Universidad Tecnológica de Bolívar
CARTAGENA DE INDIAS

Machine Learning

Support Vector Machines

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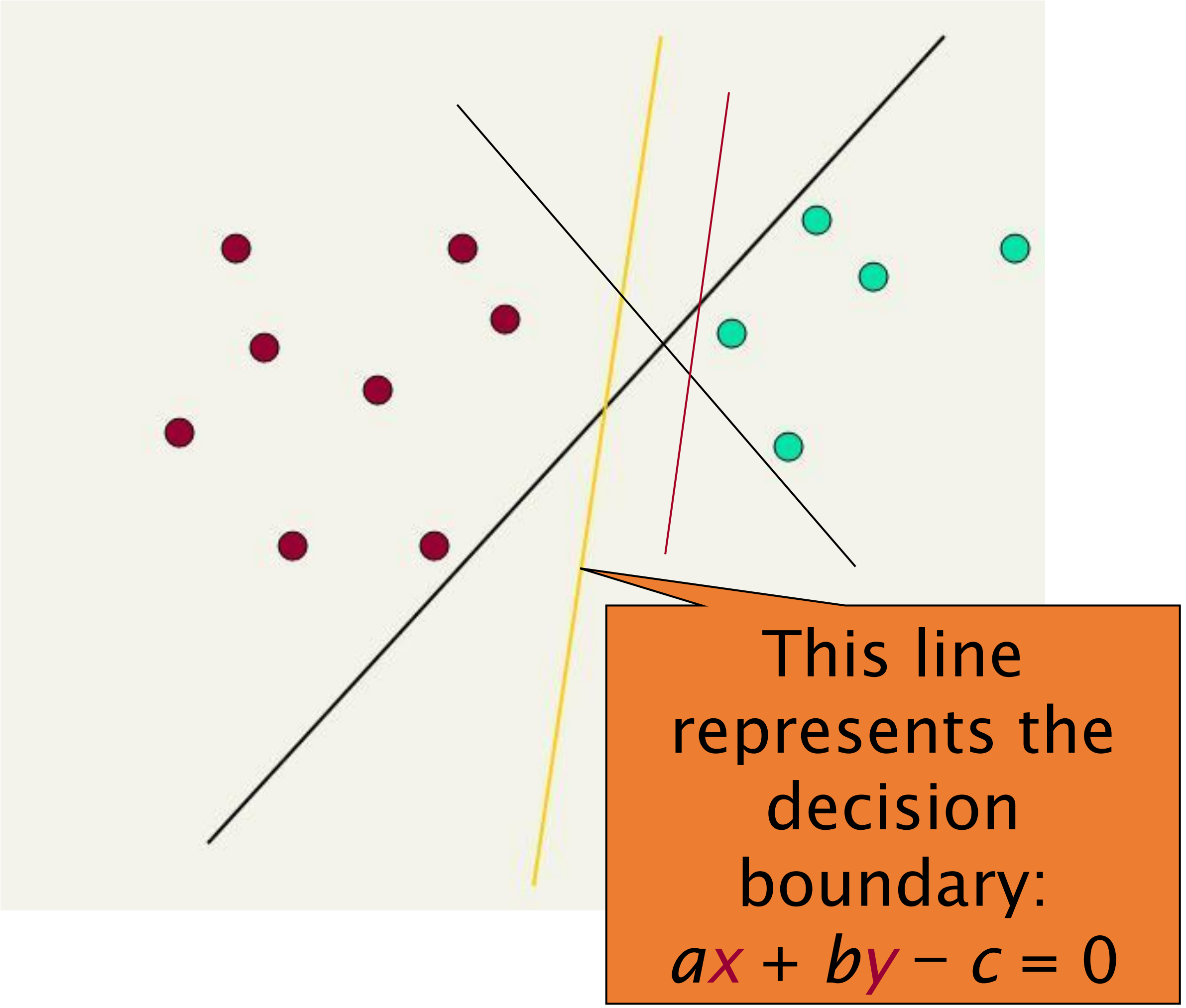
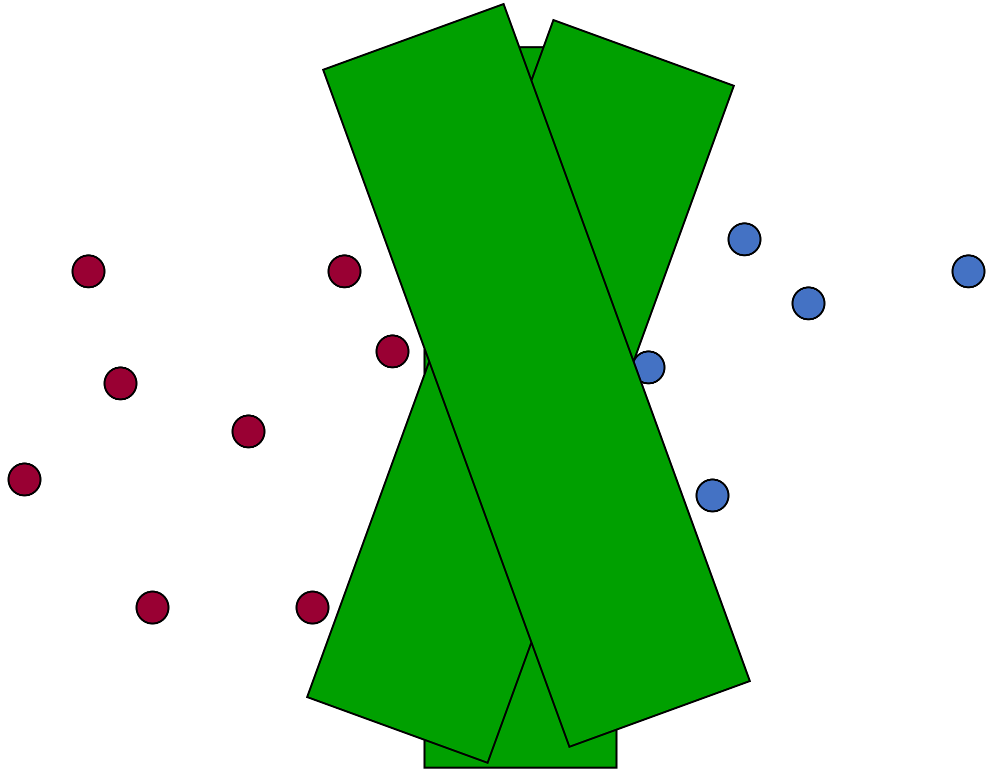
Linear classifiers: Which Hyperplane?

- Lots of possible solutions for *a, b, c.*
- Some methods find a separating hyperplane, but not the optimal one [according to some criterion of expected goodness]
  - E.g., perceptron
- Support Vector Machine (SVM) finds an optimal* solution.
  - Maximizes the distance between the hyperplane and the “difficult points” close to decision boundary
  - One intuition: if there are no points near the decision surface, then there are no very uncertain classification decisions



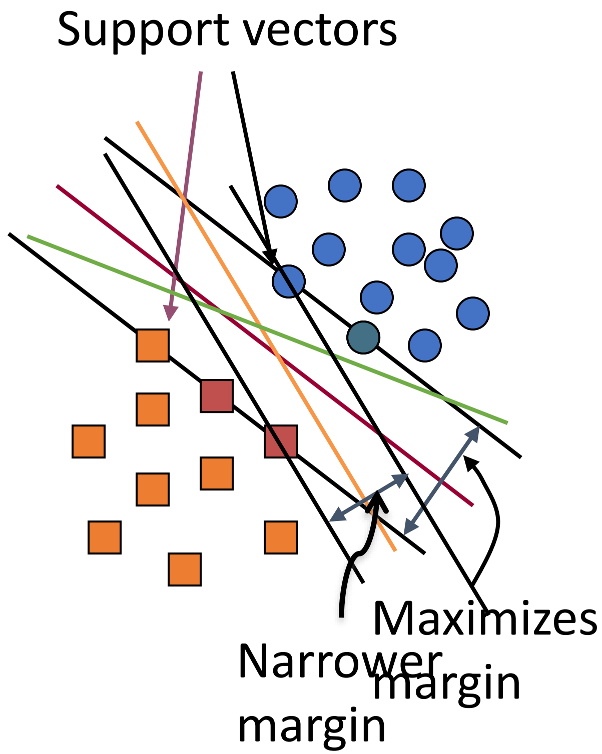
Another intuition

If you have to place a fat separator between classes, you have less choices, and so the capacity of the model has been decreased



Support Vector Machine (SVM)

- SVMs maximize the *margin* around the separating hyperplane.
  - A.k.a. large margin classifiers
- The decision function is fully specified by a subset of training samples, *the support vectors*.
- Solving SVMs is a *quadratic programming* problem
- Seen by many as the most successful current text classification method*



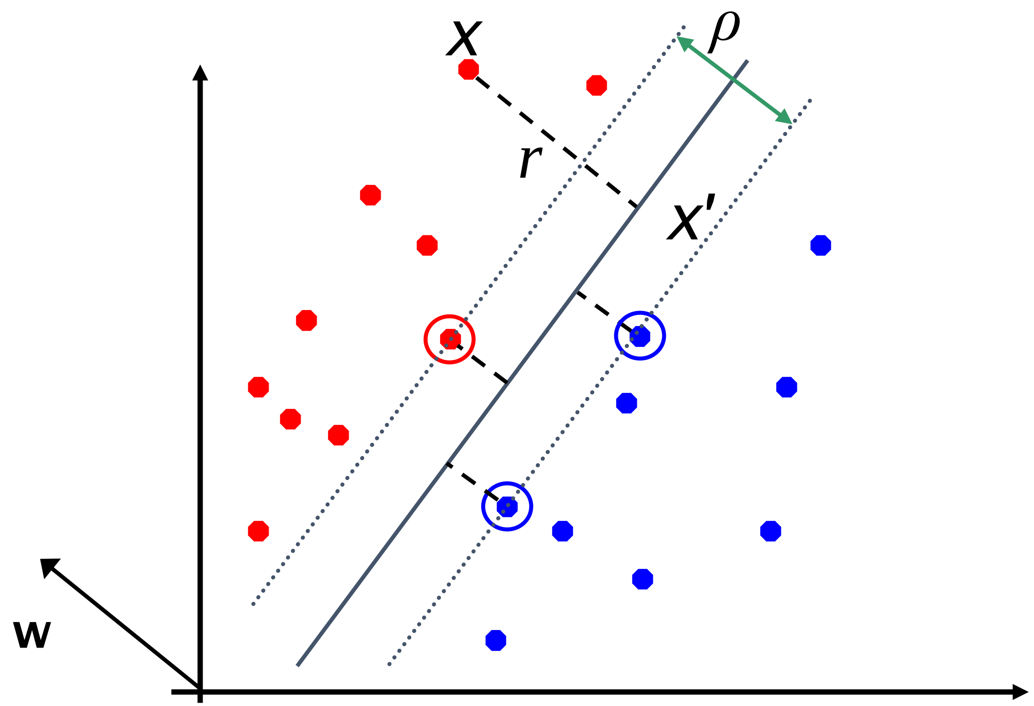
*but other discriminative methods often perform very similarly

Maximum Margin: Formalization

- **w**: decision hyperplane normal vector
- $\mathbf{x}_i$: data point *i*
- y_i: class of data point *i* (+1 or -1)   NB: Not 1/0
- Classifier is: $f(\mathbf{x}_i) = \text{sign}(\mathbf{w}^T\mathbf{x}_i + b)$
- Functional margin of $\mathbf{x}_i$ is: $y_i\,(\mathbf{w}^T\mathbf{x}_i + b)$
  - But note that we can increase this margin simply by scaling **w**, **b**….
- Functional margin of dataset is twice the minimum functional margin for any point
  - The factor of 2 comes from measuring the whole width of the margin

Geometric Margin

- Distance from example to the separator is $$r = y\frac{\mathbf{w}^T\mathbf{x}+b}{\|\mathbf{w}\|}$$
- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the width of separation between support vectors of classes.



Derivation of finding *r:*
Dotted line $\mathbf{x}'-\mathbf{x}$ is perpendicular to decision boundary so parallel to $\mathbf{w}$.
Unit vector is $\mathbf{w}/|\mathbf{w}|$, so line is $r\mathbf{w}/|\mathbf{w}|$.
$\mathbf{x}' = \mathbf{x} - yr\mathbf{w}/|\mathbf{w}|$.
$\mathbf{x}'$ satisfies $\mathbf{w}^T\mathbf{x}'+b = 0$.
So $\mathbf{w}^T(\mathbf{x} - yr\mathbf{w}/|\mathbf{w}|) + b = 0$
Recall that $|\mathbf{w}| = \text{sqrt}(\mathbf{w}^T\mathbf{w})$.
So $\mathbf{w}^T\mathbf{x} - yr|\mathbf{w}| + b = 0$
So, solving for r gives:
$r = y(\mathbf{w}^T\mathbf{x} + b)/|\mathbf{w}|$

Linear SVM Mathematically

The linearly separable case

- Assume that all data is at least distance 1 from the hyperplane, then the following two constraints follow for a training set $\{(\mathbf{x_i}, y_i)\}$

$$\mathbf{w^T x_i} + b \geq 1 \quad \text{if } y_i = 1$$

$$\mathbf{w^T x_i} + b \leq -1 \quad \text{if } y_i = -1$$

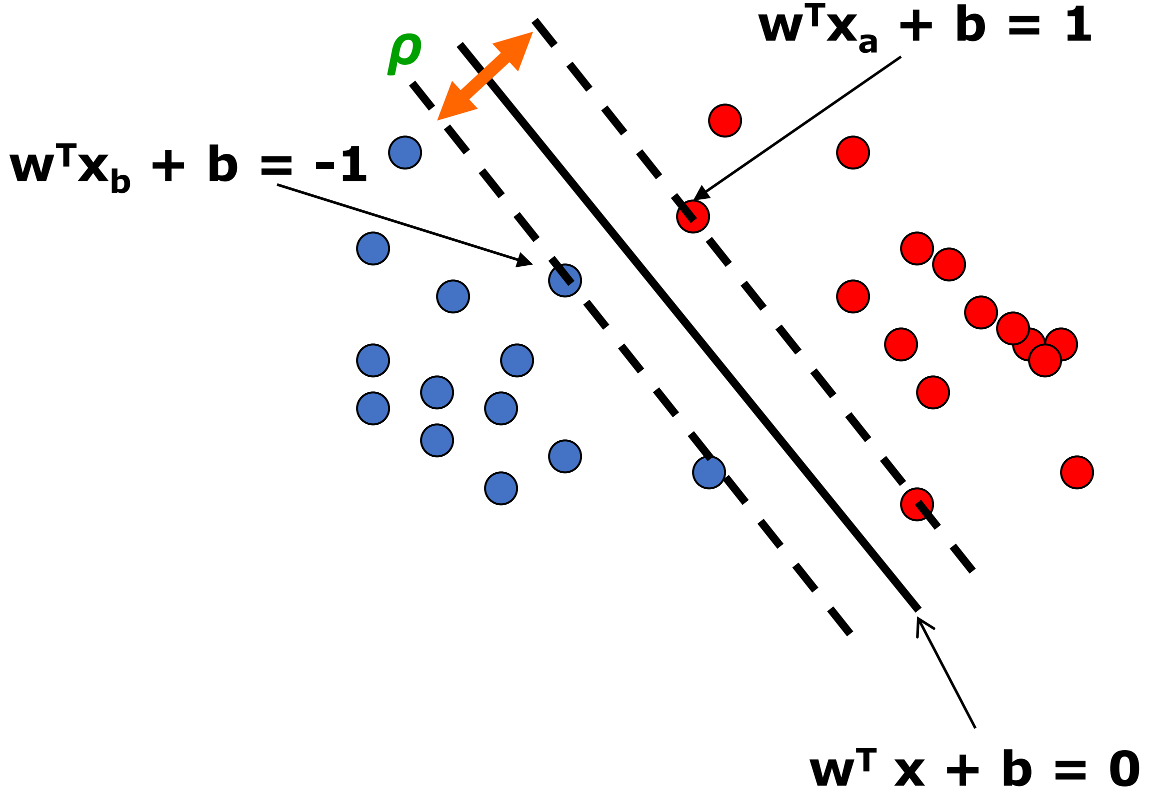
- For support vectors, the inequality becomes an equality
- Then, since each example's distance from the hyperplane is

$$r = y\frac{\mathbf{w}^T\mathbf{x} + b}{\|\mathbf{w}\|}$$

- The margin is: $r = \dfrac{2}{\|\mathbf{w}\|}$

Linear Support Vector Machine (SVM)

- **Hyperplane**
- $\mathbf{w}^T \mathbf{x} + b = 0$
- **Extra scale constraint**:
- $\min_{i=1,\dots,n} |\mathbf{w}^T \mathbf{x}_i + \mathbf{b}| = 1$
- This implies:
- $w^T(x_a - x_b) = 2$
- $\rho = ||x_a - x_b||_2 = 2/||\mathbf{w}||_2$



Linear SVMs Mathematically (cont.)

- Then we can formulate the *quadratic optimization problem:*

Find $\mathbf{w}$ and b such that

$r = \dfrac{2}{\|\mathbf{w}\|}$ is maximized; and for all $\{(\mathbf{x_i}, y_i)\}$

$\mathbf{w^T x_i} + b \geq 1$ if $y_i = 1$; $\mathbf{w^T x_i} + b \leq -1$ if $y_i = -1$

- A better formulation (min **||w||** = max 1/ **||w||**):

Find $\mathbf{w}$ and b such that

$\mathbf{\Phi(w)} = \frac{1}{2}\, \mathbf{w}^{\mathrm{T}}\mathbf{w}$ is minimized;

and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i (\mathbf{w^T x_i} + b) \geq 1$

Solving the Optimization Problem

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = ½\ \mathbf{w}^{\mathrm{T}}\mathbf{w}$ is minimized;
and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i (\mathbf{w^T x_i} + b) \geq 1$

- This is now optimizing a *quadratic* function subject to *linear* constraints
- Quadratic optimization problems are a well-known class of mathematical programming problem, and many (intricate) algorithms exist for solving them (with many special ones built for SVMs)
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every constraint in the primary problem:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i^T x_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

The Optimization Problem Solution

- The solution has the form:

$$\boxed{\mathbf{w} = \Sigma \alpha_i y_i \mathbf{x_i} \qquad b = y_k - \mathbf{w^T x_k} \text{ for any } \mathbf{x_k} \text{ such that } \alpha_k \neq 0}$$

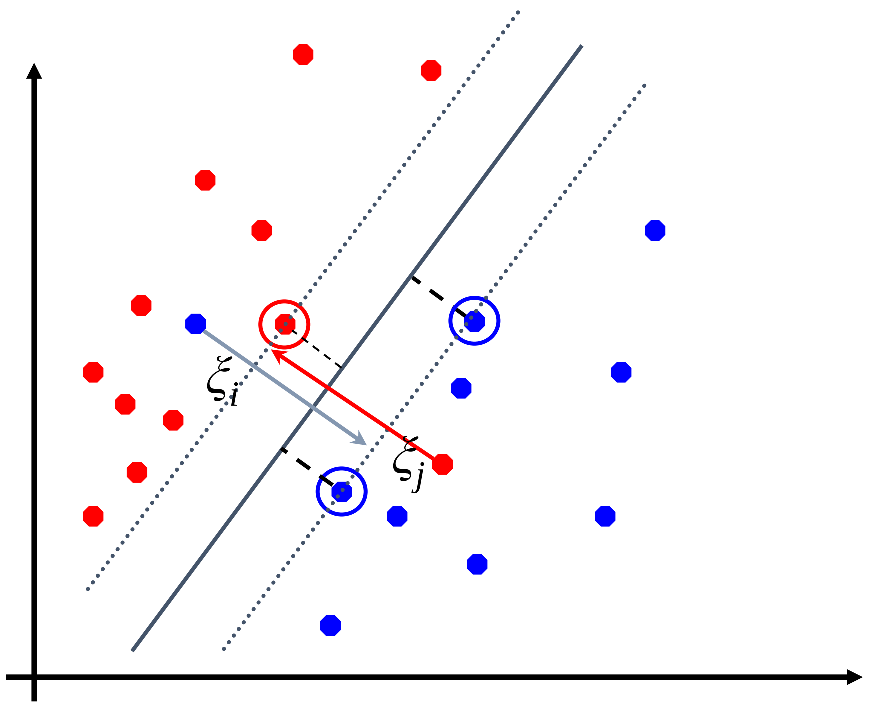
- Each non-zero α_i indicates that corresponding $\mathbf{x_i}$ is a support vector.
- Then the classifying function will have the form:

$$\boxed{f(\mathbf{x}) = \Sigma \alpha_i y_i \mathbf{x_i^T x} + b}$$

- Notice that it relies on an *inner product* between the test point $\mathbf{x}$ and the support vectors $\mathbf{x_i}$
  - We will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x_i^T x_j}$ between all pairs of training points.

Soft Margin Classification

- If the training data is not linearly separable, *slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.
- Allow some errors
    - Let some points be moved to where they belong, at a cost
- Still, try to minimize training set errors, and to place hyperplane "far" from each class (large margin)



Soft Margin Classification Mathematically

- The old formulation:

> Find $\mathbf{w}$ and b such that
> $\boldsymbol{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^{\mathrm{T}}\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
> $y_i\, (\mathbf{w^T x_i} + \mathrm{b}) \geq 1$

- The new formulation incorporating slack variables:

> Find $\mathbf{w}$ and b such that
> $\boldsymbol{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^{\mathrm{T}}\mathbf{w} + C\Sigma\xi_i$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
> $y_i\, (\mathbf{w^T x_i} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i

- Parameter *C* can be viewed as a way to control overfitting
  - A regularization term

Soft Margin Classification – Solution

- The dual problem for soft margin classification:

Find $\alpha_1 \ldots \alpha_N$ such that

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^{\mathbf{T}}\mathbf{x_j}$ is maximized and

(1) $\Sigma\alpha_i y_i = 0$

(2) $0 \leq \alpha_i \leq C$ for all α_i

- Neither slack variables ξ_i nor their Lagrange multipliers appear in the dual problem!
- Again, $\mathbf{x_i}$ with non-zero α_i will be support vectors.
- Solution to the dual problem is:

$\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x_i}$

$b = y_k(1 - \xi_k) - \mathbf{w}^{\mathbf{T}}\mathbf{x}_k$ where $k = \underset{k'}{\operatorname{argmax}}\, \alpha_{k'}$

w is not needed explicitly for classification!

$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x_i}^{\mathbf{T}}\mathbf{x} + b$

Classification with SVMs

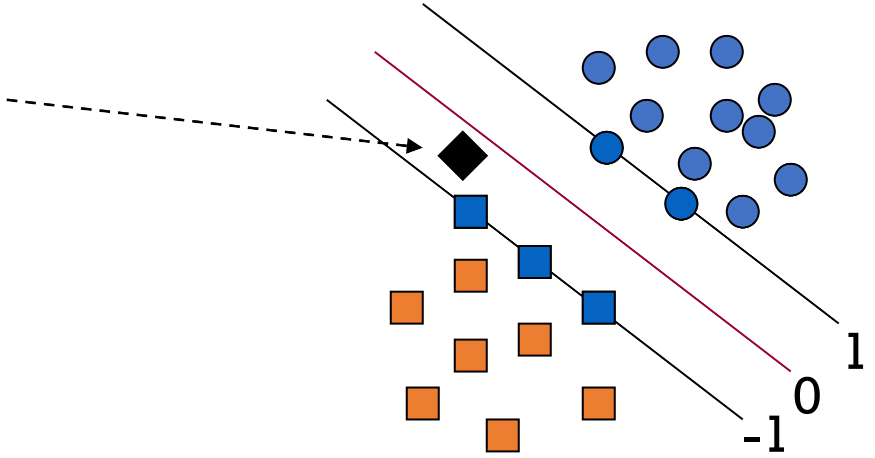
- Given a new point $\mathbf{x}$, we can score its projection onto the hyperplane normal:
  - I.e., compute score: $\mathbf{w}^T\mathbf{x} + b = \Sigma\alpha_i y_i \mathbf{x}_\mathbf{i}^T\mathbf{x} + b$
    - Decide class based on whether < or > 0

  - Can set confidence threshold t.

Score > t: yes

Score < -t: no

Else: don’t know



Linear SVMs: Summary

- The classifier is a *separating hyperplane.*
- The most "important" training points are the support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_\mathbf{i}$ are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation of the problem and in the solution, training points appear only inside inner products:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \boxed{\mathbf{x}_\mathbf{i}^\mathbf{T}\mathbf{x}_\mathbf{j}}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

$$f(\mathbf{x}) = \Sigma\alpha_i y_i \boxed{\mathbf{x}_\mathbf{i}^\mathbf{T}\mathbf{x}} + b$$