CS639:
Data Management for Data Science

Lecture 17: Linear Classifiers and Support Vector Machines

Theodoros Rekatsinas

(lecture by Ankur Goswami many slides from David Sontag)

Today's Lecture

1. Linear classifiers

2. The Perceptron Algorithm

3. Support Vector Machines

Linear classifier

- Let's simplify life by assuming:
  - Every instance is a vector of real numbers, $\mathbf{x}=(x_1,\ldots,x_n)$. (Notation: boldface **x** is a vector.)
  - There are only two classes, $y=(+1)$ and $y=(-1)$
- A <u>linear classifier</u> is vector **w** of the same dimension as **x** that is used to make this prediction:

$$\hat{y} = \mathrm{sign}(w_1 x_1 + w_2 x_2 + \ldots + w_n x_n) = \mathrm{sign}(\mathbf{w}\cdot\mathbf{x})$$

$$\mathrm{sign}(x) = \begin{cases} +1 & \text{if } x \geq 0 \\ -1 & \text{if} < 0 \end{cases}$$

Example: Linear classifier

- Imagine 3 features (spam is "positive" class):
  1. free (number of occurrences of "free")
  2. money (occurrences of "money")
  3. BIAS (intercept, always has value 1)

$$w \cdot f(x)$$

$$\sum_i w_i \cdot f_i(x)$$

x	$f(x)$	w
"free money"	BIAS : 1 free : 1 money : 1 ...	BIAS : -3 free : 4 money : 2 ...

$$(1)(-3) \; +$$
$$(1)(4) \; +$$
$$(1)(2) \; +$$
$$\cdots$$
$$= 3$$

w.f(x) > 0 ➔ SPAM!!!

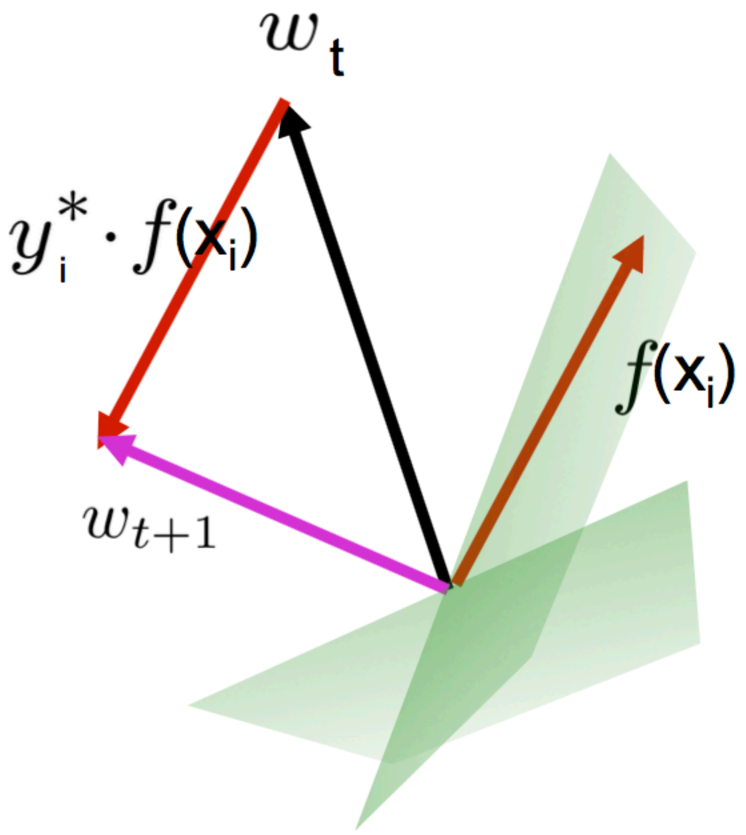
The Perceptron Algorithm to learn a Linear Classifier

- Start with weight vector = $\vec{0}$
- For each training instance (x_i,y_i*):
  - Classify with current weights

$$y_i = \begin{cases} +1 & \text{if } \; w \cdot f(x_i) \geq 0 \\ -1 & \text{if } \; w \cdot f(x_i) < 0 \end{cases}$$

  - If correct (i.e., y=y_i*), no change!
  - If wrong: update

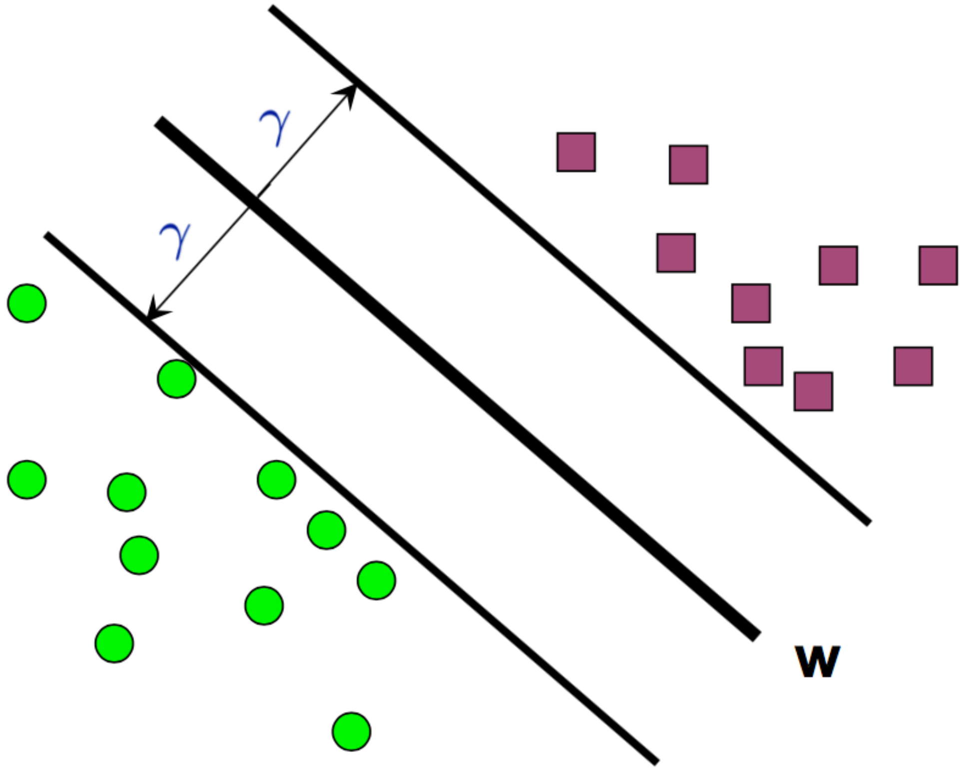
$$w = w + y_i^* f(x_i)$$



Definition: Linearly separable data

$\exists \mathbf{w}$ such that $\forall t$ $\quad y_t(\mathbf{w} \cdot \mathbf{x}_t) \geq \gamma > 0$

Called the *margin*



Equivalently, for $y_t = +1$,

$$w \cdot x_t \geq \gamma$$

and for $y_t = -1$,

$$w \cdot x_t \leq -\gamma$$

Does the perceptron algorithm work?

- Assume the data set *D* is linearly separable with margin γ, i.e.,

$$\exists \mathbf{w}^*, |\mathbf{w}^*|_2 = 1,\ \forall t, y_t \mathbf{x}_t^\top \mathbf{w}^* \geq \gamma$$

- Assume $|\mathbf{x}_t|_2 \leq R, \forall t$
- Theorem: The maximum number of mistakes made by the perceptron algorithm is bounded by R^2/γ^2

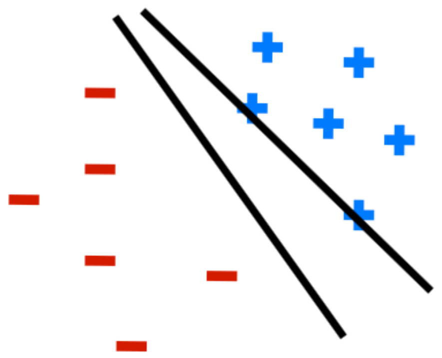
[Rong Jin]

Properties of the perceptron algorithm

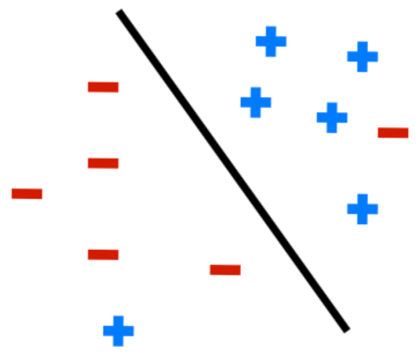
- Separability: some parameters get the training set perfectly correct

- Convergence: if the training is **linearly separable**, perceptron will eventually converge

Separable

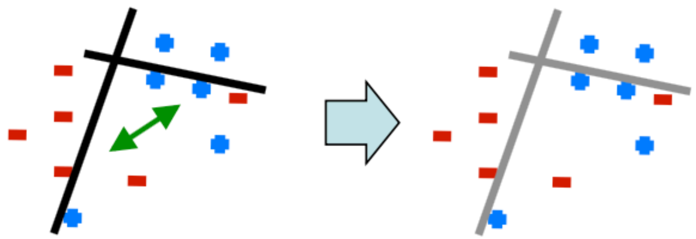


Non-Separable

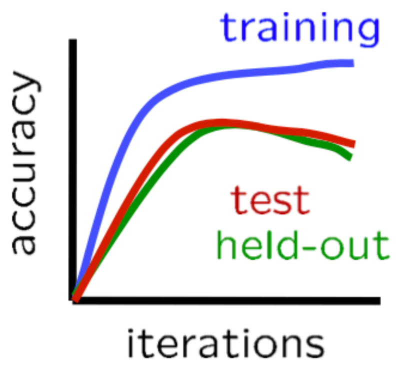


Problems with the perceptron algorithm

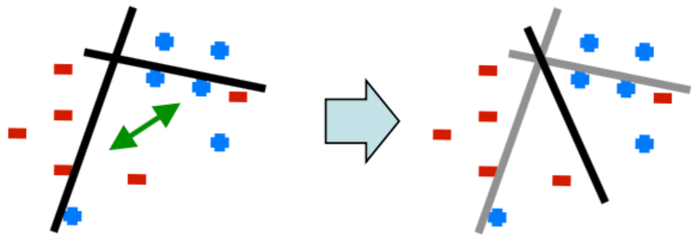
- **Noise**: if the data isn't linearly separable, no guarantees of convergence or accuracy



- Frequently the training data ***is*** linearly separable! Why?
  - When the number of features is much larger than the number of data points, there is lots of flexibility
  - As a result, Perceptron can significantly **overfit** the data **[We will see next week]**

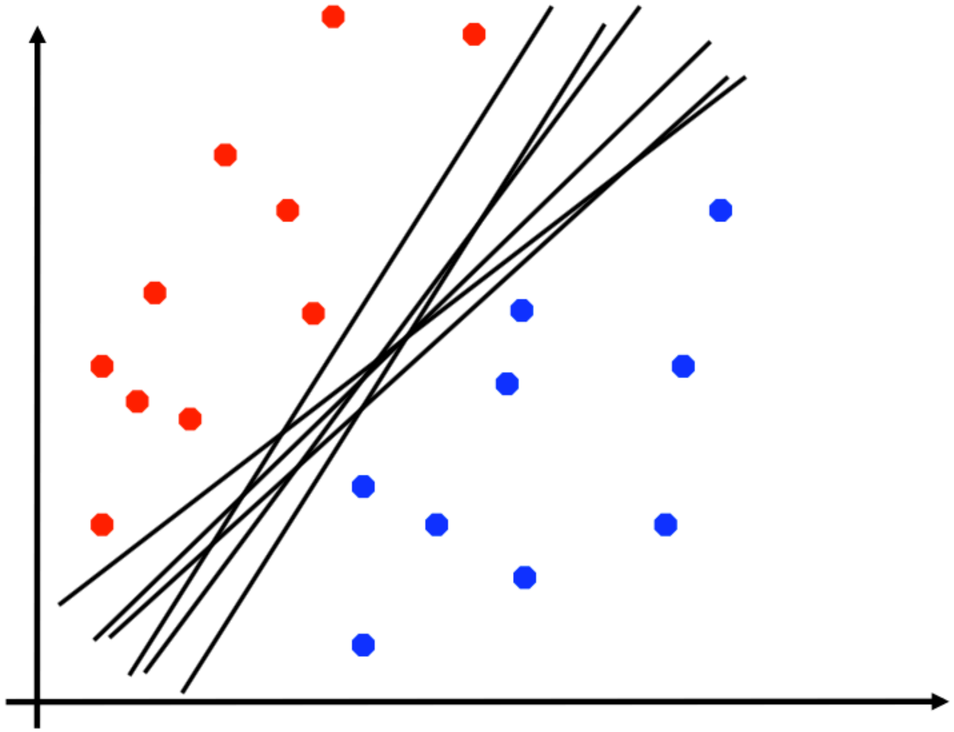


- **Averaged** perceptron is an algorithmic modification that helps with both issues
  - Averages the weight vectors across all iterations



Linear separators

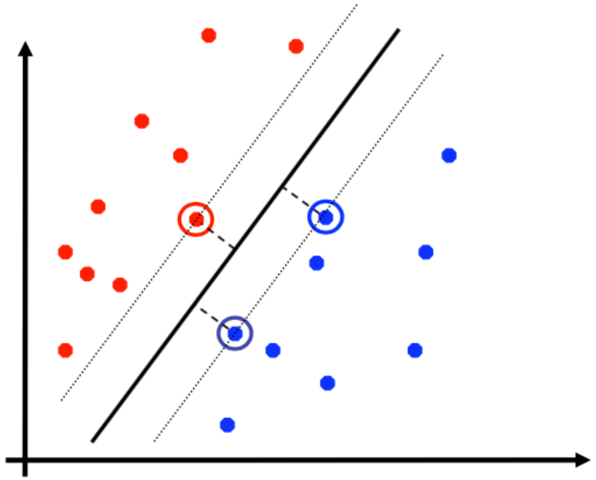
- Which of these linear separators is optimal?



Support Vector Machines

- SVMs (Vapnik, 1990's) choose the linear separator with the **largest margin**

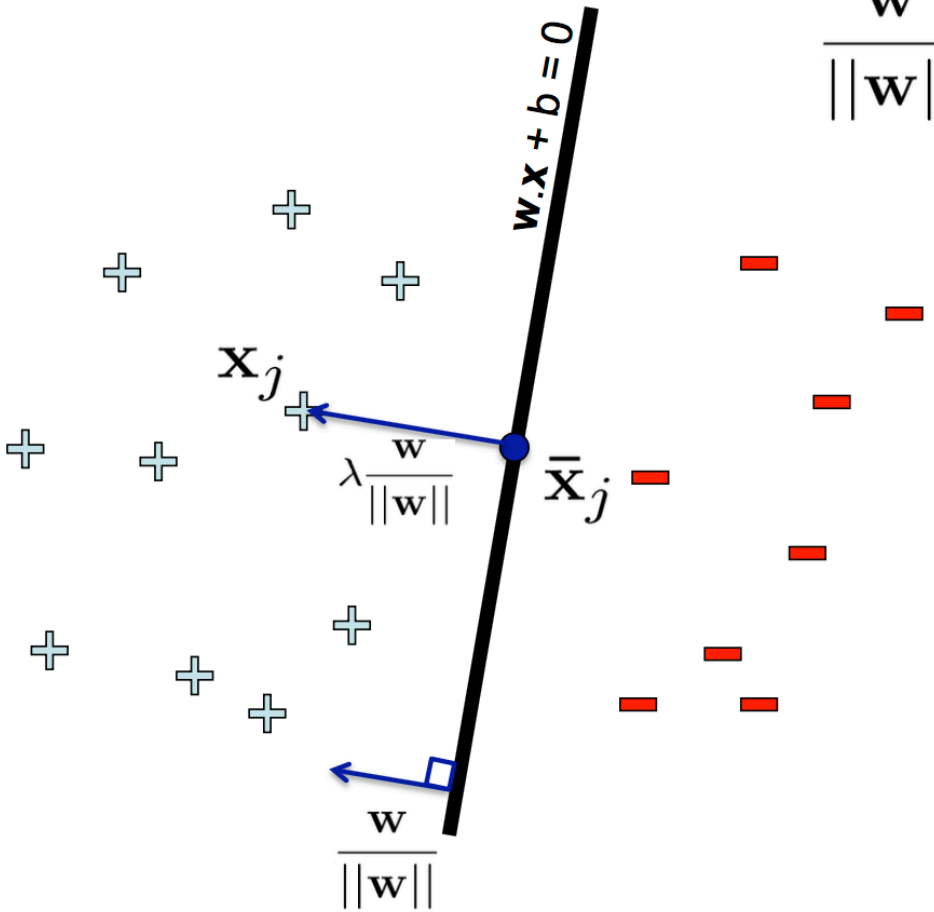
Robust to outliers!



V. Vapnik

- Good according to intuition, theory, practice
- SVM became famous when, using images as input, it gave accuracy comparable to neural-network with hand-designed features in a handwriting recognition task

Normal to a plane



$\frac{\mathbf{w}}{||\mathbf{w}||}$ -- unit vector parallel to w

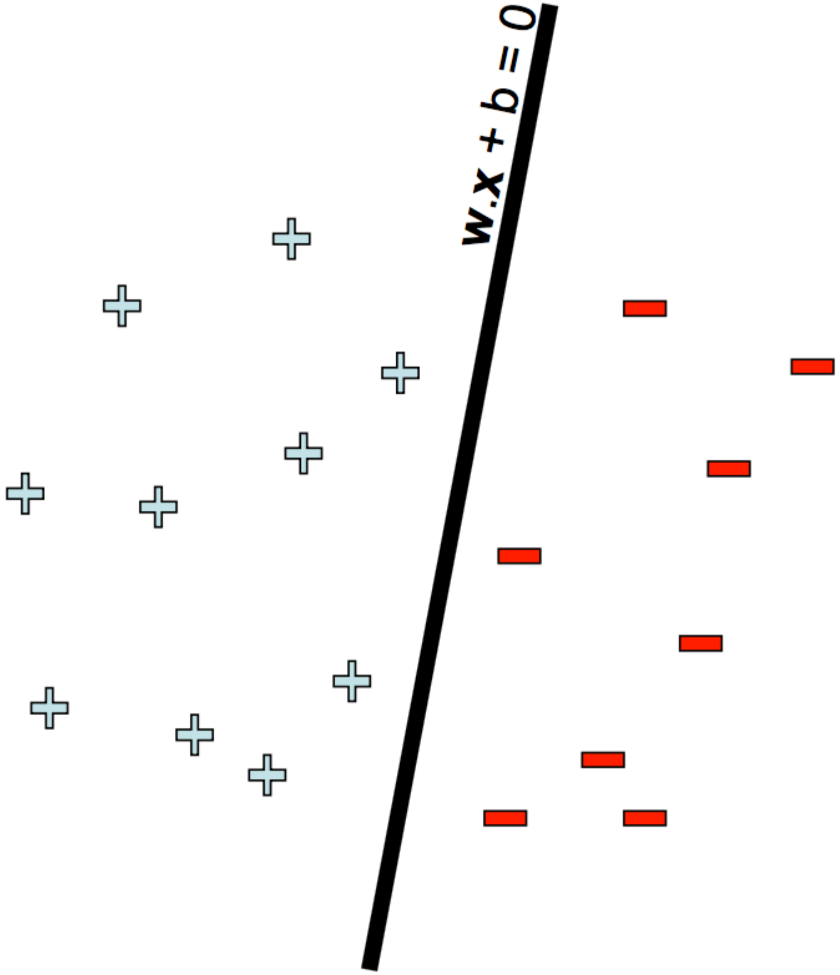
$\bar{\mathbf{x}}_j$ -- projection of x_j onto the plane

$$x_j - \bar{x}_j = \lambda \frac{w}{||w||}$$

λ is the length of the vector, i.e.

$$||x_j - \bar{x}_j|| = \frac{\lambda}{||w||}||w|| = \lambda$$

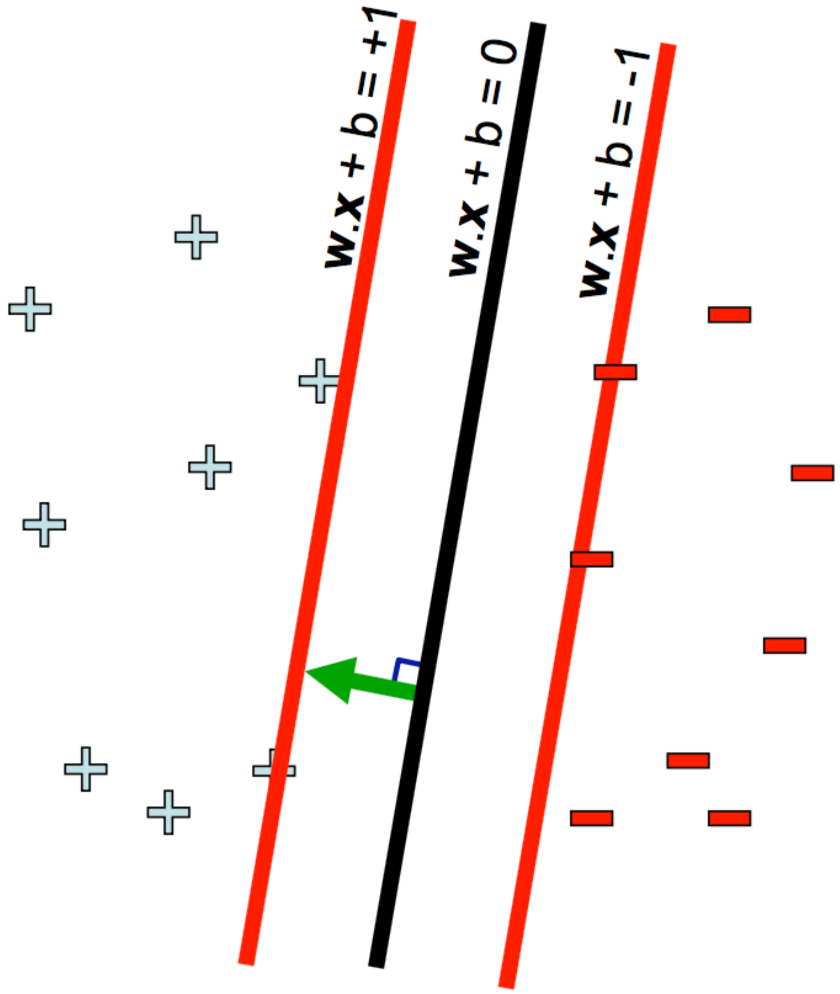
Scale invariance



Any other ways of writing the same dividing line?

- **w.x** + b = 0
- 2**w.x** + 2b = 0
- 1000**w.x** + 1000b = 0
- ….

Scale invariance



During learning, we set the scale by asking that, for all *t*,

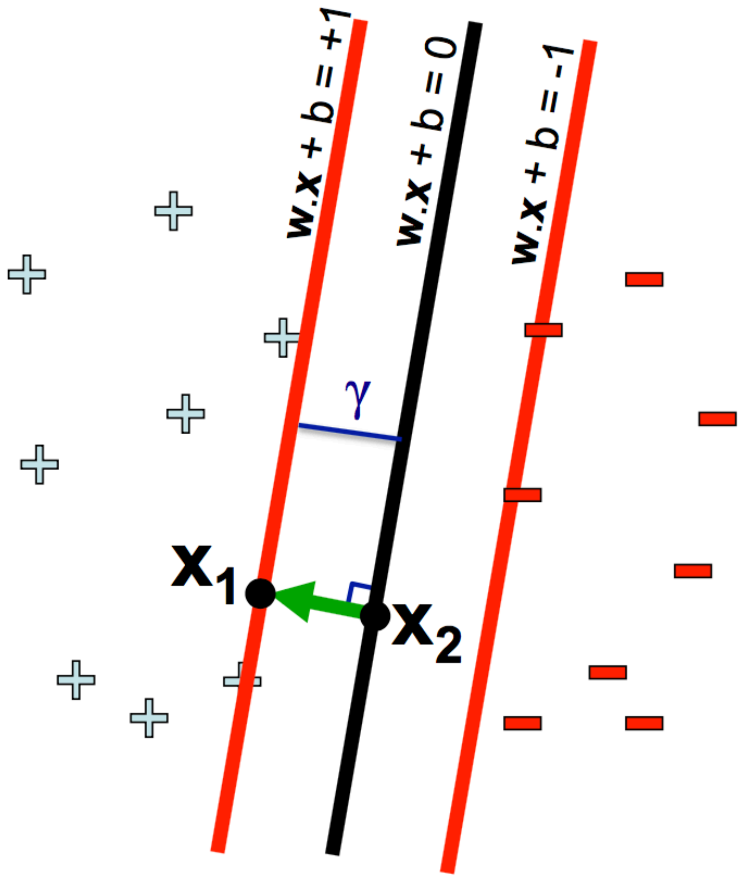
for y_t = +1, $w \cdot x_t + b \geq 1$

and for y_t = -1, $w \cdot x_t + b \leq -1$

That is, we want to satisfy all of the **linear** constraints

$$y_t \left(w \cdot x_t + b \right) \geq 1 \quad \forall t$$

What is γ as a function of **w**?



$$w \cdot x_1 + b = 1$$

$$-$$

$$w \cdot x_2 + b = 0$$

$$w \cdot (x_1 - x_2) = 1$$

Plug in

We also know that:

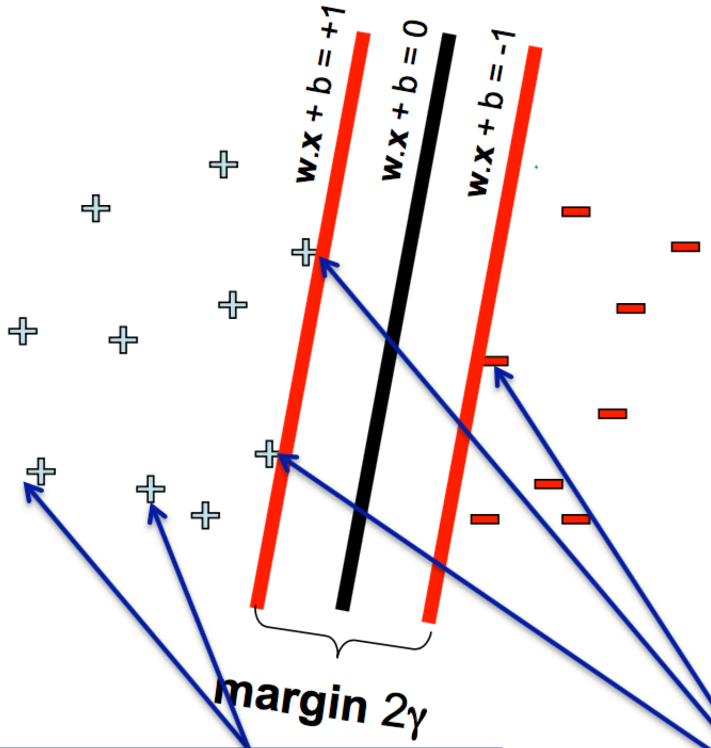
$$x_1 - x_2 = \gamma \frac{w}{||w||}$$

$$1 = w \cdot \left(\gamma \frac{w}{||w||}\right) = \frac{\gamma}{||w||} w \cdot w = \gamma ||w||$$

$$\boxed{\text{So, } \gamma = \frac{1}{||w||}}$$

Final result: can maximize margin by minimizing $||w||_2$!!!

Support Vector Machines (SVMs)



$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1, \ \forall j$$

- Example of a **convex optimization** problem
  - A quadratic program
  - Polynomial-time algorithms to solve!
- Hyperplane defined by **support vectors**
  - Could use them as a lower-dimension basis to write down line, although we haven't seen how yet
- More on these later

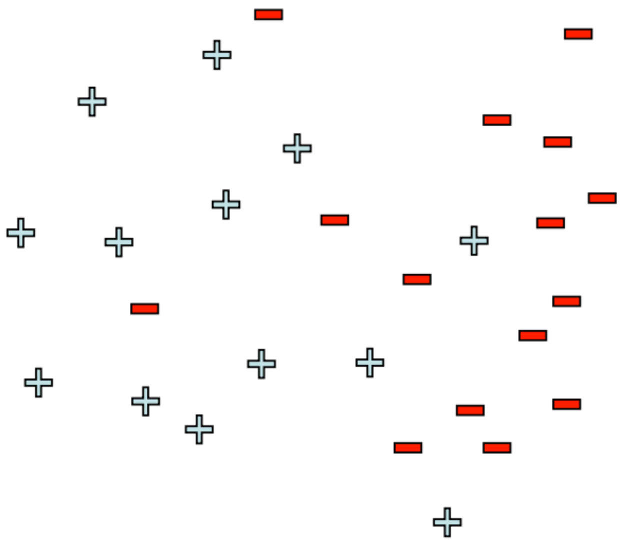
Non-support Vectors:
- everything else
- moving them will not change **w**

Support Vectors:
- data points on the canonical lines

What if the data is not separable?

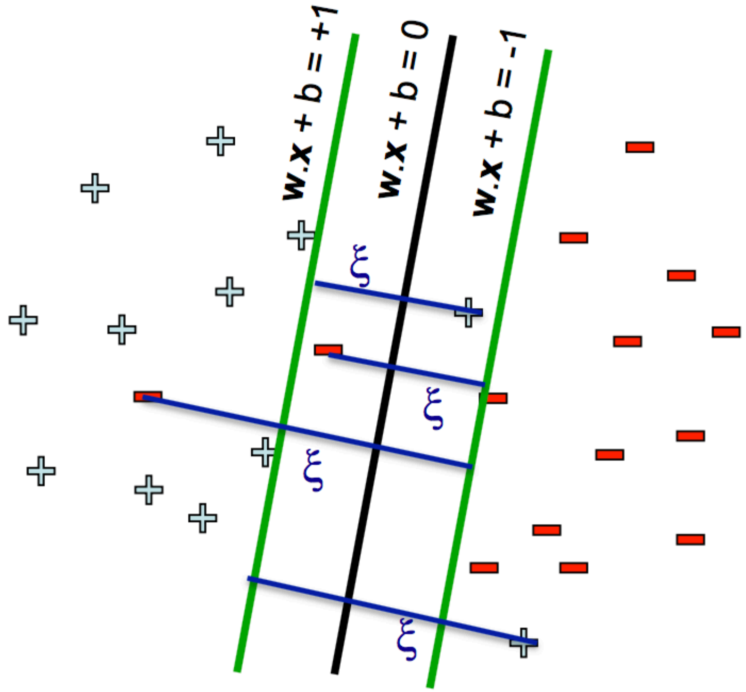
$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w} \; + \text{C } \#(\text{mistakes})$$

$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 \qquad , \forall j$$



- First Idea: Jointly minimize **w.w** and number of training mistakes
  - How to tradeoff two criteria?
  - Pick C using held-out data
- Tradeoff #(mistakes) and **w.w**
  - 0/1 loss
  - Not QP anymore
  - Also doesn't distinguish near misses and really bad mistakes
  - NP hard to find optimal solution!!!

Allowing for slack: "Soft margin" SVM



$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w} + C\,\Sigma_j\,\xi_j$$

$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j \quad ,\forall j \quad \xi_j \geq 0$$

"slack variables"

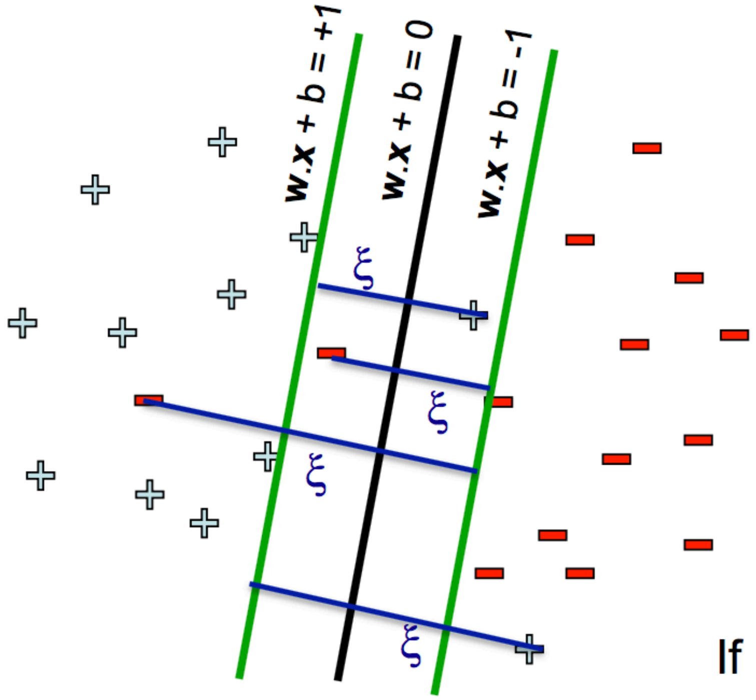
Slack penalty $C > 0$:

- $C=\infty$ → have to separate the data!
- $C=0$ → ignores the data entirely!

For each data point:

- If margin ≥ 1, don't care
- If margin < 1, pay linear penalty

Allowing for slack: "Soft margin" SVM



$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w} + C\,\Sigma_j\,\xi_j$$

$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j \quad, \forall j \quad \xi_j \geq 0$$

"slack variables"

What is the (optimal) value of ξ_j as a function of **w** and b?

If $(w \cdot x_j + b)\, y_j \geq 1$, then $\xi_j = 0$

If $(w \cdot x_j + b)\, y_j < 1$, then $\xi_j = 1 - (w \cdot x_j + b)\, y_j$

$$\xi_j = \max\left(0, 1 - (w \cdot x_j + b)\, y_j\right)$$

Sometimes written as

$$\left(1 - (w \cdot x_j + b)\, y_j\right)_+$$

Equivalent Hinge Loss Formulation

$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w} + C\,\Sigma_j\, \xi_j$$

$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j \quad , \forall j \quad \xi_j \geq 0$$

Substituting $\xi_j = \max\left(0, 1 - (w \cdot x_j + b)\, y_j\right)$ into the objective, we get:

$$\boxed{\min ||w||^2 + C \sum_j \max\left(0, 1 - (w \cdot x_j + b)\, y_j\right)}$$

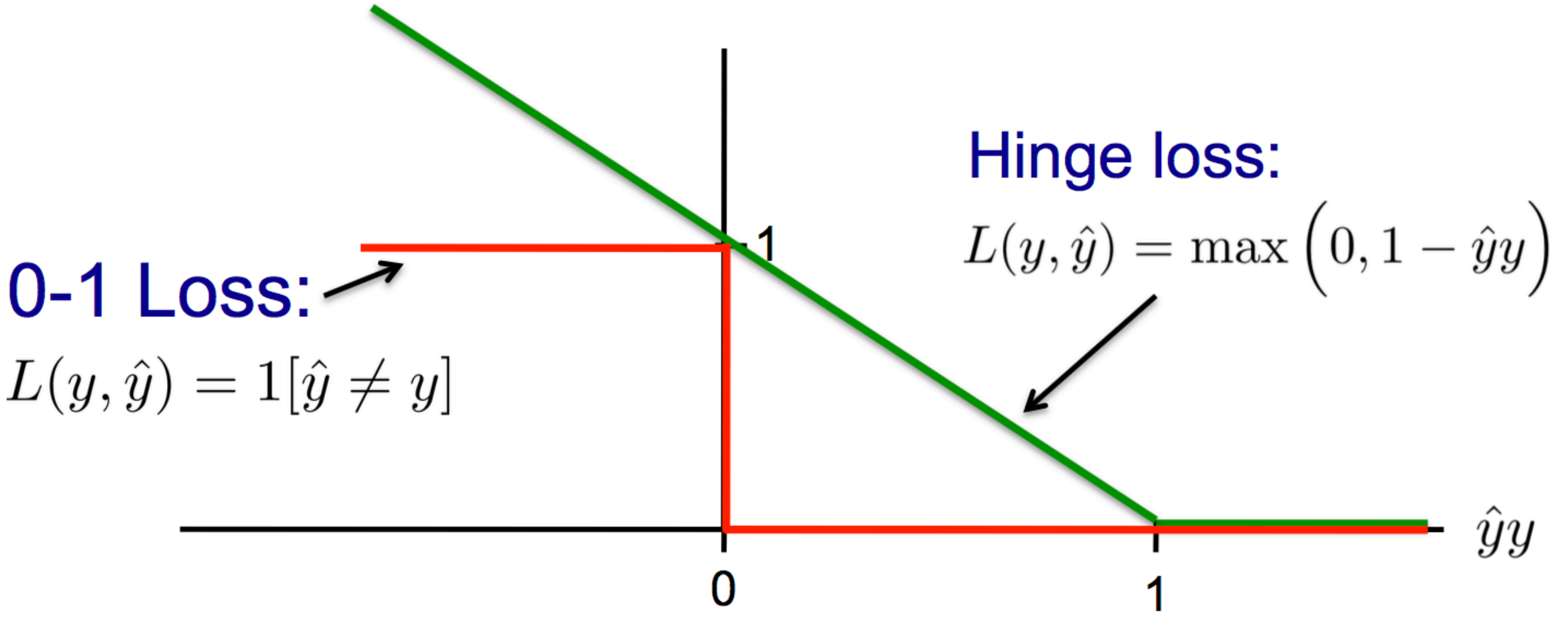
The **hinge loss** is defined as $L(y, \hat{y}) = \max\left(0, 1 - \hat{y}y\right)$

$$\min_{w,b} ||w||_2^2 + C \underline{\sum_j L(y_j, \mathbf{w} \cdot x_j + b)}$$

This is called **regularization**; used to prevent overfitting!

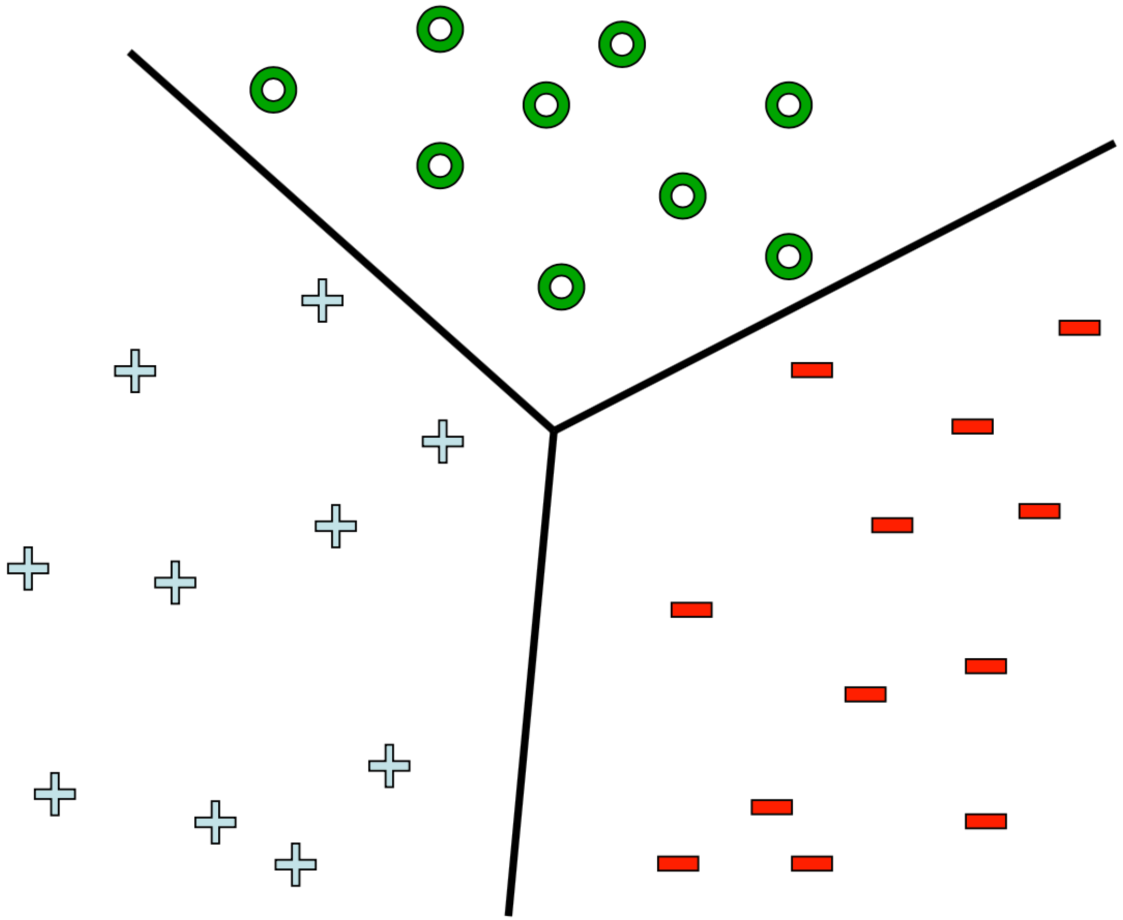
This part is empirical risk minimization, using the hinge loss

Hinge Loss vs 0-1 Loss

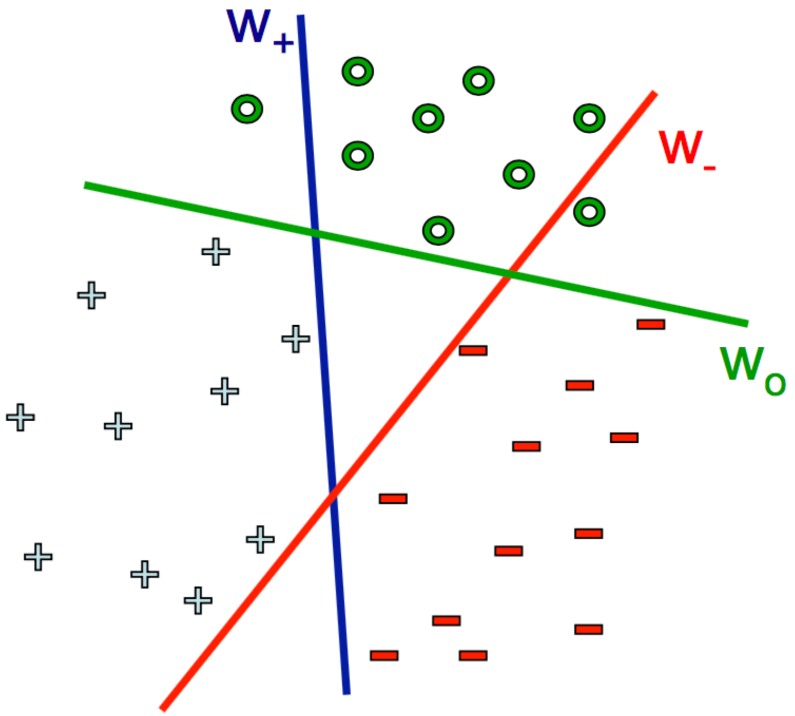


Hinge loss upper bounds 0/1 loss!

Multiclass SVM



One versus all classification



Learn 3 classifiers:

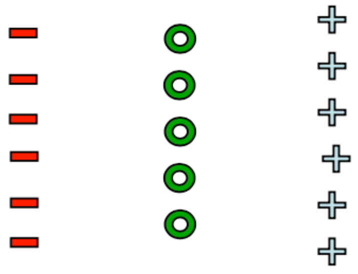
- \- vs {o,+}, weights w_-
- \+ vs {o,-}, weights w_+
- o vs {+,-}, weights w_o

Predict label using:

$$\hat{y} \leftarrow \arg\max_k \; w_k \cdot x + b_k$$

Any problems?

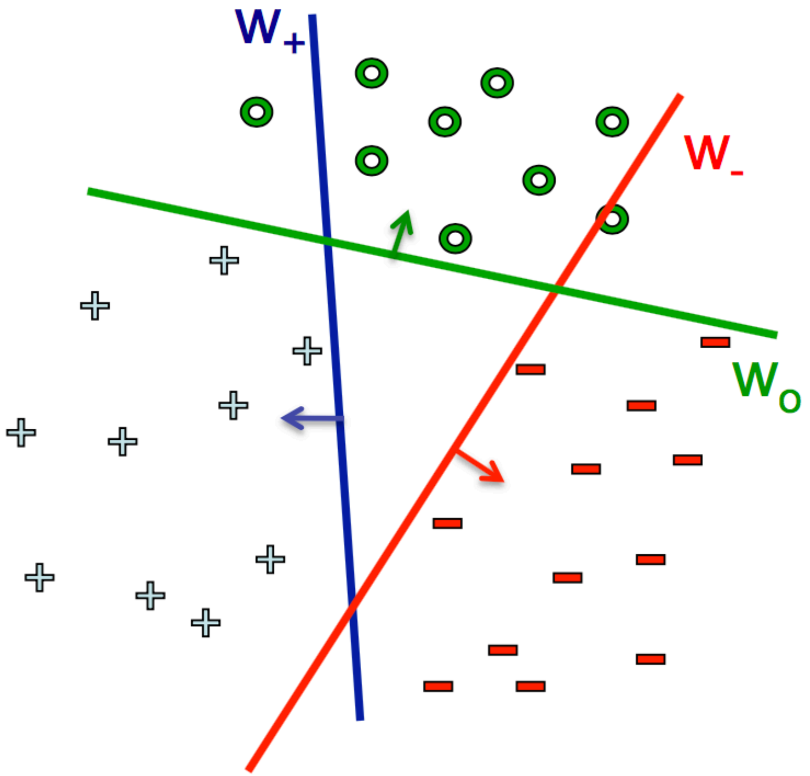
Could we learn this dataset? →



Multiclass SVM

Simultaneously learn 3 sets of weights:

- How do we guarantee the correct labels?
- Need new constraints!



The "score" of the correct class must be better than the "score" of wrong classes:

$$w^{(y_j)} \cdot x_j + b^{(y_j)} > w^{(y)} \cdot x_j + b^{(y)} \qquad \forall j,\ y \neq y_j$$

Multiclass SVM

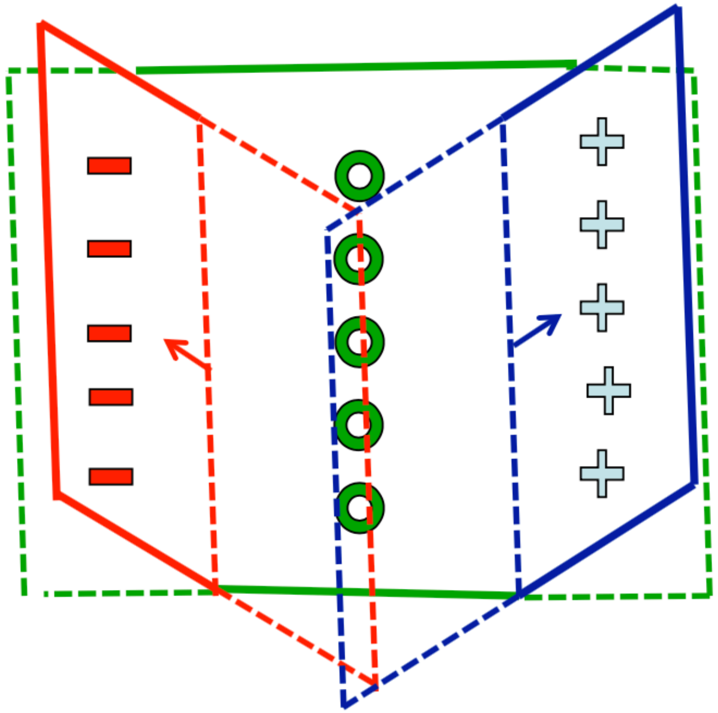
As for the SVM, we introduce slack variables and maximize margin:

$$\text{minimize}_{\mathbf{w},b} \quad \textstyle\sum_y \mathbf{w}^{(y)}.\mathbf{w}^{(y)} + C\sum_j \xi_j$$
$$\mathbf{w}^{(y_j)}.\mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y')}.\mathbf{x}_j + b^{(y')} + 1 - \xi_j, \;\; \forall y' \neq y_j, \;\; \forall j$$
$$\xi_j \geq 0, \;\; \forall j$$

To predict, we use:

$$\hat{y} \leftarrow \arg\max_k \; w_k \cdot x + b_k$$

Now can we learn it? →



What you need to know

- Perceptron mistake bound
- Maximizing margin
- Derivation of SVM formulation
- Relationship between SVMs and empirical risk minimization
  - 0/1 loss versus hinge loss
- Tackling multiple class
  - One against All
  - Multiclass SVMs