UVA CS 4774: Machine Learning

S4: Lecture 20: Support Vector Machine (Basics)

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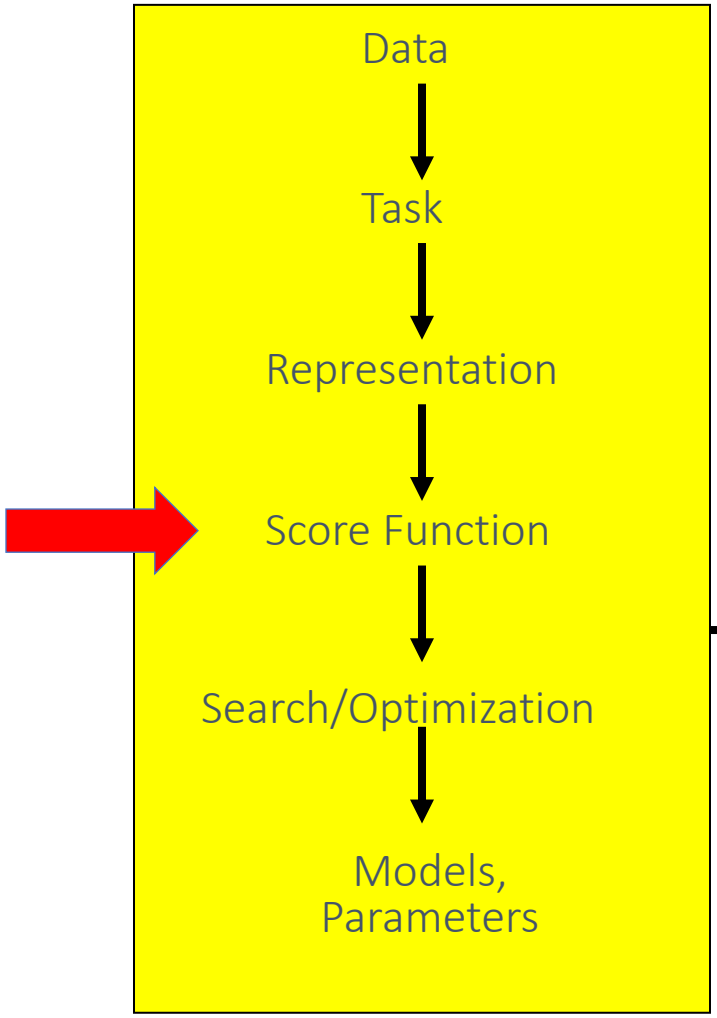
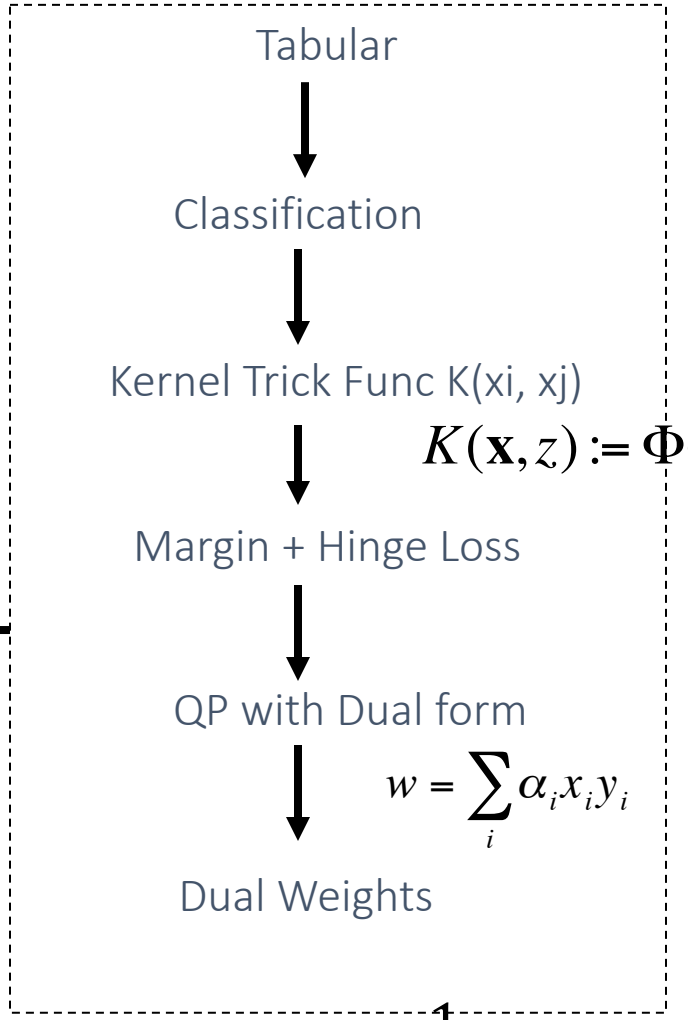
University of Virginia

Department of Computer Science

Today: Basic Support Vector Machine





$$\underset{\mathbf{w},b}{\operatorname{argmin}} \sum_{i=1}^{p} w_i^2 + \mathrm{C} \sum_{\mathrm{i}=1}^{\mathrm{n}} \varepsilon_{\mathrm{i}}$$

$$\text{subject to } \forall \mathbf{x}_i \in Dtrain : y_i \left(\mathbf{x}_i \cdot \mathbf{w} + b \right) \geq 1 - \varepsilon_{\mathrm{i}}$$

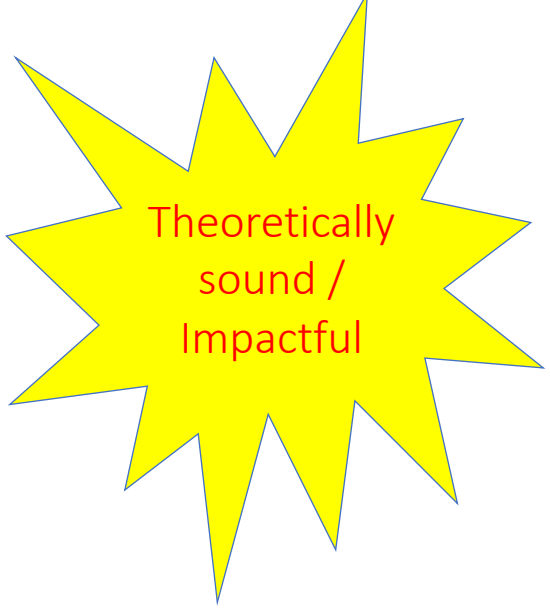
$$\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y_i} y_j \mathbf{x_i}^T \mathbf{x_j}$$

$$\sum_i \alpha_i \mathrm{y_i} = 0, \qquad \alpha_i \geq 0 \qquad \forall i$$

Today

- Support Vector Machine (SVM)
  - ✓ History of SVM
  - ✓ Large Margin Linear Classifier
  - ✓ Define Margin (M) in terms of model parameter
  - ✓ Optimization to learn model parameters (w, b)
  - ✓ Linearly Non-separable case
  - ✓ Optimization with dual form
  - ✓ Nonlinear decision boundary
  - ✓ Multiclass SVM

History of SVM



- SVM is inspired from statistical learning theory [3]
- SVM was first introduced in 1992 [1]

- SVM becomes popular because of its success in handwritten digit recognition (1994)
  - 1.1% test error rate for SVM.
  - The same as the error rates of a carefully constructed neural network, LeNet 4.
    - Section 5.11 in [2] or the discussion in [3] for details
- Regarded as an important example of "kernel methods", arguably the hottest area in machine learning 20 years ago

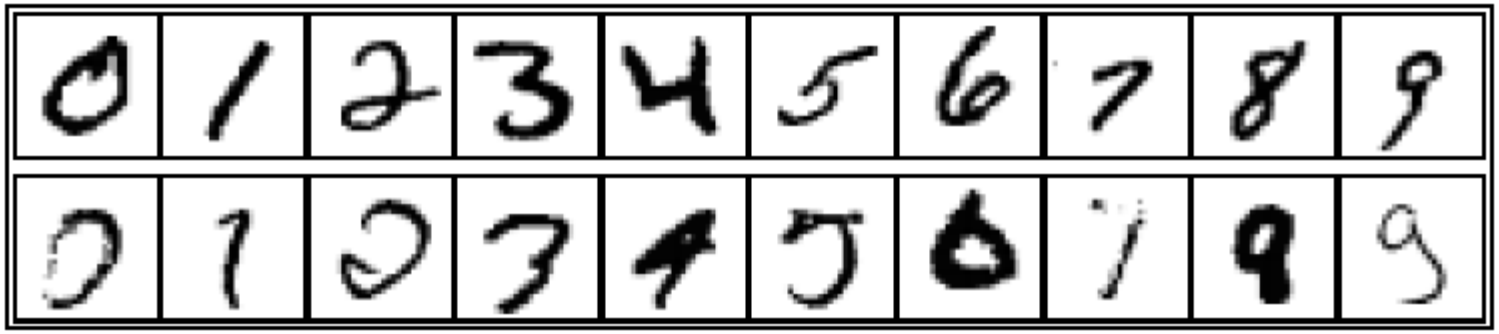
[1] B.E. Boser et al. A Training Algorithm for Optimal Margin Classifiers. Proceedings of the Fifth Annual Workshop on Computational Learning Theory 5 144-152, Pittsburgh, 1992.

[2] L. Bottou et al. Comparison of classifier methods: a case study in handwritten digit recognition. Proceedings of the 12th IAPR International Conference on Pattern Recognition, vol. 2, pp. 77-82, 1994.

[3] V. Vapnik. The Nature of Statistical Learning Theory. 2nd edition, Springer, 1999.

Handwritten digit recognition

→ MNIST (SVM) 1994



3-nearest-neighbor = 2.4% error

400–300–10 unit MLP = 1.6% error

LeNet: 768–192–30–10 unit MLP = 0.9% error

best (kernel machines, vision algorithms) ≈ 0.6% error

Applications of SVMs

- Computer Vision
- Text Categorization
- Ranking (e.g., Google searches)
- Handwritten Character Recognition
- Time series analysis
- Bioinformatics
- …….

→Lots of very successful applications!!!

Early History

- In 1950 English mathematician Alan Turing wrote a landmark paper titled "Computing Machinery and Intelligence" that asked the question: "Can machines think?"
- Further work came out of a 1956 workshop at Dartmouth sponsored by John McCarthy. In the proposal for that workshop, he coined the phrase a "study of artificial intelligence"
- 1950s
  - Samuel's checker player : start of machine learning
  - Selfridge's Pandemonium
- **1952-1969: Enthusiasm:** Lots of work on neural networks
- 1970s: Expert systems, Knowledge bases to add on rule-based inference

Adapted From Prof. Raymond J. Mooney's slides

Early History

- 1980s :
  - Advanced decision tree and rule learning
  - Valiant's PAC Learning Theory

- 1990s:
  - Reinforcement learning (RL)
  - Ensembles: Bagging, Boosting, and Stacking
  - Bayes Net learning
  - Convolutional neural network (CNN) and Recurrent neural network (RNN) were invented
  - SVM

- 2000s ~2010s
  - Support vector machines (becoming popular and dominating)
  - Kernel methods
  - Graphical models
  - Statistical relational learning
  - Transfer learning
  - Sequence labeling
  - Collective classification and structured outputs

Adapted From Prof. Raymond J. Mooney's slides

MIT Technology Review

10 Breakthrough Technologies 2013

Think of the most frustrating, intractable, or simply annoying problems you can imagine. Now think about what technology is doing to fix them. That's what we did in coming up with our annual list of 10 Breakthrough Technologies. We're looking for technologies that we believe will expand the scope of human possibilities.

Deep Learning

CNN/RNN

1990s

10 Breakthrough Technologies 2017

These technologies all have staying power. They will affect the economy and our politics, improve medicine, or influence our culture. Some are unfolding now; others will take a decade or more to develop. But you should know about all of them right now.

Deep Reinforcement Learning

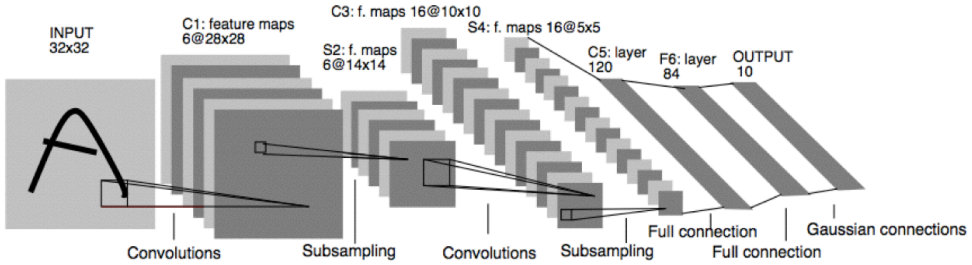
1990s~2010s

10 BREAKTHROUGH TECHNOLOGIES 2018

Generative Adversarial Network (GAN)

2010s

- 1952-1969 Enthusiasm: Lots of work on neural networks
- 1990s: Convolutional neural network (CNN) and Recurrent neural network (RNN) were invented



Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, Gradient-based learning applied to document recognition, Proceedings of the IEEE 86(11): 2278–2324, 1998.

Reason of the recent breakthroughs of deep learning:

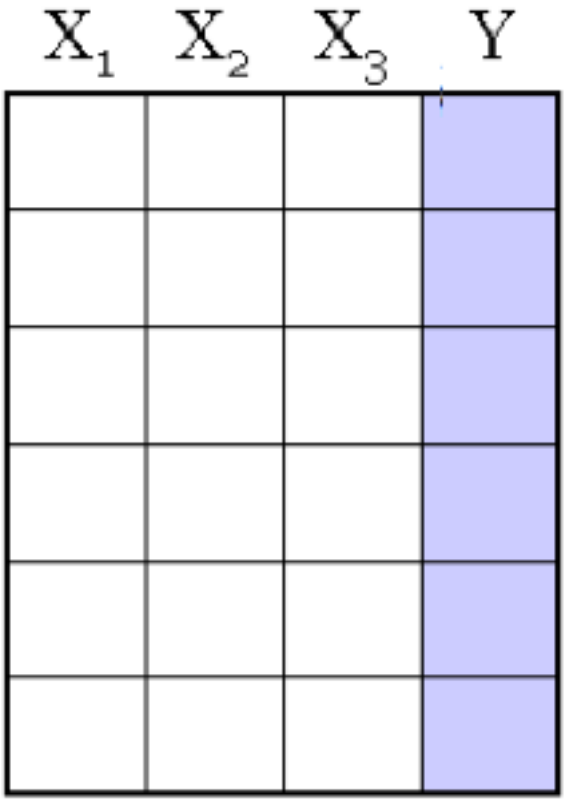
① Low Bias / High Variance

Plenty of (Labeled) Data

Advanced Computer Architecture that fits DNNs

Powerful DNN platforms / Libraries

② XgBoost → Tree Based / reduce variance



$f : X \longrightarrow Y$

$\{-1, 1\}$

Output as Binary Class: only two possibilities

- **Data***/points/instances/examples/samples/records*: [rows]
- **Features***/attributes/dimensions/independent variables/covariates/predictors/regressors*: [columns, except the last]
- **Target***/outcome/response/label/dependent variable*: special column to be predicted [last column]

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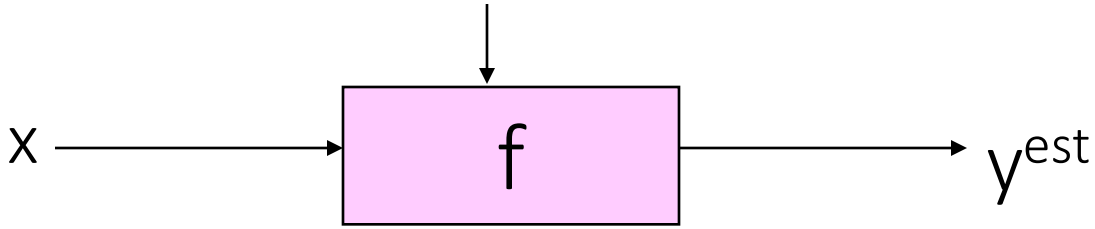
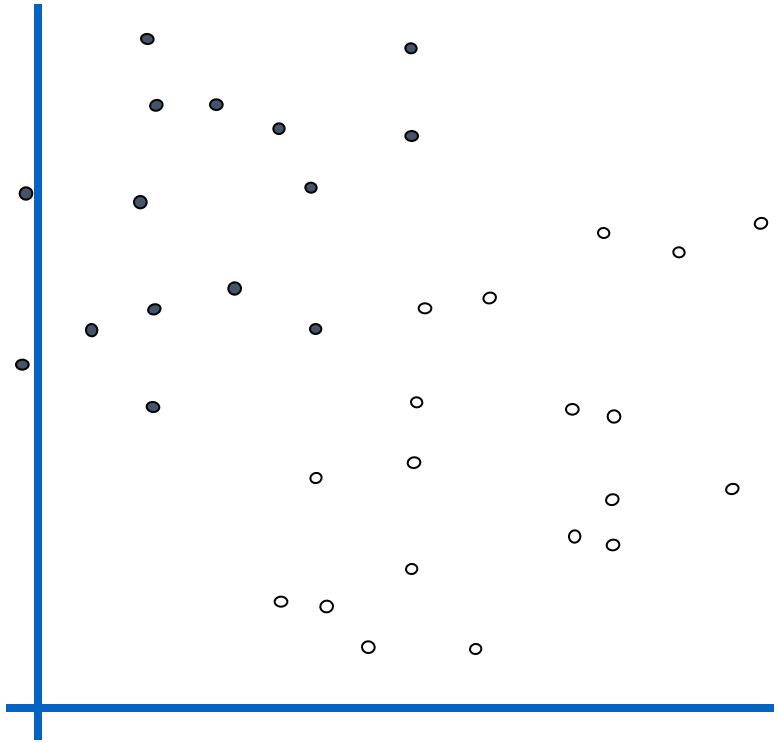
Linear Classifiers



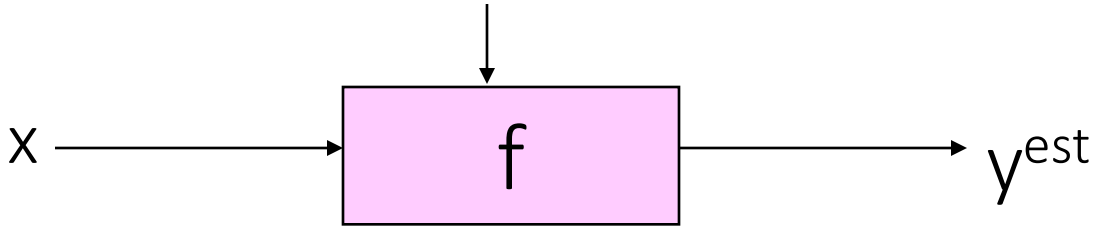
- denotes +1
- denotes -1

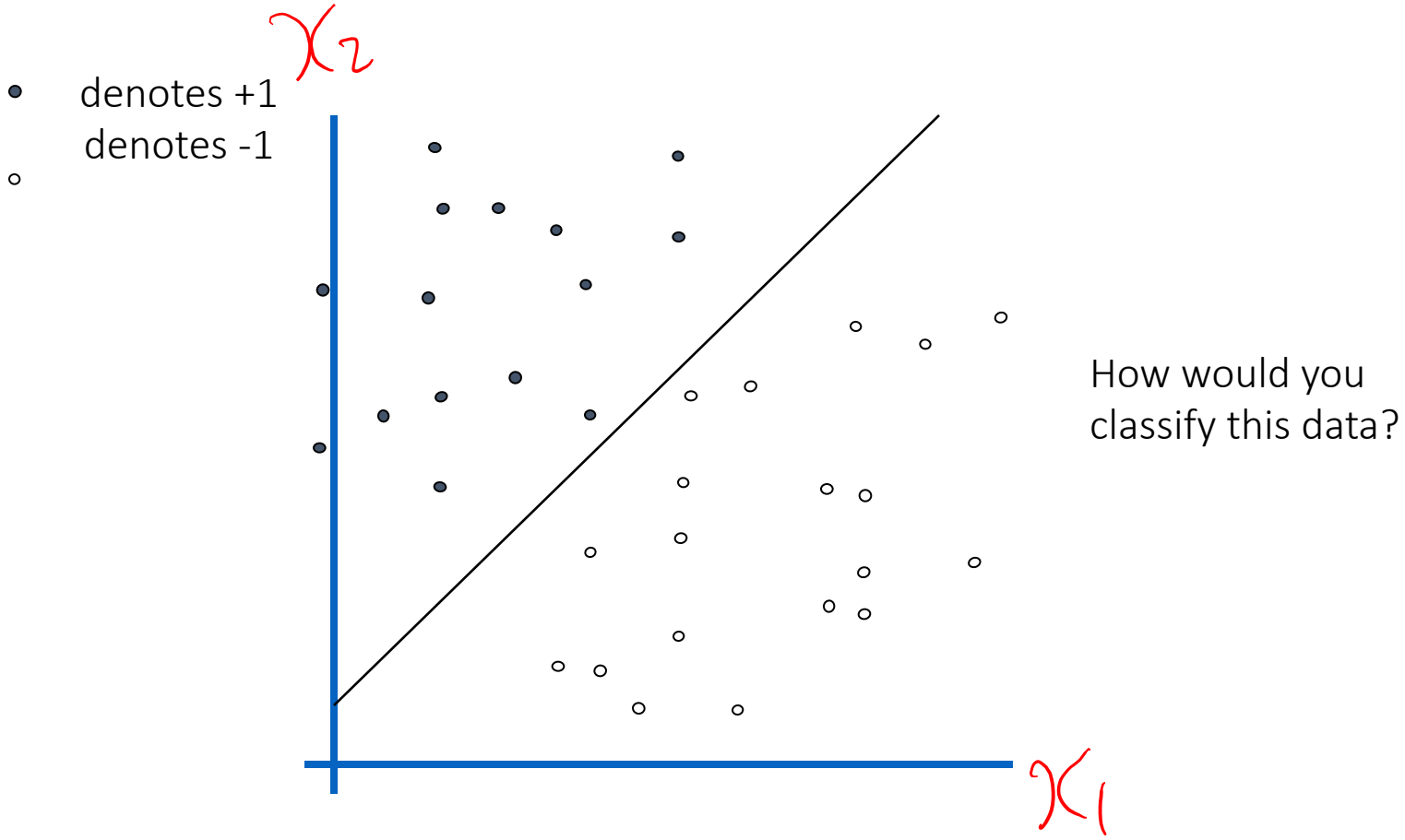


How would you classify this data?

Credit: Prof. Moore

Linear Classifiers





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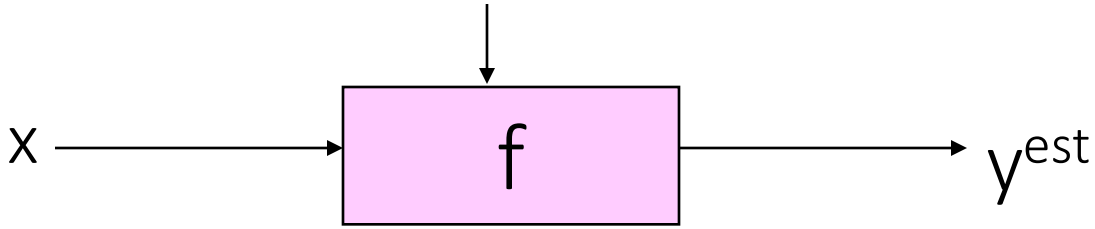

denotes +1

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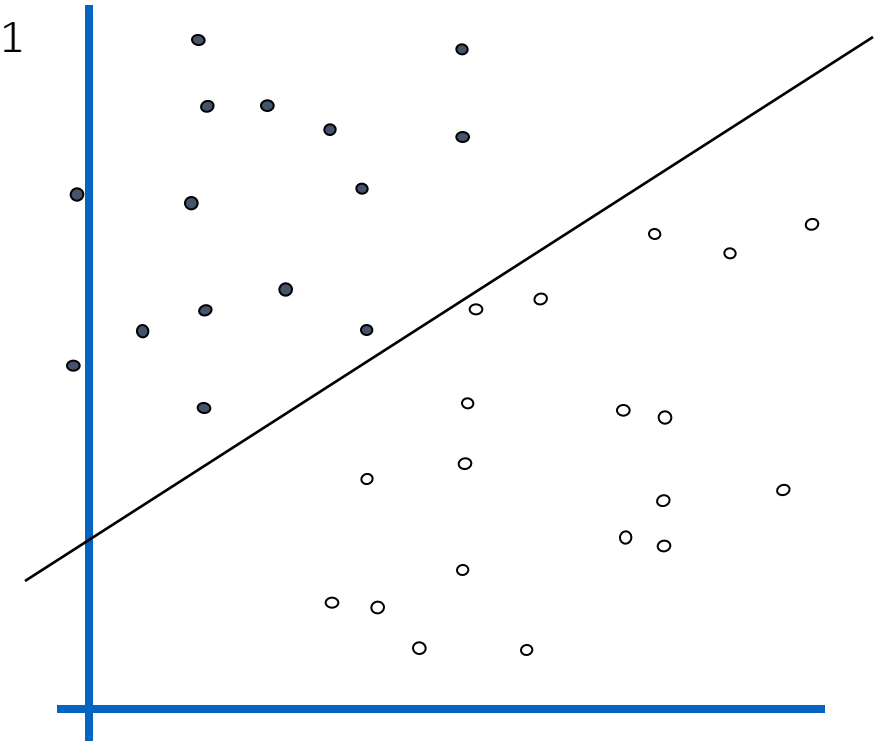

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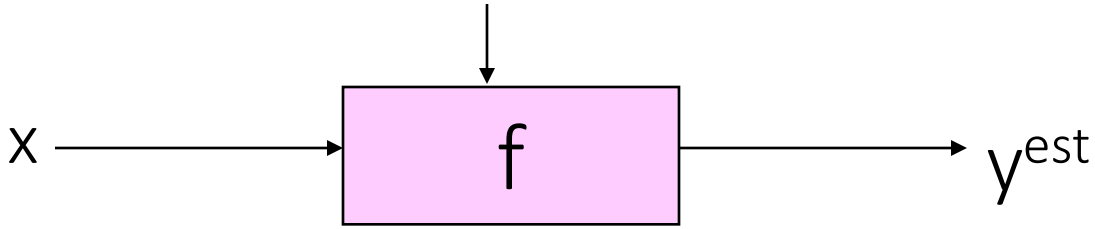
Linear Classifiers



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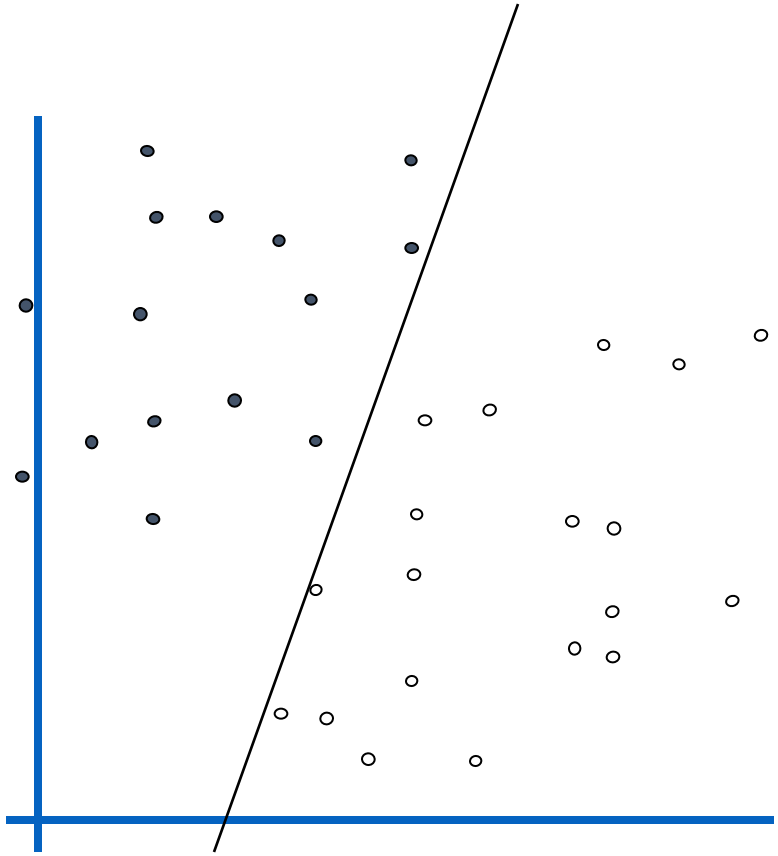

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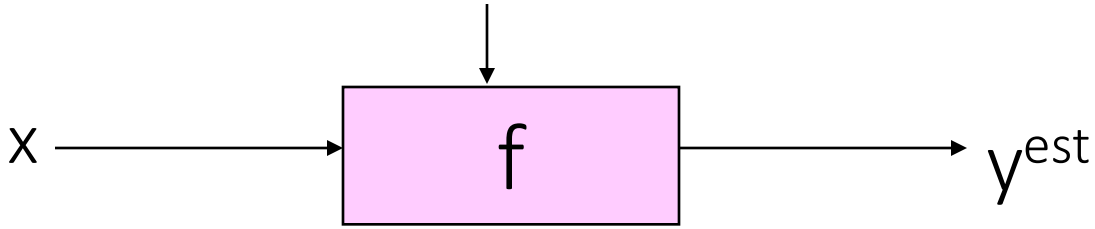
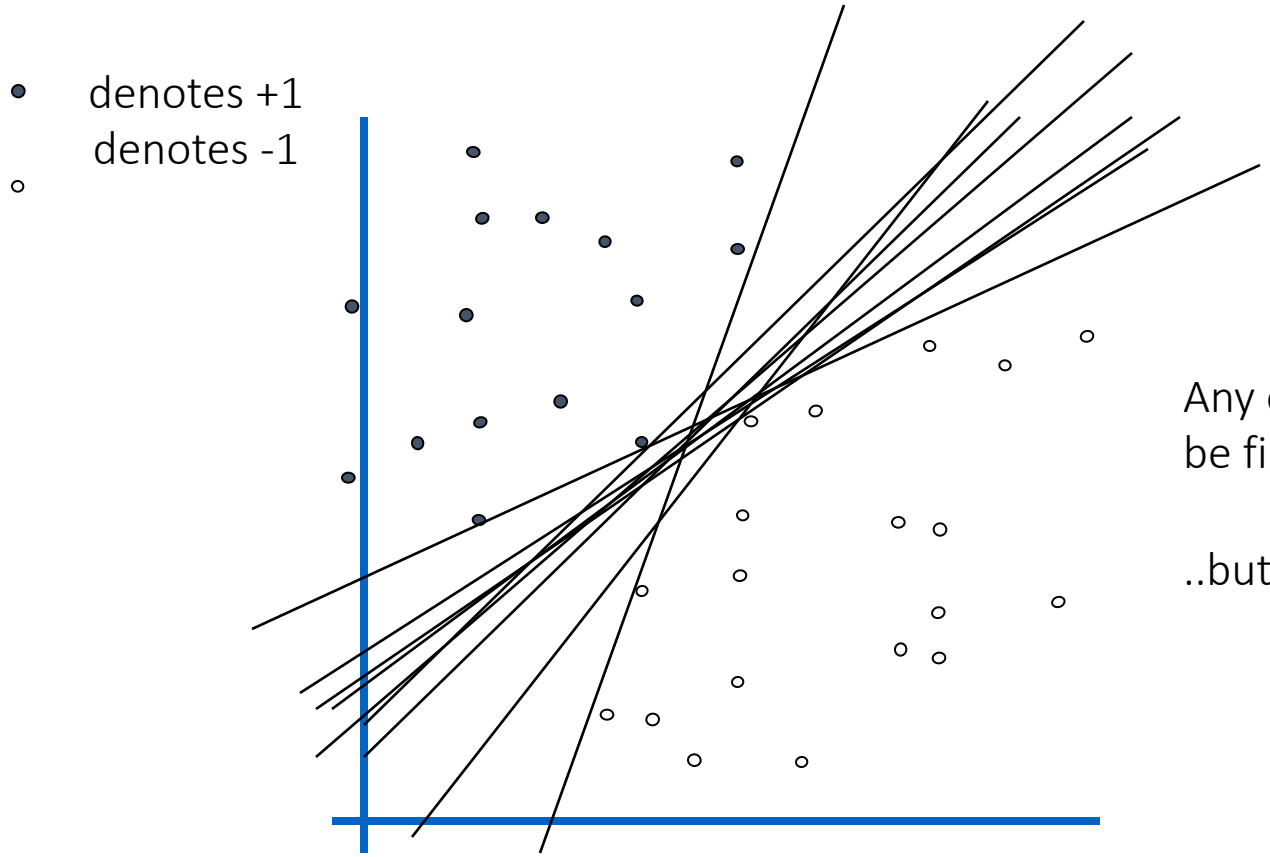
Linear Classifiers



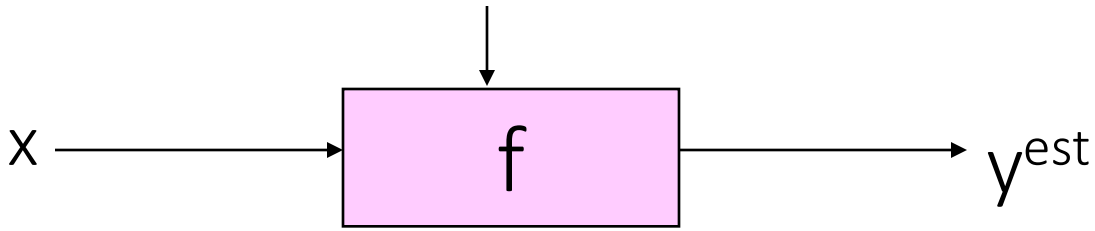


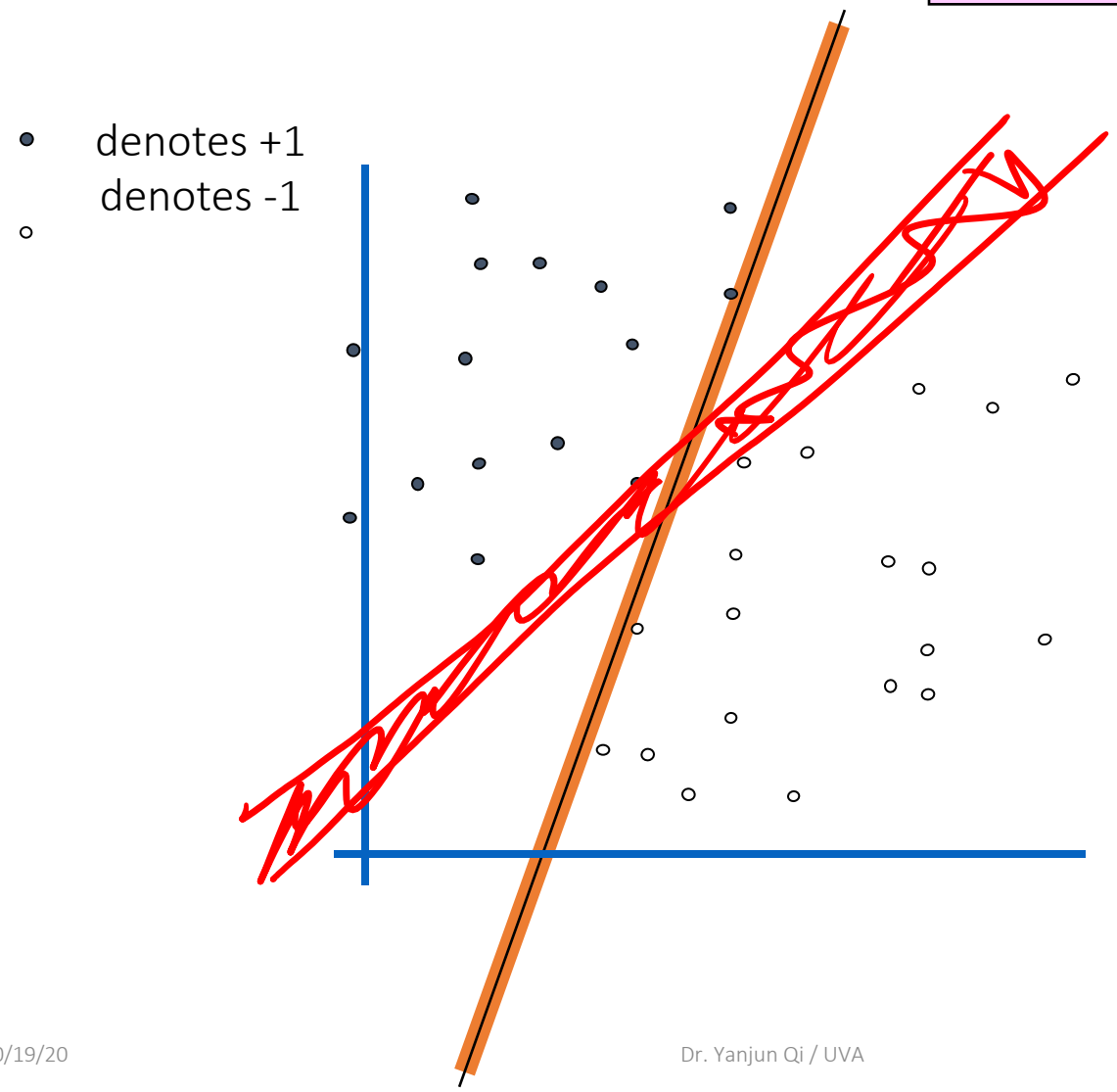
Any of these would be fine..

..but which is best?

Credit: Prof. Moore

Classifier Margin

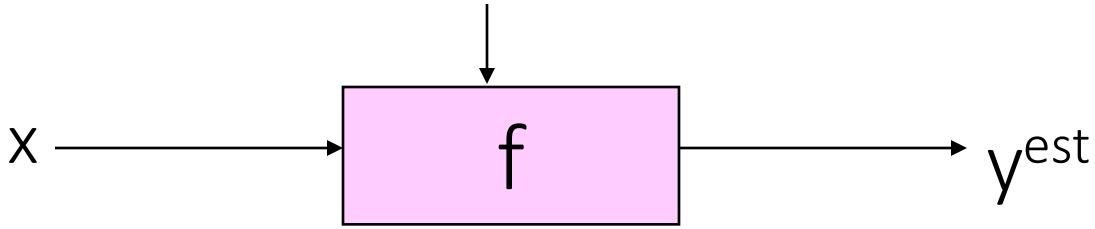


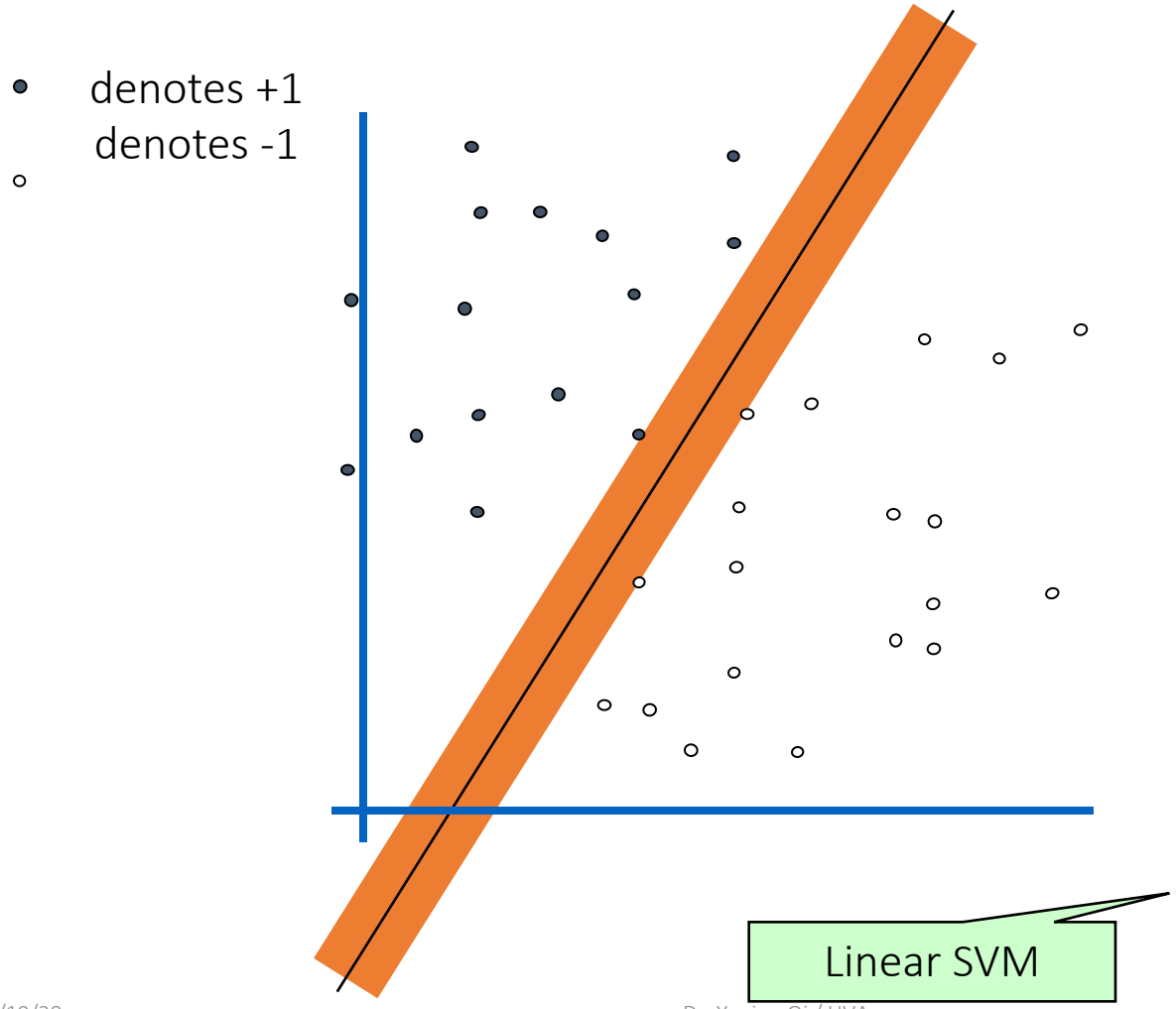


Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

Credit: Prof. Moore

Maximum Margin

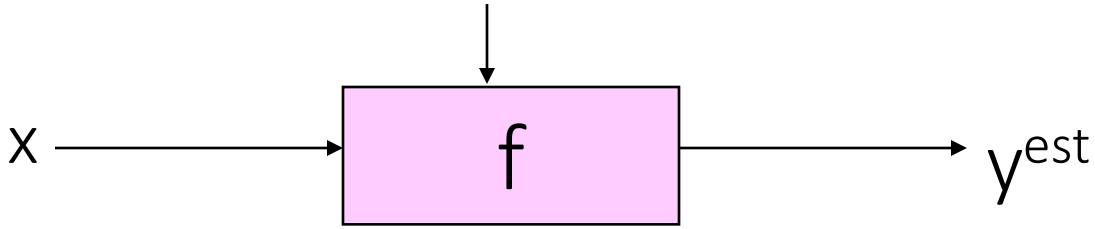


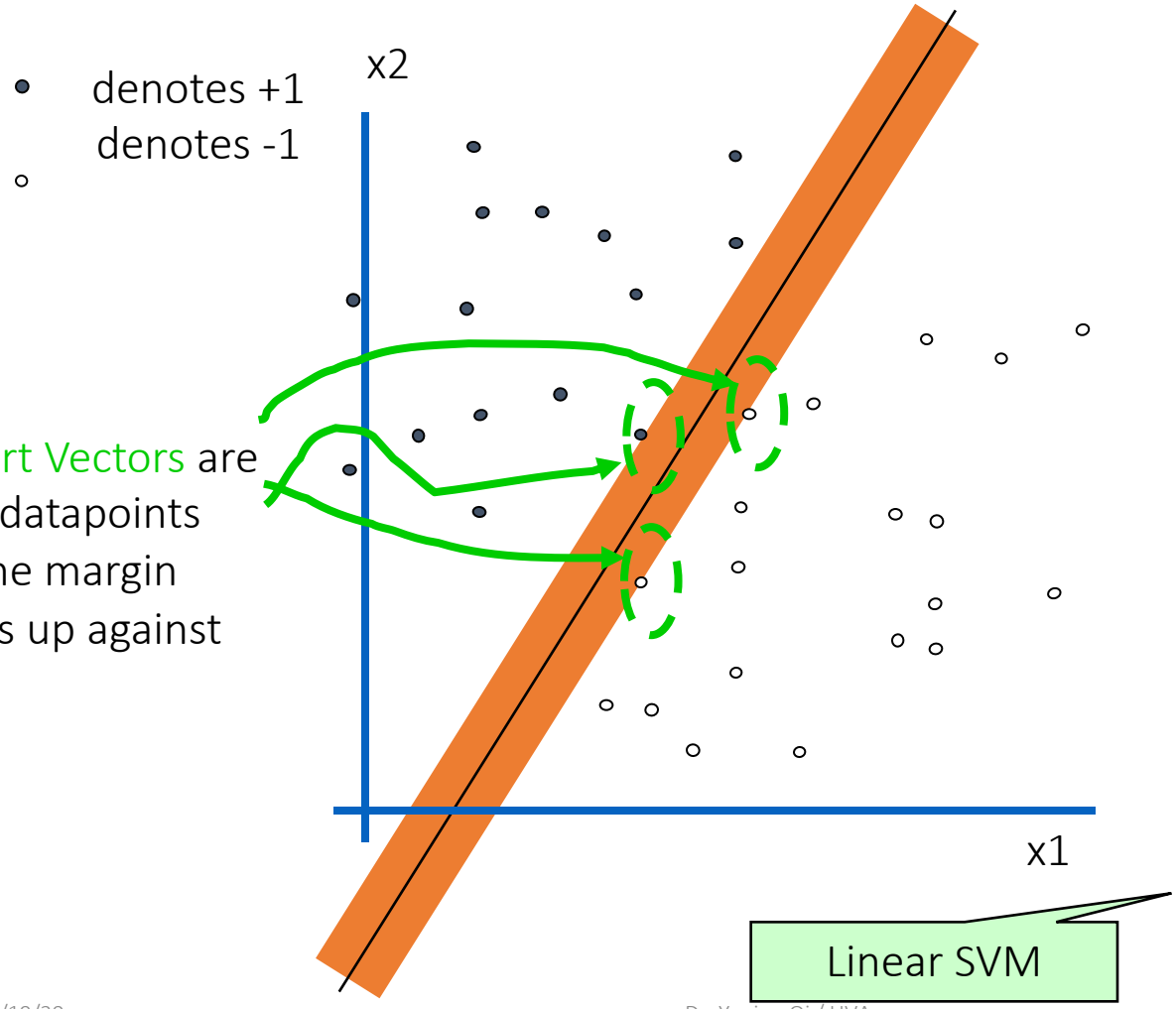


The maximum margin linear classifier is the linear classifier with the, maximum margin. This is the simplest kind of SVM (Called an LSVM)

Credit: Prof. Moore

Maximum Margin





Support Vectors are those datapoints that the margin pushes up against

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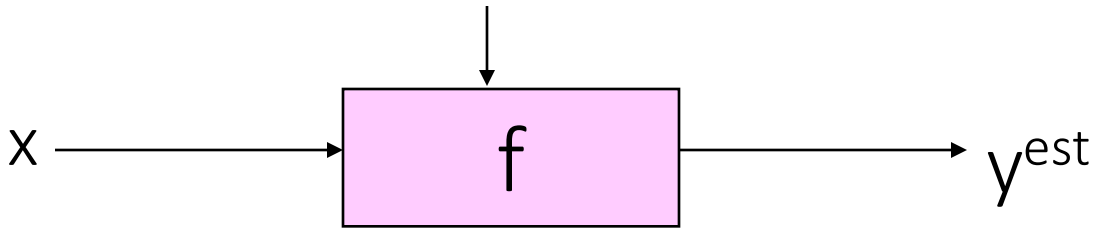
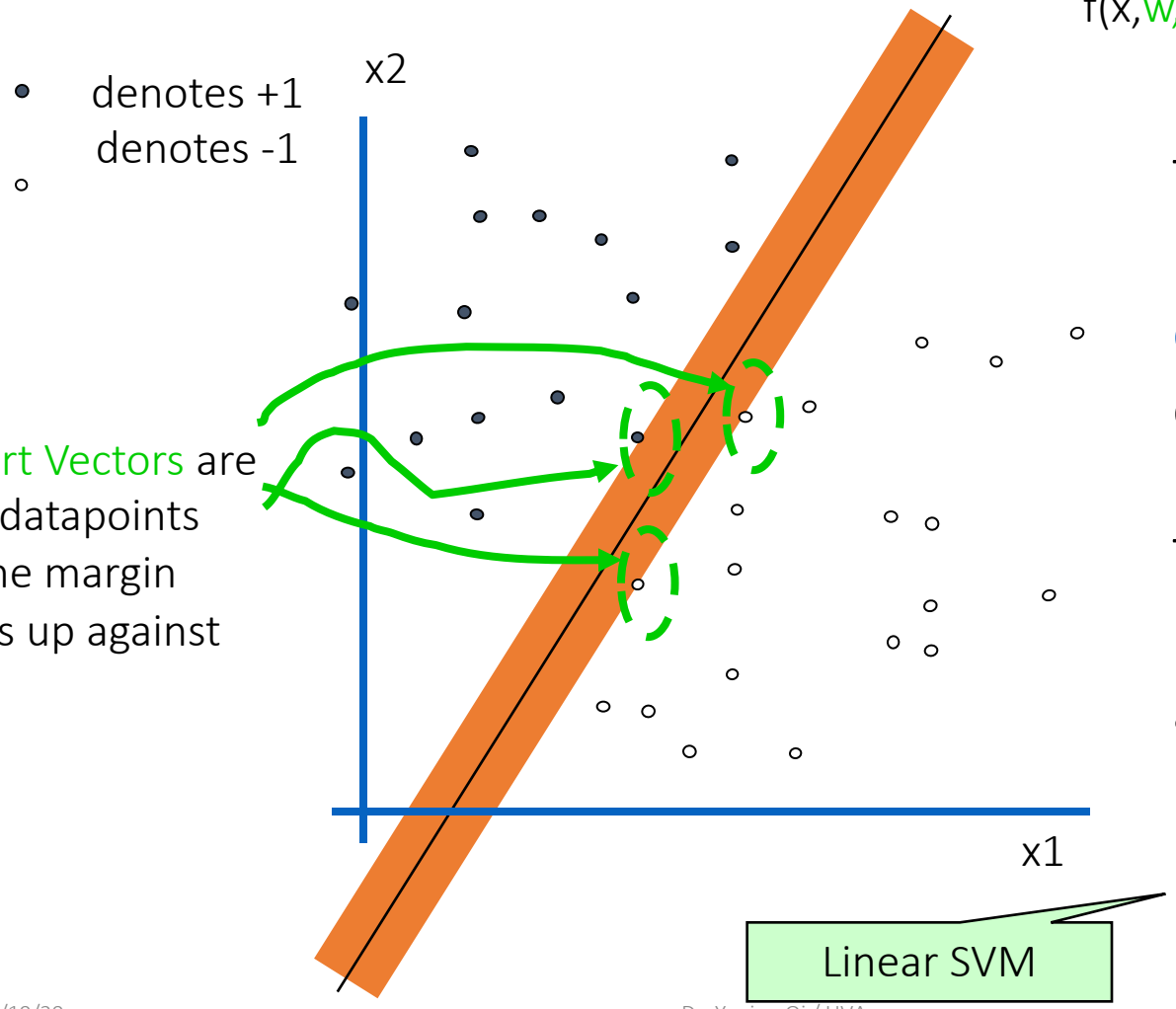
Maximum Margin



$f(x,w,b) = \text{sign}(w^T x + b)$



Support Vectors are those datapoints that the margin pushes up against

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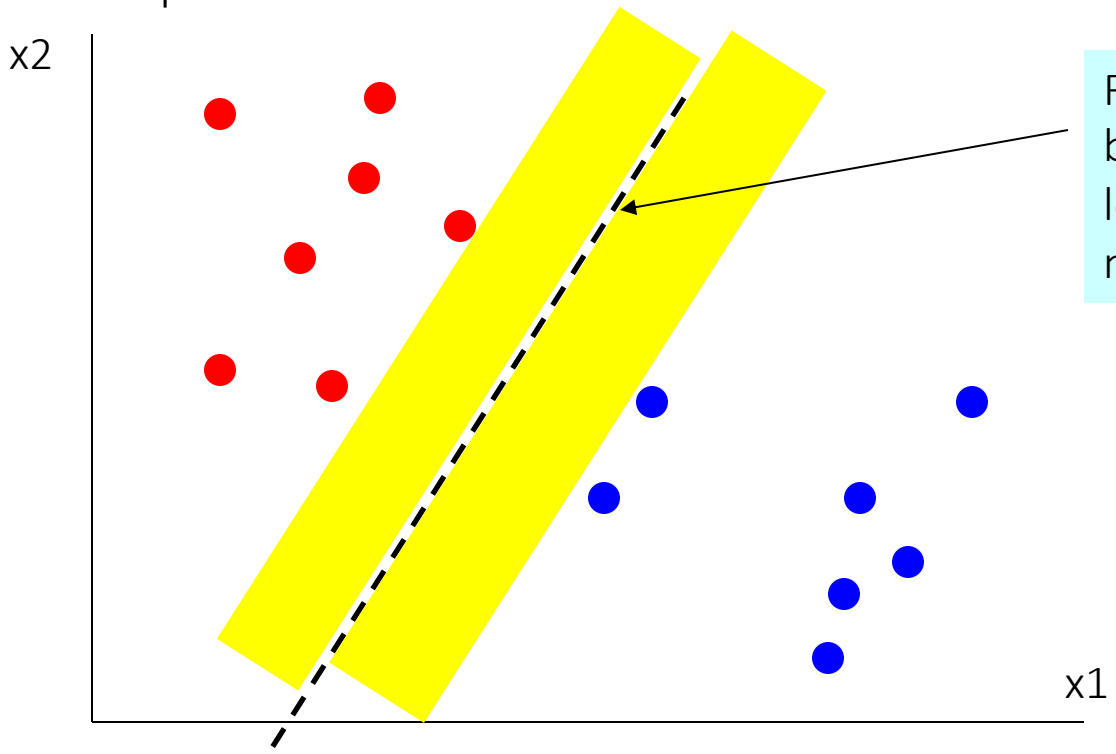
Max margin classifiers

- Instead of fitting all points, focus on boundary points
- Learn a boundary that leads to the largest margin from both sets of points



From all the possible boundary lines, this leads to the largest margin on both sides

$f(x,w,b) = \text{sign}(w^T x + b)$

Credit: Prof. Moore

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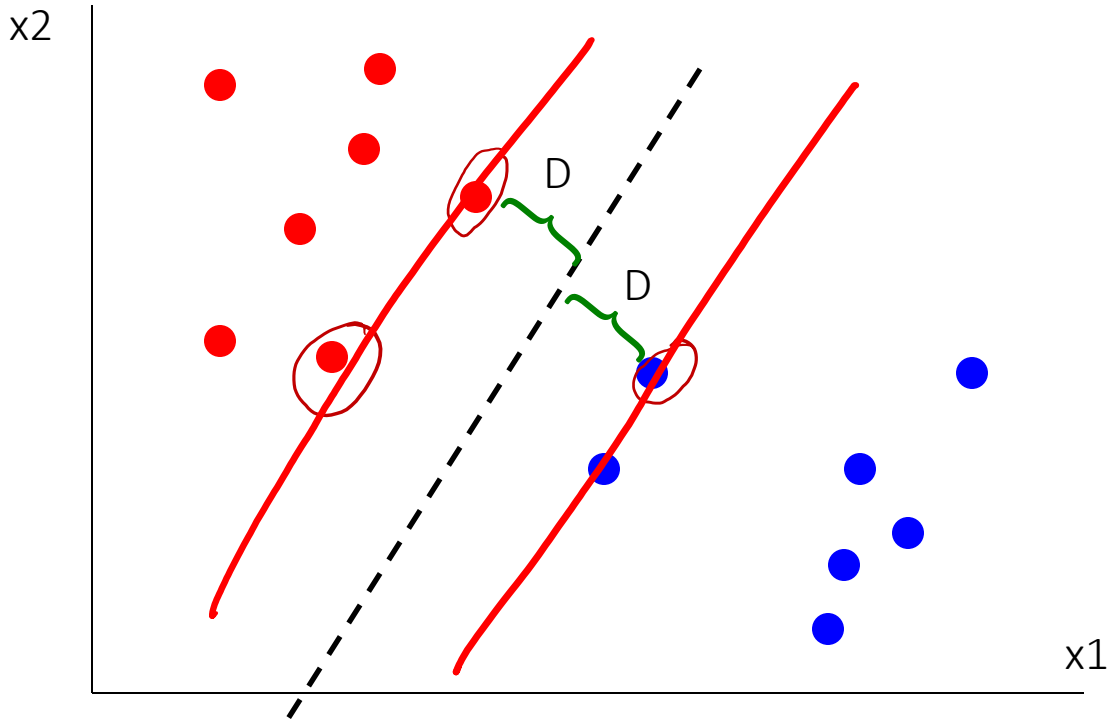

Why MAX margin?

- Intuitive, 'makes sense'
- Some theoretical support (using VC dimension)
- Works well in practice

Credit: Prof. Moore


Thank You
Thank you

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Module II

Dr. Yanjun Qi

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Department of Computer Science

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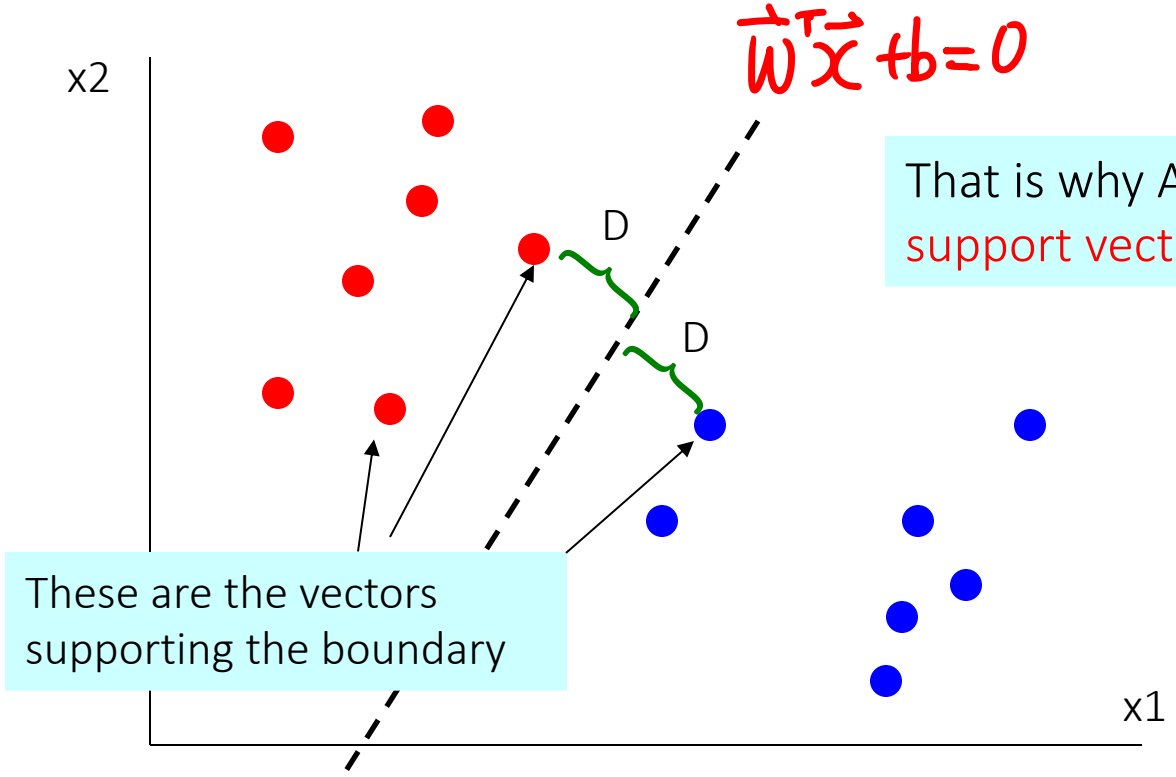
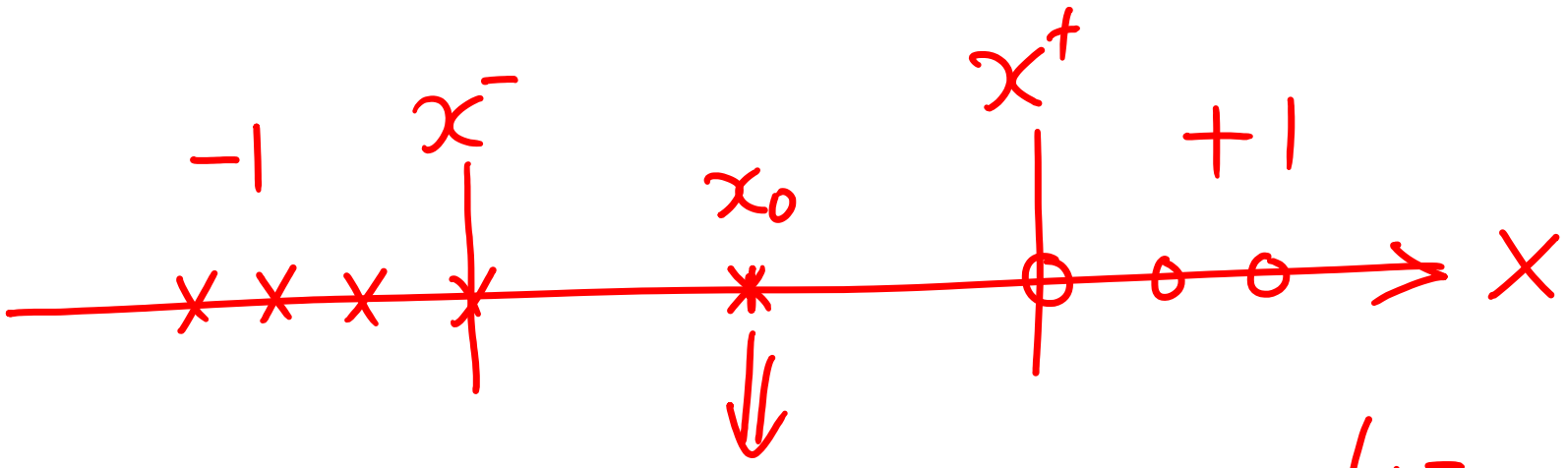


That is why Also known as linear support vector machines (SVMs)

$f(x,w,b) = \text{sign}(w^T x + b)$

Credit: Prof. Moore

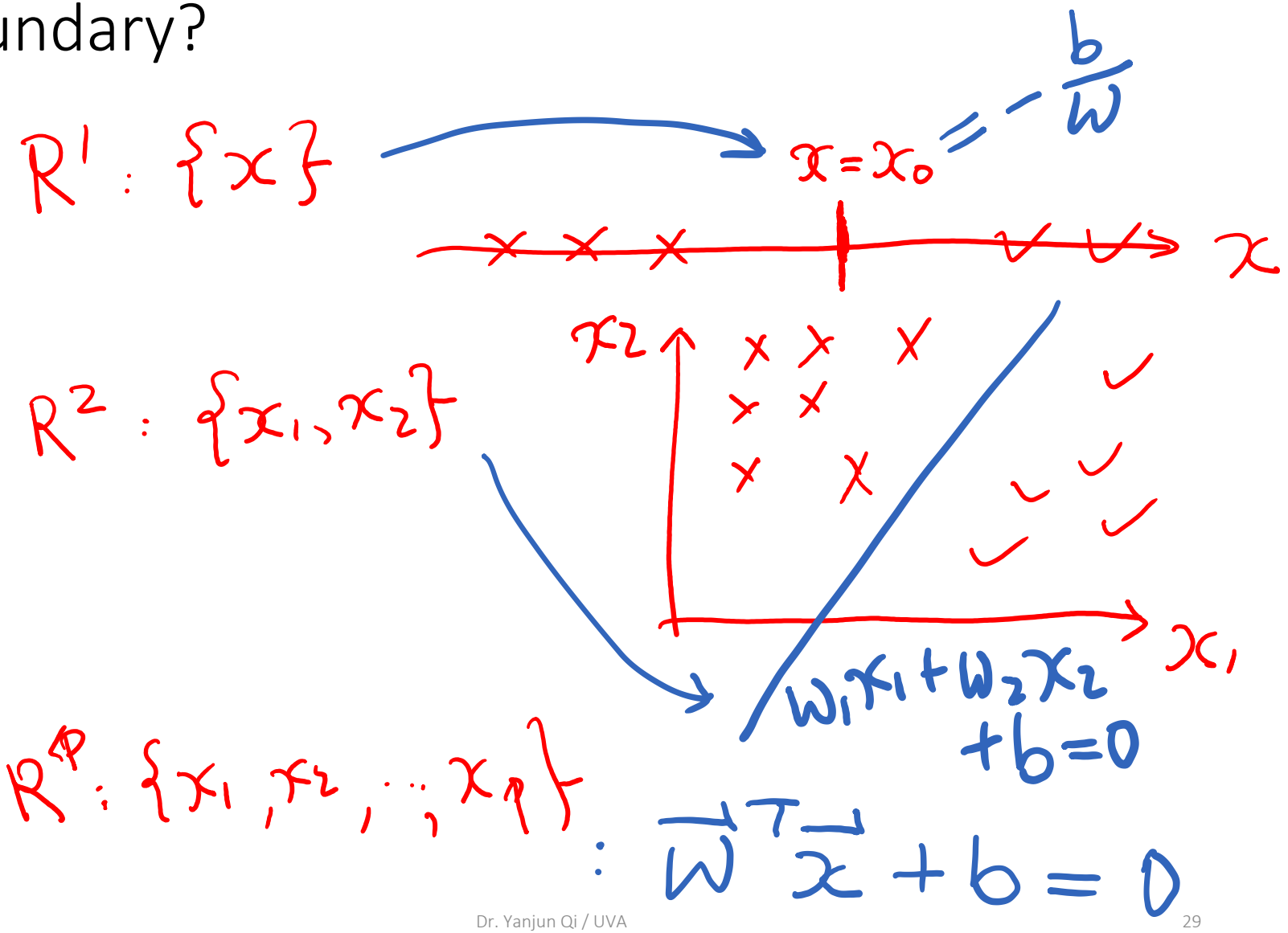
$R^1: \{x\} \rightarrow \{+1, -1\}$



$$\begin{cases} \vec{w}^T \vec{x}_0 + b = 0 \\ w^T x^- + b = -1 \\ w^T x^+ + b = 1 \end{cases}$$

$$f(x) = \text{Sign}\left(\vec{w}^T x + b\right)$$

How to represent a Linear Decision Boundary?



Review : **Affine Hyperplanes**

- https://en.wikipedia.org/wiki/Hyperplane
- Any hyperplane can be given in coordinates as the solution of a single linear (algebraic) equation of degree 1.

$[a_1x_1 + a_2x_2 + a_3x_3 + \cdots + a_px_p = -b]$, at least one $a_i \neq 0$

$\Rightarrow$ e.g. classification Boundary $\vec{w}^T\vec{x} + b = 0$

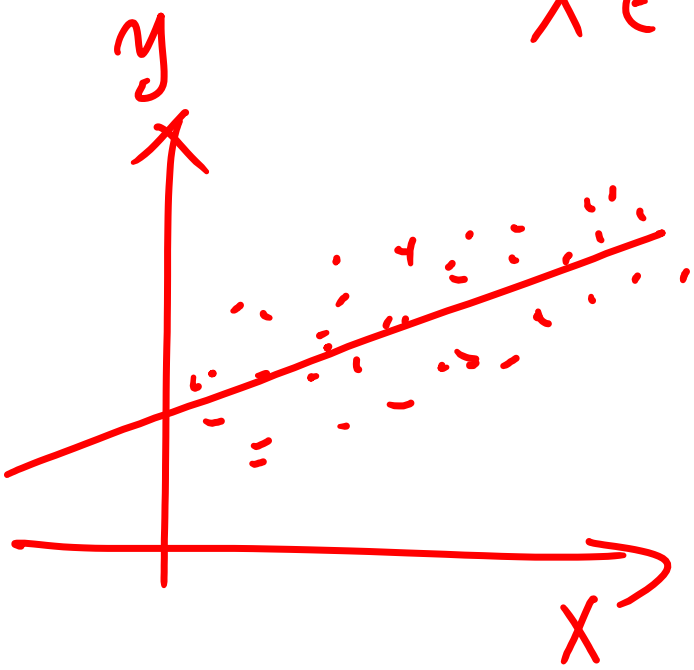
$\begin{cases} \vec{x} \in R^p \\ b \in R \end{cases}$

Q: How does this connect to linear regression?

[Regression]

$y \in R^1$

$\vec{X} \in R^p$, $p=1$ e.g.



$y = w^T x + w_0$

$-y + w^T x + w_0 = 0$

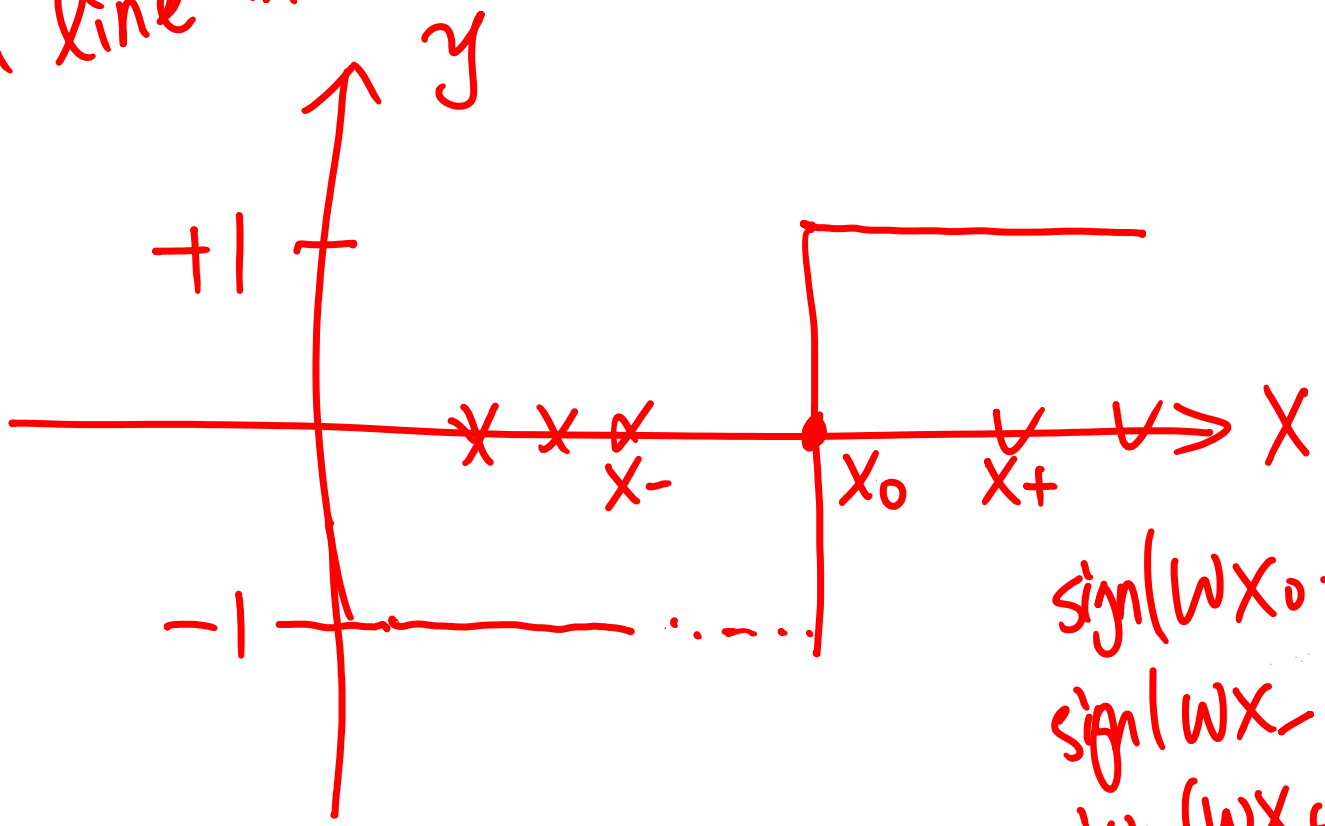
a line in (x, y) space

$p+1$

Binary Classification $y \in \{-1, 1\}$

[Decision Boundary is a line in R^p]

$X \in R^p$, $p = 1$ e.g.



(x, y)

$\text{sign}(wx_0 + b) = 0$

$\text{sign}(wx_- + b) = -1$

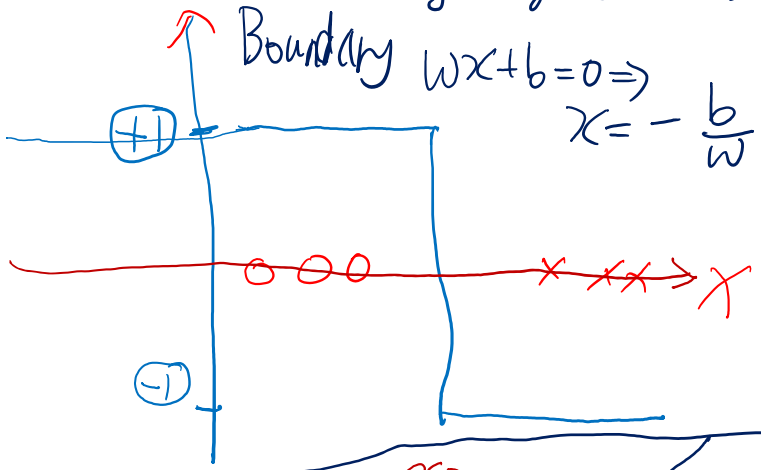
$\text{sign}(wx_+ + b) = +1$

Binary Classification

$y \in \{-1, 1\}$

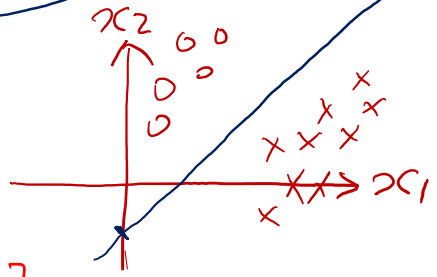
if $\Rightarrow$ 1D $[x \in R]$

$y = sign(wx+b)$



if $\Rightarrow$ 2D $[x \in R^2]$

Boundary $w^T x + b = 0$



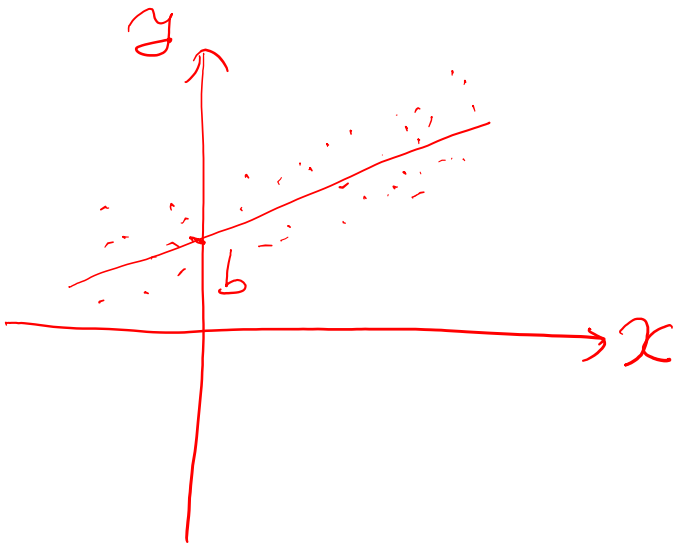
if $\Rightarrow$ P dim $[x \in R^P]$

Boundary : hyperplane

Regression

$y \in R$

if $\Rightarrow$ 1D $x \in R$



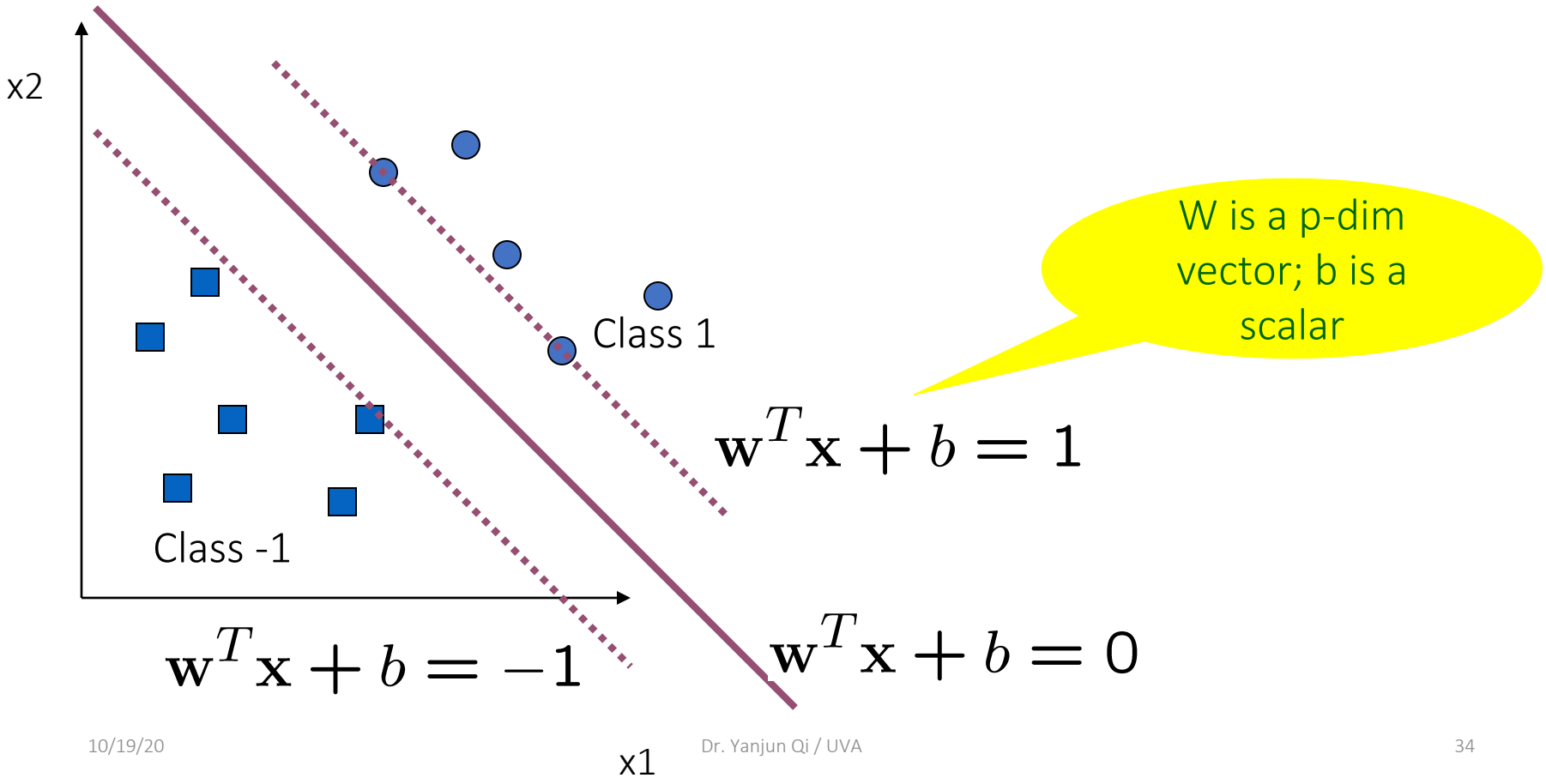
$y = wx + b$

$y = \vec{w}^T \vec{x} + b$ if $x \in R^P$

aka. $y - wx - b = 0$

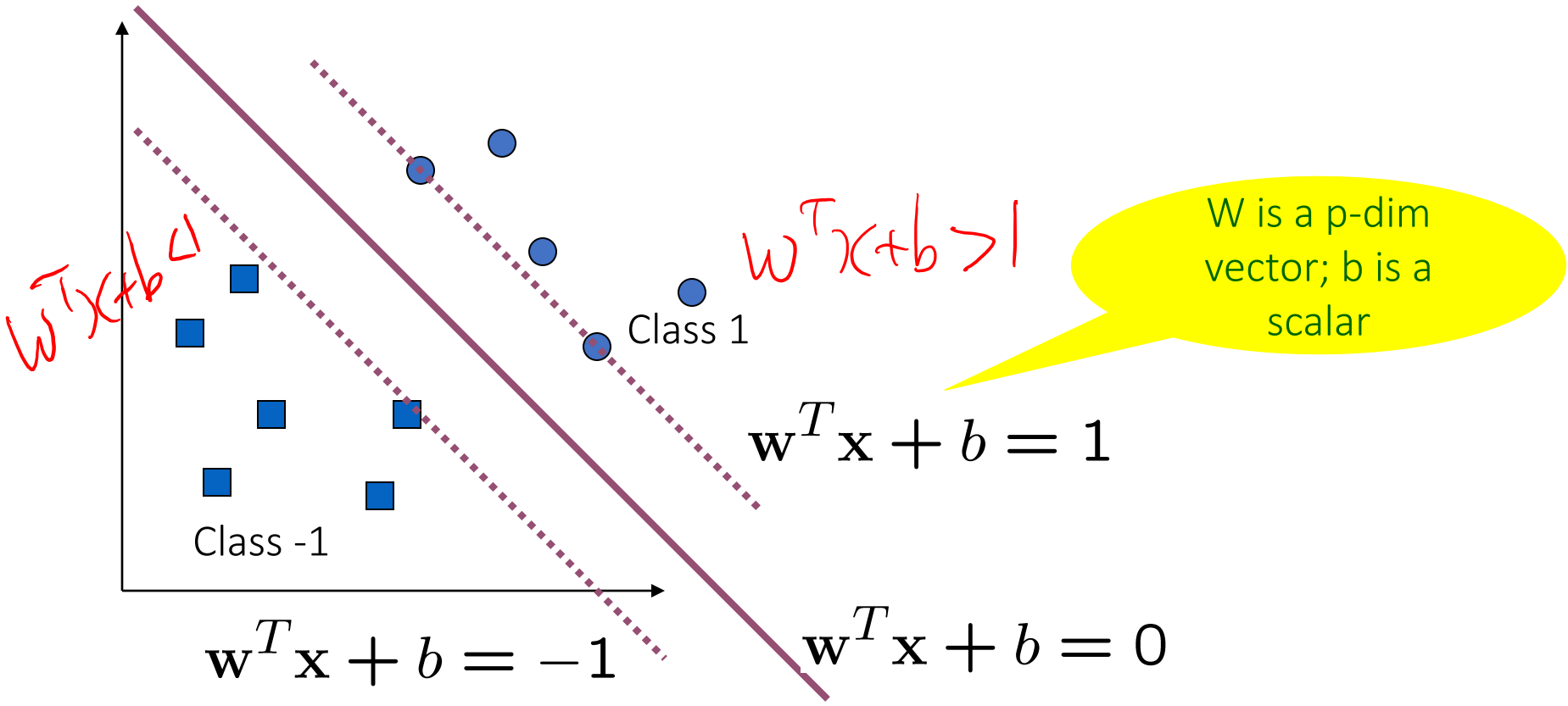
linear-line in 2-D space $\{x, y\}$

Max-margin & Decision Boundary



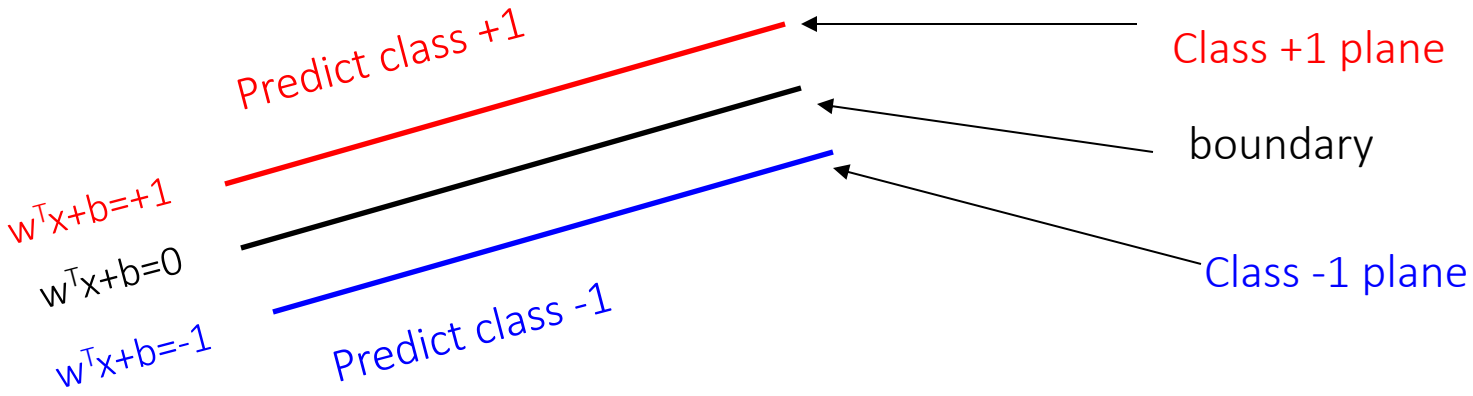
Max-margin & Decision Boundary $\mathbf{w}^T\mathbf{x} + b = 0$

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



$f(x,w,b) = \text{sign}(w^T x + b)$

Specifying a max margin classifier

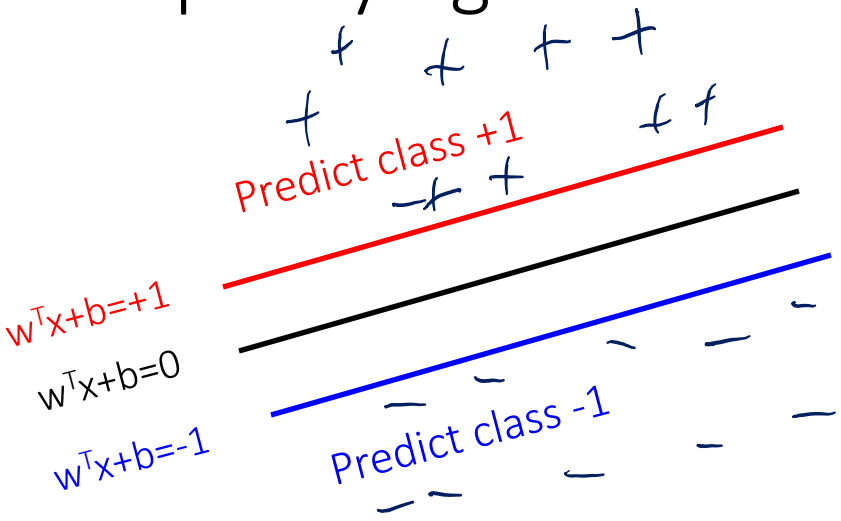


Classify as +1 if $w^T x+b >= 1$

Classify as -1 if $w^T x+b <= -1$

Undefined if $-1 < w^T x+b < 1$

Specifying a max margin classifier



Is the linear separation assumption realistic?

We will deal with this shortly, but lets assume it for now

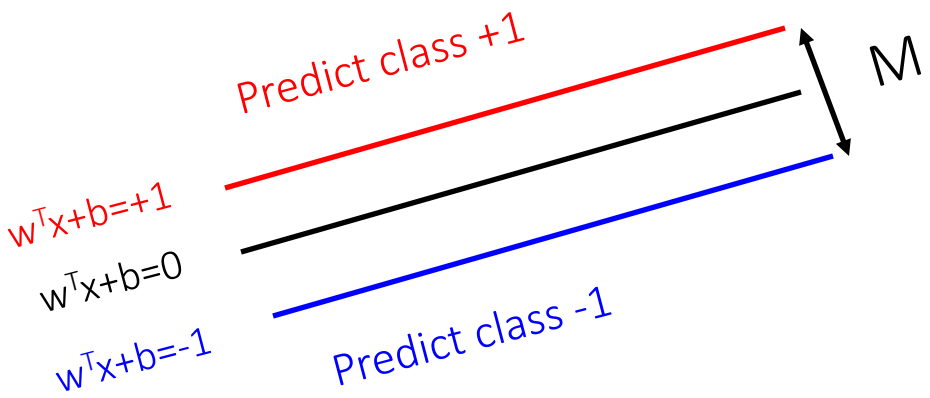
Classify as +1 if $w^T x+b >= 1$

Classify as -1 if $w^T x+b <= -1$

Undefined if $-1 < w^T x+b < 1$

Now Assuming such lines exist in our train

Maximizing the margin



Classify as +1 if $w^T x+b >= 1$

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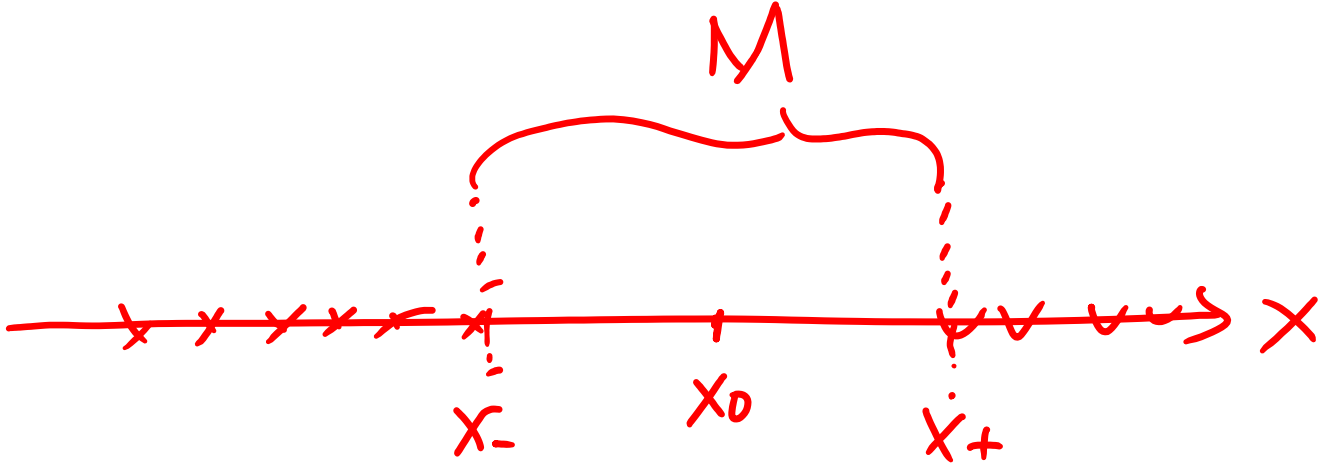
Undefined if $-1 < w^T x+b < 1$

- Let us define the width of the margin by M
- How can we encode our goal of maximizing M in terms of our parameters (w and b)?
- Lets start with a few observations

See Concrete derivations of M in Extra slides



$p = 1$

$\Rightarrow M = |x_+ - x_-|$

$= \frac{2}{w}$

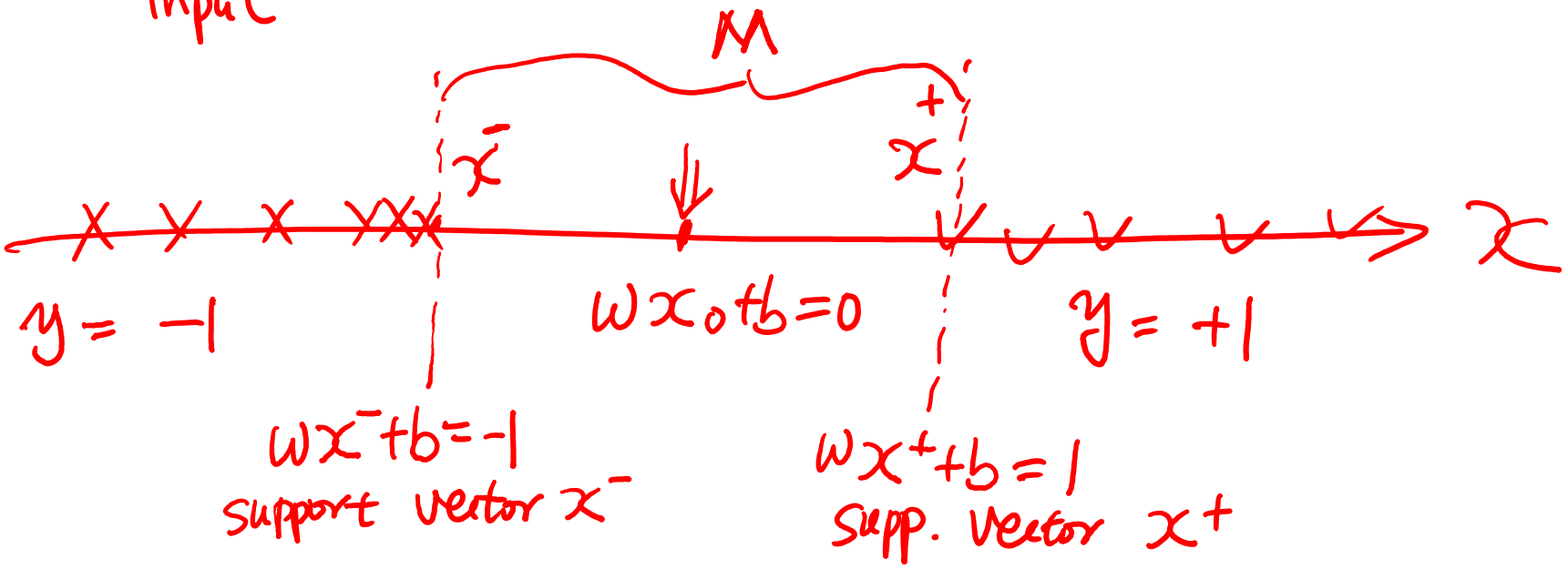
$$\begin{cases} w x_- + b = -1 \\ w x_+ + b = 1 \end{cases}$$

$\Downarrow$

$w(x_+ - x_-) = 2$

$\Rightarrow M = \frac{2}{\sqrt{w^T w}} \Rightarrow \max M \Rightarrow \min w^T w$

If 1-D input $\{x\} \rightarrow \{+1, -1\}$

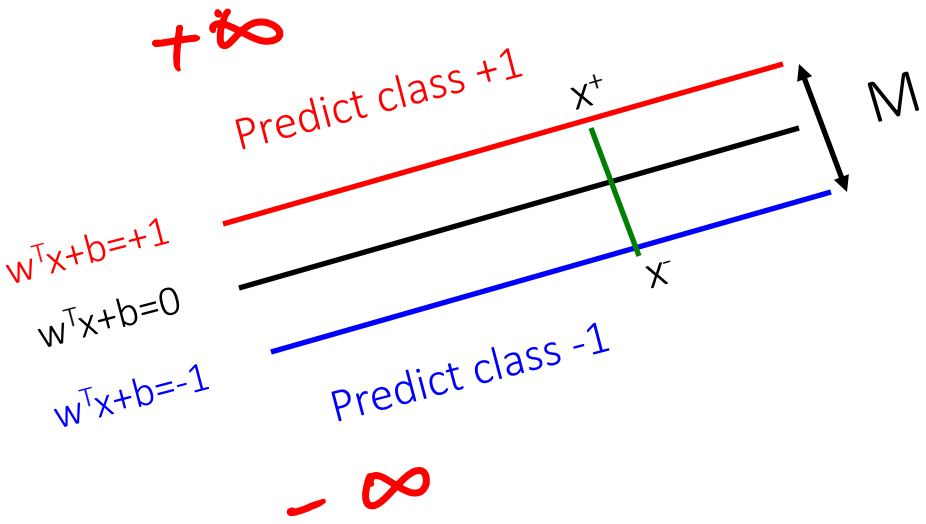


$$\Rightarrow \begin{cases} wx^- + b = -1 \\ wx^+ + b = 1 \end{cases} \Rightarrow w(x^+ - x^-) = 2$$

$$\text{margin } M = |x^+ - x^-| = \frac{2}{|w|}$$

(Interval when 1-D x)

Finding the optimal parameters



$$M = \frac{2}{\sqrt{w^T w}} = \frac{2}{||w||}$$

We can now search for the optimal parameters by finding a solution that:

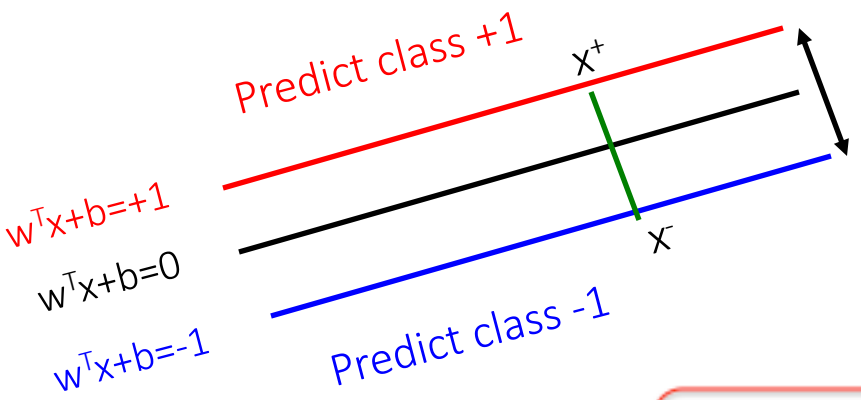
1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes $w^T w$)

Several optimization methods can be used: Gradient descent, OR SMO (see extra slides)

Today

- Support Vector Machine (SVM)
  - ✓ History of SVM
  - ✓ Large Margin Linear Classifier
  - ✓ Define Margin (M) in terms of model parameter
  - ✓ Optimization to learn model parameters (w, b)
  - ✓ Linearly Non-separable case
  - ✓ Optimization with dual form
  - ✓ Nonlinear decision boundary
  - ✓ Practical Guide

Optimization Step
i.e. learning optimal parameter for SVM

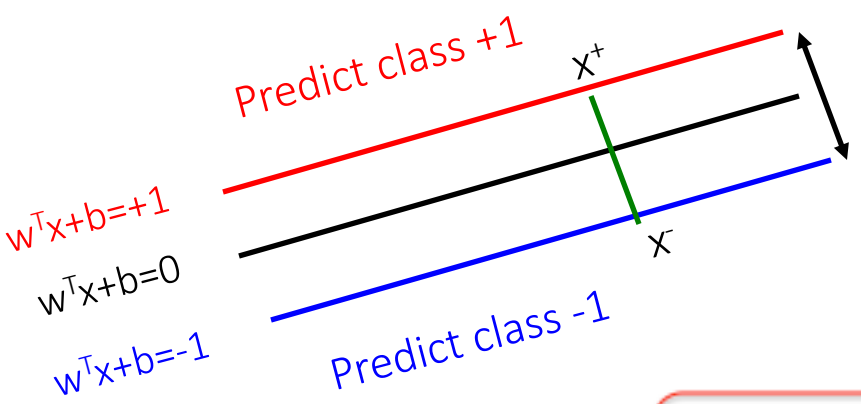


$$M = \frac{2}{\sqrt{w^T w}}$$

$$f(x,w,b) = \text{sign}(w^T x + b)$$

1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes $w^T w$)

Optimization Step
i.e. learning optimal parameter for SVM



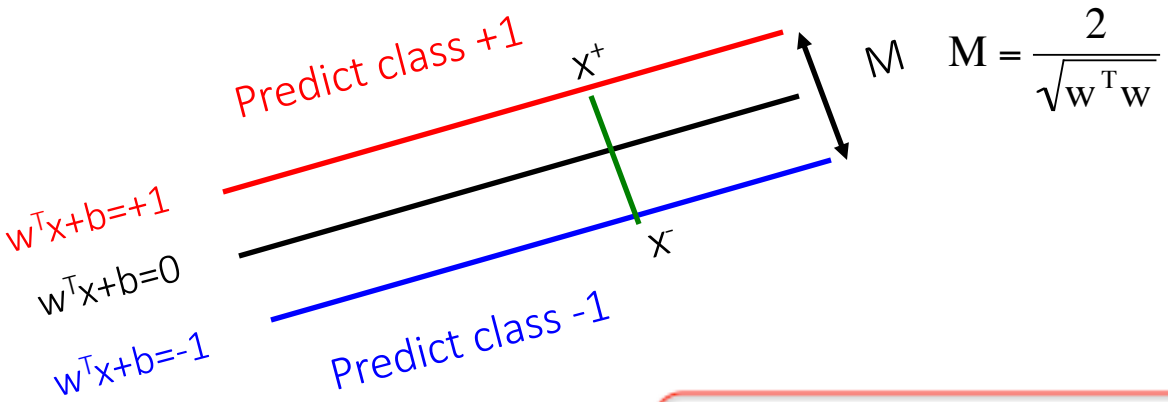
$$M = \frac{2}{\sqrt{w^T w}}$$

1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes $w^T w$)

Min $(w^T w)/2$

subject to the following constraints:

Optimization Step
i.e. learning optimal parameter for SVM



1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes $w^T w$)

Min $(w^T w)/2$

subject to the following constraints:

For all x in class + 1

$w^T x+b >= 1$

For all x in class - 1

$w^T x+b <= -1$

A total of n constraints if we have n training samples

Optimization Reformulation

$f(x,w,b) = \text{sign}(w^T x + b)$

1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes $w^T w$)

Min $(w^T w)/2$

subject to the following constraints:

For all x in class + 1

$w^T x+b >= 1$ $\quad y_i = 1$

For all x in class - 1

$w^T x+b <= -1$ $\quad y_i = -1$

A total of n constraints if we have n input samples

$\rightarrow$ pos $y_i = 1$, $w^T x_i + b \geq 1$

$y_i (w^T x_i + b) \geq 1$

$\rightarrow$ neg $y_i = -1$, $w^T x_i + b \leq -1$

$y_i (w^T x_i + b) \geq 1$

Optimization Reformulation

1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes $w^T w$)

Min $(w^T w)/2$

subject to the following constraints:

For all x in class + 1

$w^T x+b >= 1$

For all x in class - 1

$w^T x+b <= -1$

A total of n constraints if we have n input samples

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \sum_{i=1}^{p} w_i^2$$

$$\text{subject to } \forall \mathbf{x}_i \in Dtrain : y_i\left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq 1$$

$x_i^T w = w^T x_i$

Optimization Reformulation

$f(x,w,b) = \text{sign}(w^T x + b)$

1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes $w^T w$)

Min $(w^T w)/2$

subject to the following constraints:

For all x in class + 1

$w^T x+b >= 1$

For all x in class - 1

$w^T x+b <= -1$

} A total of n constraints if we have n input samples

$y_i \in \{+1, -1\}$

Quadratic Objective

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \sum_{i=1}^{p} w_i^2$$

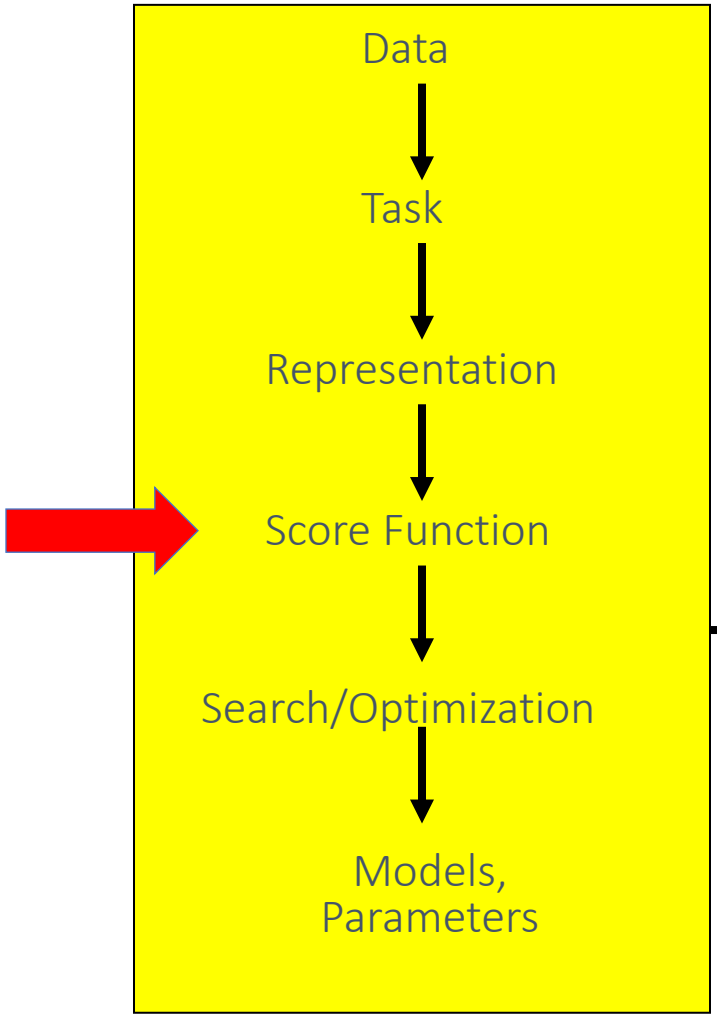
$$\text{subject to } \forall \mathbf{x}_i \in Dtrain : y_i\left(\mathbf{w}^T \mathbf{x}_i + b\right) \geq 1$$

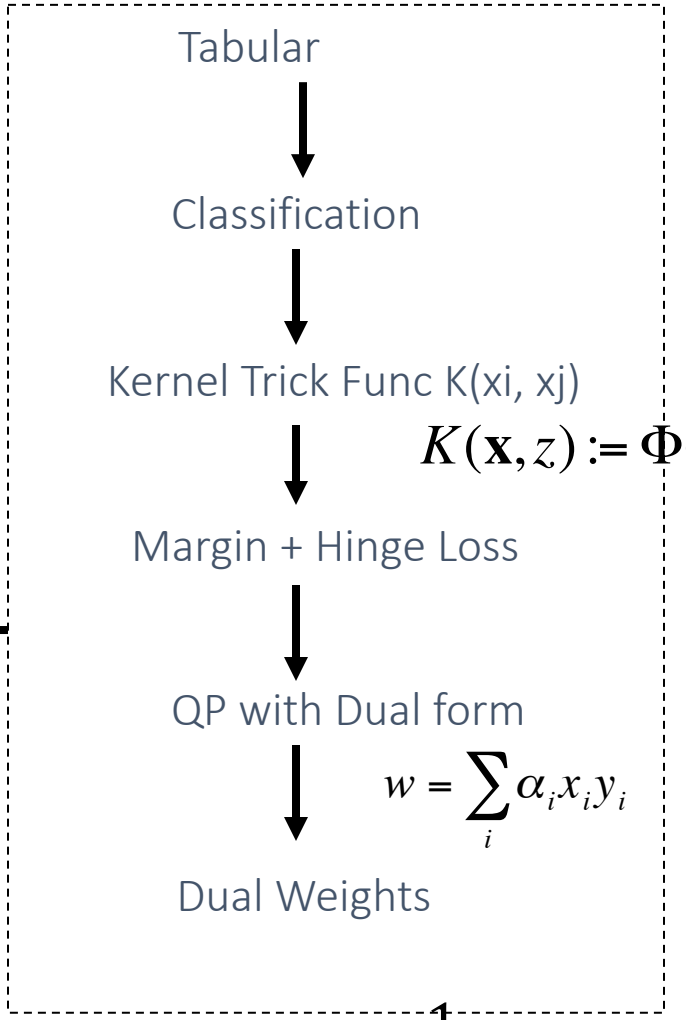
1×1 1×P P×1 1×1

1×1

Quadratic programming i.e.,
- Quadratic objective
- Linear constraints

Today: Basic Support Vector Machine





$$K(\mathbf{x}, z) := \Phi(\mathbf{x})^T \Phi(z)$$

$$w = \sum_i \alpha_i x_i y_i$$

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \sum_{i=1}^{p} w_i^2 + \mathrm{C} \sum_{\mathrm{i}=1}^{\mathrm{n}} \varepsilon_{\mathrm{i}}$$

$$\text{subject to } \forall \mathbf{x}_i \in Dtrain : y_i \left(\mathbf{x}_i \cdot \mathbf{w} + b \right) \geq 1 - \varepsilon_{\mathrm{i}}$$

$$\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y_i} y_j \mathbf{x_i}^T \mathbf{x_j}$$

$$\sum_i \alpha_i \mathrm{y_i} = 0, \qquad \alpha_i \geq 0 \qquad \forall i$$

What Next?

- Support Vector Machine (SVM)
  - ✓ History of SVM
  - ✓ Large Margin Linear Classifier
  - ✓ Define Margin (M) in terms of model parameter
  - ✓ Optimization to learn model parameters (w, b)
  - ✓ Linearly Non-separable case (soft SVM)
  - ✓ Optimization with dual form
  - ✓ Nonlinear decision boundary
  - ✓ Practical Guide

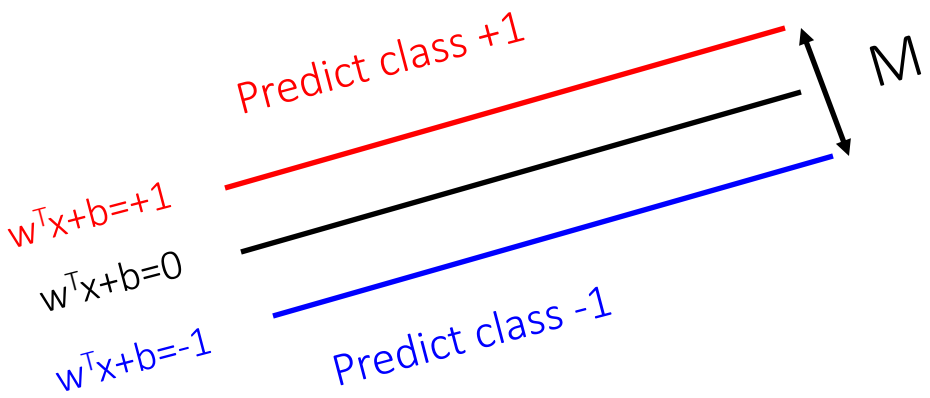

Thank You
Thank you

References

- Big thanks to Prof. Ziv Bar-Joseph and Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- Elements of Statistical Learning, by Hastie, Tibshirani and Friedman
- Prof. Andrew Moore @ CMU's slides
- Tutorial slides from Dr. Tie-Yan Liu, MSR Asia
- A Practical Guide to Support Vector Classification Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin, 2003-2010
- Tutorial slides from Stanford "Convex Optimization I — Boyd & Vandenberghe

EXTRA

How to define the width of the margin by M (EXTRA)



Classify as +1 if $w^T x+b >= 1$

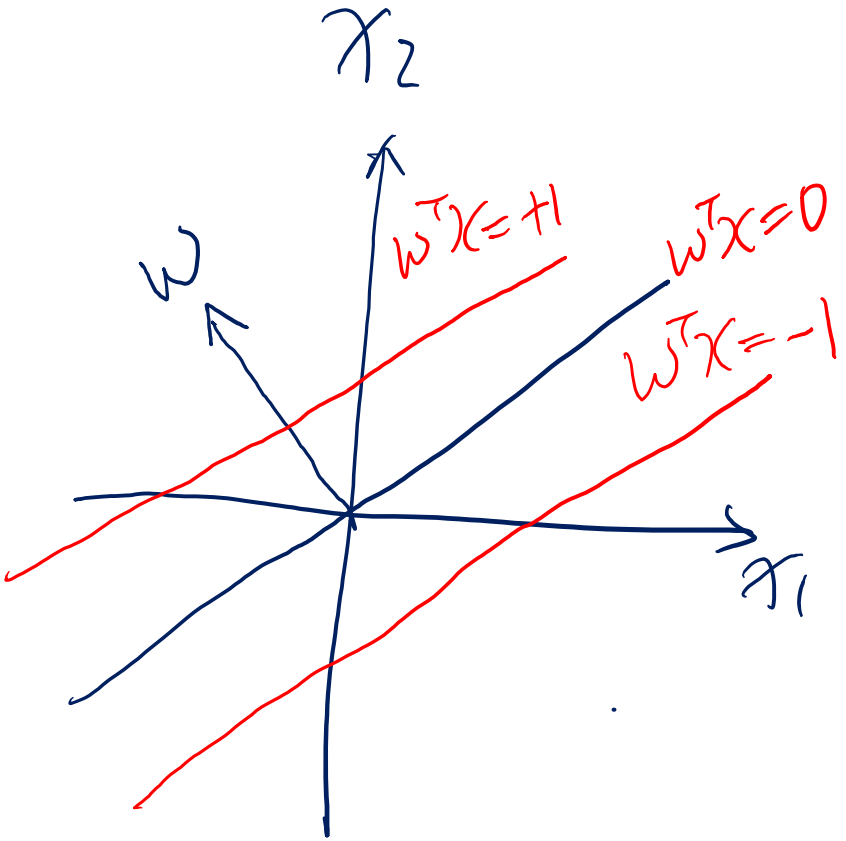
Classify as -1 if $w^T x+b <= -1$

Undefined if $-1 < w^T x+b < 1$

- Lets define the width of the margin by M
- How can we encode our goal of maximizing M in terms of our parameters (w and b)?
- Lets start with a few obsevrations

Concrete derivations of M see Extra

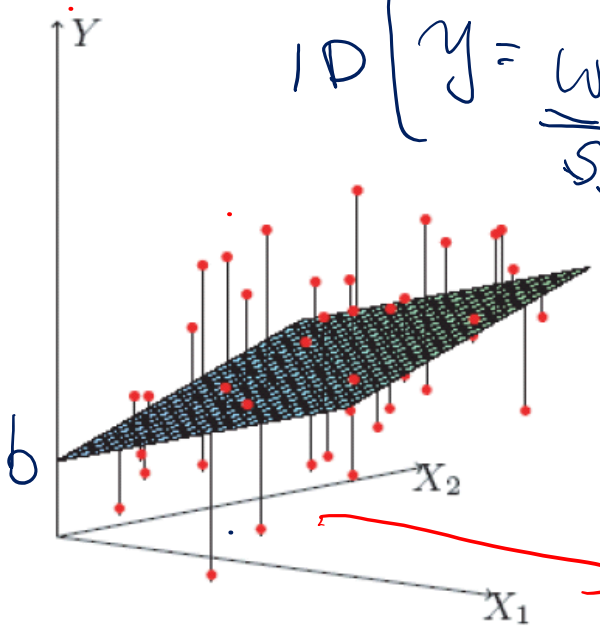
[Classification]



[Regression]

$$y = \vec{w}^T \vec{x} + b$$

$$\Delta X = \frac{\partial y}{\partial x} = \vec{w} \quad \text{slope}$$



1D $[y = wx + b]$

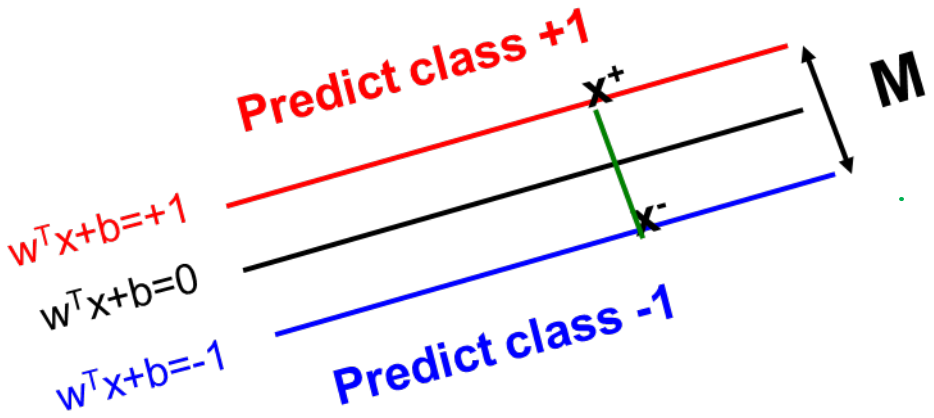
slope intercept

Bias

$\Delta X = w$

The gradient points in the direction of the greatest rate of increase of the function and its magnitude is the slope of the graph in that direction

Margin M



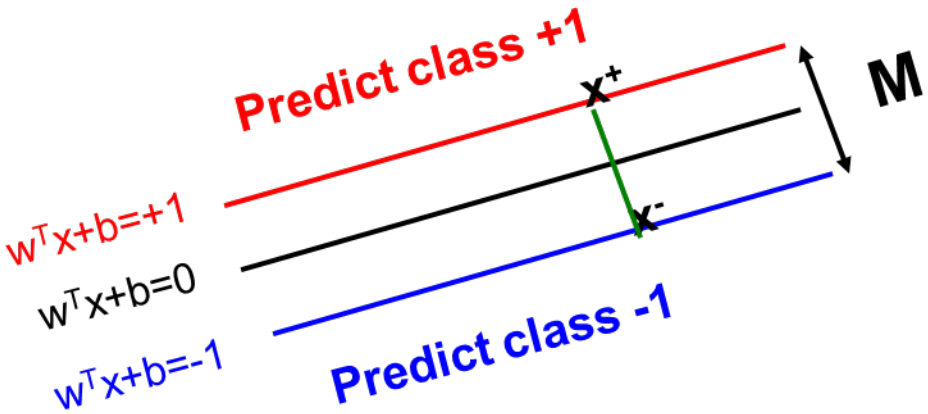
Classify as +1 if $w^Tx+b >= 1$

Classify as -1 if $w^Tx+b <= -1$

Undefined if $-1 < w^Tx+b < 1$

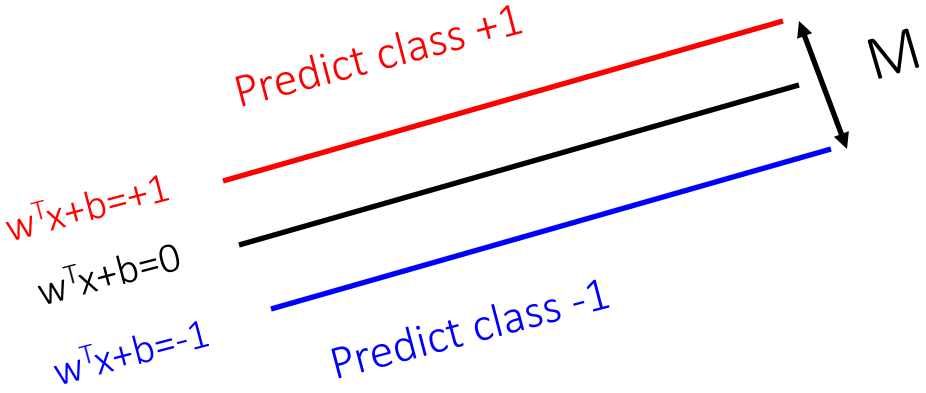
$M = |x^+ - x^-|$ length of vector $(x^+ - x^-)$

$\Rightarrow$ How to represent $(x^+ - x^-)$???



- $w^T x^+ + b = +1$
- $w^T x^- + b = -1$
- $M = | x^+ - x^- | = ?$

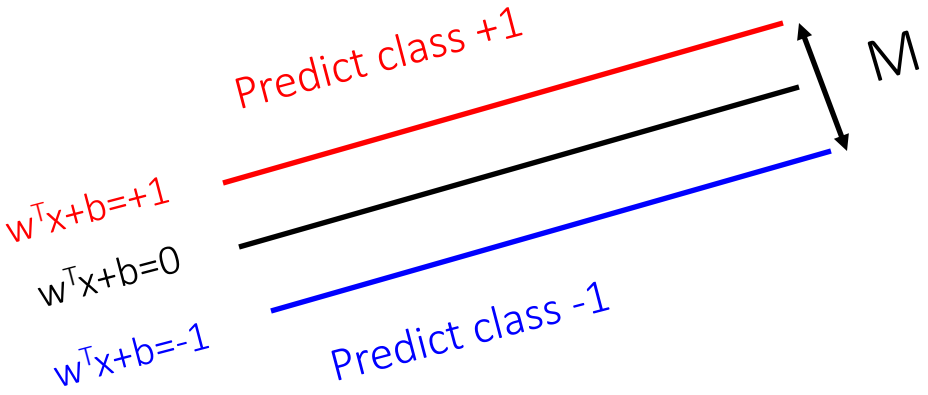
Maximizing the margin: observation-1



- Observation 1: the vector w is orthogonal to the +1 plane
- Why?

Corollary: the vector w is orthogonal to the -1 plane

Maximizing the margin: observation-1



Classify as +1 if $w^T x+b >= 1$

Classify as -1 if $w^T x+b <= -1$

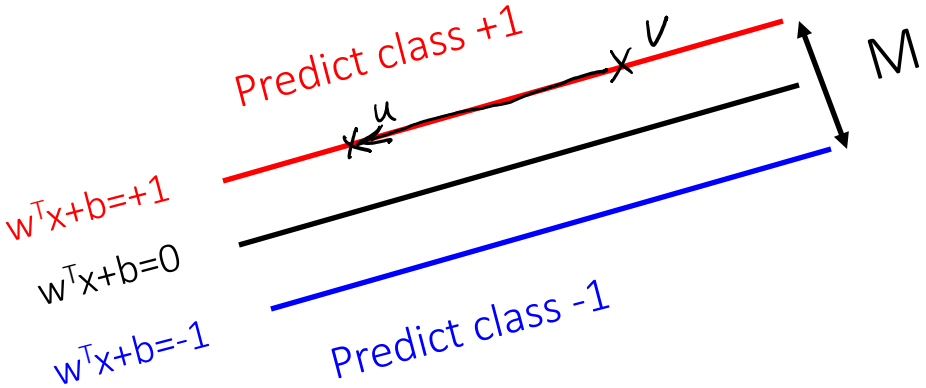
Undefined if $-1 < w^T x+b < 1$

- Observation 1: the vector w is orthogonal to the +1 plane
- Why?

Let u and v be two points on the +1 plane, then for the vector defined by u and v we have $w^T(u-v) = 0$

Corollary: the vector w is orthogonal to the -1 plane

Maximizing the margin: observation-1



Classify as +1 if $w^T x+b >= 1$

Classify as -1 if $w^T x+b <= -1$

Undefined if $-1 < w^T x+b < 1$

- Observation 1: the vector w is orthogonal to the +1 plane
- Why?

→ vector $(u-v)$ shown above

→ $w^T(u-v) = w^T u - w^T v = (1-b) - (1-b) = 0$

⇒ w orthogonal to $(u-v)$

Let u and v be two points on the +1 plane, then for the vector defined by u and v we have $w^T(u-v) = 0$

Corollary: the vector w is orthogonal to the -1 plane

Review :
Vector Product, Orthogonal, and Norm

For two vectors x and y,

$$x^T y$$

is called the (inner) vector product.

x and y are called orthogonal if

$$x^T y = 0$$

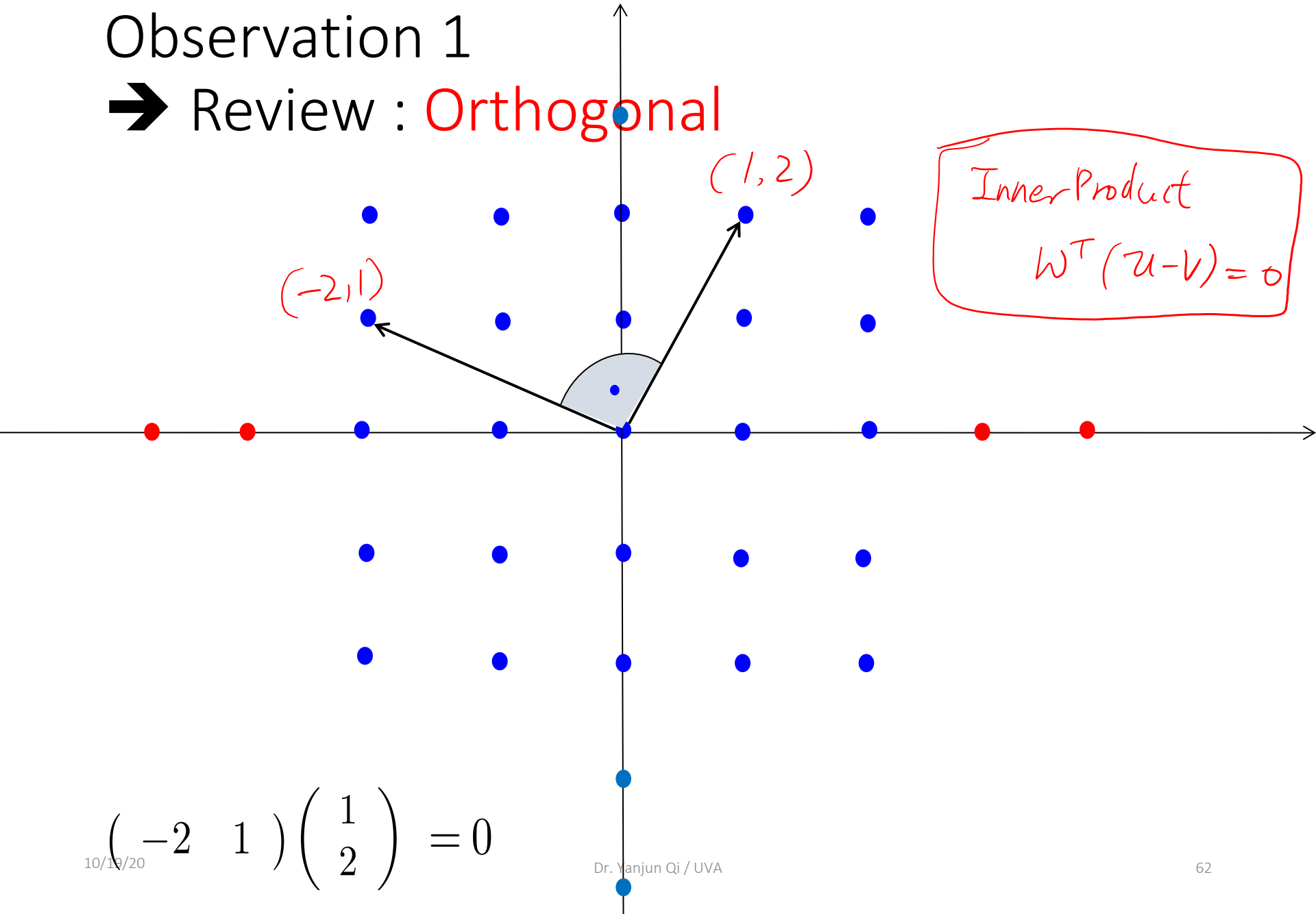
The square root of the product of a vector with itself,

$$\sqrt{x^T x}$$

is called the 2-norm ($|x|_2$), can also write as $|x|$

Observation 1

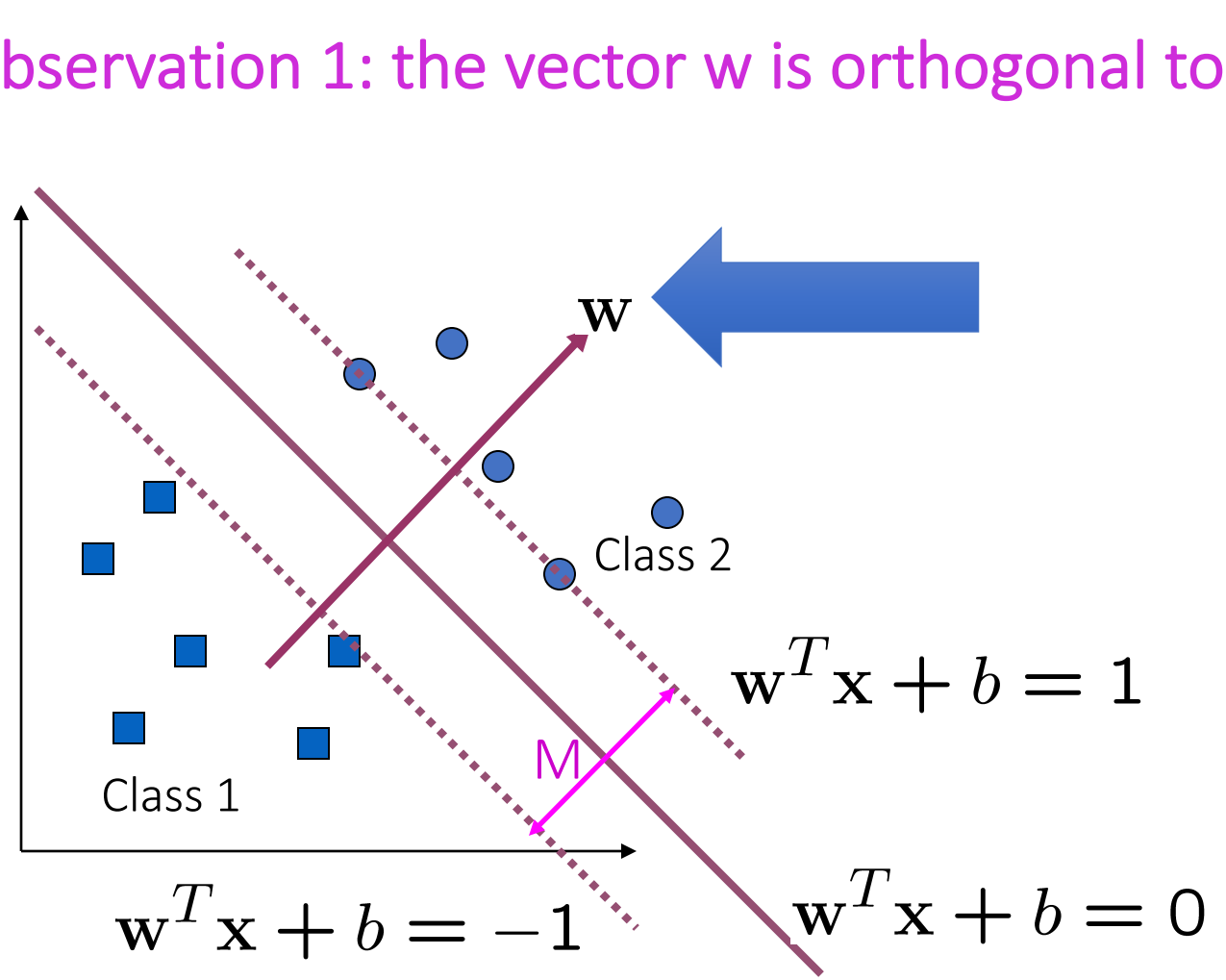
➔ Review : Orthogonal



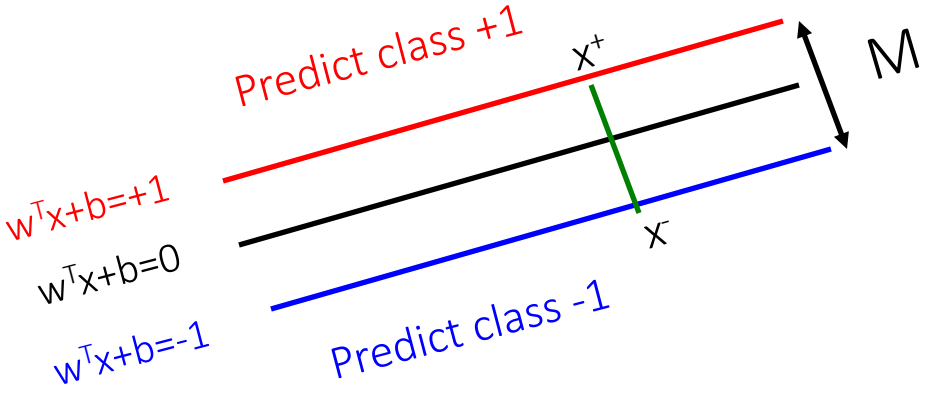
$$\begin{pmatrix} -2 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \end{pmatrix} = 0$$

Maximizing the margin: observation-1

- Observation 1: the vector w is orthogonal to the +1 plane



Maximizing the margin: observation-2



Classify as +1 if $w^Tx+b >= 1$

Classify as -1 if $w^Tx+b <= -1$

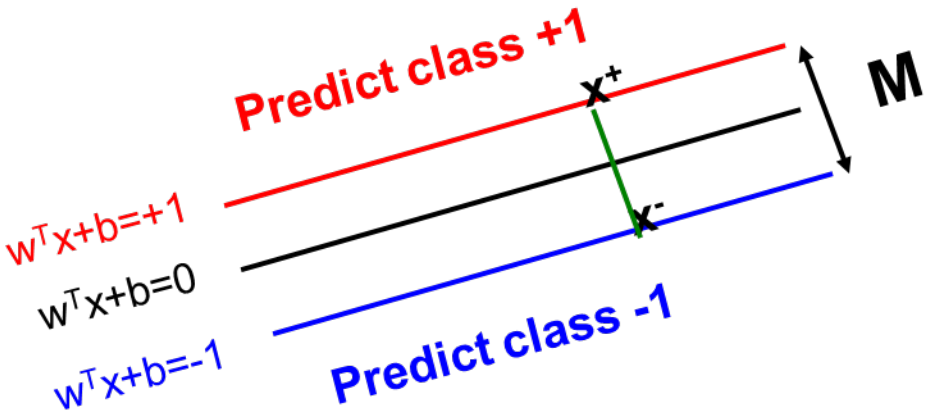
Undefined if $-1 < w^Tx+b < 1$

- Observation 1: the vector w is orthogonal to the +1 and -1 planes
- Observation 2: if x^+ is a point on the +1 plane and x^- is the closest point to x^+ on the -1 plane then

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

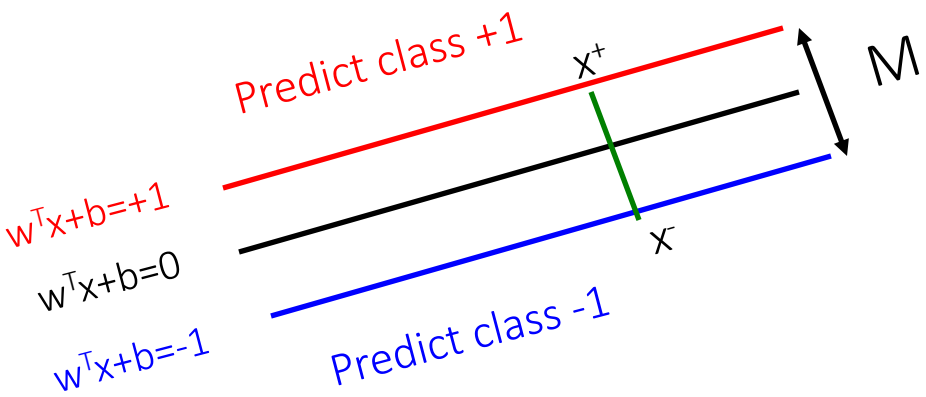
Since w is orthogonal to both planes we need to 'travel' some distance along w to get from x^+ to x^-

Putting it together



- $w^T x^+ + b = +1$
- $w^T x^- + b = -1$
- $M = | x^+ - x^- | = ?$
- $x^+ = \lambda w + x^-$

Putting it together



- $w^T x^+ + b = +1$
- $w^T x^- + b = -1$
- $x^+ = \lambda w + x^-$
- $| x^+ - x^- | = M$

We can now define M in terms of w and b

$$M = |x^+ - x^-|$$
$$= |\lambda w|$$
$$= \lambda |w|$$
$$= \lambda \sqrt{w^T w}$$
$$= \frac{2}{w^T w} \sqrt{w^T w}$$
$$\left[= \frac{2}{\sqrt{w^T w}} \right]$$

$$w^T x^+ + b = 1$$

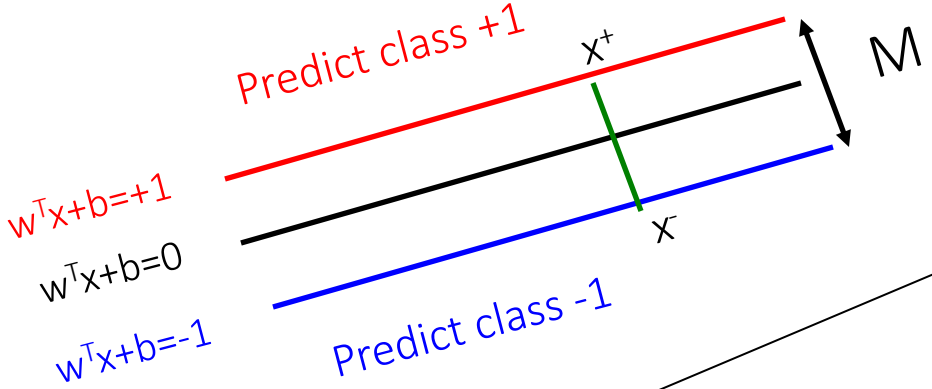
$$w^T(\lambda w + x^-) + b = +1$$

$$\lambda w^T w + \underbrace{w^T x^- + b}_{\Rightarrow -1} = 1$$

$$\lambda w^T w = 2$$

$$\Rightarrow \lambda = \frac{2}{w^T w}$$

Putting it together



- $w^T x^+ + b = +1$
- $w^T x^- + b = -1$
- $x^+ = \lambda w + x^-$
- $| x^+ - x^- | = M$

$w^T x^+ + b = +1$

=>

$w^T (\lambda w + x^-) + b = +1$

=>

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

=>

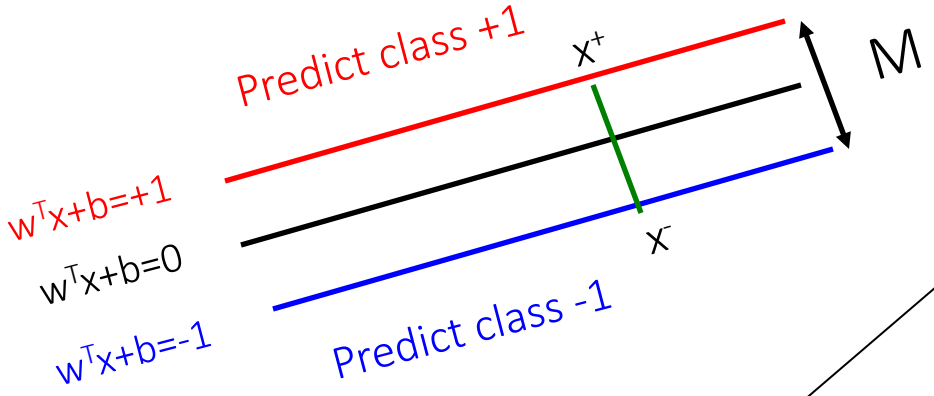
$-1 + \lambda w^T w = +1$

=>

$\lambda = 2/w^T w$

We can now define M in terms of w and b

Putting it together



- $w^T x^+ + b = +1$
- $w^T x^- + b = -1$
- $x^+ = \lambda w + x^-$
- $| x^+ - x^- | = M$
- $\lambda = 2/w^T w$

$M = |x^+ - x^-|$

=>

$$M = |\lambda w| = \lambda |w| = \lambda \sqrt{w^T w}$$

=>

$$M = 2\frac{\sqrt{w^T w}}{w^T w} = \frac{2}{\sqrt{w^T w}}$$

max (M)

$\Rightarrow$ min ($w^T w$)

We can now define M in terms of w and b