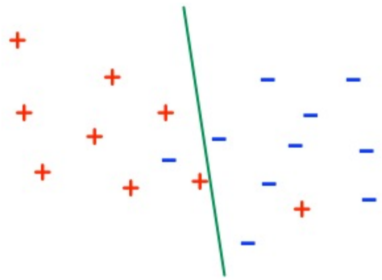
More linear classification

DSE 220

The decision boundary



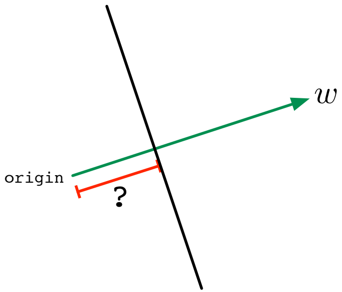
Decision boundary in $\mathbb{R}^p$ is a **hyperplane**.

- How is this boundary parametrized?
- How can we learn a hyperplane from training data?

Hyperplanes

Hyperplane $\{x : w \cdot x = b\}$

- orientation $w \in \mathbb{R}^p$
- offset $b \in \mathbb{R}$



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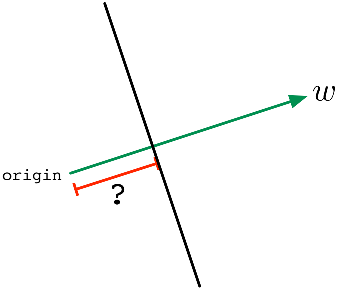

Can always normalize w to unit length:

$$(w, b) \quad \longleftrightarrow \quad \left(\widehat{w} = \frac{w}{\|w\|}, \frac{b}{\|w\|}\right)$$

$$w \cdot x = b \quad \longleftrightarrow \quad \widehat{w} \cdot x = \frac{b}{\|w\|}$$

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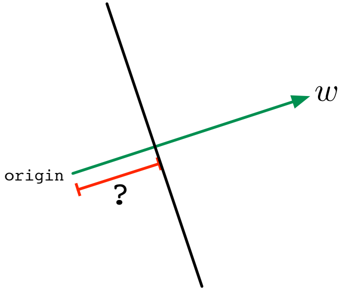

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Equivalently: all points whose projection onto $\widehat{w}$ is $b/\|w\|$.

Homogeneous linear separators

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Reduce to this case by adding an extra feature to x:

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Then $\{x : w \cdot x = b\} \equiv \{x : \widetilde{w} \cdot \widetilde{x} = 0\}$ where $\widetilde{w} = (w, -b)$.

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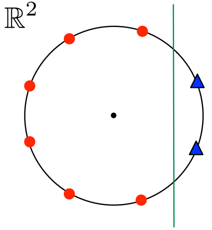

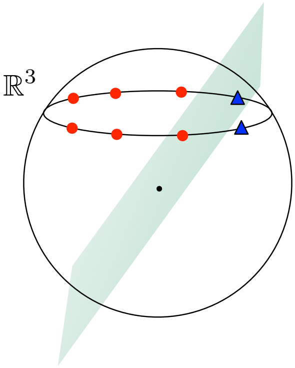

The learning problem: separable case

Input: training data $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, +1\}$

Output: linear classifier $w \in \mathbb{R}^p$ such that

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- Each data point is a linear constraint on w
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A simple alternative: **Perceptron algorithm** (Rosenblatt, 1958)

- $w = 0$
- while some (x, y) is misclassified:
  - $w = w + yx$

Perceptron: example

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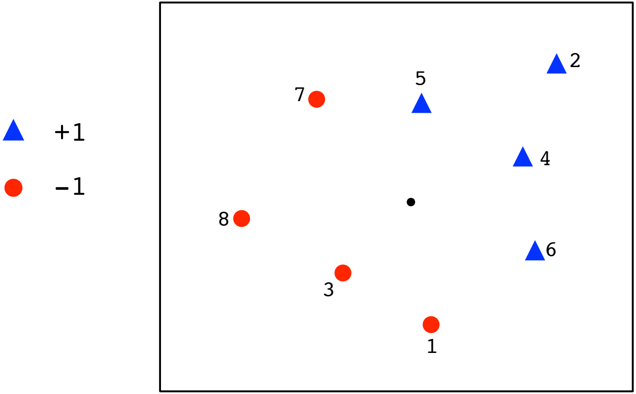

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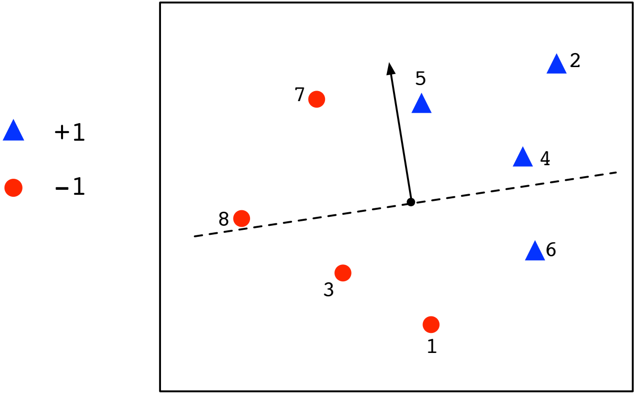

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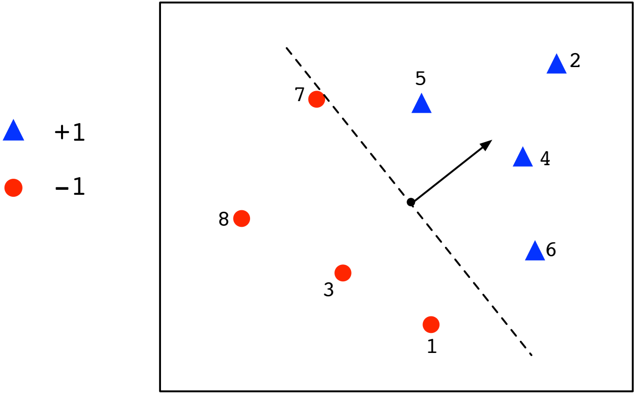

Separator: $w = -x^{(1)} + x^{(6)}$

Perceptron: convergence

Theorem: Let $R = \max \|x^{(i)}\|$. Suppose there is a unit vector w^* and some (margin) $\gamma > 0$ such that

$$y^{(i)}(w^* \cdot x^{(i)}) \geq \gamma \ \text{ for all } i.$$

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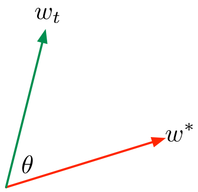
Proof idea. Let w_t be the classifier after t updates.



Track angle between w_t and w^*:

$$\cos(\angle(w_t, w^*)) = \frac{w_t \cdot w^*}{\|w\|}.$$

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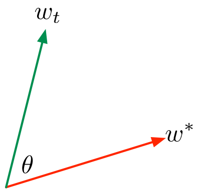

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On each mistake, when w_t is updated to w_{t+1},

- $w_t \cdot w^*$ grows significantly.
- $\|w_t\|$ does not grow much.

Perceptron convergence, cont'd

Perceptron update: if $y(w_t \cdot x) < 0$ (misclassified) then $w_{t+1} = w_t + yx$.
Target vector w^* has unit length, and margin condition $y(w^* \cdot x) \geq \gamma$.

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2. When updating w_t to w_{t+1}:

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$$w_T \cdot w^* \geq T\gamma$$
$$\|w_T\|^2 \leq TR^2$$

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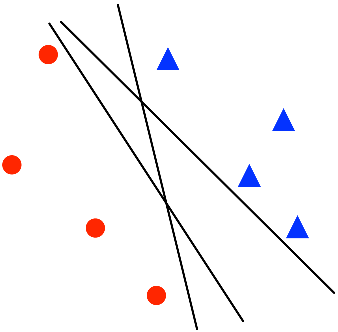
4. The angle between w_T and w^* is given by

$$\cos(\angle(w_T, w^*)) = \frac{w_T \cdot w^*}{\|w\|} \geq \frac{T\gamma}{R\sqrt{T}}.$$

This is at most 1, so $T \leq R^2/\gamma^2$.

A better separator?

For a linearly separable data set, there are in general many possible separating hyperplanes, and Perceptron is guaranteed to find one of them.



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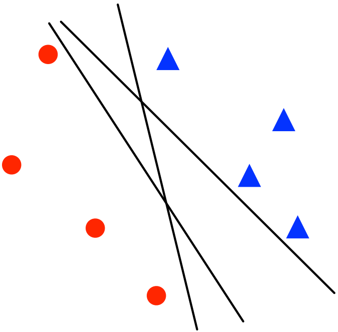

But is there a better, more systematic choice of separator? The one with the most buffer around it, for instance?

Maximizing the margin

Given training data $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, +1\}$, find $w \in \mathbb{R}^p$ and $b \in \mathbb{R}$ such that $y^{(i)}(w \cdot x^{(i)} + b) > 0$ for all i.

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By scaling w, b, can equally ask for

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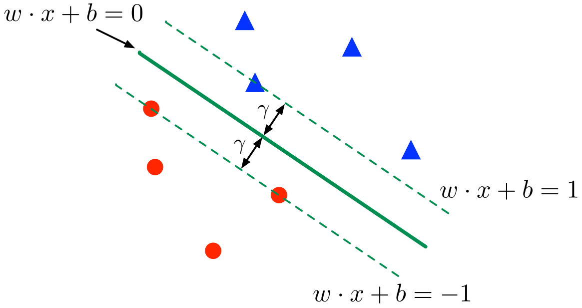

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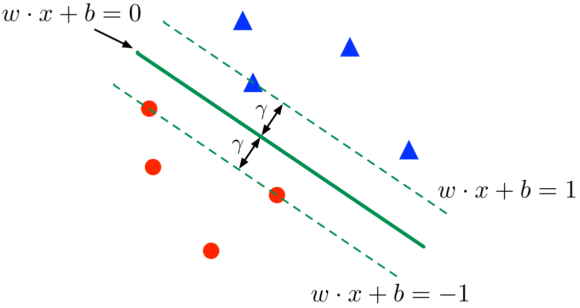
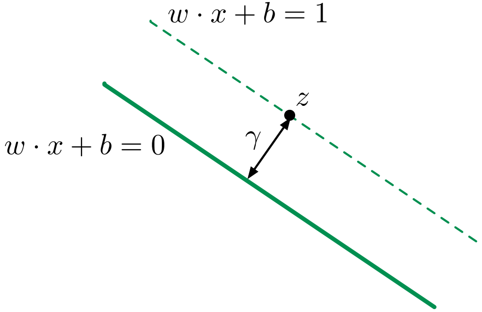


Maximize the **margin** γ.

What is the margin?

Close-up of a point z on the positive boundary.



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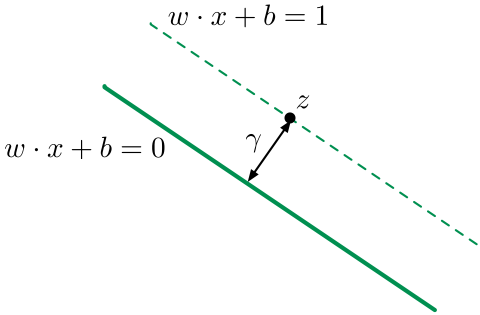

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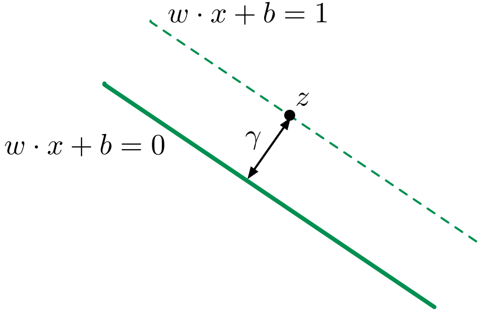

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Then $z - \gamma \widehat{w}$ is on the separator, so

$$w \cdot (z - \gamma \widehat{w}) + b = 0 \;\; \Rightarrow \;\; \gamma w \cdot \widehat{w} = w \cdot z + b = 1 \;\; \Rightarrow \;\; \gamma = 1/\|w\|$$

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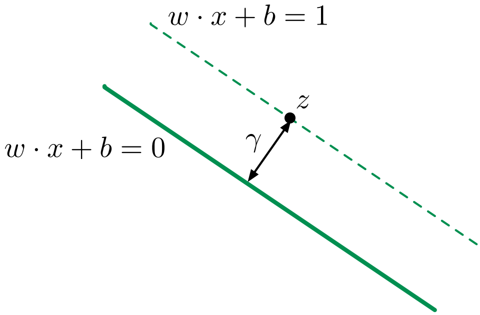

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In short: to maximize the margin, minimize $\|w\|$.

Maximum-margin linear classifier

- Given $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, +1\}$.

$$
\boxed{\begin{array}{l} (\textsc{primal}) \qquad \displaystyle\min_{w \in \mathbb{R}^p, b \in \mathbb{R}} \quad \frac{1}{2}\|w\|^2 \\ \text{s.t.:} \quad y^{(i)}(w \cdot x^{(i)} + b) \geq 1 \quad \text{for all } i = 1, 2, \ldots, n \end{array}}
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- This is a convex optimization problem:
  - Convex objective function
  - Linear constraints
- It has a dual maximization problem with the same optimum value.

$$\text{(DUAL)} \quad \max_{\alpha \in \mathbb{R}^n} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} (x^{(i)} \cdot x^{(j)})$$
$$\text{s.t.:} \quad \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$
$$\alpha \geq 0$$

Complementary slackness

$$\boxed{\begin{array}{l} (\text{PRIMAL}) \quad \displaystyle\min_{w\in\mathbb{R}^p, b\in\mathbb{R}} \quad \frac{1}{2}\|w\|^2 \\ \text{s.t.: } y^{(i)}(w \cdot x^{(i)} + b) \geq 1 \quad \text{for all } i = 1, 2, \ldots, n \end{array}}$$

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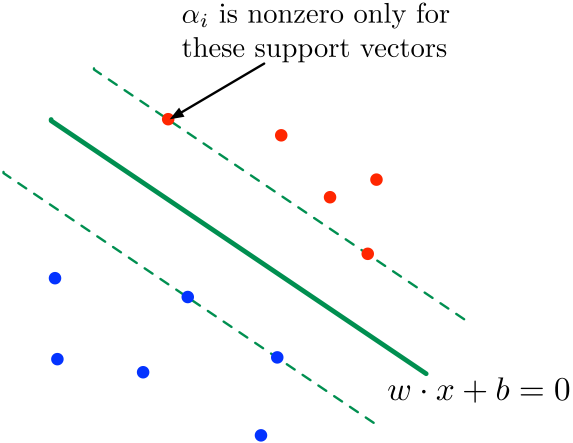
At optimality, $w = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)}$ and moreover

$$\alpha_i > 0 \quad \Rightarrow \quad y^{(i)}(w \cdot x^{(i)} + b) = 1$$

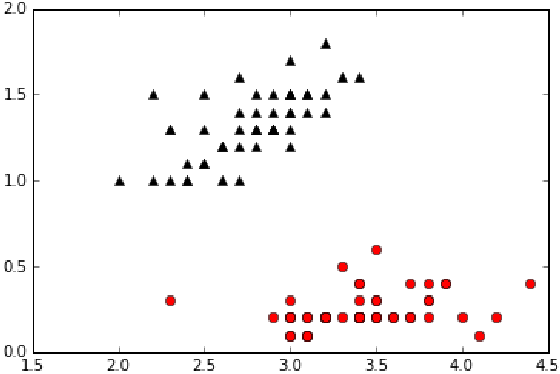
Points $x^{(i)}$ with $\alpha_i > 0$ are called **support vectors**.

Support vectors



Linear classifier $w = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)}$ is a function of just the support vectors.

Small example: Iris data set



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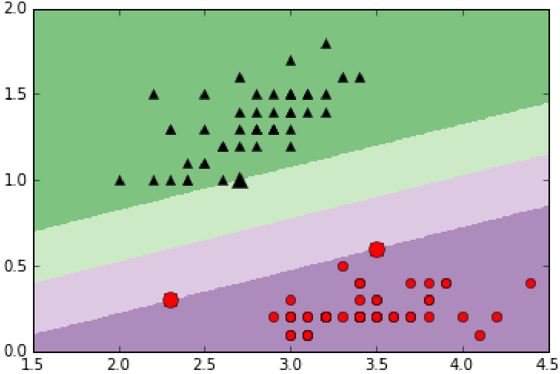
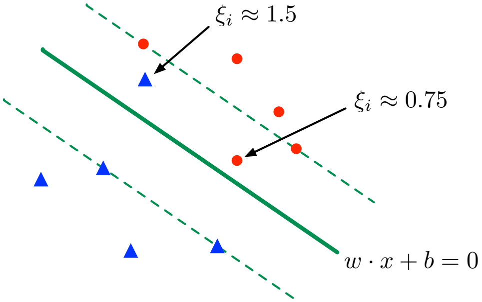


The non-separable case

Idea: allow each data point $x^{(i)}$ some slack ξ_i.

$$\boxed{\begin{array}{c} \text{(PRIMAL)} \quad \min_{w\in\mathbb{R}^p, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i \\ \text{s.t.:} \;\; y^{(i)}(w\cdot x^{(i)} + b) \geq 1 - \xi_i \quad \text{for all } i = 1,2,\ldots,n \\ \xi \geq 0 \end{array}}$$



Dual for general case

$$\text{(PRIMAL)} \quad \min_{w\in\mathbb{R}^p, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.:} \quad y^{(i)}(w\cdot x^{(i)} + b) \geq 1 - \xi_i \quad \text{for all } i = 1, 2, \ldots, n$$

$$\xi \geq 0$$

$$\text{(DUAL)} \quad \max_{\alpha\in\mathbb{R}^n} \quad \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y^{(i)}y^{(j)}(x^{(i)}\cdot x^{(j)})$$

$$\text{s.t.:} \quad \sum_{i=1}^{n}\alpha_i y^{(i)} = 0$$

$$0 \leq \alpha_i \leq C$$

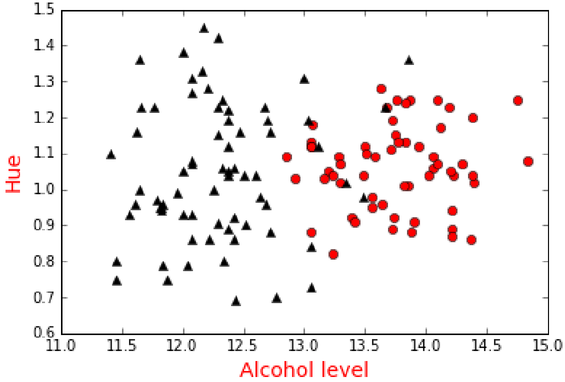
At optimality, $w = \sum_i \alpha_i y^{(i)} x^{(i)}$, with

$$0 < \alpha_i < C \quad \Rightarrow \quad y^{(i)}(w\cdot x^{(i)} + b) = 1$$

$$\alpha_i = C \quad \Rightarrow \quad y^{(i)}(w\cdot x^{(i)} + b) = 1 - \xi_i$$

Wine data set

Here $C = 1.0$



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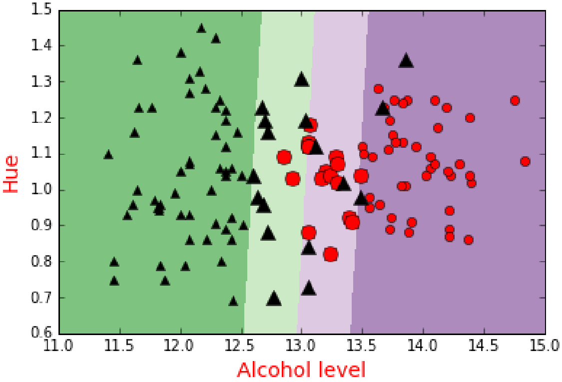
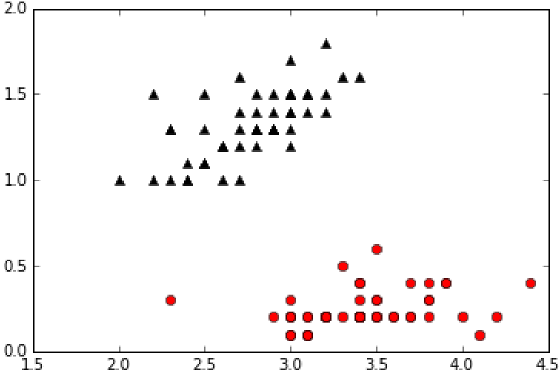


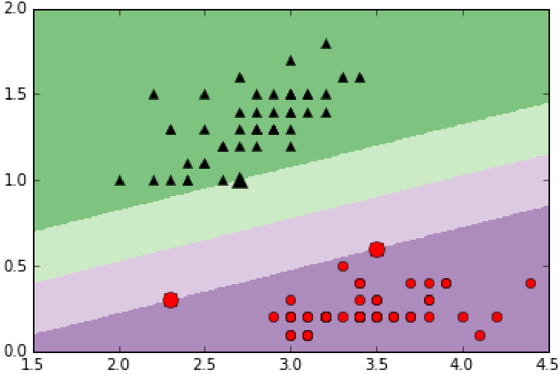
Back to Iris

$C = 10$



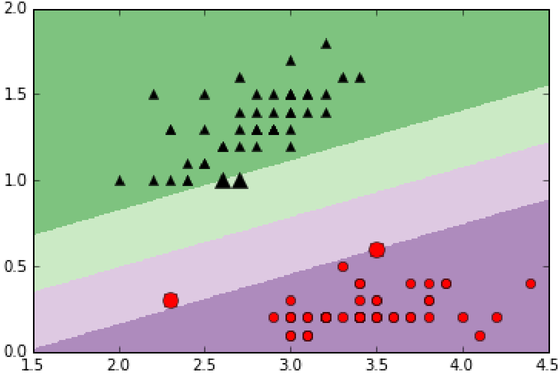
Back to Iris

$C = 10$



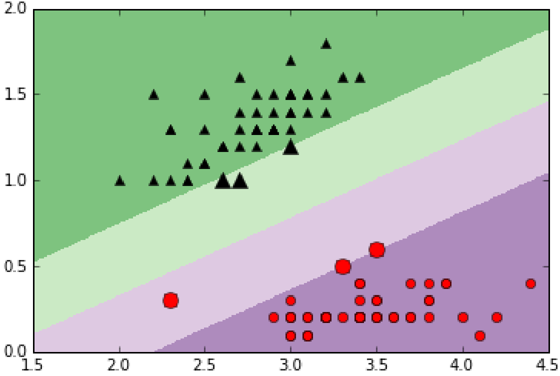
Back to Iris

$C = 3$



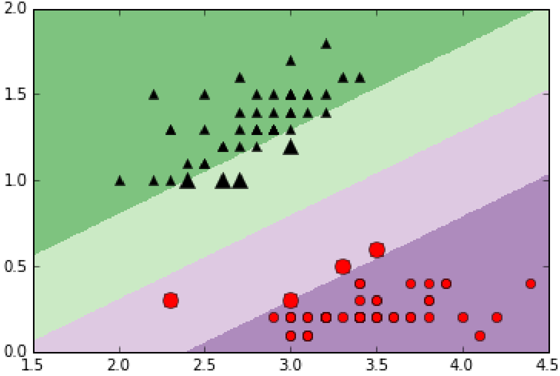
Back to Iris

$C = 2$



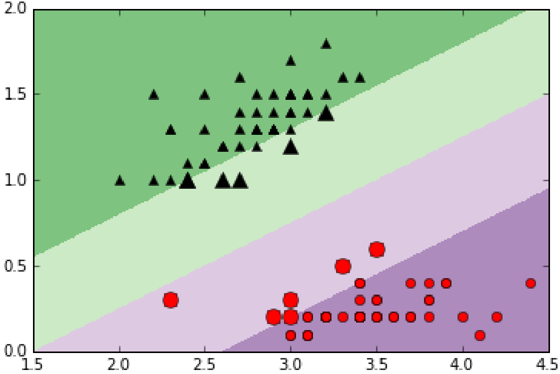
Back to Iris

$C = 1$



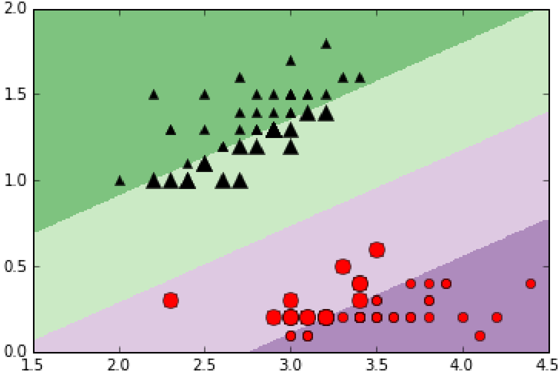
Back to Iris

$C = 0.5$



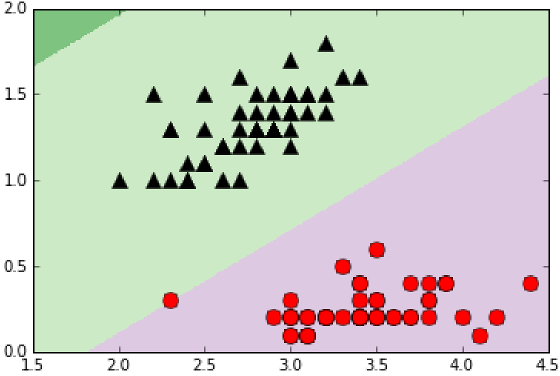
Back to Iris

$C = 0.1$



Back to Iris

$C = 0.01$



Convex surrogates for 0-1 loss

Want a separator w that misclassifies as few training points as possible.

- 0-1 loss: charge $1(y(w \cdot x) < 0)$ for each (x, y)

Problem: this is NP-hard.

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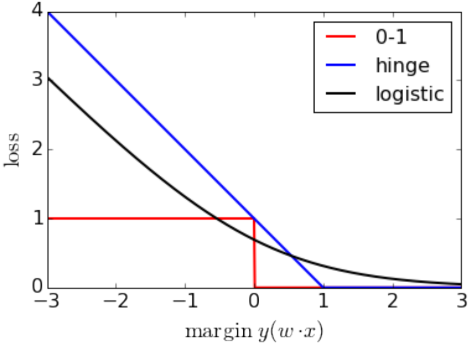

A high-level view of optimization

Unconstrained optimization

Logistic regression: find the vector $w \in \mathbb{R}^p$ that minimizes

$$L(w) = \sum_{i=1}^{n} \ln(1 + \exp(-y^{(i)}(w \cdot x^{(i)})).$$

We know how to check such problems for convexity and how to solve using gradient descent or Newton methods.

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Constrained optimization

Support vector machine: find $w \in \mathbb{R}^p$ and $b \in \mathbb{R}$ that minimize

$$L(w) = \|w\|^2$$

subject to the constraints

$$y^{(i)}(w \cdot x^{(i)} + b) \geq 1$$

What problems of this kind are easy to solve?

Constrained optimization

Write the optimization problem in a standardized form:

$$\min f_o(z)$$
$$f_i(z) \leq 0 \ \text{ for } i = 1, .., m$$
$$h_i(z) = 0 \ \text{ for } i = 1, .., n$$

Special cases that can be solved (relatively) easily:

- **Linear programs.**
  f_o, f_i, h_i are all linear functions.
- **Convex programs.**
  f_o, f_i are convex functions. The h_i are linear functions.

Example: regression with ℓ_1 loss

Given $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \mathbb{R}$, find $w \in \mathbb{R}^p$ minimizing

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Equivalently: let X be the $n \times p$ matrix with rows $x^{(i)}$, and $y = (y^{(1)}, \ldots, y^{(n)})$. Then $L(w) = \|Xw - y\|_1$.

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Optimization problem in $p + n$ variables, $w \in \mathbb{R}^p$ and $z \in \mathbb{R}^n$:

$$\min \sum_{i=1}^{n} z_i$$

$$y^{(i)} - w \cdot x^{(i)} \leq z_i, \quad i = 1, 2, \ldots, n$$

$$w \cdot x^{(i)} - y^{(i)} \leq z_i, \quad i = 1, 2, \ldots, n$$

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A linear program.

The dual of an optimization problem

Take any optimization problem, convex or not:

$$\min f_o(z)$$
$$f_i(z) \leq 0 \quad \text{for } i = 1, .., m$$
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Call this the *primal* problem.

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There is a *dual* optimization problem over $n + m$ variables:

- $\lambda \in \mathbb{R}^m$, one variable for each primal inequality
- $\nu \in \mathbb{R}^n$, one variable for each primal equality

It is a maximization problem:

$$\max g(\lambda, \nu)$$
$$\lambda \geq 0$$

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Constructing the dual is straightforward. But interpreting it is not.

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- KKT (Karush-Kuhn-Tucker) conditions.
  If the f_i and h_i are differentiable, these are first-derivative-equals-zero conditions that hold at optimality.