CPSC 340: Machine Learning and Data Mining

Multi-Class Classification

Fall 2018

Admin

- Assignment 4:
  - Due Friday of next week.

- Midterm:
  - Grades posted.
  - Can view exam during Mike or my office hours this week and next week.

Last Time: SVMs, Logistic Regression, One vs. All

- We discussed hinge loss and logistic loss for binary classification.
  - Convex approximation to number of classification errors in linear models.
  - Leads to SVMs (hinge + L2-regularization) and logistic regression (logistic).
- We discussed multi-class classification: y_i in $\{1,2,\dots,k\}$.
- One vs. all with +1/-1 binary classifier:
  - Train weights w_c to predict +1 for class 'c', -1 otherwise.

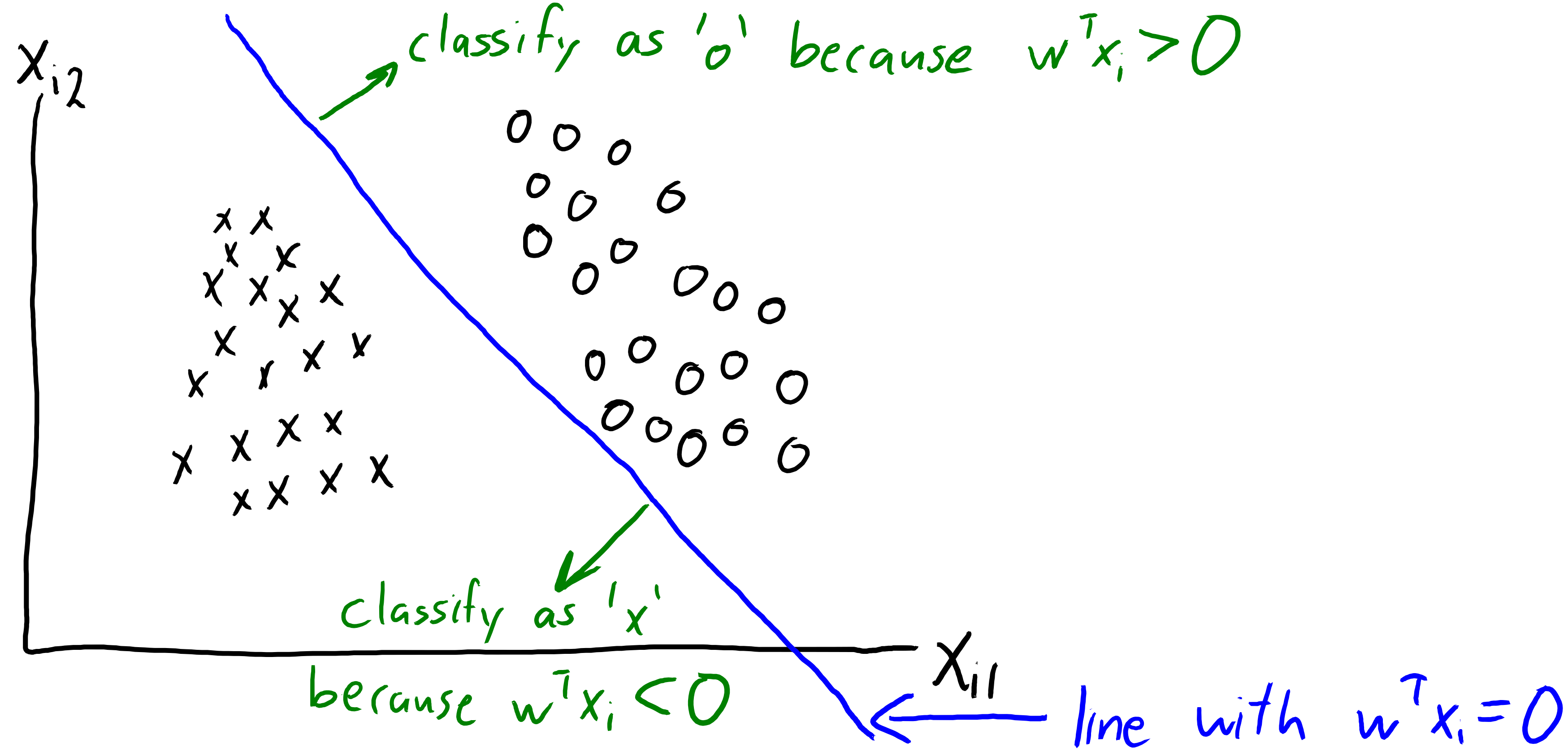
$$W = \underbrace{\begin{bmatrix} \text{---}\ w_1^T\ \text{---} \\ \text{---}\ w_2^T\ \text{---} \\ \vdots \\ \text{---}\ w_k^T\ \text{---} \end{bmatrix}}_{d} \left.\vphantom{\begin{bmatrix} a \\ a \\ a \\ a \end{bmatrix}}\right\} k$$

Each row 'c' gives weights w_c for a binary logistic regression model to predict class 'c'.

  - Predict by taking 'c' maximizing $w_c^T x_i$.
    - Problem: each w_c is only "trying to get sign right" during training.
      - Didn't train the w_c so that the largest $w_c^T x_i$ would be $\mathbf{w}_{y_i}^T x_i$.

Shape of Decision Boundaries

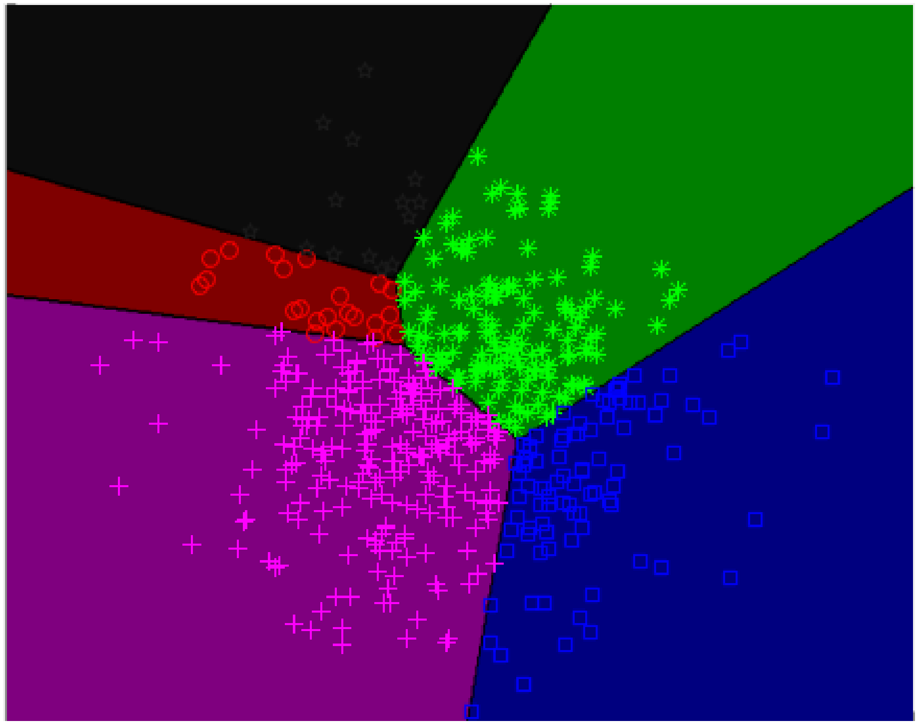
- Recall that a binary linear classifier splits space using a hyper-plane:



- Divides x_i space into 2 "half-spaces".

Shape of Decision Boundaries

- Multi-class linear classifier is intersection of these "half-spaces":
  - This divides the space into convex regions (like k-means):



"Blue" region is region where we have:

$w_{blue}^T x_i \geq w_{green}^T x_i$

$w_{blue}^T x_i \geq w_{magenta}^T x_i$

$w_{blue}^T x_i \geq w_{red}^T x_i$

$w_{blue}^T x_i \geq w_{black}^T x_i$

  - Could be non-convex with change of basis.

Multi-Class SVMs

- Can we define a loss that encourages largest $w_c^T x_i$ to be $w_{y_i}^T x_i$?
  - So when we maximizing over $w_c^T x_i$, we choose correct label y_i.
- Recall our derivation of the hinge loss (SVMs):
  - We wanted $y_i w^T x_i > 0$ for all 'i' to classify correctly.
  - We avoided non-degeneracy by aiming for $y_i w^T x_i \geq 1$.
  - We used the constraint violation as our loss: $\max\{0, 1 - y_i w^T x_i\}$.
- We can derive multi-class SVMs using the same steps…

Multi-Class SVMs

- Can we define a loss that encourages largest $w_c^T x_i$ to be $w_{y_i}^T x_i$?

We want $w_{y_i}^T x_i > w_c^T x_i$ for all 'c' that are not correct label y_i

If we penalize violation of this constraint it's degenerate.

We use $w_{y_i}^T x_i \geq w_c^T x_i + 1$ for all $c \neq y_i$ to avoid strict inequality

Equivalently: $0 \geq 1 - w_{y_i}^T x_i + w_c^T x_i$

- For here, there are two ways to measure constraint violation:

"Sum"

$$\sum_{c \neq y_i} \max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\}$$

"Max"

$$\max_{c \neq y_i} \{\max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\}\}$$

Multi-Class SVMs

- Can we define a loss that encourages largest $w_c^T x_i$ to be $w_{y_i}^T x_i$?

"Sum"

$$\sum_{c \neq y_i} \max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\}$$

"Max"

$$\max_{c \neq y_i} \{\max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\}\}$$

- For each training example 'i':
  - "Sum" rule penalizes for each 'c' that violates the constraint.
  - "Max" rule penalizes for one 'c' that violates the constraint the most.
    - "Sum" gives a penalty of 'k-1' for W=0, "max" gives a penalty of '1'.
- If we add L2-regularization, both are called multi-class SVMs:
  - "Max" rule is more popular, "sum" rule usually works better.
  - Both are convex upper bounds on the 0-1 loss.

Multi-Class Logistic Regression

- We derived binary logistic loss by smoothing a degenerate 'max'.
  - A degenerate constraint in the multi-class case can be written as:

$$w_{y_i}^T x_i \geq \max_c \{w_c^T x_i\}$$

or

$$0 \geq -w_{y_i}^T x_i + \max_c \{w_c^T x_i\}$$

- We want the right side to be as small as possible.
- Let's smooth the max with the log-sum-exp:

$$-w_{y_i}^T x_i + \log\left(\sum_{c=1}^{k} \exp(w_c^T x_i)\right)$$

  - With W=0 this gives a loss of log(k).
- This is the softmax loss, the loss for multi-class logistic regression.

Multi-Class Logistic Regression

- We sum the loss over examples and add regularization:

$$f(W) = \sum_{i=1}^{n}\Big[\underbrace{-w_{y_i}^T x_i}_{\text{Tries to make } w_c^T x_i \text{ big for the correct label}} + \underbrace{\log\Big(\sum_{c=1}^{k}\exp(w_c^T x_i)\Big)}_{\text{Approximates } \max_c\{w_c^T x_i\} \text{ so tries to make } w_c^T x_i \text{ small for all labels.}}\Big] + \underbrace{\frac{\lambda}{2}\sum_{j=1}^{d}\sum_{c=1}^{k} w_{jc}^2}_{\text{Usual } L_2\text{-regularizer on elements of 'W'}}$$

- This objective is convex (should be clear for 1^{st} and 3^{rd} terms).
  – It's differentiable so you can use gradient descent.
- When k=2, equivalent to binary logistic.
  – Not obvious at the moment.

Digression: Frobenius Norm

- We can write regularizer in matrix notation using:

$$\frac{\lambda}{2}\sum_{j=1}^{d}\sum_{c=1}^{k} w_{jc}^2 = \frac{\lambda}{2}\|W\|_F^2$$

- The Frobenius norm of a matrix 'W' is defined by:

$$\|W\|_F = \sqrt{\sum_{j=1}^{d}\sum_{c=1}^{k} w_{jc}^2}$$

(L_2-norm if you "stack" columns into one big vector)

(pause)

Motivation: Dog Image Classification

- Suppose we're classifying images of dogs into breeds:

- What if we have images where class label isn't obvious?
  - Syberian husky vs. Inuit dog?

https://www.slideshare.net/angjoo/dog-breed-classification-using-part-localization
https://ischlag.github.io/2016/04/05/important-ILSVRC-achievements

Learning with Preferences

- Do we need to throw out images where label is ambiguous?
  - We don't have the y_i.

  - We want classifier to prefer Syberian husky over bulldog, Chihuahua, etc.
    - Even though we don't know if these are Syberian huskies or Inuit dogs.
  - Can we design a loss that enforces preferences rather than "true" labels?

https://ischlag.github.io/2016/04/05/important-ILSVRC-achievements

Learning with Pairwise Preferences (Ranking)

- Instead of y_i, we're given list of (c_1,c_2) preferences for each 'i':

We want $w_{c_1}^T x_i > w_{c_2}^T x_i$ for these particular (c_1,c_2) values

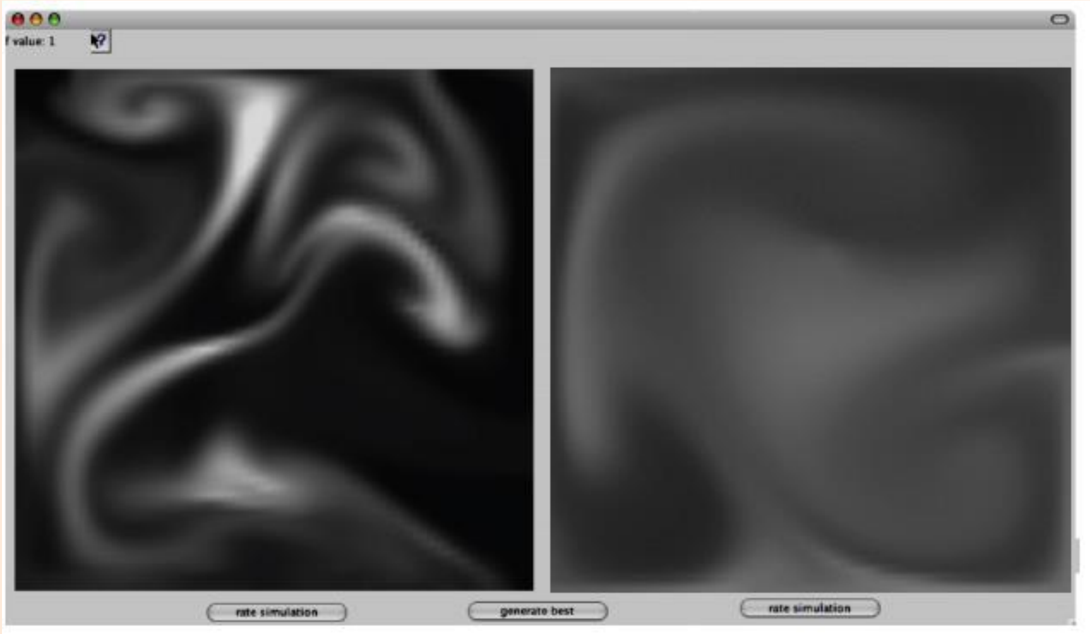
- Multi-class classification is special case of choosing (y_i,c) for all 'c'.

- By following the earlier steps, we can get objectives for this setting:

$$\sum_{i=1}^{n} \underbrace{\sum_{(c_1,c_2)} \max\{0, 1 - w_{c_1}^T x_i + w_{c_2}^T x_i\}}_{\text{"sum" version of multi-class SVM}} + \frac{\lambda}{2}\|W\|_F^2$$

Learning with Pairwise Preferences (Ranking)

- Pairwise preferences for computer graphics:
  - We have a smoke simulator, with several parameters:

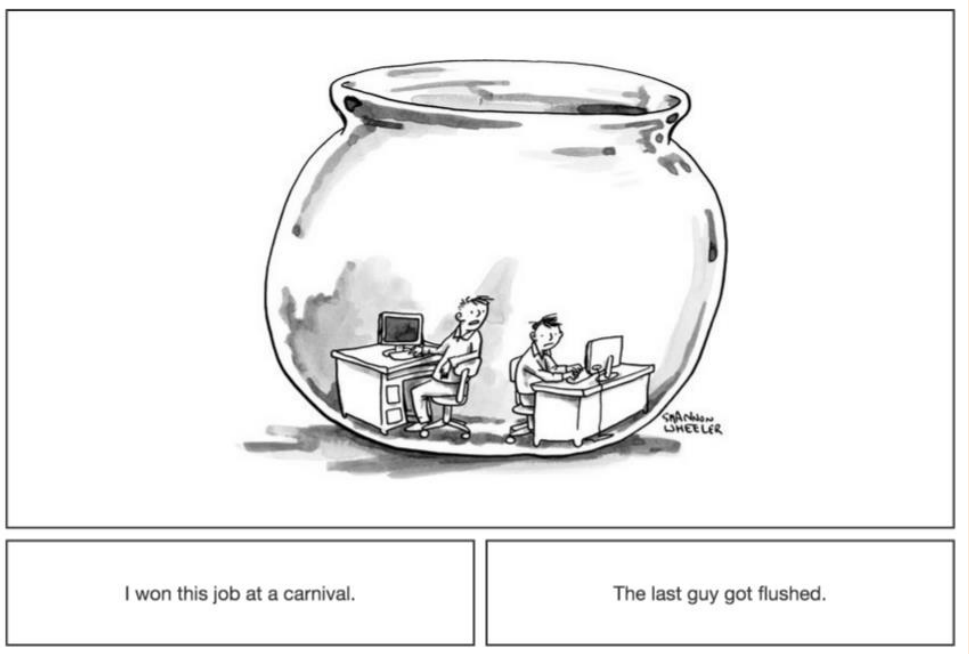


  - Don't know what the optimal parameters are, but we can ask the artist:
    - "Which one looks more like smoke"?

https://circle.ubc.ca/bitstream/handle/2429/30519/ubc_2011_spring_brochu_eric.pdf?sequence=3

Learning with Pairwise Preferences (Ranking)

- Pairwise preferences for humour:
  - New Yorker caption contest:



  - “Which one is funnier”?

https://homes.cs.washington.edu/~jamieson/resources/next.pdf

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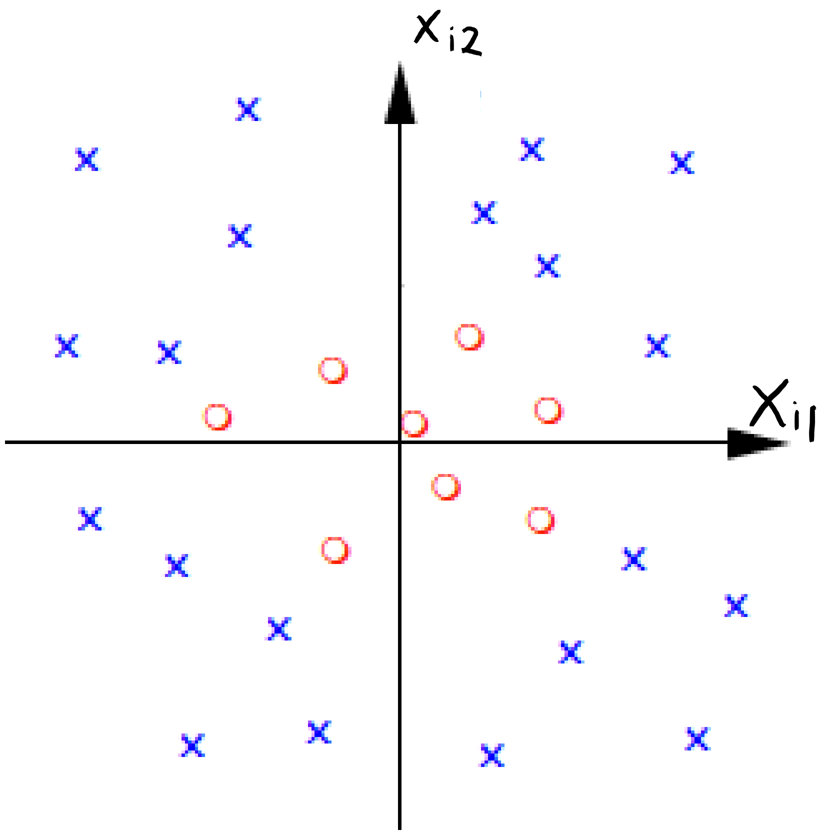
Support Vector Machines for Non-Separable

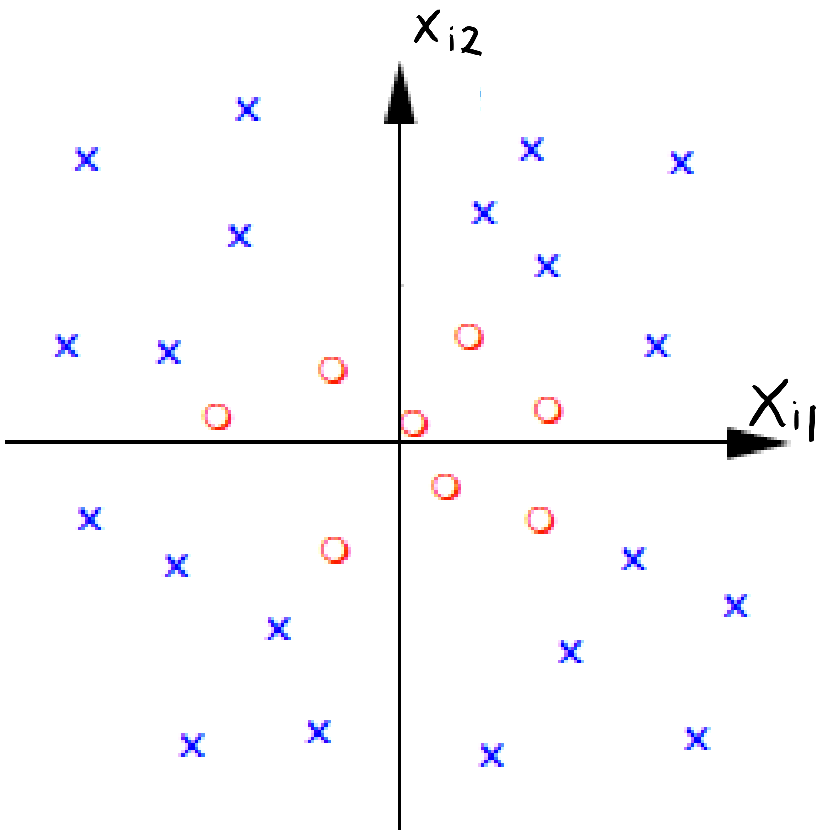
- What about data that is not even close to separable?



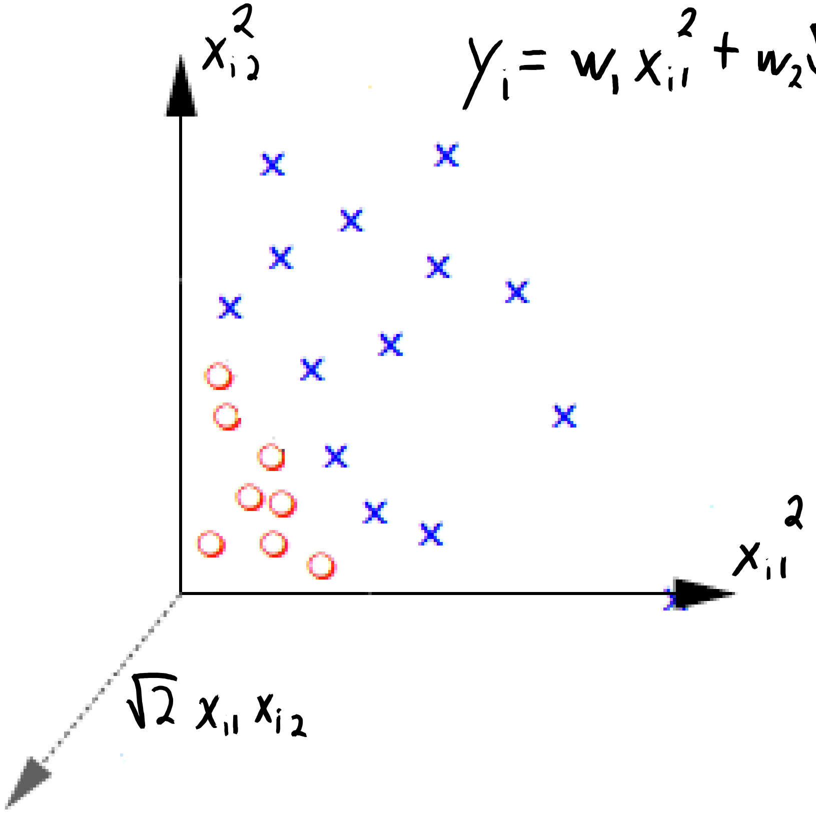
http://math.stackexchange.com/questions/353607/how-do-inner-product-space-determine-half-planes

Support Vector Machines for Non-Separable

- What about data that is not even close to separable?
  - It may be separable under change of basis (or closer to separable).



$y_i = w_1 x_{i1}^2 + w_2 \sqrt{2} x_{i1} x_{i2} + w_3 x_{i2}^2$



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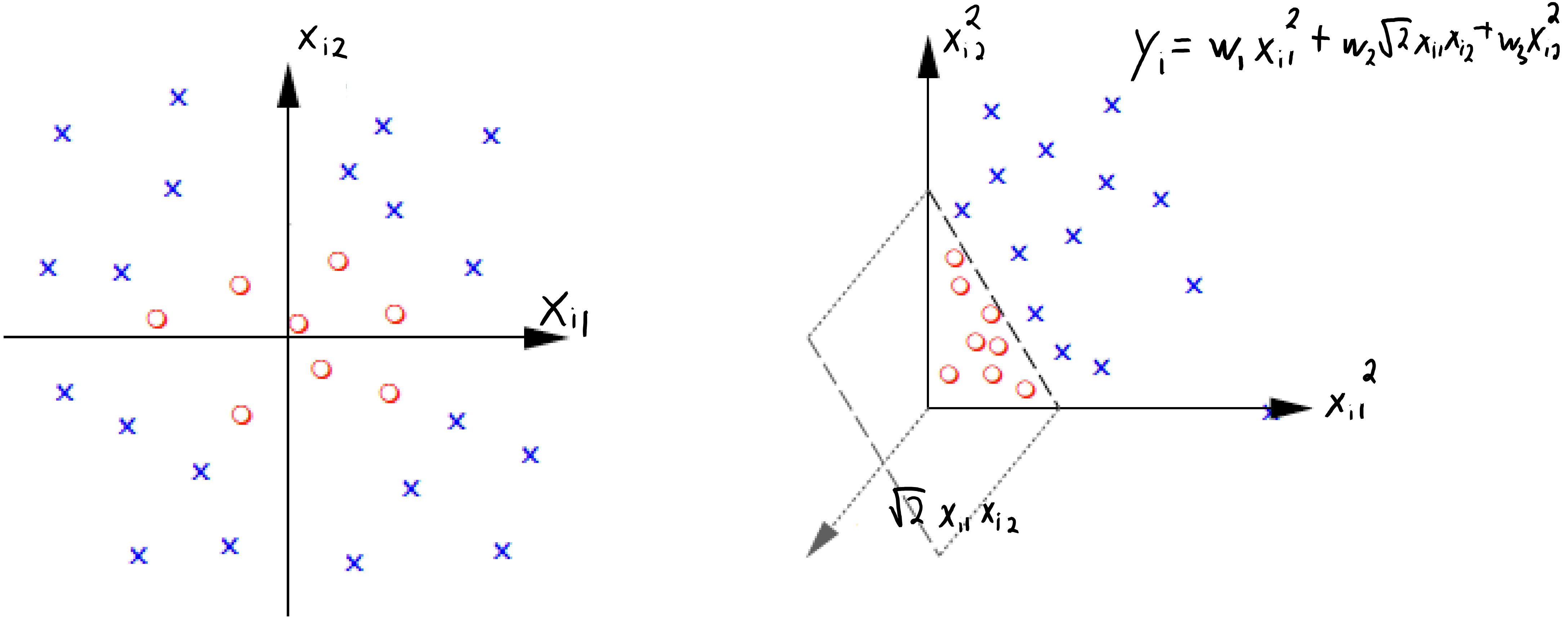

Support Vector Machines for Non-Separable

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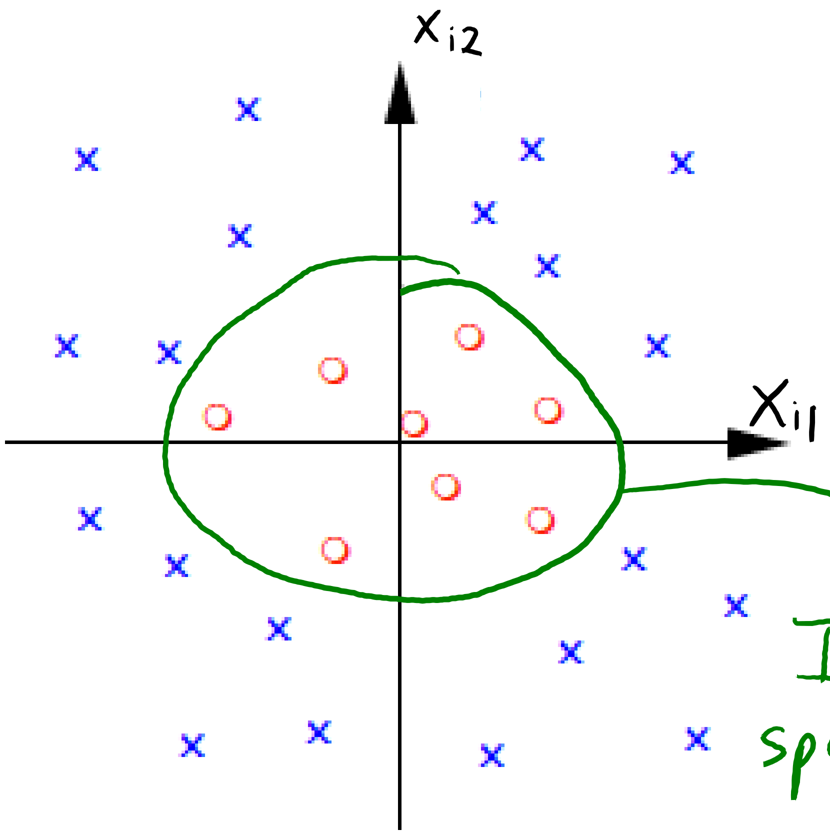
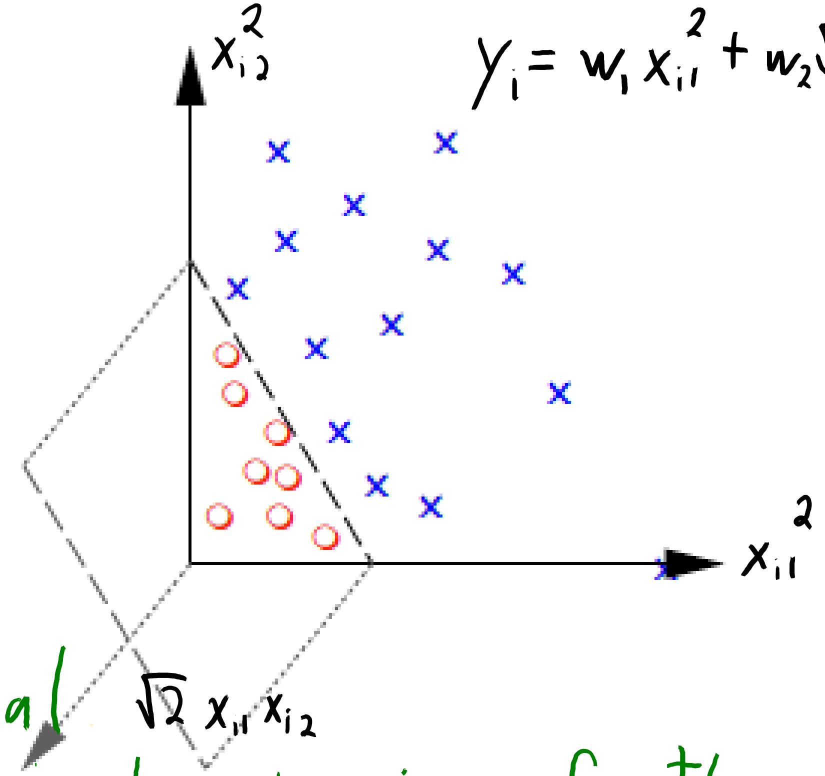
$y_i = w_1 x_{i1}^2 + w_2 \sqrt{2} x_{i1} x_{i2} + w_3 x_{i2}^2$





In original space, decision boundary is of the form,

$0 = w_1 x_{i1}^2 + w_2 \sqrt{2} x_{i1} x_{i2} + w_3 x_{i2}^2$

Multi-Dimensional Polynomial Basis

- Recall fitting polynomials when we only have 1 feature:

$$\hat{y}_i = w_0 + w_1 x_i + w_2 x_i^2$$

- We can fit these models using a change of basis:

$$X = \begin{bmatrix} 0.2 \\ -0.5 \\ 1 \\ 4 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 & 0.2 & (0.2)^2 \\ 1 & -0.5 & (-0.5)^2 \\ 1 & 1 & (1)^2 \\ 1 & 4 & (4)^2 \end{bmatrix}$$

- How can we do this when we have a lot of features?

Multi-Dimensional Polynomial Basis

- Polynomial basis for d=2 and p=2:

$$X = \begin{bmatrix} 0.2 & 0.3 \\ 1 & 0.5 \\ -0.5 & -0.1 \end{bmatrix} \longrightarrow Z = \begin{array}{c} \begin{bmatrix} 1 & 0.2 & 0.3 & (0.2)^2 & (0.3)^2 & (0.1)(0.3) \\ 1 & 1 & 0.5 & (1)^2 & (0.5)^2 & (1)(0.5) \\ 1 & 0.5 & -0.1 & (0.5)^2 & (-0.1)^2 & (-0.5)(-0.1) \end{bmatrix} \\ \begin{array}{cccccc} \text{bias} & x_{i1} & x_{i2} & (x_{i1})^2 & (x_{i2})^2 & (x_{i1})(x_{i2}) \end{array} \end{array}$$

- With d=4 and p=3, the polynomial basis would include:
  - Bias variable and the x_{ij}: 1, x_{i1}, x_{i2}, x_{i3}, x_{i4}.
  - The x_{ij} squared and cubed: $(x_{i1})^2$, $(x_{i2})^2$, $(x_{i3})^2$, $(x_{i4})^2$, $(x_{i1})^3$, $(x_{i2})^3$, $(x_{i3})^3$, $(x_{i4})^3$.
  - Two-term interactions: $x_{i1}x_{i2}$, $x_{i1}x_{i3}$, $x_{i1}x_{i4}$, $x_{i2}x_{i3}$, $x_{i2}x_{i4}$, $x_{i3}x_{i4}$.
  - Cubic interactions: $x_{i1}x_{i2}x_{i3}$, $x_{i2}x_{i3}x_{i4}$, $x_{i1}x_{i3}$,x_{i4}, $x_{i1}x_{i2}x_{i4}$,
    $x_{i1}^2x_{i2}$, $x_{i1}^2x_{i3}$, $x_{i1}^2x_{i4}$, $x_{i1}x_{i2}^2$, $x_{i2}^2x_{i3}$, $x_{i2}^2x_{i4}$, $x_{i1}x_{i3}^2$, $x_{i2}x_{i3}^2$,$x_{i3}^2x_{i4}$, $x_{i1}x_{i4}^2$, $x_{i2}x_{i4}^2$, $x_{i3}x_{i4}^2$.

Kernel Trick

- If we go to degree p=5, we'll have O(d^5) quintic terms:

$$x_{i1}^5,\ x_{i1}^4 x_{i2},\ x_{i1}^4 x_{i3},\ \dots,\ x_{i1}^4 x_{id},\ x_{i1}^3 x_{i2}^2,\ x_{i1}^3 x_{i3}^2,\ \dots,\ x_{i1}^3 x_{id}^2,\ \dots,\ x_{i2}^5,\ x_{i2}^4 x_{i3},\ \dots\dots,\ x_{id}^5$$

- For large 'd' and 'p', storing a polynomial basis is intractable!
  - 'Z' has k=O(d^p) columns, so it does not fit in memory.

- Today: efficient polynomial basis for L2-regularized least squares.
  - Main tools: the "other" normal equations and the "kernel trick".

The "Other" Normal Equations

- Recall the L2-regularized least squares objective with basis 'Z':

$$f(v) = \frac{1}{2}\|Zv - y\|^2 + \frac{\lambda}{2}\|v\|^2$$

- We showed that the minimum is given by

$$v = (\underbrace{Z^T Z + \lambda I}_{k \times k})^{-1} Z^T y$$

(in practice you still solve the linear system, since inverse can be numerically unstable – see CPSC 302)

- With some work (bonus), this can equivalently be written as:

$$v = Z^T (\underbrace{Z Z^T + \lambda I}_{n \times n})^{-1} y$$

- This is faster if n << k:
  - Cost is $O(n^2k + n^3)$ instead of $O(nk^2 + k^3)$.
  - But for the polynomial basis, this is still too slow since $k = O(d^p)$.

The "Other" Normal Equations

- With the "other" normal equations we have $v = Z^T(ZZ^T + \lambda I)^{-1}y$
- Given test data $\tilde{X}$, predict $\hat{y}$ by forming $\tilde{Z}$ and then using:

$$\begin{aligned}\hat{y} &= \tilde{Z}v \\ &= \underbrace{\tilde{Z}Z^T}_{\tilde{K}}(\underbrace{ZZ^T}_{K} + \lambda I)^{-1}y \\ \underset{t\times 1}{} &= \underbrace{\tilde{K}}_{t\times n}\underbrace{(K + \lambda I)^{-1}}_{n\times n}\underbrace{y}_{n\times 1}\end{aligned}$$

- Notice that if you have K and $\widetilde{K}$ then you do not need Z and $\tilde{Z}$.
- Key idea behind "kernel trick" for certain bases (like polynomials):
  - We can efficiently compute K and $\widetilde{K}$ even though forming Z and $\tilde{Z}$ is intractable.

Gram Matrix

- The matrix $K = ZZ^T$ is called the Gram matrix K.

$$K = ZZ^T = \underbrace{\begin{bmatrix} — & z_1^T & — \\ — & z_2^T & — \\ & \vdots & \\ — & z_n^T & — \end{bmatrix}}_{Z} \underbrace{\begin{bmatrix} | & | & & | \\ z_1 & z_2 & \cdots & z_n \\ | & | & & | \end{bmatrix}}_{Z^T}$$

$$= \underbrace{\begin{bmatrix} z_1^T z_1 & z_1^T z_2 & \cdots & z_1^T z_n \\ z_2^T z_1 & z_2^T z_2 & \cdots & z_2^T z_n \\ \vdots & & \ddots & \vdots \\ z_n^T z_1 & z_n^T z_2 & \cdots & z_n^T z_n \end{bmatrix}}_{n} \Big\} n$$

- K contains the dot products between all training examples.
  - Similar to ‘Z’ in RBFs, but using dot product as “similarity” instead of distance.

Gram Matrix

- The matrix $\tilde{K} = \tilde{Z}Z^T$ has dot products between train and test examples:

$$\tilde{K} = \tilde{Z}Z^T = \underbrace{\begin{bmatrix} \text{---} & \tilde{z}_1^T & \text{---} \\ \text{---} & \tilde{z}_2^T & \text{---} \\ & \vdots & \\ \text{---} & \tilde{z}_t^T & \text{---} \end{bmatrix}}_{\tilde{Z}} \underbrace{\begin{bmatrix} | & | & & | \\ z_1 & z_2 & \cdots & z_n \\ | & | & & | \end{bmatrix}}_{Z^T}$$

$$= \underbrace{\begin{bmatrix} \tilde{z}_1^T z_1 & \tilde{z}_1^T z_2 & \cdots & \tilde{z}_1^T z_n \\ \tilde{z}_2^T z_1 & \tilde{z}_2^T z_2 & \cdots & \tilde{z}_2^T z_n \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{z}_t^T z_n & \tilde{z}_t^T z_2 & \cdots & \tilde{z}_t^T z_n \end{bmatrix}}_{n} \left.\vphantom{\begin{bmatrix} a \\ a \\ a \\ a \end{bmatrix}}\right\} t$$

- Kernel function: $k(x_i, x_j) = z_i^T z_j$.
  - Computes dot product between in basis ($z_i^T z_j$) using original features x_i and x_j.

Kernel Trick

To apply linear regression, I only need to know K and $\tilde{K}$

Use x_i to form z_i

Use x_j to form z_j

compute $z_i^T z_j$

set $k_{ij} = z_i^T z_j$

$$K = \underbrace{\begin{bmatrix} \quad & \quad & \quad \\ & & \\ & & \end{bmatrix}}_{\text{Final result is } n \times n \text{ (no matter how large } z_i \text{ is)}}$$

Kernel Trick

To apply linear regression, I <u>only</u> need to know K and $\tilde{K}$

Use x_i ~~to form z_i~~

Use x_j ~~to form z_j~~

~~compute $z_i^T z_j$~~

~~set $k_{ij} = z_i^T z_j$~~

$K = $

Directly compute k_{ij} from x_i and x_j

Final result is $n \times n$ (no matter how large z_i is)

Linear Regression vs. Kernel Regression

Linear Regression

Training

1. Form basis Z from X.
2. Compute $\underbrace{v}_{k \times 1} = (Z^T Z + \lambda I)^{-1} (Z^T y)$

Testing

1. Form basis $\tilde{Z}$ from $\tilde{X}$
2. Compute $\hat{y} = \underbrace{\tilde{Z}}_{t \times k} \underbrace{v}_{k \times 1}$

Kernel Regression

Training:

1. Form inner products K from X.
2. Compute $\underbrace{u}_{n \times 1} = (K + \lambda I)^{-1} y$

Testing:

1. Form inner products $\tilde{K}$ from X and $\tilde{X}$

Non-parametric

2. Compute $\hat{y} = \underbrace{\tilde{K}}_{t \times n} \underbrace{u}_{n \times 1}$

(Everything you need to know about Z and $\tilde{Z}$ is contained within K and $\tilde{K}$)

Summary

- Multi-class SVMs measure violation of classification constraints.
- Softmax loss is a multi-class version of logistic loss.
- High-dimensional bases allows us to separate non-separable data.
- “Other” normal equations are faster when $n < d$.

- Next time: how do we train on all of Gmail?

Bonus Slide: Equivalent Form of Ridge Regression

Note that $\hat{X}$ and Y are the same on the left and right side, so we only need to show that

$$(X^T X + \lambda I)^{-1} X^T = X^T (X X^T + \lambda I)^{-1}. \tag{1}$$

A version of the matrix inversion lemma (Equation 4.107 in MLAPP) is

$$(E - F H^{-1} G)^{-1} F H^{-1} = E^{-1} F (H - G E^{-1} F)^{-1}.$$

Since matrix addition is commutative and multiplying by the identity matrix does nothing, we can re-write the left side of (1) as

$$(X^T X + \lambda I)^{-1} X^T = (\lambda I + X^T X)^{-1} X^T = (\lambda I + X^T I X)^{-1} X^T = (\lambda I - X^T(-I)X)^{-1} X^T = -(\lambda I - X^T(-I)X)^{-1} X^T(-I)$$

Now apply the matrix inversion with $E = \lambda I$ (so $E^{-1} = \left(\frac{1}{\lambda}\right) I$), $F = X^T$, $H = -I$ (so $H^{-1} = -I$ too), and $G = X$:

$$-(\lambda I - X^T(-I)X)^{-1} X^T(-I) = -(\frac{1}{\lambda}) I X^T (-I - X \left(\frac{1}{\lambda}\right) X^T)^{-1}.$$

Now use that $(1/\alpha)A^{-1} = (\alpha A)^{-1}$, to push the $(-1/\lambda)$ inside the sum as $-\lambda$,

$$-(\frac{1}{\lambda}) I X^T (-I - X \left(\frac{1}{\lambda}\right) X^T)^{-1} = X^T (\lambda I + X X^T)^{-1} = X^T (X X^T + \lambda I)^{-1}.$$