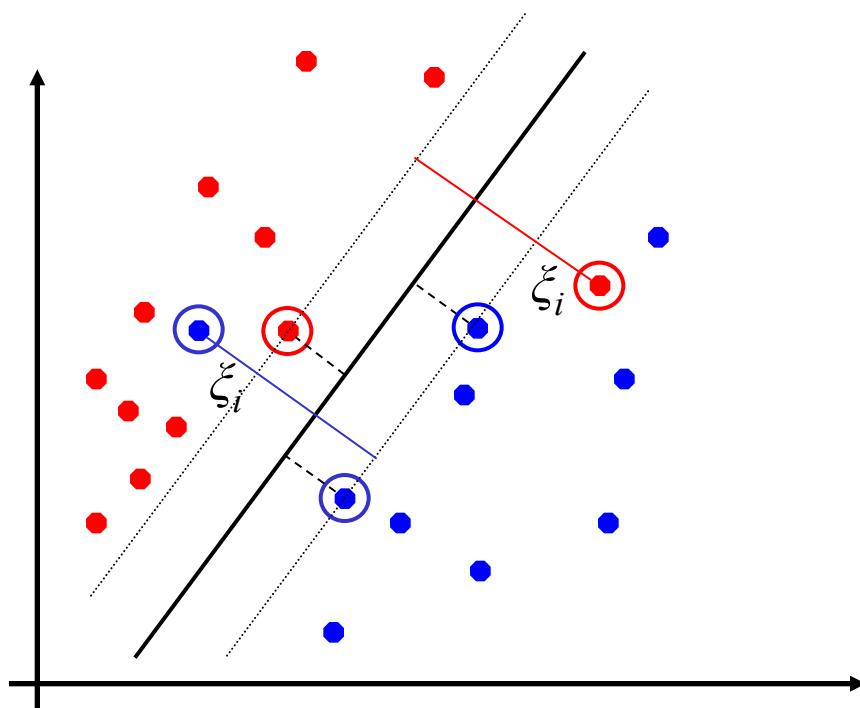
$$\begin{aligned}\tilde{w} &= \sum_{i=1}^3 \alpha_i \tilde{s}_i \\ &= -3.5 \times \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + 0.75 \times \begin{pmatrix} 3 \\ 1 \\ 1 \end{pmatrix} + 0.75 \times \begin{pmatrix} 3 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ -2 \end{pmatrix}\end{aligned}$$

- The bias b and w are:

$$w = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } b = -2$$

Soft Margin Classification

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



Soft Margin Classification Mathematically

- The old formulation:

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

- Modified formulation incorporates slack variables:

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

- 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.

Soft Margin Classification – Solution

- Dual problem is identical to separable case (would *not* be identical if the 2-norm penalty for slack variables $C\sum\xi_i^2$ was used in primal objective, we would need additional Lagrange multipliers for slack variables):

Find $\alpha_1 \dots \alpha_N$ such that

$\mathbf{Q}(\mathbf{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and

$$(1) \quad \sum \alpha_i y_i = 0$$

$$(2) \quad 0 \leq \alpha_i \leq C \text{ for all } \alpha_i$$

- Again, \mathbf{x}_i with non-zero α_i will be support vectors.
- Solution to the dual problem is:

$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i$$

$$b = y_k(1 - \xi_k) - \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x}_k \quad \text{for any } k \text{ s.t. } \alpha_k > 0$$

Again, we don't need to compute \mathbf{w} explicitly for classification:

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b$$