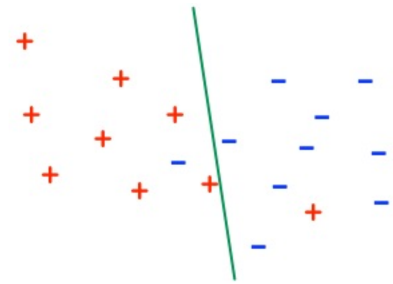
More linear classification

CSE 250B

The decision boundary



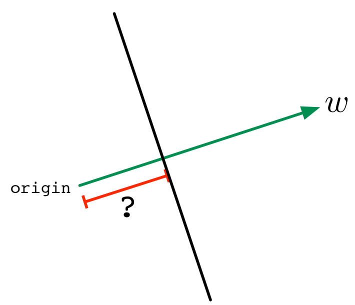
Decision boundary in $\mathbb{R}^p$ is a **hyperplane**.

- 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 $b \in \mathbb{R}$



Can always normalize w to unit length:

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

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

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

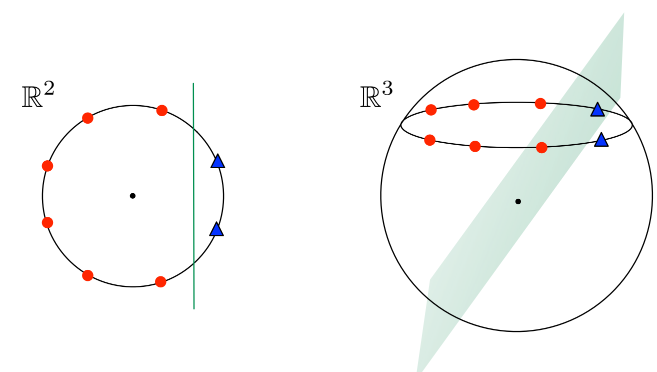
Homogeneous linear separators

Hyperplanes that pass through the origin have no offset, $b = 0$.

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

$$\widetilde{x} = (x, 1) \in \mathbb{R}^{p+1}$$

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



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

$$y^{(i)}(w \cdot x^{(i)}) > 0 \quad \text{for } i = 1, 2, \ldots, n$$

This is linear programming:

- Each data point is a linear constraint on w
- Want to find w that satisfies all these constraints

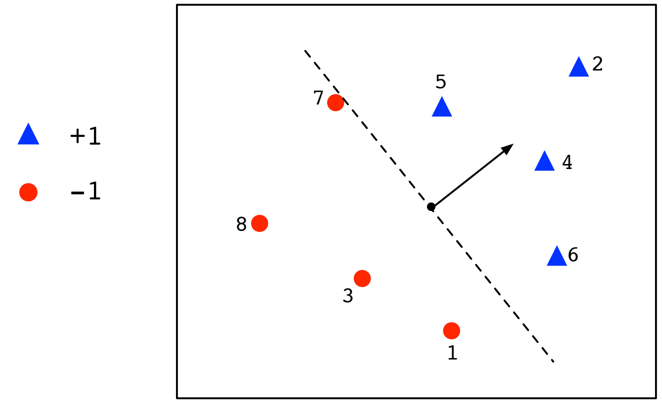
But we won't use generic linear programming methods, such as simplex.

A simple alternative: **Perceptron algorithm** (Rosenblatt, 1958)

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

Perceptron: example

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



Separator: $w = 0 w = -x^{(1)} w = -x^{(1)} + x^{(6)}$

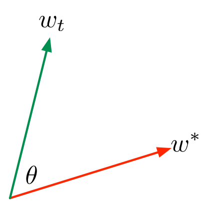
Perceptron: convergence

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

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

Then the Perceptron algorithm converges after at most R^2/γ^2 updates.

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



Track angle between w_t and w^*:

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

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 $y(w^* \cdot x) \geq \gamma$.

1. Initial vector $w_0 = 0$.
2. When updating w_t to w_{t+1}:

$$w_{t+1} \cdot w^* = (w_t + yx) \cdot w^* = w_t \cdot w^* + y(w^* \cdot x) \geq w_t \cdot w^* + \gamma$$
$$\|w_{t+1}\|^2 = \|w_t + yx\|^2 = \|w_t\|^2 + \|x\|^2 + 2y(w_t \cdot x) \leq \|w_t\|^2 + R^2$$

3. After T updates, we have

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

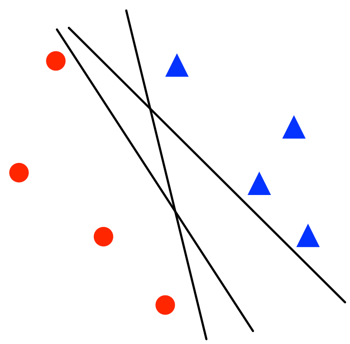
4. The angle between w_T and w^* is given by

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

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.



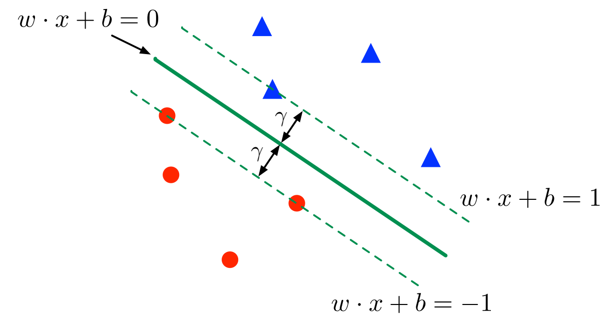
But is there a better, more systematic choice of separator? The one with the most buffer around it, for instance?

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.

By scaling w, b, can equally ask for

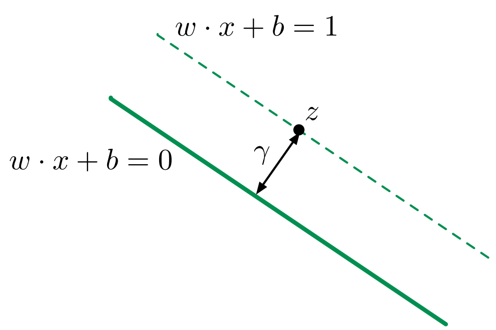
$$y^{(i)}(w \cdot x^{(i)} + b) \geq 1 \quad \text{for all } i.$$



Maximize the **margin** γ.

What is the margin?

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



Let $\widehat{w}$ be the unit vector in the direction of w, i.e. $\widehat{w} = w/\|w\|$.
Then $z - \gamma\widehat{w}$ is on the separator, so

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

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

Maximum-margin linear classifier

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

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

- This is a convex optimization problem:
  - Convex objective function
  - Linear constraints
- It has a dual maximization problem with the same optimum value.

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

Complementary slackness

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

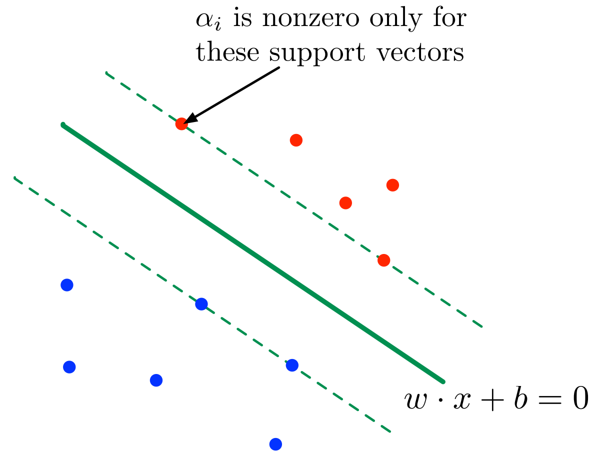
$$\text{(DUAL)} \quad \max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} (x^{(i)} \cdot x^{(j)})$$
$$\text{s.t.:} \quad \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$
$$\alpha \geq 0$$

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

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

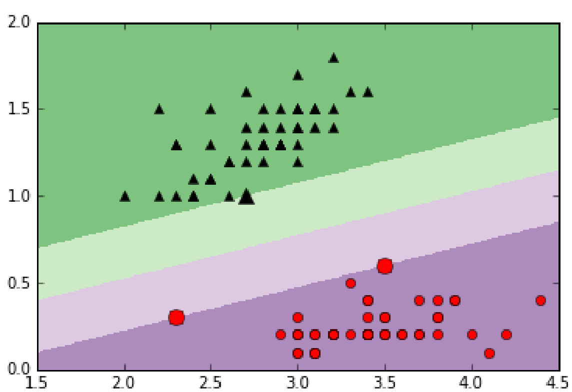
Points $x^{(i)}$ with $\alpha_i > 0$ are called **support vectors**.

Support vectors



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

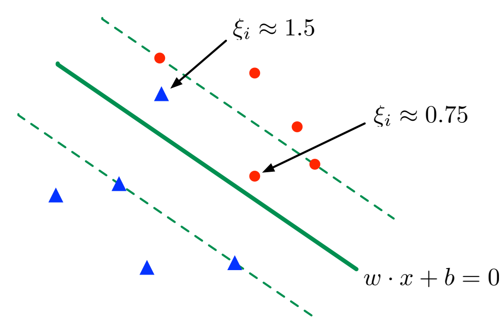
Small example: Iris data set



The non-separable case

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

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



Dual for general case

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

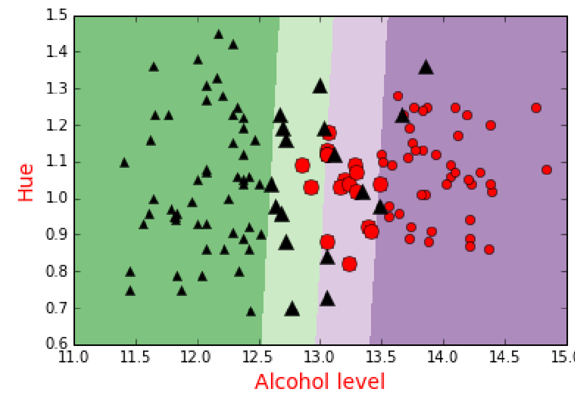
$$\text{(DUAL)} \quad \max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} (x^{(i)} \cdot x^{(j)})$$
$$\text{s.t.: } \sum_{i=1}^n \alpha_i y^{(i)} = 0$$
$$0 \leq \alpha_i \leq C$$

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

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

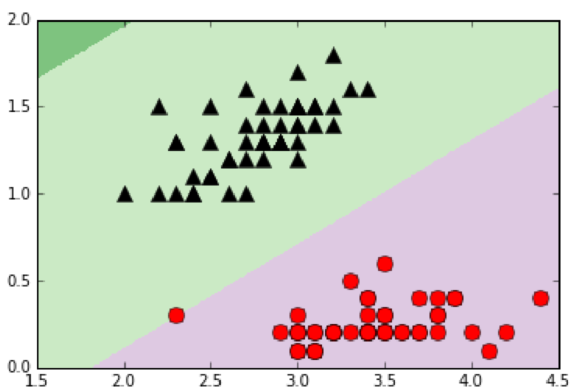
Wine data set

Here $C = 1.0$



Back to Iris

$C = 0.01$



Convex surrogates for 0-1 loss

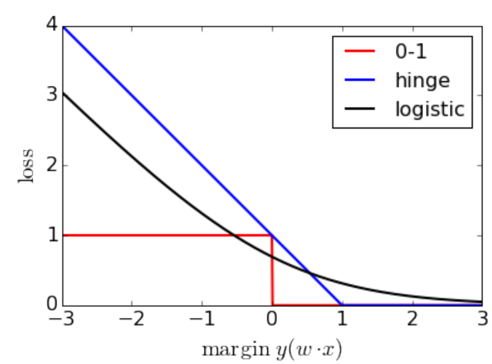
Want a separator w that misclassifies as few training points as possible.

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

Problem: this is NP-hard.

Instead, use **convex** loss functions.

- Hinge loss (SVM): charge $(1 - y(w \cdot x))_+$
- Logistic loss: charge $\ln(1 + e^{-y(w \cdot x)})$



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.

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:

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

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

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

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

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

$$\begin{aligned} &\min \sum_{i=1}^{n} z_i \\ y^{(i)} - w \cdot x^{(i)} &\leq z_i, \quad i = 1, 2, \ldots, n \\ w \cdot x^{(i)} - y^{(i)} &\leq z_i, \quad i = 1, 2, \ldots, n \end{aligned}$$

A linear program.

The dual of an optimization problem

Take any optimization problem, convex or not:

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

Call this the *primal* problem.

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:

$$\begin{aligned} &\max g(\lambda, \nu) \\ &\lambda \geq 0 \end{aligned}$$

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

Duality and complementary slackness

Let z^* and λ^*, ν^* be the optimal primal and dual solutions.

- Weak duality.
  Dual solution is at most the primal solution: $g(\lambda^*, \nu^*) \le f_o(z^*)$.
- Strong duality.
  If primal problem is convex then (almost always, with an easily checkable condition) the primal and dual solutions are equal.
- Complementary slackness.
  If primal and dual solutions are equal, then for any $i = 1, \ldots, m$,

$$\lambda_i^* > 0 \;\Rightarrow\; f_i(z^*) = 0.$$

- 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.