Kernels and Support Vector Machines

Machine Learning – CSE446

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November 1, 2016

Announcements:

- Project Milestones coming up
- HW2
  - You've implemented GD, SGD, etc…
- HW3 posted this week.
  - Let's get state of the art on MNIST!
  - It'll be collaborative

$\leq 1.2\%$

next class:

review

- Today:
  - Review: the perceptron, margins, and separability
  - Kernels & SVMs

Support Vector Machines (Two Ideas Mixed up)

- 1) An attempt to better optimize the classification loss?
  - Questionable?
  - Latent SVMs are interesting.
- 2) Kernels
  - Warp the feature space
  - This idea is actually more general

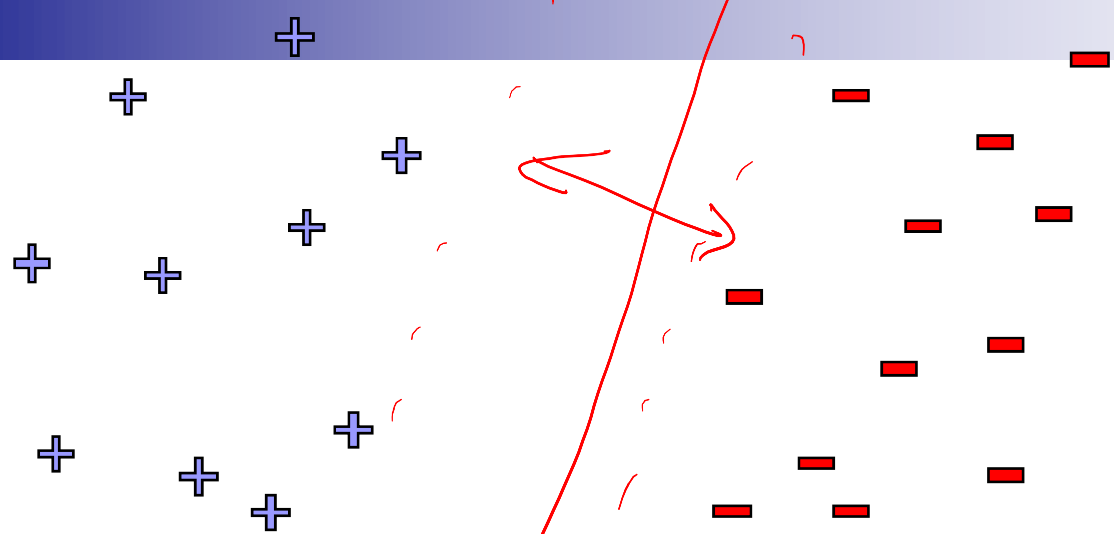
good lesson:

polished released code

e.g. lib-svm

- The success of SVMS?

Linear Separability: More formally, Using Margin



$\frac{1}{\|w_*\|}$

- Data linearly separable, if there exists
  - a vector $\quad \exists\ w_*$
  - a margin $\quad \forall t \qquad y_t(w_* \cdot x_t) \geq 1$
- Such that

Perceptron Analysis: Linearly Separable Case

- Theorem [Block, Novikoff]:
  - Given a sequence of labeled examples:
  - Each feature vector has bounded norm: $\|X_t\| \leq 1$
  - If dataset is linearly separable:

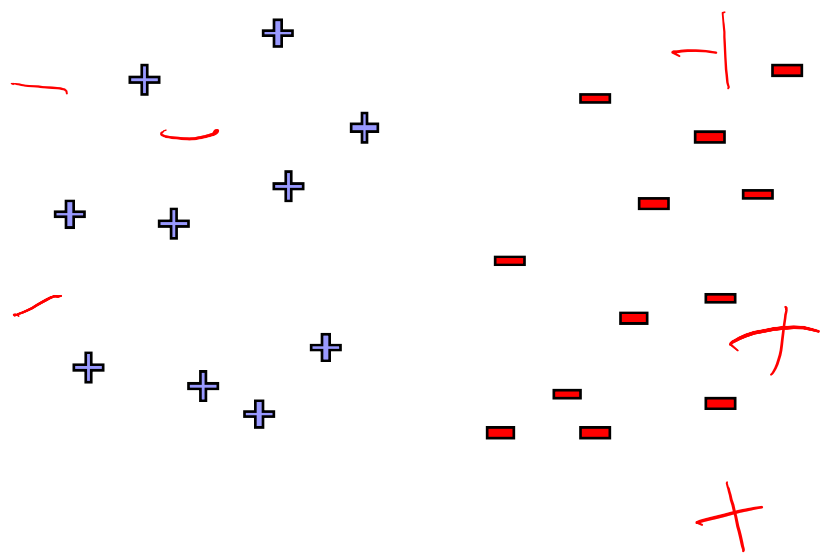
(satisfying margin assumption)

- Then the number of mistakes made by the online perceptron on any such sequence is bounded by

$$\|w_*\|^2$$

Beyond Linearly Separable Case

- Perceptron algorithm is super cool!
  - No assumption about data distribution!
    - Could be generated by an oblivious adversary, no need to be iid
  - Makes a fixed number of mistakes, and it's done for ever!
    - Even if you see infinite data
- However, real world not linearly separable
  - Can't expect never to make mistakes again



Kernels

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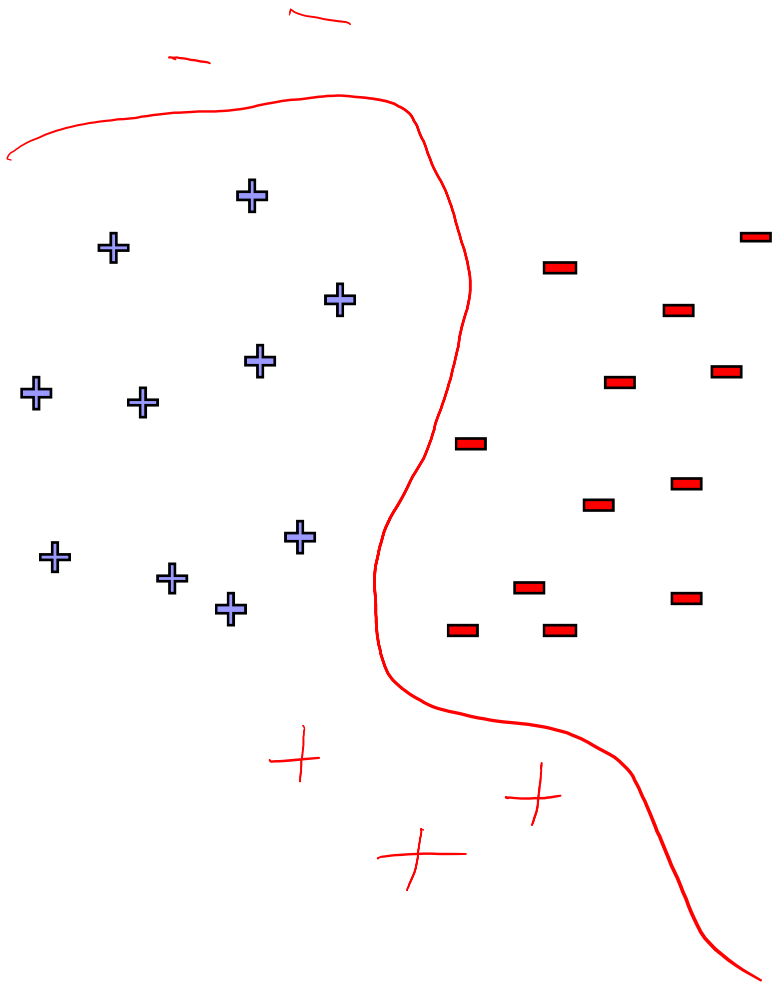
What if the data is not linearly separable?



Use features of features of features of features….

$$\Phi(\mathbf{x}) : R^m \mapsto F$$

$m=1$

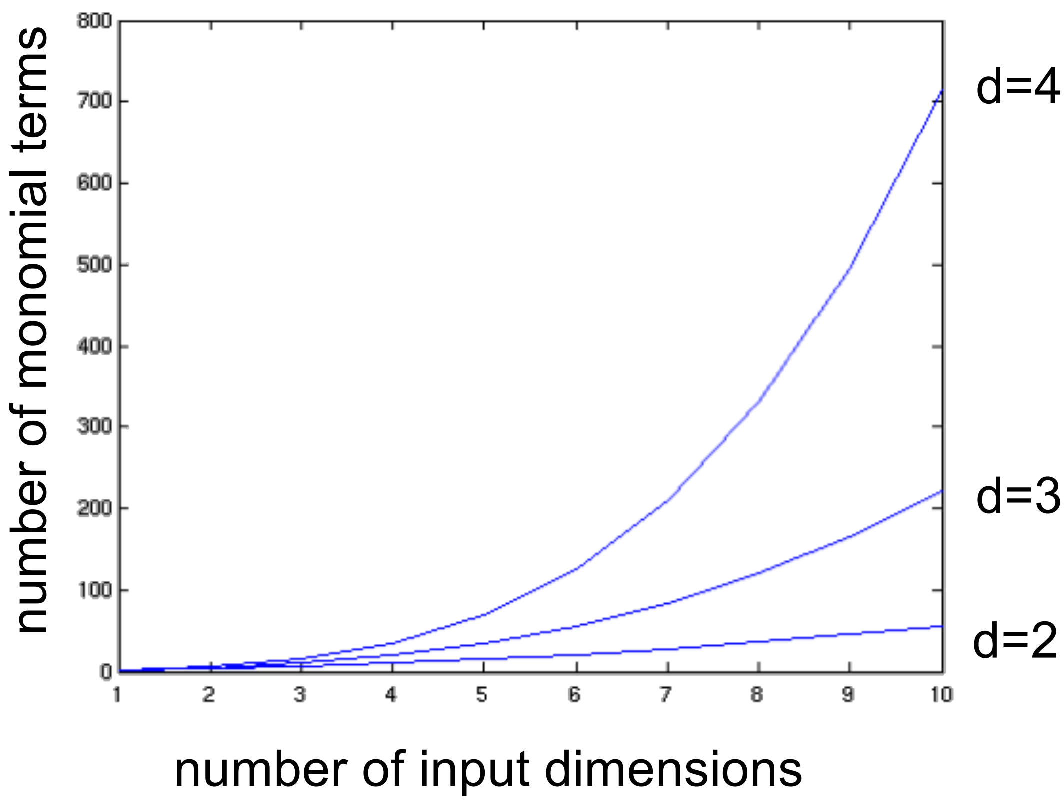
$$\phi(x) = \begin{pmatrix} x \\ x^2 \\ x^3 \\ \sqrt{x} \\ \vdots \\ \vdots \end{pmatrix}$$

Feature space can get really large really quickly!

Higher order polynomials

$$\text{num. terms} = \binom{d+m-1}{d} = \frac{(d+m-1)!}{d!(m-1)!}$$

m – input features
d – degree of polynomial



grows fast!
d = 6, m = 100
about 1.6 billion terms

Perceptron Revisited

- Given weight vector $w^{(t)}$, predict point $\mathbf{x}$ by:

$\sum y^{(j)} \phi(x^{(j)})$

- Mistake at time t: $w^{(t+1)} \leftarrow w^{(t)} + y^{(t)} x^{(t)}$

- Thus, write weight vector in terms of mistaken data points only:
  - Let $M^{(t)}$ be time steps up to t when mistakes were made:

$w^{(t)} = \sum_{j \text{ s.t. mistake made}} y^{(j)} x^{(j)}$

- Prediction rule now:

$\operatorname{sign}(w^{(t)} \cdot x) = \operatorname{sign}\left(\sum_{j \in M(t)} y^{(j)} x^{(j)} \cdot x\right)$

- When using high dimensional features:

$\operatorname{sign}(w^{(t)} \phi(x)) = \operatorname{sign}\left(\sum_{j \in M(t)} y^{(j)} \phi(x^{j}) \cdot \phi(x)\right)$

Dot-product of polynomials

$u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$

$\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) =$ polynomials of degree exactly d

$d = 1$ $\phi(u) \cdot \phi(v) = \vec{u} \cdot \vec{v}$

$\phi(u) = u$

$d = 2$ $\phi(u) = \begin{pmatrix} u_1^2 \\ u_2^2 \\ u_1 u_2 \\ u_2 u_1 \end{pmatrix}$ $\phi(u) \cdot \phi(v) = u_1^2 v_1^2 + 2 u_1 u_2 + u_2^2 v_2^2$

$= (u \cdot v)^2$

for general d (same construction $\phi(u) \cdot \phi(v) = (u \cdot v)^d$

"Kernel trick"

Finally the Kernel Trick!!! (Kernelized Perceptron

define

$K(x, x') = \phi(x) \cdot \phi(x')$

- Every time you make a mistake, remember $(x^{(t)}, y^{(t)})$

- Kernelized Perceptron prediction for $\mathbf{x}$:

$$sign(\mathbf{w}^{(t)} \cdot \phi(\mathbf{x})) = \sum_{j \in M^{(t)}} y^{(j)} \phi(\mathbf{x}^{(j)}) \cdot \phi(\mathbf{x})$$

$$= \sum_{j \in M^{(t)}} y^{(j)} k(\mathbf{x}^{(j)}, \mathbf{x})$$

Polynomial kernels

- All monomials of degree d in O(d) operations:

$$\Phi(\mathbf{u})\cdot\Phi(\mathbf{v}) = (\mathbf{u}\cdot\mathbf{v})^d = \text{polynomials of degree exactly d}$$

- How about all monomials of degree up to d?
  - Solution 0: concatenate them

    $$\phi(u)\cdot\phi(v) = \sum_{i=0}^{d} \binom{d}{i} (u\cdot v)^i$$

  - Better solution:

better solution

$$1 + (u\cdot v)^1 + (u\cdot v)^2 + (v\cdot u)^1 = (u\cdot v+1)^2$$

get all polynomials up to d with $K(u,v) = (u\cdot v+1)^d$

Common kernels

- Polynomials of degree exactly d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^d$$

- Polynomials of degree up to d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^d$$

- Gaussian (squared exponential) kernel

Radial Basis Function.

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||^2}{2\sigma^2}\right)$$

- Sigmoid

$$K(\mathbf{u}, \mathbf{v}) = \tanh(\eta \mathbf{u} \cdot \mathbf{v} + \nu)$$

Mercer's Theorem

- When do we have a Kernel K(x,x')?
- Definition 1: when there exists an embedding ϕ

$$K(x,x') = \phi(x)\cdot\phi(x')$$

- Mercer's Theorem:
  - K(x,x') is a valid kernel if and only if K is a positive semi-definite.
  - PSD in the following sense:

$M \in \mathbb{R}^{\ell\times\ell}$

$\forall \ell$

$\forall\ u_1 \ldots u_\ell$ let $M_{ij} = K(u_i, u_j)$

the M must be pos. semi-definite

$\forall$ "functions" f $\int f(x) K(x,x') f(x') \, dx\, dx' \geq 0$

Support Vector Machines

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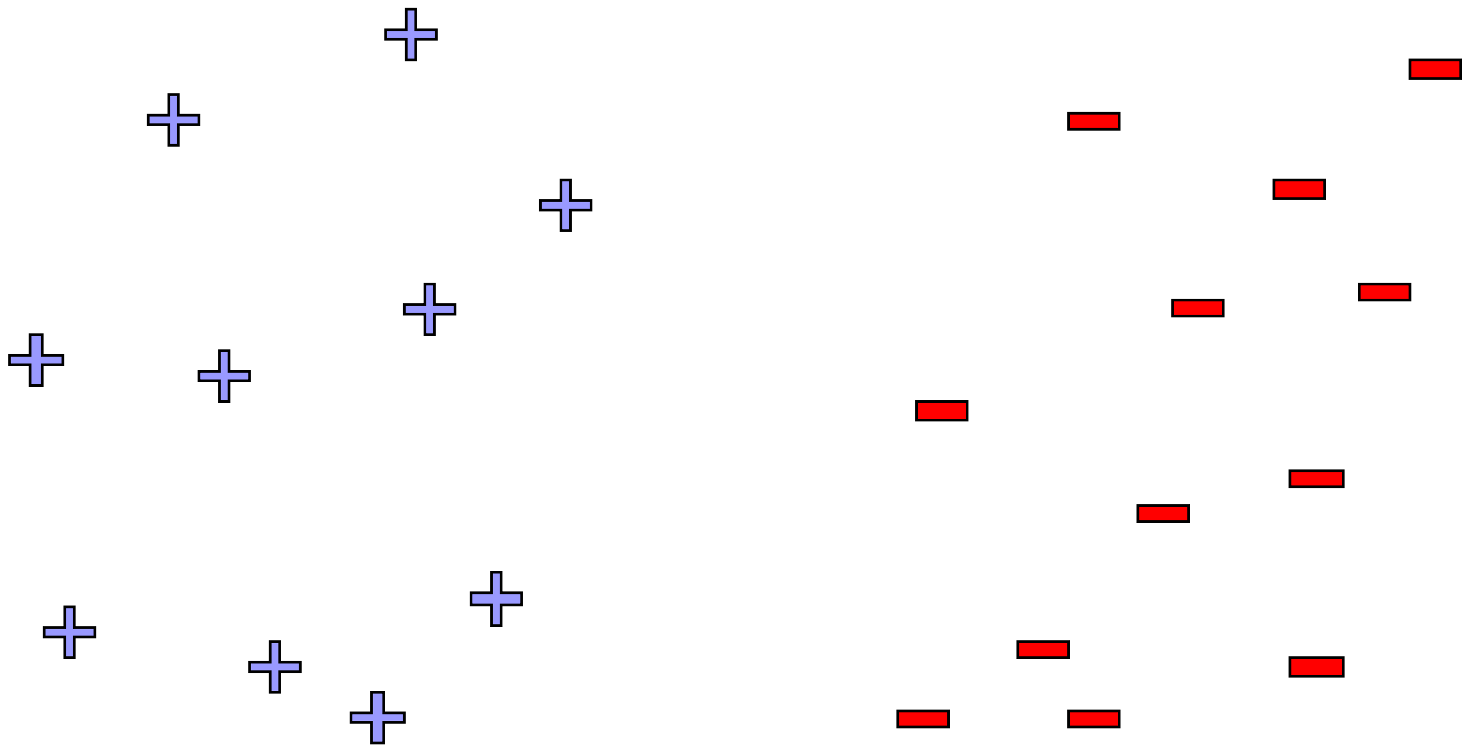
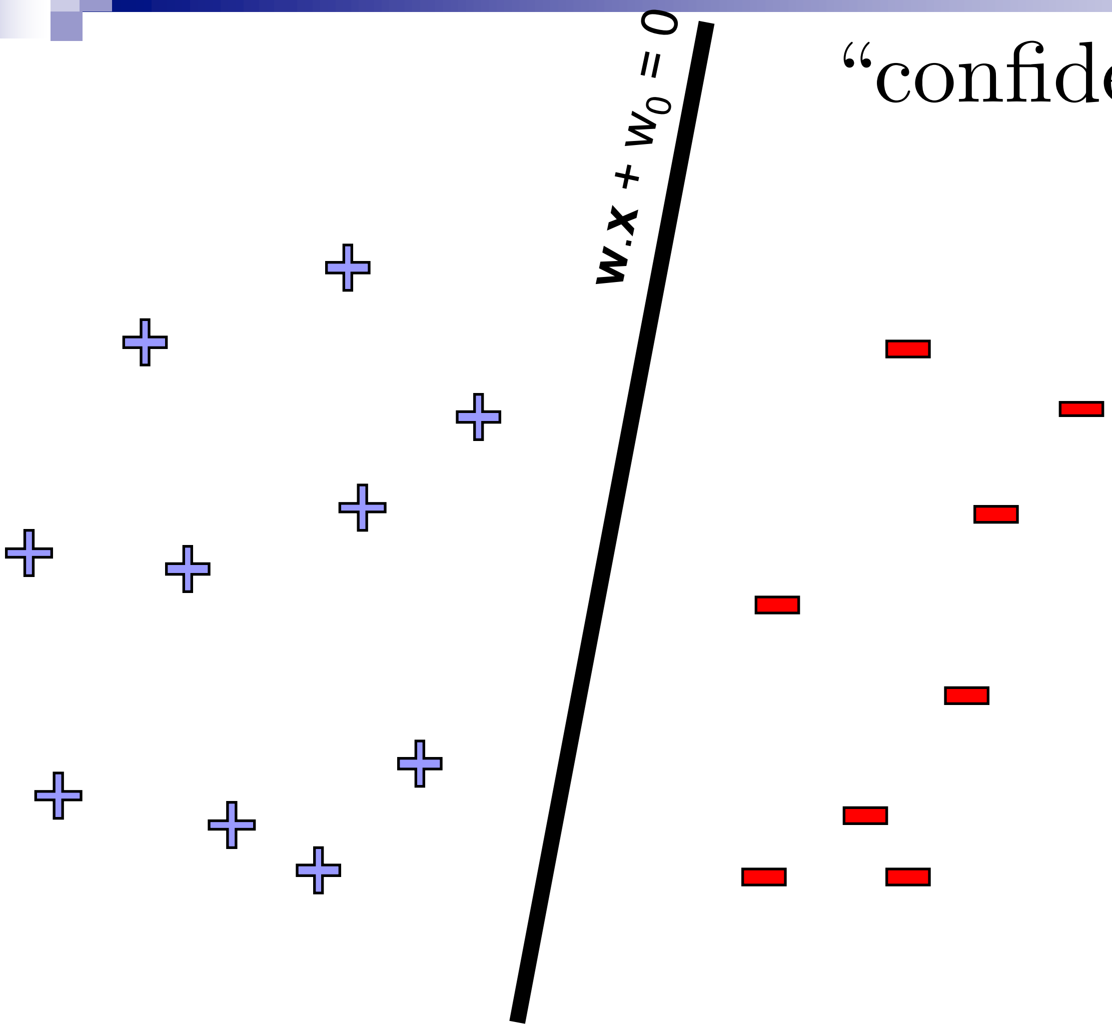
Linear classifiers – Which line is better?

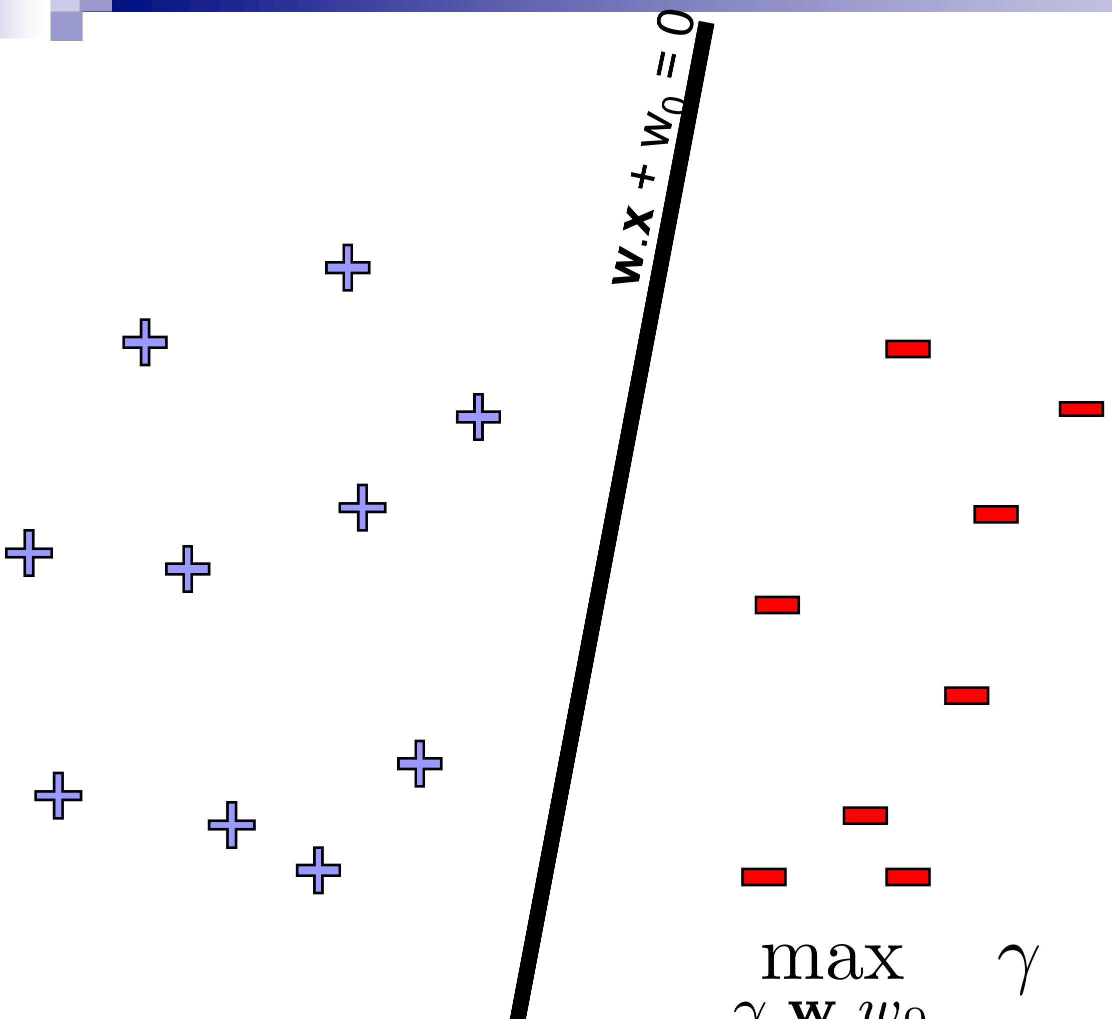


Pick the one with the largest margin!



$$\text{“confidence”} = y^j(\mathbf{w} \cdot \mathbf{x}^j + w_0)$$

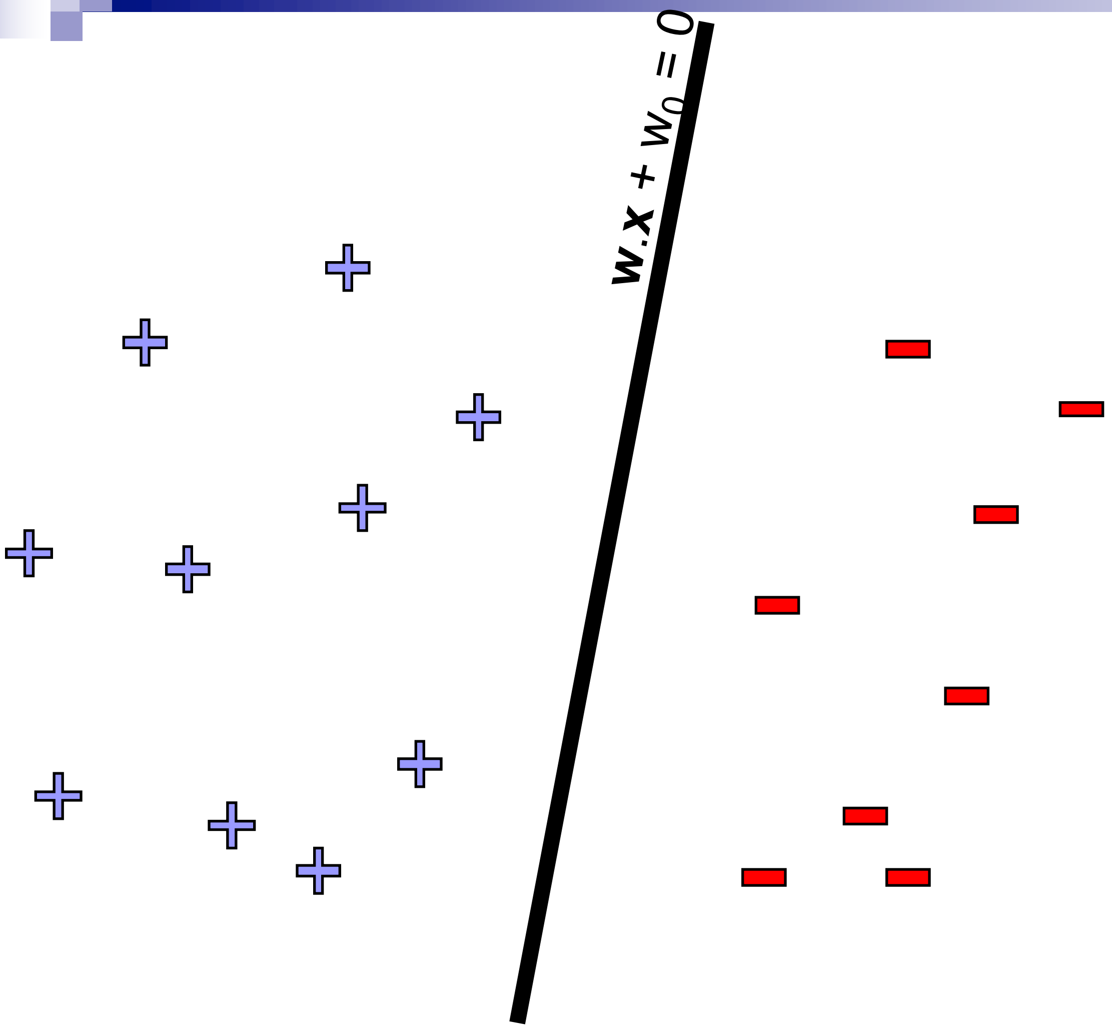
Maximize the margin



$$\max_{\gamma,\mathbf{w},w_0} \quad \gamma$$

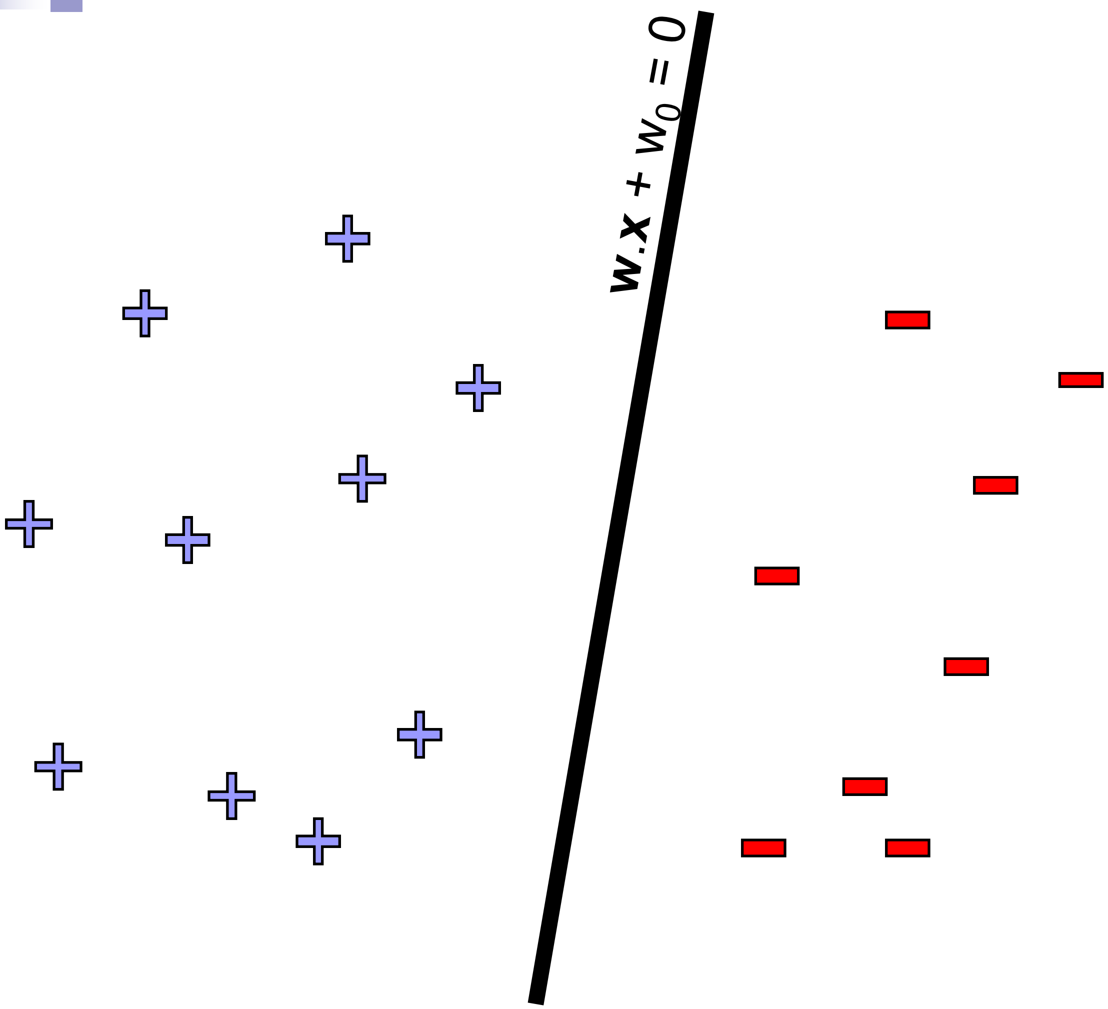
$$y^j(\mathbf{w}\cdot\mathbf{x}^j + w_0) \geq \gamma, \forall j \in \{1,\ldots,N\}$$

But there are many planes…



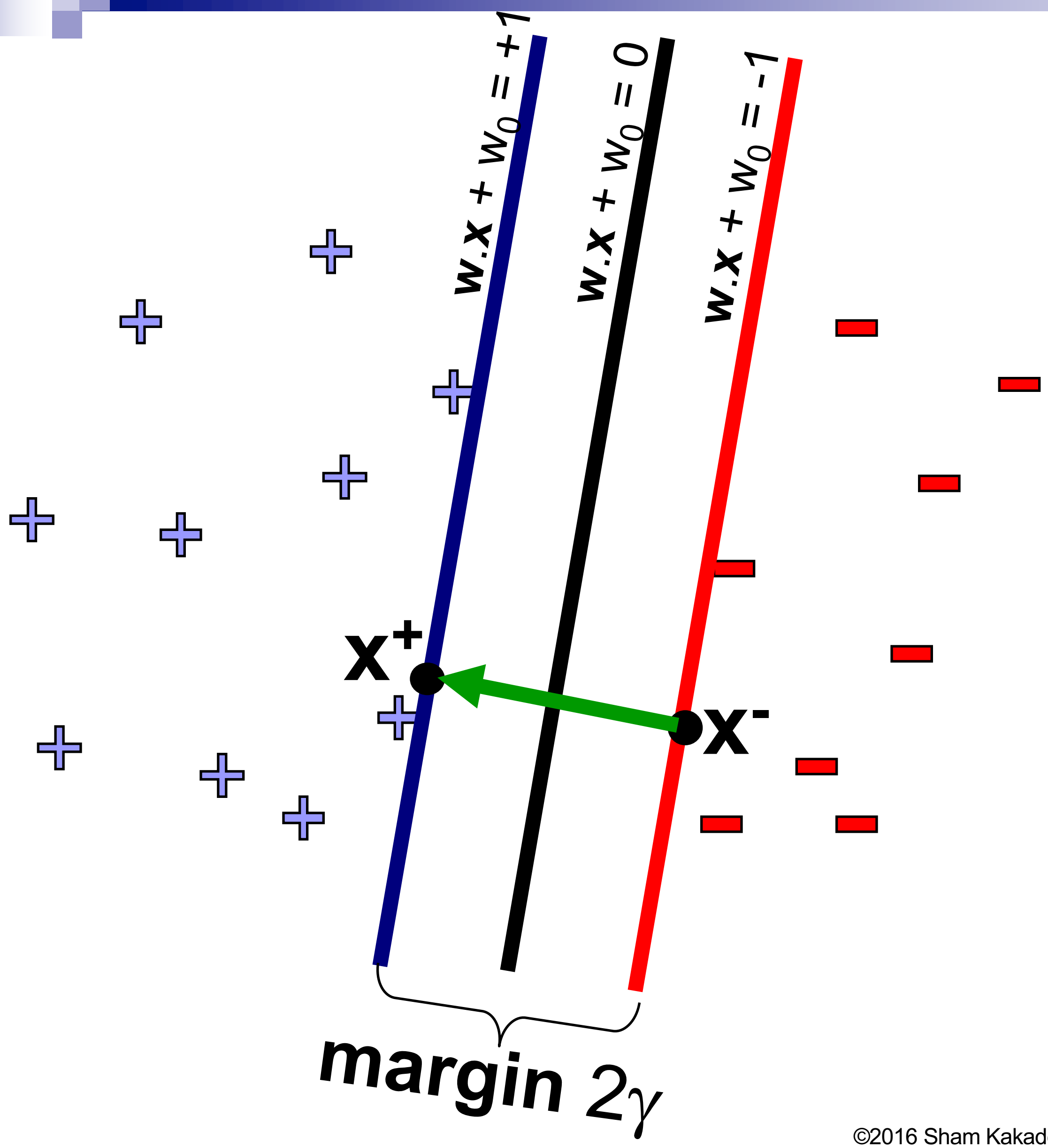
Review: Normal to a plane

$$\mathbf{x}^j = \bar{\mathbf{x}}^j + \alpha \frac{\mathbf{w}}{||\mathbf{w}||}$$

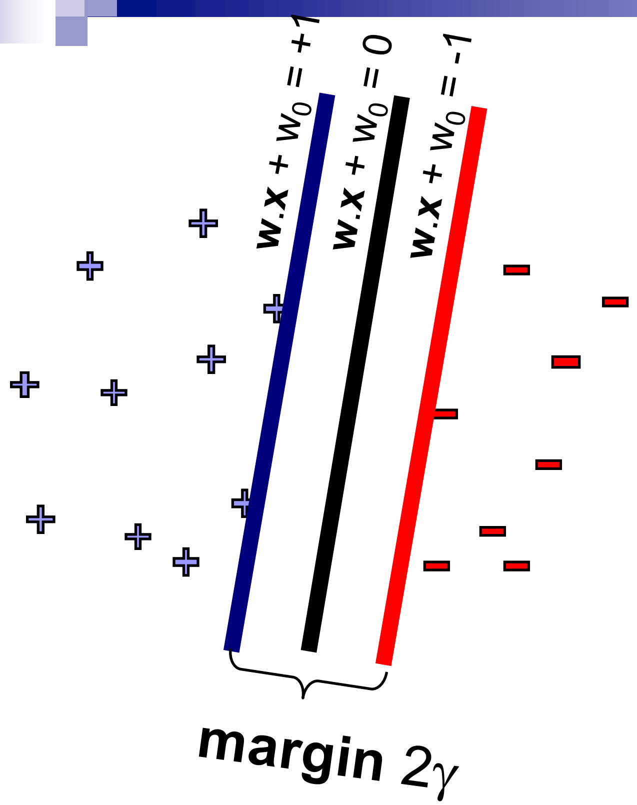


A Convention: Normalized margin – Canonical hyperplanes

$$\mathbf{x}^j = \bar{\mathbf{x}}^j + \alpha \frac{\mathbf{w}}{||\mathbf{w}||}$$



Margin maximization using canonical hyperplanes



Unnormalized problem:

$$\max_{\gamma, \mathbf{w}, w_0} \quad \gamma$$

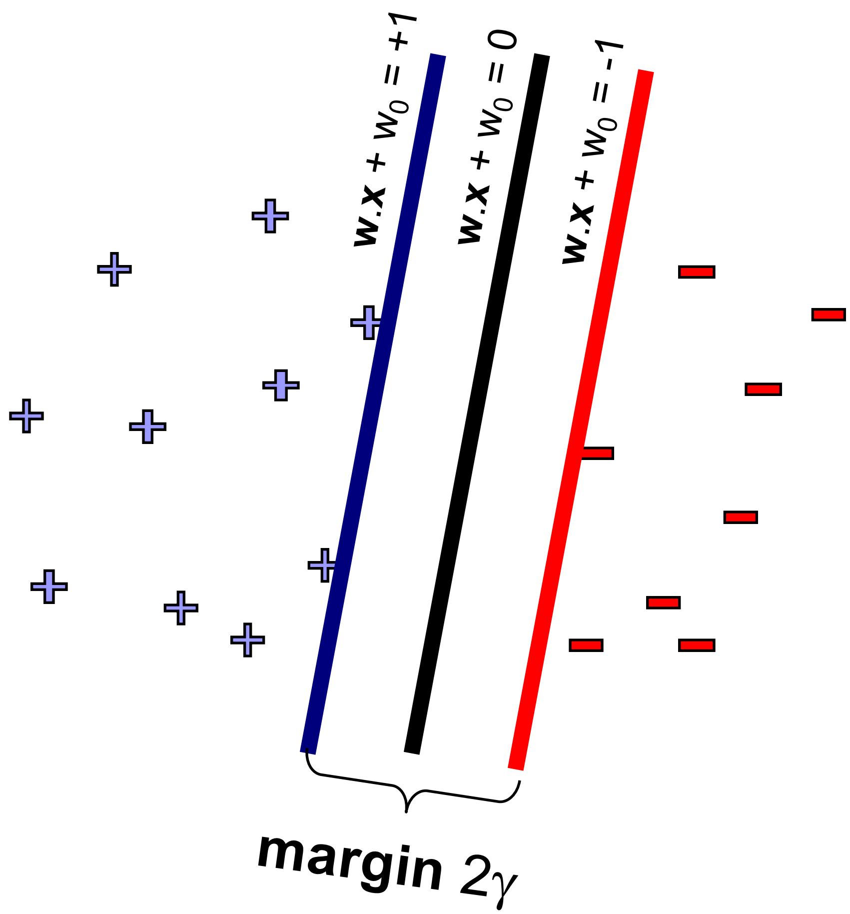
$$y^j(\mathbf{w} \cdot \mathbf{x}^j + w_0) \geq \gamma, \forall j \in \{1, \ldots, N\}$$

Normalized Problem:

$$\min_{\mathbf{w}, w_0} \quad ||w||_2^2$$

$$y^j(\mathbf{w} \cdot \mathbf{x}^j + w_0) \geq 1, \forall j \in \{1, \ldots, N\}$$

Support vector machines (SVMs)



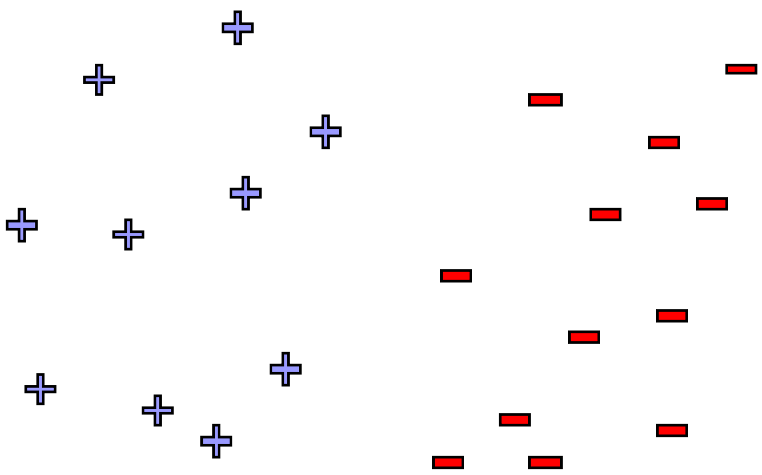
$$\min_{\mathbf{w},w_0} \quad ||w||_2^2$$

$$y^j(\mathbf{w}\cdot\mathbf{x}^j + w_0) \geq 1, \forall j \in \{1,\ldots,N\}$$

- Solve efficiently by many methods, e.g.,
  - quadratic programming (QP)
    - Well-studied solution algorithms
  - Stochastic gradient descent
- Hyperplane defined by support vectors

What if the data is not linearly separable?

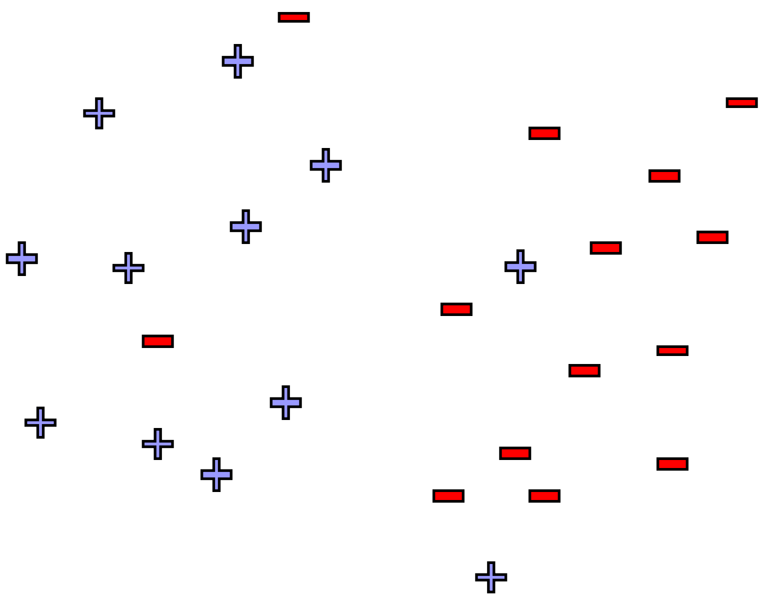
Use features of features of features of features….



What if the data is still not linearly separable?

$$\min_{\mathbf{w},w_0} \quad ||w||_2^2$$

$$y^j(\mathbf{w}\cdot\mathbf{x}^j + w_0) \geq 1 \qquad ,\forall j$$



- If data is not linearly separable, some points don't satisfy margin constraint:
- How bad is the violation?
- Tradeoff margin violation with ||**w**||:

SVMs for Non-Linearly Separable meet my friend the Perceptron…

- Perceptron was minimizing the hinge loss:

$$\sum_{j=1}^{N}\left(-y^j(\mathbf{w}\cdot\mathbf{x}^j+w_0)\right)_+$$

- SVMs minimizes the regularized hinge loss!!

$$||\mathbf{w}||_2^2+C\sum_{j=1}^{N}\left(1-y^j(\mathbf{w}\cdot\mathbf{x}^j+w_0)\right)_+$$

Stochastic Gradient Descent for SVMs

- Perceptron minimization:

$$\sum_{j=1}^{N} \left(-y^j(\mathbf{w} \cdot \mathbf{x}^j + w_0)\right)_+$$

- SGD for Perceptron:

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + \mathbb{1}\left[y^{(t)}(\mathbf{w}^{(t)} \cdot \mathbf{x}^{(t)}) \leq 0\right] y^{(t)}\mathbf{x}^{(t)}$$

- SVMs minimization:

$$||\mathbf{w}||_2^2 + C\sum_{j=1}^{N} \left(1 - y^j(\mathbf{w} \cdot \mathbf{x}^j + w_0)\right)_+$$

- SGD for SVMs:

SVMs vs logistic regression

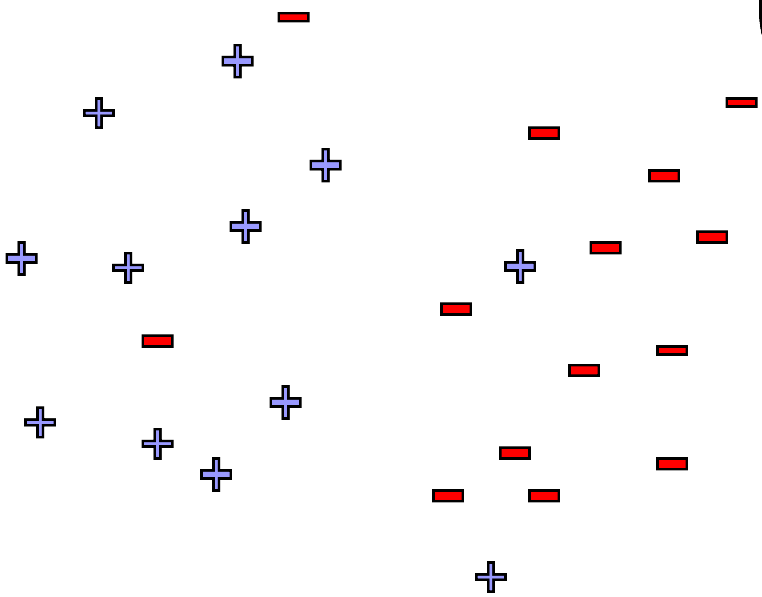
- We often want probabilities/confidences (logistic wins here)
- For classification loss, they are comparable
- Multiclass setting:
  - Softmax naturally generalizes logistic regression
  - SVMs have
- What about good old least squares?

Multiple Classes

- One can generalize the hinge loss
  - If no error (by some margin) -> no loss
  - If error, penalize what you said against the best
- SVMs vs logistic regression
  - We often want probabilities/confidences (logistic wins here)
  - For classification loss, they are
- Latent SVMs
  - When you have many classes it's difficult to do logistic regression
- 2) Kernels
  - Warp the feature space

Slack variables – Hinge loss

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



- If margin ¸ 1, don’t care
- If margin < 1, pay linear penalty

Side note: What's the difference between SVMs and logistic regression?

SVM:

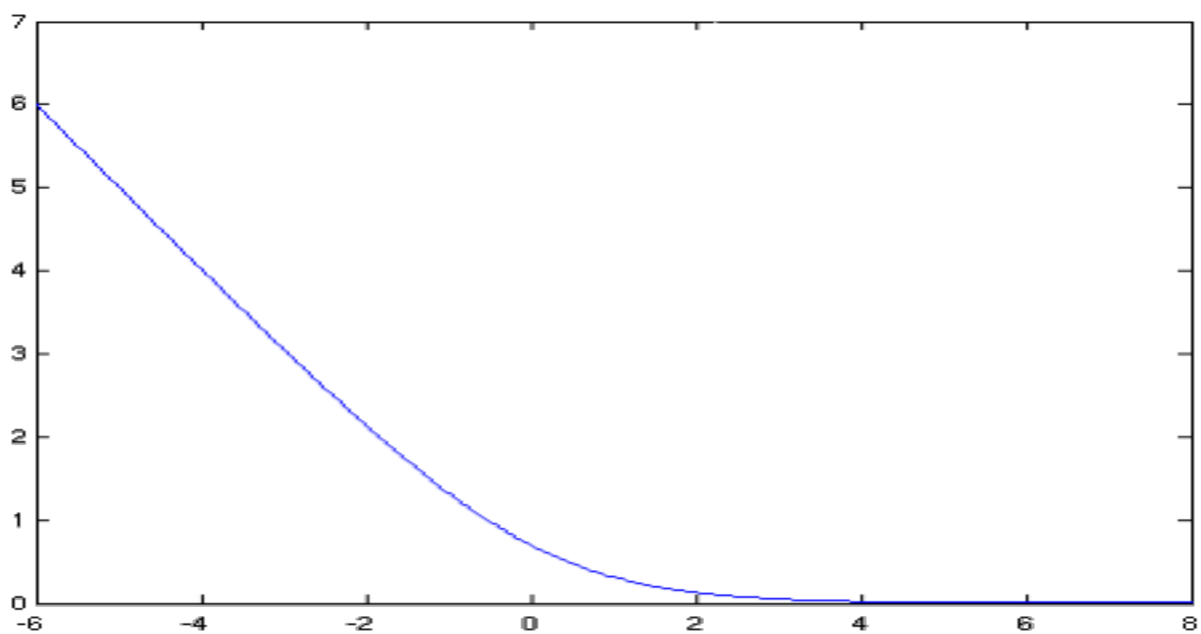
$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w} + C\sum_j \xi_j$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j, \ \ \forall j$$
$$\xi_j \geq 0, \ \ \forall j$$

Logistic regression:

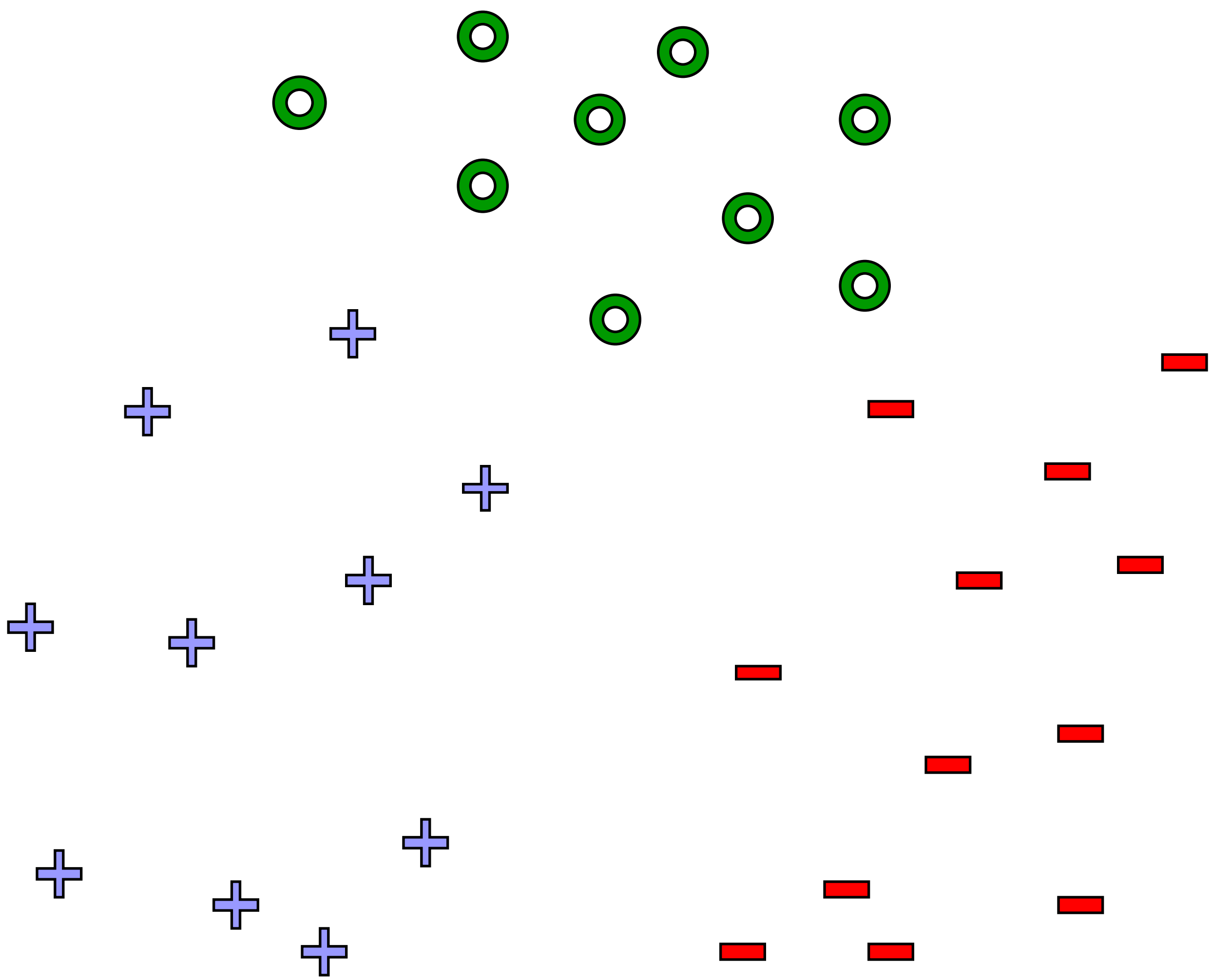
$$P(Y = 1 \mid x, \mathbf{w}) \ = \ \frac{1}{1 + e^{-(\mathbf{w}.\mathbf{x}+b)}}$$

Log loss:

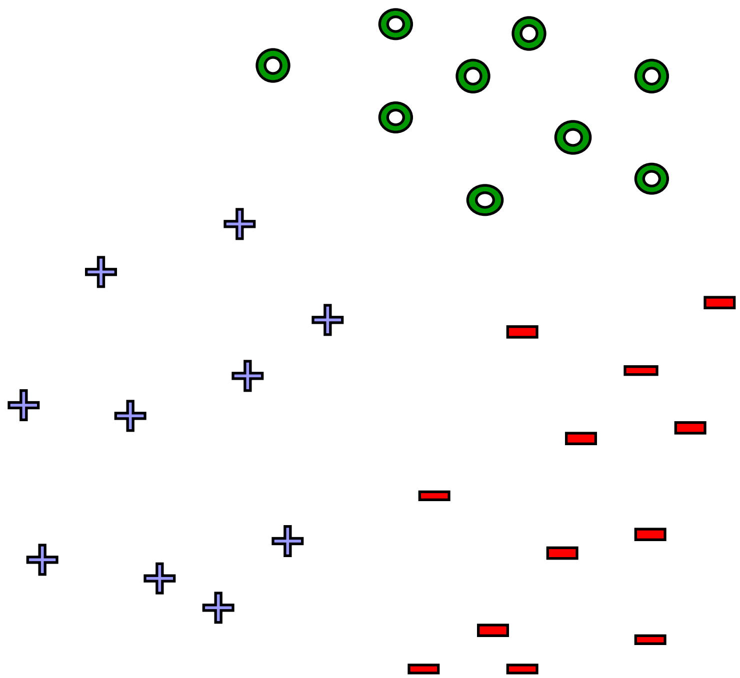
$$-\ln P(Y = 1 \mid x, \mathbf{w}) \ = \ \ln\left(1 + e^{-(\mathbf{w}.\mathbf{x}+b)}\right)$$



What about multiple classes?



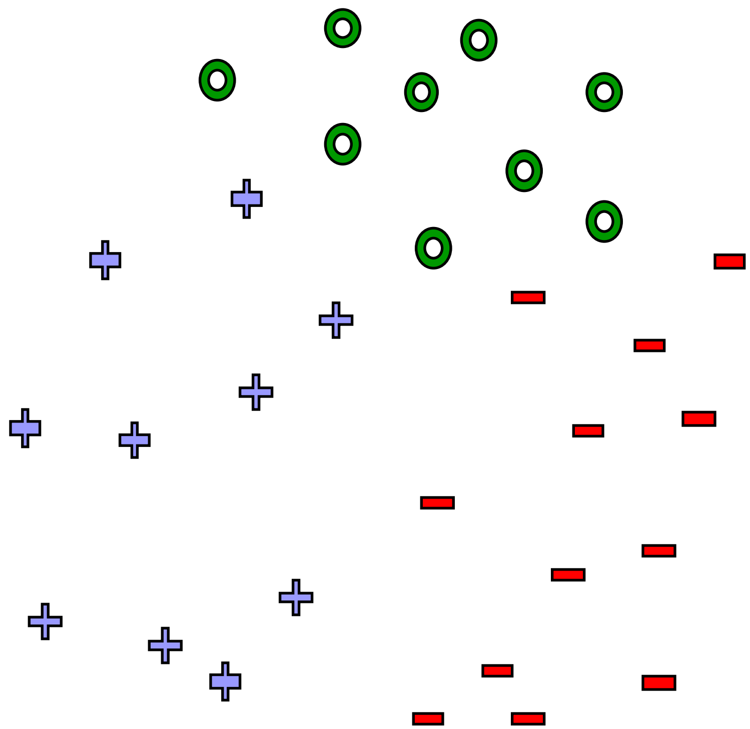
One against All



Learn 3 classifiers:

Learn 1 classifier: Multiclass SVM

Simultaneously learn 3 sets of weights



$$\mathbf{w}^{(y_j)}.\mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y')}.\mathbf{x}_j + b^{(y')} + 1, \ \forall y' \neq y_j, \ \forall j$$

Learn 1 classifier: Multiclass SVM

$$\text{minimize}_{\mathbf{w},b} \quad \sum_y \mathbf{w}^{(y)}.\mathbf{w}^{(y)} + C\sum_j \xi_j$$

$$\mathbf{w}^{(y_j)}.\mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y')}.\mathbf{x}_j + b^{(y')} + 1 - \xi_j, \;\; \forall y' \neq y_j, \;\; \forall j$$

$$\xi_j \geq 0, \;\; \forall j$$