Kernels

Machine Learning – CSE446
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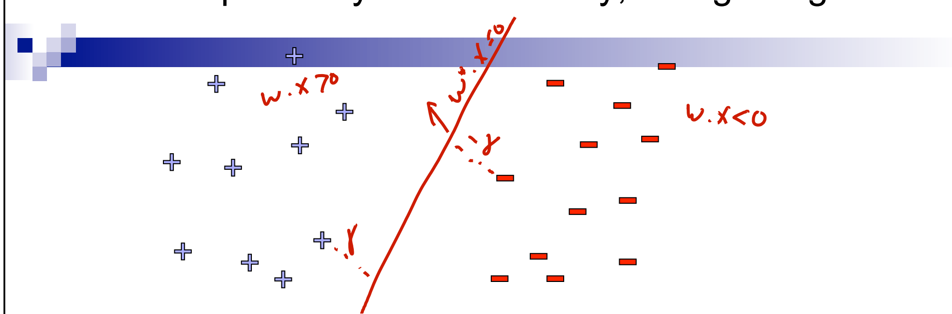
October 28, 2013

Linear Separability: More formally, Using Margin



- Data linearly separable, if there exists
  - a vector $\exists\, w^*,\ \|w^*\| = 1$
  - a margin $\gamma > 0$
- Such that all points are at least γ away from $w.x = 0$

$\forall t$: if $y^{(t)} = +1,\ w^*.x^{(t)} \geq \gamma$; Linearly separable:
$y^{(t)} = -1,\ w^*.x^{(t)} \leq -\gamma$; $y^{(t)}\, w^*.x^{(t)} \geq \gamma$

Perceptron Analysis: Linearly Separable Case

- Theorem [Block, Novikoff]:
  - Given a sequence of labeled examples: $(x^{(1)}, y^{(1)}) \ldots (x^{(T)}, y^{(T)})$ — not iid
  - Each feature vector has bounded norm: $\forall t \; \|x^{(t)}\| \leq R$
  - If dataset is linearly separable:

$$\exists w^*, \|w^*\| = 1, \; \forall t \quad y^{(t)} w^* \cdot x^{(t)} \geq \gamma \quad \text{for } \gamma > 0$$

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

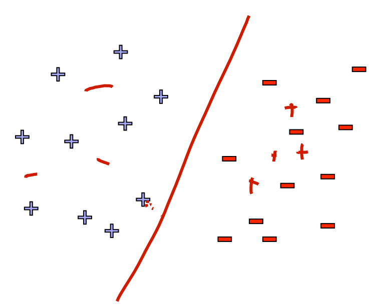
$$\left(\frac{R}{\gamma}\right)^2$$

Wow!! :)

constant, doesn't grow with T !! :)

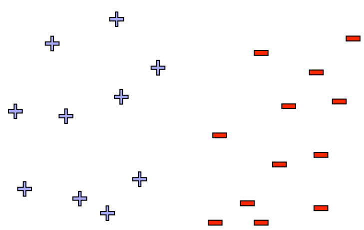
Beyond Linearly Separable Case

- 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
  - Analysis extends to non-linearly separable case
  - Very similar bound, see Freund & Schapire
  - Converges, but ultimately may not give good accuracy (make many many many mistakes)



& if data is very very non-linearly separable

What if the data is not linearly separable?



Use features of features of features of features….

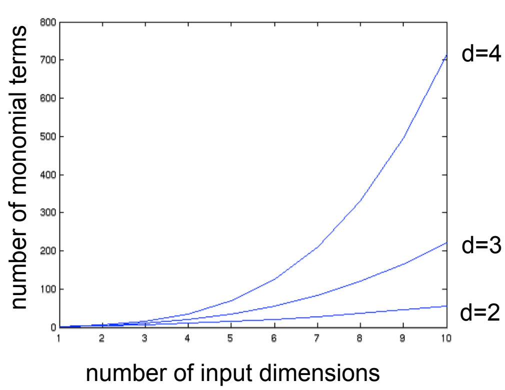
$$\Phi(\mathbf{x}) : R^m \mapsto F$$

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 **x** by:
- 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:
- Prediction rule now:
- When using high dimensional features:

Dot-product of polynomials

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

Finally the Kernel Trick!!! (Kernelized Perceptron

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

- Kernelized Perceptron prediction for **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:
  - Better solution:

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

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

- Sigmoid

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

What you need to know

- Notion of online learning
- Perceptron algorithm
- Mistake bounds and proofs
- The kernel trick
- Kernelized Perceptron
- Derive polynomial kernel
- Common kernels
- In online learning, report averaged weights at the end

Your Midterm…

- Content: Everything up to last Wednesday (Perceptron)…
- Only 80mins, so arrive early and settle down quickly, we'll start and end on time
- "Open book"
  - Textbook, Books, Course notes, Personal notes
- Bring a calculator that can do log ☺
- No:
  - Computers, tablets, phones, other materials, internet devices, wireless telepathy or wandering eyes…
- The exam:
  - Covers key concepts and ideas, work on understanding the big picture, and differences between methods

Support Vector Machines

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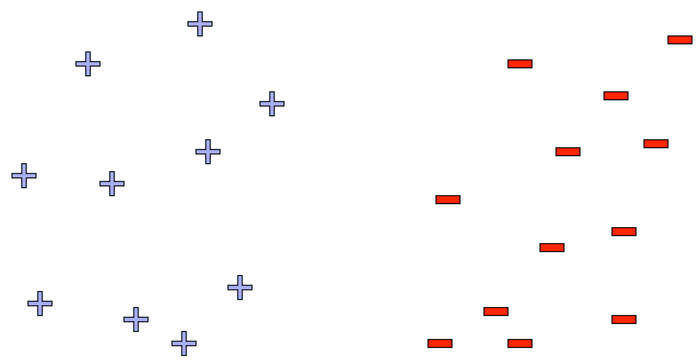
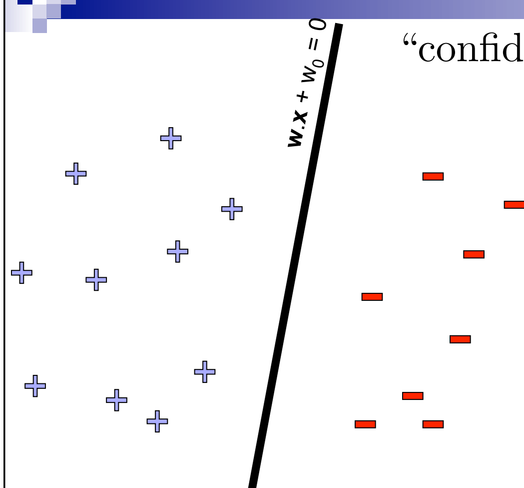
Linear classifiers – Which line is better?

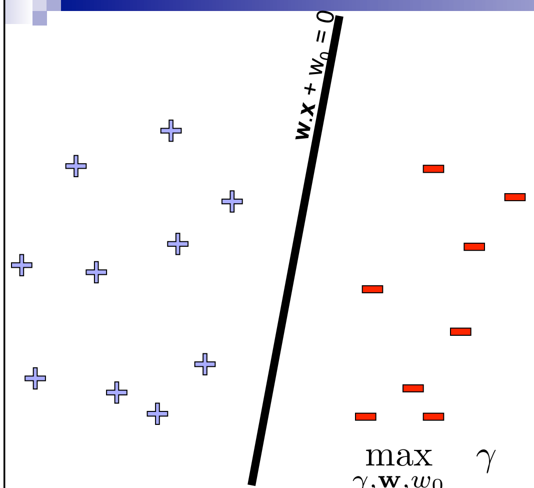


Pick the one with the largest margin!

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



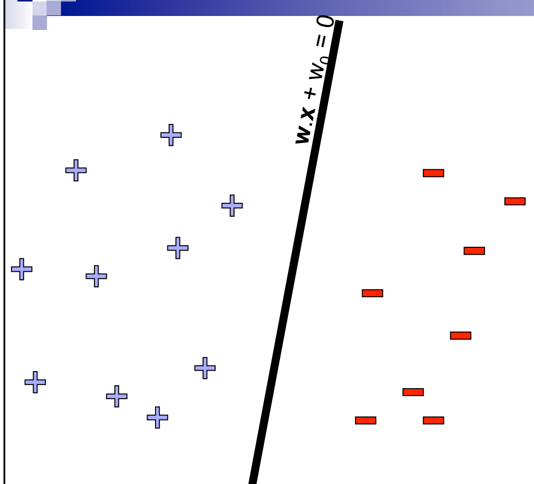
Maximize the margin



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

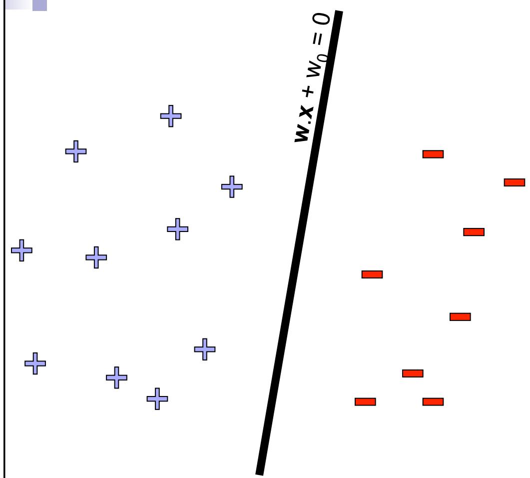
$$y^j(\mathbf{w} \cdot \mathbf{x}^j + w_0) \geq \gamma, \forall j \in \{1, \ldots, N\}$$

But there are many planes…



Review: Normal to a plane

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



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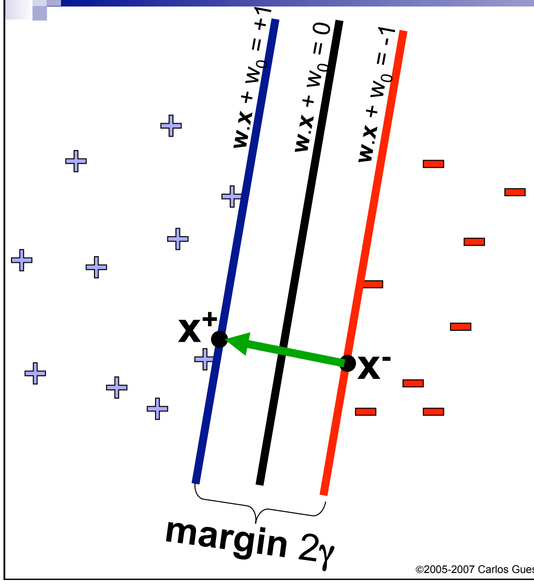
A Convention: Normalized margin – Canonical hyperplanes

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



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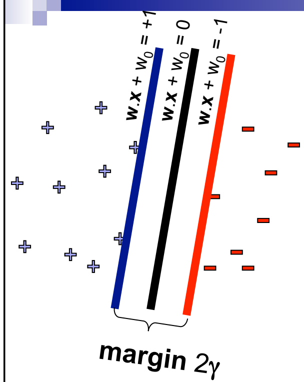
Margin maximization using canonical hyperplanes



Unnormalized problem:

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

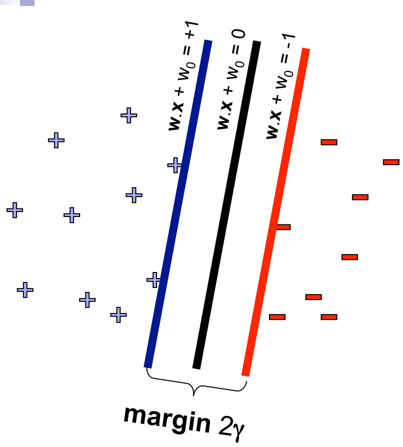
$$y^j(\mathbf{w}\cdot\mathbf{x}^j + w_0) \geq \gamma, \forall j \in \{1,\ldots,N\}$$

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)



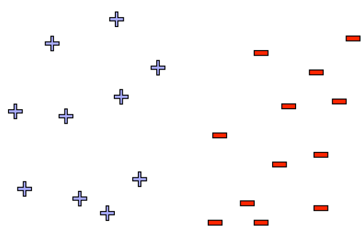
$$\min_{\mathbf{w},w_0} \quad ||w||_2^2$$

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

- 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….



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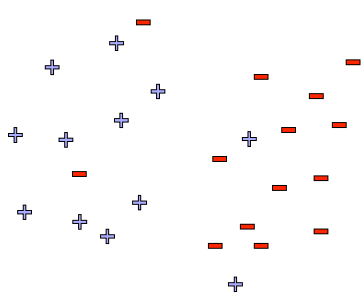
What if the data is still not linearly separable?

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

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



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

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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:

What you need to know

- Maximizing margin
- Derivation of SVM formulation
- Non-linearly separable case
  - Hinge loss
  - A.K.A. adding slack variables
- SVMs = Perceptron + L2 regularization
- Can also use kernels with SVMs
- Can optimize SVMs with SGD
  - Many other approaches possible