Machine Learning: Chenhao Tan

University of Colorado Boulder

LECTURE 16

Slides adapted from Jordan Boyd-Graber, Chris Ketelsen

Logistics

- Homework 3 is due on Sunday!

Overview

A little bit of history

Linear classifiers and margin

Hard-margin SVM
- Formulation
- Theoretical Guarantees

Outline

Outline of CSCI 4622

We've already covered stuff in blue!

- Problem formulations: classification, regression
- Supervised techniques: decision trees, nearest neighbors, perceptron, linear models, neural networks, support vector machine, kernel methods
- Unsupervised techniques: clustering, linear dimensionality reduction
- "Meta-techniques": ensembles, expectation-maximization
- Understanding ML: limits of learning, practical issues, bias & fairness
- Recurring themes: (stochastic) gradient descent

History lesson

- 1962: Rosenblatt, Principles of Neurodynamics: Perceptrons and the Theory of Brain Mechanisms
  - First neuron-based learning algorithm
  - “Could learning anything that you could program”

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  - First neuron-based learning algorithm
  - “Could learning anything that you could program”
- 1969: Minsky & Papert, Perceptron: An Introduction to Computational Geometry
  - First real complexity analysis
  - Showed, in principle, many things that perceptrons can’t learn to do
  - Shut down any interest in neural networks

History lesson

- 1986: Rumelhart, Hinton & Williams, Back Propagation
  - Overcame many difficulties raised by Minsky et al.
  - Neural networks wildly popular again (for a while)

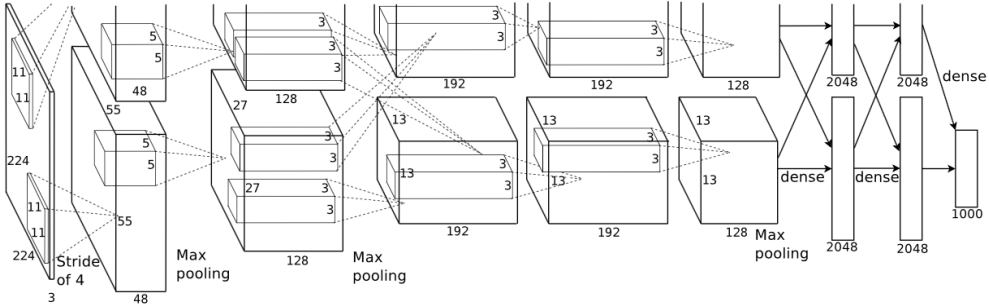
History lesson

- 1999-2005
  - Shift to Bayesian Methods
    - Best ideas from neural networks
    - Direct statistical computing
  - Support Vector Machines
    - Nice mathematical properties
    - Kernel tricks
  - A few people still playing with NNs
    - Bengio
    - Hinton
    - LeCun

History lesson

- 2005-2010
  - Core group continues to make improvements
  - Various tricks to make NNs practical
- 2010-present
  - BOOM!

AlexNet



Krizhevsky et al. [2012]

History lesson

Question: Why? What made neural networks amazing again?

- Massive datasets
- Computing power
- Algorithmic improvements

History lesson

Machine learning has a short history, but seems cyclic.
What is next?

Outline

Linear classifiers

We have already seen several:

- Logistic regression
- Perceptron

Definition: A linear classifier makes decisions by computing a linear combination of features of the form $\boldsymbol{w}^T\boldsymbol{x} + b$ and then classifies based on

$$\boldsymbol{w}^T\boldsymbol{x} + b \geq 0.$$

The decision boundary between the two classes is defined by $\boldsymbol{w}^T\boldsymbol{x} + b = 0$.

We estimate the weights and bias using the training data.

A linear classifier in 1D

- A linear classifier in 1D is a point x described by the equation $\boldsymbol{w}_1\boldsymbol{x}_1 = -b$.

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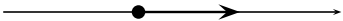

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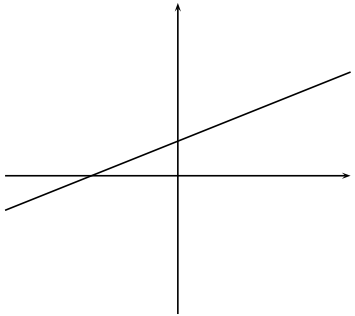
A linear classifier in 2D



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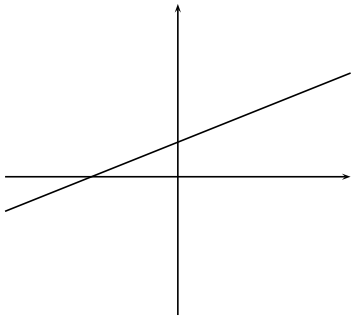

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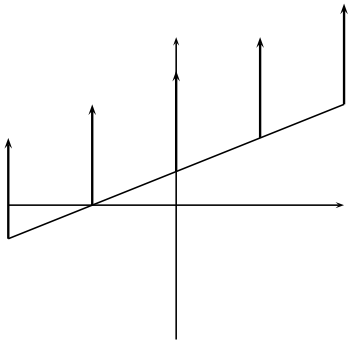

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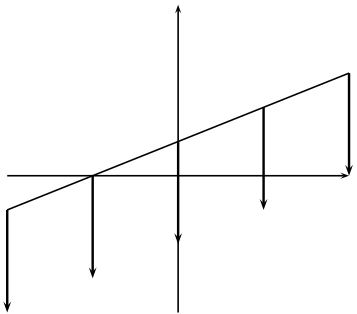

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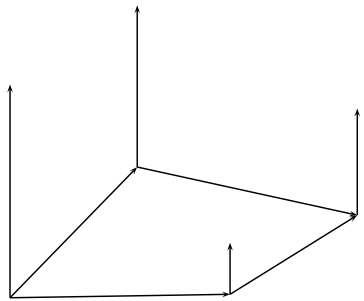
A linear classifier in 3D



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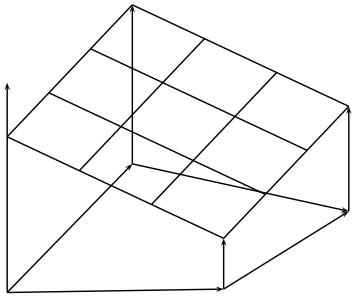

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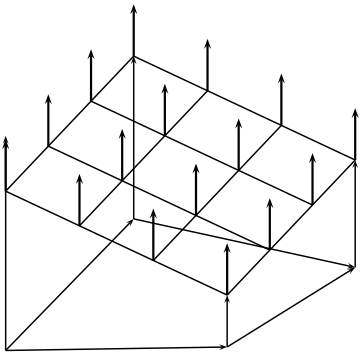

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- Points $(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ with $\boldsymbol{w}_1\boldsymbol{x}_1 + \boldsymbol{w}_2\boldsymbol{x}_2 + \boldsymbol{w}_3\boldsymbol{x}_3 \geq -b$ are in the class c.

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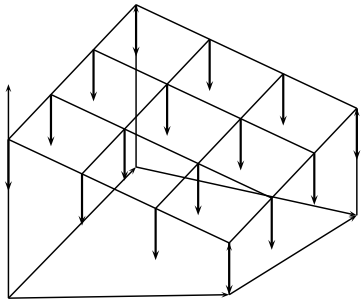

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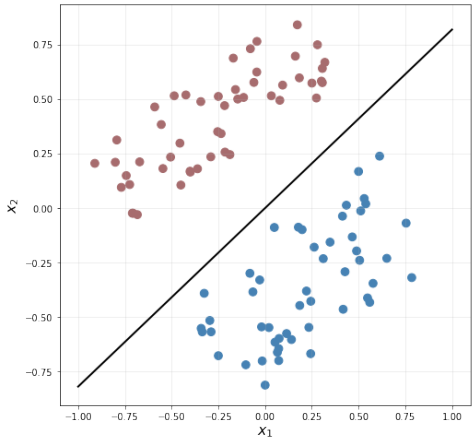
Pictorial definition of margin

Assuming that the dataset is separable, margin is defined as the smallest distance from any data point to the decision boundary.



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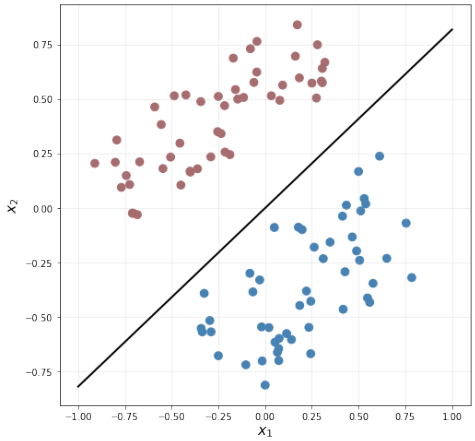
What is the margin of the classifier on the right?



Outline

Which hyperplane?

- For linearly separable training sets: there are **infinitely** many separating hyperplanes.
- They all separate the training set perfectly . . .
- . . . but they behave differently on test data.
- Error rates on new data are low for some, high for others.
- How do we find a low-error separator?

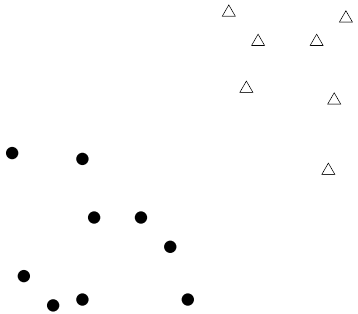
Support vector machines

SVMs: A kind of large-margin classifier

Find a decision boundary between two classes that is maximally far from any point in the training data (possibly discounting some points as outliers or noise).

Support Vector Machines

- 2-class training data



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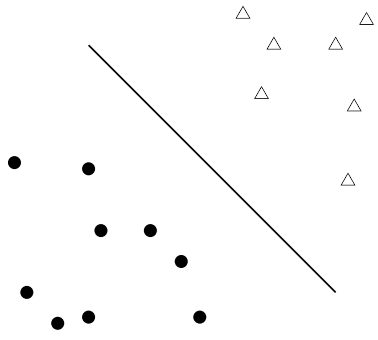

Support Vector Machines

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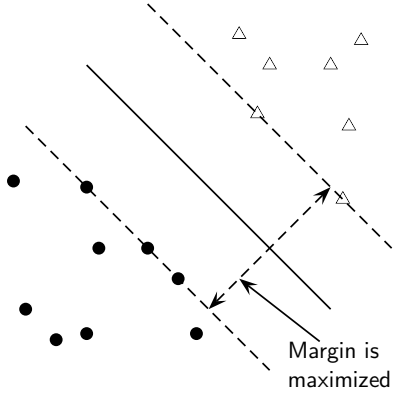
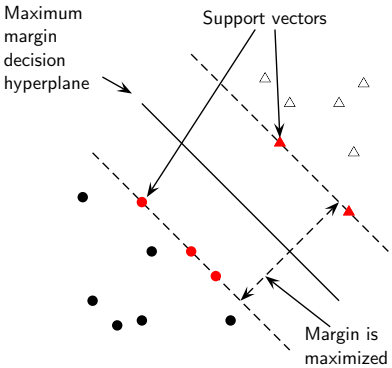
- criterion: being maximally far away from any data point → determines classifier **margin**



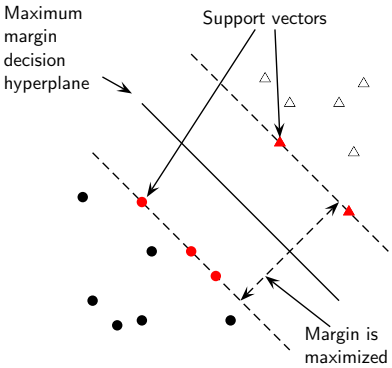
Support Vector Machines

- 2-class training data
- decision boundary $\rightarrow$ **linear separator**
- criterion: being maximally far away from any data point $\rightarrow$ determines classifier **margin**
- linear separator position defined by **support vectors**
- other points have no impact on the decision boundary



Why maximize the margin?

- Points near decision surface $\rightarrow$ uncertain classification decisions
- A classifier with a large margin is always confident
- Gives classification safety margin (measurement or variation)
- Increased ability to correctly generalize to test data



Equation

- Equation of a hyperplane

$$\boldsymbol{w} \cdot \boldsymbol{x} + b = 0$$

- Distance of a point to hyperplane

$$\frac{|\boldsymbol{w} \cdot \boldsymbol{x} + b|}{||\boldsymbol{w}||}$$

- The margin ρ is given by

$$\rho \equiv \min_{(\boldsymbol{x},y) \in S} \frac{|\boldsymbol{w} \cdot \boldsymbol{x} + b|}{||\boldsymbol{w}||} \equiv \frac{1}{||\boldsymbol{w}||}$$

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This is because for any point on the marginal hyperplane, we can let $|\boldsymbol{w} \cdot x + b| = 1$, and we would like to maximize the margin ρ.

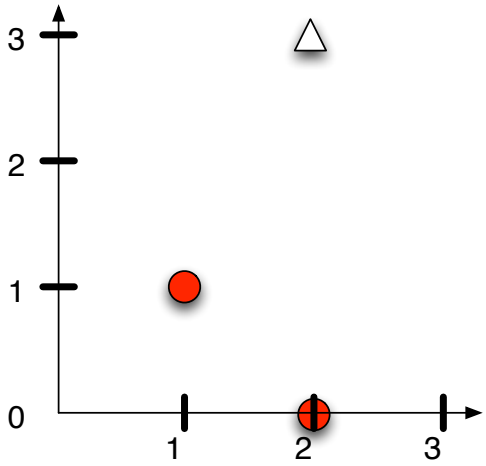
Optimization Problem

We want to find a weight vector $\boldsymbol{w}$ and bias b that optimize

$$\min_{\boldsymbol{w},b} \frac{1}{2}||\boldsymbol{w}||^2$$

subject to $y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) \geq 1, \forall \boldsymbol{i} \in [1, n]$.

Find the maximum margin hyperplane



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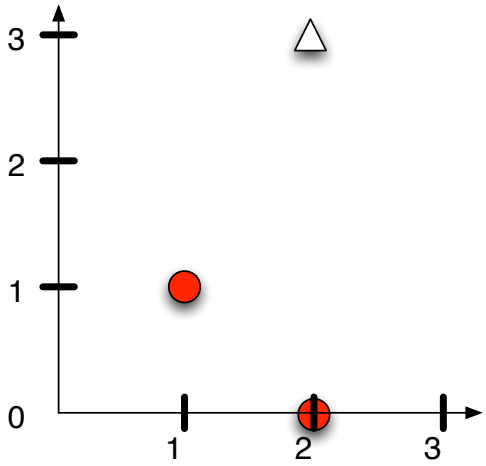

Which are the support vectors?

Walk through example: building an SVM over the data shown

Working geometrically:

- Set up system of equations

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Working geometrically:

- Set up system of equations

$$
\begin{aligned}
w_1 + w_2 + b &= -1 \\
\frac{3}{2} w_1 + 2 w_2 + b &= 0 \\
2 w_1 + 3 w_2 + b &= +1
\end{aligned}
$$

Walk through example: building an SVM over the data shown

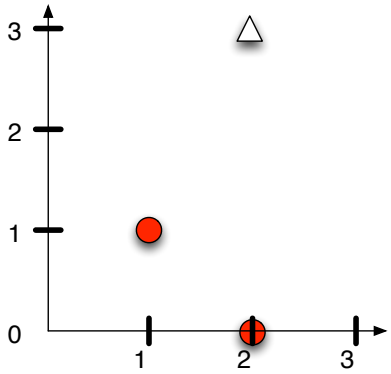
Working geometrically:

- Set up system of equations

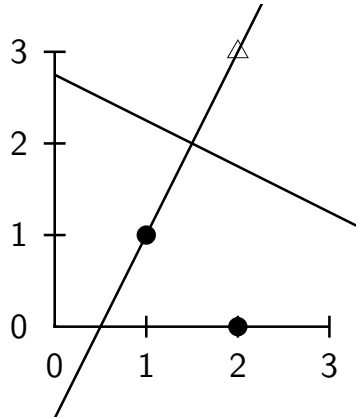
$$w_1 + w_2 + b = -1$$
$$\frac{3}{2}w_1 + 2w_2 + b = 0$$
$$2w_1 + 3w_2 + b = +1$$

The SVM decision boundary is:

$$0 = \frac{2}{5}x + \frac{4}{5}y - \frac{11}{5}$$



Canonical form



$$w_1 x_1 + w_2 x_2 + b = 0$$

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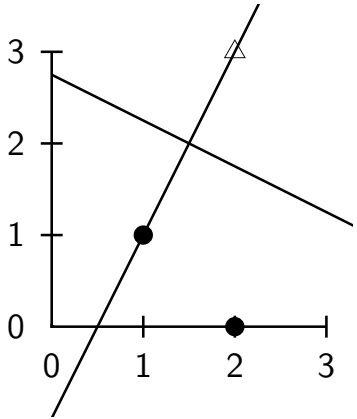

$$.4x_1 + .8x_2 - 2.2 = 0$$

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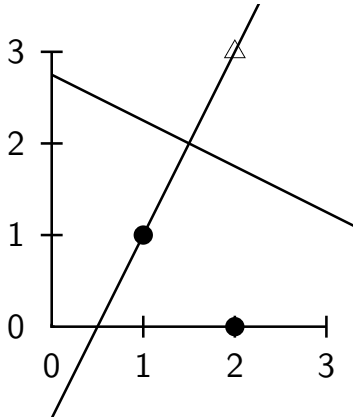

$.4x_1 + .8x_2 - 2.2 = 0$

- $.4 \cdot 1 + .8 \cdot 1 - 2.2 = -1$
- $.4 \cdot \frac{3}{2} + .8 \cdot 2 - 2.2 = 0$
- $.4 \cdot 2 + .8 \cdot 3 - 2.2 = +1$

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- Distance to closest point

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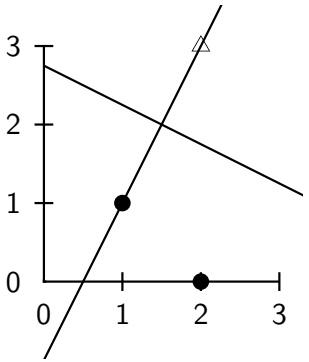
$$\frac{1}{||w||}=\frac{1}{\sqrt{\left(\frac{2}{5}\right)^2+\left(\frac{4}{5}\right)^2}}=\frac{1}{\sqrt{\frac{20}{25}}}=\frac{5}{\sqrt{5}\sqrt{4}}=\frac{\sqrt{5}}{2}$$



$$\frac{2}{5}x+\frac{4}{5}y-\frac{11}{5}=0$$

Theoretical evidence that suggests SVMs will Work

- Leave-one-out error

Leave One Out Error (sketch)

Leave one out error is the error by using one point as your test set (averaged over all such points).

$$\hat{R}_{LOO} = \frac{1}{m} \sum_{i=1}^{m} \mathbb{1} \left[h_{s-\{x_i\}} \neq y_i \right] \tag{1}$$

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This serves as an unbiased estimate of generalization error for samples of size $m - 1$:

Leave One Out Error (sketch)

Leave-one-out error is bounded by the number of support vectors.

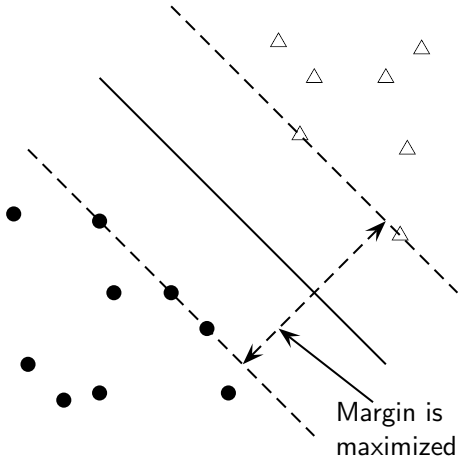
$$\mathbb{E}_{S\sim D^{m-1}}\left[R(h_s)\right] \leq \mathbb{E}_{S\sim D^m}\left[\frac{N_{SV}(S)}{m}\right] \tag{2}$$

Consider the held out error for x_i.

- If x_i was not a support vector, the answer doesn't change.
- If x_i was a support vector, it could change the answer; this is when we can have an error.

There are N_{SV} support vectors and thus N_{SV} possible errors.

Pictorial proof



References

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. ImageNet Classification with Deep Convolutional Neural Networks. In *Proceedings of the 25th International Conference on Neural Information Processing Systems*, 2012.