香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning
Lecture 6

# Support Vector Machines

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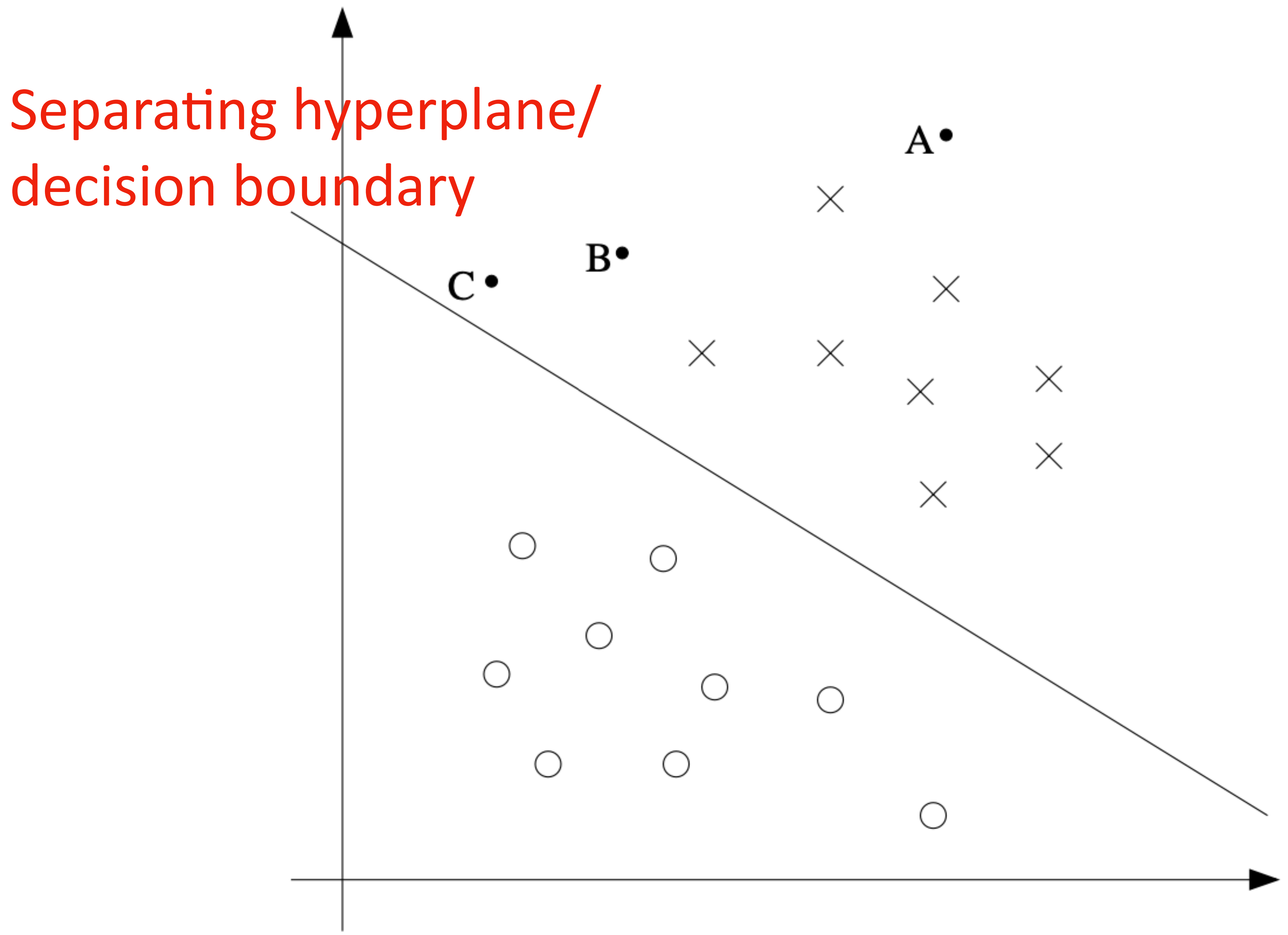
# Recap: Support Vector Machines



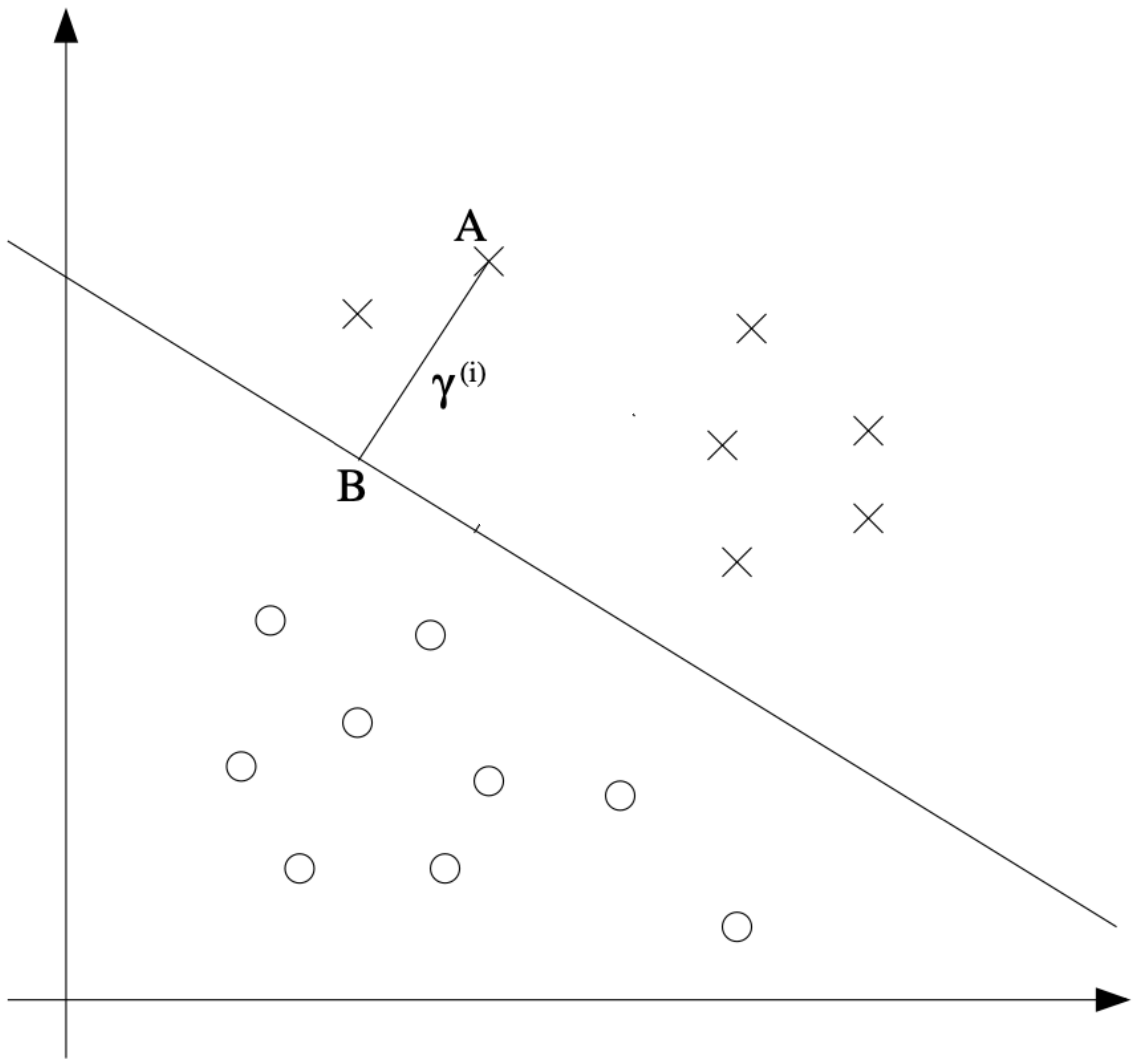
# Recap: Notations

Consider a binary classification problem, with the input feature $x$ and $y \in \{-1, 1\}$ (instead of $\{0, 1\}$), the classifier is:

$$h_{w,b}(x) = g(w^T x + b).$$

$$g(z) = 1 \text{ if } z \geq 0, \text{ and } g(z) = -1$$

# Recap: Geometric Margin




What is the geometric margin?

# Recap: Functional Margin

Given a training example $(x^{(i)}, y^{(i)})$

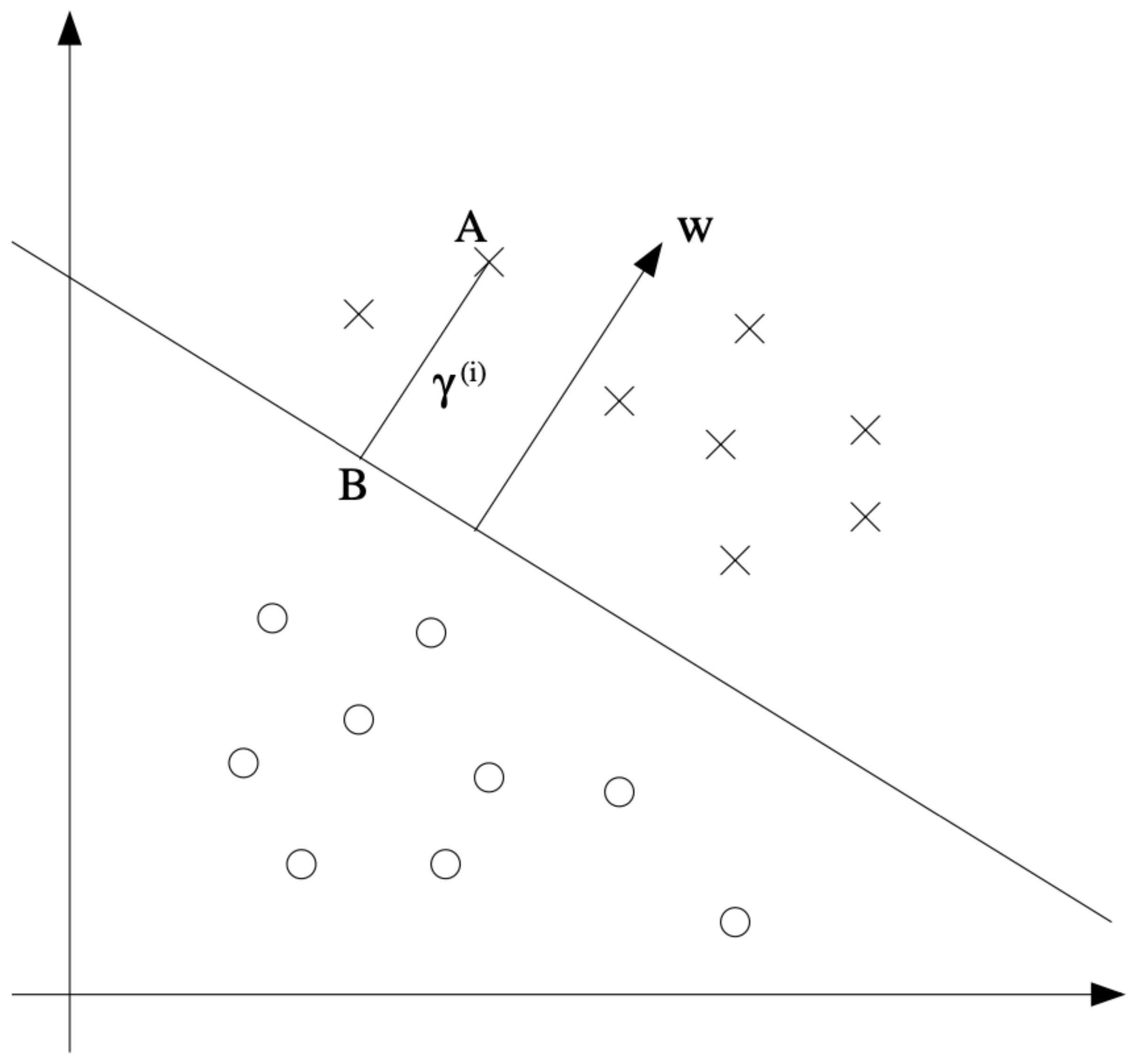
$$\hat{\gamma}^{(i)} = y^{(i)}(w^T x^{(i)} + b).$$

Given a training set $S = \{(x^{(i)}, y^{(i)}); i = 1,\ldots,n\}$

$$\hat{\gamma} = \min_{i=1,\ldots,n} \hat{\gamma}^{(i)}$$

Functional margin changes rescaling parameters, making it a bad objective, e.g. when w->2w, b->2b, the functional margin changes while the separating plane does not really change

# Recap: Geometric Margin




$$w^T\left(x^{(i)} - \gamma^{(i)}\frac{w}{||w||}\right) + b = 0.$$

$$\gamma^{(i)} = \frac{w^T x^{(i)} + b}{||w||} = \left(\frac{w}{||w||}\right)^T x^{(i)} + \frac{b}{||w||}$$

Generally

$$\gamma^{(i)} = y^{(i)}\left(\left(\frac{w}{||w||}\right)^T x^{(i)} + \frac{b}{||w||}\right)$$

# Recap: Geometric Margin

Given a training set $S = \{(x^{(i)}, y^{(i)}); i = 1,\ldots,n\}$

$$\gamma = \min_{i=1,\ldots,n} \gamma^{(i)}$$

# Recap: The Optimization Problem

Rewrite

$$\max_{w,b} \min_{i=1,\dots,n} \gamma^{(i)} \quad \Rightarrow \quad \max_{\gamma,w,b} \ \gamma$$

$$\text{s.t.} \quad y^{(i)}\left(\left(\frac{w}{\|w\|}\right)^T x^{(i)} + \frac{b}{\|w\|}\right) \geq \gamma, \ i = 1, \cdots, n$$

Linear constraint

$$\Rightarrow \quad \max_{\hat{\gamma},w,b} \quad \frac{\hat{\gamma}}{||w||}$$

$$\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq \hat{\gamma}, \quad i = 1, \dots, n$$

Infinite solutions, as $\hat{\gamma}$ can be at any scale without changing the classifier

||w|| is not easy to deal with, non-convex objective

# Recap: The Optimization Problem

$$\max_{\hat{\gamma},w,b} \quad \frac{\hat{\gamma}}{||w||}$$
$$\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq \hat{\gamma}, \quad i = 1, \ldots, n$$

Add constraint $\hat{\gamma} = 1$

$$\min_{w,b} \quad \frac{1}{2}||w||^2$$
$$\text{s.t.} \quad y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad i = 1, \ldots, n$$

This is a standard quadratic problem that can be directly solved with quadratic problem solvers

Assumption: the training dataset is linearly separable

# The Dual Problem in Optimization

In optimization, sometimes the primal optimization is hard to solve, then we may find a related alternative optimization problem that can be solved more easily, to solve the orignal problem in an indirect way

# Quadratic Program

$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}||w||^2 \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad i = 1, \ldots, n \end{aligned}$$

This is already a standard convex opt problem that is ready to be solved, why are we doing all the rest of things?

# Lagrange Duality — Lagrange Multiplier

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & h_i(w) = 0, \quad i = 1, \dots, l. \end{aligned}$$

$$\mathcal{L}(w, \beta) = f(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

Solve $w, \beta$

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0; \quad \frac{\partial \mathcal{L}}{\partial \beta_i} = 0,$$

# Lagrange Multiplier: Example

$$\begin{aligned} &\min_{x,y} 5x - 3y \\ \text{s.t.} \quad &x^2 + y^2 = 136 \end{aligned}$$

# Generalized Lagrangian

Primal optimization problem

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \leq 0, \quad i = 1, \ldots, k \\ & h_i(w) = 0, \quad i = 1, \ldots, l. \end{aligned}$$

Generalized Lagrangian

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

# Generalized Lagrangian

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

$$\theta_{\mathcal{P}}(w) \quad = \quad \max_{\alpha, \beta \,:\, \alpha_i \geq 0} f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

$$\theta_{\mathcal{P}}(w) = \begin{cases} f(w) & \text{if } w \text{ satisfies primal constraints} \\ \infty & \text{otherwise.} \end{cases}$$

# Generalized Lagrangian

Consider this optimization problem

$$\min_w \theta_{\mathcal{P}}(w) = \min_w \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta)$$

It has exactly the same solution as our original problem

$$p^* = \min_w \theta_{\mathcal{P}}(w)$$

# The Dual Problem in Optimization

In optimization, sometimes the primal optimization is hard to solve, then we may find a related alternative optimization problem that can be solved more easily, to solve the orignal problem in an indirect way

# The Dual Problem

$$\theta_{\mathcal{D}}(\alpha, \beta) = \min_{w} \mathcal{L}(w, \alpha, \beta)$$

The dual optimization problem

$$\max_{\alpha, \beta \,:\, \alpha_i \geq 0} \theta_{\mathcal{D}}(\alpha, \beta) = \max_{\alpha, \beta \,:\, \alpha_i \geq 0} \min_{w} \mathcal{L}(w, \alpha, \beta)$$

The primal optimization problem

$$\min_{w} \theta_{\mathcal{P}}(w) = \min_{w} \max_{\alpha, \beta \,:\, \alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta)$$

What is the relation of the two problems?

# The Dual Problem

$$\mathcal{L}(w,b,\alpha) = \frac{1}{2}||w||^2 - \sum_{i=1}^{n} \alpha_i \left[ y^{(i)}(w^T x^{(i)} + b) - 1 \right]$$

The dual optimization problem

$$\max_{\alpha,\beta\,:\,\alpha_i \geq 0} \theta_{\mathcal{D}}(\alpha,\beta) = \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \min_{w} \mathcal{L}(w,\alpha,\beta)$$

$$\nabla_w \mathcal{L}(w,b,\alpha) = w - \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} = 0 \qquad w = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} \qquad \frac{\partial}{\partial b}\mathcal{L}(w,b,\alpha) = \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\boxed{\theta(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)})^T x^{(j)}}$$

# The Dual Problem

$$\theta(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)})^T x^{(j)}$$

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \ldots, n$$

$$\nabla_w \mathcal{L}(w, b, \alpha) = w - \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} = 0 \qquad w = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} \qquad \frac{\partial}{\partial b} \mathcal{L}(w, b, \alpha) = \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

What is the relation between solving this dual problem and solving the original problem

# The Dual Problem

$$d^* = \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \min_w \mathcal{L}(w,\alpha,\beta) \leq \min_w \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \mathcal{L}(w,\alpha,\beta) = p^*$$

$$\max_x \min_y f(x,y) \leq \min_y \max_x f(x,y)$$

Under certain conditions: $d^* = p^*$ Zero-duality Gap

What are the conditions?

# Slater's Condition

$$\begin{aligned} \min_w \quad & f(w) \\ \text{s.t.} \quad & g_i(w) \leq 0, \quad i = 1, \ldots, k \\ & h_i(w) = 0, \quad i = 1, \ldots, l. \end{aligned}$$

- f(w) and g(w) are convex
- $h_i(w)$ is affine (i.e. linear)
- $g_i(w)$ are strictly feasible for all i, which means there exists some w so that $g_i(w) < 0$ for all i

If slater's condition holds, then $d* = p*$

The primal optimization problem of SVM satisfies the slater's condition

# KKT Conditions

Denote the solution to the primal problem as $w^*$, the solution to the dual problem as $\alpha^*, \beta^*$, then zero duality gap is sufficient and necessary (i.e. equivalent) to satisfy KKT Conditions:

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

$$\boxed{\begin{aligned} \frac{\partial}{\partial w_i}\mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, \quad i = 1, \ldots, d \\ \frac{\partial}{\partial \beta_i}\mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, \quad i = 1, \ldots, l \end{aligned}}$$

Normal Lagrange multiplier equations

$$\alpha_i^* g_i(w^*) = 0, \quad i = 1, \ldots, k$$

$$\boxed{\begin{aligned} g_i(w^*) &\leq 0, \quad i = 1, \ldots, k \\ \alpha^* &\geq 0, \quad i = 1, \ldots, k \end{aligned}}$$

The original constraints

# KKT Conditions

Denote the solution to the primal problem as $w*$, the solution to the dual problem as $\alpha*, \beta*$, then zero duality gap is sufficient and necessary (i.e. equivalent) to satisfy KKT Conditions:

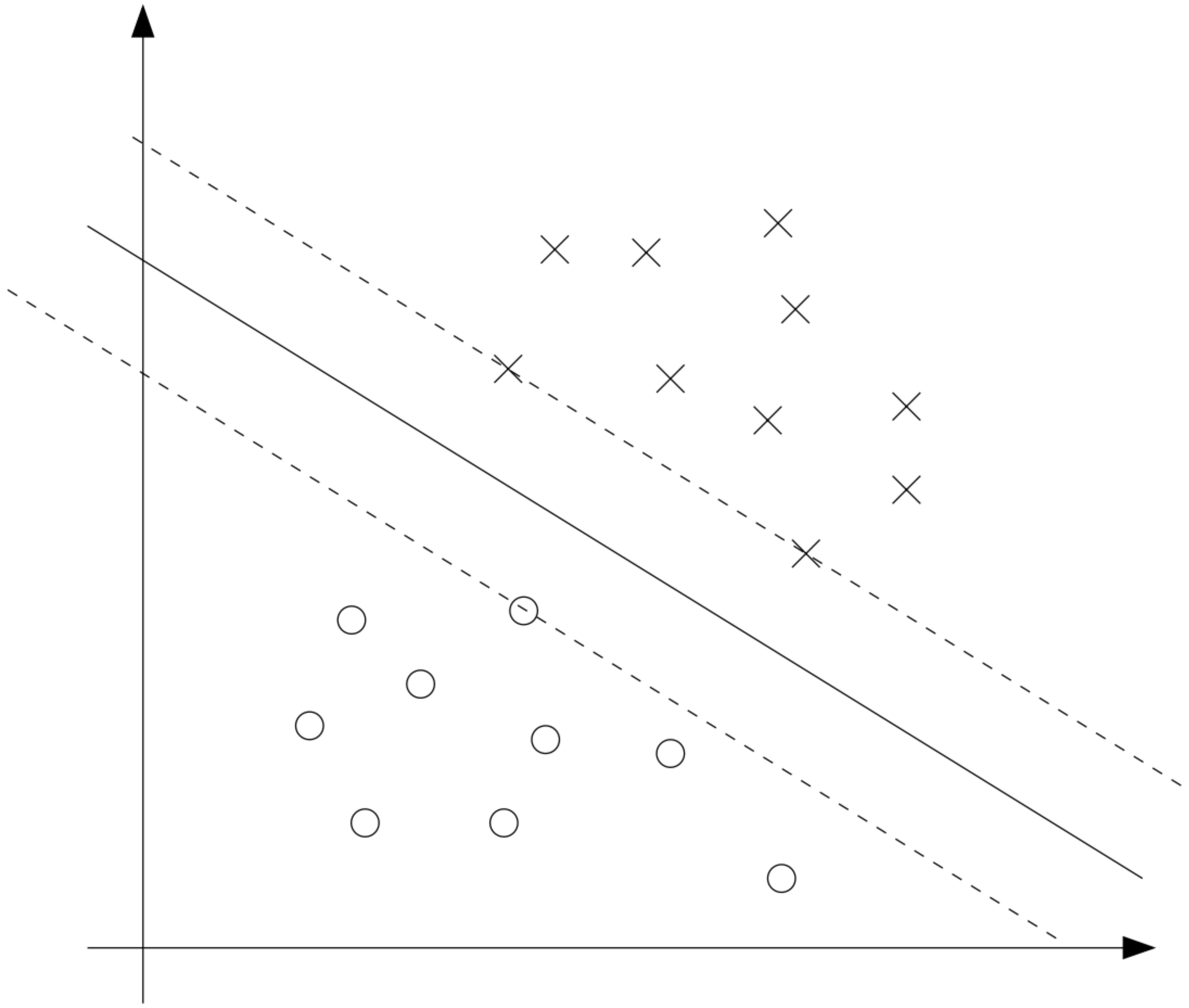
$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

$$\begin{aligned} \frac{\partial}{\partial w_i} \mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, \quad i = 1, \ldots, d \\ \frac{\partial}{\partial \beta_i} \mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, \quad i = 1, \ldots, l \\ \boxed{\alpha_i^* g_i(w^*) = 0, \quad i = 1, \ldots, k} \\ g_i(w^*) &\leq 0, \quad i = 1, \ldots, k \\ \alpha^* &\geq 0, \quad i = 1, \ldots, k \end{aligned}$$

If $\alpha_i^* > 0$, then $g_i(w^*) = 0$, the inequality is actually equality

# Supporting Vectors

$$\alpha_i^* g_i(w^*) \;=\; 0, \;\; i = 1, \ldots, k$$



Only the 3 points have non-zero $\alpha_i$, and they are called supporting vectors

# Lagrangian for SVM

$$\mathcal{L}(w,b,\alpha) = \frac{1}{2}||w||^2 - \sum_{i=1}^{n} \alpha_i \left[ y^{(i)}(w^T x^{(i)} + b) - 1 \right]$$

The dual optimization problem

$$\max_{\alpha,\beta\,:\,\alpha_i \geq 0} \theta_{\mathcal{D}}(\alpha,\beta) = \max_{\alpha,\beta\,:\,\alpha_i \geq 0} \min_{w} \mathcal{L}(w,\alpha,\beta)$$

$$\nabla_w \mathcal{L}(w,b,\alpha) = w - \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} = 0 \qquad w = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} \qquad \frac{\partial}{\partial b}\mathcal{L}(w,b,\alpha) = \sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\boxed{\theta(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)})^T x^{(j)}}$$

# The Dual Problem of SVM

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j=1}^n y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)}, x^{(j)}\rangle$$

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \ldots, n$$

$$\sum_{i=1}^n \alpha_i y^{(i)} = 0,$$

Kernel is all we need!

After solving $\alpha$ (we'll talk about how later)

$$w = \sum_{i=1}^n \alpha_i y^{(i)} x^{(i)}$$

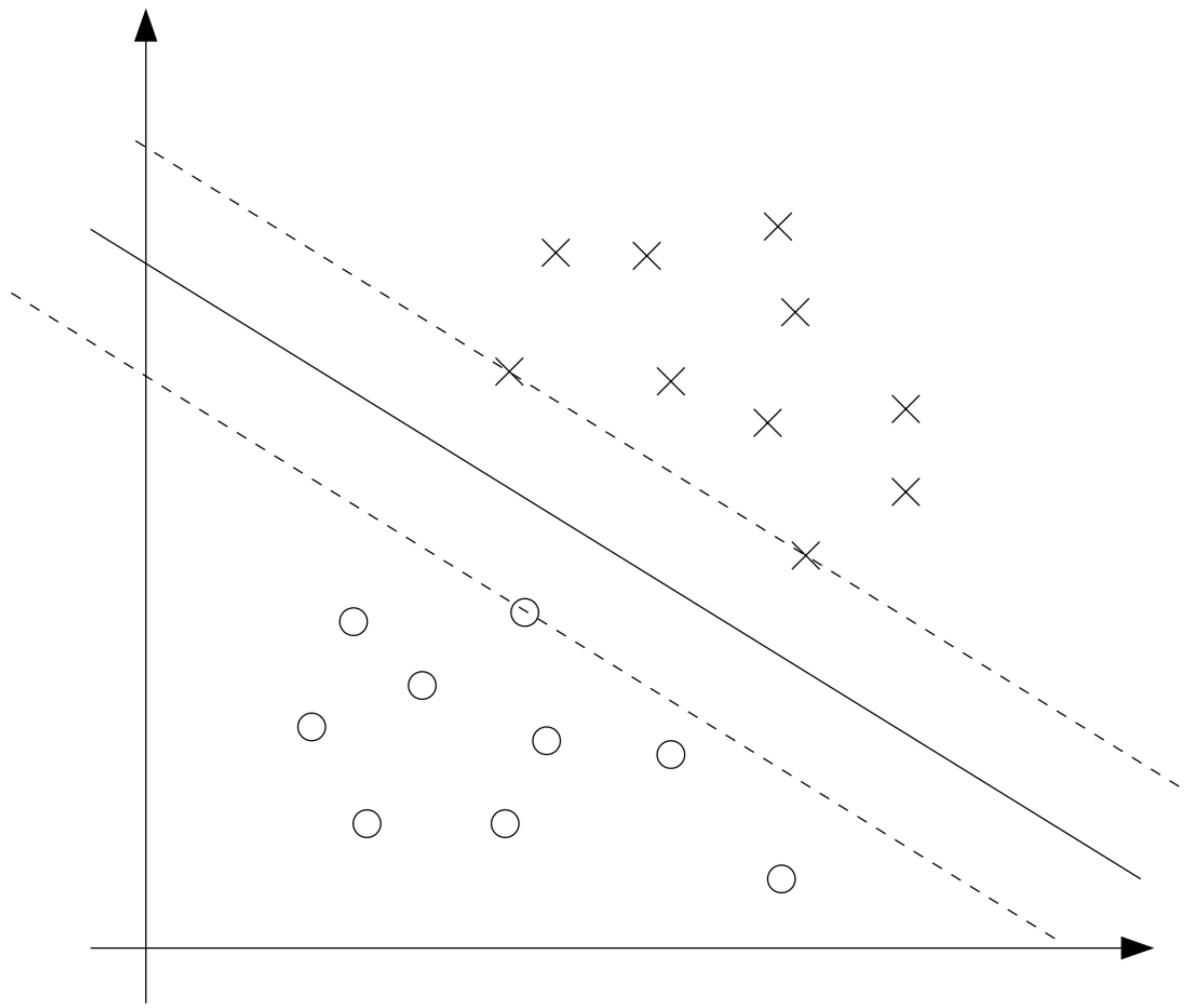
From KKT Conditions

$$b^* = -\frac{\max_{i:y^{(i)}=-1} {w^*}^T x^{(i)} + \min_{i:y^{(i)}=1} {w^*}^T x^{(i)}}{2}$$

From the original constraints

# Inference

$$
\begin{aligned}
w^T x + b &= \left( \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} \right)^T x + b \\
&= \sum_{i=1}^{n} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b.
\end{aligned}
$$

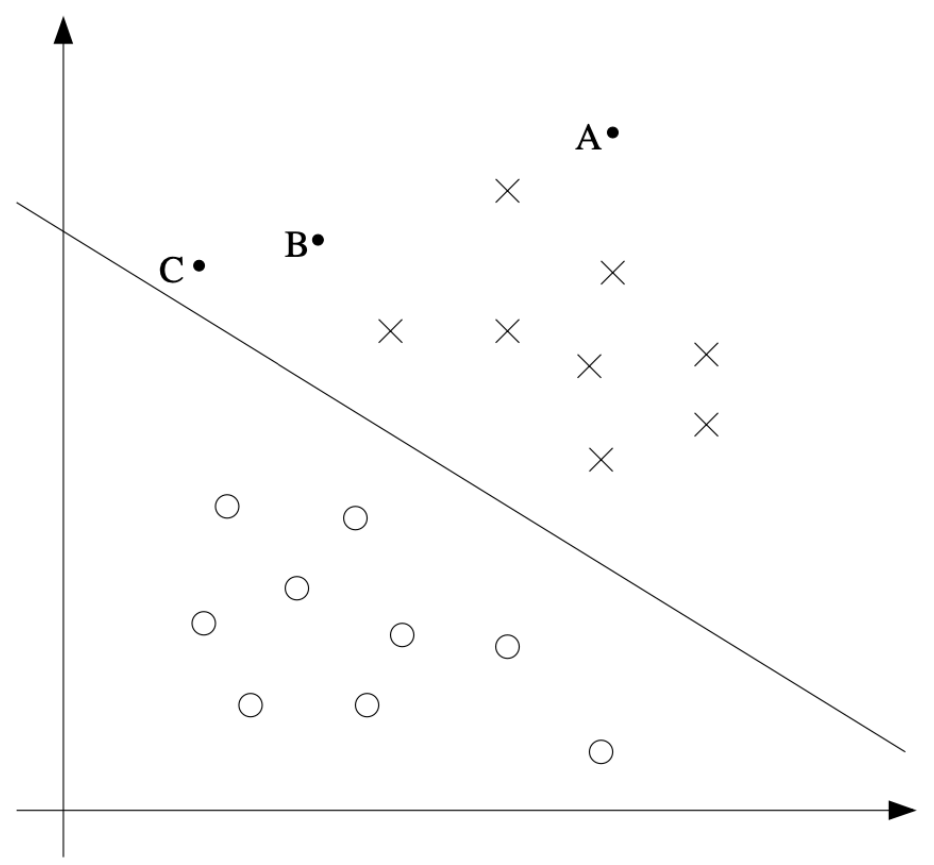


We never need to really compute w

$$
\alpha_i^* g_i(w^*) \;=\; 0, \quad i = 1, \ldots, k
$$

Most $\alpha_i$ are 0, only the supporting examples will influence the final prediction

# Review of the High-Level Logic




$$h_{w,b}(x) = g(w^T x + b).$$

Maximize geometric margin

Problem rewriting

Quadratic Optimization Problem

Finding a related optimization problem that is easier

Dual optimization problem

$$\gamma^{(i)} = y^{(i)}\left(\left(\frac{w}{||w||}\right)^T x^{(i)} + \frac{b}{||w||}\right)$$

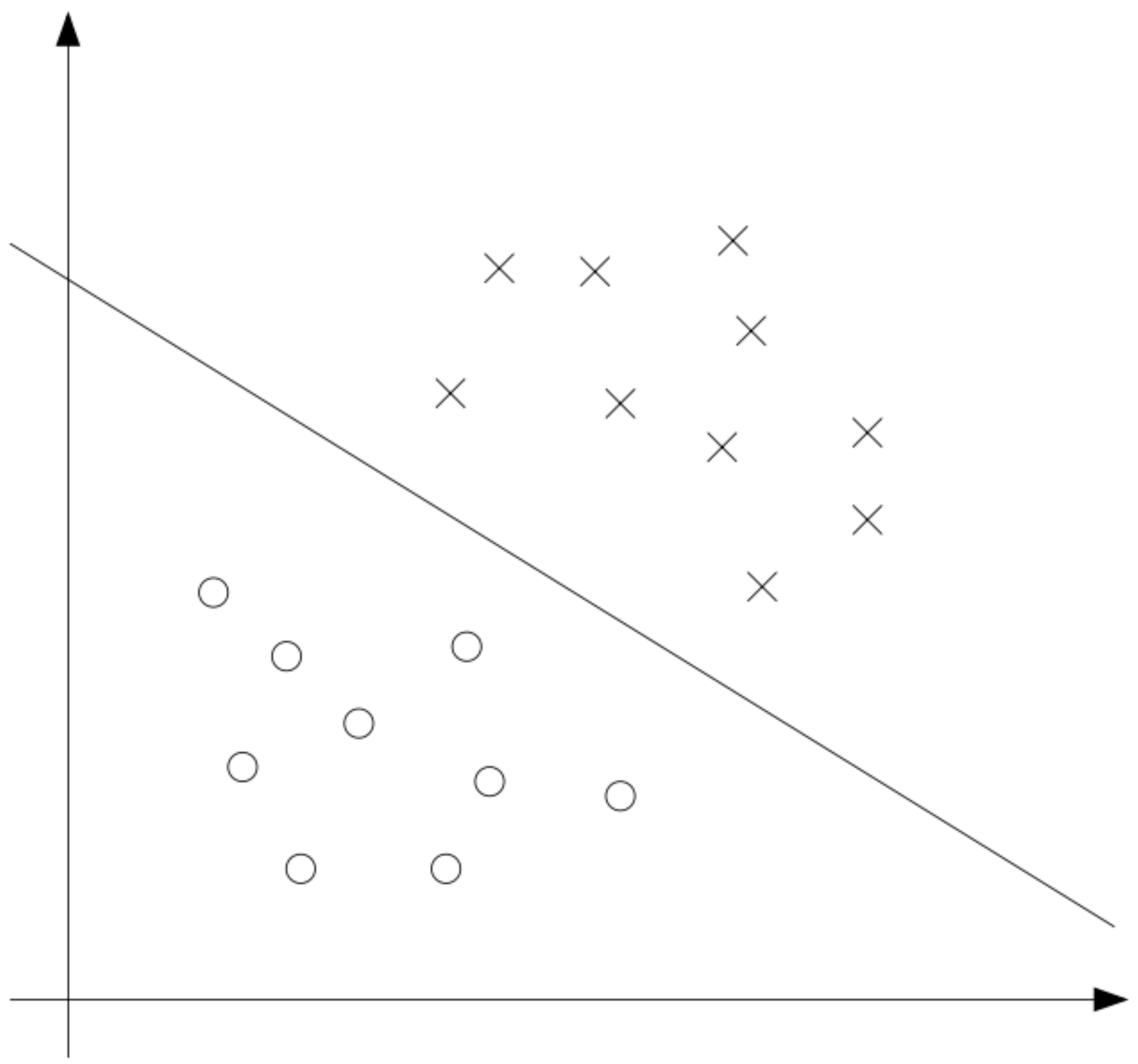
$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}||w||^2 \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad i = 1, \ldots, n \end{aligned}$$

Not suitable for non-linear cases (high-dim feature map)

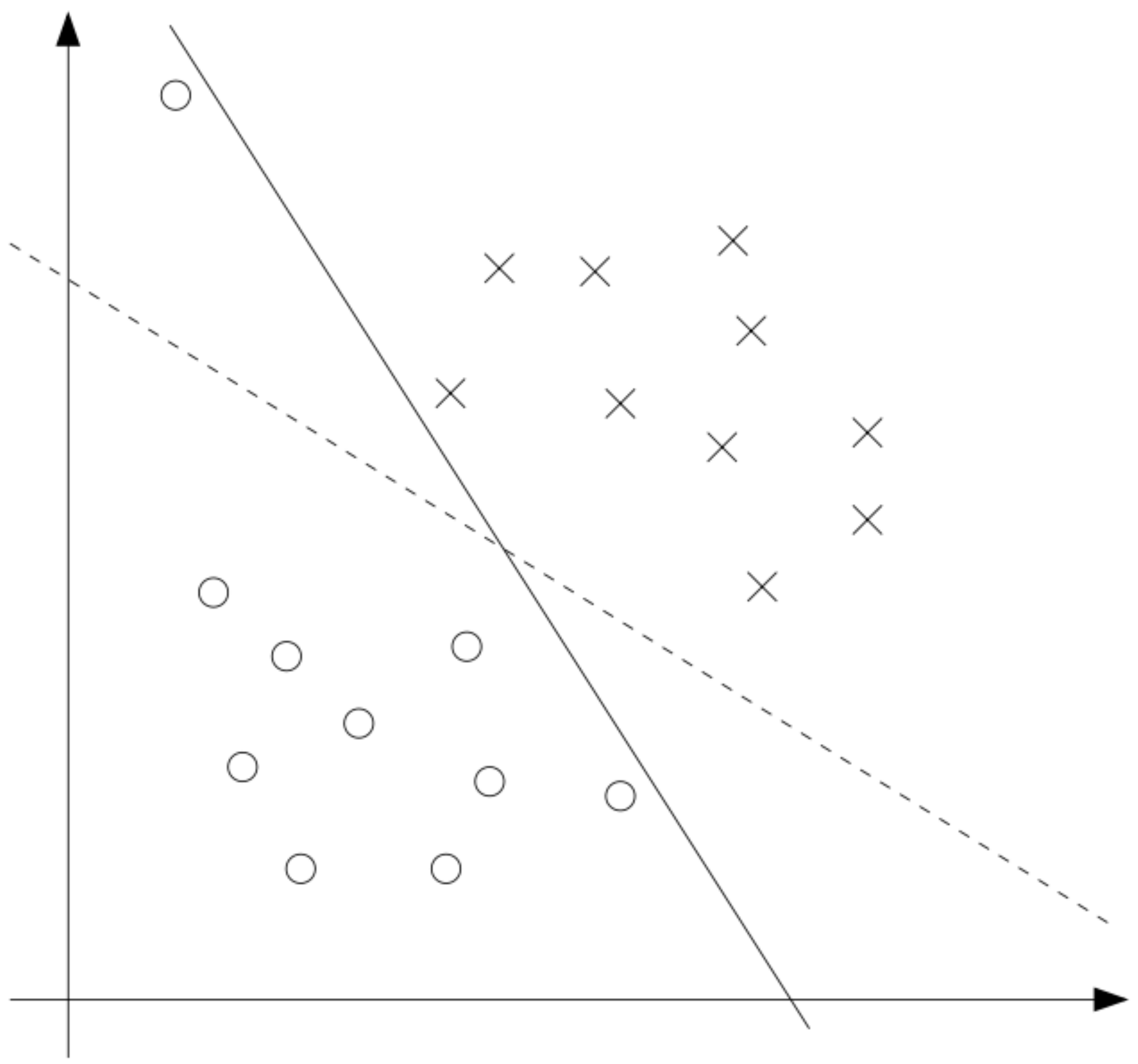
$$\begin{aligned} \max_\alpha \quad & W(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j=1}^n y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\ \text{s.t.} \quad & \alpha_i \geq 0, \quad i = 1, \ldots, n \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \end{aligned}$$

Kernel makes it very flexible in non-linear cases!

# The Non-Separable Case



Linearly Separable



Linearly Non-Separable

# The Non-Separable Case

Primal opt problem:

$$\begin{aligned} \min_{\gamma,w,b} \quad & \frac{1}{2}||w||^2 + C\sum_{i=1}^{n}\xi_i \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i, \quad i = 1,\ldots,n \\ & \xi_i \geq 0, \quad i = 1,\ldots,n. \end{aligned}$$

Dual opt problem

$$\begin{aligned} \max_{\alpha} \quad & W(\alpha) = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)}, x^{(j)}\rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \quad i = 1,\ldots,n \\ & \sum_{i=1}^{n}\alpha_i y^{(i)} = 0, \end{aligned}$$

# Thank You!
# Q & A