# Large-Scale Machine Learning: SVM

Mining of Massive Datasets

Jure Leskovec, Anand Rajaraman, Jeff Ullman
Stanford University

http://www.mmds.org

# New Topic: Machine Learning!

| High dim. data | Graph data | Infinite data | Machine learning | Apps |
|---|---|---|---|---|
| Locality sensitive hashing | **PageRank,** SimRank | Filtering data streams | SVM | Recommen der systems |
| Clustering | Community Detection | Web advertising | Decision Trees | Association Rules |
| Dimensional ity reduction | Spam Detection | Queries on streams | Perceptron, kNN | Duplicate document detection |

# Supervised Learning

- **Example: Spam filtering**

| | viagra | learning | the | dating | nigeria | $spam?$ |
|---|---|---|---|---|---|---|
| $\vec{x}_1 = ($ | 1 | 0 | 1 | 0 | 0 ) | $y_1 = 1$ |
| $\vec{x}_2 = ($ | 0 | 1 | 1 | 0 | 0 ) | $y_2 = -1$ |
| $\vec{x}_3 = ($ | 0 | 0 | 0 | 0 | 1 ) | $y_3 = 1$ |

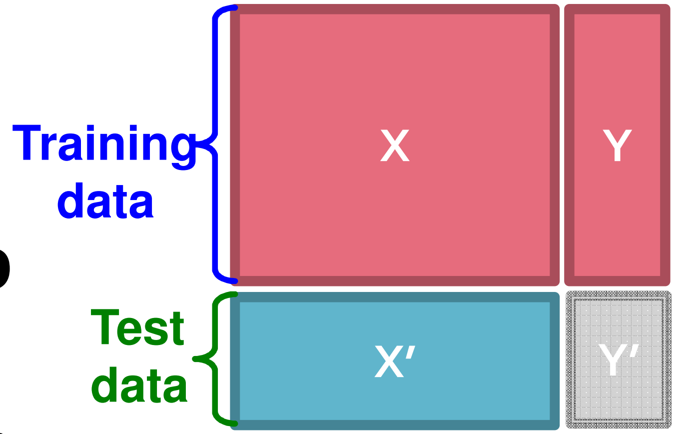
- **Instance space x ∈ X** (|**X**|= **n** data points)
  - **Binary or real-valued feature vector *x* of word occurrences**
  - ***d*** features (words + other things, **d**~100,000)
- **Class y ∈ Y**
  - ***y***: Spam (+1), Ham (-1)
- **Goal: Estimate** a function **f(x)** so that ***y = f(x)***

# More generally: Supervised Learning

- **Would like to do prediction:**
  **estimate** a function **f(x)** so that ***y = f(x)***
- **Where *y* can be:**
  - **Real number**: Regression
  - **Categorical: Classification**
  - **Complex object:**
    - Ranking of items, Parse tree, etc.
- **Data is labeled:**
  - Have many pairs **{(x, y)}**
    - **x** … vector of binary, categorical, real valued features
    - **y** … class ({+1, -1}, or a real number)

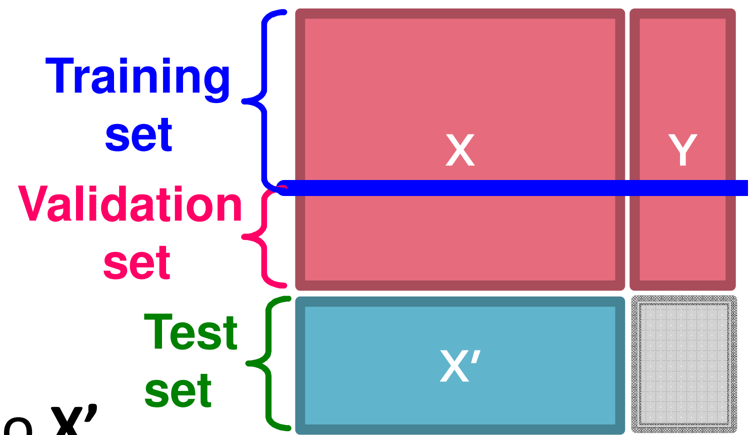
# Supervised Learning

- **Task:** Given data **(X,Y)** build a model **f()** to predict **Y'** based on **X'**
- **Strategy: Estimate $y = f(x)$ on $(X, Y)$. Hope that the same $f(x)$ also works to predict unknown $Y'$**
  - The **"hope"** is called **generalization**
    - **Overfitting: If f(x) predicts well Y but is unable to predict Y'**
  - **We want to build a model that <u>generalizes</u> well to unseen data**
    - But Jure, how can we well on data we have never seen before?!?




# Supervised Learning

- **Idea:** **Pretend we do not know the data/labels we actually do know**
  - Build the model **f(x)** on the training data
    See how well **f(x)** does on the test data
    - If it does well, then apply it also to **X'**



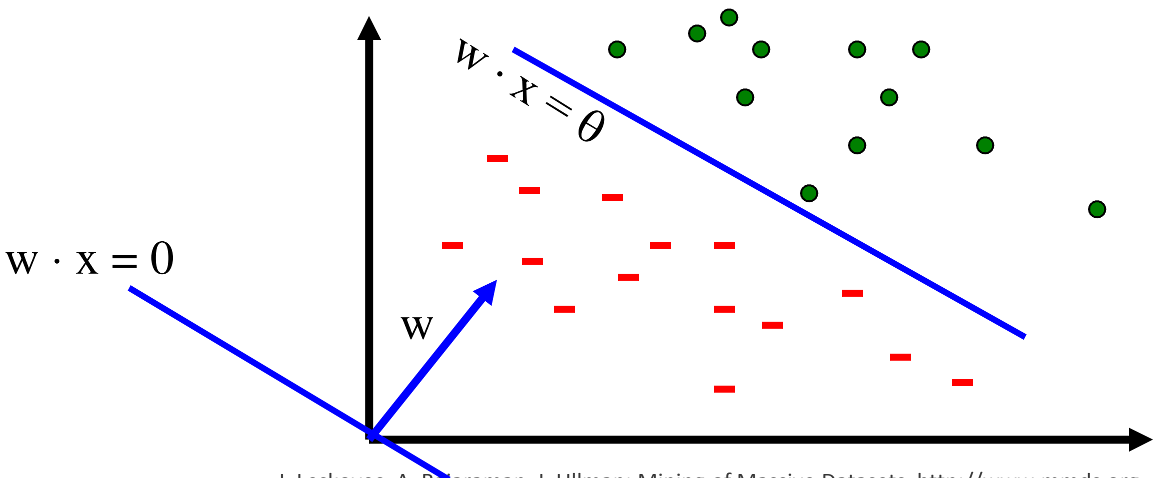

- **Refinement: Cross validation**
  - Splitting into training/validation set is brutal
  - Let's split our data **(X,Y)** into 10-folds (buckets)
  - Take out 1-fold for validation, train on remaining 9
  - Repeat this 10 times, report average performance

# 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**

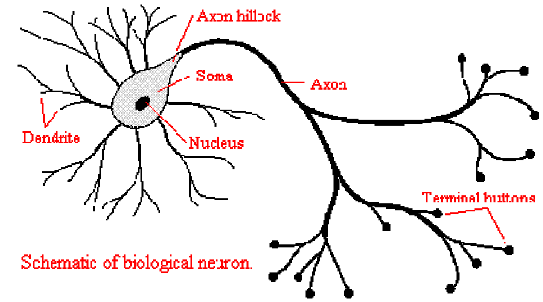
**Note:**

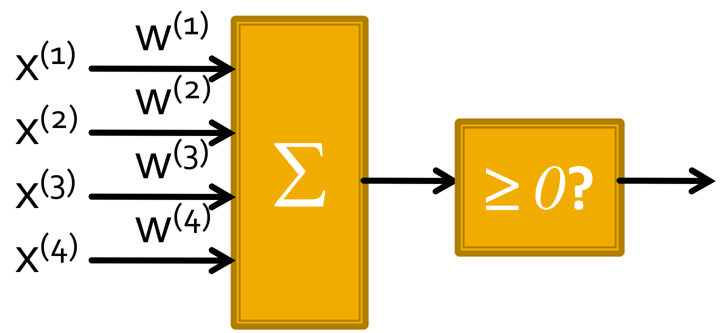
$$\mathbf{x} \rightarrow \langle \mathbf{x}, 1 \rangle \quad \forall \mathbf{x}$$

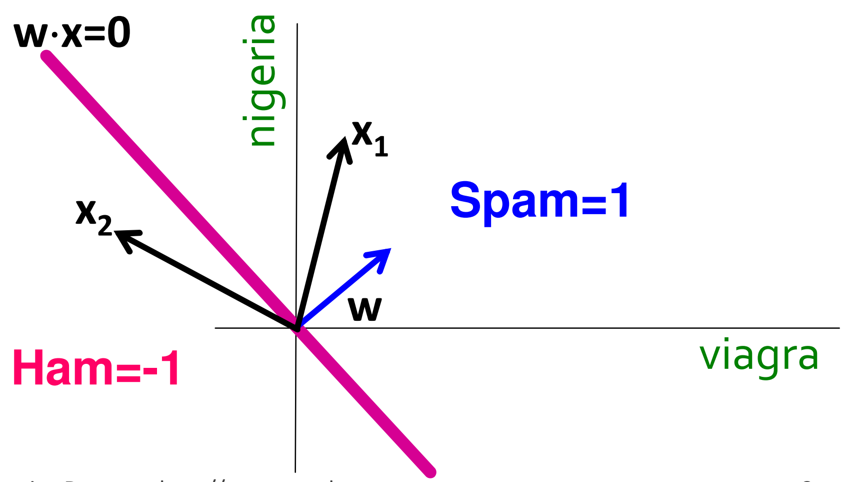
$$\mathbf{w} \rightarrow \langle \mathbf{w}, -\theta \rangle$$

# Perceptron [Rosenblatt '58]

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



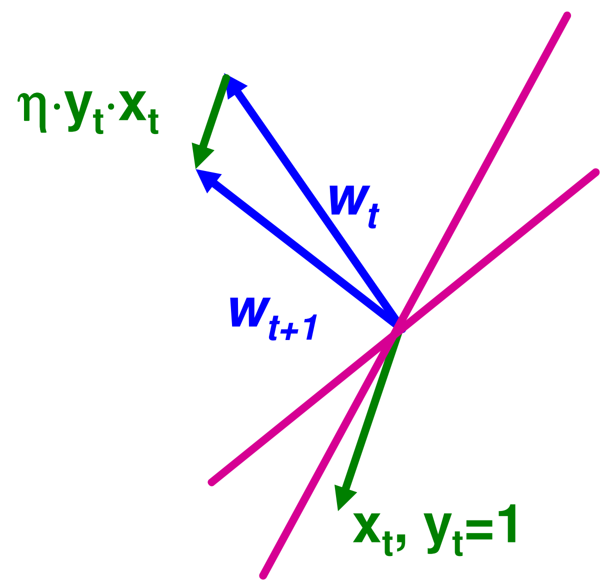
# Perceptron

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 $w_t$

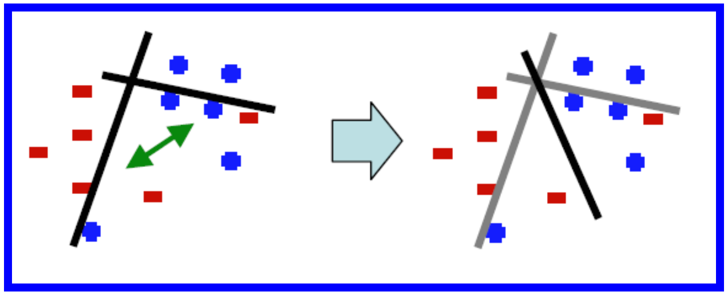
$$w_{t+1} = w_t + \eta \cdot y_t \cdot x_t$$

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

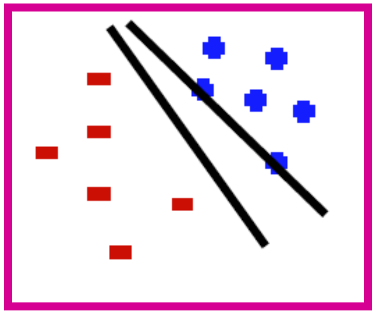


# Perceptron: The Good and the Bad

- **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



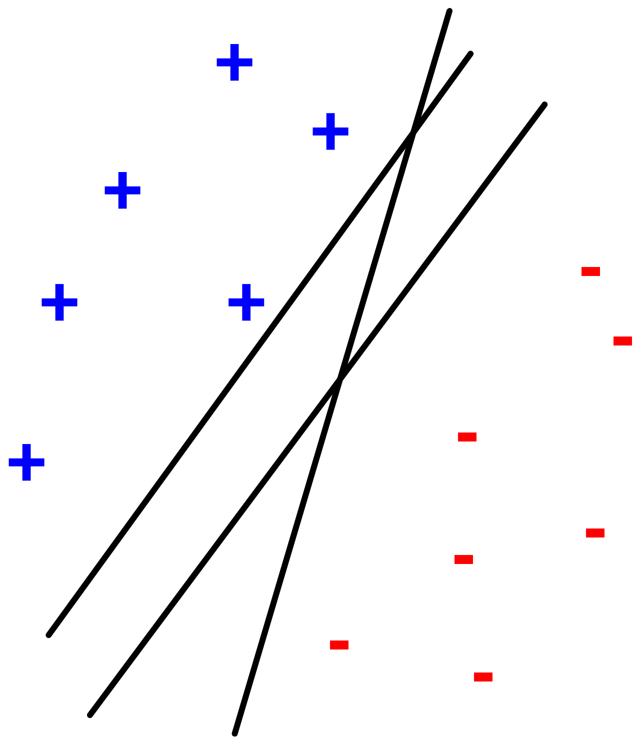
# Updating the Learning Rate

- **Perceptron will oscillate and won't converge**
- **So, when to stop learning?**
- **(1)** Slowly decrease the learning rate $\eta$
  - A classic way is to: $\eta$ **= $c_1$/(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**



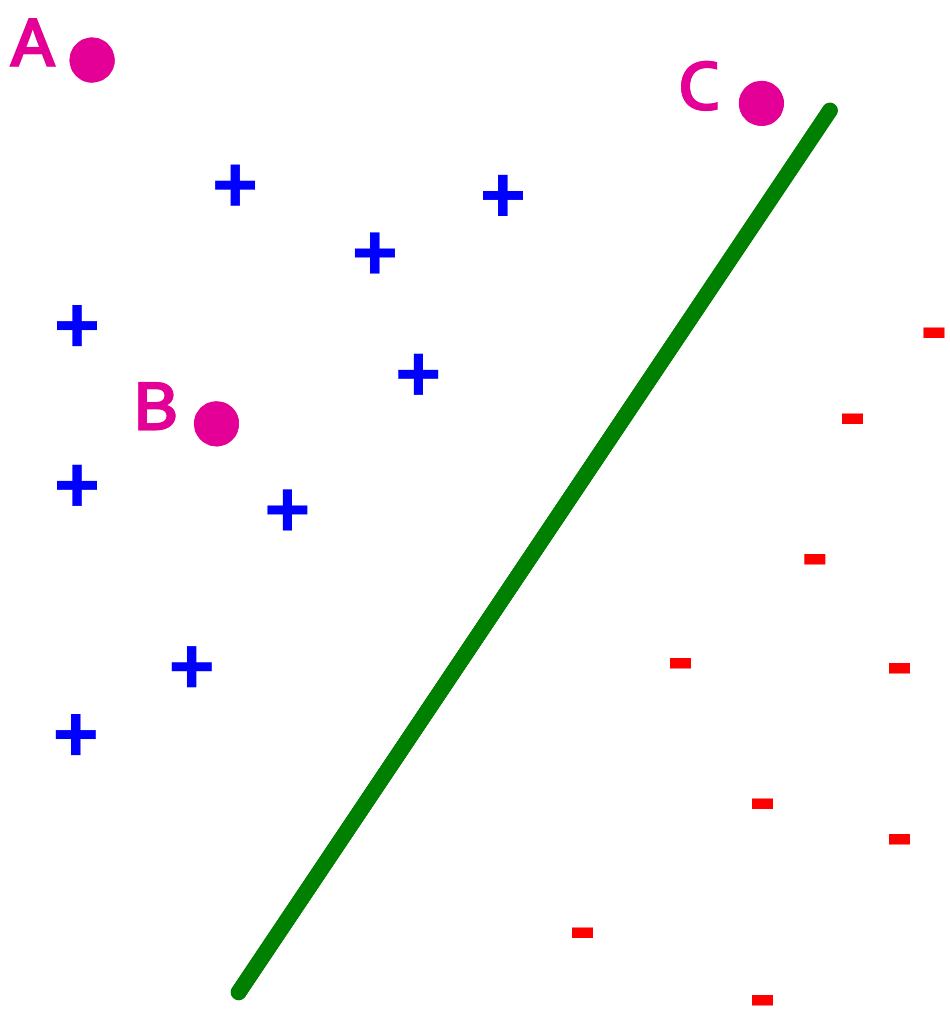

**Data:**

- **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*)?**

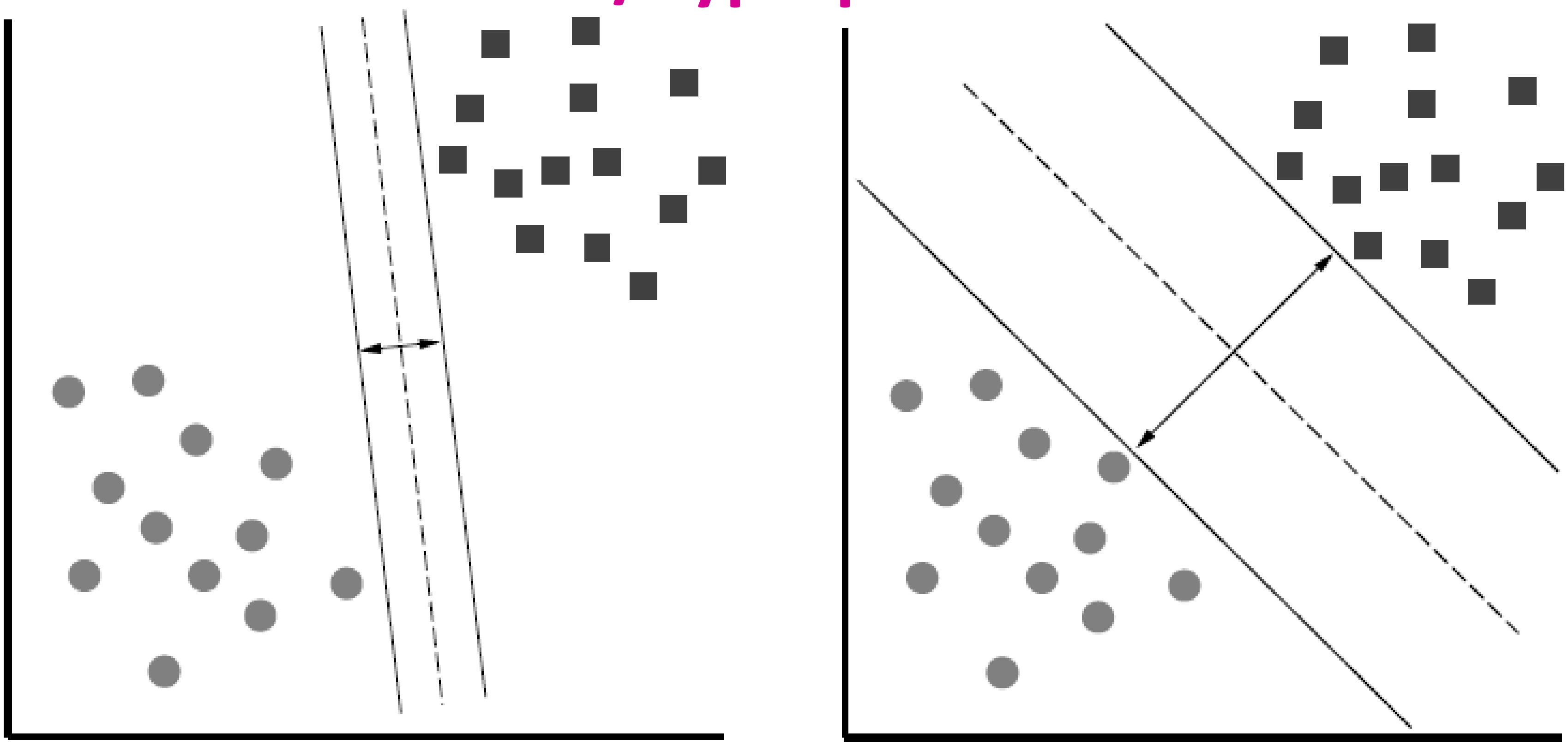
# Largest Margin




- **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 $\gamma$: Distance of closest example from the decision line/hyperplane**

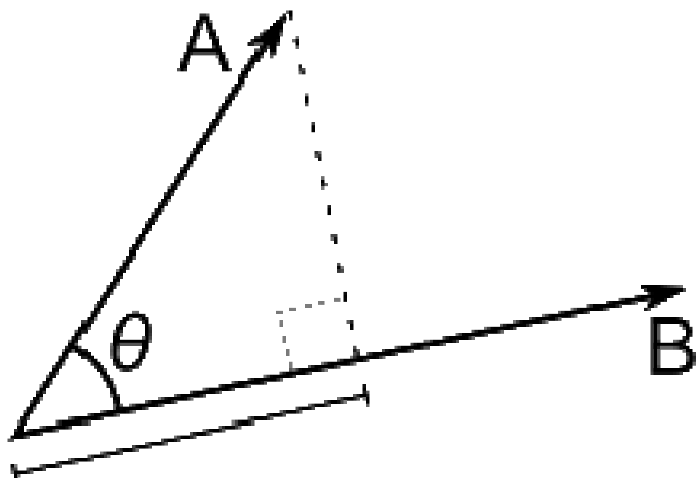


The reason we define margin this way is due to theoretical convenience and existence of generalization error bounds that depend on the value of margin.

# Why maximizing $\gamma$ a good idea?

- **Remember: Dot product**

$$A \cdot B = \|A\| \cdot \|B\| \cdot \cos\theta$$

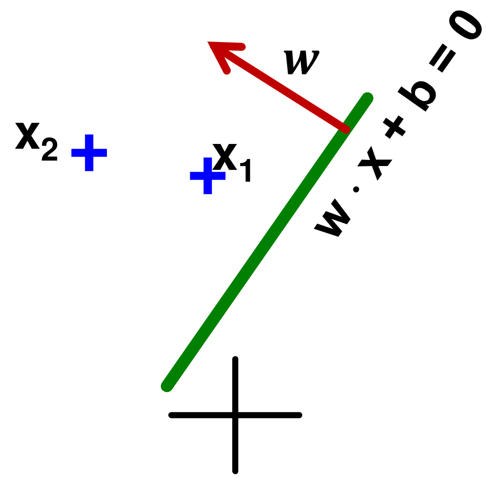


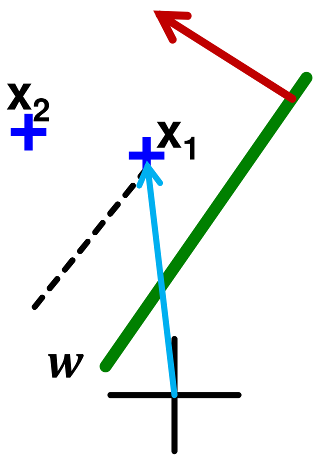

$$\|A\| cos\theta$$

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

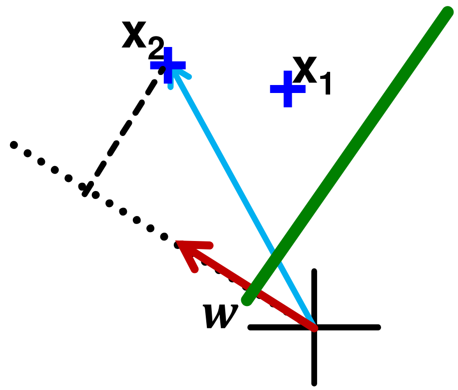
# Why maximizing $\gamma$ a good idea?

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



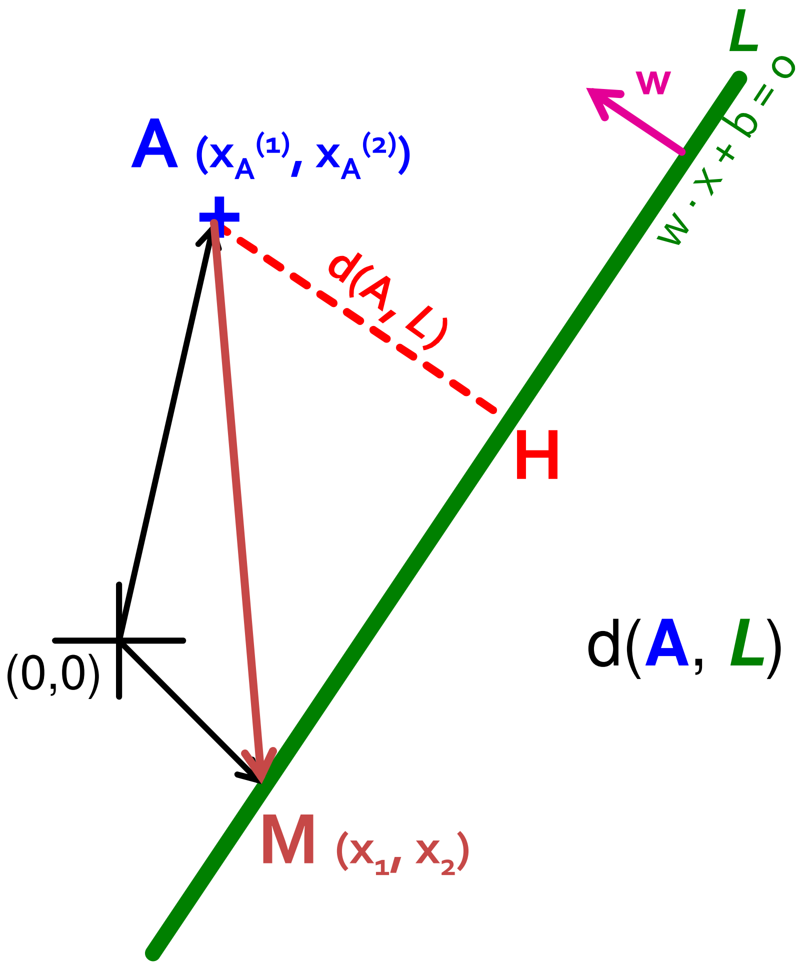

In this case
$\gamma_1 \approx \|w\|^2$




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

- **So, $\gamma$ roughly corresponds to the margin**
  - Bigger $\gamma$ bigger the separation

# What is the margin?



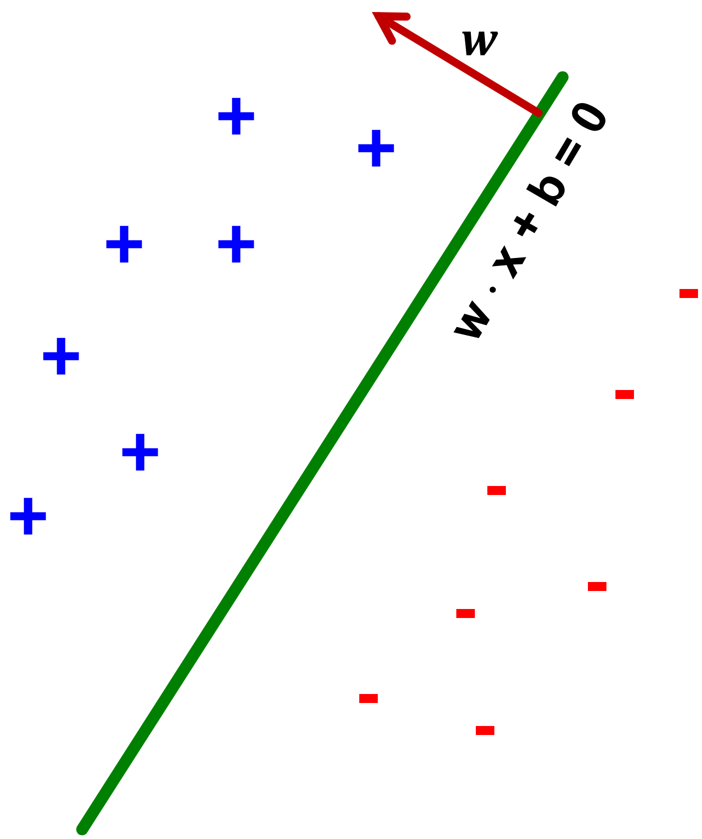

Note we assume $\|w\|_2 = 1$

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

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

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

# Largest Margin




- Prediction = $\mathbf{sign}(w \cdot x + b)$
- "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**

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

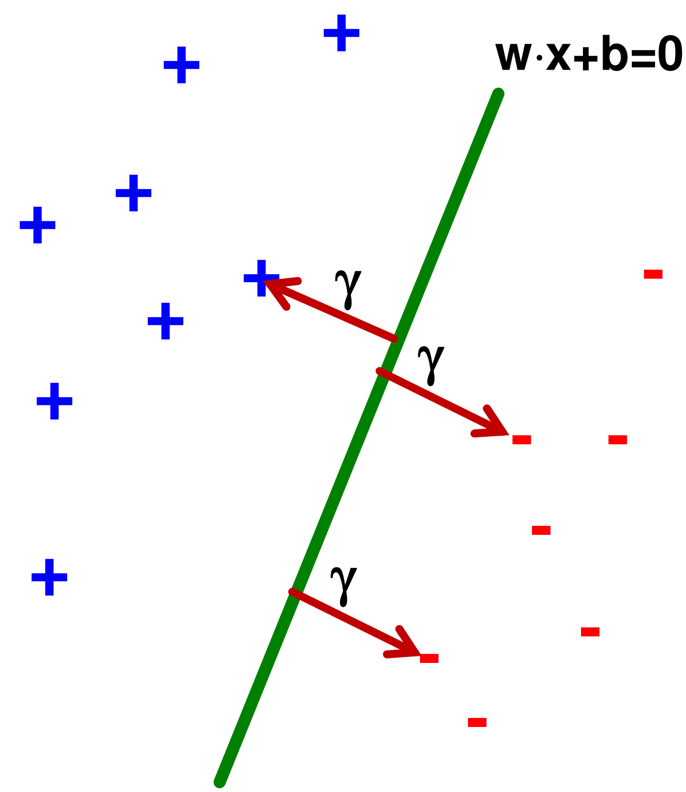
$$s.t. \forall i,\ y_i (w \cdot x_i + b) \geq \gamma$$

# Support Vector Machine

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

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

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



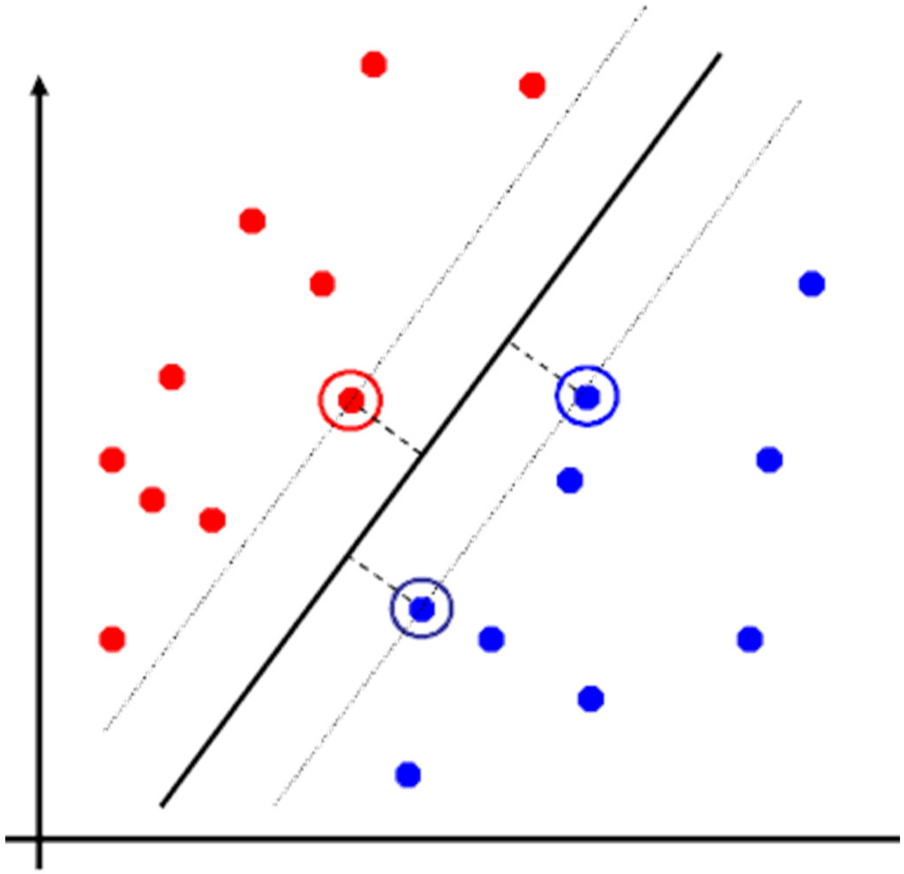
Maximizing the margin

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

# 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)

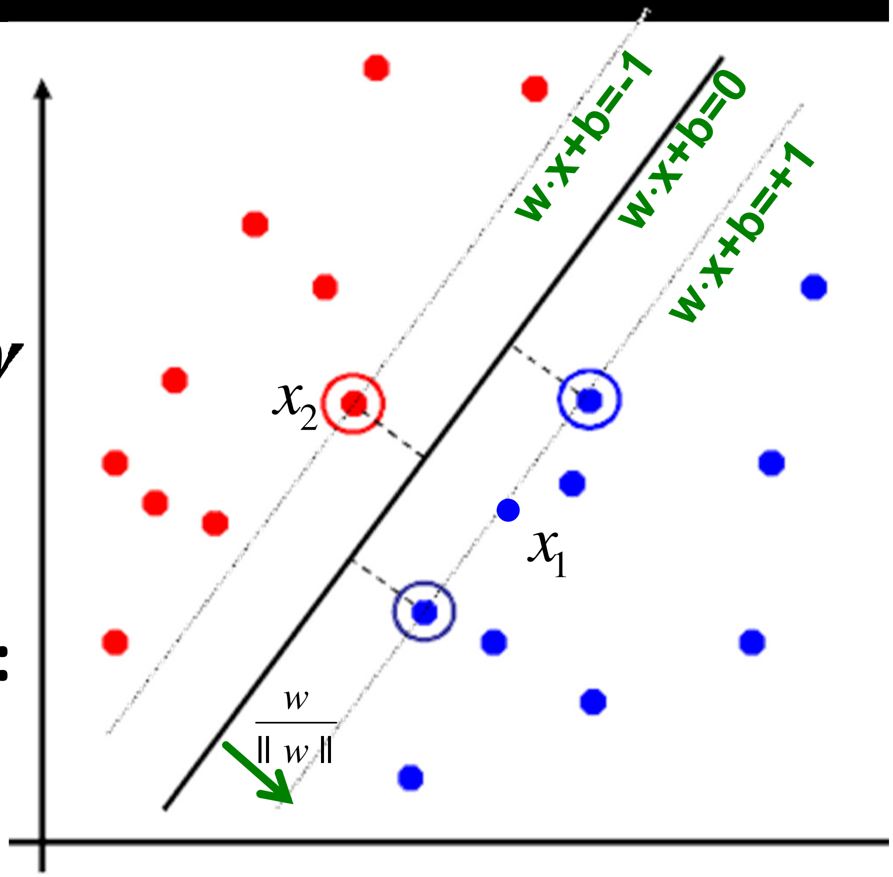


# Canonical Hyperplane: Problem

- **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*:**

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

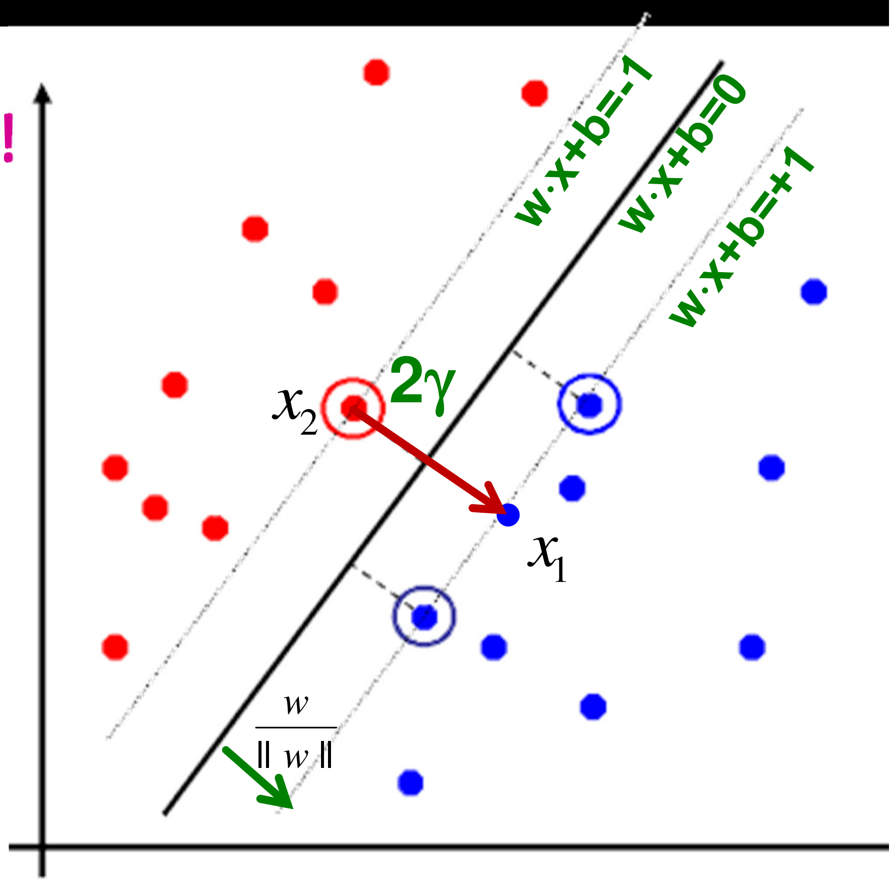
  - Let's also require **support vectors $\boldsymbol{x}_j$** to be on the plane defined by: $\boldsymbol{w}\cdot\boldsymbol{x}_j + \boldsymbol{b} = \pm\mathbf{1}$




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

# Canonical Hyperplane: Solution

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




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

**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!**

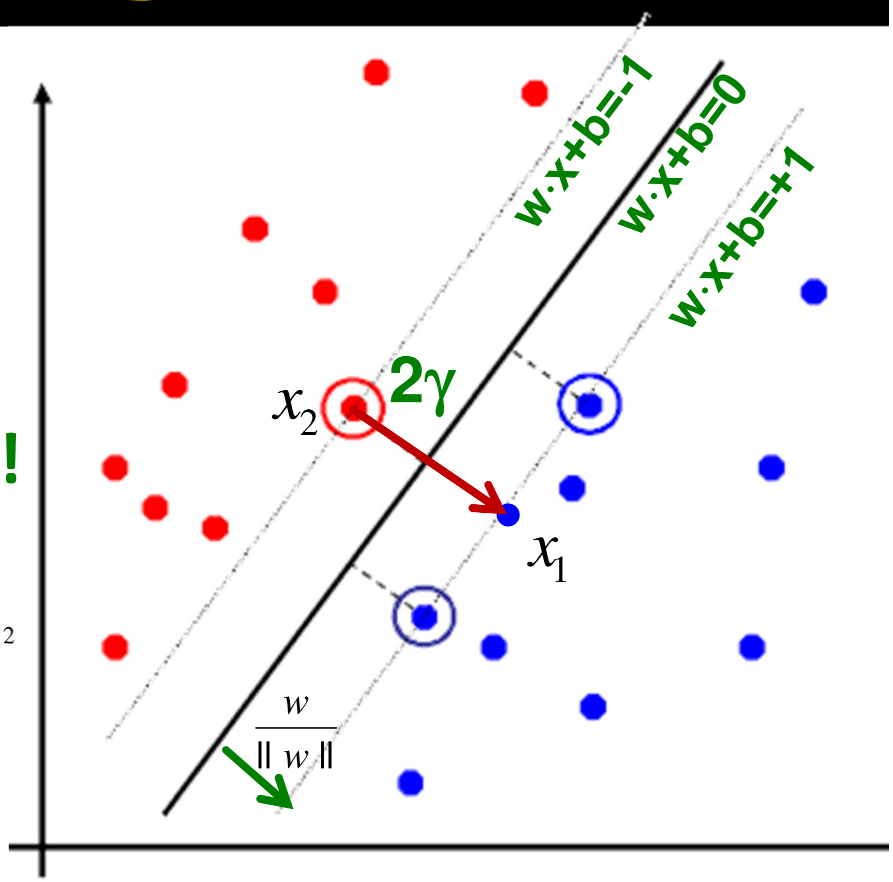
- **We normalized and...**

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

- **Then:**

$$\min_w \tfrac{1}{2} \| w \|^2$$

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



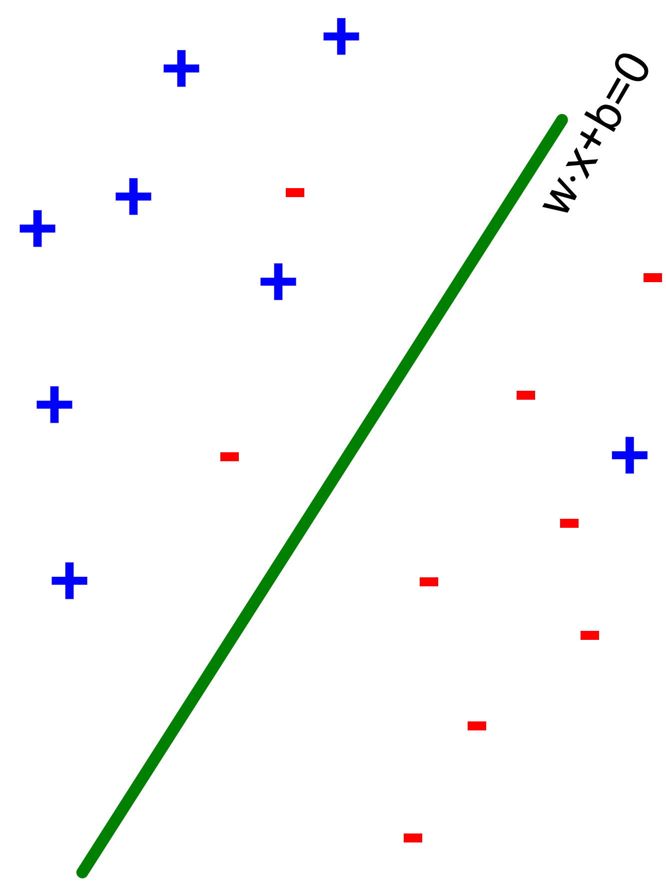

**This is called SVM with "hard" constraints**

# Non-linearly Separable Data

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

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

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




- **How to penalize mistakes?**
  - **All mistakes are not equally bad!**

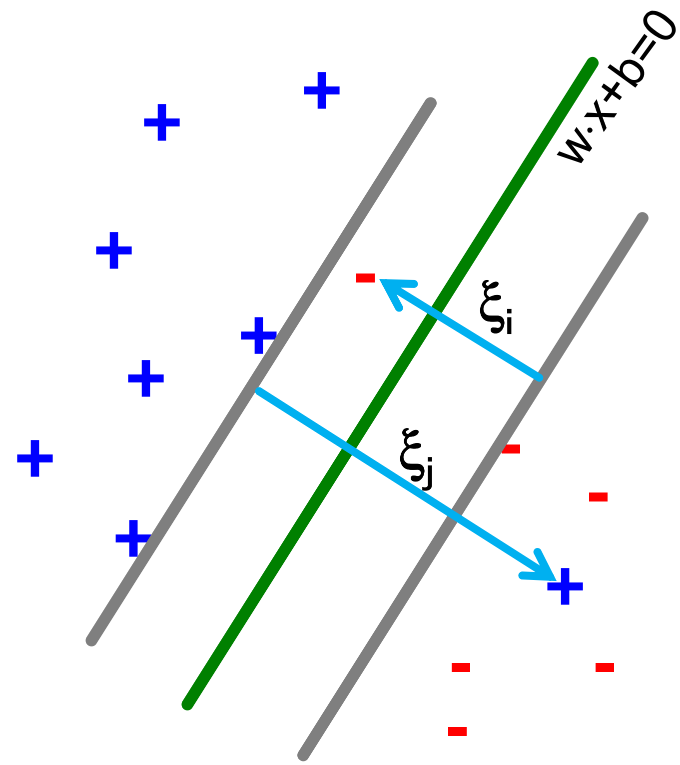
# Support Vector Machines

- **Introduce slack variables $\xi_i$**

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

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

- If point $\boldsymbol{x_i}$ is on the wrong side of the margin then get penalty $\xi_i$



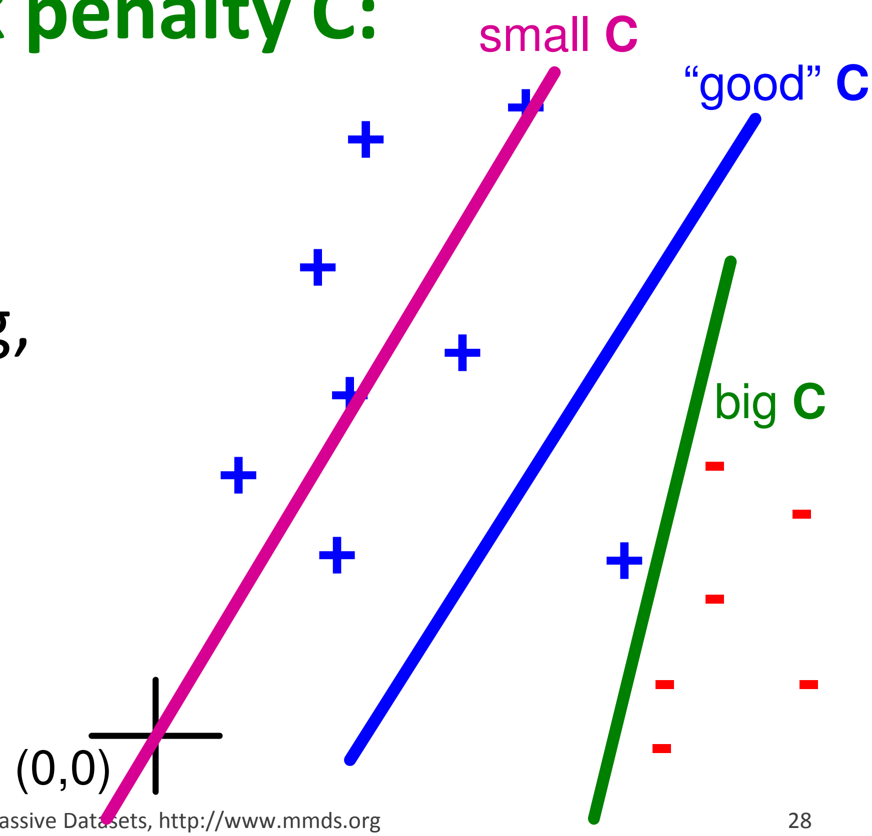

**For each data point:**
If margin ≥ 1, don't care
If margin < 1, pay linear penalty

# Slack Penalty *C*

$$\min_w \tfrac{1}{2}\|w\|^2 + C \cdot (\#\text{number of mistakes})$$

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

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



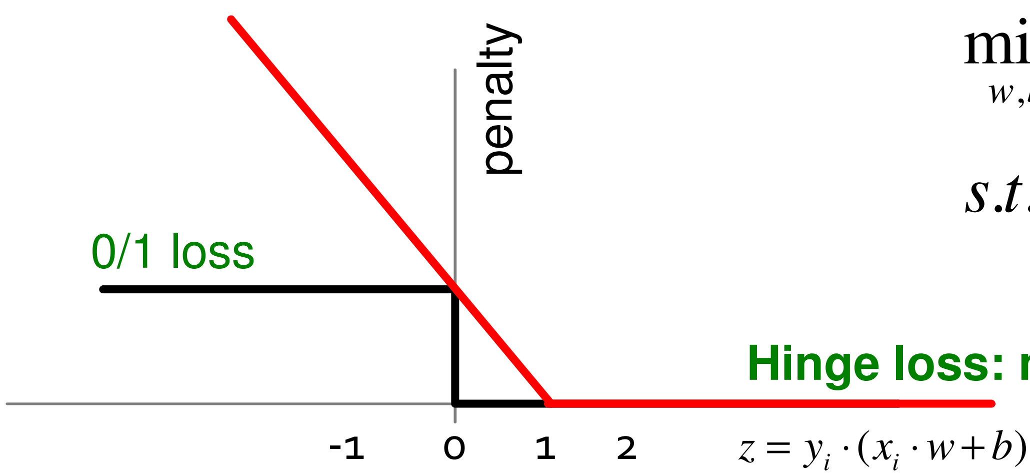
# Support Vector Machines

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

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

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?

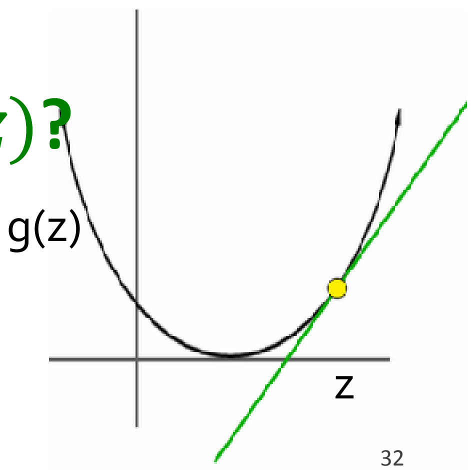
- **Want to estimate w, b!**
- **Alternative approach:**
  - **Want to minimize *f(w,b)*:**

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

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

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

- **Side note:**
  - **How to minimize convex functions $g(z)$?**
  - Use gradient descent: **$\min_z g(z)$**
  - 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 $\nabla$(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:** $\nabla f^{(j)} = \frac{\partial f(w,b)}{\partial w^{(j)}} = w^{(j)} + C\sum_{i=1}^{n} \frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$
  - **Update:**

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

$\eta$…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?

We just had:

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

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

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

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:** $w^{(j)} \leftarrow w^{(j)} - \eta\, \nabla f^{(j)}(x_i)$

# Support Vector Machines: Example

# Example: Text categorization

- **Example by Leon Bottou:**
  - **Reuters RCV1** document corpus
    - Predict a category of a document
      - One **vs.** the rest classification
  - ***n* = 781,000** training examples (documents)
  - 23,000 test examples
  - ***d* = 50,000** features
    - One feature per word
    - Remove stop-words
    - Remove low frequency words

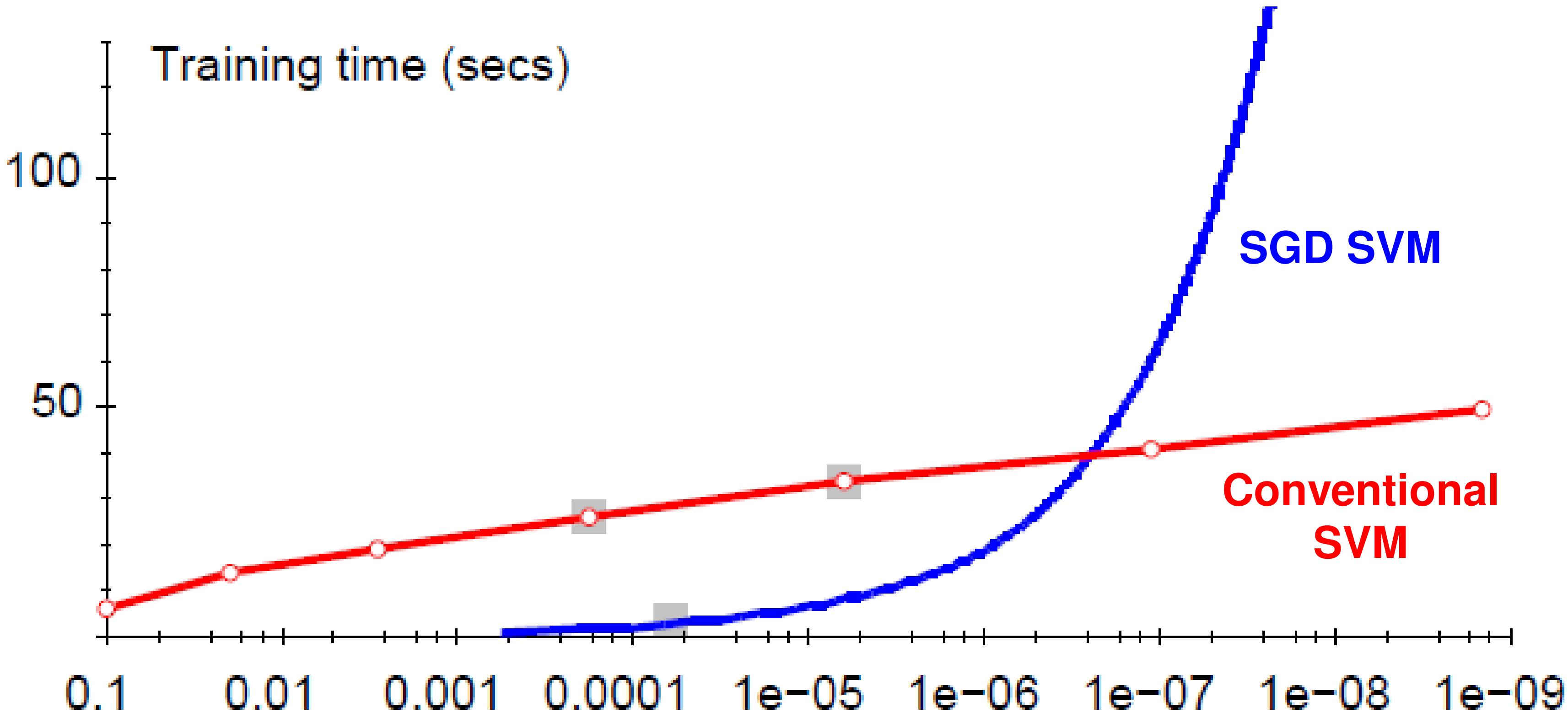
# Example: Text categorization

- **Questions:**
  - **(1)** Is **SGD** successful at minimizing ***f(w,b)***?
  - **(2)** How quickly does **SGD** find the min of ***f(w,b)***?
  - **(3)** What is the error on a test set?

| | *Training time* | *Value of f(w,b)* | *Test error* |
|---|---|---|---|
| Standard SVM | 23,642 secs | 0.2275 | 6.02% |
| "Fast SVM" | 66 secs | 0.2278 | 6.03% |
| **SGD SVM** | 1.4 secs | 0.2275 | 6.02% |

**(1)** SGD-SVM is successful at minimizing the value of ***f(w,b)***
**(2)** SGD-SVM is super fast
**(3)** SGD-SVM test set error is comparable

# Optimization "Accuracy"

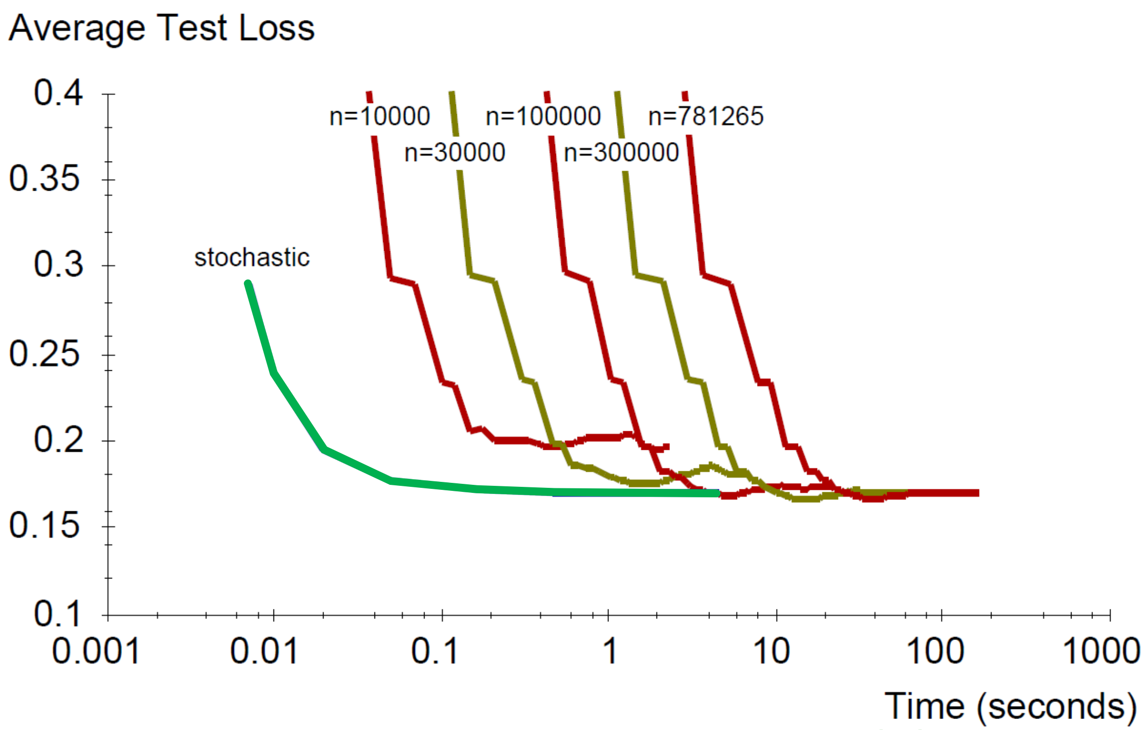



**Optimization quality: | *f(w,b) – f (w^opt,b^opt)* |**

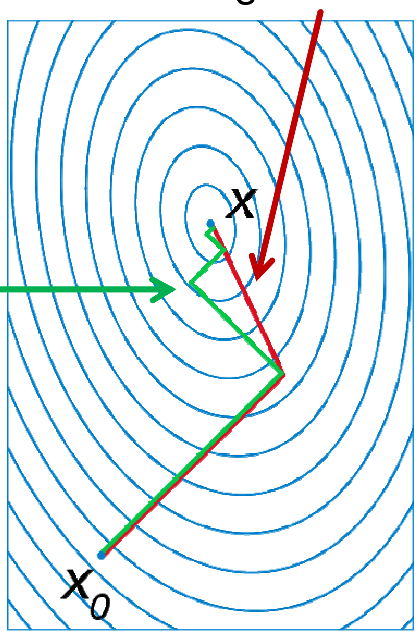
For optimizing *f(w,b) within reasonable* quality
*SGD-SVM* is super fast

# SGD vs. Batch Conjugate Gradient

- **SGD** on full dataset vs. **Conjugate Gradient** on a sample of ***n*** training examples




**Theory says: Gradient descent** converges in linear time $\boldsymbol{k}$. **Conjugate gradient** converges in $\sqrt{\boldsymbol{k}}$.




$\boldsymbol{k}$… condition number

**Bottom line:** Doing a simple (but fast) SGD update many times is better than doing a complicated (but slow) CG update a few times

# Practical Considerations

- **Need to choose learning rate η and $t_0$**

$$w_{t+1} \leftarrow w_t - \frac{\eta_t}{t+t_0}\left(w_t + C\frac{\partial L(x_i, y_i)}{\partial w}\right)$$

- **Leon suggests:**
  - Choose $\mathbf{t_0}$ so that the expected initial updates are comparable with the expected size of the weights
  - Choose η:
    - Select a **small subsample**
    - Try various rates η (e.g., 10, 1, 0.1, 0.01, …)
    - Pick the one that most reduces the cost
    - Use η for next 100k iterations on the full dataset

# Practical Considerations

- **Sparse Linear SVM:**
  - **Feature vector $x_i$ is sparse (contains many zeros)**
    - Do not do: $\boldsymbol{x_i} = [0,0,0,1,0,0,0,0,5,0,0,0,0,0,0,\ldots]$
    - But represent $\mathbf{x_i}$ as a sparse vector $\mathbf{x_i}$**=[*(4,1), (9,5),* …]**
  - **Can we do the SGD update more efficiently?**

$$w \leftarrow w - \eta\left(w + C\frac{\partial L(x_i, y_i)}{\partial w}\right)$$

  - **Approximated in 2 steps:**

$$w \leftarrow w - \eta C \frac{\partial L(x_i, y_i)}{\partial w}$$

**cheap**: $\boldsymbol{x_i}$ is sparse and so few coordinates ***j*** of ***w*** will be updated

$$w \leftarrow w(1-\eta)$$

**expensive**: ***w*** is not sparse, all coordinates need to be updated

# Practical Considerations

- **Solution 1:** $\boldsymbol{w} = \boldsymbol{s} \cdot \boldsymbol{v}$
  - Represent vector ***w*** as the product of scalar ***s*** and vector ***v***
  - Then the update procedure is:
    - ***(1)*** $\boldsymbol{v} = \boldsymbol{v} - \eta C \frac{\partial L(x_i, y_i)}{\partial w}$
    - ***(2)*** $\boldsymbol{s} = \boldsymbol{s}(1 - \eta)$
- **Solution 2:**
  - Perform only step **(1)** for each training example
  - Perform step **(2)** with lower frequency and higher $\eta$

**Two step update procedure:**

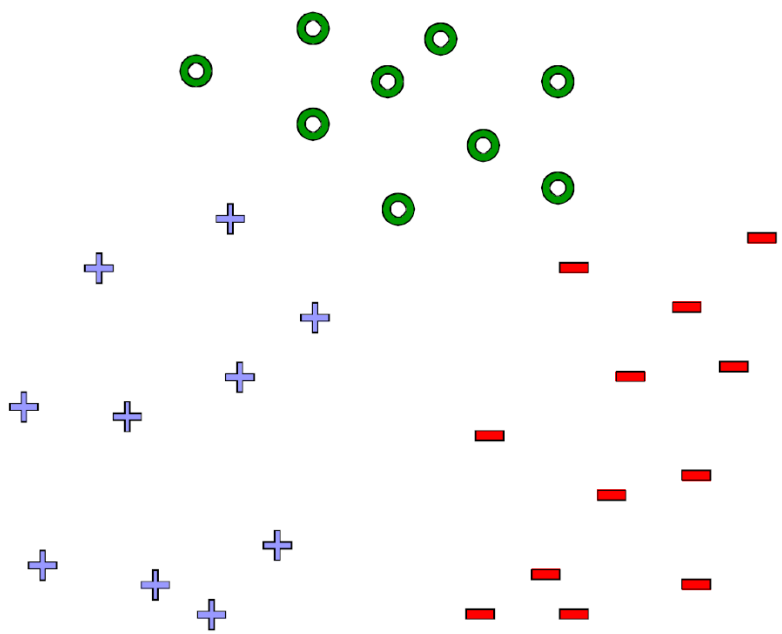
**(1)** $w \leftarrow w - \eta C \frac{\partial L(x_i, y_i)}{\partial w}$

**(2)** $w \leftarrow w(1 - \eta)$

# Practical Considerations

- **Stopping criteria:**
  **How many iterations of SGD?**
  - **Early stopping with cross validation**
    - Create a validation set
    - Monitor cost function on the validation set
    - Stop when loss stops decreasing
  - **Early stopping**
    - Extract two disjoint subsamples **A** and **B** of training data
    - Train on **A**, stop by validating on **B**
    - Number of epochs is an estimate of ***k***
    - Train for ***k*** epochs on the full dataset

# What about multiple classes?



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

  Obtain:

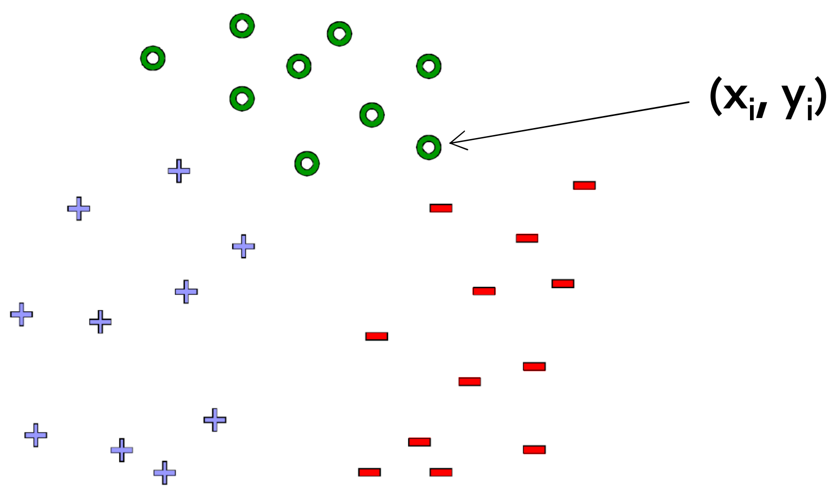
  $\mathbf{w}_+\, b_+,\ \ \mathbf{w}_-\, b_-,\ \ \mathbf{w}_o\, b_o$
- **How to classify?**
- Return class *c*

  $$\arg\max_c\ w_c\, x + b_c$$

# Learn 1 classifier: Multiclass SVM

- **Idea 2: Learn 3 sets of weights simoultaneously!**
  - For each class ***c*** estimate $\boldsymbol{w_c}$, $\boldsymbol{b_c}$
  - **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:**

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

$$w_{y_i}\cdot x_i + b_{y_i} \ge w_c \cdot x_i + b_c + 1 - \xi_i \qquad \forall c \neq y_i, \forall i$$

$$\xi_i \ge 0, \forall i$$

  - 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**