Support Vector Machines

Machine Learning – CSE446
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Announcements:

- Project Milestones coming up neural net
- No class Thurs, Nov 10 LS
- HW2 ≤ 2.5%
  - Let's figure it out…
- HW3 posted this week.
  - Let's get state of the art on MNIST!
  - It'll be collaborative
- Today:
  - Review: Kernels
  - SVMs
  - Generalization/review

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Kernels

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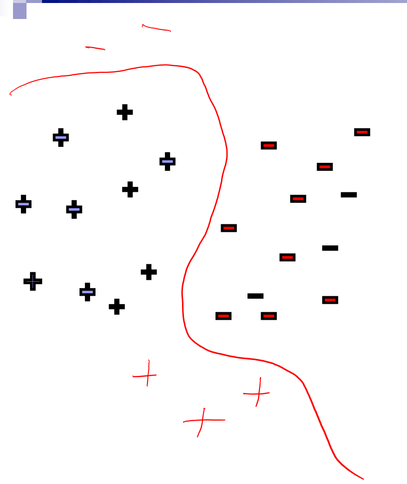
What if the data is not linearly separable?



Use features of features of features of features….

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

$m=1$

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

Feature space can get really large really quickly!

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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

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

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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:

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

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

the M must be pos. semi-definite

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

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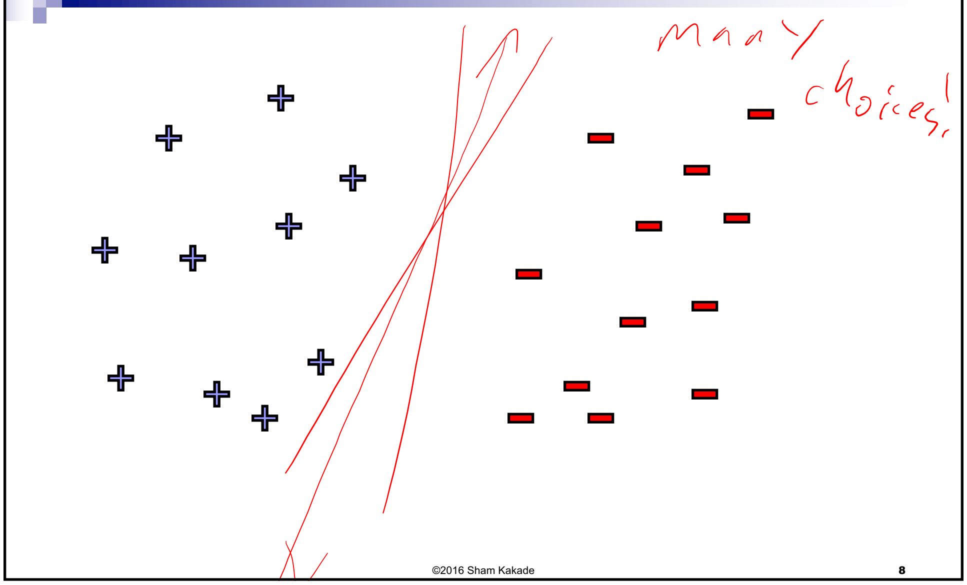
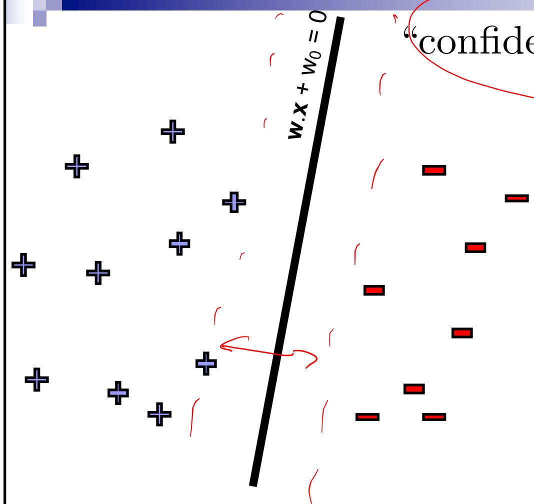
Linear classifiers – Which line is better?

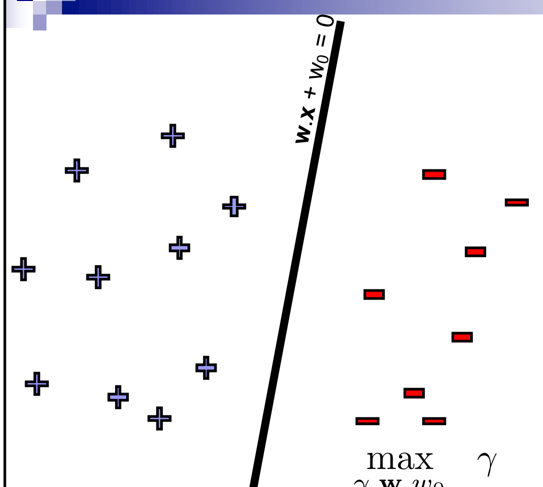


Pick the one with the largest margin!

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



Maximize the margin

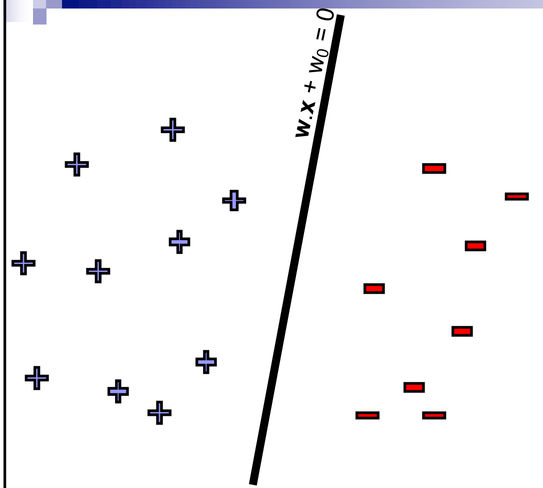


$\|w\| = 1.$

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

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

But there are many planes…



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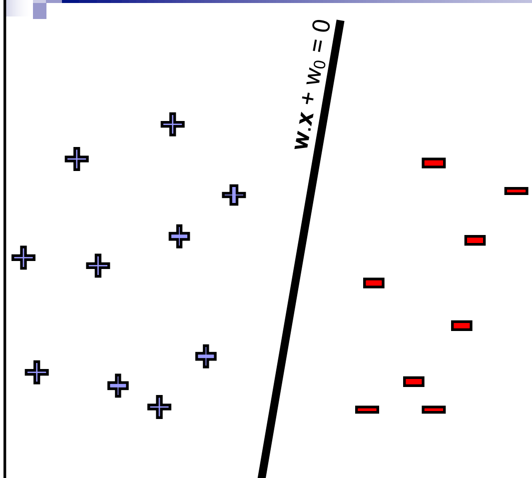
Review: Normal to a plane

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



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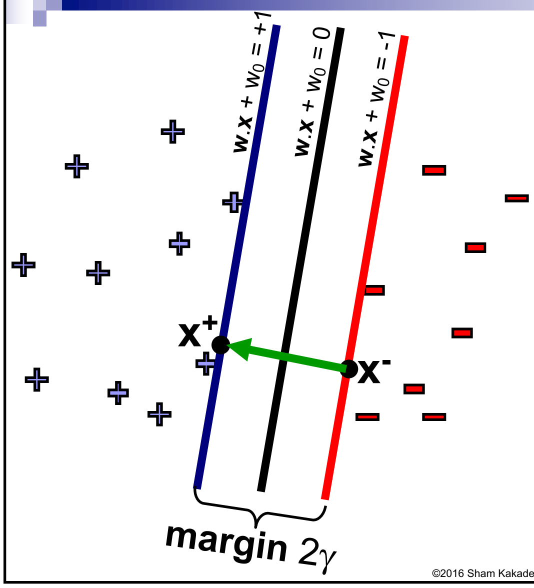
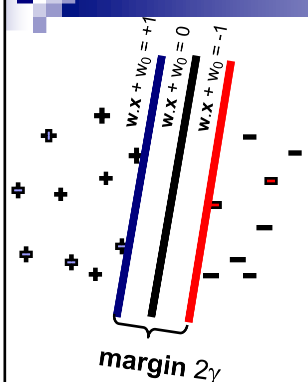
A Convention: Normalized margin – Canonical hyperplanes

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



Margin maximization using canonical hyperplanes



Unnormalized problem:

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

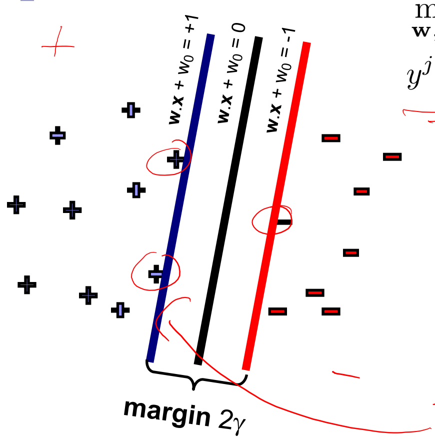
$$y^j(\mathbf{w}\cdot\mathbf{x}^j + w_0) \geq \gamma, \forall j \in \{1,\ldots,N\}$$

Normalized Problem:

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

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

Support vector machines (SVMs)



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

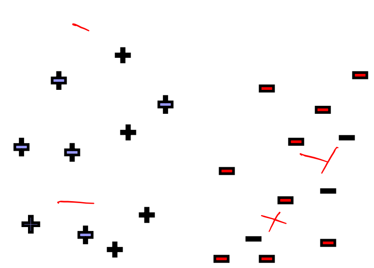
$w = [w, w_0)$

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

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

support vectors

What if the data is not linearly separable?

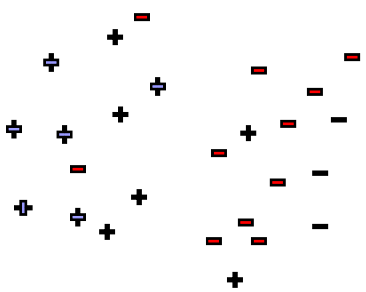


Use features of features of features of features….

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…

$$[x]_+ = \begin{cases} x & \text{if } x>0 \\ 0 & \text{else} \end{cases}$$

- 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!!

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

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

logistic wins

- We often want probabilities/confidences (logistic wins here)
- For classification loss, they are comparable

my opinion

- Multiclass setting:
  - Softmax naturally generalizes logistic regression
  - SVMs have a generalization.

win for logistic

- 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

SVMs can be reasonable with many classes (if partition difficult to compute for softmax)

Generalization/Model Comparisons

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What method should I use?

- Linear regression, logistic, SVMs?
- No regularization? Ridge? L1?

- I ran SGD without any regularization and it was ok?

Generalization

- You get N samples.
- You learn a classifier/regression f^.

- How close are you to optimal?

$$L(f^\wedge)-L(f^*) < ???$$

- (We can look at the above in expectation or with 'high' probability).

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Finite Case:

- You get N samples.
- You learn a classifier/regressor f^ among K classifiers:

$$L(f^\wedge)-L(f^*) < \sqrt{\frac{\log\left(\frac{K}{\delta}\right)}{N}}$$

with probability $\geq 1-\delta$

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Linear Regression

- N samples, d dimensions.
- L is the square loss.
- w^ is the least squares estimate.

$$L(w\hat{})-L(w^*) < O(d/N)$$

- Need about N=O(d) samples

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Sparse Linear Regression

- N samples, d dimensions, L is the square loss.
- f^ is best fit line which only uses k features (computationally intractable)

$$L(w\hat{})-L(w^*) < k\log(d)/N$$

- true of Lasso under stronger assumptions: "incoherence"
- When do like sparse regression??
  - When we believe there are a few of GOOD features.

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Learning a Halfspace

- You get N samples, in D dimensions.
- L is the 0/1 loss.
- ~~f^~~ is the empirical risk minimizer (computationally infeasible to compute)

$\hat{w}$

$$L(w^\wedge)-L(w^*) < \sqrt{d \log(N)/N}$$

- Need N=O(d) samples

"VC theory"

What about Regularization?

- Let's look at (dual) constrained problem
- Minimize:

$$\min L^\wedge(w)$$
$$\text{such } ||w||_{??} < W_+$$

- Where L^ is our training error.

Optimization and Regularization?

- I did SGD without regularization and it was fine?
- "Early stopping" implicitly regularizes (in L2)

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L2 Regularization

- Assume $||w||_2 < W_2$ $||x||_2 < R_2$
- L is some convex loss (logistic,hinge,square)
- w^ is the constrained minimizer (computationally tractable to compute)

$$L(w\hat{}) - L(w^*) < W_2 R_2 / \sqrt{N}$$

- DIMENSION FREE "margin" Bound!

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L1 Regularization

- Assume $||w||_1 < W_1$ $||x||_\infty < R_\infty$
- L is some convex loss (logistic,hinge,square)
- w^ is the constrained minimizer (computationally tractable to compute)

$$L(w\hat{})-L(w^*)<\frac{W_1 R_\infty log(d)}{\sqrt{N}}$$

- Promotes sparsity, one can think of W1 as the "sparsity level/k" (mild dimension dependence, log(d).

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