CPSC 340: Machine Learning and Data Mining

Kernel Methods

Fall 2016

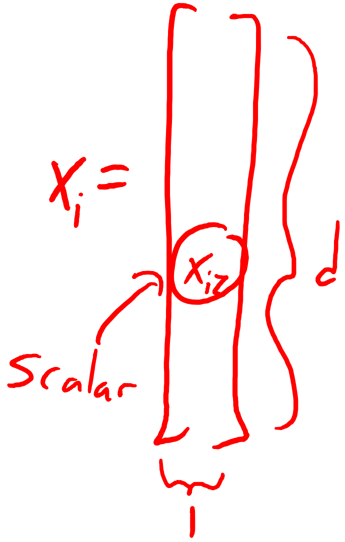
Admin

- Assignment 2:
  – Solution posted.
- Assignment 3:
  – Due Wednesday (before midnight anywhere on Earth).
  – Solutions released next Wednesday after class (last possible late class).
- Midterm on Friday October 28.
  – Midterm from last year and list of topics posted (covers Assignments 1-3)
  – In class, 55 minutes, closed-book, cheat sheet: 2-pages each double-sided.

Part 3 Review

- Focus of Part 3 is linear models:
  - Supervised learning where prediction is linear combination of features:

$$y_i = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id}$$
$$= w^T x_i$$



- Change of basis: replace features x_i with z_i:
  - Add a bias variable (feature that is always one).
  - Polynomial basis.
  - Radial basis functions (non-parametric basis).
- Regression:
  - Target y_i is numerical.
  - Testing whether (yhat == y_i) doesn't make sense.

Good fit that doesn't exactly pass through any point.

Part 3 Review

- Alternate error functions for regression:
  - Squared error: $$\frac{1}{2}\sum_{i=1}^{n}(w^Tx_i - y_i)^2 \quad \text{or} \quad \frac{1}{2}\|Xw - y\|^2$$
    - Can find optimal 'w' by solving linear system.
  - L_1-norm and L_∞-norm errors: $$\|Xw - y\|_1 \qquad \|Xw - y\|_\infty$$
    - More/less robust to outliers.
- L2-regularization:
  - Adding a penalty on the L2-norm of 'w' to decrease overfitting:

$$f(w) = \|Xw - y\|_1 + \frac{\lambda}{2}\|w\|^2$$

Part 3 Review

- Gradient descent:
  - Can we used to find a local minimum of a smooth function.
- L_1-norm and L_∞-norm errors are convex but non-smooth:
  - But we can smooth them using Huber and log-sum-exp functions.
- Convex functions:
  - Special functions where all local minima are global minima.
  - Simple rules for showing that a function is convex.

Last Time: Classification using Regression

- Binary classification using sign of linear models:

  Fit model $y_i = w^T x_i$ and predict using $\text{sign}(w^T x_i)$

  $y_i \to +1, -1$

- Problems with existing errors:
  - If $y_i = +1$ and $w^T x_i = +100$, then squared error $(w^T x_i - y_i)^2$ is huge.
  - Hard to minimize training error ("0-1 loss") in terms of 'w'.
- Motivates convex approximations to 0-1 loss:
  - Logistic loss (logistic regression): $\sum_{i=1}^{n} \log(1 + \exp(-y_i w^T x_i)) + \frac{\lambda}{2}\|w\|^2$
  - Hinge loss (support vector machine): $\sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\} + \frac{\lambda}{2}\|w\|^2$

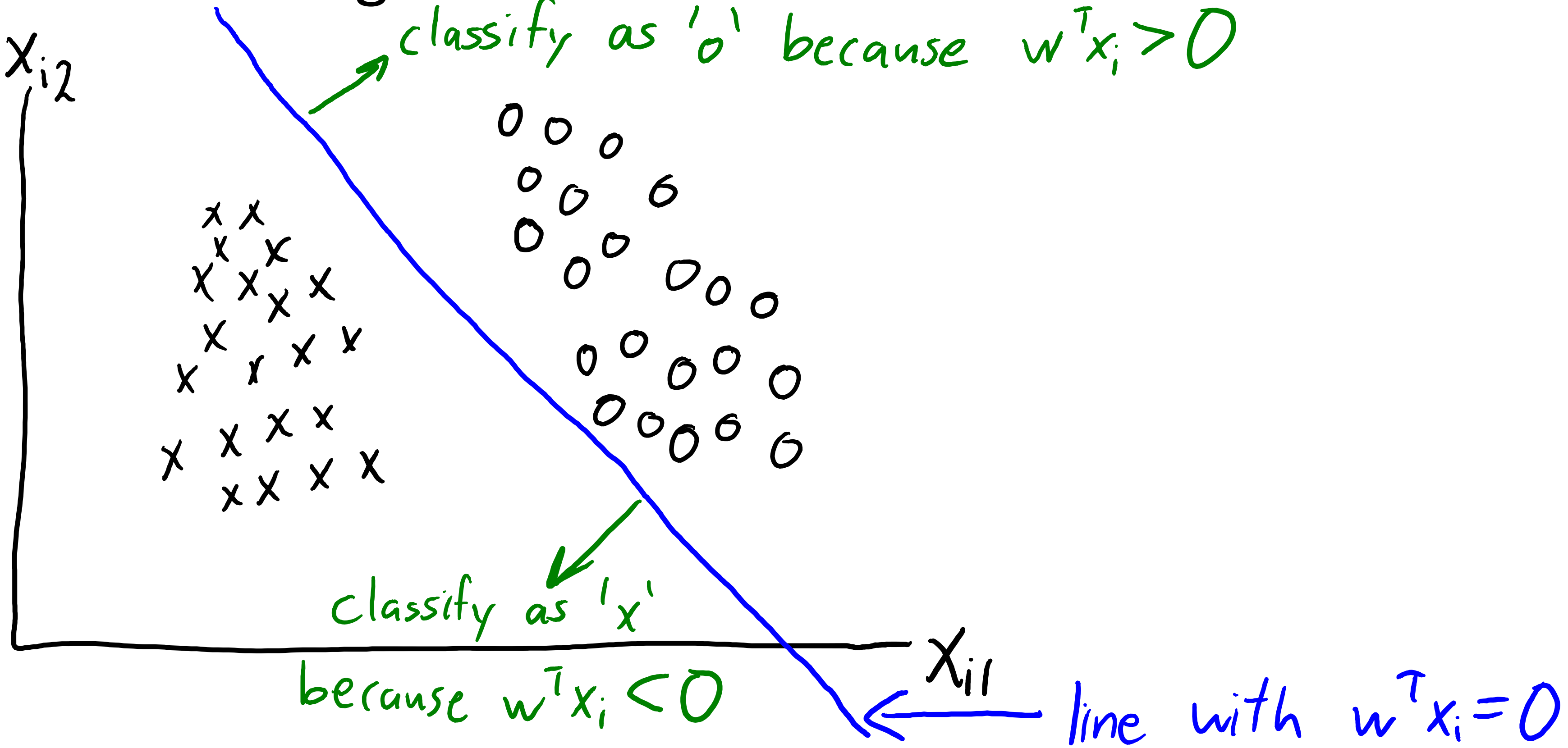
Last Time: Classification using Regression

- Can minimize smooth/convex logistic loss using gradient descent.
  - There are also efficient methods for support vector machines (SVMs).
- Logistic regression and SVMs are used EVERYWHERE!
  - Fast training and testing, weights w_j are easy to understand.
  - With high-dimensional features and regularization, often good test error.
    - Otherwise, often good test error with RBF basis and regularization.

- Some random questions you might be asking:
  - Can we use a polynomial basis with more than 1 feature?
  - Why didn't we do the "textbook" derivation of logistic/SVM?
  - How do we train on all of Gmail?
  - Did we miss feature selection?

2D View of Linear Classifiers

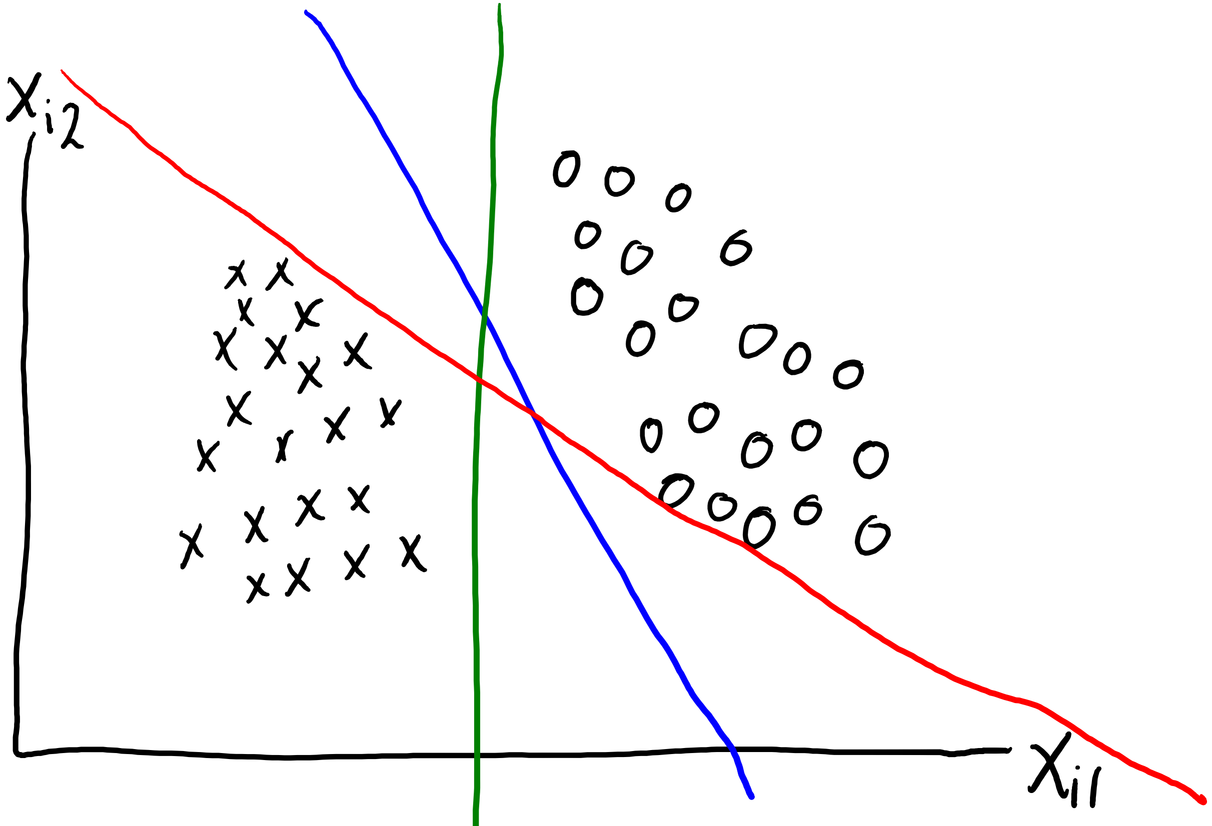
- 2D Visualization of linear regression for classification:



- “Linearly separable”: a perfect linear classifier exists.

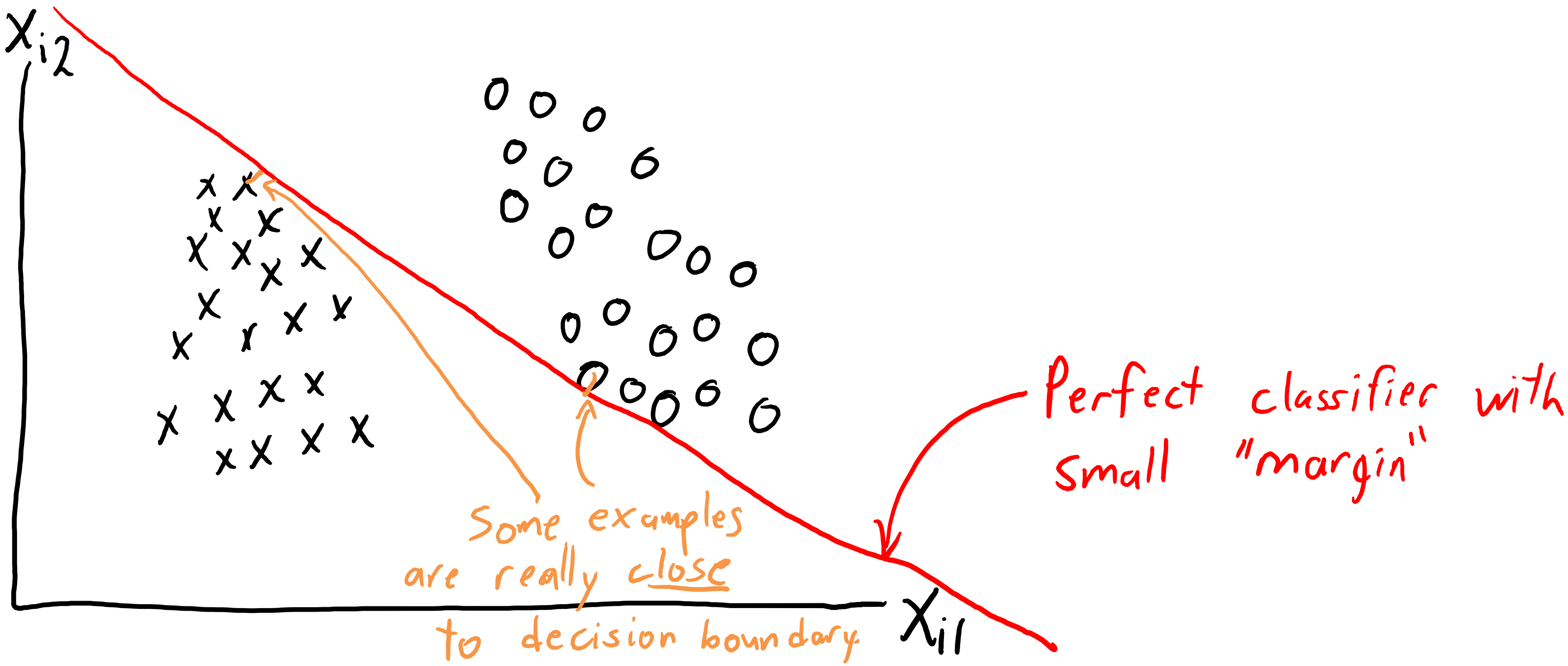
Maximum-Margin Classifier

- Consider a linearly-separable dataset.
  - "Perceptron" algorithm finds *some* classifier with zero error.
  - But are all zero-error classifiers equally good?



Maximum-Margin Classifier

- Consider a linearly-separable dataset.
  - Maximum-margin classifier: choose the farthest from both classes.



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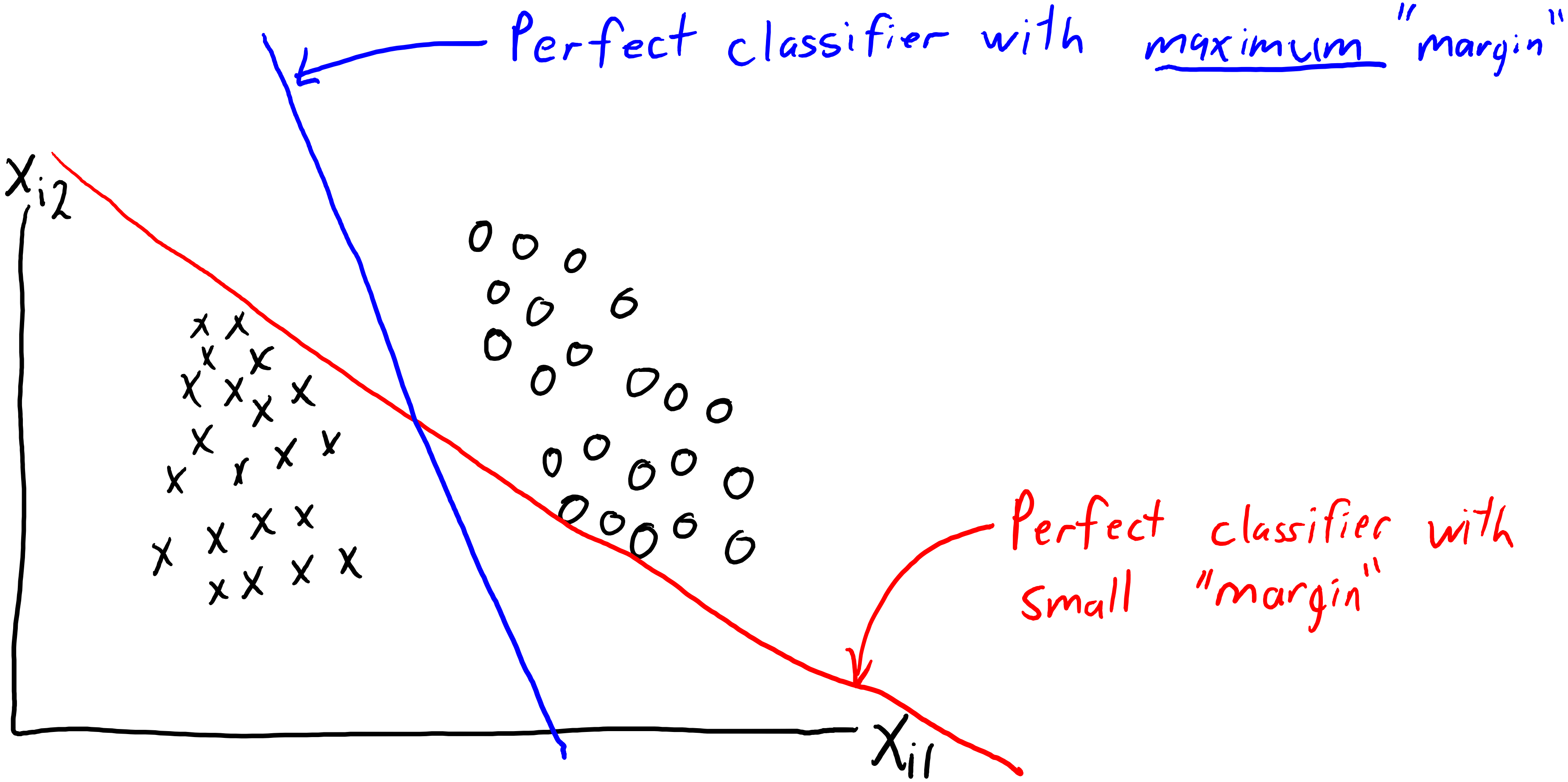

Maximum-Margin Classifier

- Consider a linearly-separable dataset.
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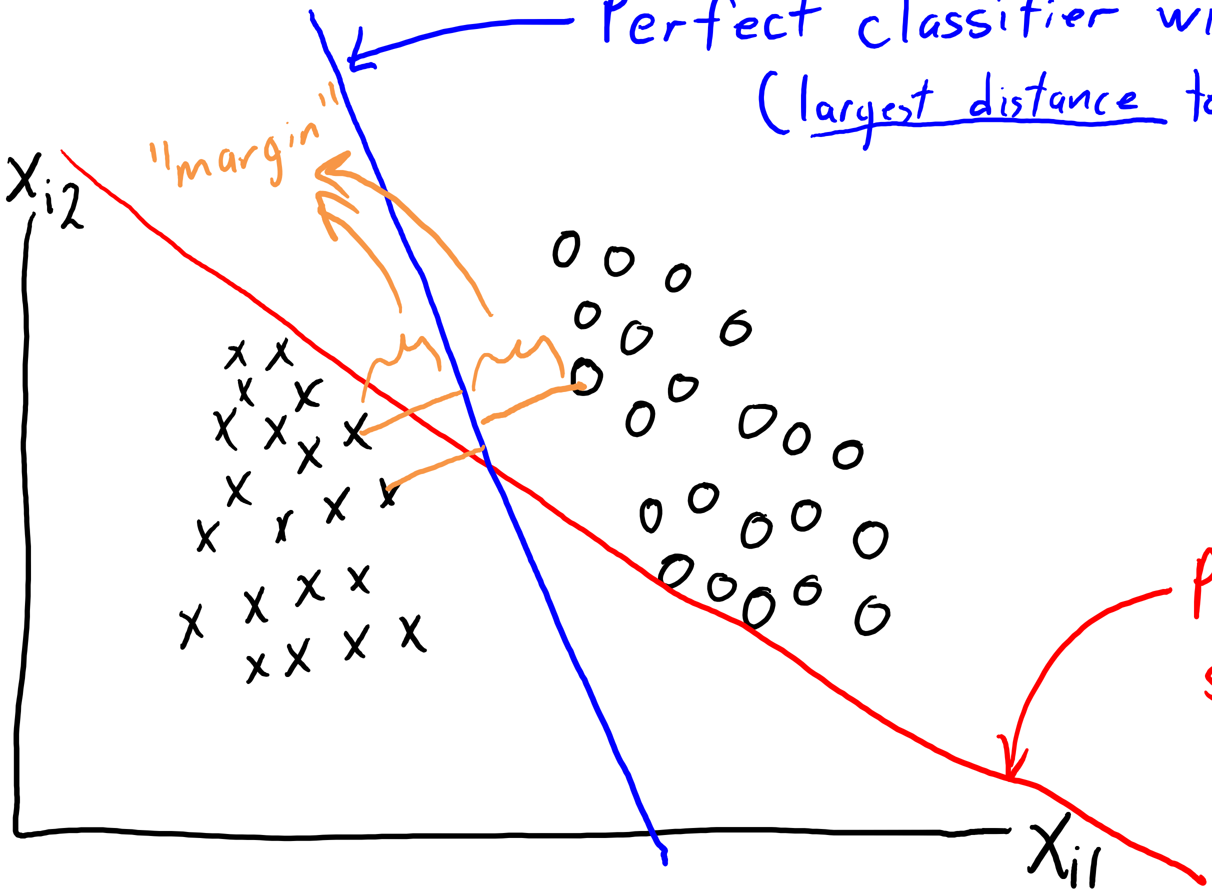
Why maximize margin?

If test is close to training data, then max margin leaves more "room" before we make an error.



Maximum-Margin Classifier

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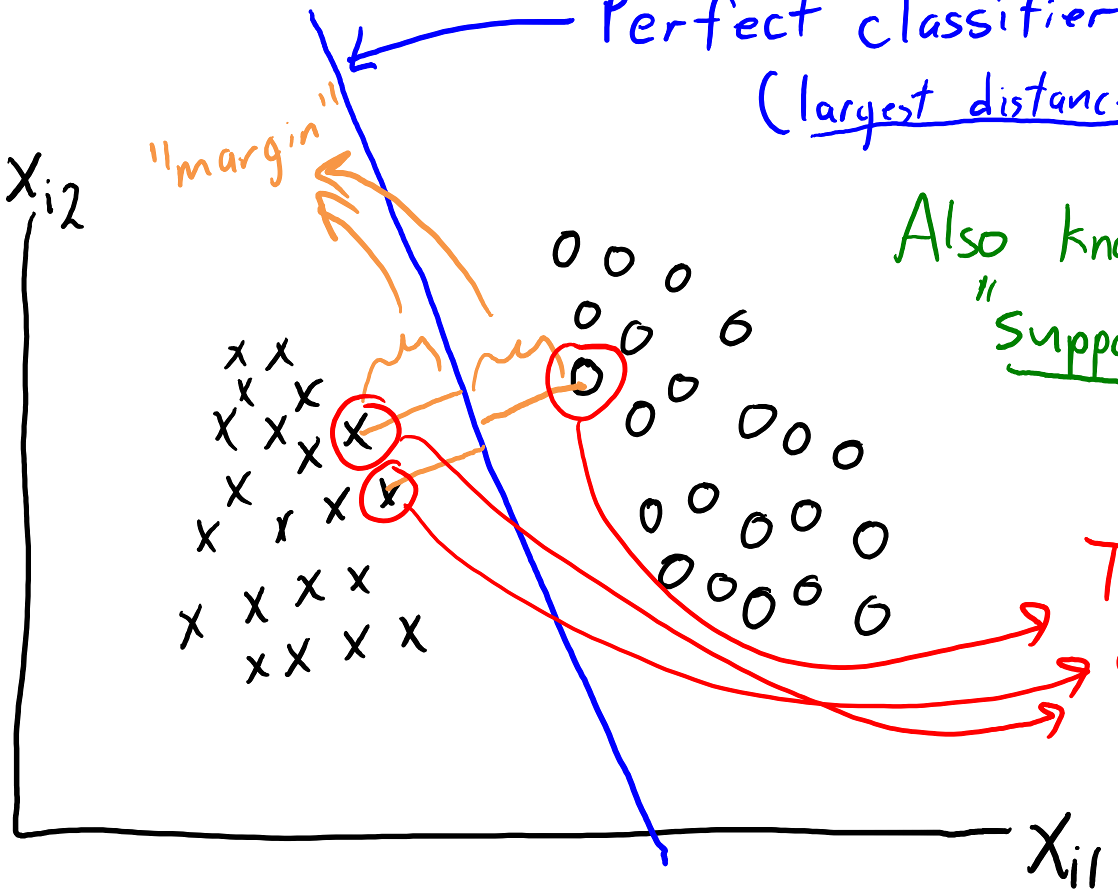
Perfect classifier with maximum "margin"
(largest distance to closest examples)

Also known as a "support vector machine"



The examples that are closest are called "support vectors"

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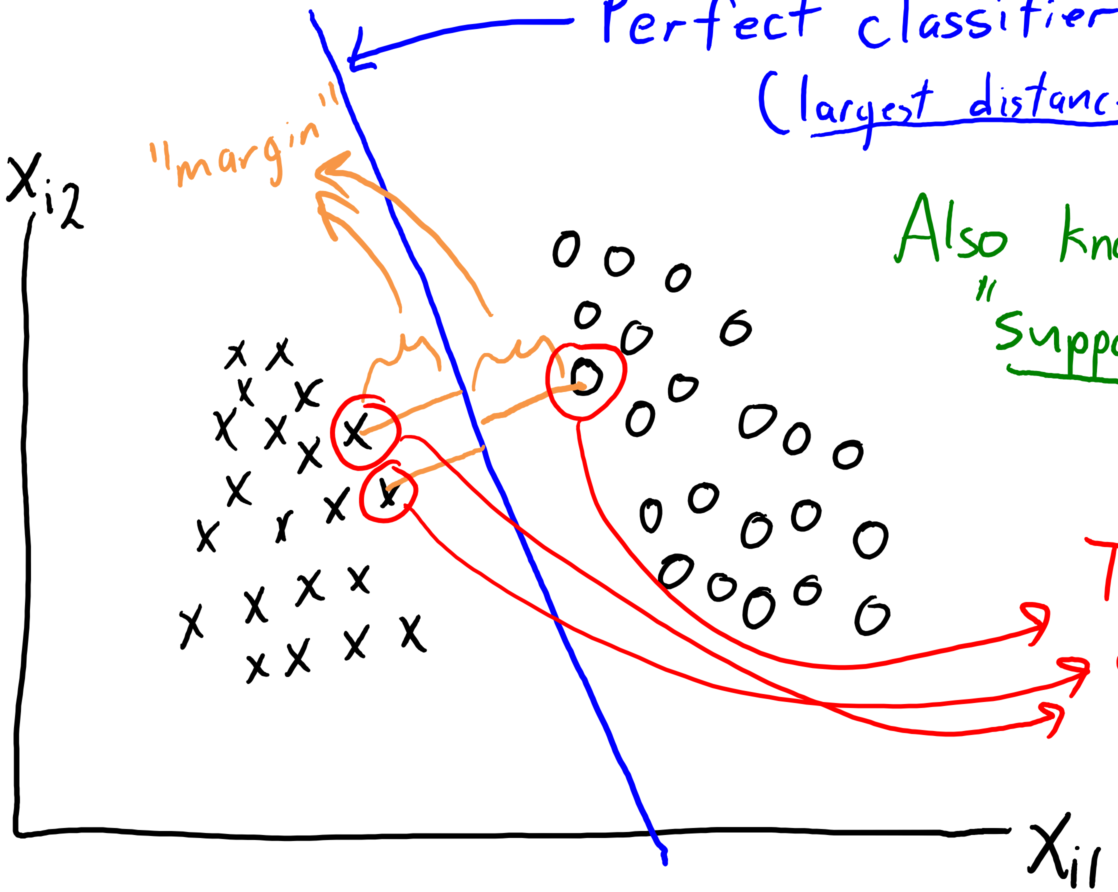

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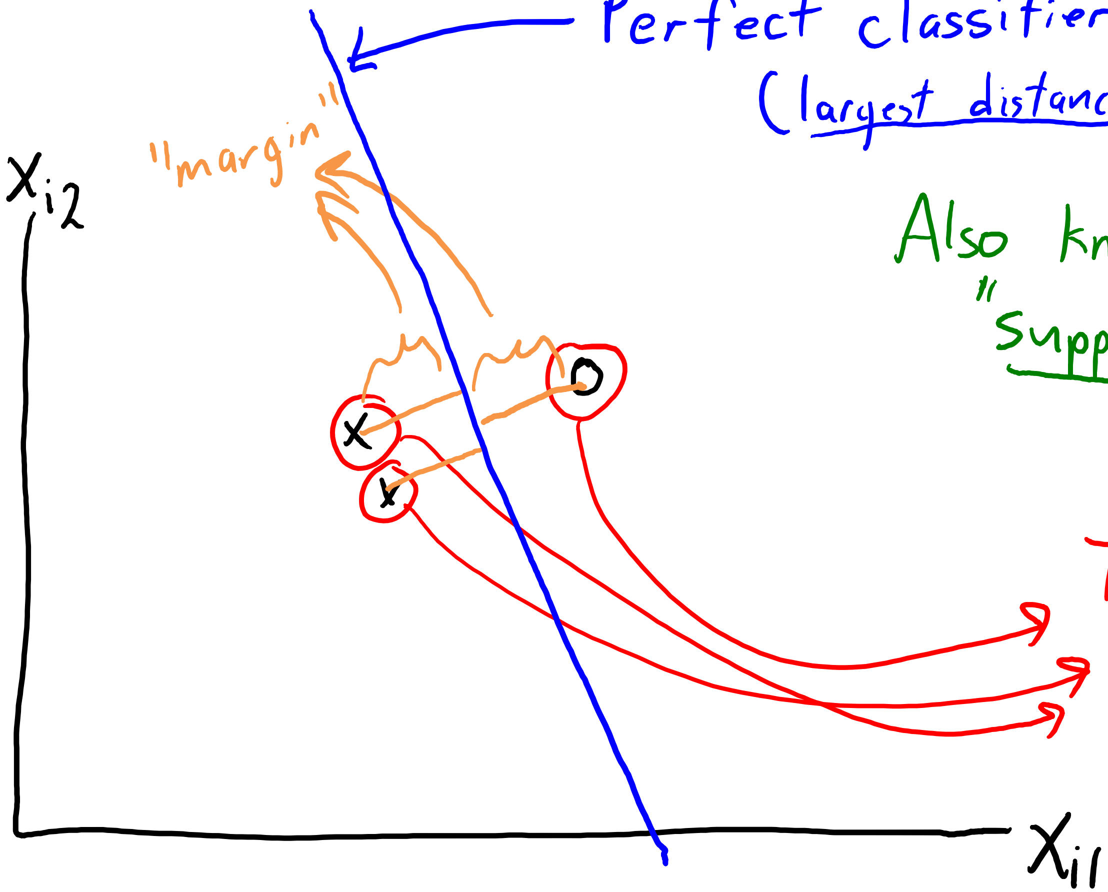

You could throw away the other examples and get the same classifier.

The examples that are closest are called "support vectors"

Support Vector Machines

- For linearly-separable data, support vector machine (SVM) minimizes:

$$f(w) = \frac{1}{2}\|w\|^2$$

  – Subject to the constraints that: (see Wikipedia or ML textbooks)

$$\left.\begin{aligned} w^T x_i &\geq 1 \quad \text{for } y_i = 1 \\ w^T x_i &\leq -1 \quad \text{for } y_i = -1 \end{aligned}\right\}$$

Or we can write both cases as

$$y_i w^T x_i \geq 1$$

- For non-separable data, try to minimize violation of constraints:

We want $y_i w^T x_i \geq 1$

or equivalently $0 \geq 1 - y_i w^T x_i$

Since we can't satisfy this for all 'i', let's add "slack" $\beta_i \geq 0$ to each constraint:

$$\beta_i \geq 1 - y_i w^T x_i$$

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- For non-separable data, we usually define SVMs as minimum of:

$$f(w) = \sum_{i=1}^{n} \underbrace{\max\{0, 1 - y_i w^T x_i\}} + \underbrace{\frac{\lambda}{2} \|w\|^2}$$

Hinge loss for example 'i':

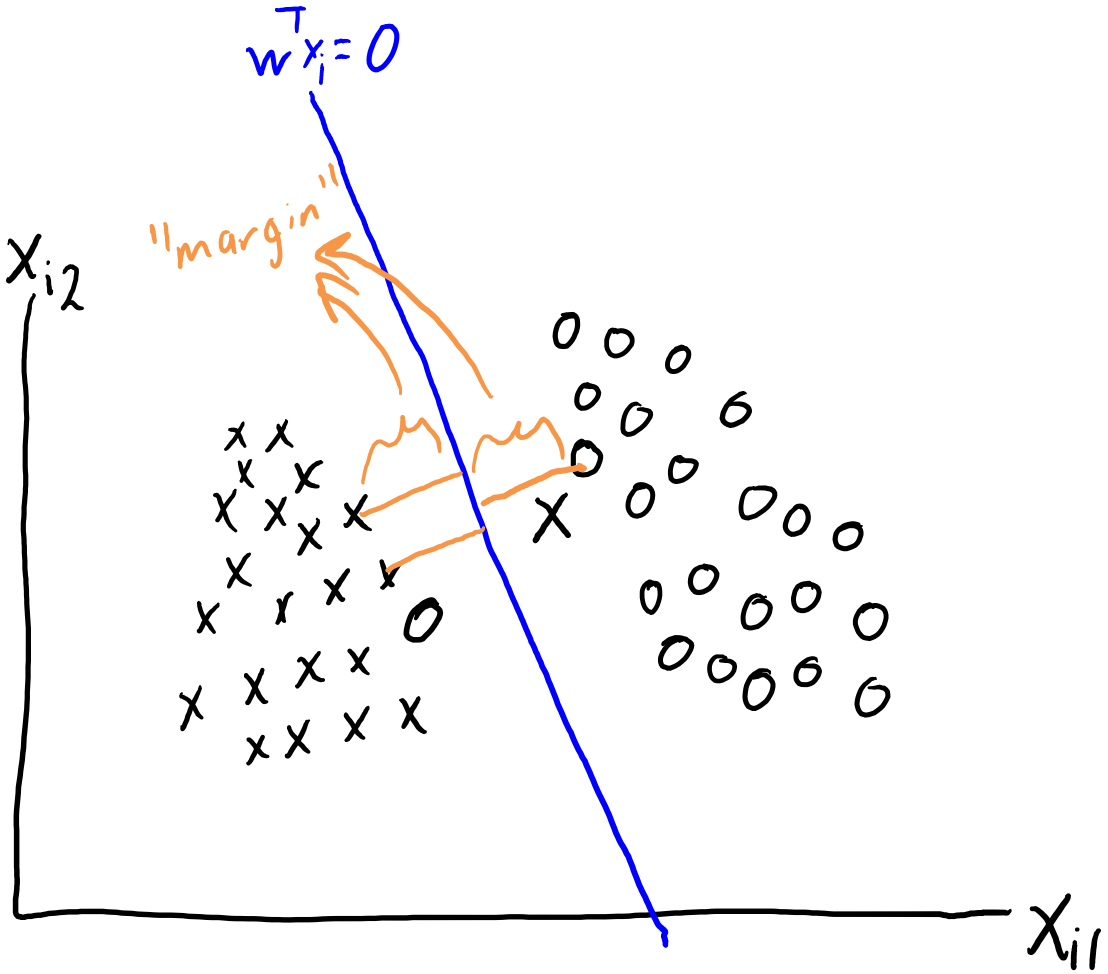
it's the amount we violate $y_i w^T x_i \geq 1$

"slack"

Original SVM objective: encourages large margin.

Support Vector Machines for Non-Separable

- Non-separable case:



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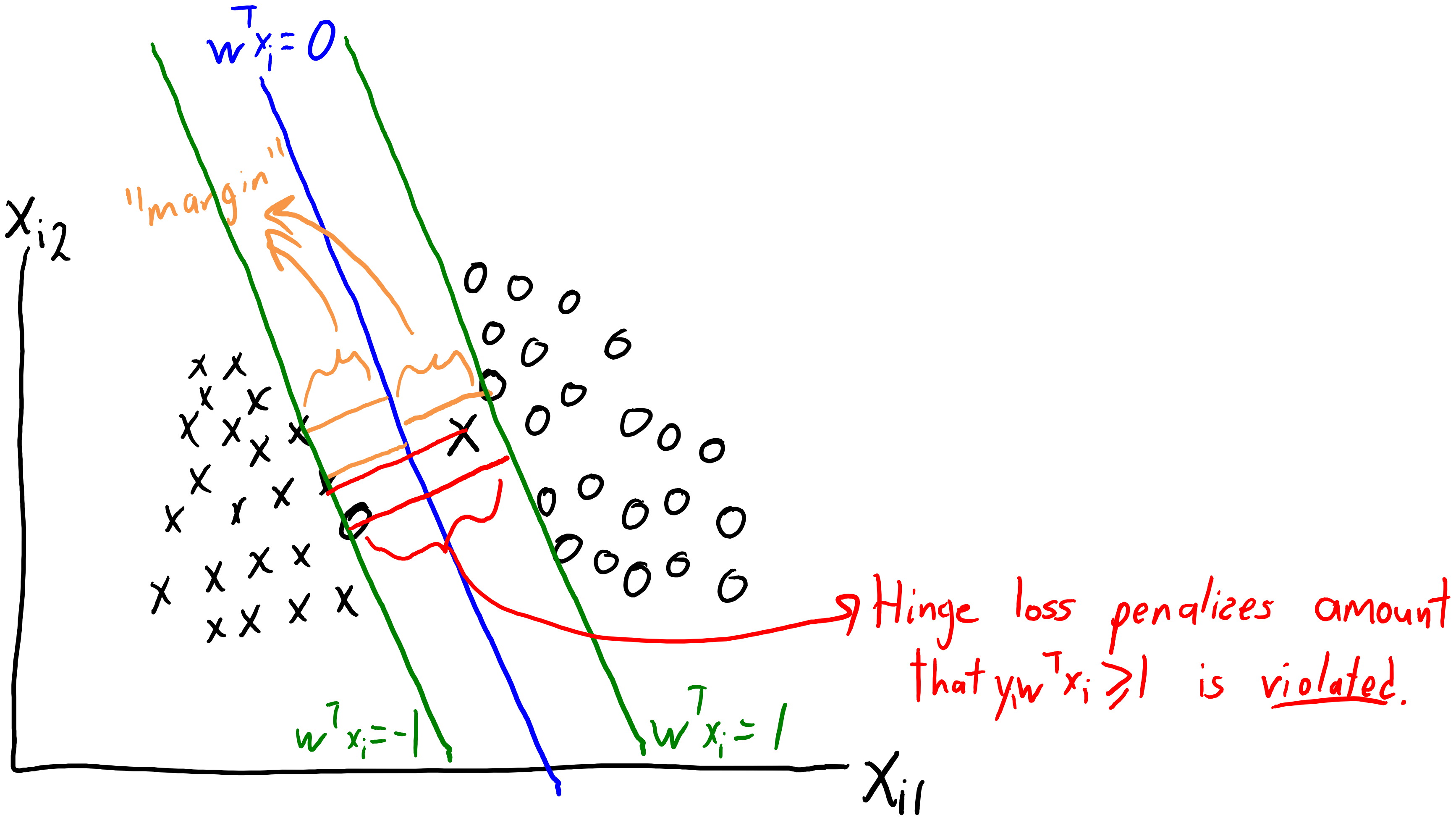

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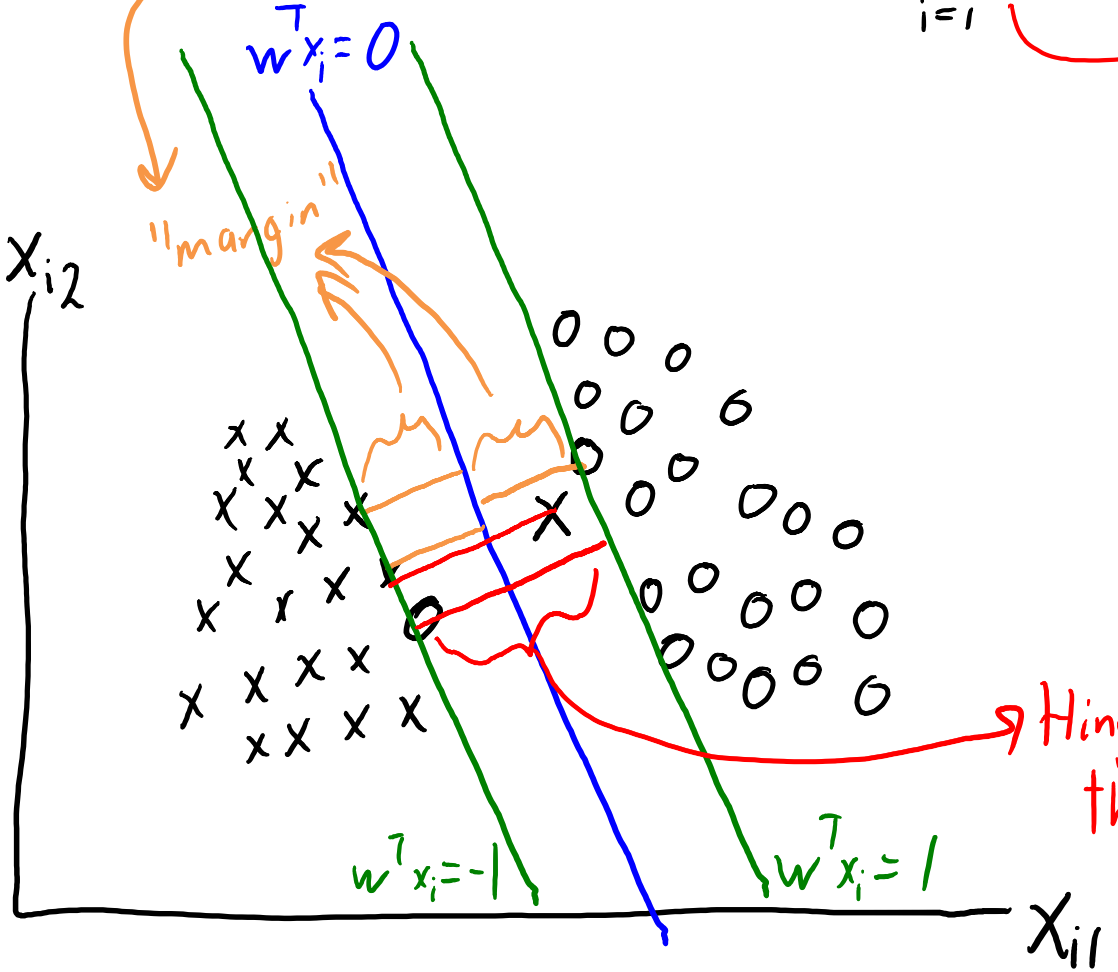
$$f(w) = \underbrace{\sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\}} + \frac{\lambda}{2}\|w\|^2$$

Logistic regression can be viewed as smooth approximation to SVMs.

But, no concept of "support vectors" with logistic loss.



λ controls trade-off between having large margin and classifying examples correctly.

Hinge loss penalizes amount that $y_i w^T x_i \geq 1$ is violated.

Support Vector Machines for Non-Separable

- Non-separable case:

$$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\} + \frac{\lambda}{2}\|w\|^2$$

Support vectors are examples 'i' where $1 - y_i w^T x_i \geq 0$

Hinge loss penalizes amount that $y_i w^T x_i \geq 1$ is violated.

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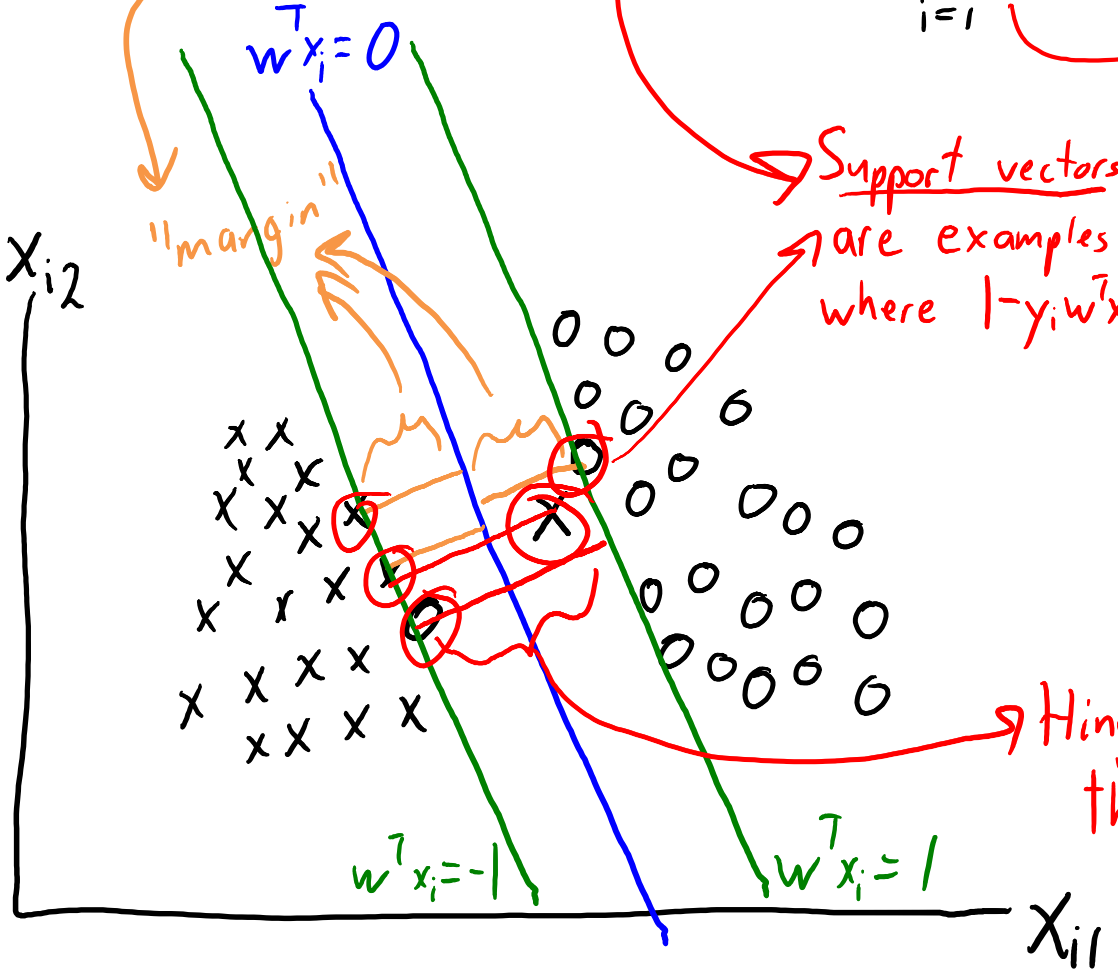

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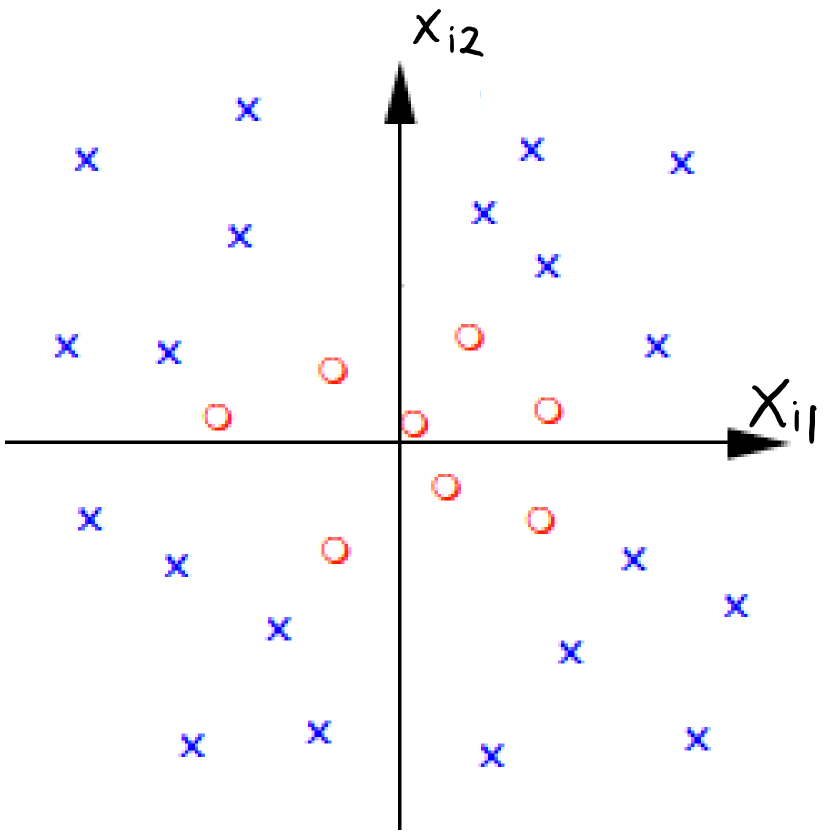
Support Vector Machines for Non-Separable

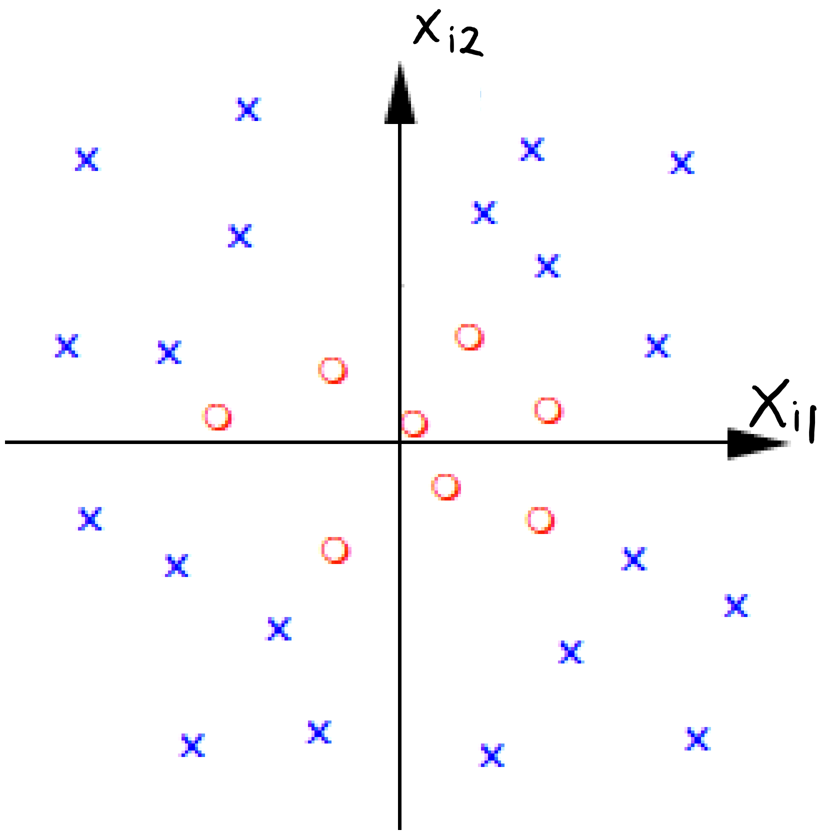
- What about data that is not even close to separable?

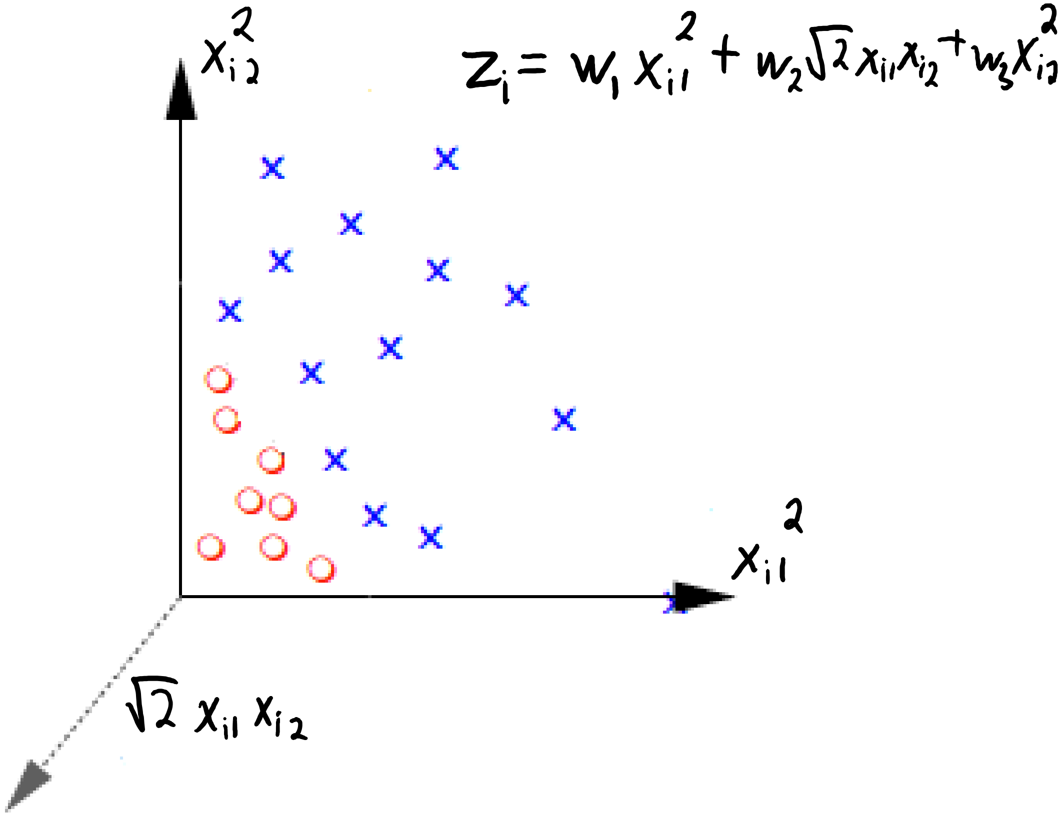


http://math.stackexchange.com/questions/353607/how-do-inner-product-space-determine-half-planes

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).





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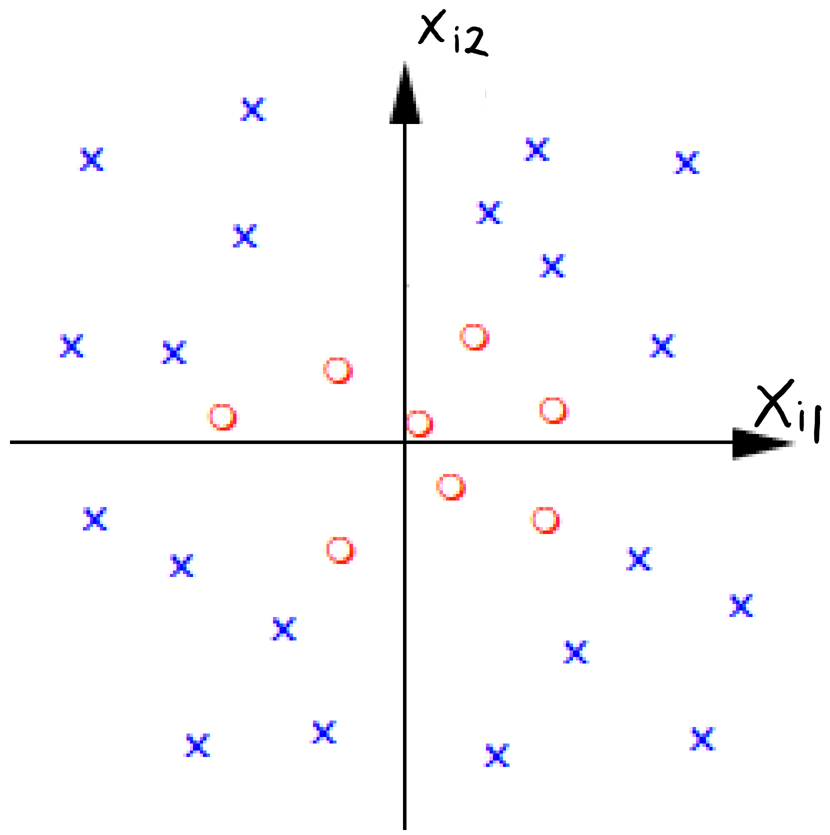

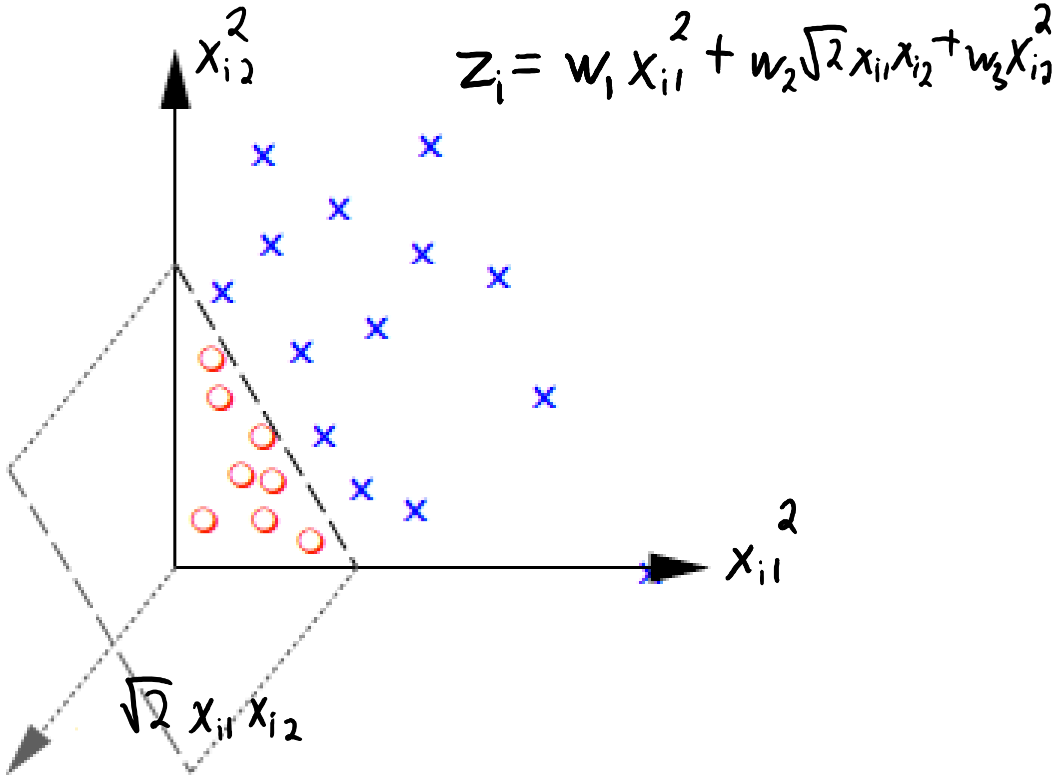

Multi-Dimensional Polynomial Basis

- Recall fitting polynomials when we only have 1 feature:

$$y_i = w_0 + w_1 x_i + w_2 x_i^2$$

- 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

- Approach 1: use polynomial basis for each variable.

$$X = \begin{bmatrix} 0.2 & 0.3 \\ 1 & 0.5 \\ -0.5 & -0.1 \end{bmatrix} \longrightarrow Z = \begin{bmatrix} \underbrace{\begin{matrix} 1 \\ 1 \\ 1 \end{matrix}}_{\text{bias}} & \underbrace{\begin{matrix} 0.2 & (0.2)^2 \\ 1 & (1)^2 \\ 0.5 & (0.5)^2 \end{matrix}}_{\text{quadratic function of } x_{i1}} & \underbrace{\begin{matrix} 0.3 & (0.3)^2 \\ 0.5 & (0.5)^2 \\ -0.1 & (-0.1)^2 \end{matrix}}_{\text{quadratic function of } x_{i2}} \end{bmatrix}$$

- But this is restrictive:
  - We should allow terms like '$x_{i1}x_{i2}$' that depend on feature interaction.
  - But number of terms in X_{poly} is huge:
    - Degree-5 polynomial basis has $O(d^5)$ terms:

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

- If reasonable 'n', we can do this efficiently using the kernel trick.

Equivalent Form of Ridge Regression

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

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

- We showed that the solution is given by:

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

- Using a "matrix inversion lemma" we can re-write this as:

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

- This is faster if n << d:
  - Z^TZ is 'd' by 'd' while ZZ^T is 'n' by 'n'.

Predictions using Equivalent Form

- Given test data $\hat{X}$, predict $\hat{y}$ by forming and $\hat{Z}$ using:

$$\hat{y} = \hat{Z}w \leftarrow w = Z^T(ZZ^T + \lambda I)^{-1}y$$

$$= \underbrace{\hat{Z}Z^T}_{\hat{K}}(\underbrace{ZZ^T}_{K} + \lambda I)^{-1}y$$

$$= \hat{K}(K + \lambda I)^{-1}y$$

- Key observation behind kernel trick:
  - Predictions $\hat{y}$ only depend on features through K and $\hat{K}$.
  - If we have function that computes K and $\hat{K}$, we don't need the features.

Gram Matrix

- The Gram matrix 'K' is defined by:

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

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

- 'K' contains the inner products between all training examples.

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- 'K' contains the inner products between all training examples.
- '$\hat{K}$' contains the inner products between training and test examples.
- Kernel trick:
  - I want to use a basis z_i that is too huge to store.
  - But I only need z_i to compute $K = ZZ^T$ and $\hat{K} = \hat{Z}Z^T$.
  - I can use this basis if I have a kernel function that computes $k(x_i,x_j) = z_i^T z_j$.

Polynomial Kernel

- Consider two examples x_i and x_j for a 2-dimensional dataset:

$$x_i = (x_{i1}, x_{i2}) \qquad x_j = (x_{j1}, x_{j2})$$

- And consider a particular degree-2 basis:

$$z_i = (x_{i1}^2, \sqrt{2}\, x_{i1}x_{i2}, x_{i2}^2) \qquad z_j = (x_{j1}^2, \sqrt{2}\, x_{j1}x_{j2}, x_{j2}^2)$$

- We can compute inner product $z_i^T z_j$ without forming z_i and z_j:

$$z_i^T z_j = x_{i1}^2 x_{j1}^2 + (\sqrt{2}\, x_{i1} x_{i2})(\sqrt{2}\, x_{j1} x_{j2}) + x_{i2}^2 x_{j2}^2$$

$$= x_{i1}^2 x_{j1}^2 + 2 x_{i1} x_{i2} x_{j1} x_{j2} + x_{i1}^2 x_{i2}^2$$

$$= (\underbrace{x_{i1} x_{j1} + x_{i2} x_{j2}}_{x_i^T x_j})^2 \qquad \text{"completing the square"}$$

$$= (x_i^T x_j)^2 \leftarrow \text{No } \underline{\text{need}} \text{ for } z_i \text{ to compute } z_i^T z_j$$

Summary

- Support vector machines maximize margin to nearest data points.
- High-dimensional bases allows us to separate non-separable data.
- Kernel trick allows us to use high-dimensional bases efficiently.

- Next time:
  - How could we train on all of Gmail?