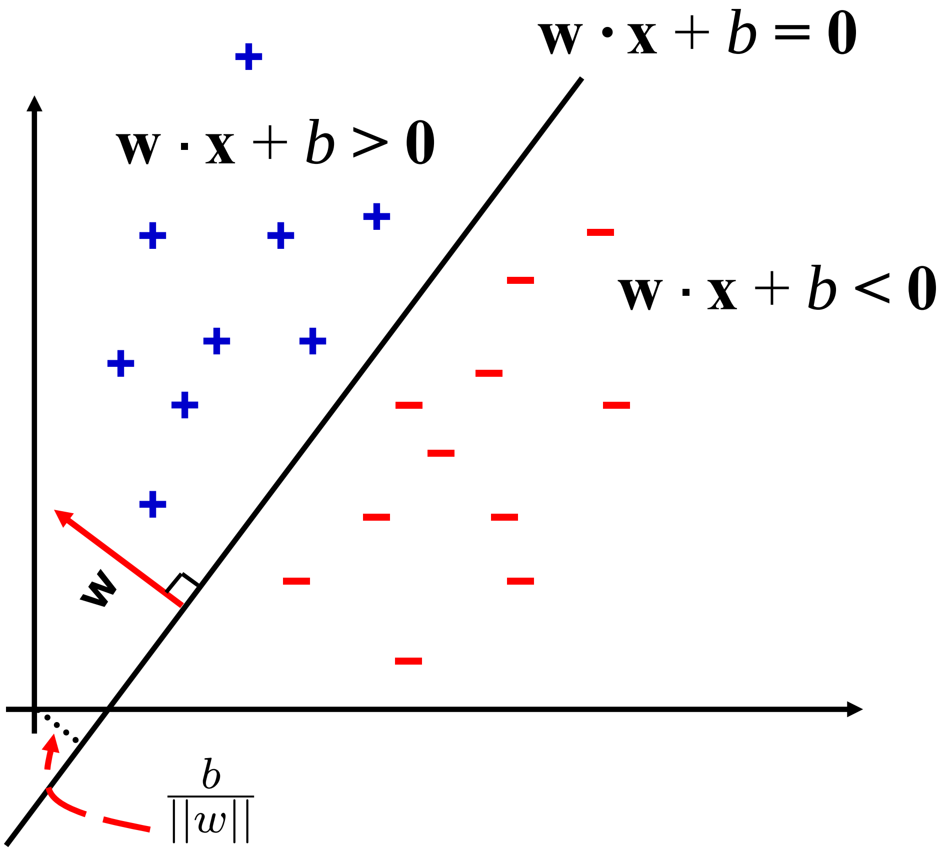
Support Vector Machines

Perceptron Revisited: Linear Separators

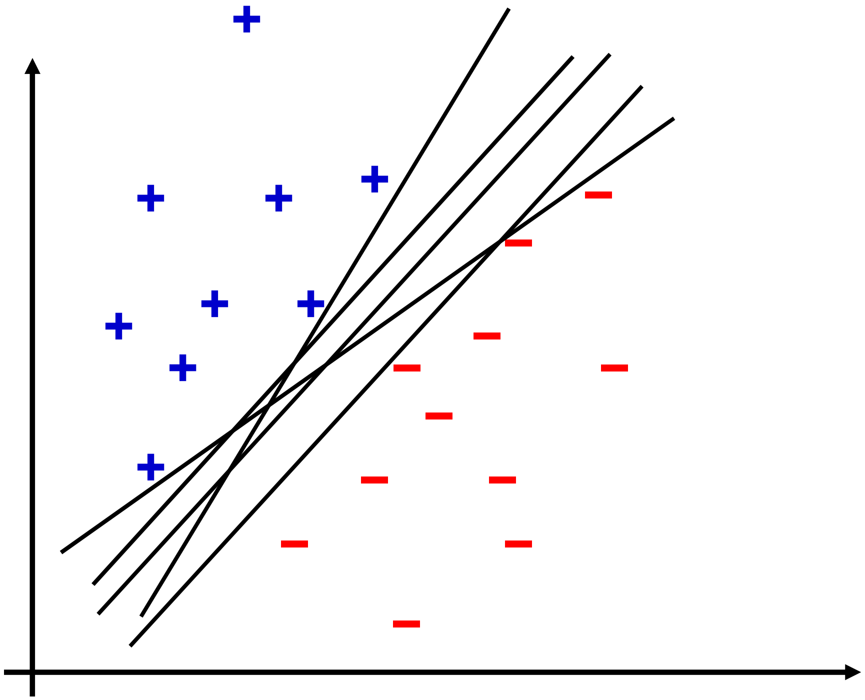
- Binary classification can be viewed as the task of separating classes in feature space:



$$f(\mathbf{x}) = \text{sign}(\mathbf{w}\cdot\mathbf{x}+b)$$

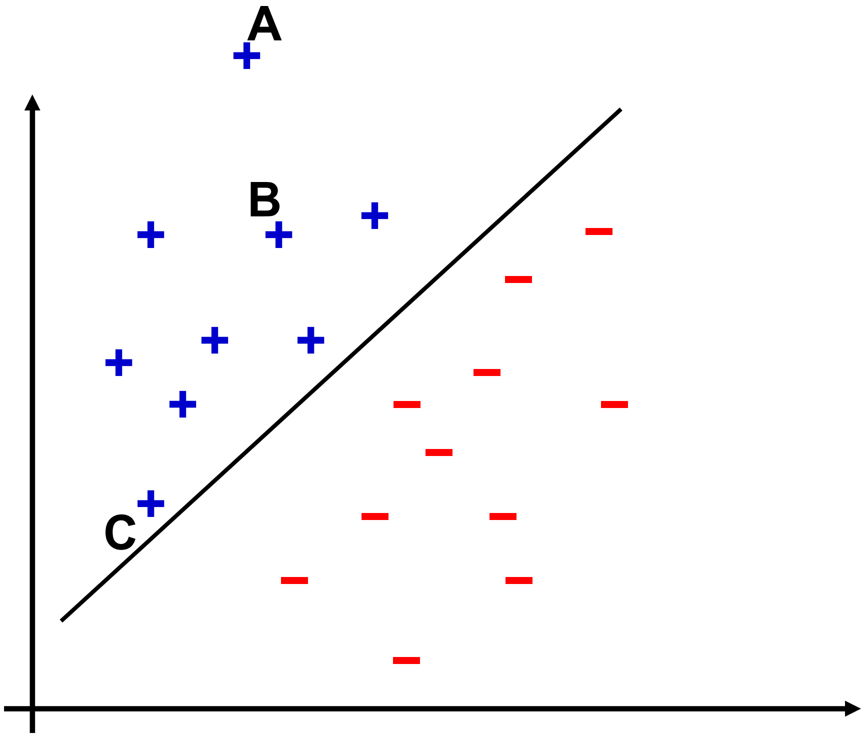
Linear Separators

- Which of the linear separators is optimal?



Intuition of Margin

- Consider points A, B, and C
- We are quite confident in our prediction for A because it is far from the decision boundary.
- In contrast, we are not so confident in our prediction for C because a slight change in the decision boundary may flip the decision.



Given a training set, we would like to make all predictions correct and confident! This leads to the concept of margin.

Functional Margin

- Given a linear classifier parameterized by (**w**, *b*), we define its functional margin w.r.t training example ($\mathbf{x}^i$, y^i) is defined as:

$$\hat{\gamma}^i = y^i(\mathbf{w} \cdot \mathbf{x}^i + b)$$

Note that $\hat{\gamma}^i > 0$ if classified correctly

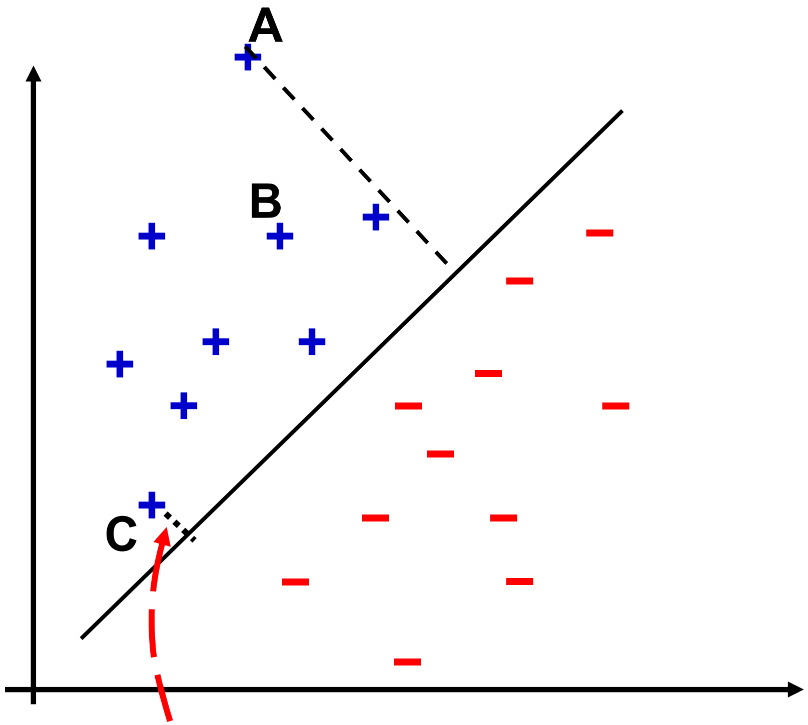
- If we rescale (**w**, *b*) by a factor α, functional margin gets multiplied by α
  - we can make it arbitrarily large without change anything meaningful
  - Instead, we will look at ***geometric margin***

Geometric Margin

- The geometric margin of (**w**, *b*) w.r.t. $\mathbf{x}^{(i)}$ is based on its distance to the decision surface

- This can be captured by:

$$\gamma^i = \frac{y^i(\mathbf{w} \cdot \mathbf{x}^i + b)}{\|\mathbf{w}\|}$$



- Given training set $S=\{(\boldsymbol{x}^i, y^i): i=1,\ldots, N\}$, the geometric margin of the classifier w.r.t. *S* is

$$\gamma = \min_{i=1 \cdots N} \gamma^{(i)}$$

Points closest to the boundary are called Support vectors – we will see that these are the points that really matters

Maximum Margin Classifier

- Given a linearly separable training set S={($\boldsymbol{x}^{(i)}$, $y^{(i)}$): $i=1,\ldots,N$}, we would like to find a linear classifier with maximum margin.
- This can be represented as an optimization problem.

$$\max_{\mathbf{w},b,\gamma} \gamma$$

$$\text{subject to}: \; y^{(i)} \frac{(\mathbf{w} \cdot \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|} \geq \gamma, \quad i = 1, \cdots, N$$

Nasty optimization problem! Let’s make it look nicer!

- Let $\gamma' = \gamma \cdot \|w\|$, this is equivalent to

$$\max_{\mathbf{w},b,\gamma'} \frac{\gamma'}{\|\mathbf{w}\|}$$

$$\text{subject to}: \; y^{i} (\mathbf{w} \cdot \mathbf{x}^{i} + b) \geq \gamma', \quad i = 1, \cdots, N$$

Maximum Margin Classifier

- Note that rescaling **w** and *b* by (1/γ') will not change the classifier, we can thus further reformulate the optimization problem

$$\max_{\mathbf{w},b} \frac{\gamma'}{\|\mathbf{w}\|}$$
$$\text{subject to: } \; y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq \gamma', \quad i = 1,\cdots,N$$

$$\Downarrow$$

$$\max_{\mathbf{w},b} \frac{1}{\|\mathbf{w}\|} \;\; (\text{or equivalently } \min_{\mathbf{w},b}\|\mathbf{w}\|^2)$$
$$\text{subject to: } \; y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1, \quad i = 1,\cdots,N$$

Maximizing the geometric margin is equivalent to minimizing the magnitude of **w** subject to maintaining a functional margin of at least 1

Solving the Optimization Problem

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

$$\text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1, \quad i = 1,\cdots,N$$

- This results in a ***quadratic optimization problem*** with *linear inequality constraints.*
- This is a well-known class of mathematical programming problems for which several (non-trivial) algorithms exist.
  - One could solve for w using any of these methods
- We will see that it is useful to first formulate an equivalent dual optimization problem and solve it instead
  - This requires a bit of machinery

Aside: Constrained Optimization

- To solve the following optimization problem

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{subject to} \quad g_i(\mathbf{x}) \leq 0 \quad \text{for } i = 1, \ldots, m$$

- Consider the following function known as the Lagrangian

$$\mathcal{L}(x, \alpha) = f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x})$$

- Under certain conditions it can be shown that for a solution x' to the above problem we have

$$f(x') = \underbrace{\min_x \max_\alpha \mathcal{L}(x, \alpha)}_{\text{Primal form}} = \underbrace{\max_\alpha \min_x \mathcal{L}(x, \alpha)}_{\text{Dual form}}$$

$$\text{subject to } \alpha_i \geq 0$$

Back to the Original Problem

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$

$$\text{subject to}: 1 - y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \le 0, \quad i = 1, \cdots, N$$

- The Lagrangian is

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}\cdot\mathbf{w} + \sum_{i=1}^{N}\alpha_i\{1 - y^i(\mathbf{w}\cdot\mathbf{x}^i + b)\}, \text{ subject to } \alpha_i \ge 0$$

- We want to solve $\max_{\alpha} \min_{w,b} \mathcal{L}(w, b, \alpha) \;\; s.t. \;\; \alpha_i \ge 0$

- Setting the gradient of $\mathcal{L}$ w.r.t. **w** and b to zero, we have

$$\mathbf{w} - \sum_{i=1}^{N}\alpha_i y^i \mathbf{x}^i = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{N}\alpha_i y^i \mathbf{x}^i$$

$$\sum_{i=1}^{N}\alpha_i y^i = 0$$

The Dual Problem

- If we substitute $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y^i \mathbf{x}^i$ to $\mathcal{L}$, we have

$$
\begin{aligned}
L(\boldsymbol{\alpha}) &= \frac{1}{2}\mathbf{w}\cdot\mathbf{w} - \sum_{i=1}^{N} \alpha_i \{y^i(\mathbf{w}\cdot\mathbf{x}^i + b) - 1\} \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i\alpha_j y^i y^j < \mathbf{x}^i \cdot \mathbf{x}^j > - \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i\alpha_j y^i y^j < \mathbf{x}^i \cdot \mathbf{x}^j > - b\sum_{i=1}^{N}\alpha_i y^i + \sum_{i=1}^{N}\alpha_i \\
&= \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i\alpha_j y^i y^j < \mathbf{x}^i \cdot \mathbf{x}^j >
\end{aligned}
$$

- Note that $\sum_{i=1}^{N} \alpha_i y^i = 0$
- This is a function of α_i only

The Dual Problem

- The new objective function is in terms of α_i only
- It is known as the dual problem: if we know all α_i, we know **w**
- The original problem is known as the primal problem
- The objective function of the dual problem needs to be maximized!
- The dual problem is therefore:

$$\max L(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y^i y^j < \mathbf{x}^i \cdot \mathbf{x}^j >$$

$$\text{subject to} \quad \alpha_i \geq 0, i = 1, \ldots, n, \qquad \sum_{i=1}^{N} \alpha_i y^i = 0$$

Properties of α_i when we introduce the Lagrange multipliers

The result when we differentiate the original Lagrangian w.r.t. b

The Dual Problem

$$\max L(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y^i y^j < \mathbf{x}^i \cdot \mathbf{x}^j >$$

$$\text{subject to} \quad \alpha_i \geq 0, i = 1, \ldots, n, \qquad \sum_{i=1}^{N} \alpha_i y^i = 0$$

- This is also quadratic programming (QP) problem
  - A global maximum of α_i can always be found
- **w** can be recovered by $\mathbf{w} = \sum_{i=1}^{N} \alpha_i y^i \mathbf{x}^i$
- b can also be recovered as well (wait for a bit)

Characteristics of the Solution

- Many of the α_i are zero
  - **w** is a linear combination of only a small number of data points
- In fact, optimization theory requires that the solution to satisfy the following KKT conditions:

$$\alpha_i \geq 0, i = 1, \ldots, n,$$

$$y^i(\sum_{j=1}^{N} \alpha_i y^j < \mathbf{x}^j \cdot \mathbf{x}^i > + \mathrm{b}) \geq 1$$

Functional margin ≥ 1

$$\alpha_i \{y^i(\sum_{j=1}^{N} \alpha_i y^j < \mathbf{x}^j \cdot \mathbf{x}^i > + \mathrm{b}) - 1\} = 0$$

α_i is nonzero only when functional margin = 1

- $\mathbf{x}_i$ with non-zero α_i are called support vectors (SV)
  - The decision boundary is determined only by the SV
  - Let t_j (j=1, ..., s) be the indices of the s support vectors. We can write

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y^{t_j} \mathbf{x}^{t_j}$$

Solve for b

- Note that we know that for support vectors the functional margin = 1
- We can use this information to solve for b
- We can use any support vector to achieve this

$$y^i\left(\sum_{j=1}^{s} \alpha_{t_j} y^{t_j} < \mathbf{x}^{t_j} \cdot \mathbf{x}^i > + \mathrm{b}\right) = 1$$

- A numerically more stable solution is to use all support vectors (details in the book)

Classifying new examples

- For classifying with a new input **z**
  - Compute $\mathbf{w}^T\mathbf{x} + b = \sum_{j=1}^{s} \alpha_{t_j} y^{t_j} < \mathbf{x}^{t_j} \cdot \mathbf{x} > + b$ and classify **z** as positive if the sum is positive, and negative otherwise
  - Note: **w** need not be formed explicitly, rather we can classify z by taking a weighted sum of the inner products with the support vectors

    (useful when we generalize from inner product to kernel functions later)

The Quadratic Programming Problem

- Many approaches have been proposed
  - Loqo, cplex, etc. (see http://www.numerical.rl.ac.uk/qp/qp.html)
- Most are "interior-point" methods
  - Start with an initial solution that can violate the constraints
  - Improve this solution by optimizing the objective function and/or reducing the amount of constraint violation
- For SVM, sequential minimal optimization (SMO) seems to be the most popular
  - A QP with two variables is trivial to solve
  - Each iteration of SMO picks a pair of (α_i, α_j) and solve the QP with these two variables; repeat until convergence
- In practice, we can just regard the QP solver as a "black-box" without bothering how it works

A Geometrical Interpretation