Large-Scale Machine Learning (2)

CS547 Machine Learning for Big Data

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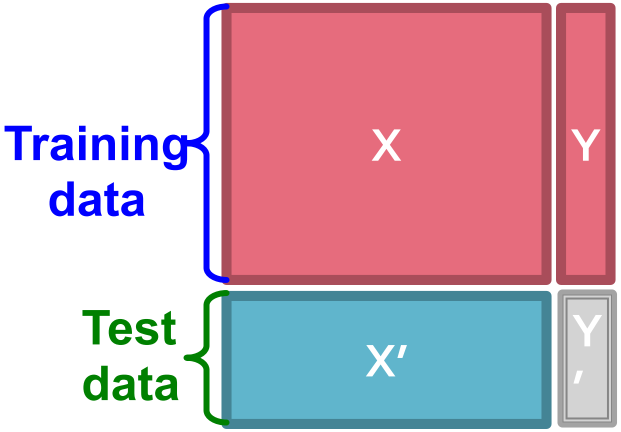
Supervised Learning

- **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

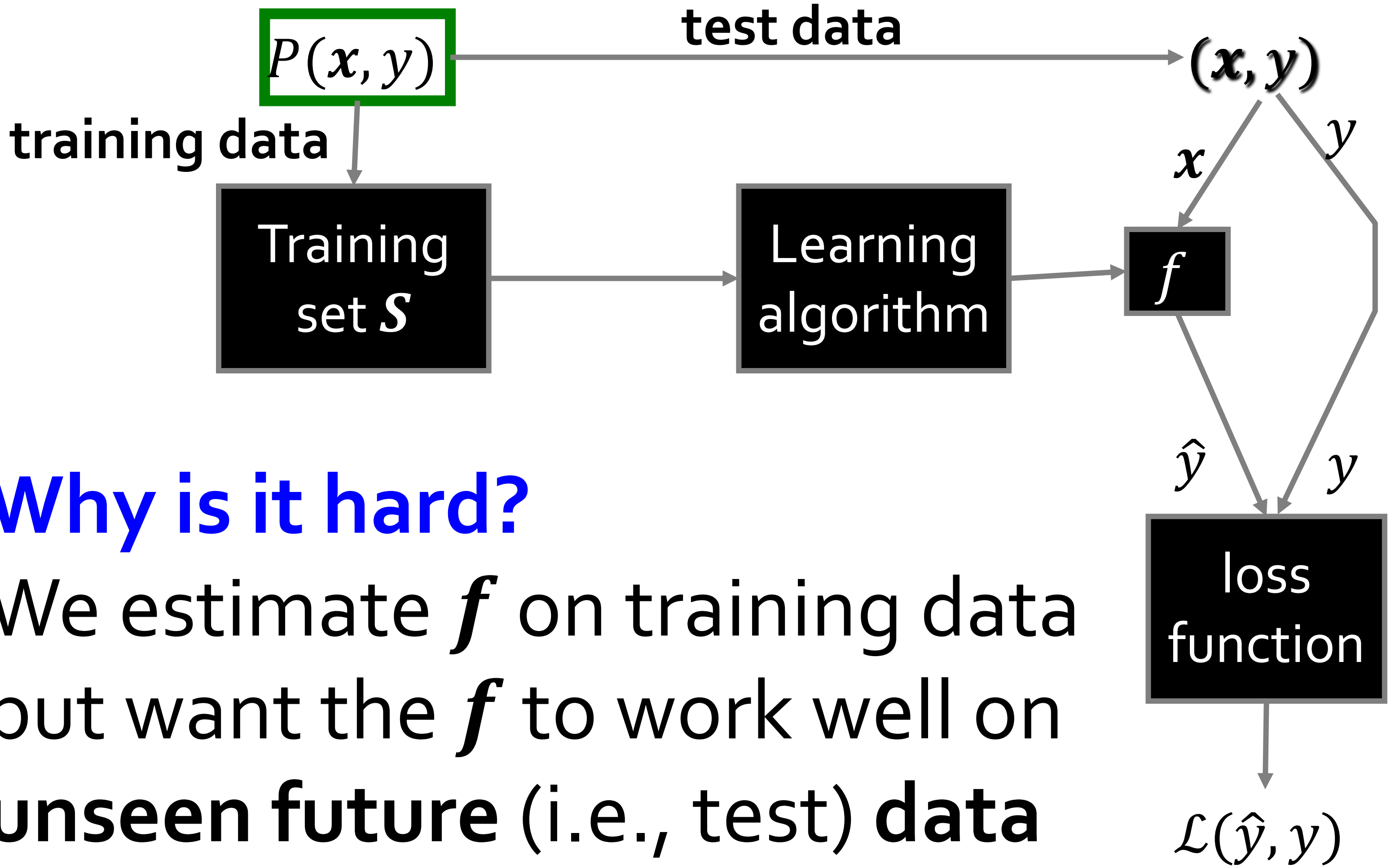
- **Task:** Given data **(X,Y)** build a model **f()** to predict **Y'** based on **X'**
- **Strategy:** **Estimate $y = f(x)$ on (X, Y).**
  Hope that the same $f(x)$ also works to predict unknown Y'
  - The **"hope"** is called **generalization**
    - **Overfitting:** **If f(x) predicts well Y but is unable to predict Y'**
  - **We want to build a model that <u>generalizes</u> well to unseen data**



Formal Setting

- **1)** Training data is drawn independently at random according to unknown probability distribution $P(\boldsymbol{x}, y)$
- **2)** The learning algorithm analyzes the examples and produces a classifier $\boldsymbol{f}$
- Given **new** data $(\boldsymbol{x}, y)$ drawn from $\boldsymbol{P}$, the classifier is given $\boldsymbol{x}$ and predicts $\widehat{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{x})$
- The **loss** $\boldsymbol{\mathcal{L}}(\widehat{\boldsymbol{y}}, \boldsymbol{y})$ is then measured
- **Goal of the learning algorithm:**
  Find $\boldsymbol{f}$ that minimizes **expected loss** $\boldsymbol{E_P}[\boldsymbol{\mathcal{L}}]$

Formal Setting



Why is it hard?

We estimate $\boldsymbol{f}$ on training data but want the $\boldsymbol{f}$ to work well on **unseen future** (i.e., test) **data**

Minimizing the Loss

- **Goal:** **Minimize the expected loss**

$$\min_f \mathbb{E}_{\mathrm{P}}[\mathcal{L}]$$

- **But, we don't have access to P but only to training sample D:**

$$\min_f \mathbb{E}_{\mathrm{D}}[\mathcal{L}]$$

- **So, we minimize the average loss on the training data:**

$$\min_f J(f) = \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(f(x_i), y_i)$$

Problem: Just memorizing the training data gives us a perfect model (with zero loss)

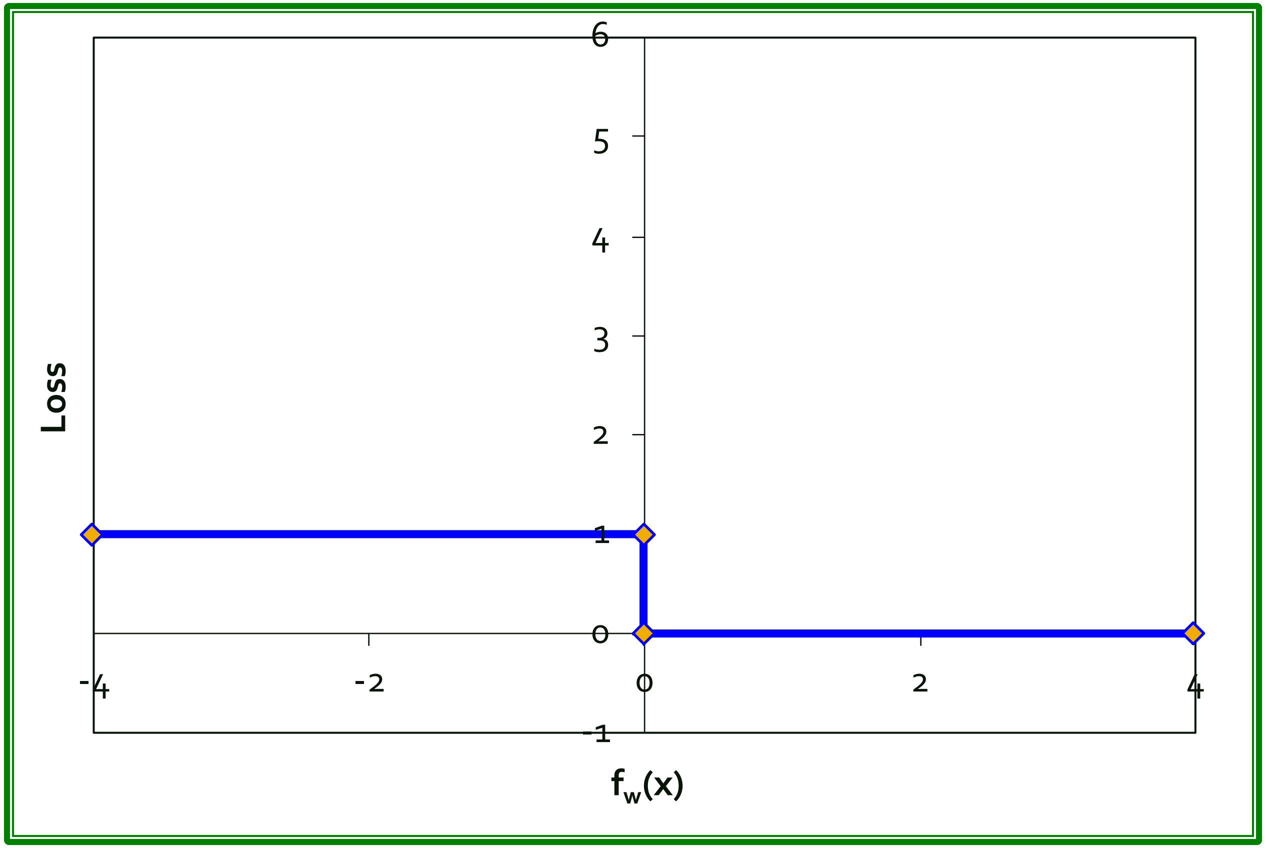
ML == Optimization

- **Given:**
  - A set of **N** training examples
    - $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  - A loss function $\boldsymbol{\mathcal{L}}$
- **Choose the model:** $\boldsymbol{f_w(x) = w \cdot x + b}$
- **Find:**
  - The weight vector w that minimizes the **expected loss on the training data**

$$J(f) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(w \cdot x_i + b, y_i)$$

Problem: Loss

- **Problem:** Step-wise Constant 0-1-Loss function



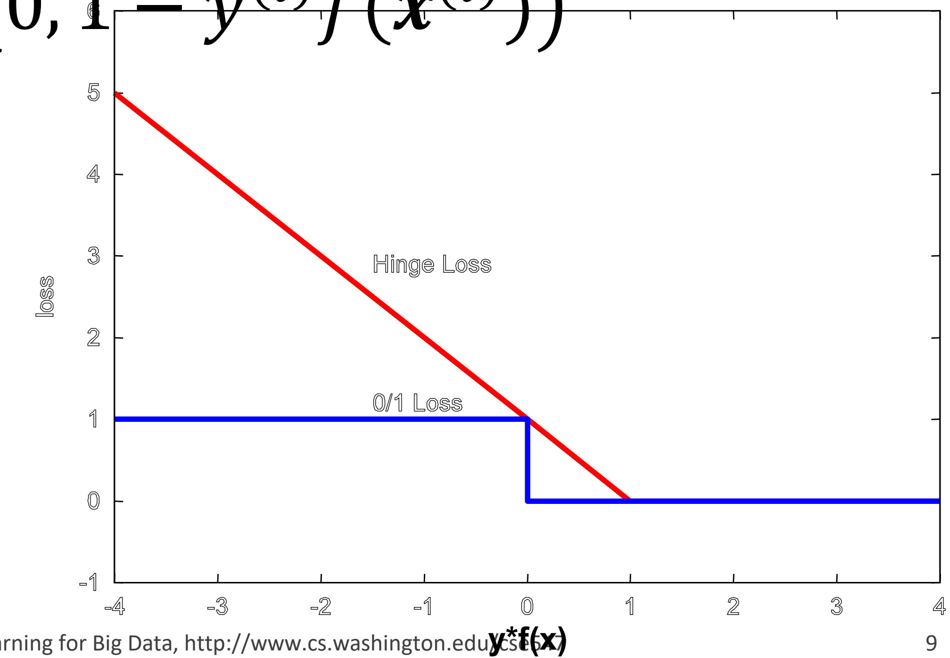
Derivative is either 0 or not differentiable

Approximating the Loss

- **Approximating the expected loss by a smooth function**
  - Replace the original objective function by a surrogate loss function. E.g., **hinge loss**:

$$\tilde{J}(\boldsymbol{w}) = \frac{1}{N}\sum_{i=1}^{N} \max\left(0, 1 - y^{(i)} f\left(\boldsymbol{x}^{(i)}\right)\right)$$

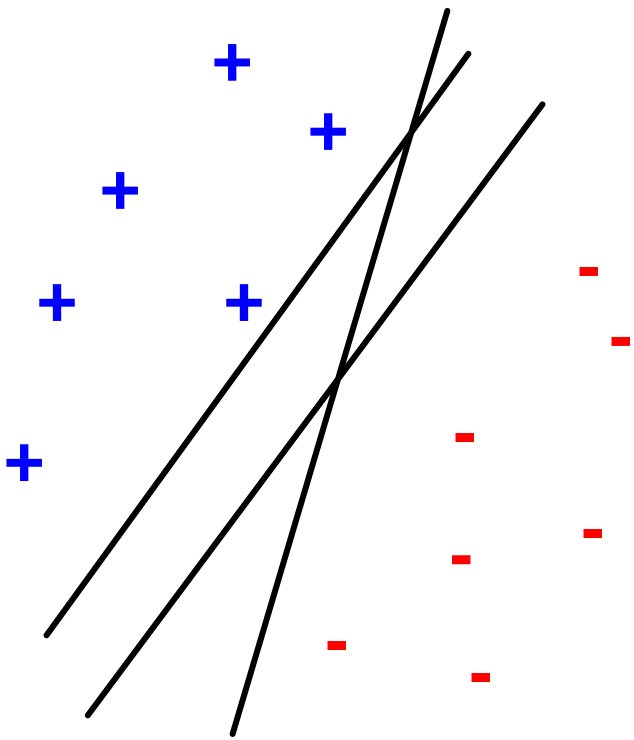
When $y = 1$:



Support Vector Machines

Support Vector Machines

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



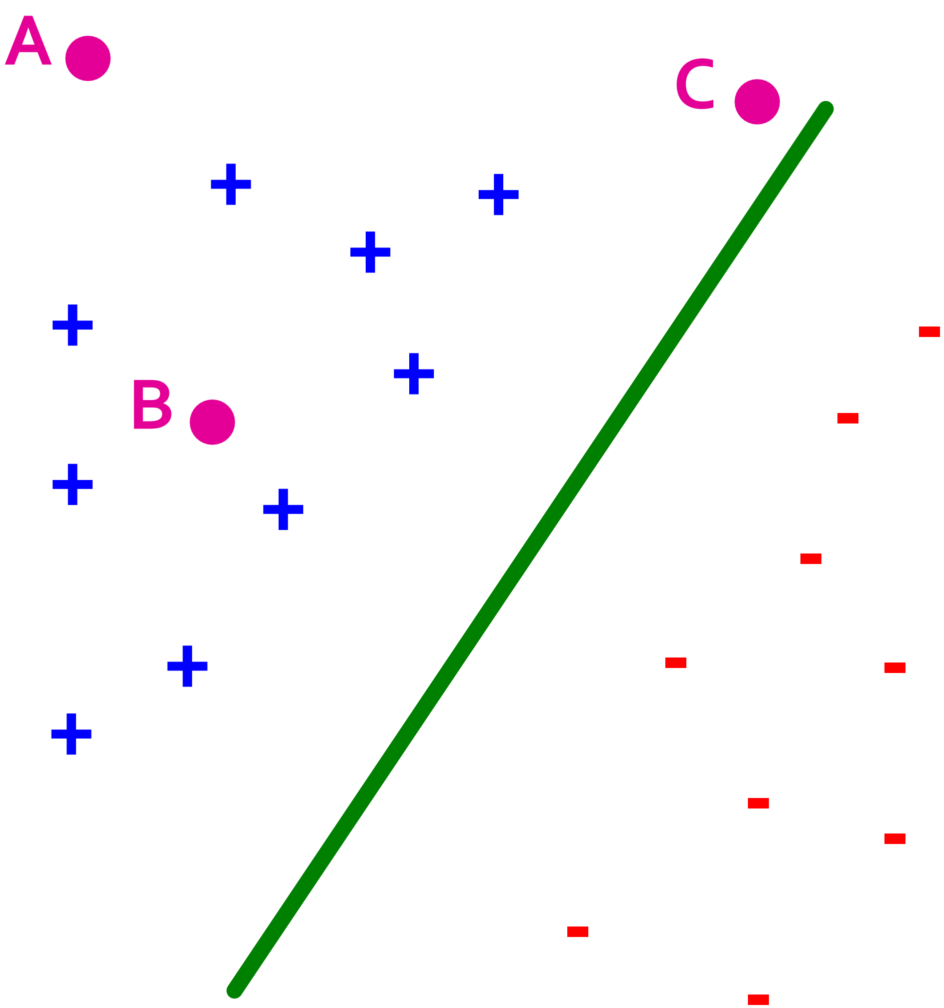
Data:

- **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,b*)?

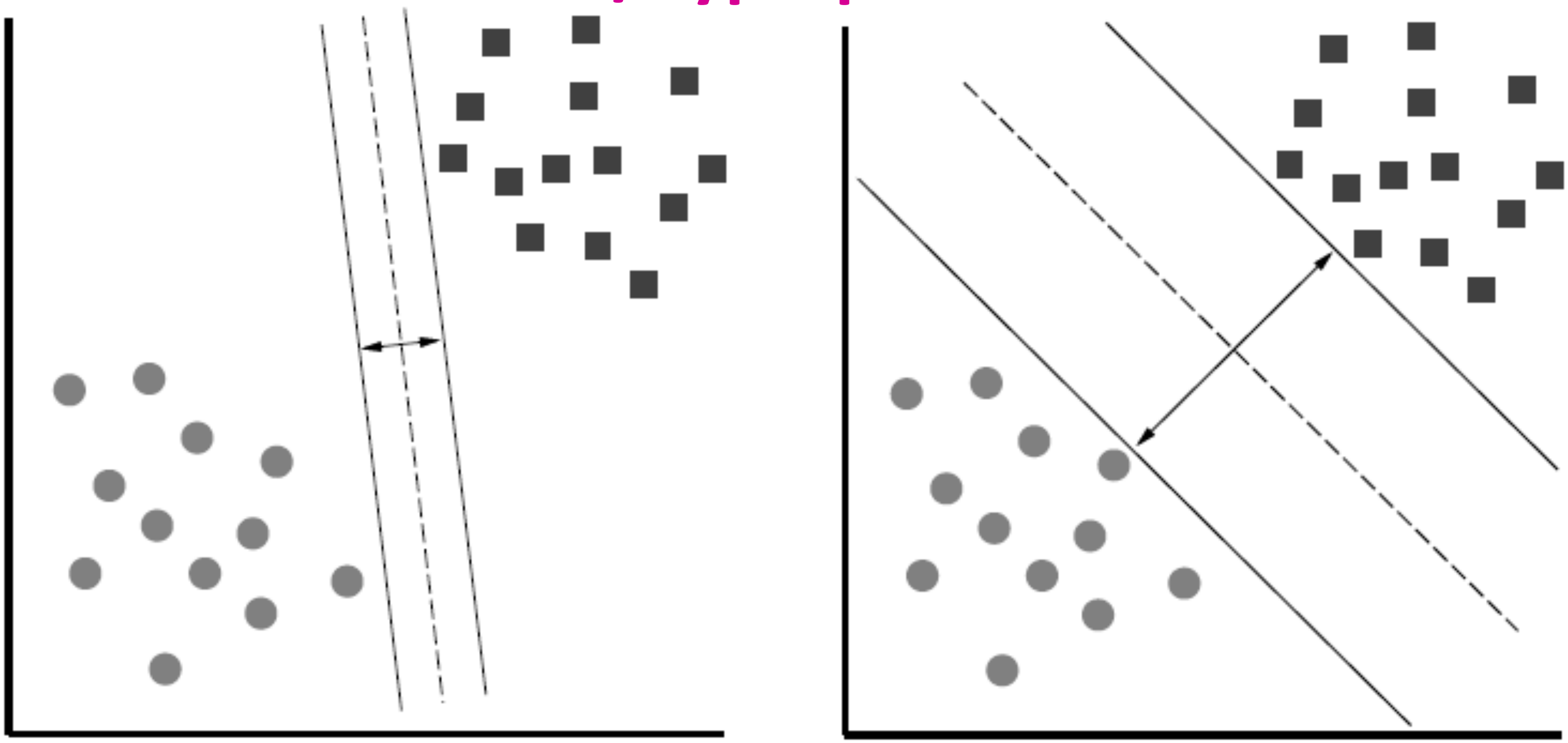
Maximum Margin



- **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**

Maximum Margin

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

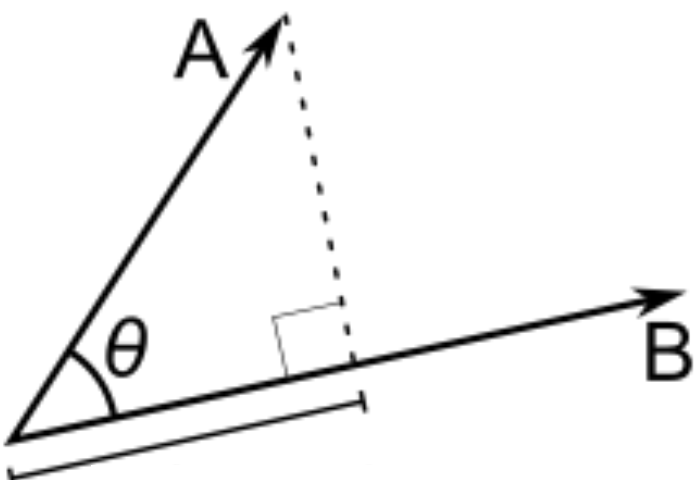


The reason we define margin this way is due to theoretical convenience and existence of generalization error bounds that depend on the value of margin.

Why maximizing γ a good idea?

- **Remember: The Dot product**

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



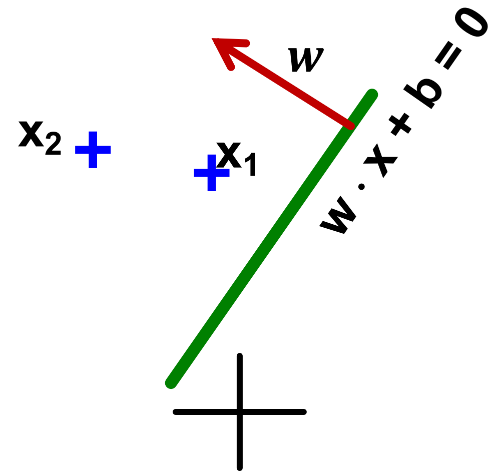
$$\|\boldsymbol{A}\|\boldsymbol{cos\theta}$$

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

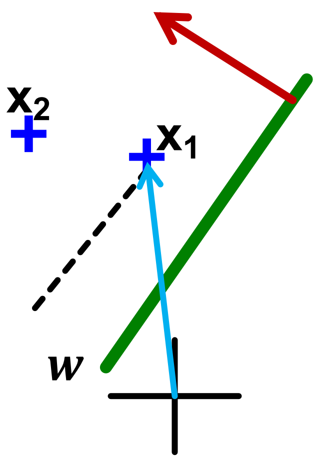
Why maximizing γ a good idea?

- **Dot product**

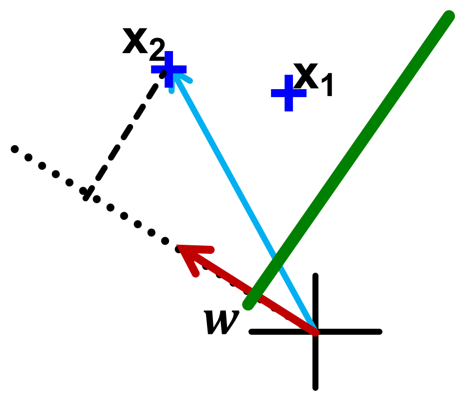
  $$A \cdot B = \|A\| \|B\| \cos\theta$$



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



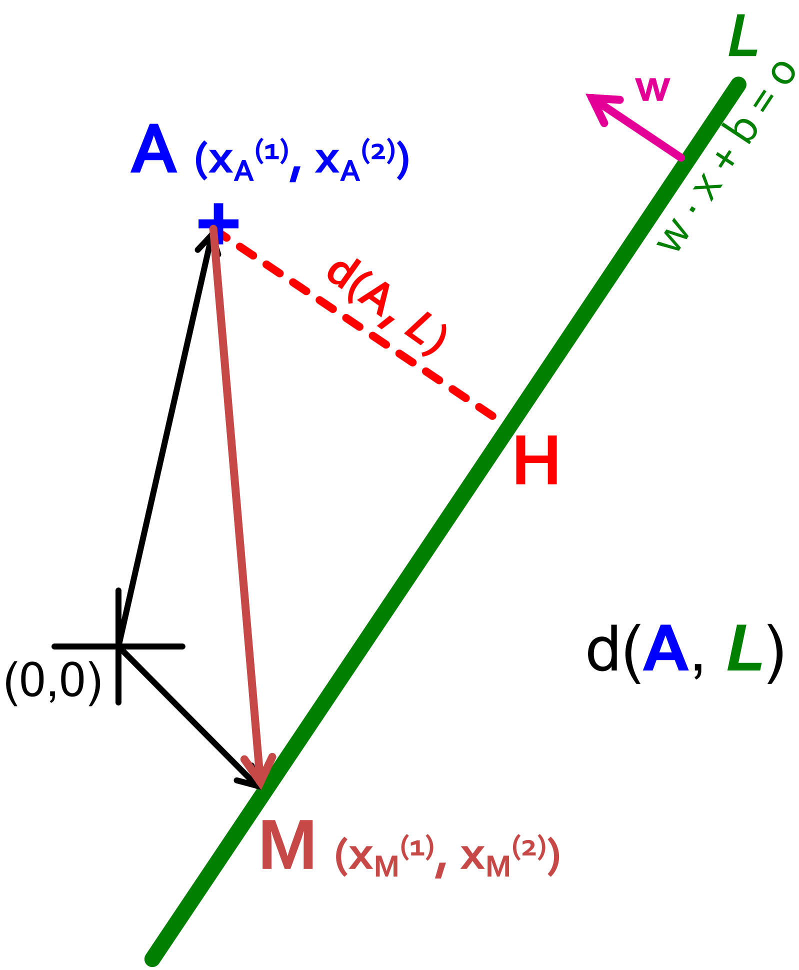
In this case
$\gamma_1 \approx \|w\|^2$



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

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

What is the margin?



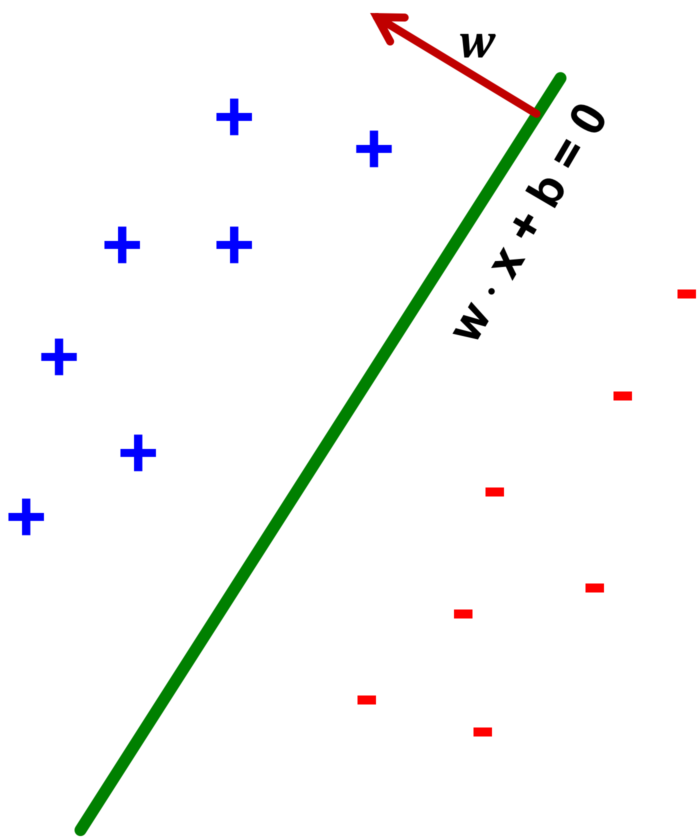
Note we assume $\|w\|_2 = 1$

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

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

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:**

$$\max_{w,b} \min_i \gamma_i$$

- **Can rewrite as**

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

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

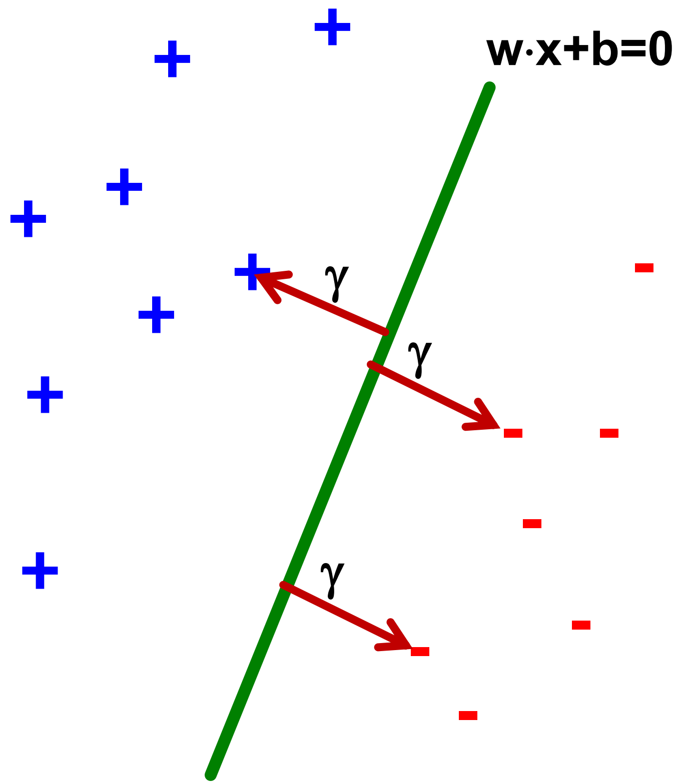
Support Vector Machine

- **Maximize the margin:**
  - **Good according to intuition, theory (c.f. "VC dimension") and practice**

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

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

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

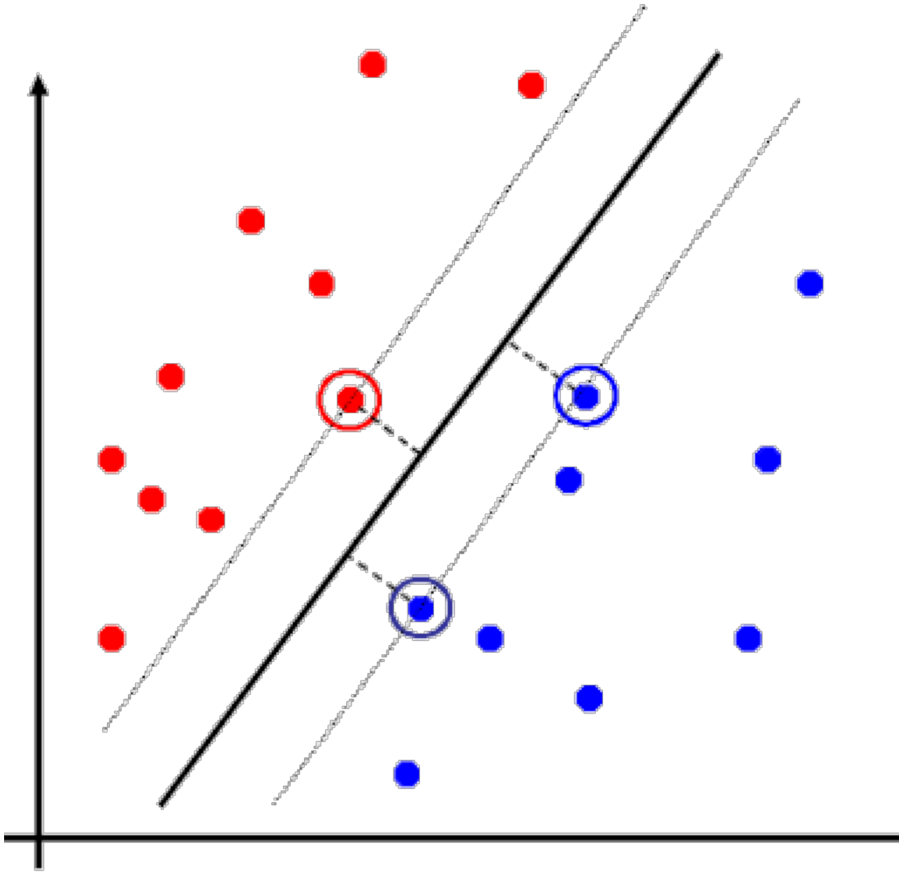


Maximizing the margin

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)



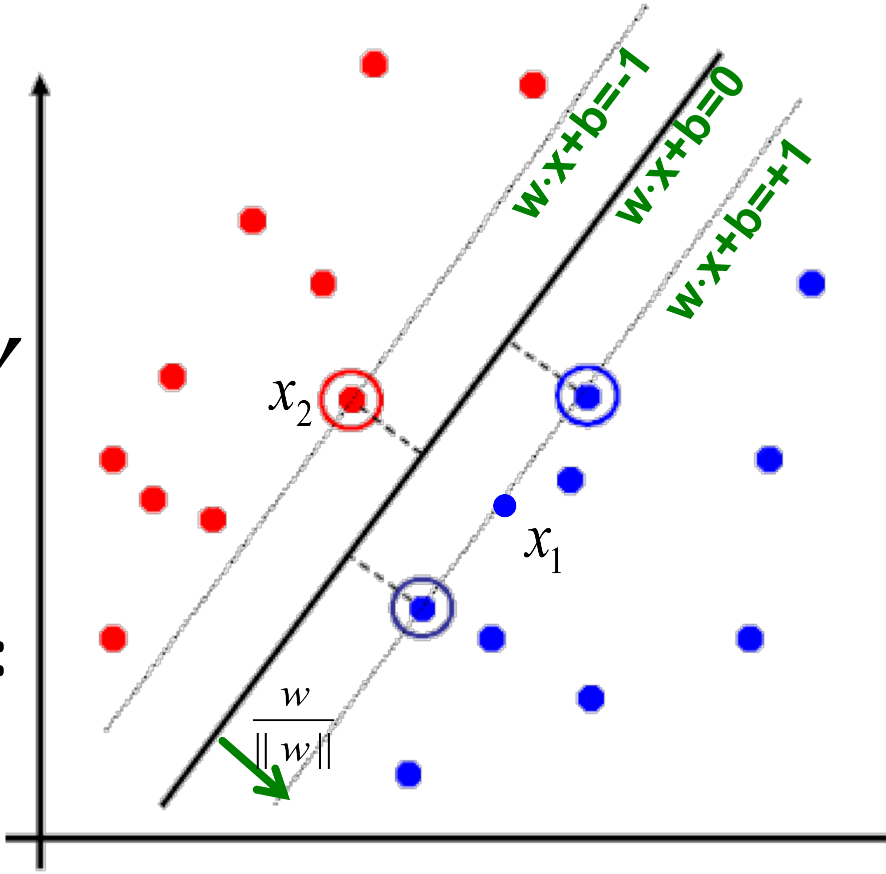
Canonical Hyperplane: Problem

- **Problem:**
  - Let $(\boldsymbol{w}\cdot\boldsymbol{x}+\boldsymbol{b})\boldsymbol{y}=\boldsymbol{\gamma}$
    then $(2\boldsymbol{w}\cdot\boldsymbol{x}+2\boldsymbol{b})\boldsymbol{y}=2\boldsymbol{\gamma}$
    - 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:

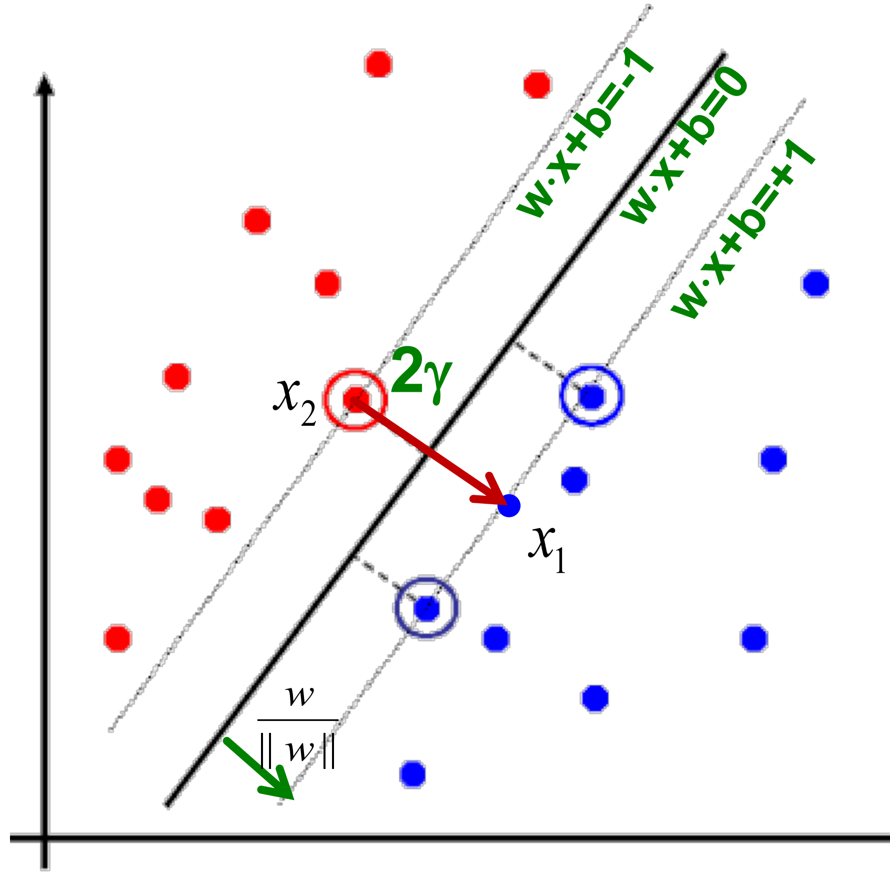
$$\boldsymbol{w}\cdot\boldsymbol{x}_j+\boldsymbol{b}=\pm\mathbf{1}$$



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

Canonical Hyperplane: Solution

- **Want to maximize margin!**
- **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:
$\mathrm{w} \cdot \mathrm{w} = \|w\|^2$

Maximizing the Margin

- **We started with**

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

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

But *w* can be arbitrarily large!

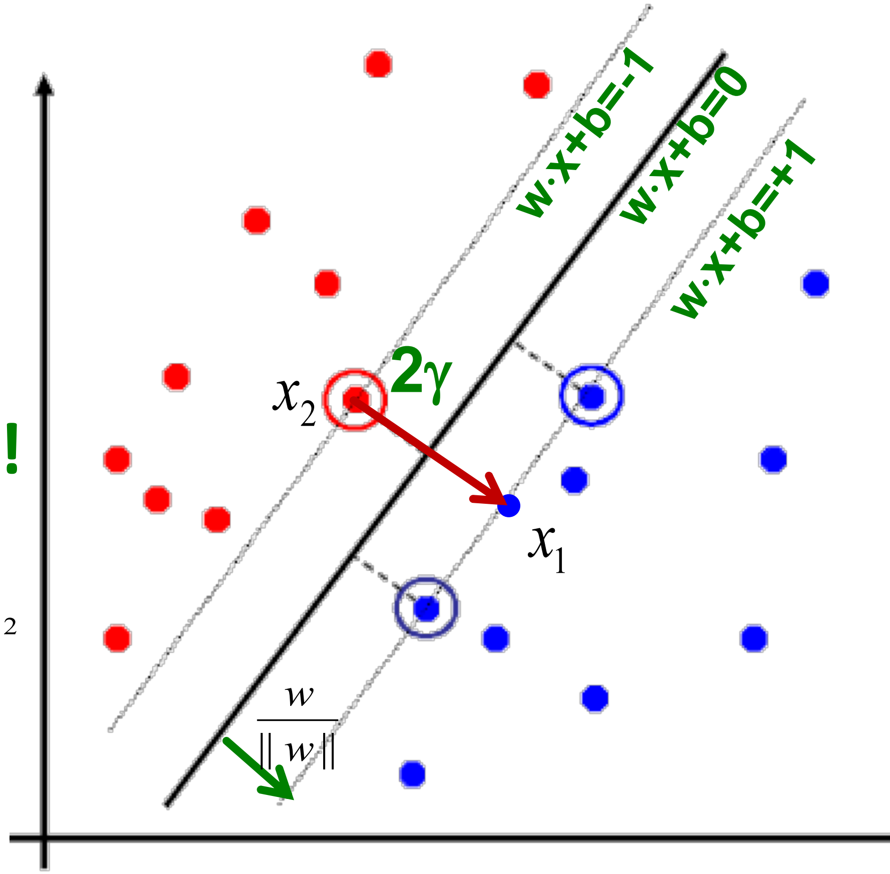
- **We normalized and...**

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

- **Then:**

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

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



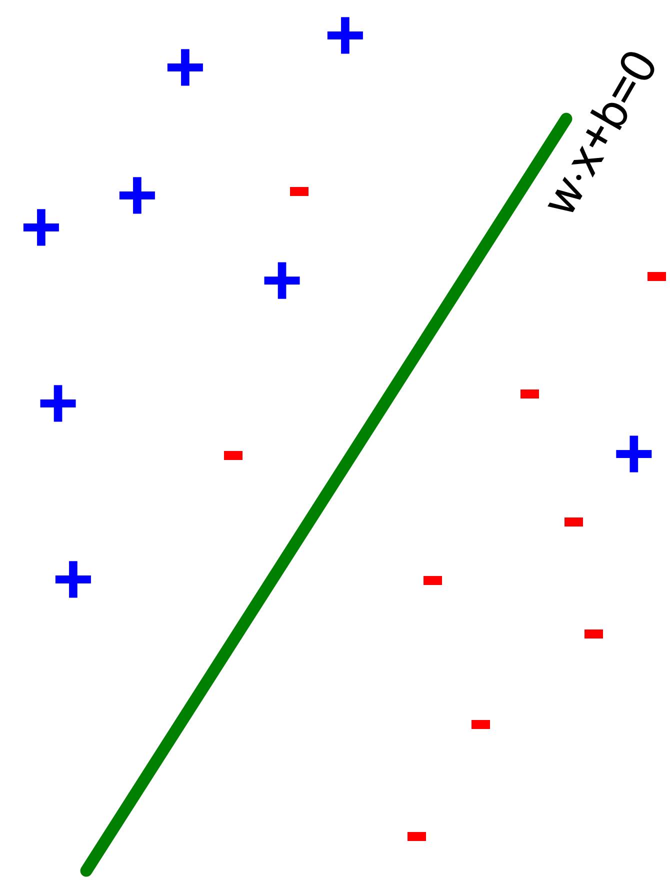
This is called SVM with "hard" constraints

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!**

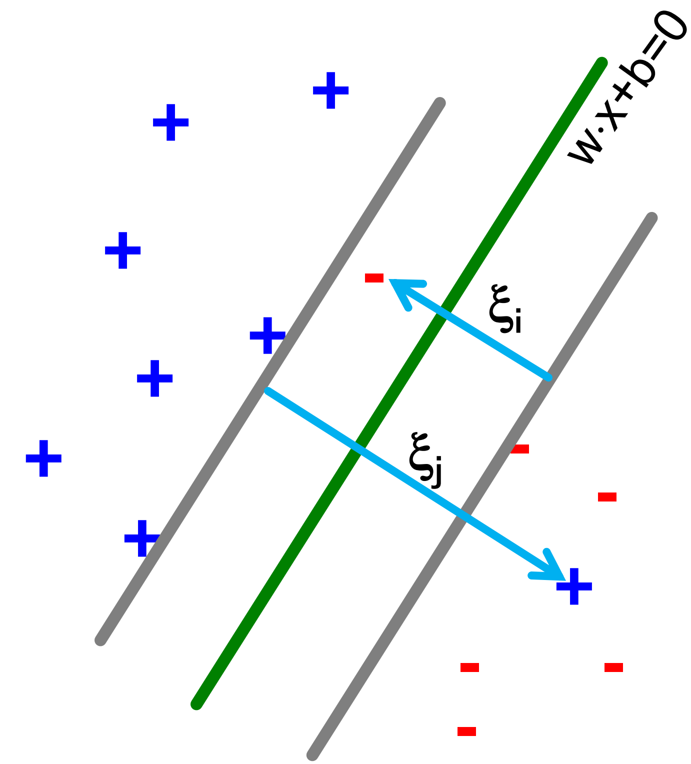
Support Vector Machines

- **Introduce slack variables 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 $\boldsymbol{x_i}$ is on the wrong side of the margin then get penalty ξ_i



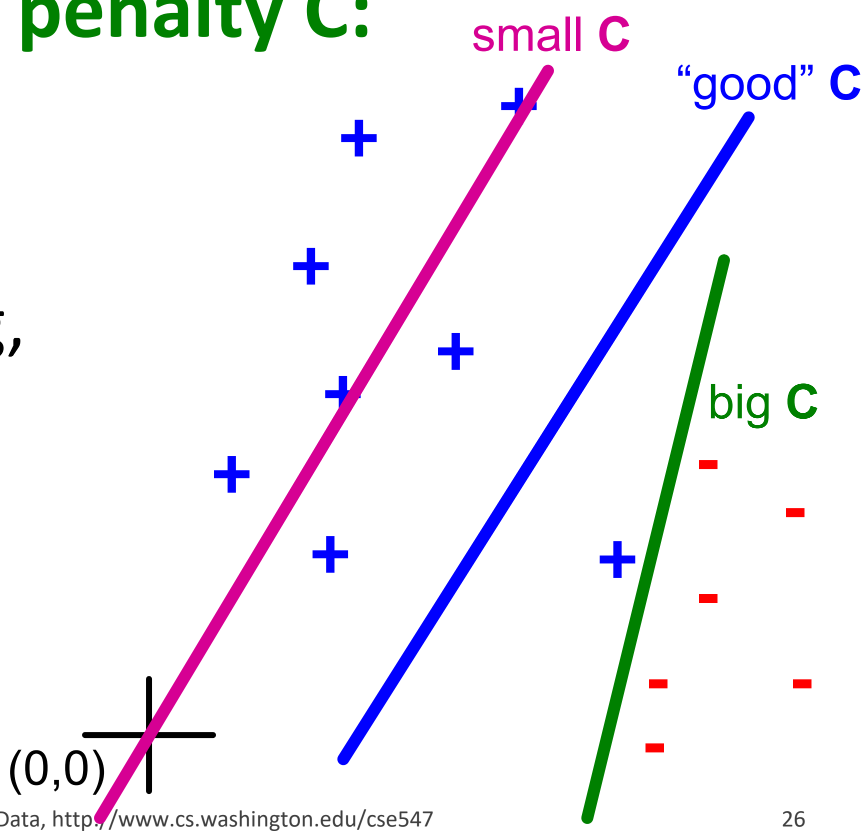
For each data point:
If margin ≥ 1, don't care
If margin < 1, pay linear penalty

Slack Penalty C

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

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

- **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**

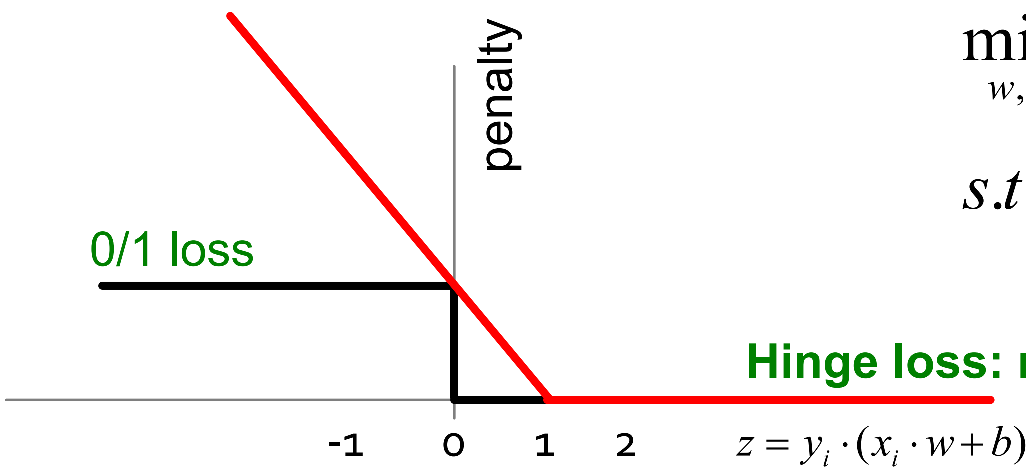
$$\arg\min_{w,b} \underbrace{\tfrac{1}{2} w \cdot w}_{\text{Margin}} + C \cdot \underbrace{\sum_{i=1}^{n} \max\{0, 1 - y_i (w \cdot x_i + b)\}}_{\text{Empirical loss L (how well we fit training data)}}$$

Regularization parameter

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

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

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



How do we obtain the Natural Form?

- Previously $$\min_{w,b} \ \tfrac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i$$ $$s.t.\forall i, y_i \cdot (w \cdot x_i + b) \geq 1 - \xi_i$$

- Solve for ξ: $$\xi_i \geq 1 - y_i \cdot (w \cdot x_i + b)$$ $$\xi_i \geq 0$$ $$\Rightarrow \xi_i \geq \max(0, 1 - y_i \cdot (w \cdot x_i + b))$$

- Natural form:

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

Support Vector Machines:
How to estimate the parameters?

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 minimize *J(w,b)*:**

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

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

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

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

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

SVM: How to estimate *w*?

- **Gradient descent:**

Iterate until convergence:

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

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

η…learning rate parameter
C… regularization parameter

SVM: How to estimate *w*?

We just had:

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

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

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

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

- **Stochastic gradient descent:**

Iterate until convergence:

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

Other variations of GD

- **Batch Gradient Descent**
  - Calculates error for each example in the training dataset, but updated model **only after** all examples have been evaluated (i.e., end of training epoch)
  - **PROS**: fewer updates, more stable error gradient
  - **CONS**: usually requires whole dataset in memory, slower than SGD
- **Mini-Batch Gradient Descent**
  - Like BGD, but using smaller batches of training data. Balance between robustness of SGD, and efficiency of BGD.

Support Vector Machines: Example

Example: Text categorization

- **Dataset:**
  - **Reuters RCV1** news 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

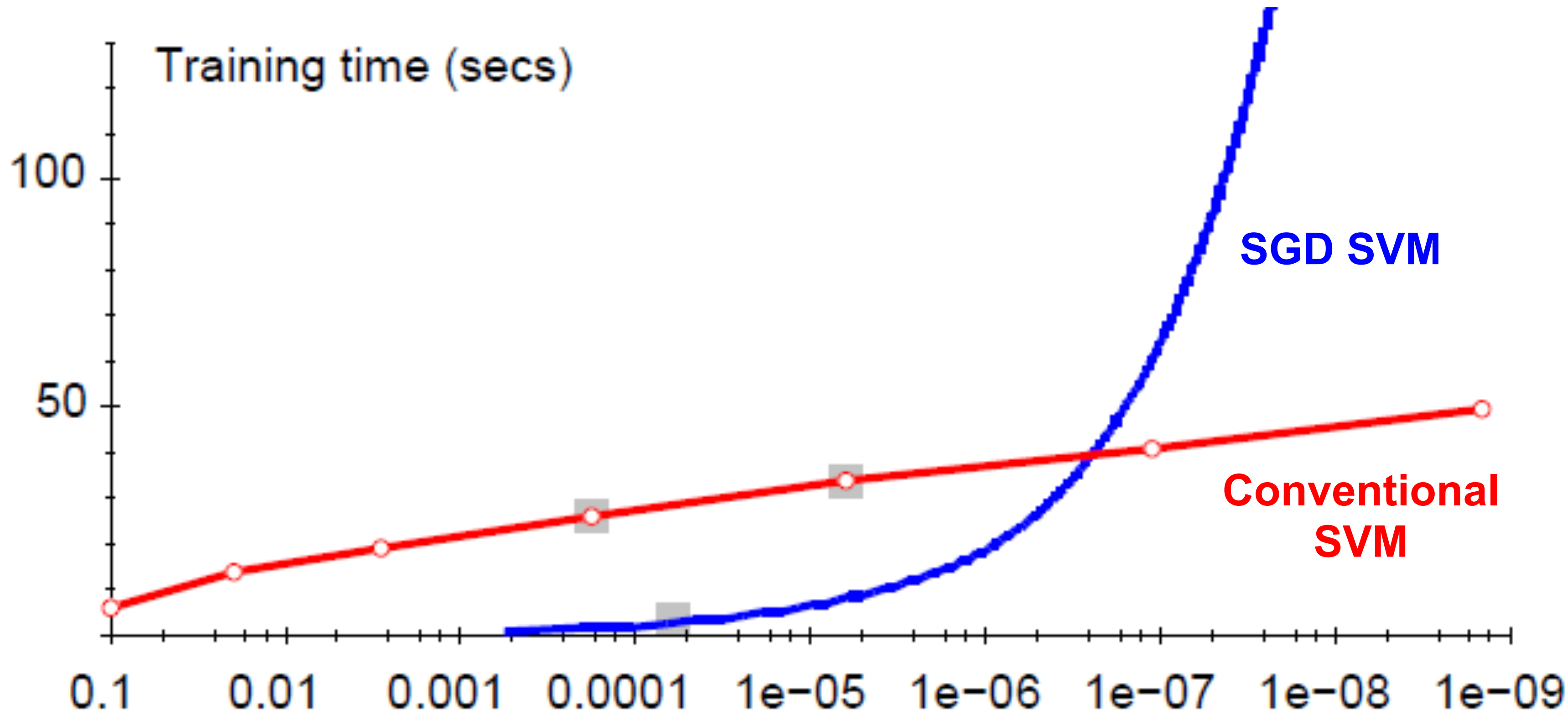
Example: Text categorization

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

	Training time	*Value of J(w,b)*	*Test error*
Standard SVM	23,642 secs	0.2275	6.02%
"Fast Linear 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 ***J(w,b)***
(2) SGD-SVM is super fast
(3) SGD-SVM test set error is comparable

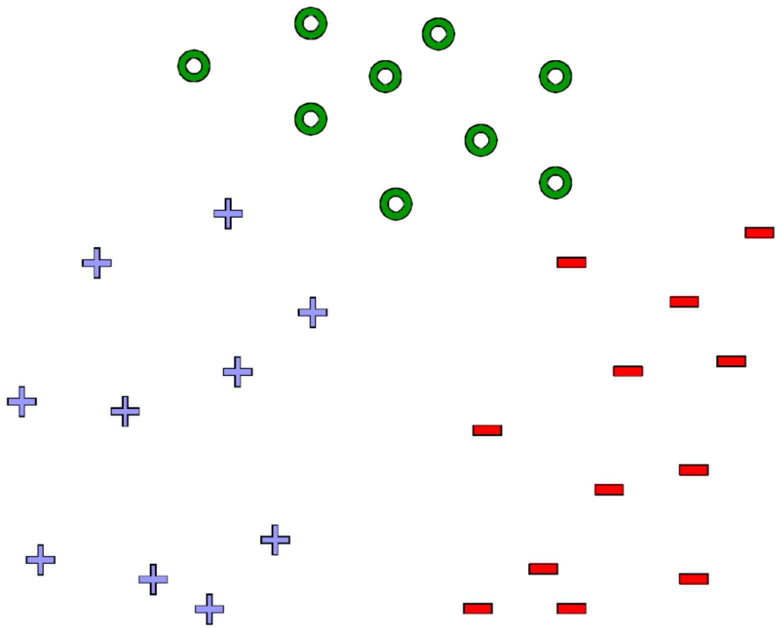
Optimization "Accuracy"



Optimization quality: | *J(w,b)* – *J* (w^{opt},b^{opt}) |

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

What about multiple classes?



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

  Obtain:

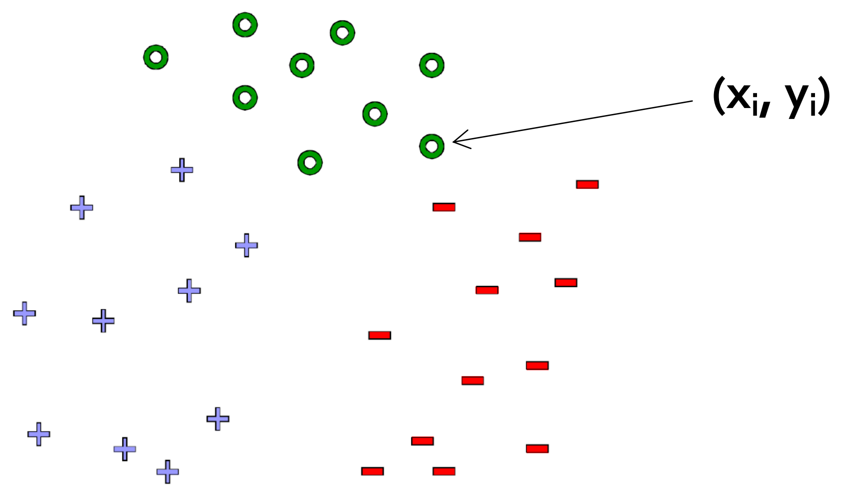
  $\mathbf{w_+\, b_+,\;\; w_-\, b_-,\;\; w_o\, b_o}$
- **How to classify?**
- Return class *c*

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

Learn 1 classifier: Multiclass SVM

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

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

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

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

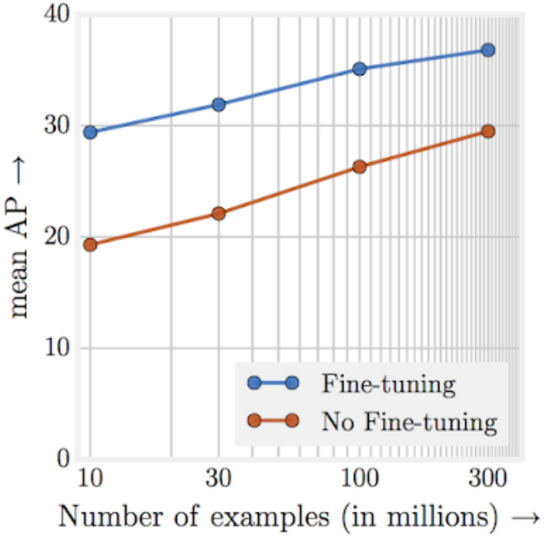
  - To obtain parameters ***w_c*, *b_c*** (for each class ***c***) we can use similar techniques as for 2 class **SVM**

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

ML Parallelization

Why Large-Scale ML?

- **The Unreasonable Effectiveness of Data**
  - In 2017, Google revisited a 15-year-old experiment on the effect of data and model size in ML, focusing on the latest Deep Learning models in computer vision
- **Findings:**
  - Performance increases logarithmically **based on volume of training data**
  - Complexity of modern ML models (i.e., deep neural nets) allows for even **further performance gains**



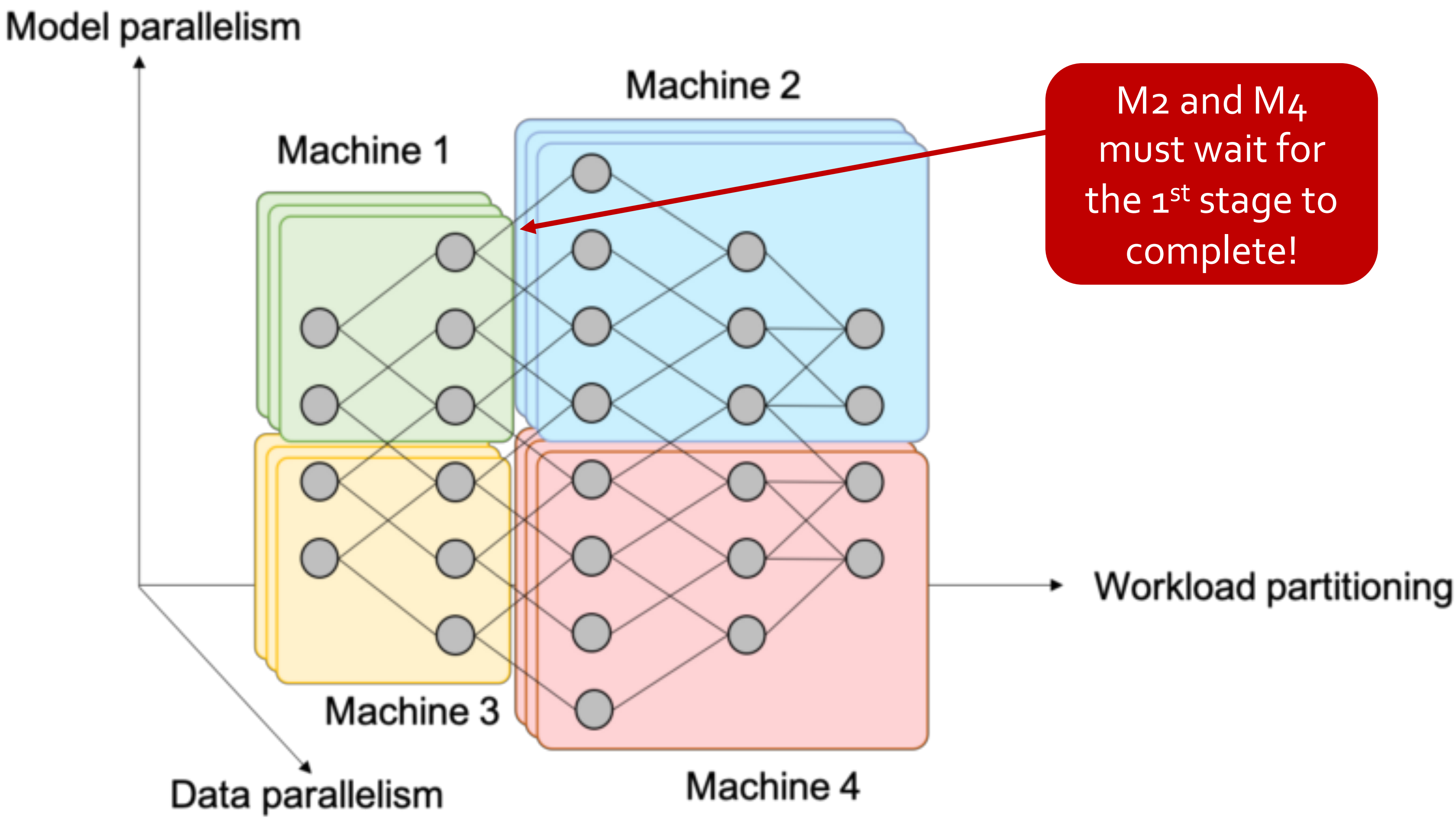
- **Large datasets + large ML models => amazing results!!**

"Revisiting Unreasonable Effectiveness of Data in Deep Learning Era": https://arxiv.org/abs/1707.02968

Recap

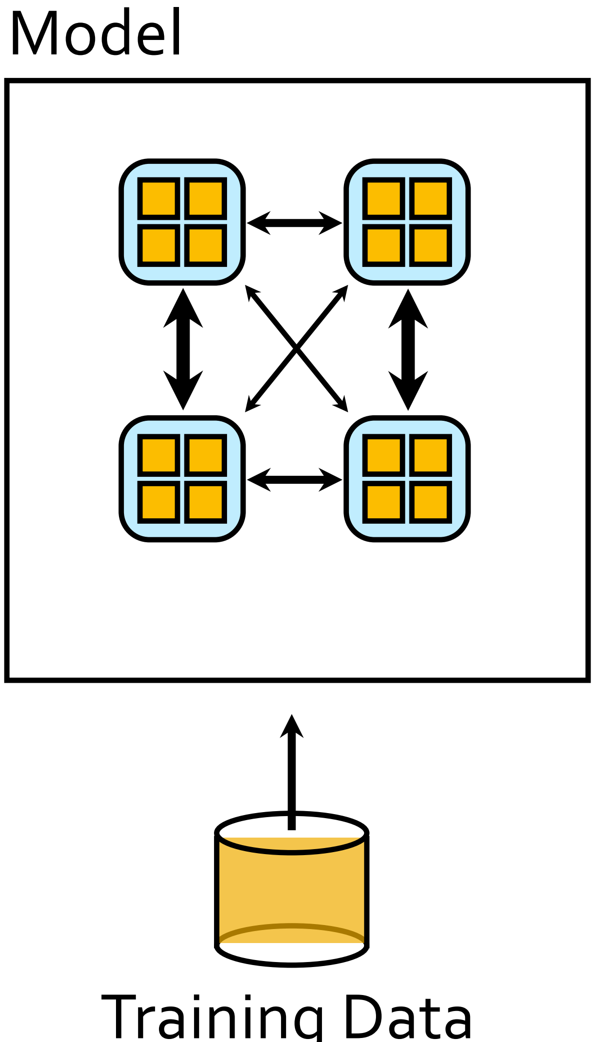
- Last lecture: Decision Trees (and PLANET) as a prime example of **Data Parallelism** in ML
- Today's lecture: Multiclass SVMs, Neural Networks (especially Deep ones), etc. can leverage both **Data Parallelism and Model Parallelism**
  - State-of-the-art Deep Neural Networks for visual recognition tasks (e.g., ImageNet challenge) can have **more than 100 million parameters!**

Parallelization overview

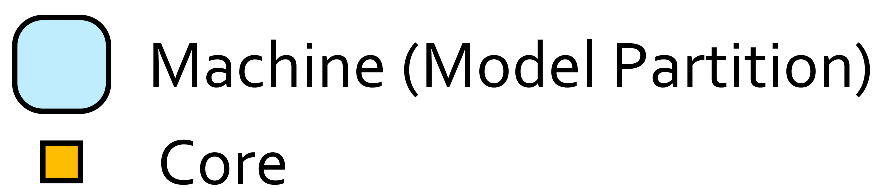


M2 and M4 must wait for the 1st stage to complete!

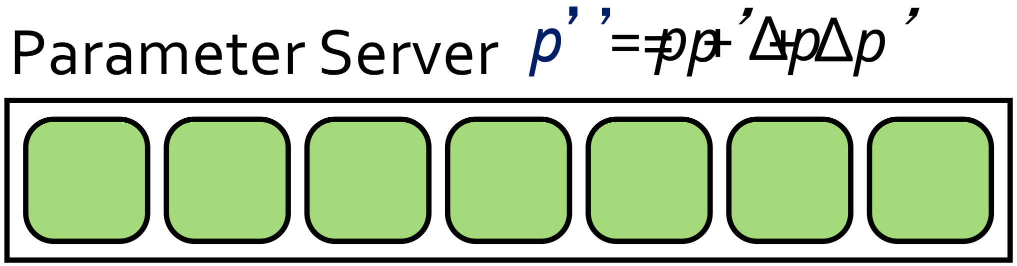
Parallelization overview

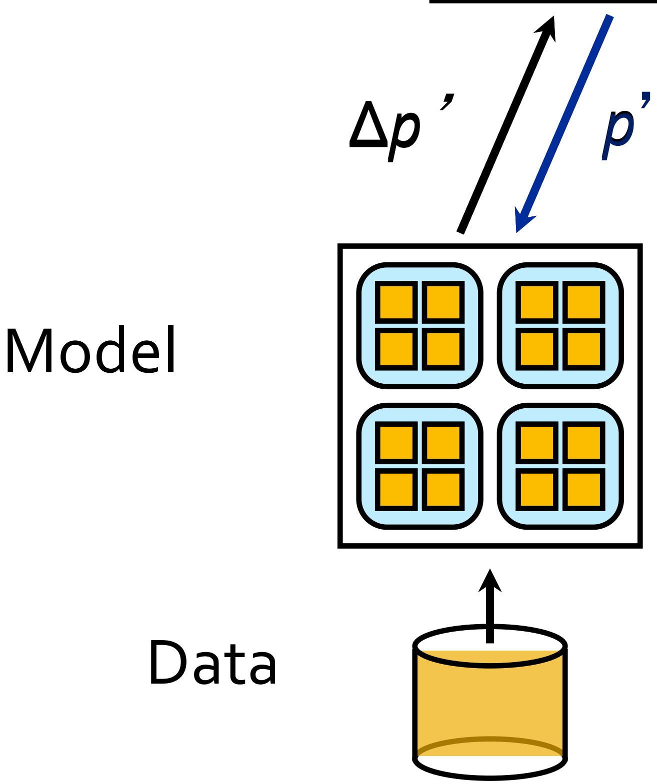


- Unsupervised or Supervised Objective
- Minibatch Stochastic Gradient Descent (SGD)
- Model parameters sharded by partition
- 10s, 100s, or 1000s of cores per model



Parameter Server

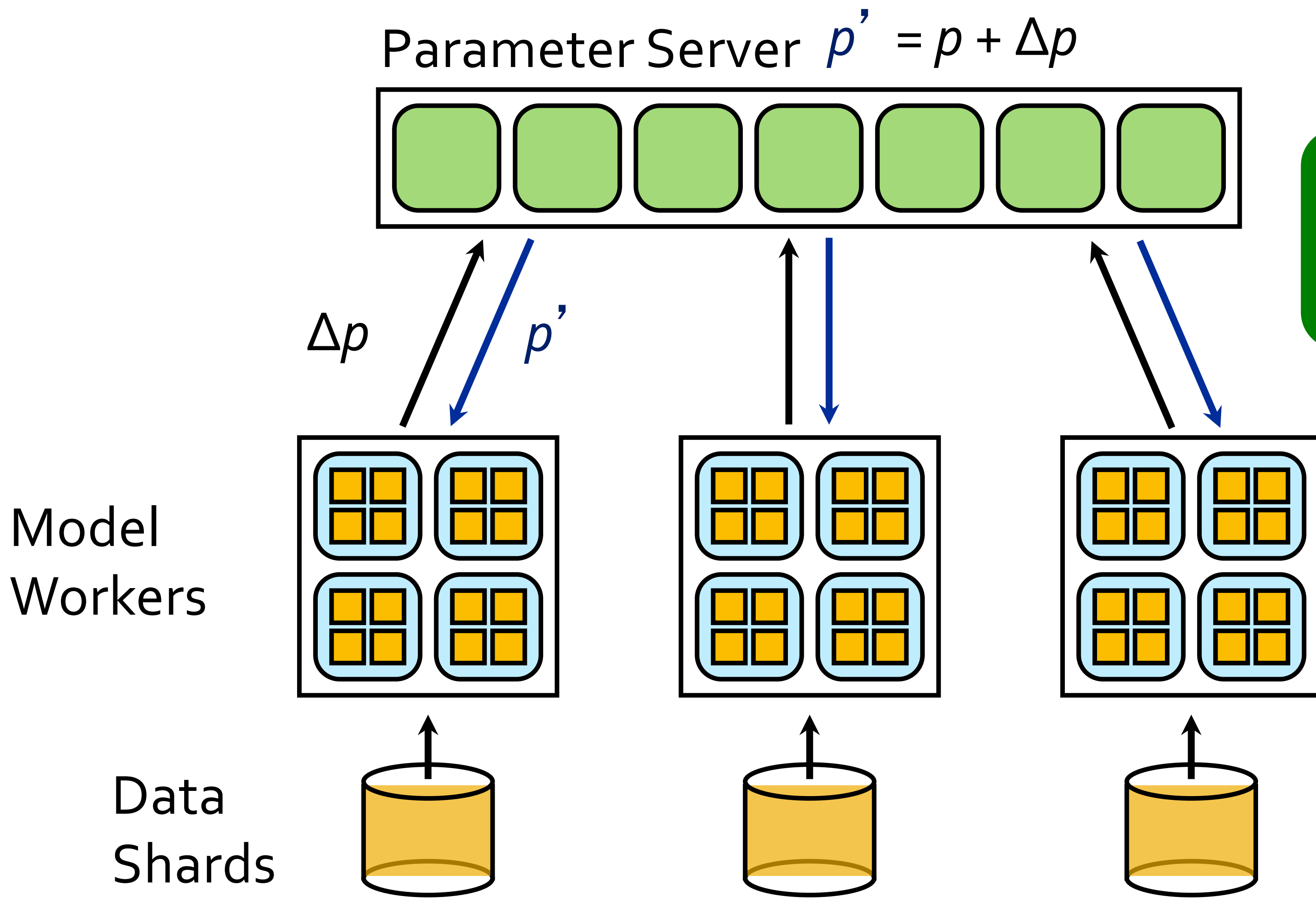




- Parameter Server: Key/Value store
- **Keys** index the model parameters (e.g., weights)
- **Values** are the parameters of the ML model (e.g., a neural network)

- **Systems challenges:**
  - **High bandwidth**
  - **Synchronization**
  - **Fault tolerance**

Parameter Server



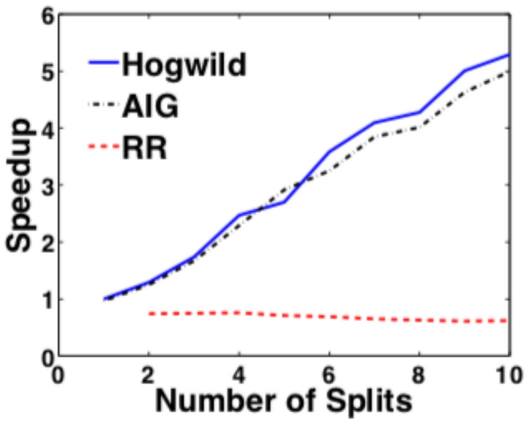
Why do **parallel updates** work?

Async SGD

- **Key idea:** don't synchronize, just **overwrite** parameters opportunistically from multiple workers (i.e., servers)
  - Same implementation as SGD, **just without locking!**

- In theory, Async SGD converges, but a slower rate than the serial version.
- In practice, when gradient updates are sparse (i.e., high dimensional data), **same convergence!**

RR is a super optimized version of online Gradient Descent, but with synchonization



- Recht et al. "[HOGWILD!: A Lock-Free Approach to Parallelizing Stochastic Gradient Descent]()", 2011

HOGWILD!

Initialize w in shared memory `// in parallel, do`

for $i = \{1, \ldots, p\}$ **do** <= P is the number of partitions / processors

  while *TRUE* **do**

    if *stopping criterion met* **then**

      break

    end

SGD

    Sample j from $1, \ldots, n$ uniformly at random.

    Compute $f_j(w)$ and $\nabla f_j(w)$ using whatever w is currently available.

    Let e_j denote non-zero indices of x_i

    for $k \in e_j$ **do**

      $w_{(k)} \leftarrow w_{(k)} - \alpha \left[\nabla F_j(w)\right]_{(k)}$

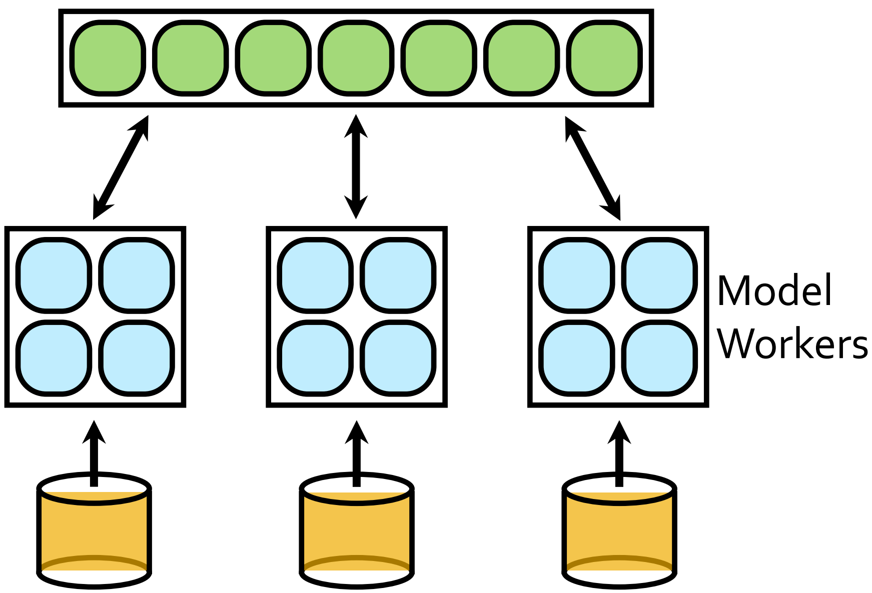
Component-wise gradient updates
(relies on sparsity)

    end

  end

end

Asynchronous Distributed SGD



- Google, "[Large Scale Distributed Deep Networks]" [2012]
- All ingredients together:
  - Model and Data parallelism
  - Async SGD
- Dawn of modern Deep Learning

From an engineering standpoint, this is much better than a single model with the same number of total machines:

- Synchronization boundaries involve fewer machines
- Better robustness to individual slow machines
- Makes forward progress even during evictions/restarts