Fall 2022 ECEN 758
Data Mining & Analysis
Support Vector Machines

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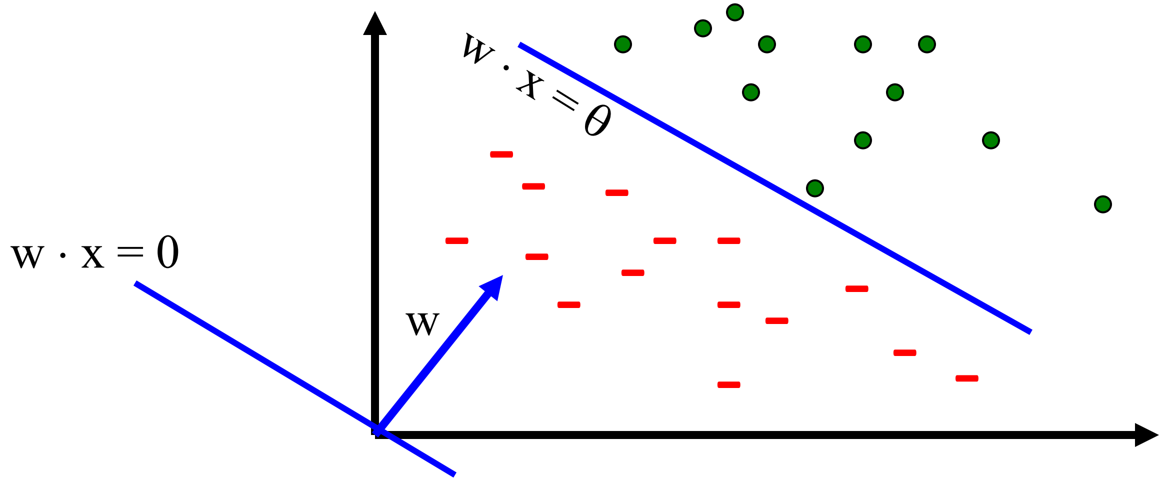
Mining of Massive Datasets, http://www.mmds.org

Linear models for classification

- **Binary classification:**

$$f(\mathbf{x}) = \begin{cases} +1 & \text{if} \quad \mathbf{w}^{(1)}\,\mathbf{x}^{(1)} + \mathbf{w}^{(2)}\,\mathbf{x}^{(2)} + \ldots \mathbf{w}^{(d)}\,\mathbf{x}^{(d)} \geq \theta \\ -1 & \text{otherwise} \end{cases}$$

- **Input: Vectors x_j and labels y_j**
  - Vectors x_j are real valued where $\|x\|_2 = 1$
- **Goal: Find vector $w = (w^{(1)}, w^{(2)}, \ldots, w^{(d)})$**
  - Each $w^{(i)}$ is a real number



Decision boundary is **linear**

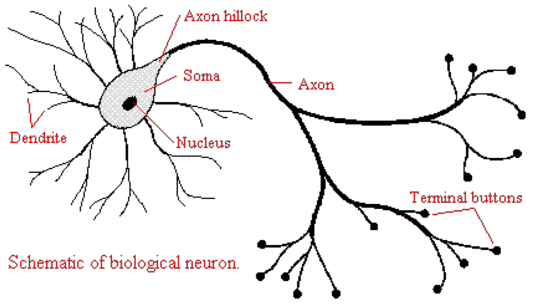
Note:

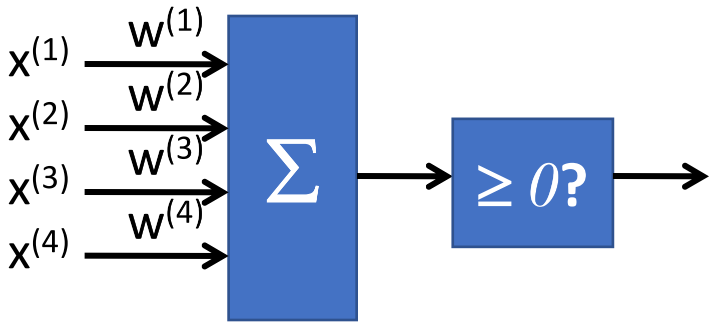
$$\mathbf{x} \rightarrow \langle \mathbf{x}, 1 \rangle \quad \forall \mathbf{x}$$

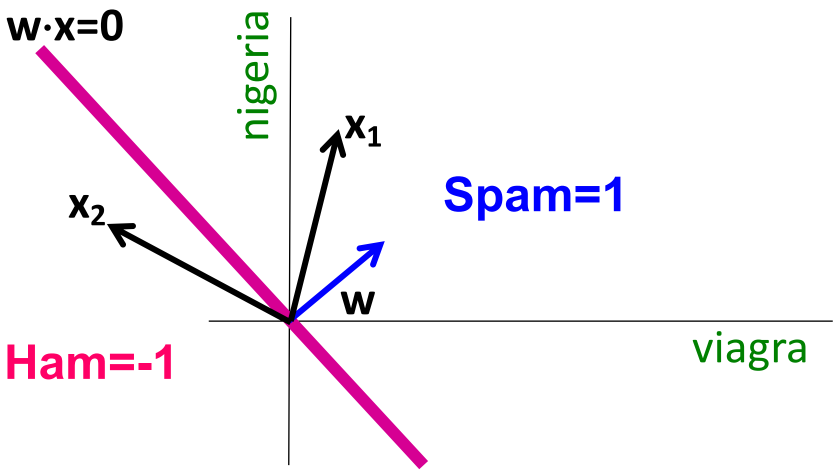
$$\mathbf{w} \rightarrow \langle \mathbf{w}, -\theta \rangle$$

Perceptron [Rosenblatt '58]

- **(Very) loose motivation: Neuron**
- **Inputs are feature values**
- **Each feature has a weight w_i**
- **Activation is the sum:**
  - $f(x) = \sum_i^d w^{(i)} x^{(i)} = w \cdot x$
- **If the *f(x)* is:**
  - **Positive:** Predict **+1**
  - **Negative:** Predict **-1**







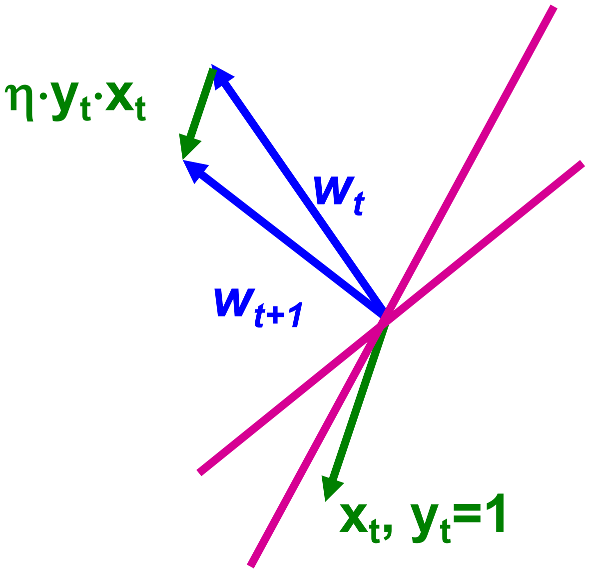
Perceptron

Note that the Perceptron is a conservative algorithm: it ignores samples that it classifies correctly.

- **Perceptron: $y' = sign(w \cdot x)$**
- **How to find parameters w?**
  - Start with $w_0 = 0$
  - Pick training examples x_t **one by one**
  - Predict class of x_t using current w_t
    - $y' = sign(w_t \cdot x_t)$
  - **If y' is correct (i.e., $y_t = y'$)**
    - No change: $w_{t+1} = w_t$
  - **If y' is wrong:** Adjust w_t

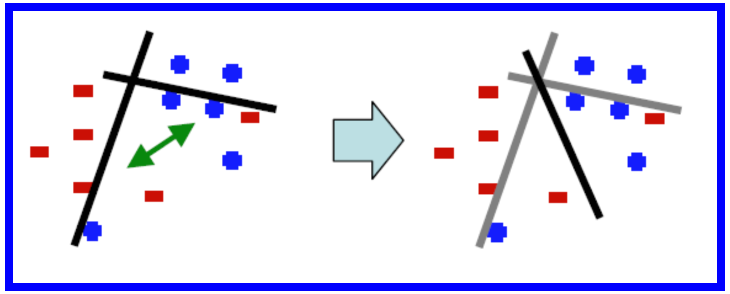
$$w_{t+1} = w_t + \eta \cdot y_t \cdot x_t$$

- η is the learning rate parameter
- x_t is the t-th training example
- y_t is true t-th class label ({+1, -1})

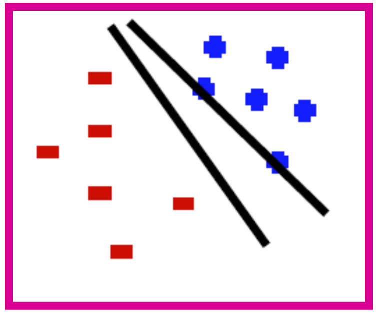


Perceptron: The Good and the Bad

- **Good: Perceptron convergence theorem:**
  - If there exist a set of weights that are consistent (i.e., the data is linearly separable) the Perceptron learning algorithm will converge
- **Bad: Never converges:**
  If the data is not separable weights dance around indefinitely



- **Bad: Mediocre generalization:**
  - Finds a “barely” separating solution



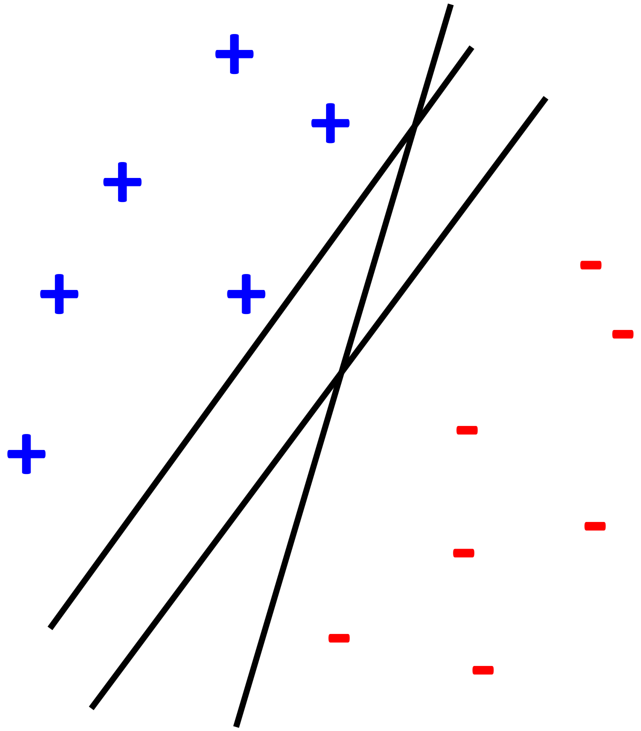
Updating the Learning Rate

- **Perceptron will oscillate and won't converge**
- **So, when to stop learning?**
- **(1) Slowly decrease the learning rate η**
  - A classic way is to: $\eta = \mathbf{c_1/(t + c_2)}$
    - But, we also need to determine constants $\mathbf{c_1}$ and $\mathbf{c_2}$
- **(2) Stop when the training error stops chaining**
- **(3) Have a small test dataset and stop when the test set error stops decreasing**
- **(4) Stop when we reached some maximum number of passes over the data**

Support Vector Machines

Support Vector Machines

- **Want to separate "+" from "-" using a line**



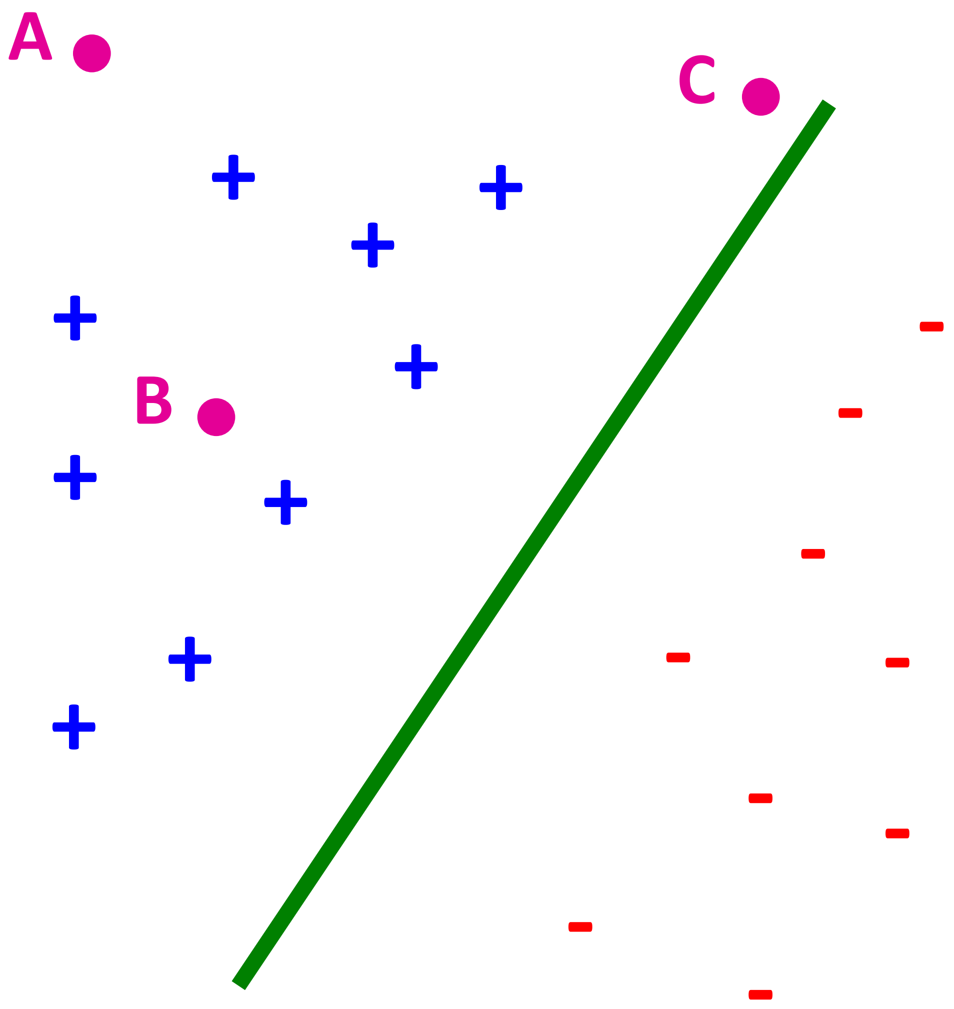
Data:

- **Training examples:**
  - **$(x_1, y_1) \ldots (x_n, y_n)$**
- **Each example *i*:**
  - **$x_i = (x_i^{(1)}, \ldots , x_i^{(d)})$**
    - $x_i^{(j)}$ is real valued
  - **$y_i \in \{ -1, +1 \}$**
- **Inner product:**

$$\boldsymbol{w} \cdot \boldsymbol{x} = \sum_{j=1}^{d} w^{(j)} \cdot x^{(j)}$$

Which is best linear separator (defined by *w*)?

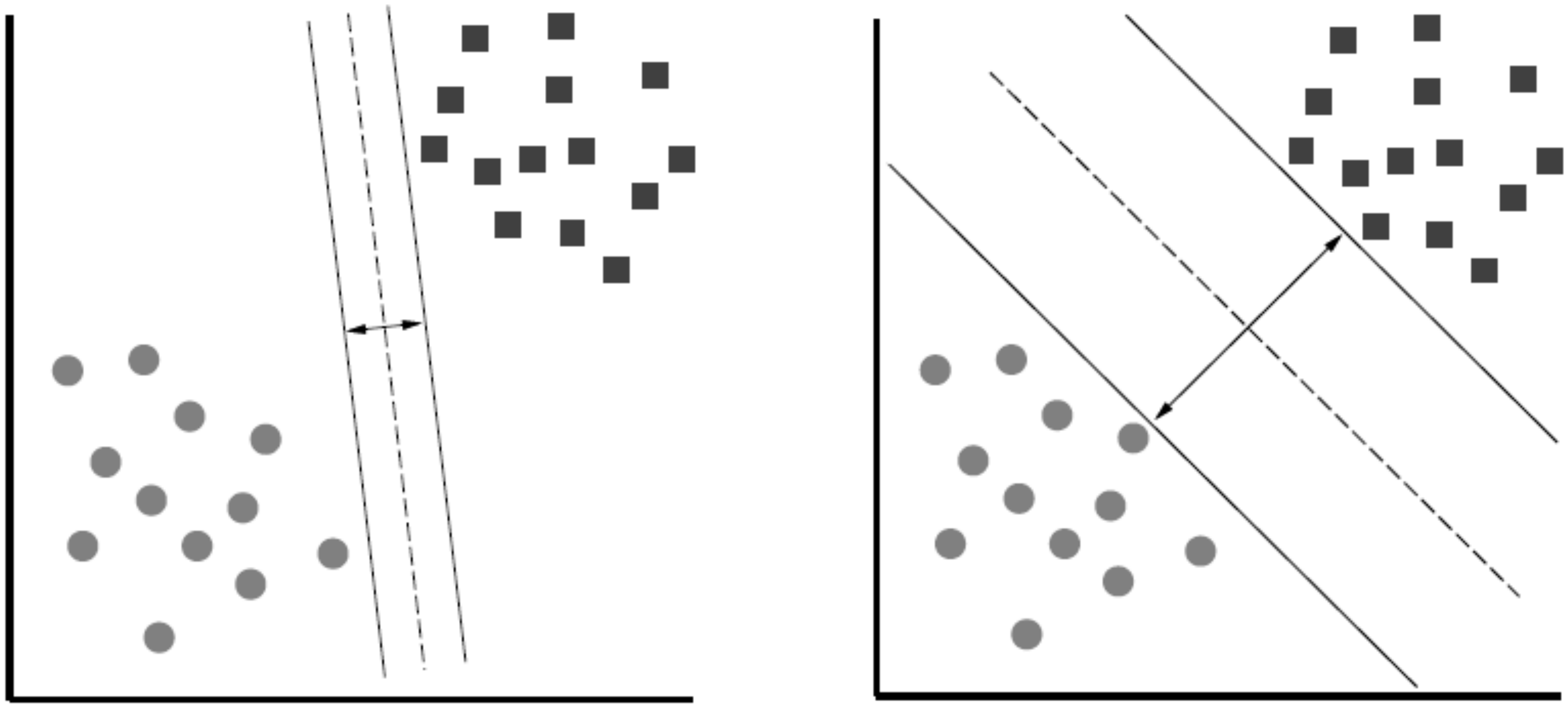
Largest Margin



- **Distance from the separating hyperplane corresponds to the "confidence" of prediction**
- **Example:**
  - We are more sure about the class of **A** and **B** than of **C**

Largest Margin

- **Margin γ: Distance of closest example from the decision line/hyperplane**



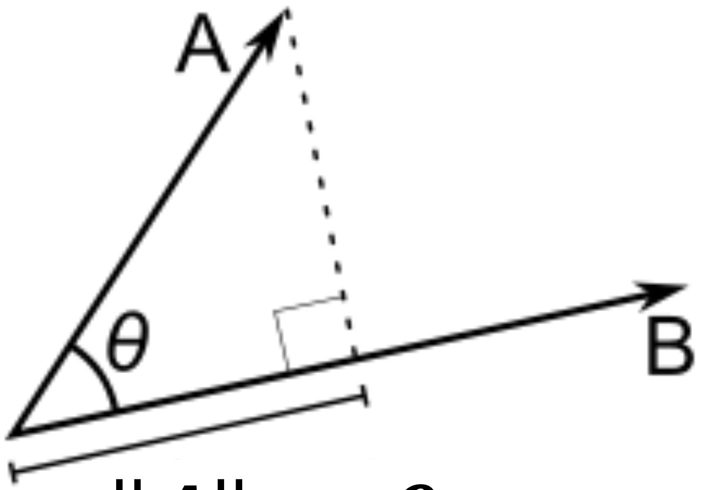
The reason we define margin this way is due to theoretical convenience and existence of generalization error bounds that depend on the value of margin.

Why maximizing $\boldsymbol{\gamma}$ a good idea?

- **Remember: Dot product**

  $$\boldsymbol{A \cdot B = \|A\| \cdot \|B\| \cdot \cos\theta}$$

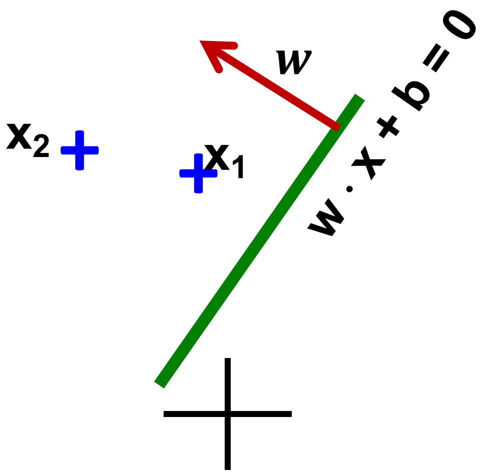
$$\|A\| = \sqrt{\sum_{j=1}^{d} (A^{(j)})^2}$$

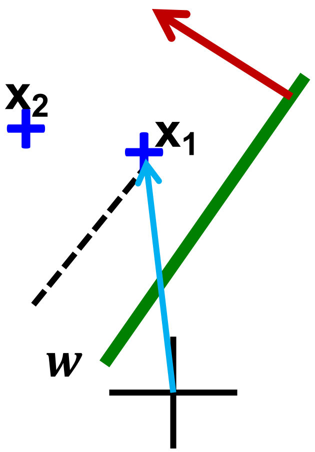


$$\|A\| cos\theta$$

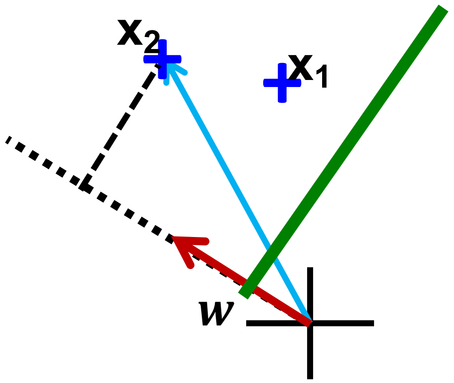
Why maximizing $\boldsymbol{\gamma}$ a good idea?

- **Dot product**
  $$\boldsymbol{A \cdot B = \|A\|\|B\| \cos\theta}$$
- **What is $\boldsymbol{w \cdot x_1}$, $\boldsymbol{w \cdot x_2}$?**





In this case
$\gamma_1 \approx \|w\|^2$



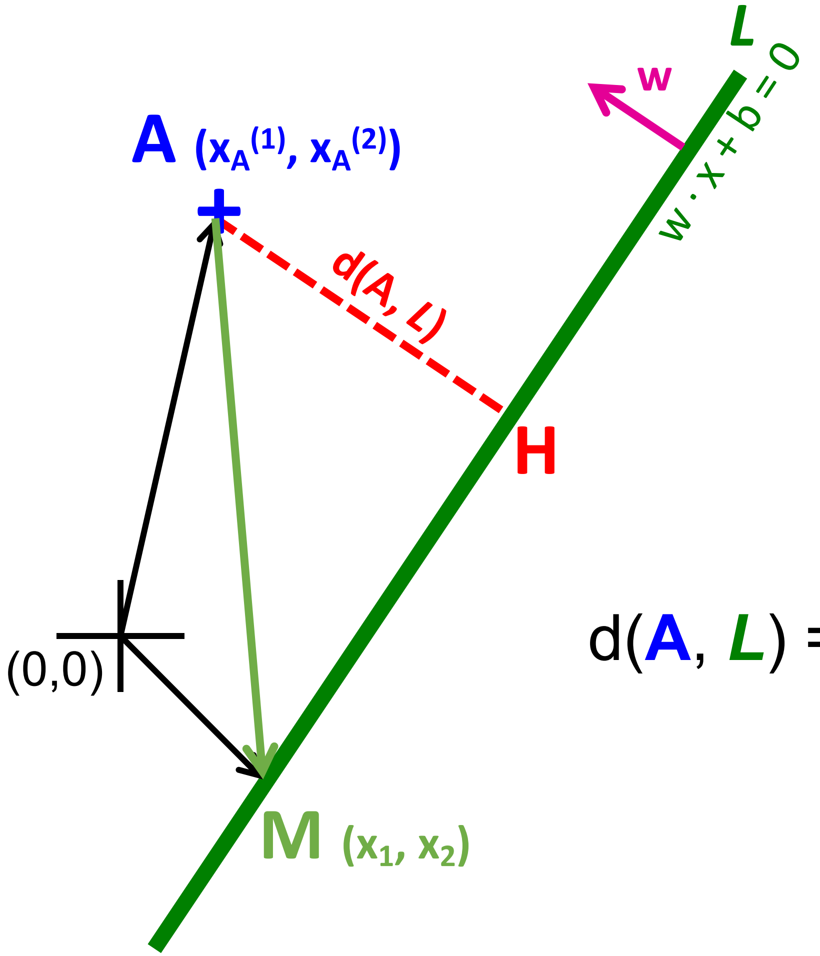
In this case
$\gamma_2 \approx 2\|w\|^2$

- **So, γ roughly corresponds to the margin**
  - Bigger γ bigger the separation

What is the margin?

Note we assume $\|w\|_2 = 1$

- **Let:**
  - **Line L**: **w·x+b** = $w^{(1)}x^{(1)}+w^{(2)}x^{(2)}+b=0$
  - **w** = $(w^{(1)}, w^{(2)})$
  - **Point A** = $(x_A^{(1)}, x_A^{(2)})$
  - **Point M** on a line = $(x_M^{(1)}, x_M^{(2)})$

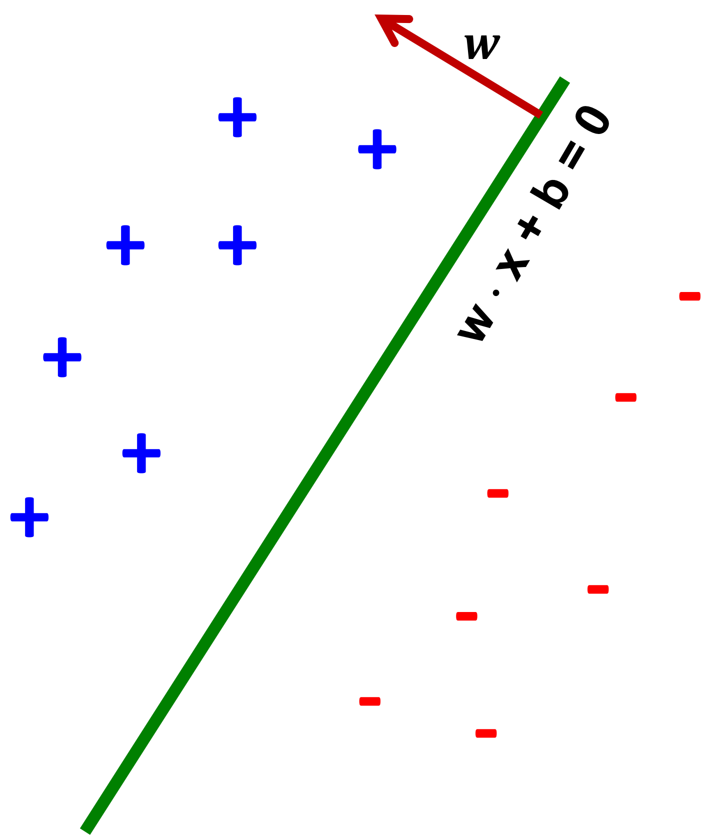


$$
\begin{aligned}
d(A, L) &= |AH| \\
&= |(A-M) \cdot w| \\
&= |(x_A^{(1)} - x_M^{(1)})\, w^{(1)} + (x_A^{(2)} - x_M^{(2)})\, w^{(2)}| \\
&= x_A^{(1)} w^{(1)} + x_A^{(2)} w^{(2)} + b \\
&= w \cdot A + b
\end{aligned}
$$

Distance from a point to a line

Remember $x_M^{(1)}w^{(1)} + x_M^{(2)}w^{(2)} = -b$ since **M** belongs to line **L**

Largest Margin



- **Prediction = sign($w \cdot x + b$)**
- **"Confidence" = $(w \cdot x + b)\, y$**
- **For i-th datapoint:**

$$\gamma_i = (w \cdot x_i + b) y_i$$

- **Want to solve:**

$$\max_{w} \min_{i} \gamma_i$$

- **Can rewrite as**

$$\max_{w,\gamma} \gamma$$

$$s.t. \forall i, y_i (w \cdot x_i + b) \geq \gamma$$

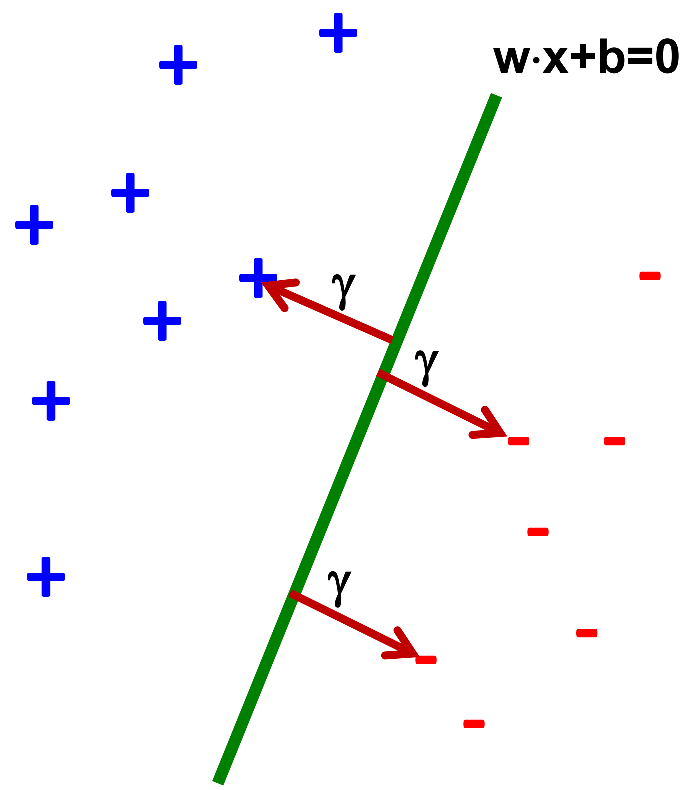
Support Vector Machine

- **Maximize the margin:**
  - **Good according to intuition, theory (VC dimension) & practice**

$$\max_{w,\gamma} \gamma$$

$$s.t. \forall i, y_i (w \cdot x_i + b) \geq \gamma$$

  - **γ is margin … distance from the separating hyperplane**

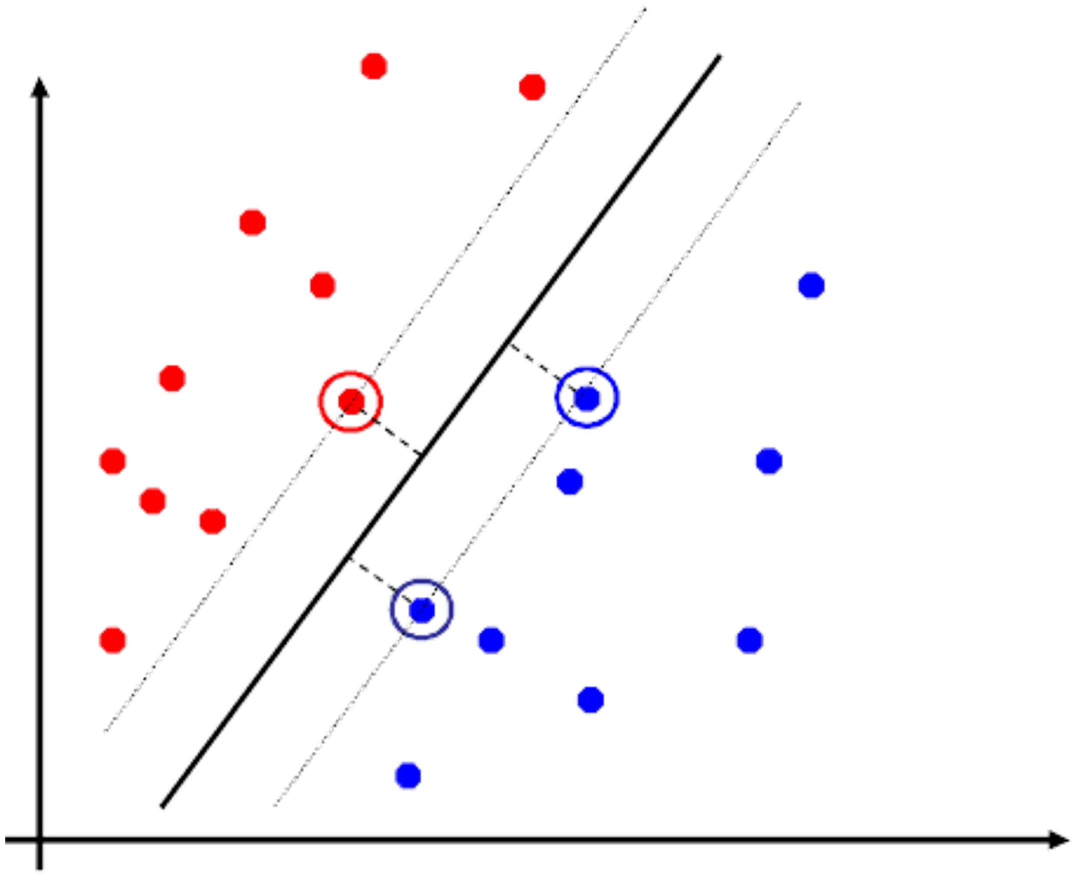


Maximizing the margin

Support Vector Machines: Deriving the margin

Support Vector Machines

- **Separating hyperplane is defined by the support vectors**
  - Points on **+/-** planes from the solution
  - If you knew these points, you could ignore the rest
  - Generally, $d+1$ support vectors (for d dim. data)

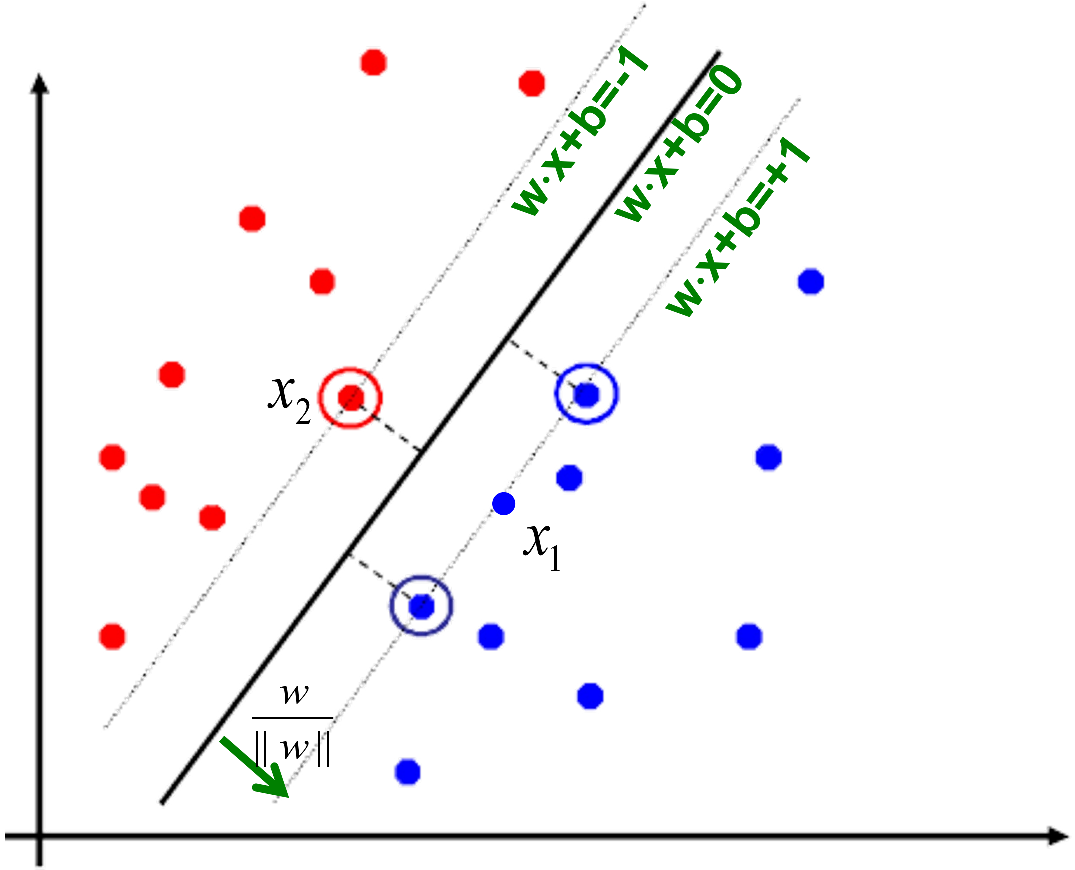


Canonical Hyperplane: Problem

- **Problem:**
  - Let $(\boldsymbol{w}\cdot\boldsymbol{x} + \boldsymbol{b})\boldsymbol{y} = \boldsymbol{\gamma}$
    then $(\mathbf{2}\boldsymbol{w}\cdot\boldsymbol{x} + \mathbf{2}\boldsymbol{b})\boldsymbol{y} = \mathbf{2}\boldsymbol{\gamma}$
    - Scaling ***w*** increases margin!
- **Solution:**
  - **Work with normalized *w*:**

$$\boldsymbol{\gamma} = \left(\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}\cdot\boldsymbol{x} + \boldsymbol{b}\right)\boldsymbol{y}$$

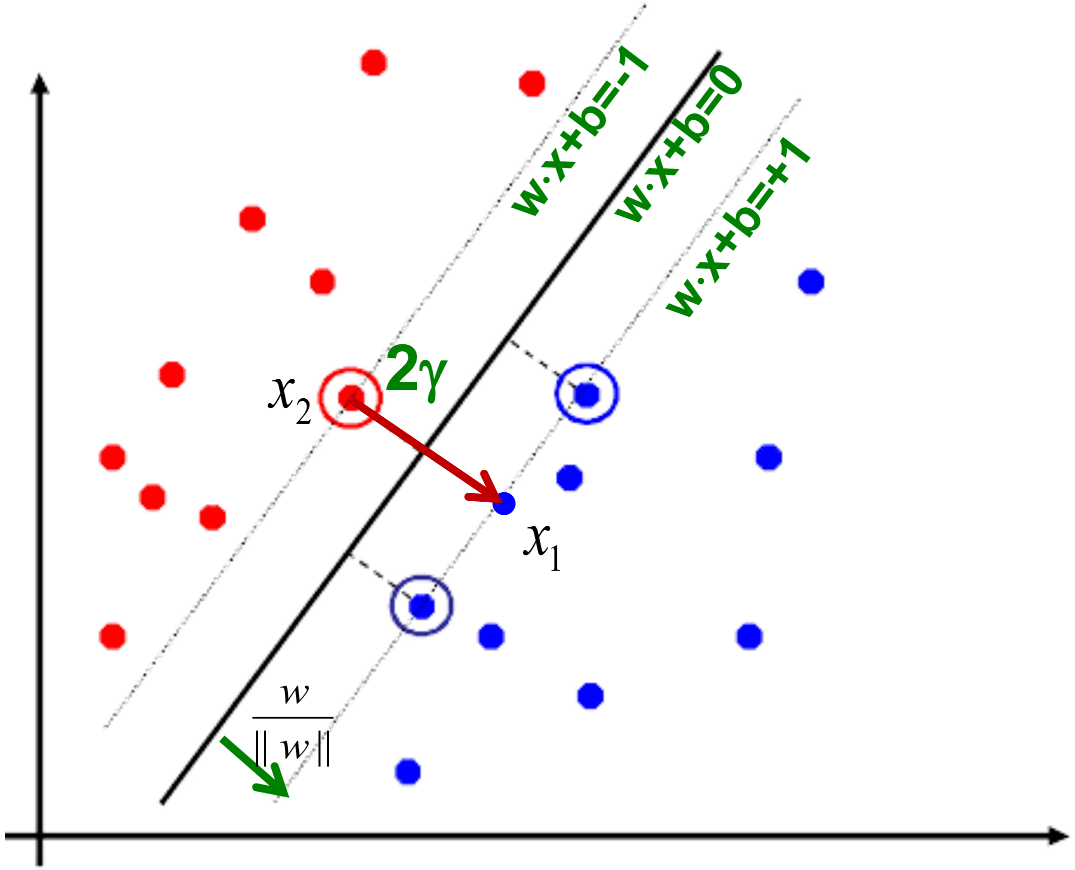
  - Let's also require **support vectors $\boldsymbol{x_j}$** to be on the plane defined by: $\boldsymbol{w}\cdot\boldsymbol{x_j} + \boldsymbol{b} = \pm\mathbf{1}$



$$\|w\| = \sqrt{\sum_{j=1}^{d}(w^{(j)})^2}$$

Canonical Hyperplane: Solution

- **Want to maximize margin γ!**
- **What is the relation between x_1 and x_2?**
  - $\boldsymbol{x_1 = x_2 + 2\gamma \frac{w}{||w||}}$
  - **We also know:**
    - $\boldsymbol{w \cdot x_1 + b = +1}$
    - $\boldsymbol{w \cdot x_2 + b = -1}$
- **So:**
  - $\boldsymbol{w \cdot x_1 + b = +1}$
  - $\boldsymbol{w\left(x_2 + 2\gamma \frac{w}{||w||}\right) + b = +1}$
  - $\boldsymbol{\underbrace{w \cdot x_2 + b}_{-1} + 2\gamma \frac{w \cdot w}{||w||} = +1}$



$$\boxed{\Rightarrow \gamma = \frac{\|w\|}{w \cdot w} = \frac{1}{\|w\|}}$$

Note: $w \cdot w = \|w\|^2$

Maximizing the Margin

- **We started with**

$$\max_{w,\gamma} \gamma$$
$$s.t. \forall i, y_i(w \cdot x_i + b) \geq \gamma$$

But *w* can be arbitrarily large!

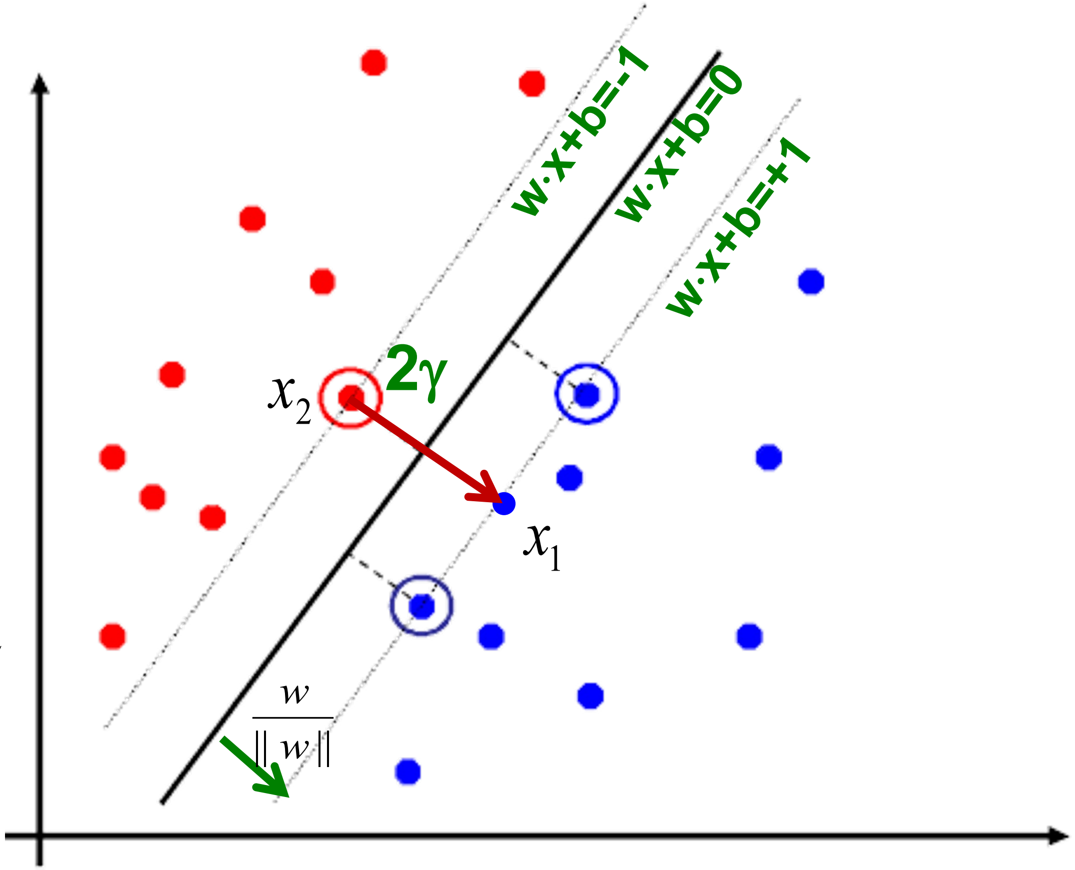
- **We normalized and...**

$$\arg\max \gamma = \arg\max \frac{1}{\|w\|} = \arg\min \|w\| = \arg\min \tfrac{1}{2}\|w\|^2$$

- **Then:**

$$\min_w \tfrac{1}{2} \| w \|^2$$
$$s.t. \forall i, y_i(w \cdot x_i + b) \geq 1$$

This is called SVM with "hard" constraints

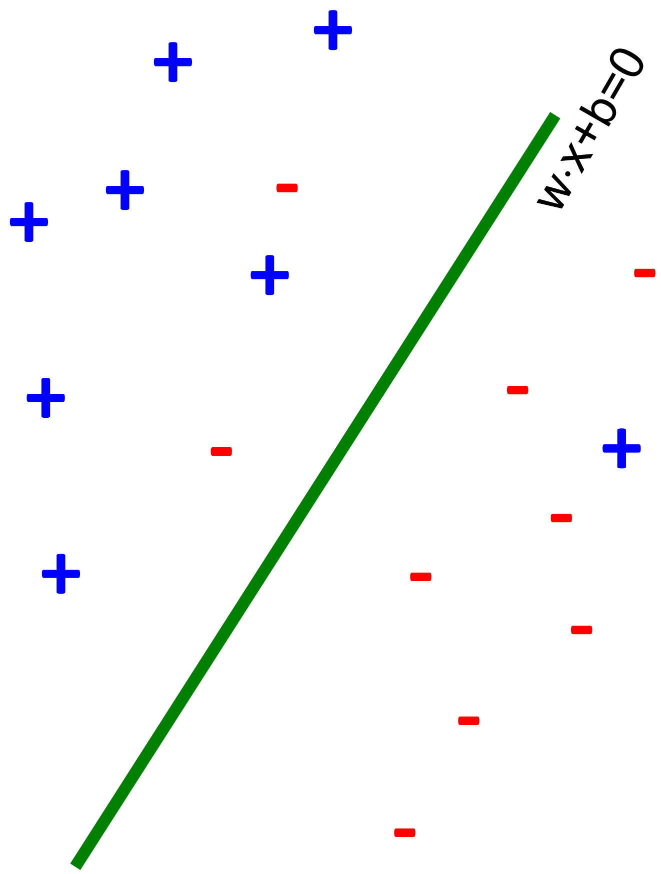


Non-linearly Separable Data

- **If data is not separable introduce penalty:**

$$\min_w \tfrac{1}{2}\|w\|^2 + C \cdot (\#\text{number of mistakes})$$
$$s.t. \forall i, y_i(w \cdot x_i + b) \geq 1$$

  - Minimize $\|w\|^2$ plus the number of training mistakes
  - Set ***C*** using cross validation



- **How to penalize mistakes?**
  - **Not all mistakes are equally bad!**

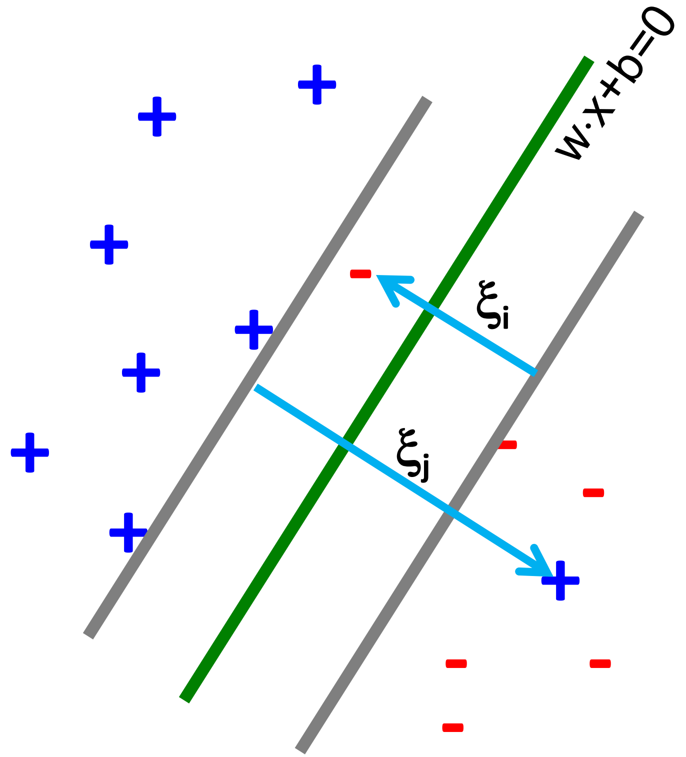
Support Vector Machines

- **Introduce slack variables ξ_i**

$$\min_{w,b,\xi_i \geq 0} \tfrac{1}{2}\|w\|^2 + C \cdot \sum_{i=1}^{n} \xi_i$$

$$s.t. \forall i, y_i (w \cdot x_i + b) \geq 1 - \xi_i$$

- **If point x_i is on the wrong side of the margin then get penalty ξ_i**

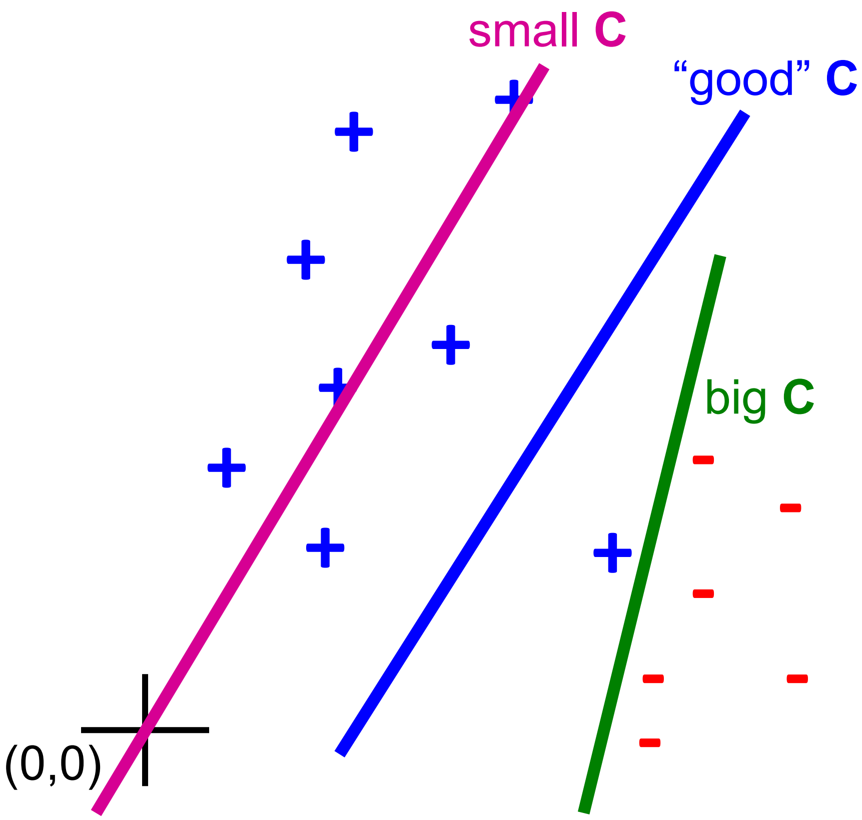


For each data point:
If margin ≥ 1, don't care
If margin < 1, pay linear penalty

Slack Penalty $\boldsymbol{C}$

$$\min_w \tfrac{1}{2}\|w\|^2 + \mathrm{C}\cdot(\#\text{number of mistakes})$$
$$s.t.\forall i, y_i(w\cdot x_i + b)\geq 1$$

- **What is the role of slack penalty C:**
  - **C=∞:** Only want to **w, b** that separate the data
  - **C=0:** Can set ξ_i to anything, then **w=0** (basically ignores the data)



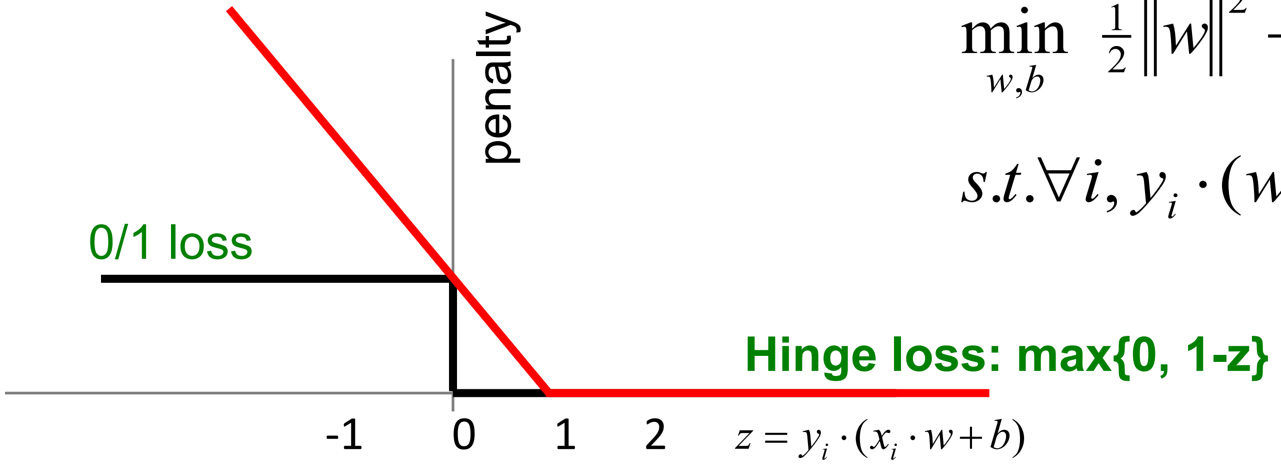
Support Vector Machines

- **SVM in the "natural" form**

$$\arg\min_{w,b} \tfrac{1}{2} \underbrace{w \cdot w}_{\text{Margin}} + C \cdot \sum_{i=1}^{n} \underbrace{\max\{0, 1 - y_i(w \cdot x_i + b)\}}_{\text{Empirical \textbf{loss L} (how well we fit training data)}}$$

Regularization parameter

- **SVM uses "Hinge Loss":**



$$\min_{w,b} \tfrac{1}{2}\|w\|^2 + C\sum_{i=1}^{n} \xi_i$$

$$s.t. \forall i, y_i \cdot (w \cdot x_i + b) \geq 1 - \xi_i$$

Support Vector Machines:
How to compute the margin?

SVM: How to estimate *w*?

$$\min_{w,b} \ \tfrac{1}{2} w \cdot w + C \cdot \sum_{i=1}^{n} \xi_i$$

$$s.t. \forall i, y_i \cdot (x_i \cdot w + b) \geq 1 - \xi_i$$

- **Want to estimate *w* and *b*!**
  - **Standard way:** Use a solver!
    - **Solver:** software for finding solutions to "common" optimization problems
- **Use a quadratic solver:**
  - Minimize quadratic function
  - Subject to linear constraints
- **Problem: Solvers are inefficient for big data!**

SVM: How to estimate *w*?

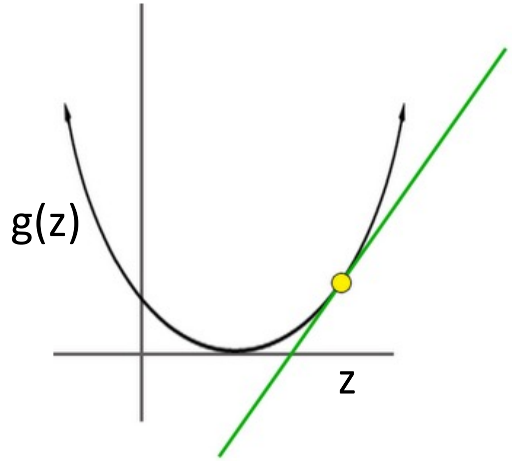
- **Want to estimate w, b!**
- **Alternative approach:**
  - **Want to minimize *f(w,b)*:**

$$\min_{w,b} \tfrac{1}{2} w \cdot w + C \sum_{i=1}^{n} \xi_i$$

$$s.t. \forall i, y_i \cdot (x_i \cdot w + b) \geq 1 - \xi_i$$

$$f(w,b) = \tfrac{1}{2} w \cdot w + C \cdot \sum_{i=1}^{n} \max\left\{0, 1 - y_i \left(\sum_{j=1}^{d} w^{(j)} x_i^{(j)} + b\right)\right\}$$

- **Side note:**
  - **How to minimize convex functions $g(z)$?**
  - Use gradient descent: $\mathbf{\min_z g(z)}$
  - Iterate: $\mathbf{z_{t+1} \leftarrow z_t - \eta \nabla g(z_t)}$



SVM: How to estimate *w*?

- **Want to minimize *f(w,b)*:**

$$f(w,b) = \tfrac{1}{2}\sum_{j=1}^{d}\left(w^{(j)}\right)^2 + C\sum_{i=1}^{n}\underbrace{\max\left\{0, 1 - y_i\left(\sum_{j=1}^{d} w^{(j)} x_i^{(j)} + b\right)\right\}}_{\text{Empirical loss } L(x_i\, y_i)}$$

- **Compute the gradient ∇(j) w.r.t. $w^{(j)}$**

$$\nabla f^{(j)} = \frac{\partial f(w,b)}{\partial w^{(j)}} = w^{(j)} + C\sum_{i=1}^{n}\frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$$

$$\frac{\partial L(x_i, y_i)}{\partial w^{(j)}} = 0 \qquad \text{if } y_i(\mathrm{w}\cdot x_i + b) \geq 1$$

$$= -y_i x_i^{(j)} \qquad \text{else}$$

SVM: How to estimate *w*?

- **Gradient descent:**

Iterate until convergence:

- **For j = 1 … d**
  - **Evaluate:** $\nabla f^{(j)} = \dfrac{\partial f(w,b)}{\partial w^{(j)}} = w^{(j)} + C\sum_{i=1}^{n} \dfrac{\partial L(x_i, y_i)}{\partial w^{(j)}}$
  - **Update:**

    $\mathbf{w}^{(j)} \leftarrow \mathbf{w}^{(j)} - \eta \nabla \mathbf{f}^{(j)}$

η…learning rate parameter
C… regularization parameter

- **Problem:**
  - **Computing $\nabla f^{(j)}$ takes O(n) time!**
    - **n** … size of the training dataset

SVM: How to estimate *w*?

- **Stochastic Gradient Descent**
  - Instead of evaluating gradient over all examples evaluate it for each **individual** training example

We just had:

$$\nabla f^{(j)} = w^{(j)} + C \sum_{i=1}^{n} \frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$$

$$\nabla f^{(j)}(x_i) = w^{(j)} + C \cdot \frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$$

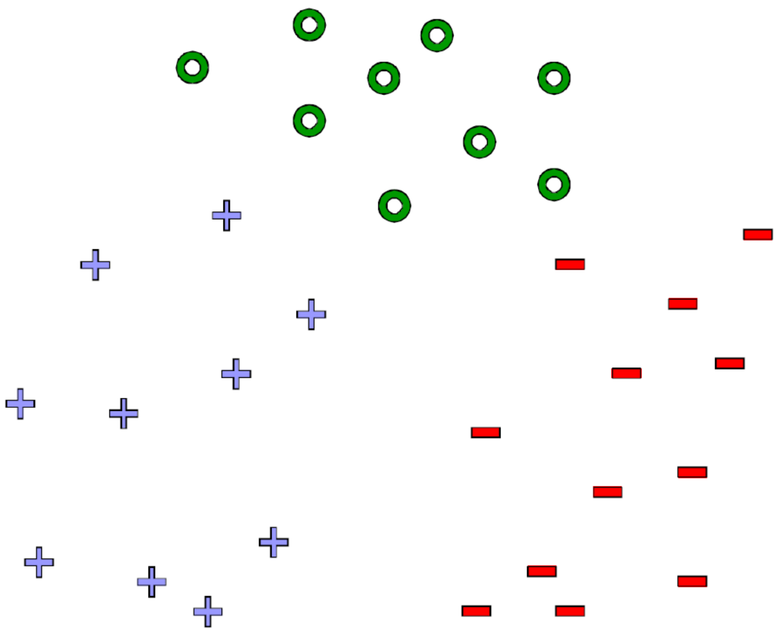
Notice: no summation over ***i*** anymore

- **Stochastic gradient descent:**

Iterate until convergence:

- **For i = 1 … n**
  - **For j = 1 … d**
    - **Compute:** $\nabla f^{(j)}(x_i)$
    - **Update:** $w^{(j)} \leftarrow w^{(j)} - \eta \nabla f^{(j)}(x_i)$

What about multiple classes?



- **Idea 1:**
  One against all
  Learn 3 classifiers
  - **+ vs. {o, -}**
  - **- vs. {o, +}**
  - **o vs. {+, -}**

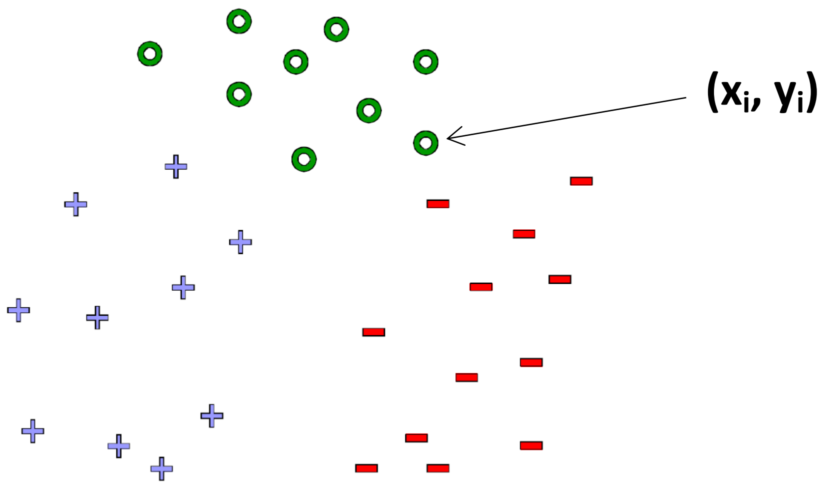
  Obtain:

  $\mathbf{w_+ b_+,\ w_- b_-,\ w_o b_o}$
- **How to classify?**
- **Return class *c***
  $\mathbf{\arg\max_c\ w_c x + b_c}$

Learn 1 classifier: Multiclass SVM

- **Idea 2: Learn 3 sets of weights simultaneously!**
  - For each class ***c*** estimate ***w_c, b_c***
  - **Want the correct class to have highest margin:**

$$\mathbf{w}_{y_i}\,\mathbf{x}_i + \mathbf{b}_{y_i} \geq 1 + \mathbf{w}_c\,\mathbf{x}_i + \mathbf{b}_c \quad \forall c \neq y_i \;, \forall i$$



Multiclass SVM

- **Optimization problem:**

$$\min_{w,b} \ \tfrac{1}{2}\sum_{\mathrm{c}} \|w_c\|^2 + C\sum_{i=1}^{n} \xi_i \qquad \forall c \neq y_i, \forall i$$

$$w_{y_i} \cdot x_i + b_{y_i} \geq w_c \cdot x_i + b_c + 1 - \xi_i \qquad \xi_i \geq 0, \forall i$$

  - To obtain parameters $\boldsymbol{w_c}$, $\boldsymbol{b_c}$ (for each class $\boldsymbol{c}$)
    we can use similar techniques as for 2 class **SVM**

- **SVM is widely perceived a very powerful learning algorithm**