Machine Learning (CS 181): 10. Max-Margin Methods

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Spring 2017

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Credit

Credit: A. Zisserman (Oxford) for slides throughout this deck.

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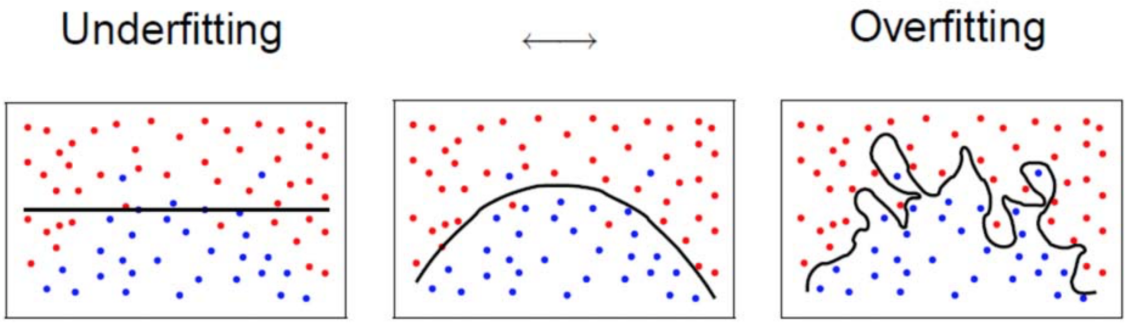
Goal: Good Generalization Performance

Minimize expected 0/1 classification error on unseen data.



Work with discriminant-based classifiers:

$$\hat{y} = \begin{cases} 1 & \text{if } h(\mathbf{x}; \mathbf{w}, w_0) > 0 \\ \text{-1} & \text{o.w.} \end{cases}$$

Neural Networks: Review

Learn non-linear function $h(\mathbf{x}; \mathbf{w}, w_0, \mathbf{W}^1, \mathbf{w}_0^1)$. If $h > 0$, predict $+1$ else predict -1.

- Adaptive basis functions through optimization of weights, use of non-linear activations.
- Outstanding performance on many problems.
- Some drawbacks:
  - Non-convex (dragons!)... can use stochastic gradient descent, but not well understood and long training time
  - Adding domain knowledge is an art
  - Hard to interpret, complex representation

Max-margin methods

Learn function $h(\mathbf{x}; \mathbf{w}, w_0)$ (non-linear when used together with basis functions). If $h(\mathbf{x}; \mathbf{w}, w_0) > 0$, predict $+1$ else predict -1.

- Convex. Can train via gradient descent (or other standard methods), will find global minimum.
- Coherent theory ("max margin")
- Can readily engineer new basis functions ("kernel engineering")
- Can obtain a succinct representation (thus, relatively interpretable.)
- The best performance

Max-margin methods

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- Coherent theory ("max margin")
- Can readily engineer new basis functions ("kernel engineering")
- Can obtain a succinct representation (thus, relatively interpretable.)
- ~~The best performance~~ Very good performance (!)

Applications of SVMs

- Face and object recognition $\leftarrow \leftarrow \leftarrow \leftarrow \leftarrow \leftarrow \leftarrow$ see this later
- Predicting a cancer type from cell samples
- Fake news characterization
- Predict the function of proteins

Especially suited to problems with non-linear interactions between features because handle basis functions very nicely (next lecture!).

Review: Binary Classification

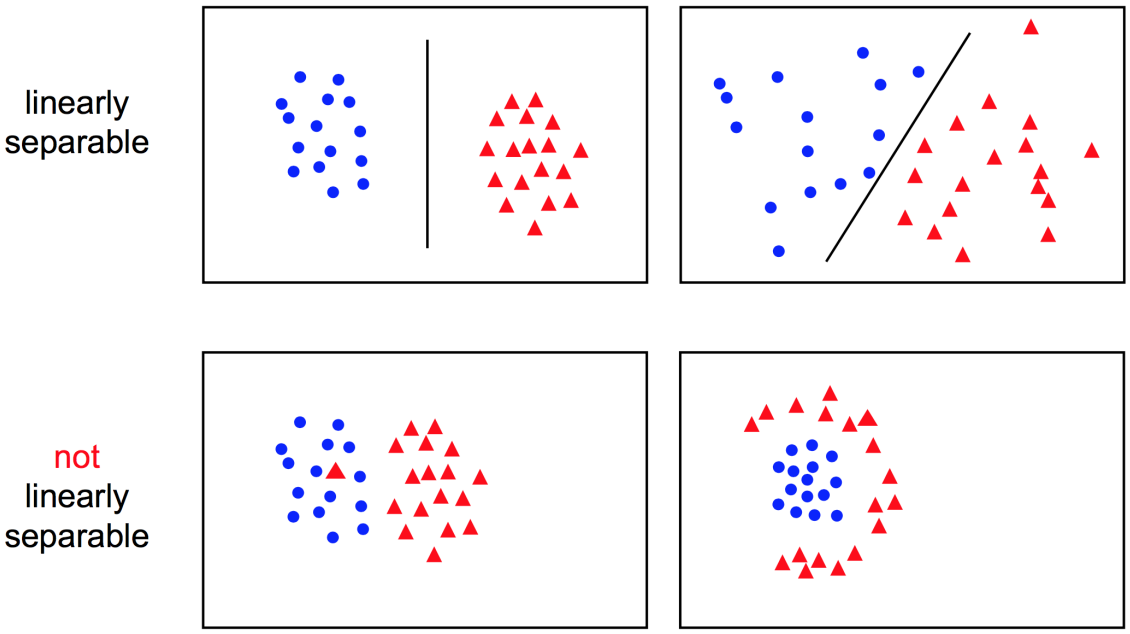
Training data $(\mathbf{x}_i, y_i)$ for $i = 1, \ldots, n$, $\mathbf{x}_i \in \mathbb{R}^m$, and $y_i \in \{-1, 1\}$, learn a discriminant function $h(\mathbf{x}; \mathbf{w}, w_0)$ such that

$$\hat{y} = \begin{cases} 1 & \text{if } h(\mathbf{x}; \mathbf{w}, w_0) > 0 \\ \text{-1} & \text{o.w.} \end{cases}$$

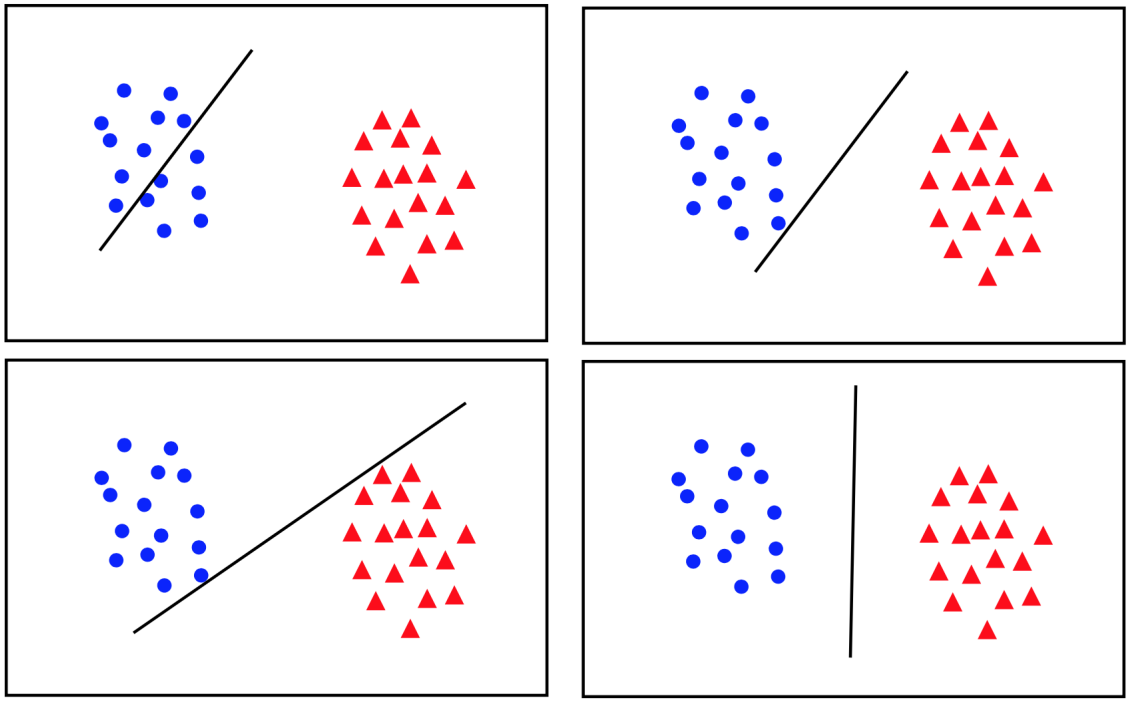
Decision boundary:

$$\mathcal{S} = \{\mathbf{x} \in \mathbb{R}^m \ : \ \mathbf{w}^\top \mathbf{x} + w_0 = 0\}$$

Linear separability (assume for now)

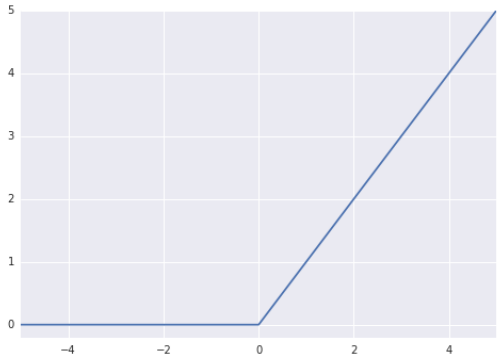


What's a good decision boundary?



Review: Perceptron Algorithm

Hinge loss function (-ve example, x-axis is $h(\mathbf{x}; \mathbf{w}, w_0) = \mathbf{w}^\top \mathbf{x} + w_0$):

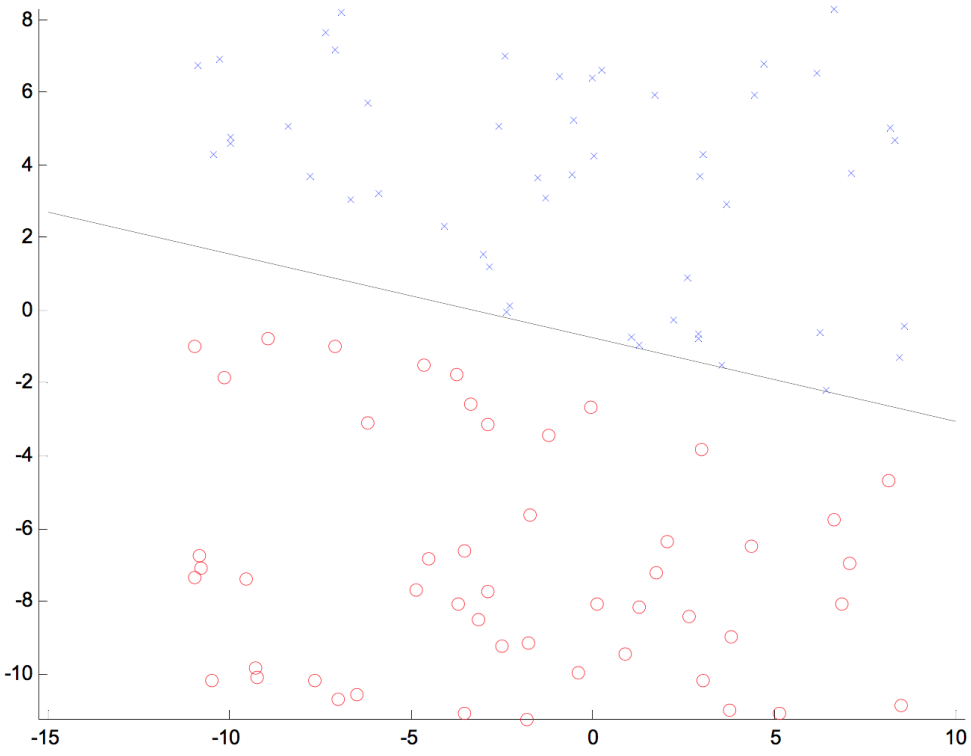


When summed up over all training data:

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} f_{relu}(-h(\mathbf{x}_i; \mathbf{w}, w_0) y_i) = \sum_{i=1: y_i \neq \hat{y}_i}^{n} -y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)$$

Convex, but can overshoot. Only guaranteed to converge if data is linearly seperable, and convergence can be slow.

Percptron also finds "bad" decision boundaries



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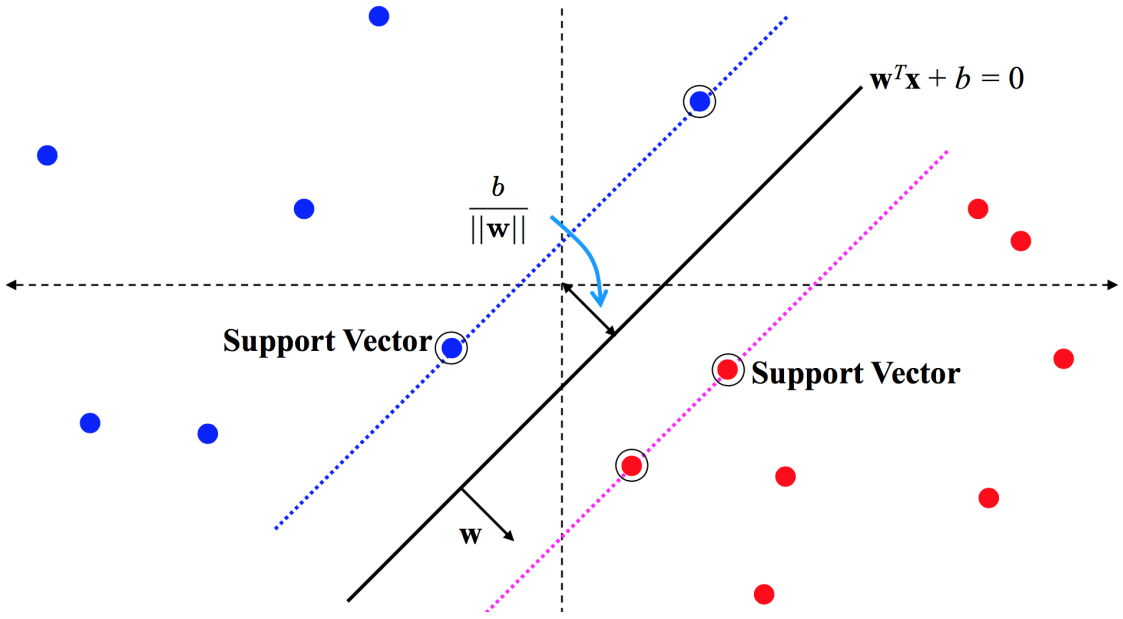
Max-margin methods

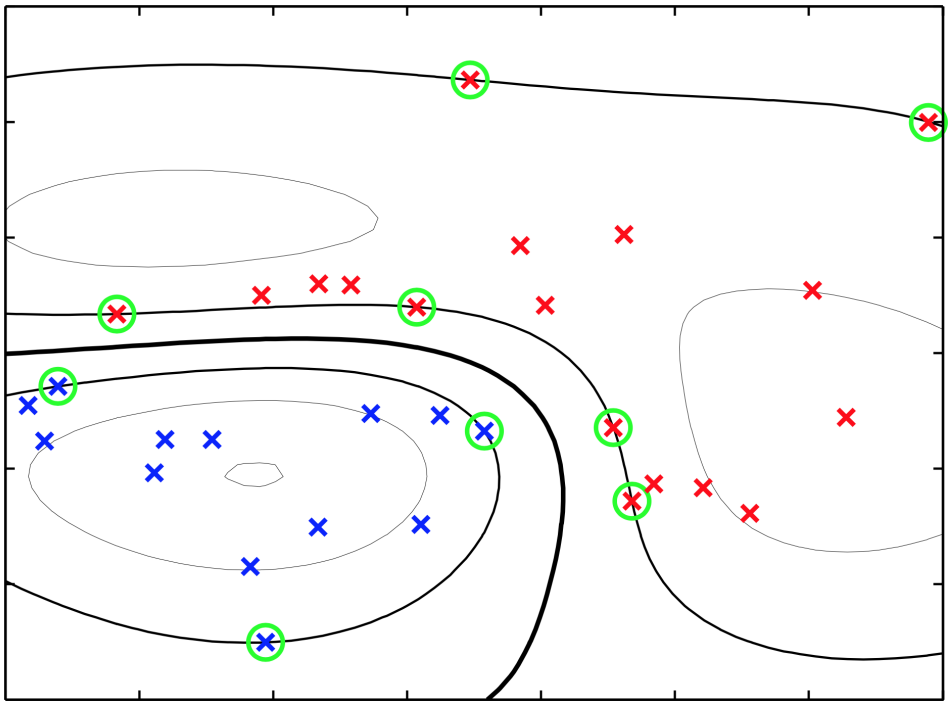


[read b as w_0.][also ignore 'support vectors' for now!]

"margin" == min dist. to decision boundary. Maximize this!

Max-margin + Basis functions

Linear separator in higher dimensional space is non-linear in $\mathbb{R}^2$:



Training problem (informal)

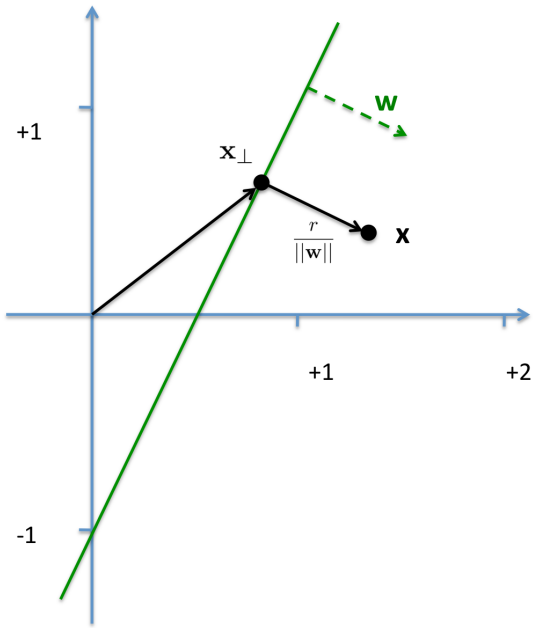
- Binary classification, with $\mathbf{x}_i \in \mathbb{R}^m$ and $h(\mathbf{x}; \mathbf{w}, w_0) = \mathbf{w}^\top \mathbf{x} + w_0$. Label $y_i \in \{-1, +1\}$
- $$\hat{y} = \begin{cases} 1 & \text{if } h(\mathbf{x}; \mathbf{w}, w_0) \geq 0 \\ \text{-1} & \text{o.w.} \end{cases}$$
- For now: assume data is linearly separable.
- Goal: Find $\mathbf{w}$ to correctly classify examples, and maximize margin on data D.
- Margin = min dist to decision boundary across all examples in D.

Example: Distance to decision boundary

Suppose $\mathbf{x} \in \mathbb{R}^2$

$h(\mathbf{x}; \mathbf{w}, w_0) = 2x_1 - x_2 - 1.$

$||\mathbf{w}|| = \sqrt{\mathbf{w}^\top \mathbf{w}} = \sqrt{5}.$



Write example $\mathbf{x}$ as

$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{||\mathbf{w}||}, \tag{1}$$

where $\mathbf{x}_\perp$ is projection of $\mathbf{x}$ onto the boundary, and r is the distance.

Solving for distance to decision boundary

We want signed, normalized, orthogonal distance from an example $\mathbf{x}$ to decision boundary associated with $(\mathbf{w}, w_0)$.

Calculate as:

$$\begin{aligned}
\mathbf{x} &= \mathbf{x}_\perp + r\frac{\mathbf{w}}{||\mathbf{w}||} \\
\Leftrightarrow \quad \mathbf{w}^\top \mathbf{x} &= \mathbf{w}^\top \mathbf{x}_\perp + r\frac{\mathbf{w}^\top \mathbf{w}}{||\mathbf{w}||} \\
\Leftrightarrow \quad h(\mathbf{x}; \mathbf{w}, w_0) - w_0 &= -w_0 + r||\mathbf{w}|| \\
\Leftrightarrow \quad r &= \frac{h(\mathbf{x}; \mathbf{w}, w_0)}{||\mathbf{w}||}
\end{aligned}$$

Lovely! A simple expression. Also, if $r > 0$, predict 1; predict -1 otherwise.

Defining the Margin of a Classifier

The "margin" for an example is the absolute value of distance r. Can write as:

Definition (Margin on an example)

The margin of a classifier on a correctly classified example $(\mathbf{x}_i, y_i)$ is

$$margin(\mathbf{x}_i) = y_i \times r = \frac{y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)}{||\mathbf{w}||} \quad (\geq 0)$$

Definition (Margin on data)

The margin of a classifer on data D is the minimum margin over correctly classified examples $(\mathbf{x}_i, y_i) \in D$.

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The Max Margin Training Problem

$$\max_{\mathbf{w},w_0}\left[\min_i \frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)\right] \qquad \text{[P1]}$$

Yikes! Non-linear in $\mathbf{w}$, and ugly "max min" structure.

Note: this formulation will find a discriminant that separates the data when one exists, because $y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)$ is negative if a point is missclassified, and thus $\max\min$ wants to push these errors to be positive.

Simplifying (1 of 3)

$$\max_{\mathbf{w},w_0}\left[\min_{i=1\ldots n} \frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)\right] \qquad \text{[P1]}$$

We have:

- Separable, and thus in solution, margin $\frac{y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)}{||\mathbf{w}||} > 0$ for all i
- Margin $\frac{y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)}{||\mathbf{w}||}$ is invariant to multiplying $(\mathbf{w}, w_0)$ by any $\beta > 0$.

Therefore, it does not preclude any solutions to rewrite as:

$$\max_{\mathbf{w},w_0}\left[\min_{i=1\ldots n} \frac{1}{||\mathbf{w}||} y_i(\mathbf{w}^\top \mathbf{x}_i + w_0)\right] \qquad \text{[P2]}$$

$$\text{s.t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1, \quad \text{for all } i$$

Simplifying (2 of 3)

$$\max_{\mathbf{w},w_0} \frac{1}{||\mathbf{w}||} \min_{i=1\ldots n} y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \qquad \text{[P2]}$$
$$\text{s.t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1, \quad \text{for all } i$$

is equivalent to

$$\max_{\mathbf{w},w_0} \frac{1}{||\mathbf{w}||} \qquad \text{[P3]}$$
$$\text{s.t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1, \quad \text{for all } i$$

(1) By the β scaling argument, it would not preclude any solutions to restrict [P2] to insist at least one constraint is binding (i.e., hold with equality in an optimal solution).
(2) Optimal solution to [P3] will achieve this, and thus also solve [P2] since objective is the same amongst solutions where at least one constraint is binding.

Simplifying (3 of 3)

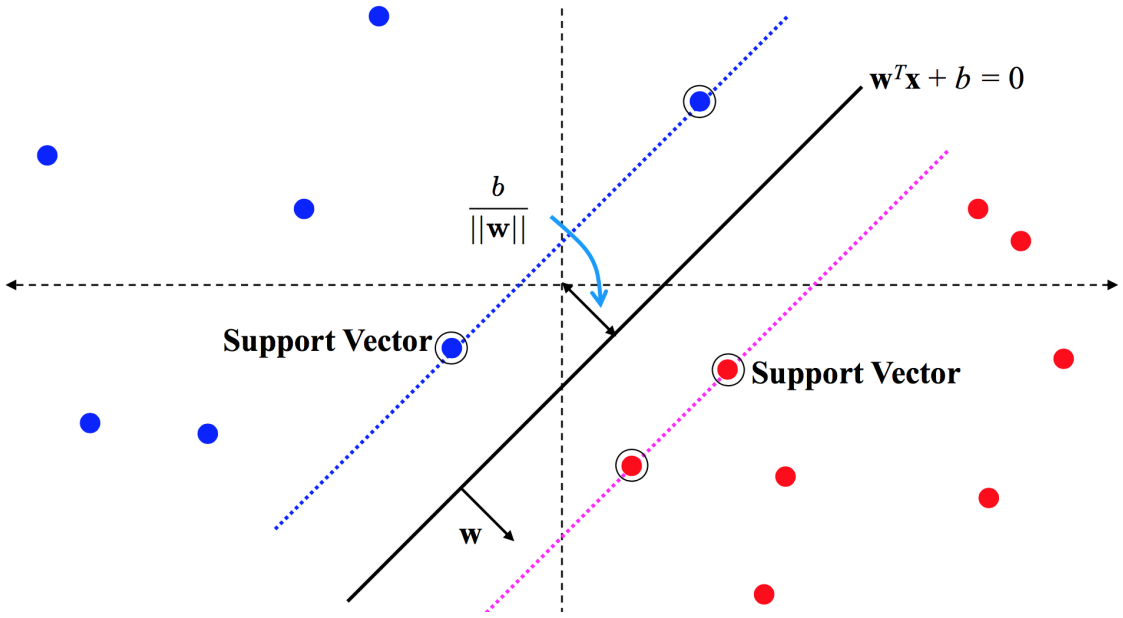
$$\max_{\mathbf{w},w_0} \frac{1}{||\mathbf{w}||} \qquad \text{[P3]}$$
$$\text{s.t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1, \quad \text{for all } i$$

Can rewrite as:

$$\min_{\mathbf{w},w_0} \frac{1}{2}||\mathbf{w}||^2 \qquad \text{[P4]}$$
$$\text{s.t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1, \quad \text{for all } i$$

Nice! This is convex and differentiable, with linear constraints (a "quadratic program"). Can solve via gradient descent. Obtain global minimum. [Note: the margin on the data will be $1/||\mathbf{w}||$ since one or more constraints will be binding.]

Interpretation: Max-Margin Solution



[read b as w_0.][also ignore 'support vectors' for now!]

Normalization: bottom margin boundary has $\mathbf{w}^\top \mathbf{x} + w_0 = +1$, top has $\mathbf{w}^\top \mathbf{x} + w_0 = -1$. "margin region" == between margin boundaries.

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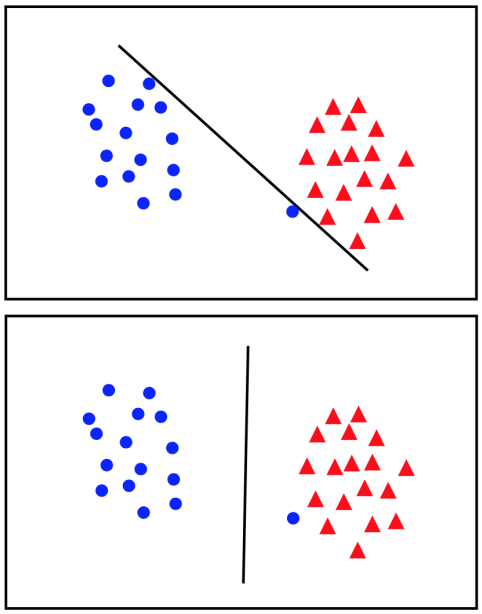
Linear separability revisited.

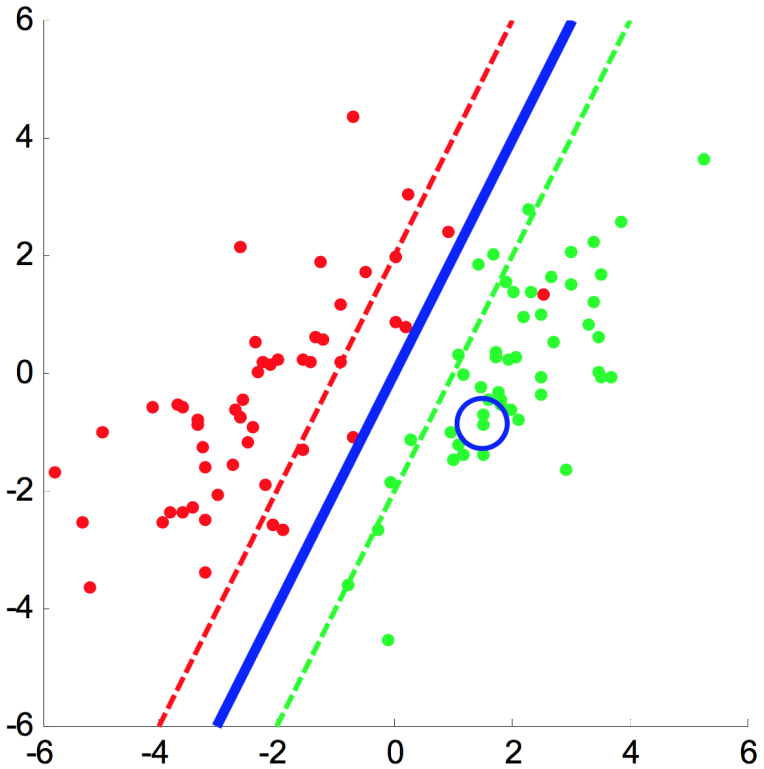


• the points can be linearly separated but there is a very narrow margin

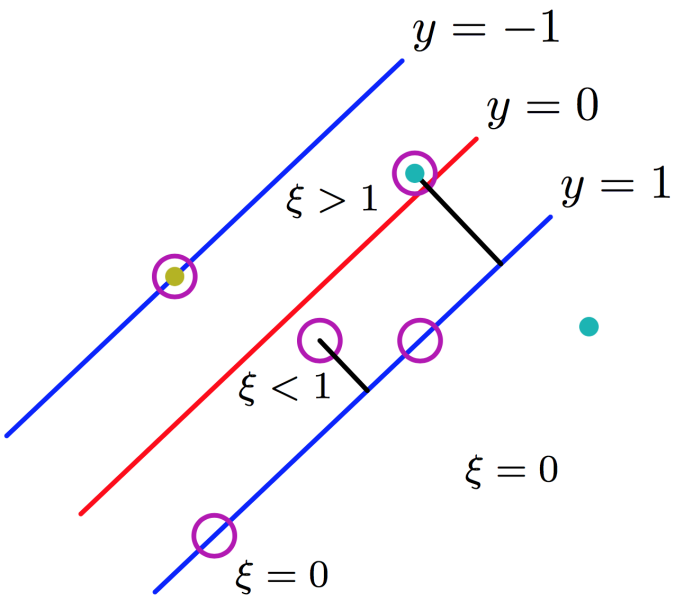
• but possibly the large margin solution is better, even though one constraint is violated

In general there is a trade off between the margin and the number of mistakes on the training data

Moreover, training data may not be linearly separable!



A relaxed formulation



[read y as h] Introduce variable $\xi_i \geq 0$, for each i, which represents how much example i is on "wrong side" of margin boundary. If $\xi_i = 0$ then it is ok. If $0 < \xi_i < 1$ it is correctly classified, but with a smaller margin than $1/||\mathbf{w}||$. If $\xi_i > 1$ then it is incorrectly classified.

The Soft Margin Formulation

$$\min_{\mathbf{w},w_0} \frac{1}{2}||\mathbf{w}||^2 \qquad \text{[P4]}$$

$$\text{s.t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1$$

$$\min_{\mathbf{w},w_0} \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n} \xi_i \qquad \text{[P5]}$$

$$\text{s.t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

For example correctly classified but with $(0 < \xi_i < 1)$, [P5] will "pretend" the margin is still $1/||\mathbf{w}||$ and that $y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) \geq 1$. [P5] also allows $\mathbf{x}_i$ to be misclassified, with $(\xi_i > 1)$.

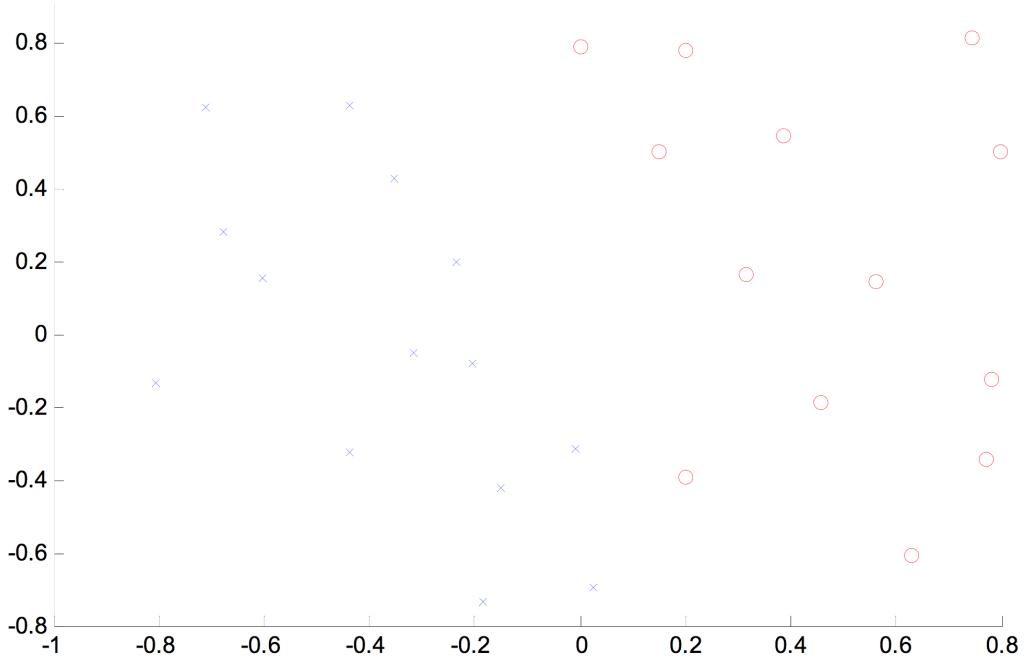
Constant $C > 0$ is a regularization parameter:

- small C, can ignore constraints, get larger margin.
- large C, constraints hard to ignore, get smaller margin.
- $C = \infty$ enforces all constraints.

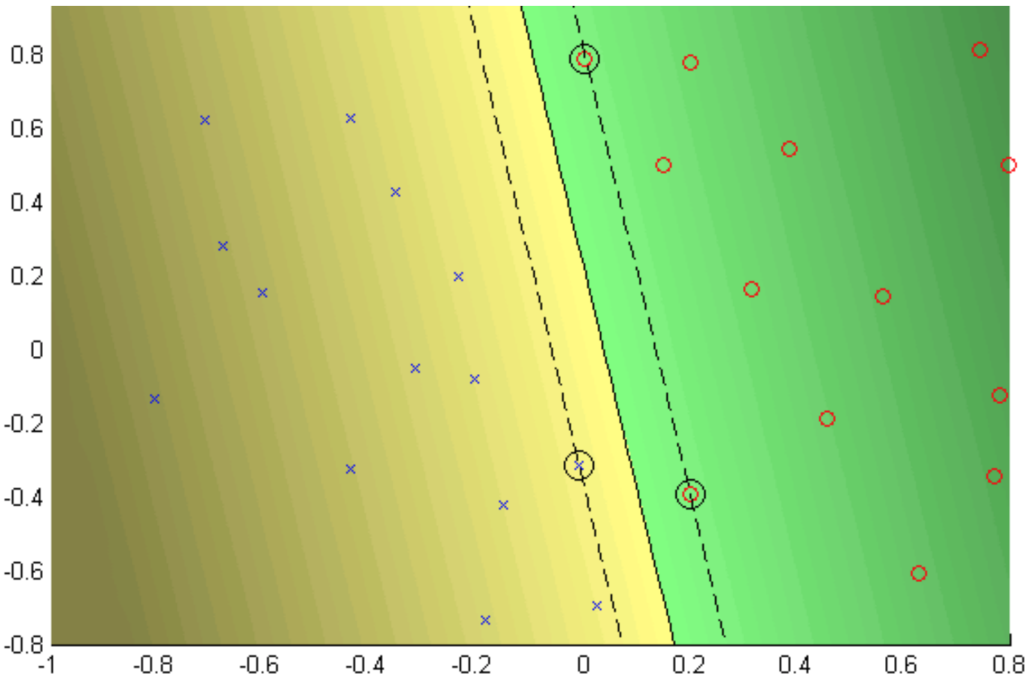
Set C via cross-validation (careful, larger is less regularization).

Example: Soft Margin Classifier

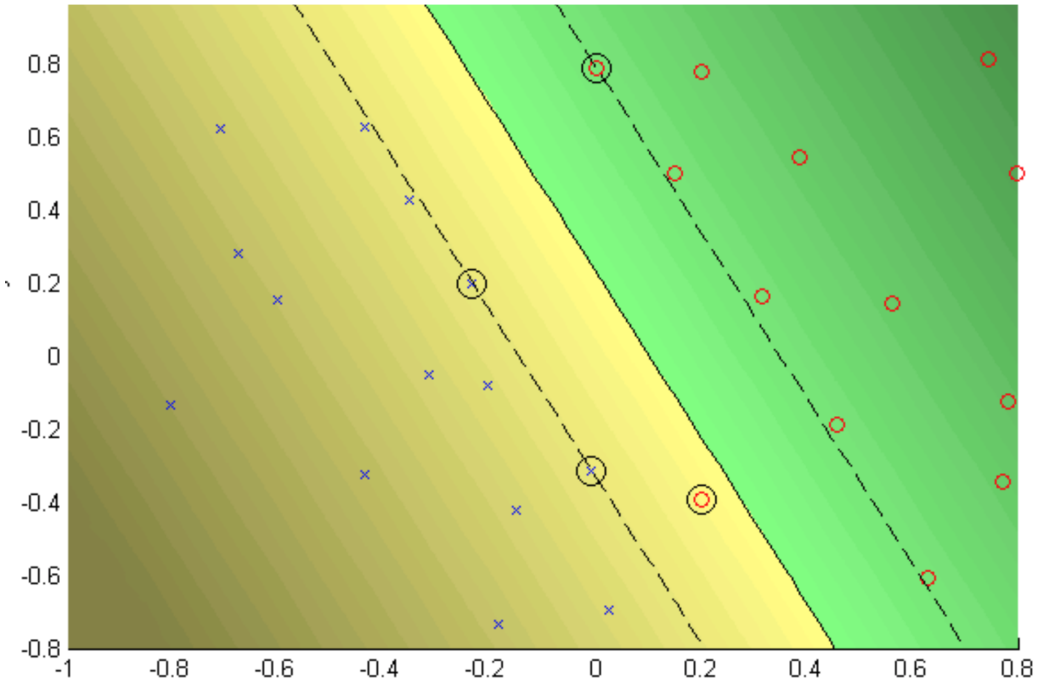
Data linearly seperable, but only with a small margin.



$C =$ Infinity (hard margin)



$C = 10$ (soft margin)



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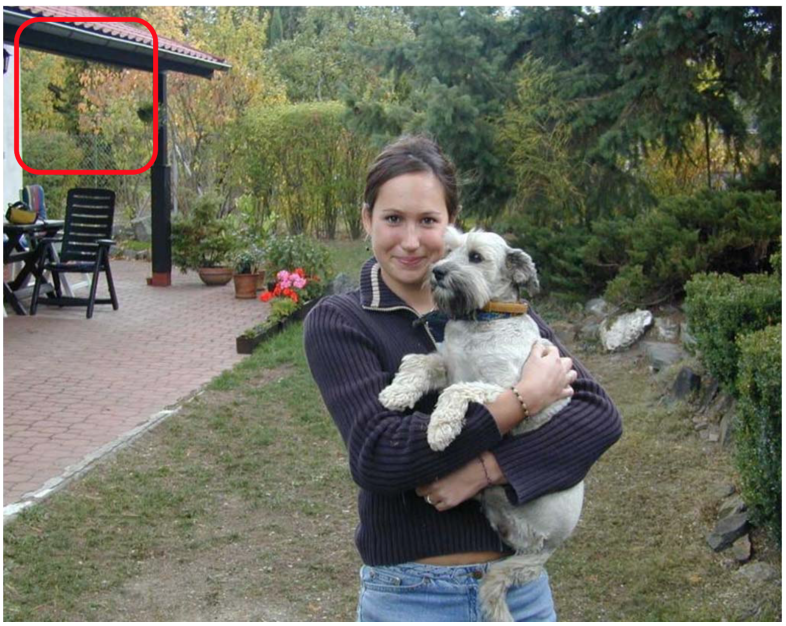
Application: Pedestrian detection in computer vision

Objective: detect standing humans in an image window.

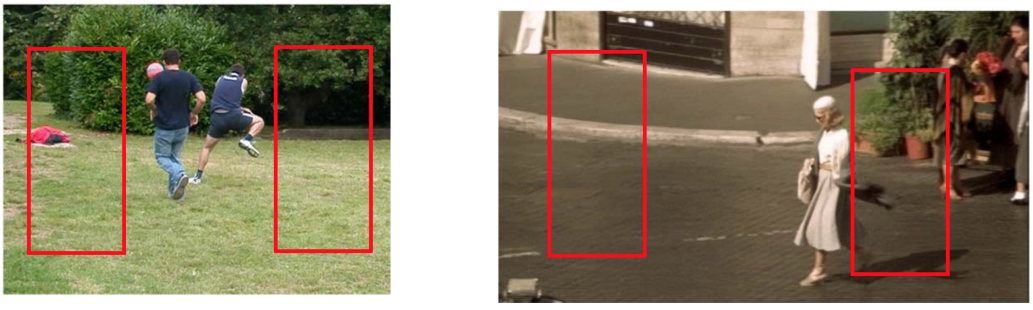


[Dalal and Triggs'05]

Training data and features

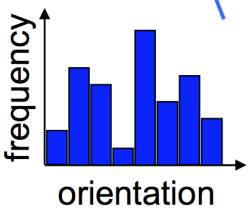
- Positive window examples

- Negative window examples



Feature encoding: Histogram of oriented gradients (HOG)

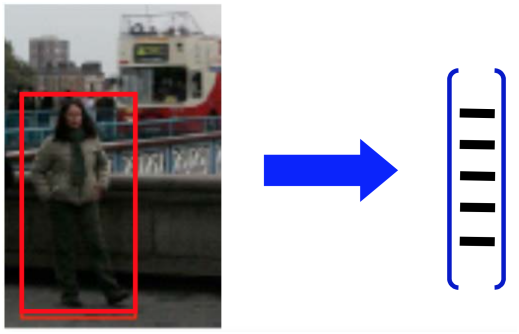
- tile window into 8 x 8 pixel cells
- each cell represented by HOG



Number features is $d = 16 \times 8$ (tiling) $\times 8$ (orientations) $= 1024$.

Max-margin algorithm

Represent each example window by a HOG feature vector



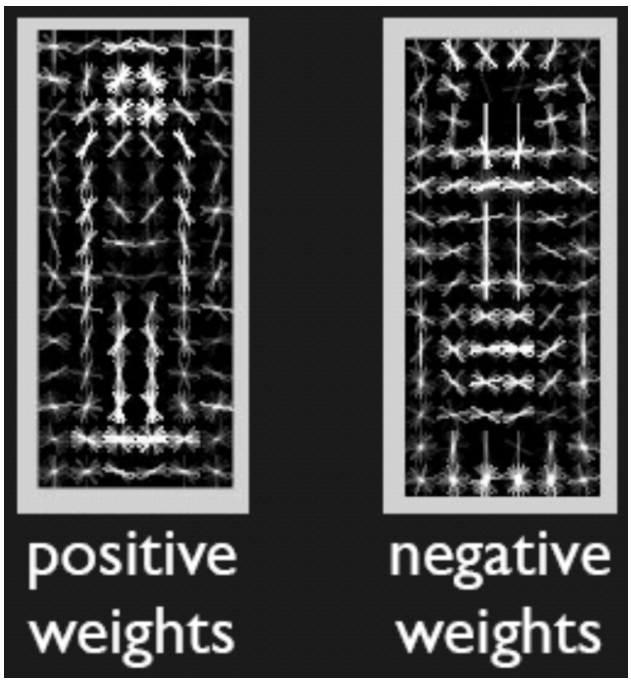
and so, example is $\mathbf{x}_i \in \mathbb{R}^{1024}$

Train a Support Vector Machine. Predict a standing human based on

$$\hat{y} = \begin{cases} 1 & \text{if } h(\mathbf{x}; \mathbf{w}, w_0) > 0 \\ -1 & \text{o.w.} \end{cases}$$

Prediction on a new example

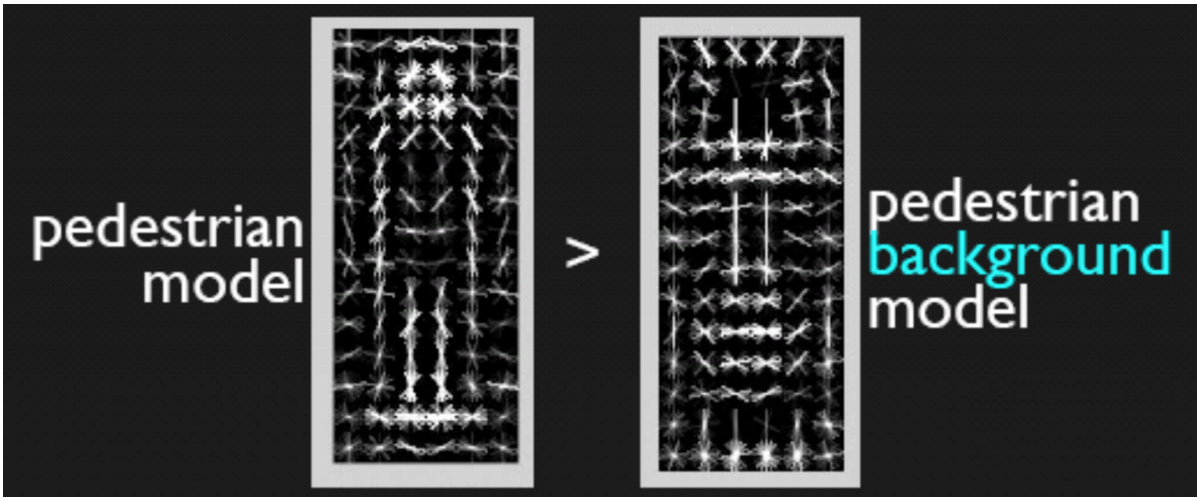
Example Weights in Trained Model



[graphic: D. Ramanan]

Interpretation of the Classifier

Will predict a standing human if:



[graphic: D. Ramanan]

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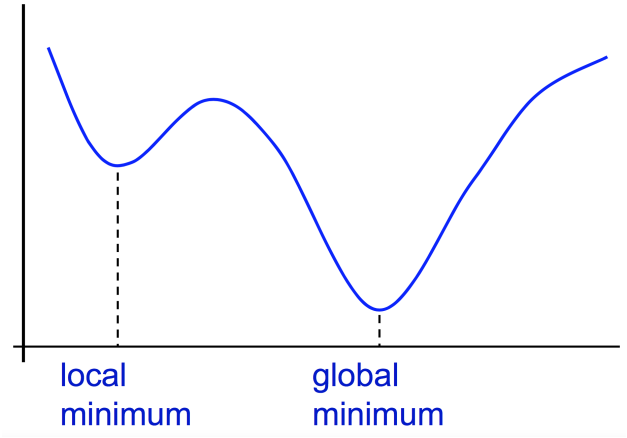
The Soft-Margin Optimization Problem

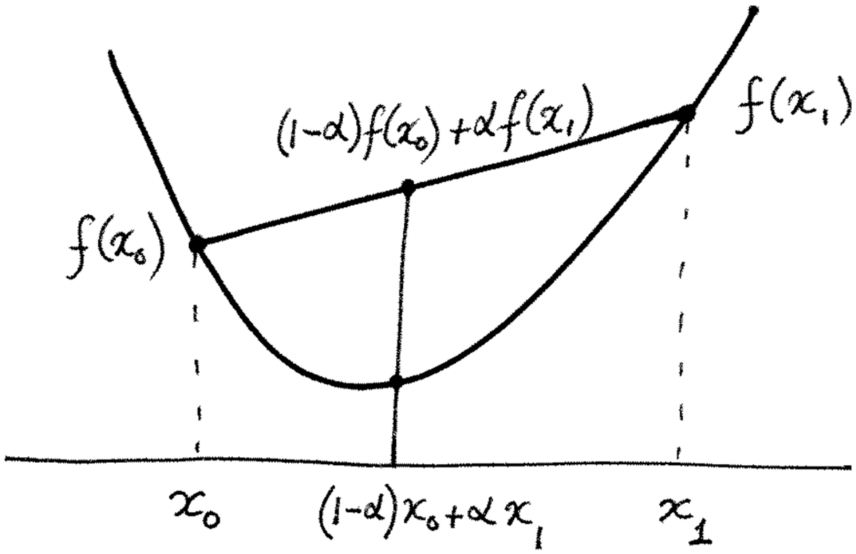
We ended up here:

$$\min_{\mathbf{w},w_0} C\sum_{i=1}^{n}\max(0,1-y_i(\mathbf{w}^\top\mathbf{x}_i+w_0))+\frac{1}{2}||\mathbf{w}||^2 \qquad \text{[P5]}$$

Is this loss function convex (i.e., will a locally optimal point be globally optimal?)

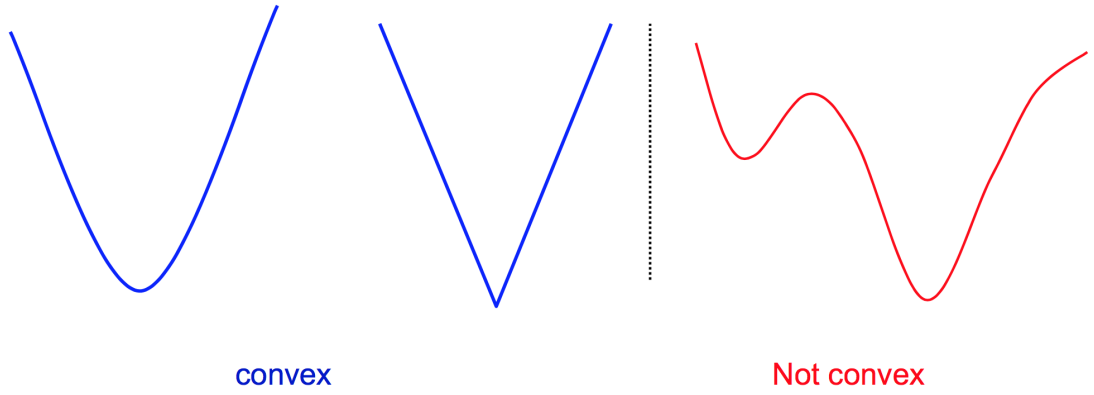


Review: Convex functions



Line joining $(x_0, f(x_0))$ and $(x_1, f(x_1))$ lies above the function graph.

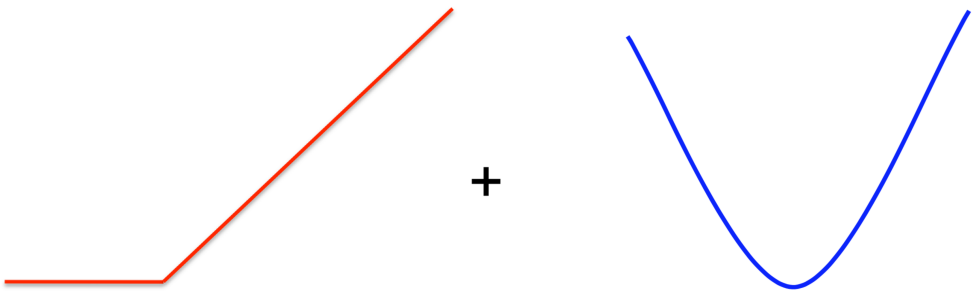
Example functions



Fact: A non-negative sum of convex functions is convex.

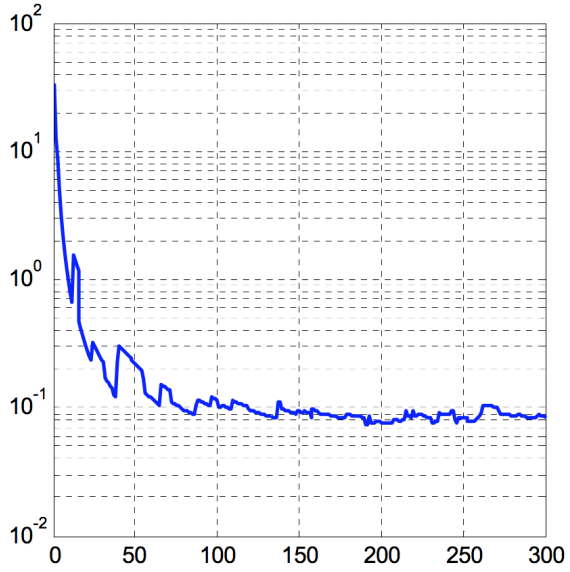
The Soft-Margin Loss function

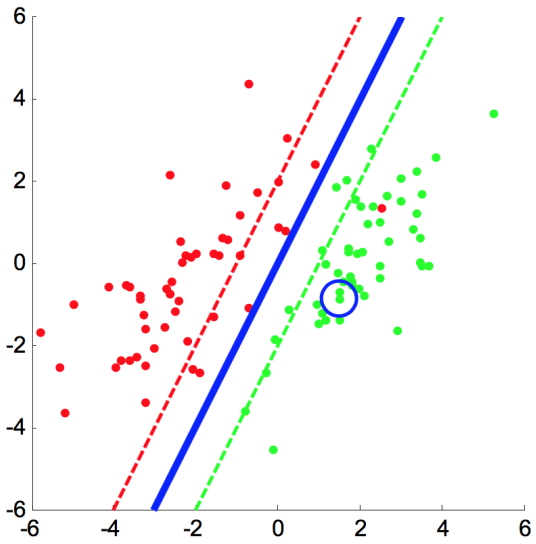
$$\min_{\mathbf{w},w_0} C\sum_{i=1}^{n}\max(0,1-y_i(\mathbf{w}^\top\mathbf{x}_i+w_0))+\frac{1}{2}||\mathbf{w}||^2$$



Convex! Can derive SGD updates to optimize.

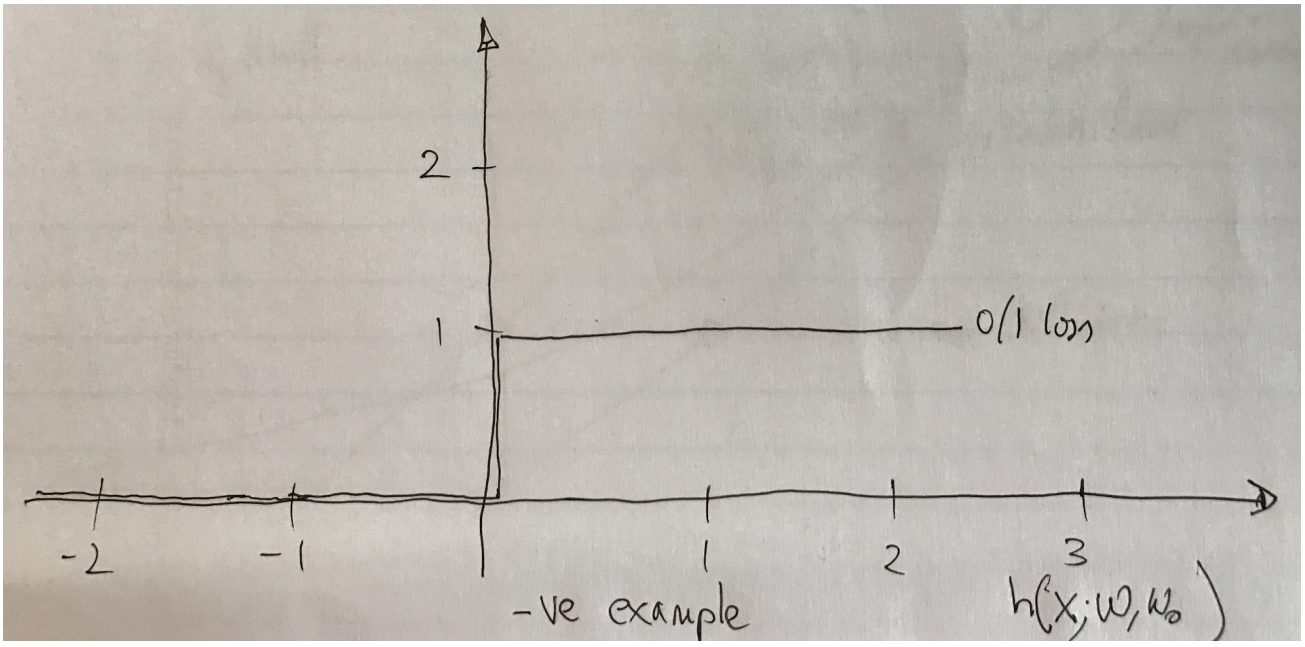
SGD based, Soft-margin training



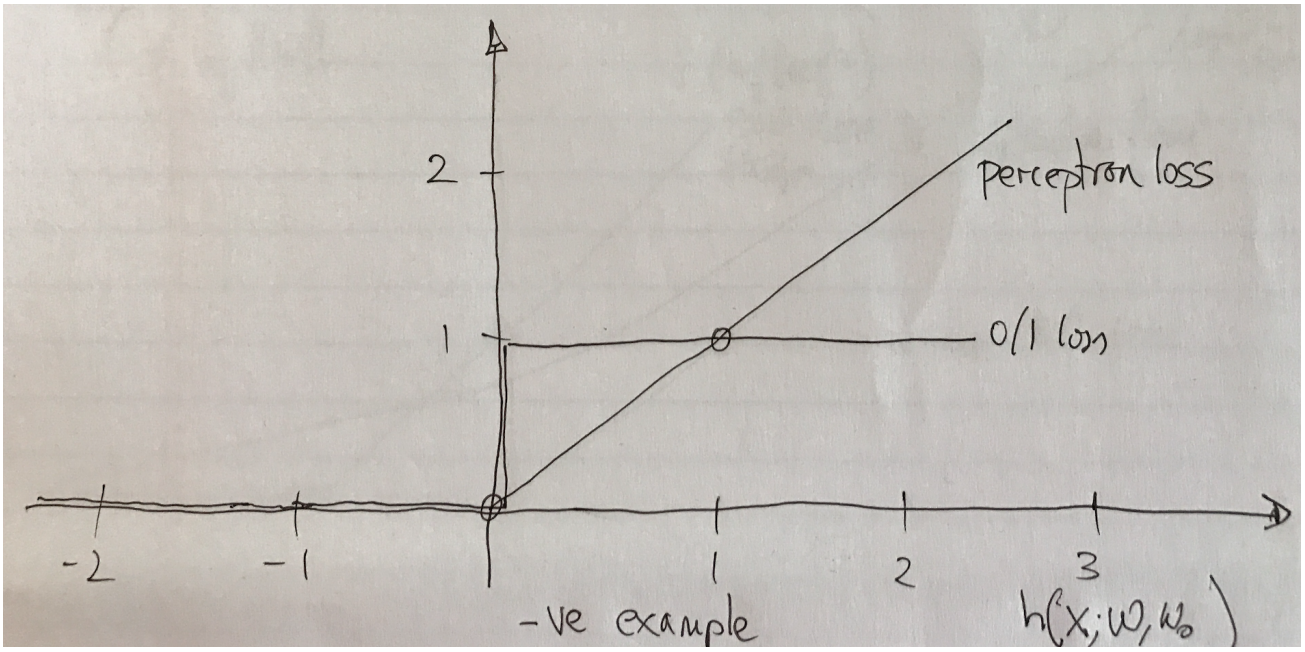


Pegasos algorithm, Shalev-Shwartz et al. 2011.

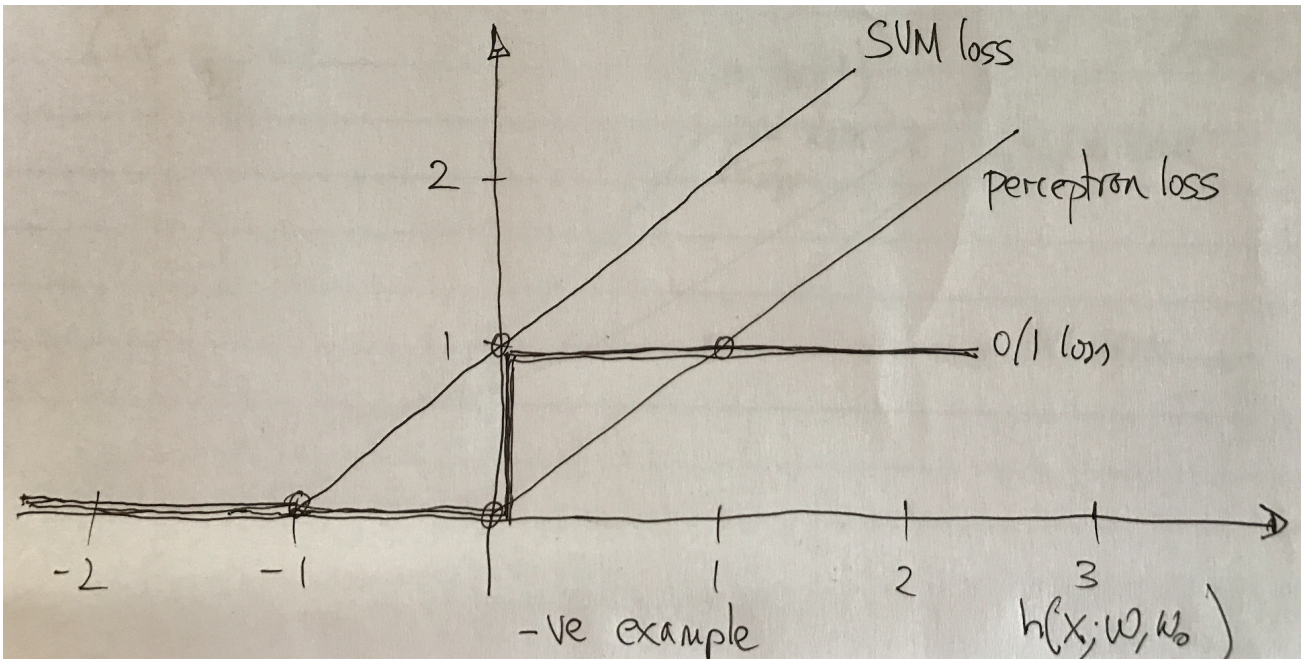
Comparing Loss Functions



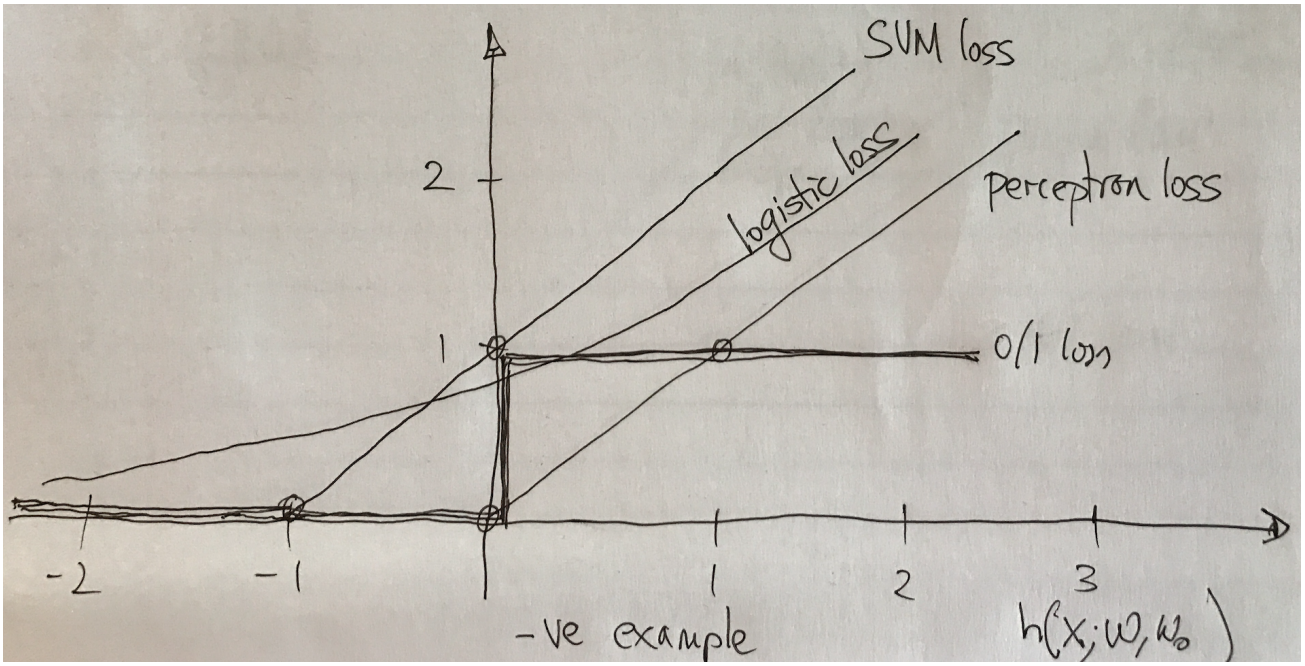
Comparing Loss Functions



Comparing Loss Functions



Comparing Loss Functions



Next class

- Limitation of current formulation is that $\mathbf{w} \in \mathbb{R}^m$ and m may be very large (espcially if $m \to d$ following basis transform).
- Can solve [P5] via a dual formulation.
- Allows for the "kernel trick." A beautiful way to work with basis functions.
- Leads to the "dual form of the predictor", which is a succinct representation via "support vectors."
- Understanding kernel functions.