Large Scale Machine Learning: SVMs

CS246: Mining Massive Datasets
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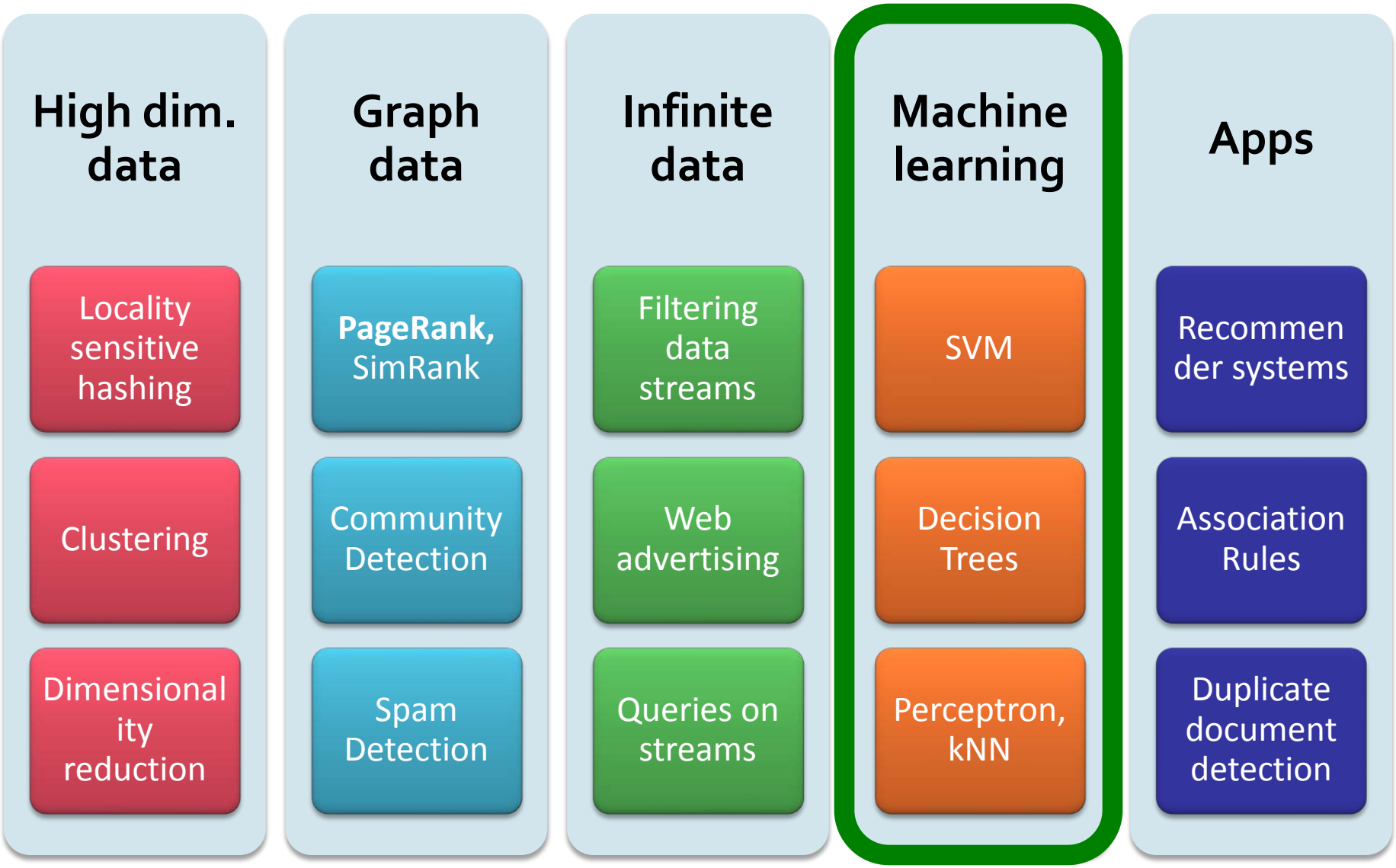
http://cs246.stanford.edu

New Topic: Graph Data!



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 $)$	$y_3 = 1$

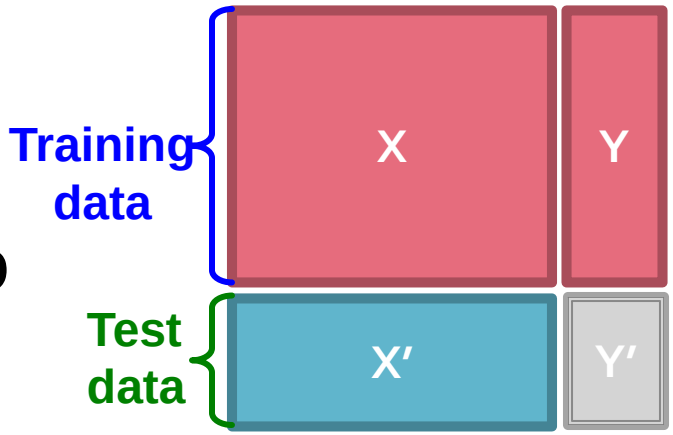
- **Instance space x ∈ X** (|**X**| = **n** data points)
  - **Binary or real-valued feature vector *x* of word occurrences**
  - ***d*** features (words + other things, **d**~100,000)
- **Class y ∈ Y**
  - ***y***: Spam (+1), Ham (-1)
- **Goal: Estimate** a function **f(x)** so that ***y = f(x)***

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

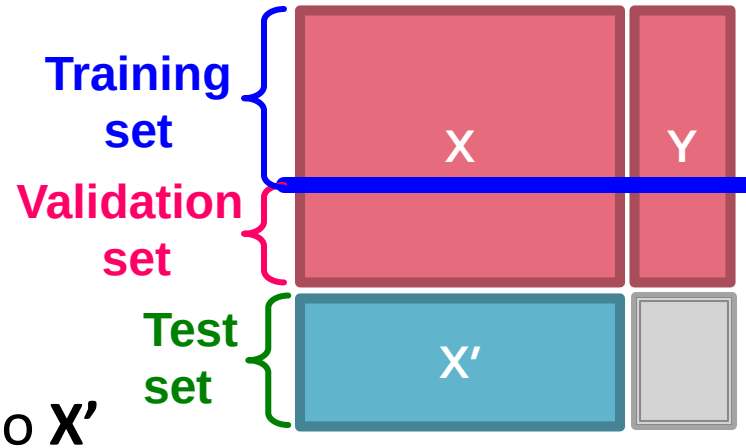
- **Task:** Given data **(X,Y)** build a model **f()** to predict **Y'** based on **X'**
- **Strategy:** **Estimate $y = f(x)$ on (X, Y).**
  Hope that the same $f(x)$ also works to predict unknown Y'



  - 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 generalizes 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'**



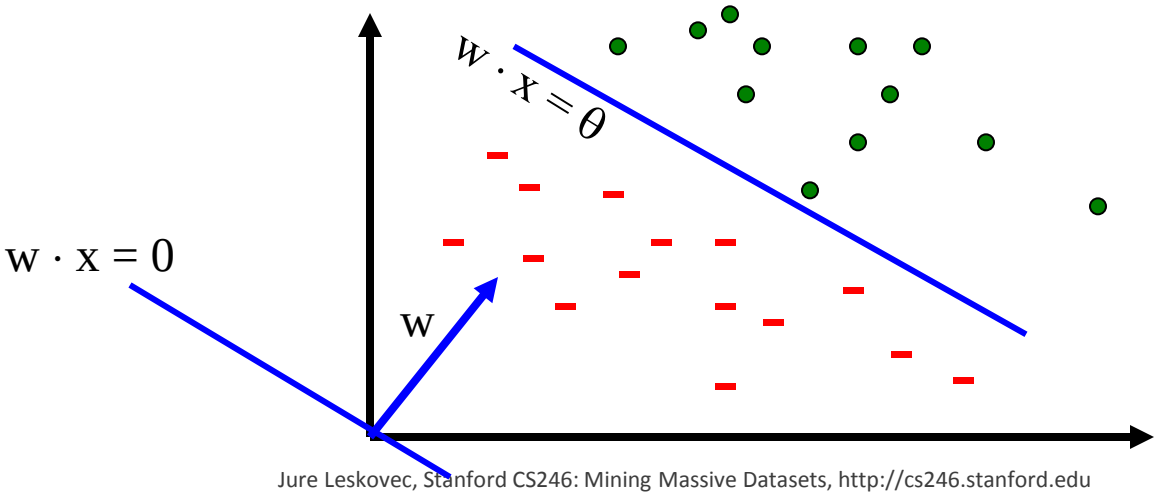
- **Refinement: Cross validation**
  - Splitting into training/validation set is brutal
  - Let's split our data **(X,Y)** into 10-folds (buckets)
  - Take out 1-fold for validation, train on remaining 9
  - Repeat this 10 times, report average performance

Linear models for classification

- **Binary classification:**

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

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



Decision boundary is **linear**

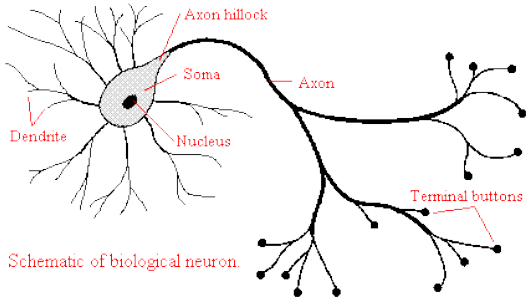
Note:

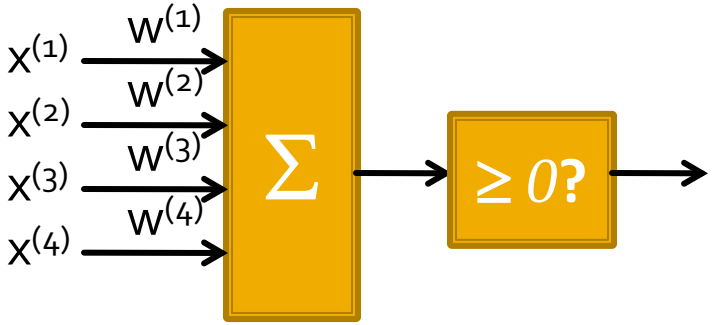
$$\mathbf{x} \rightarrow \langle \mathbf{x}, 1 \rangle \quad \forall \mathbf{x}$$

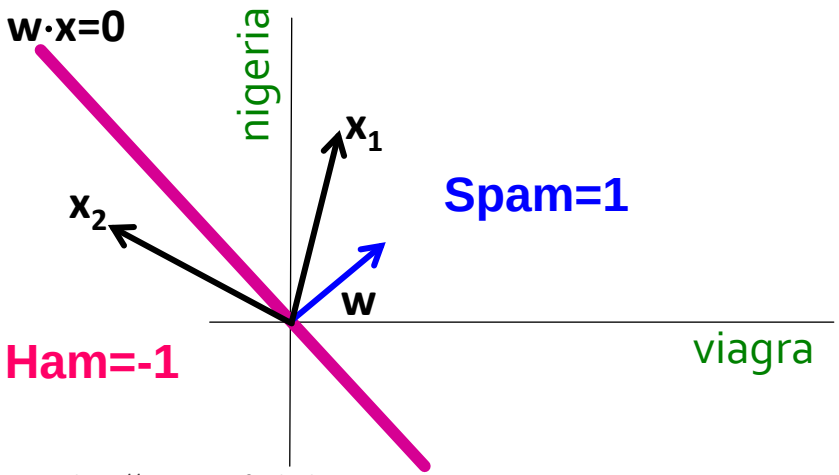
$$\mathbf{w} \rightarrow \langle \mathbf{w}, -\theta \rangle$$

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**







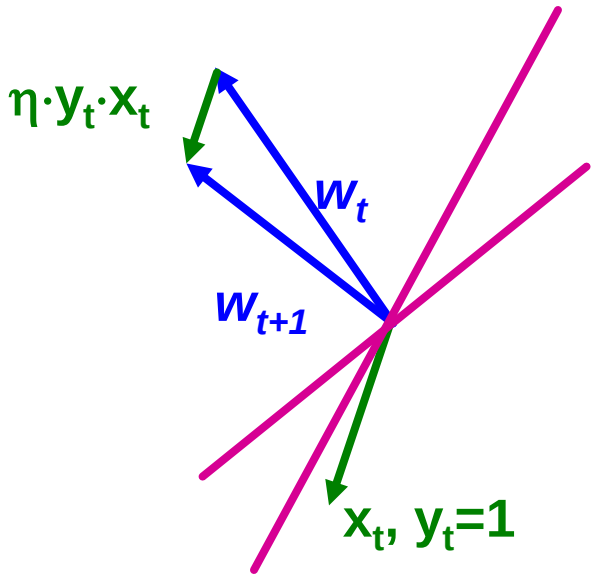
Perceptron

- **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

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

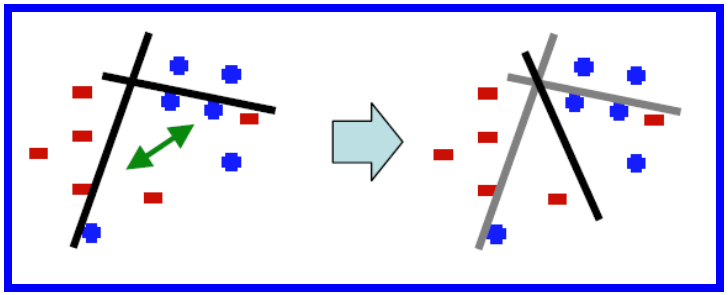
  - η is the learning rate parameter
  - x_t is the t-th training example
  - y_t is true t-th class label ({+1, -1})

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

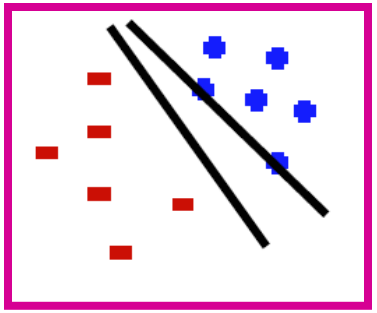


Perceptron: The Good and the Bad

- **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



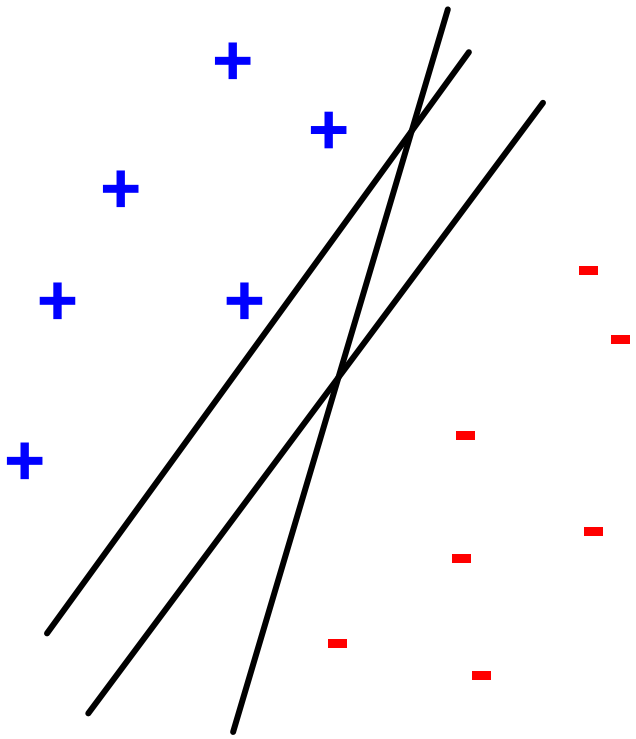
Updating the Learning Rate

- **Perceptron will oscillate and won't converge**
- **So, when to stop learning?**
- **(1)** Slowly decrease the learning rate η
  - A classic way is to: $\eta = c_1/(t + c_2)$
    - But, we also need to determine constants c_1 and 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



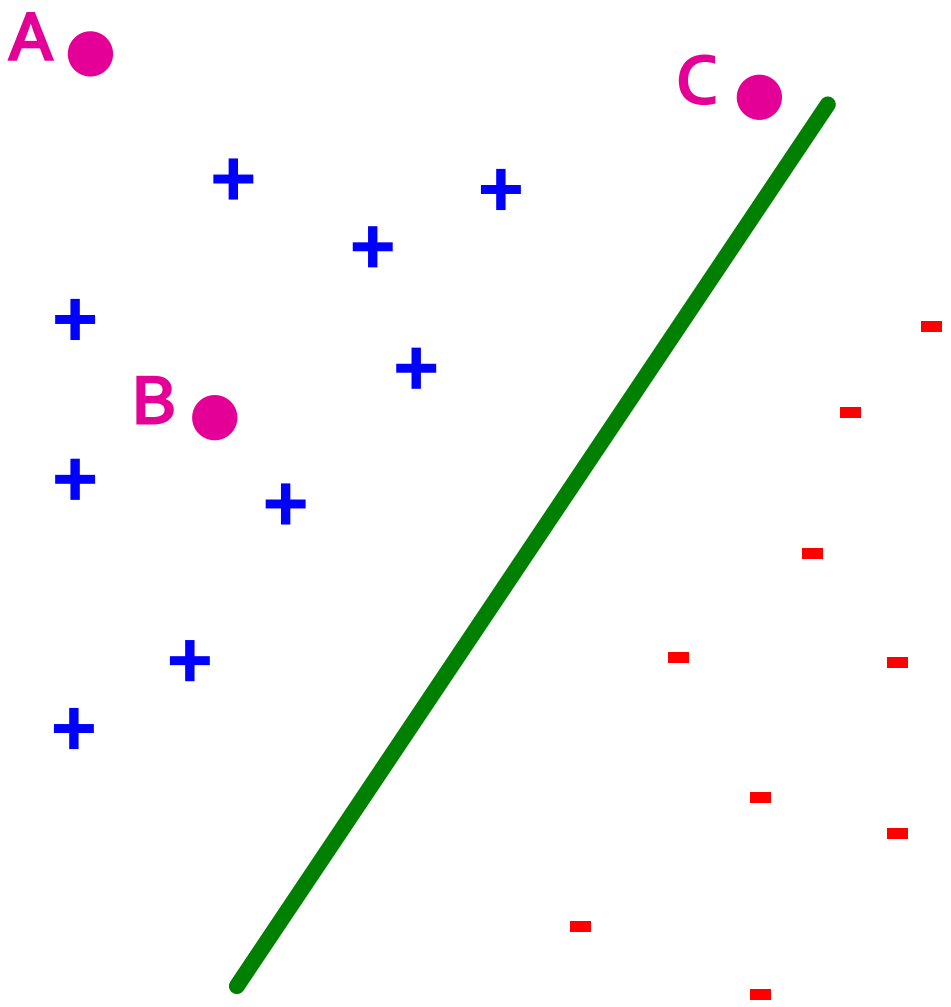
Data:

- **Training examples:**
  - $(x_1, y_1) \dots (x_n, y_n)$
- **Each example *i*:**
  - $x_i = (x_i^{(1)}, \dots , x_i^{(d)})$
    - $x_i^{(j)}$ 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*)?

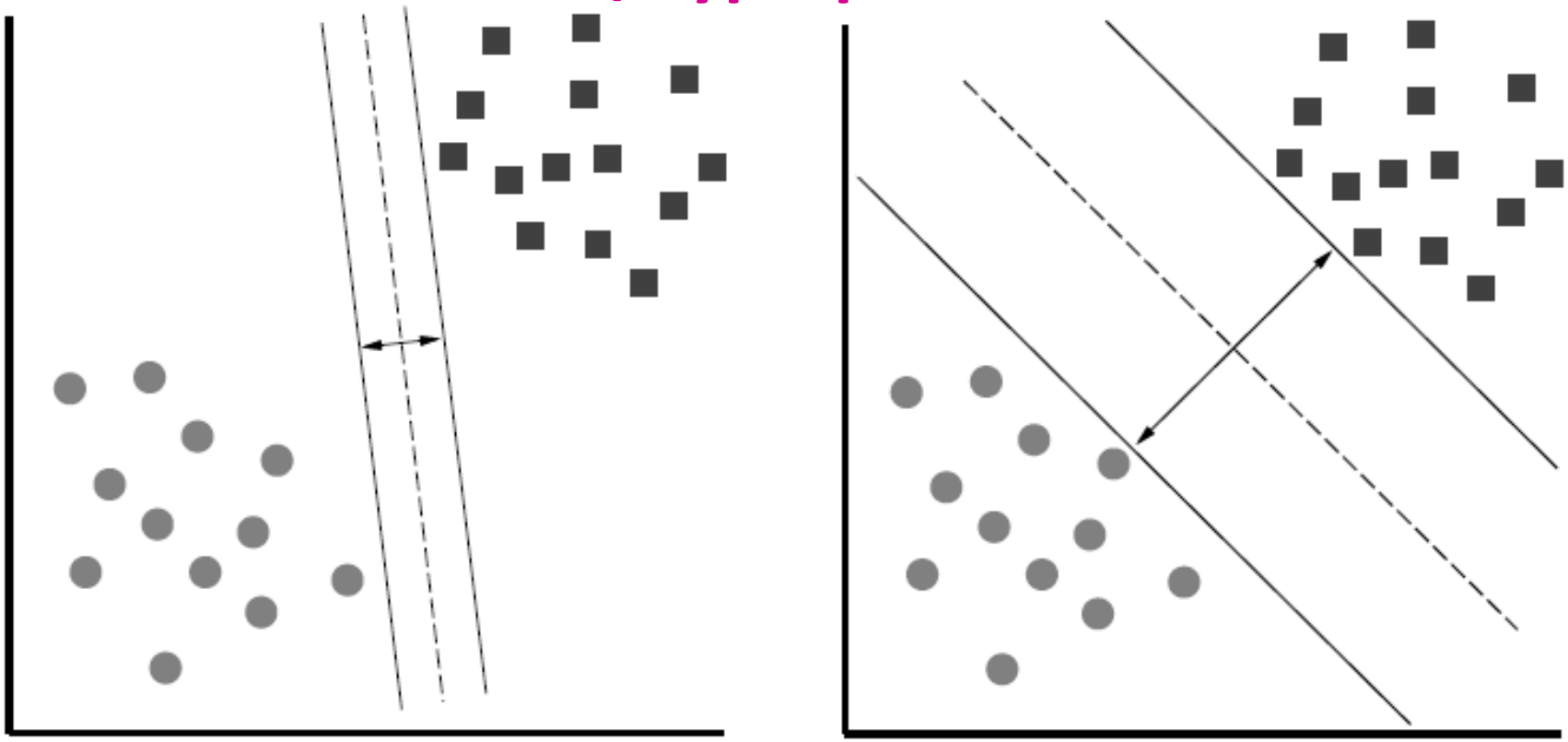
Largest Margin



- **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**

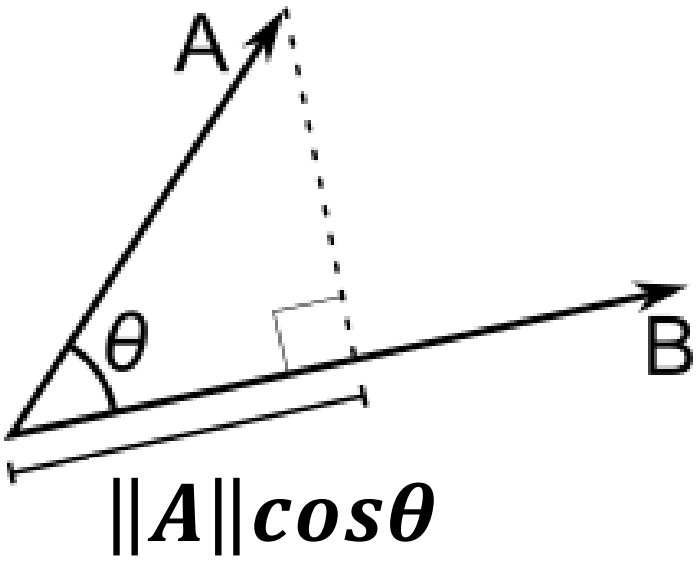


The reason we define margin this way is due to theoretical convenience and existence of generalization error bounds that depend on the value of margin.

Why maximizing γ a good idea?

- **Remember: Dot product**

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



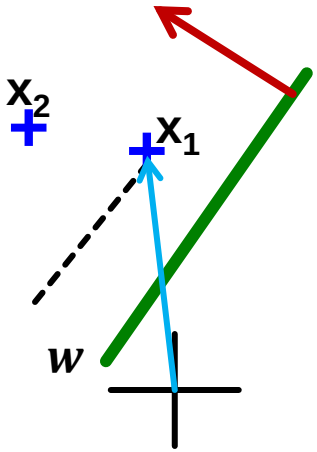
$$||\boldsymbol{A}|| = \sqrt{\sum_{j=1}^{d} (\boldsymbol{A^{(j)}})^2}$$

Why maximizing γ a good idea?

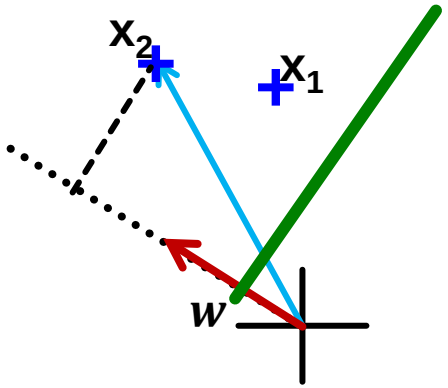
- **Dot product**

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

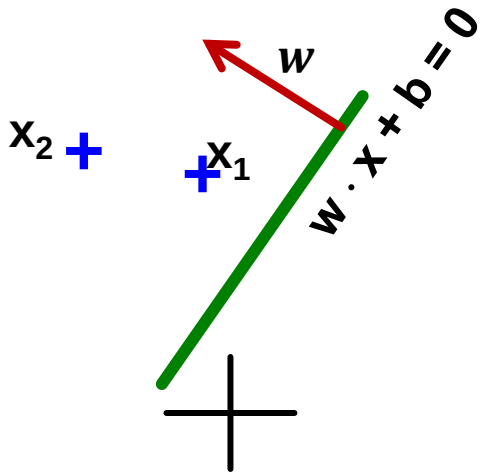
- **What is $w \cdot x_1$, $w \cdot x_2$?**



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

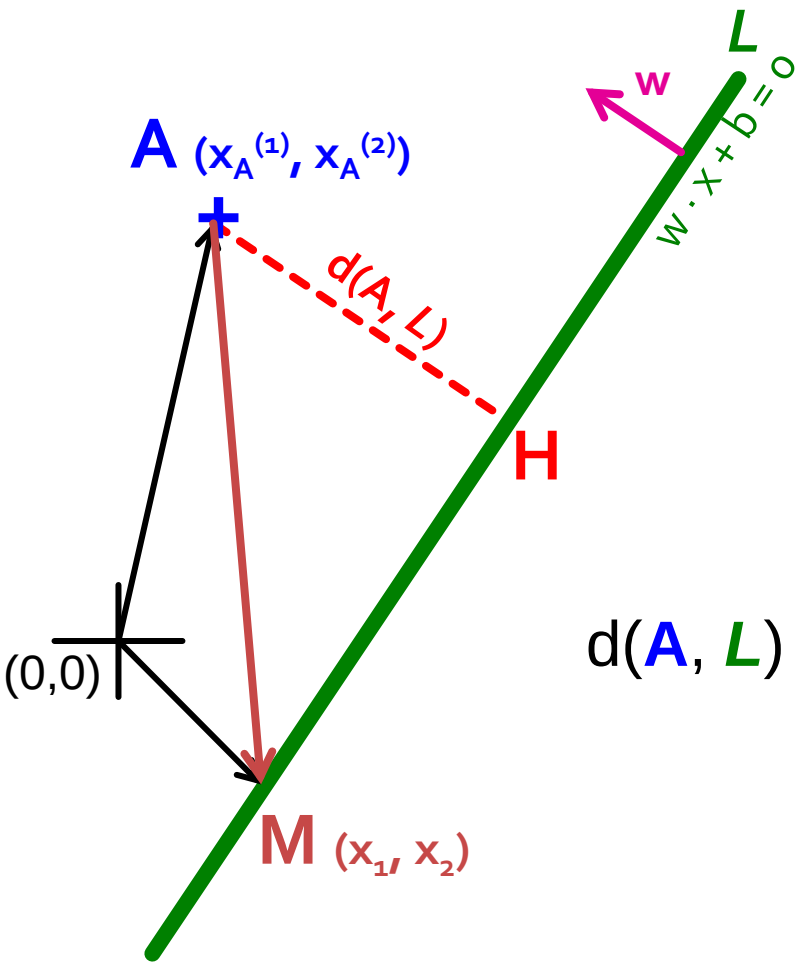


In this case
$\gamma_2 \approx 2\|w\|^2$



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

What is the margin?



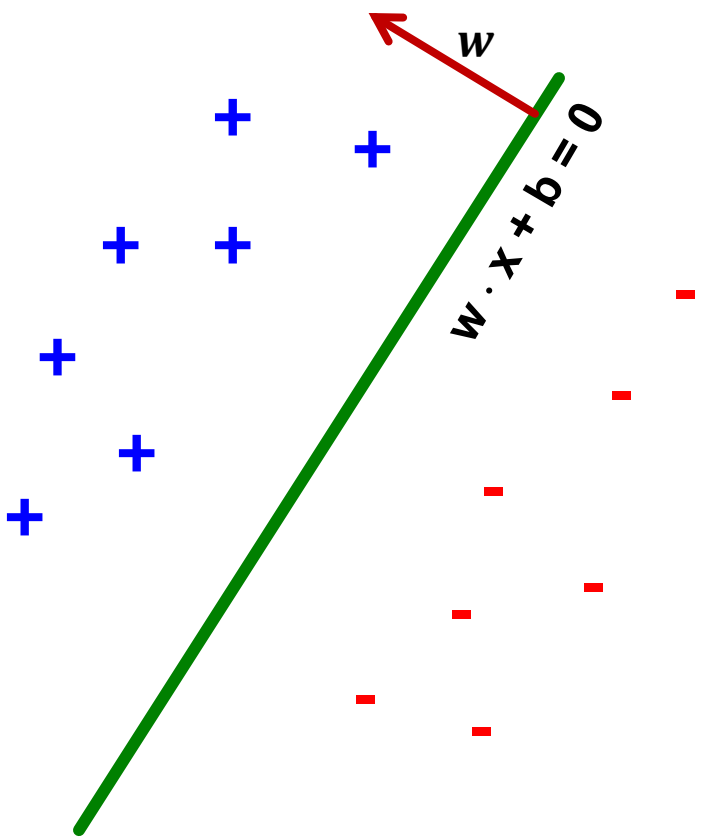
Note we assume $\|w\|_2 = 1$

- **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 $= (x_M^{(1)}, x_M^{(2)})$

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

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

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

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

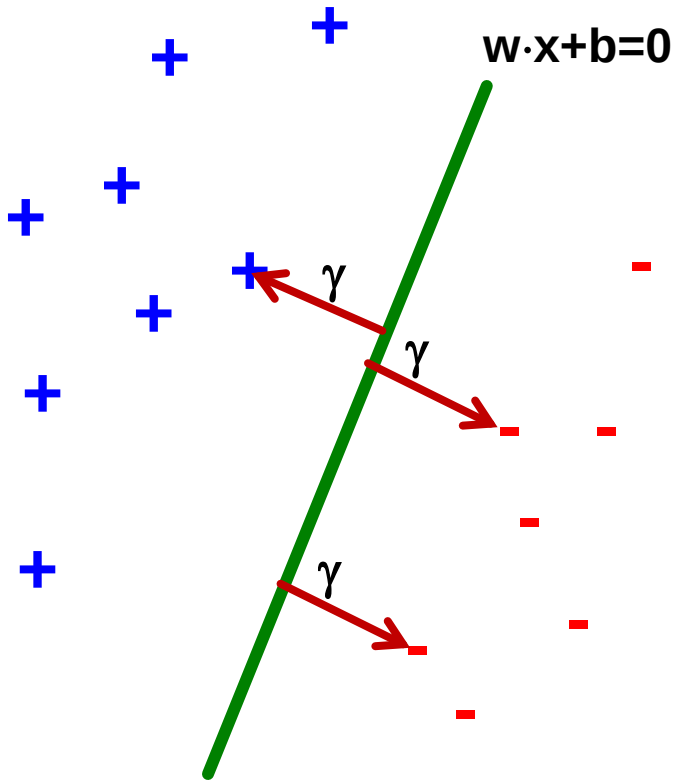
Support Vector Machine

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

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

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

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

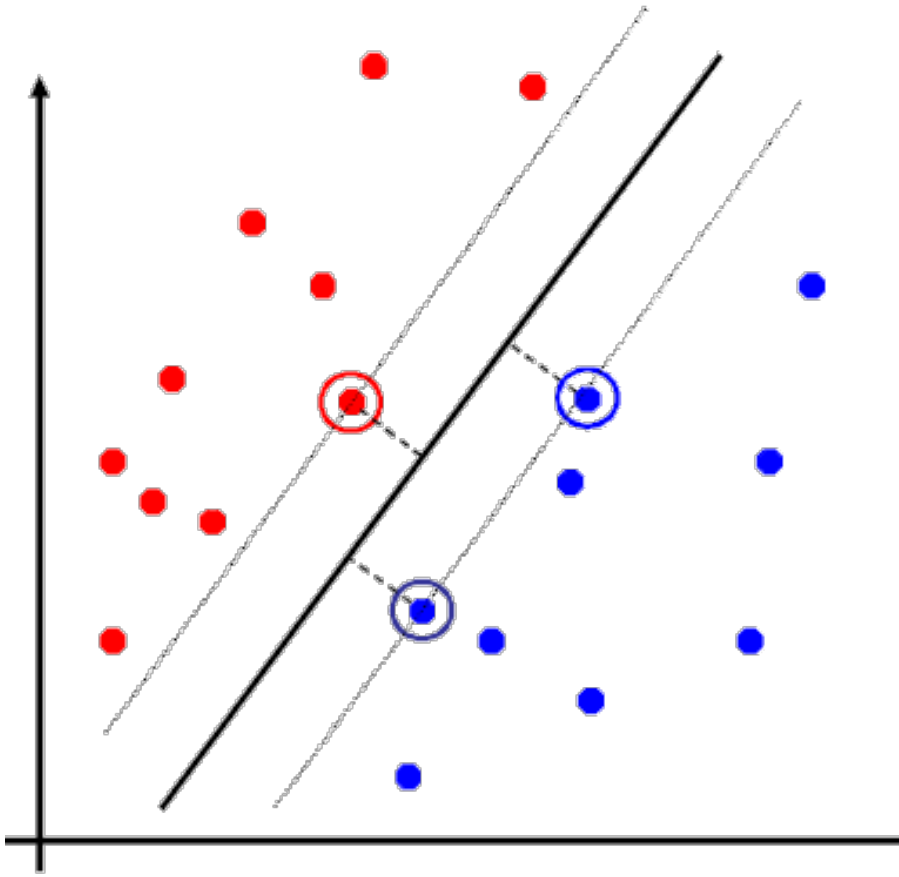


Maximizing the margin

Support Vector Machines: Deriving the margin

Support Vector Machines

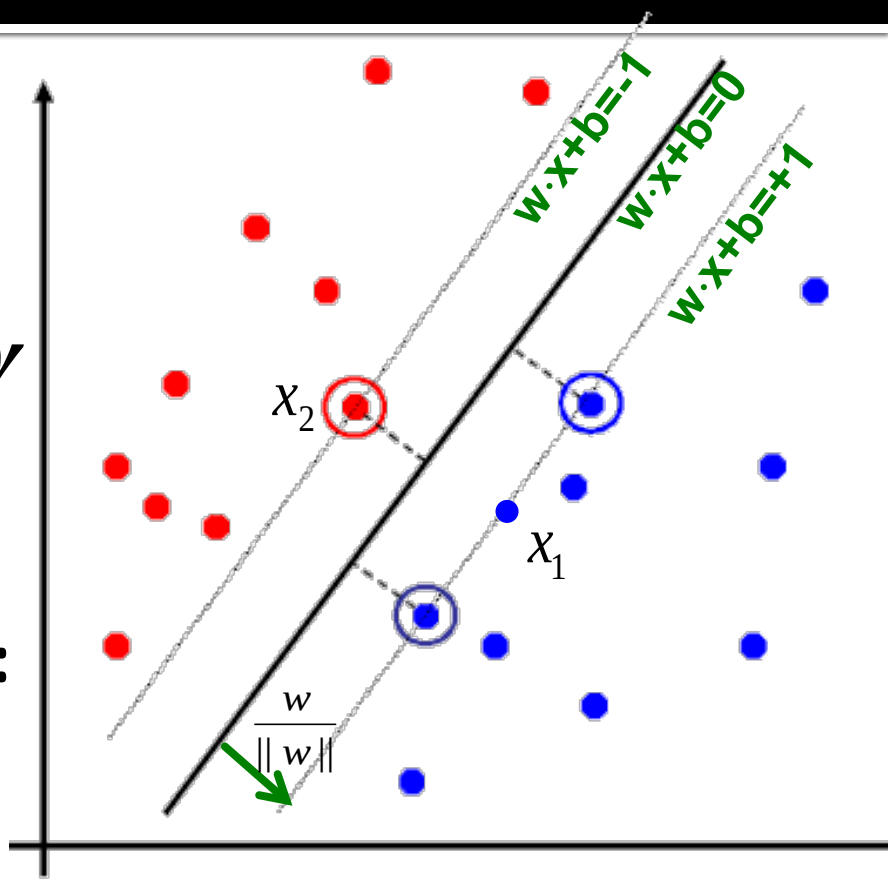
- **Separating hyperplane is defined by the support vectors**
  - Points on +/- planes from the solution
  - If you knew these points, you could ignore the rest
  - Generally, $d+1$ support vectors (for d dim. data)



Canonical Hyperplane: Problem

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

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

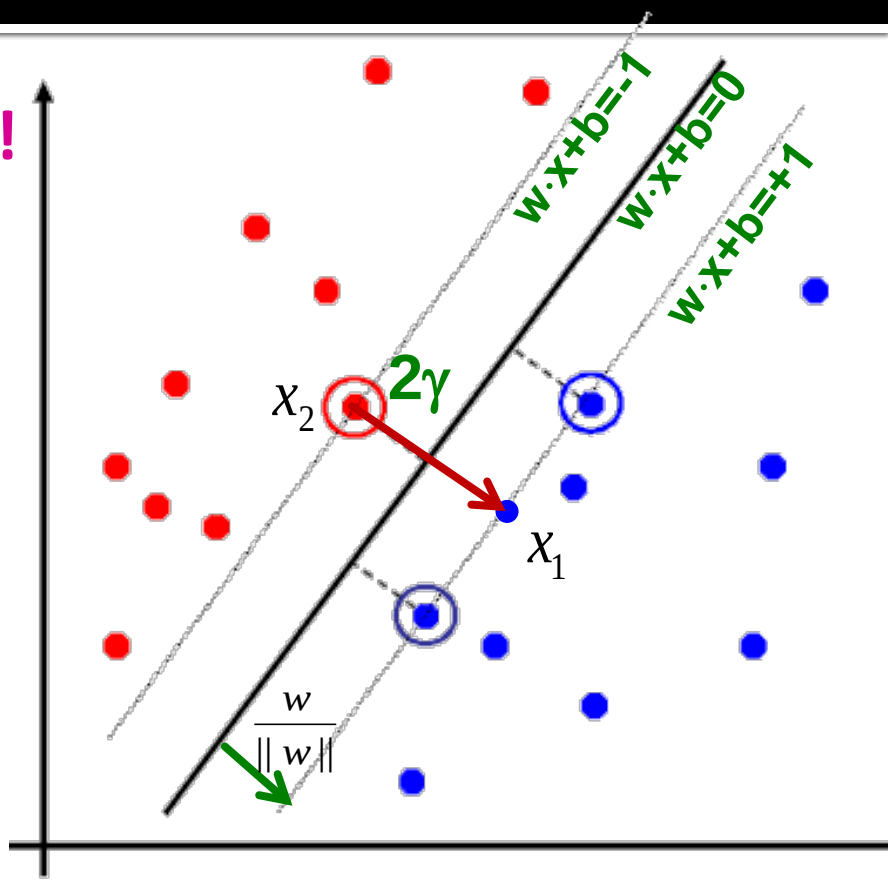


  - Let's also require **support vectors $\boldsymbol{x_j}$** to be on the plane defined by:
    $\boldsymbol{w}\cdot\boldsymbol{x_j}+\boldsymbol{b}=\pm\boldsymbol{1}$

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

Canonical Hyperplane: Solution

- Want to maximize margin γ!
- What is the relation between x_1 and x_2?
  - $x_1 = x_2 + 2\gamma \frac{w}{||w||}$
  - 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...**

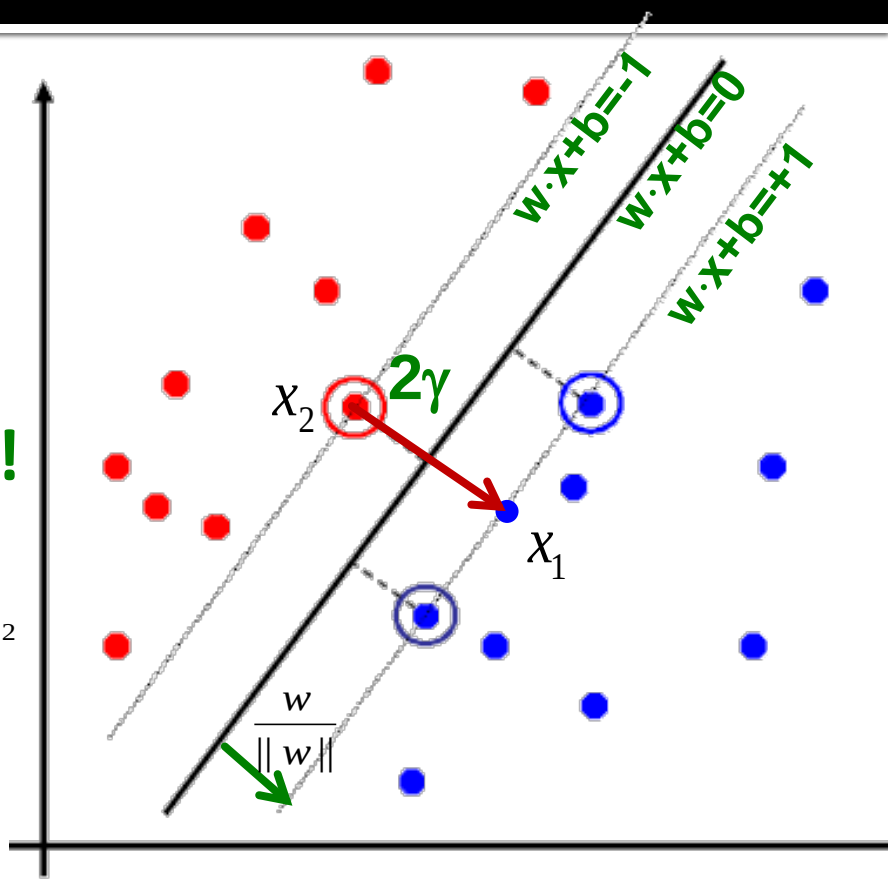
$$\arg\max \gamma = \arg\max \frac{1}{\|w\|} = \arg\min \|w\| = \arg\min \tfrac{1}{2}\|w\|^2$$

- **Then:**

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

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

This is called SVM with "hard" constraints



Non-linearly Separable Data

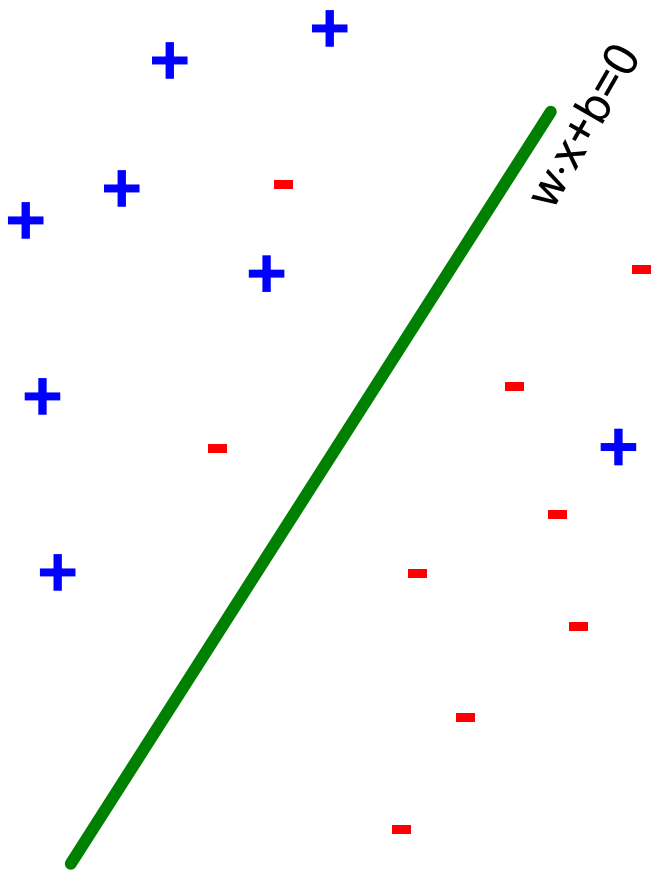
- **If data is not separable introduce penalty:**

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

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

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

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



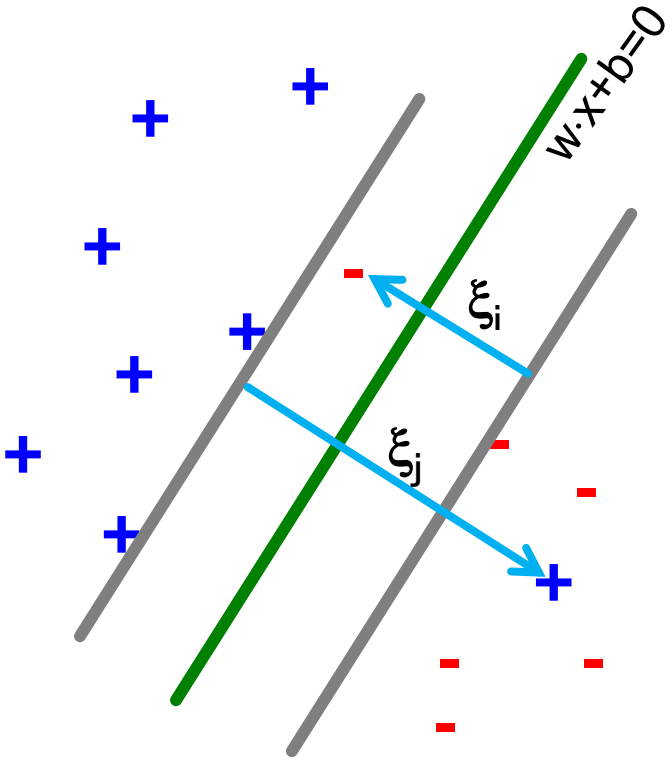
Support Vector Machines

- **Introduce slack variables ξ_i**

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

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

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



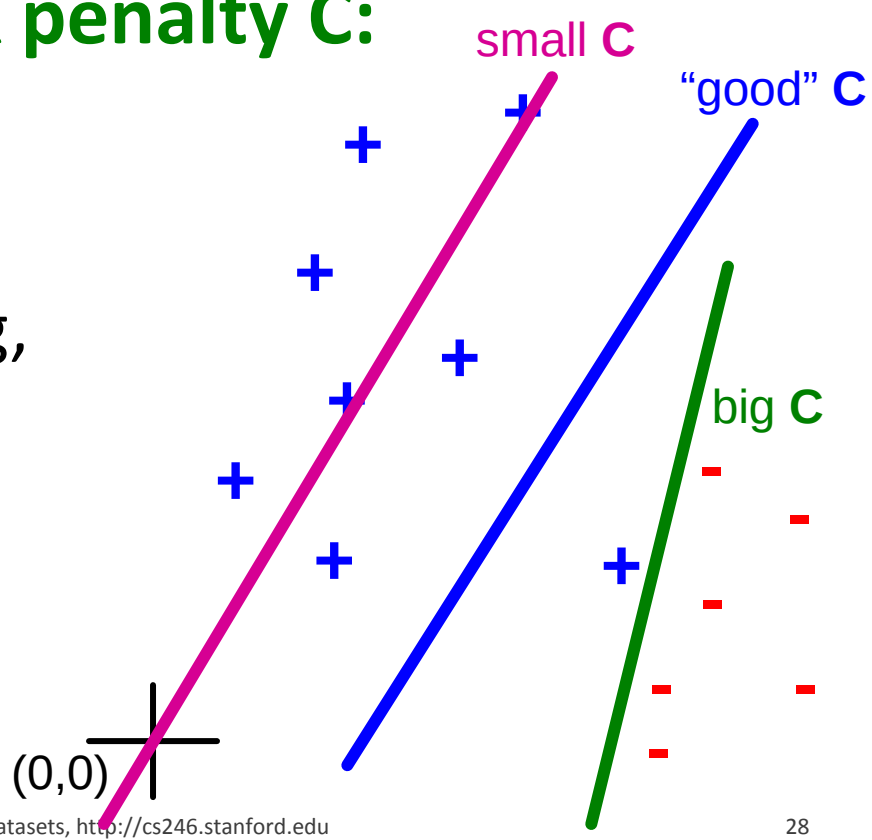
For each data point:
If margin ≥ 1, don't care
If margin < 1, pay linear penalty

Slack Penalty C

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

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

- **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**

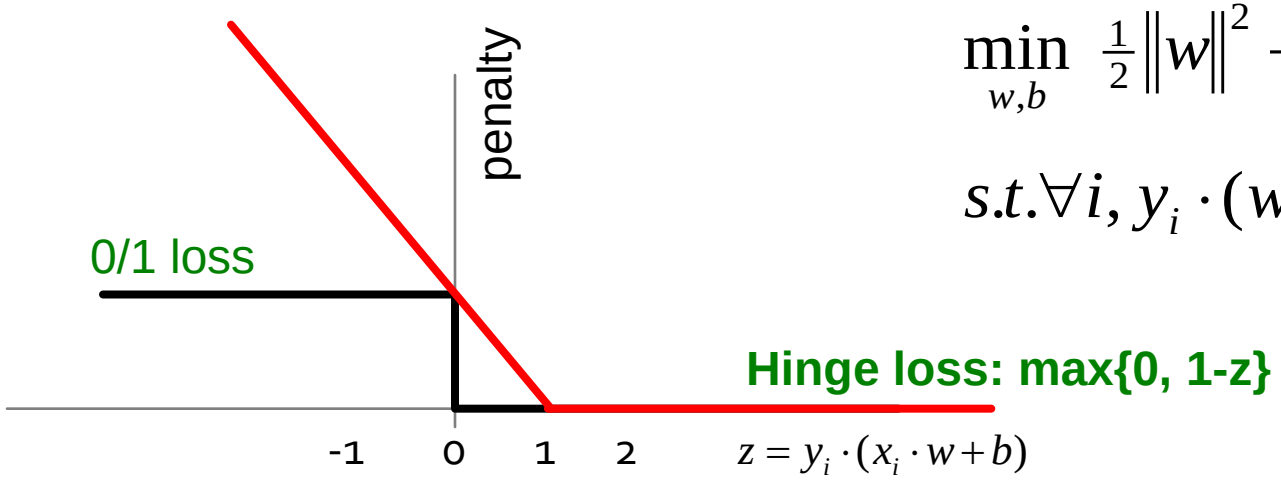
$$\arg\min_{w,b} \ \tfrac{1}{2} w \cdot w + C \cdot \sum_{i=1}^{n} \max\{0, 1 - y_i (w \cdot x_i + b)\}$$

Margin

Regularization parameter

Empirical **loss L** (how well we fit training data)

- **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?

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

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

- **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?

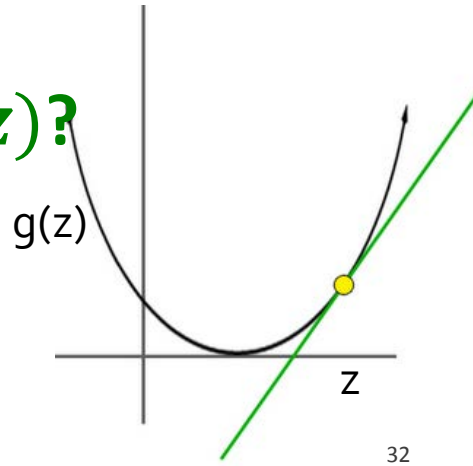
- **Want to estimate w, b!**
- **Alternative approach:**
  - **Want to minimize *f(w,b)*:**

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

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

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

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



SVM: How to estimate w?

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

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

Empirical loss $L(x_i\, y_i)$

- **Compute the gradient ∇(j) w.r.t. *w(j)***

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

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

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

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:**

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

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?

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

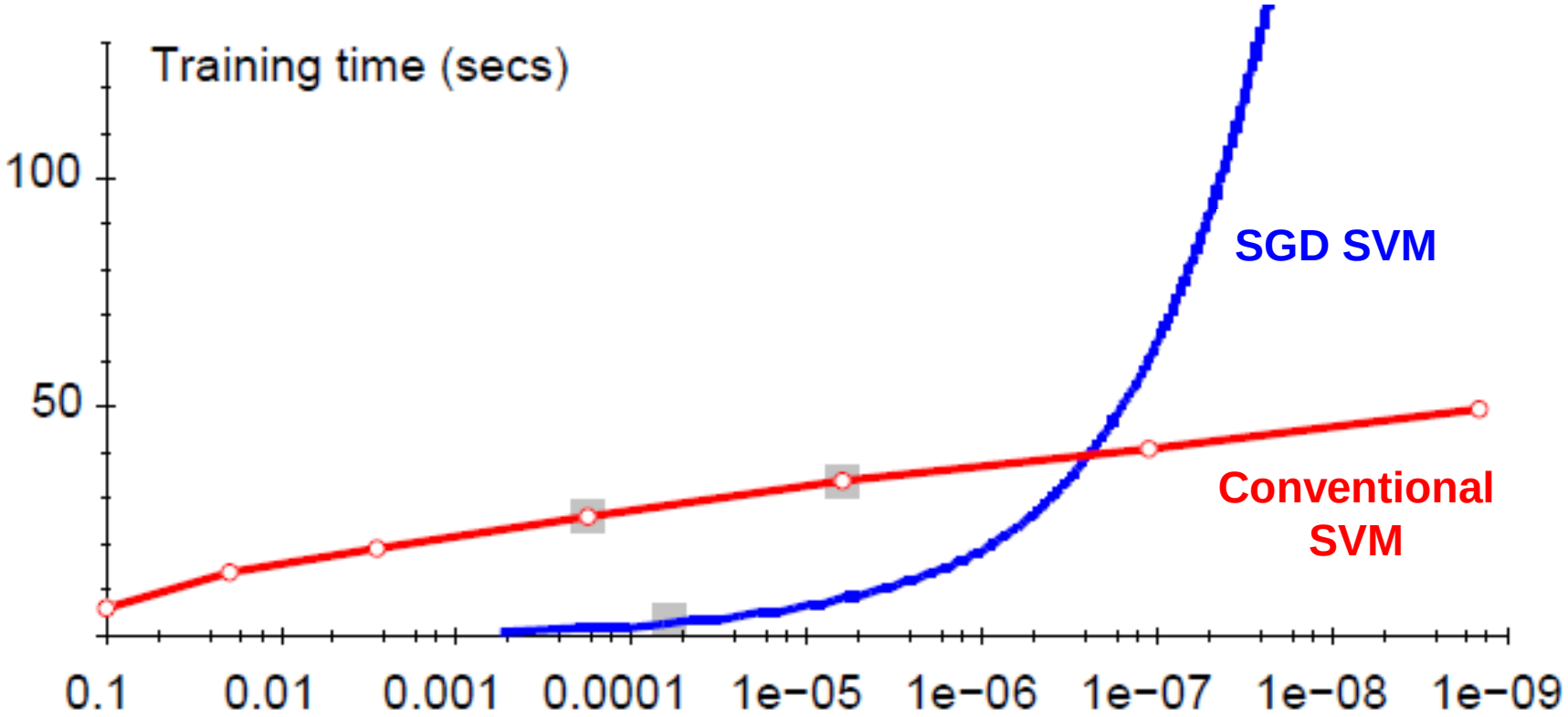
Example: Text categorization

- **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"

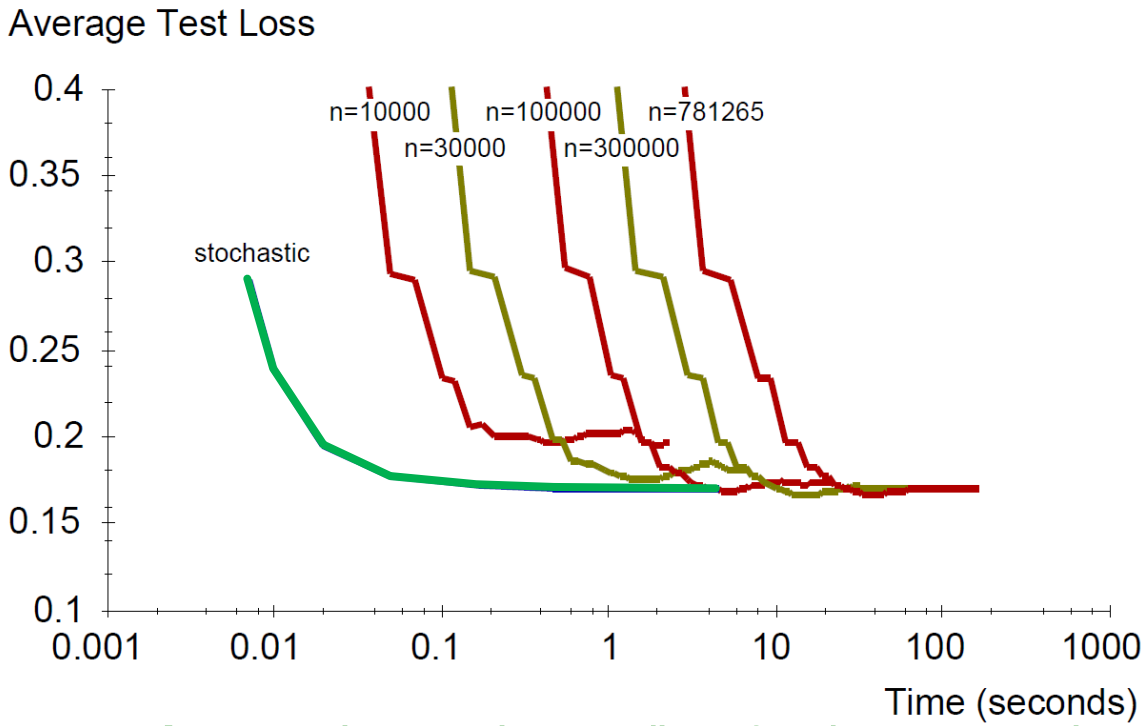


Optimization quality: $| f(w,b) - f(w^{opt},b^{opt}) |$

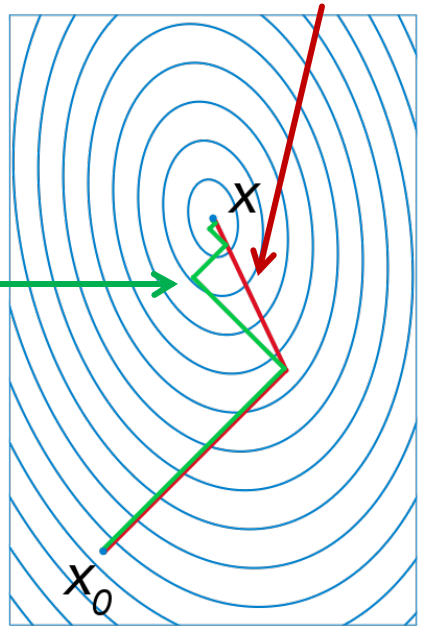
For optimizing *f(w,b) within reasonable* quality
SGD-SVM is super fast

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 k. **Conjugate gradient** converges in $\sqrt{k}$.



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

- **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,…]
    - 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:** $\boldsymbol{w = s \cdot v}$
  - Represent vector $\boldsymbol{w}$ as the product of scalar $\boldsymbol{s}$ and vector $\boldsymbol{v}$
  - Then the update procedure is:
    - $\boldsymbol{(1)\ v = v - \eta C \frac{\partial L(x_i, y_i)}{\partial w}}$
    - $\boldsymbol{(2)\ s = s(1 - \eta)}$

Two step update procedure:

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

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

- **Solution 2:**
  - Perform only step **(1)** for each training example
  - Perform step **(2)** with lower frequency and higher η

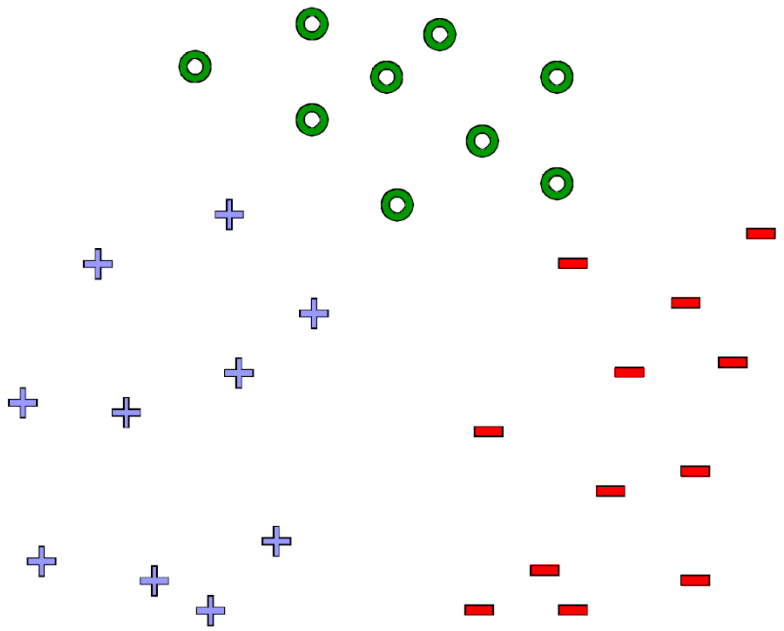
Practical Considerations

- **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:

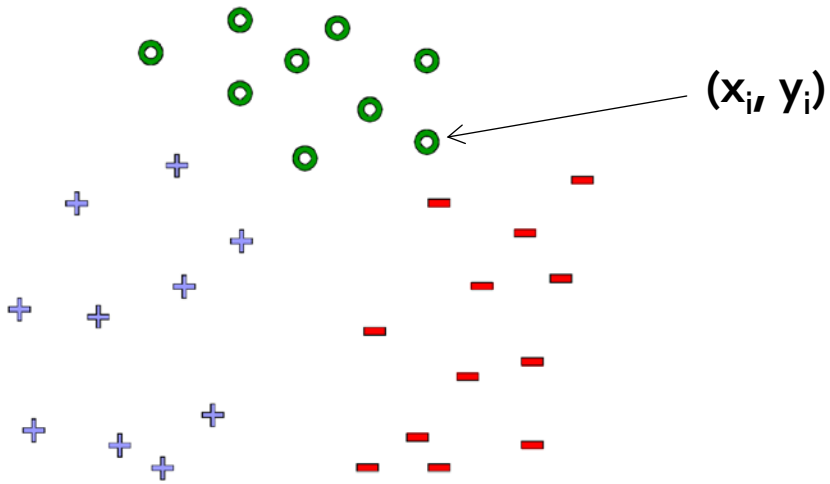
  $\mathbf{w_+ b_+,\ w_- b_-,\ w_o b_o}$
- **How to classify?**
- Return class *c*

  $\mathbf{\arg\max_c\ w_c x + b_c}$

Learn 1 classifier: Multiclass SVM

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

$$w_{y_i} x_i + b_{y_i} \geq 1 + w_c x_i + b_c \quad \forall c \neq y_i \;, \forall i$$



Multiclass SVM

- **Optimization problem:**

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

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

$$\xi_i \geq 0, \forall i$$

  - 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**