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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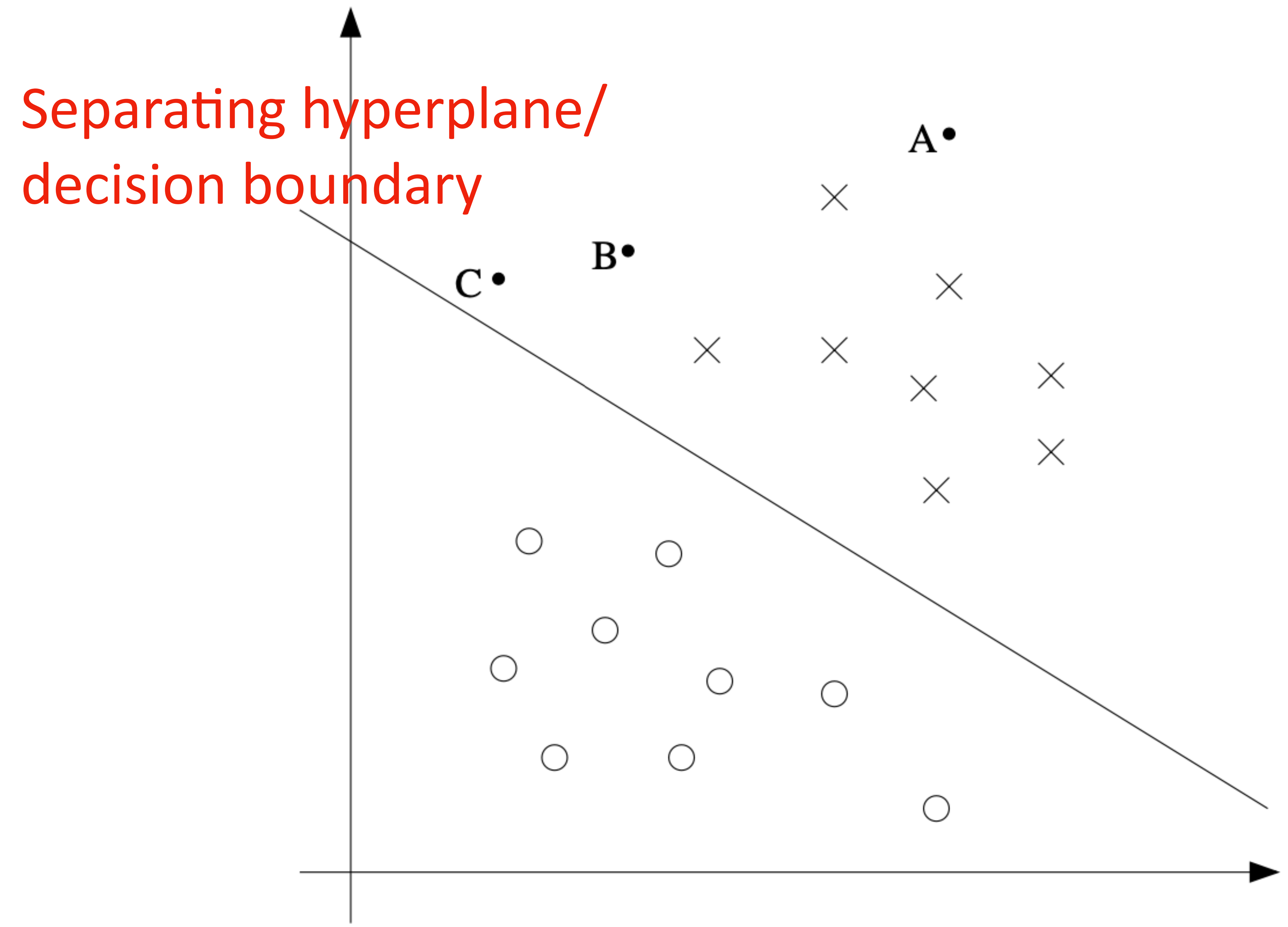
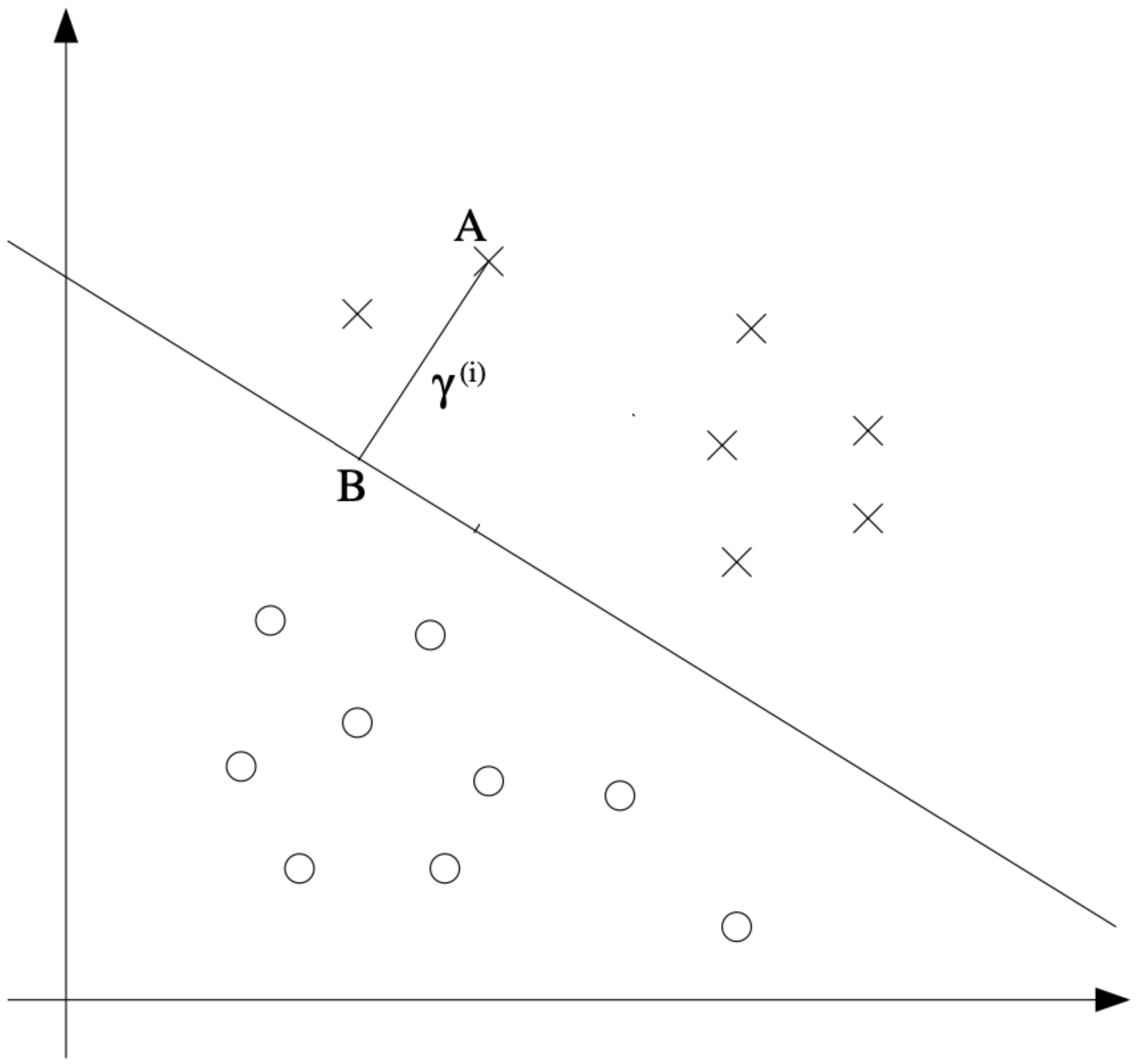
Recap: Support Vector Machines



Recap: 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

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

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

Rewrite ⟹

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

Linear constraint ⟹

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

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 $\hat{\gamma} = 1$

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

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

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

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

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

Generalized Lagrangian

Primal optimization problem

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 α^*, β^*, then zero duality gap is sufficient and necessary (i.e. equivalent) to satisfy KKT Conditions:

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

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

Normal Lagrange multiplier equations

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:

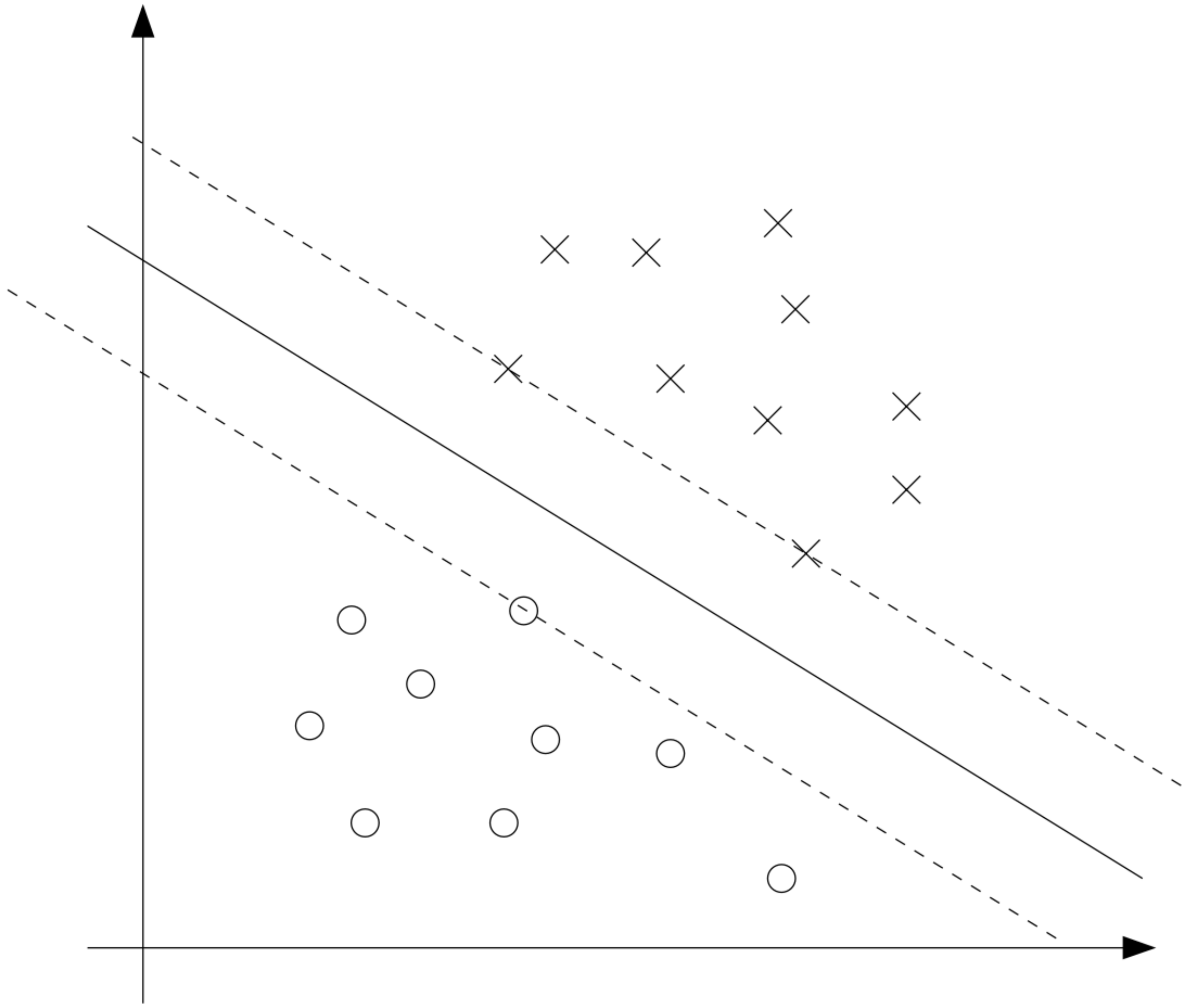
$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

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

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

Supporting Vectors

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



Only the 3 points have non-zero α_i, and they are called supporting vectors

The Dual Problem of SVM

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

Kernel is all we need!

After solving α (we'll talk about how later)

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

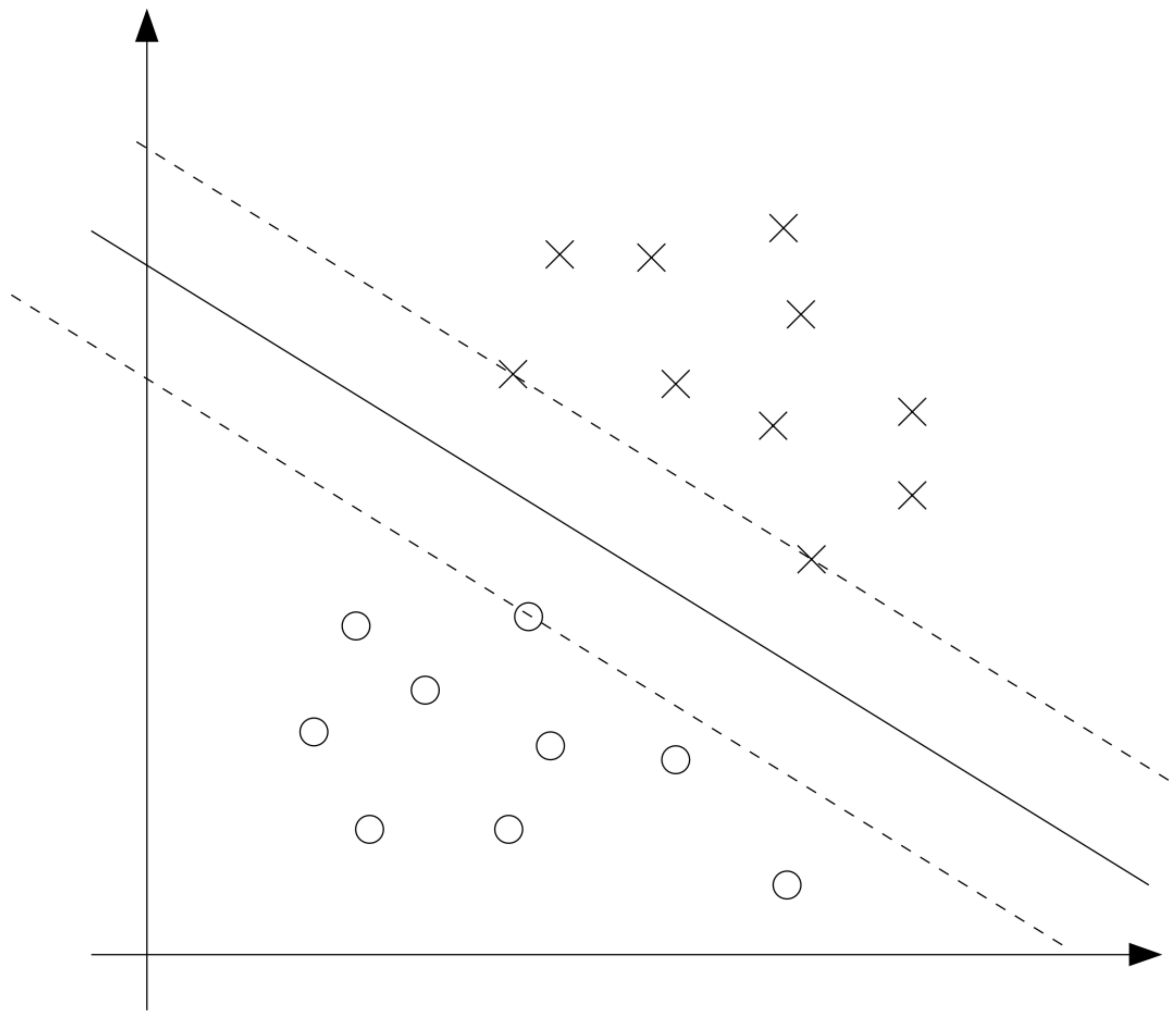
From KKT Conditions

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

From the original constraints

Inference

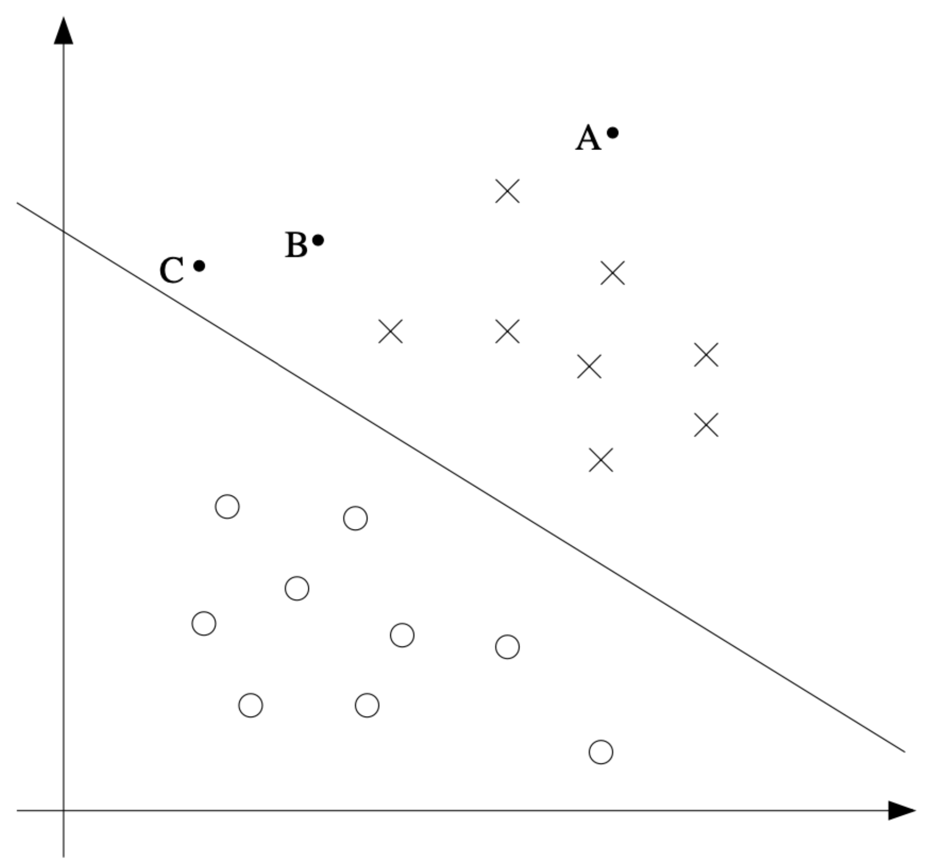
$$w^T x + b = \left(\sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} \right)^T x + b$$
$$= \sum_{i=1}^{n} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b.$$



We never need to really compute w

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

Most α_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**

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

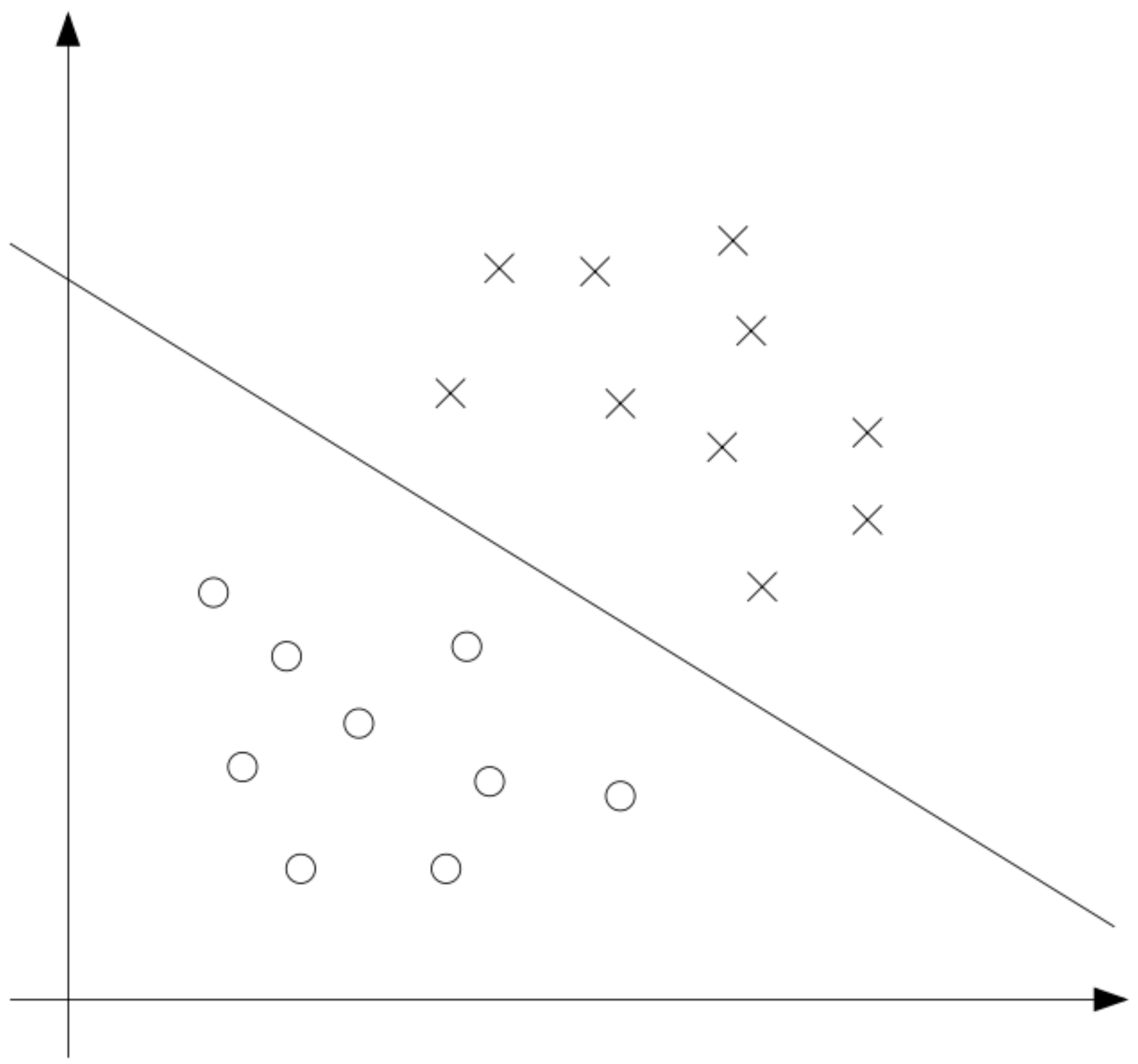
$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}||w||^2 \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad i = 1, \ldots, n \end{aligned}$$

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

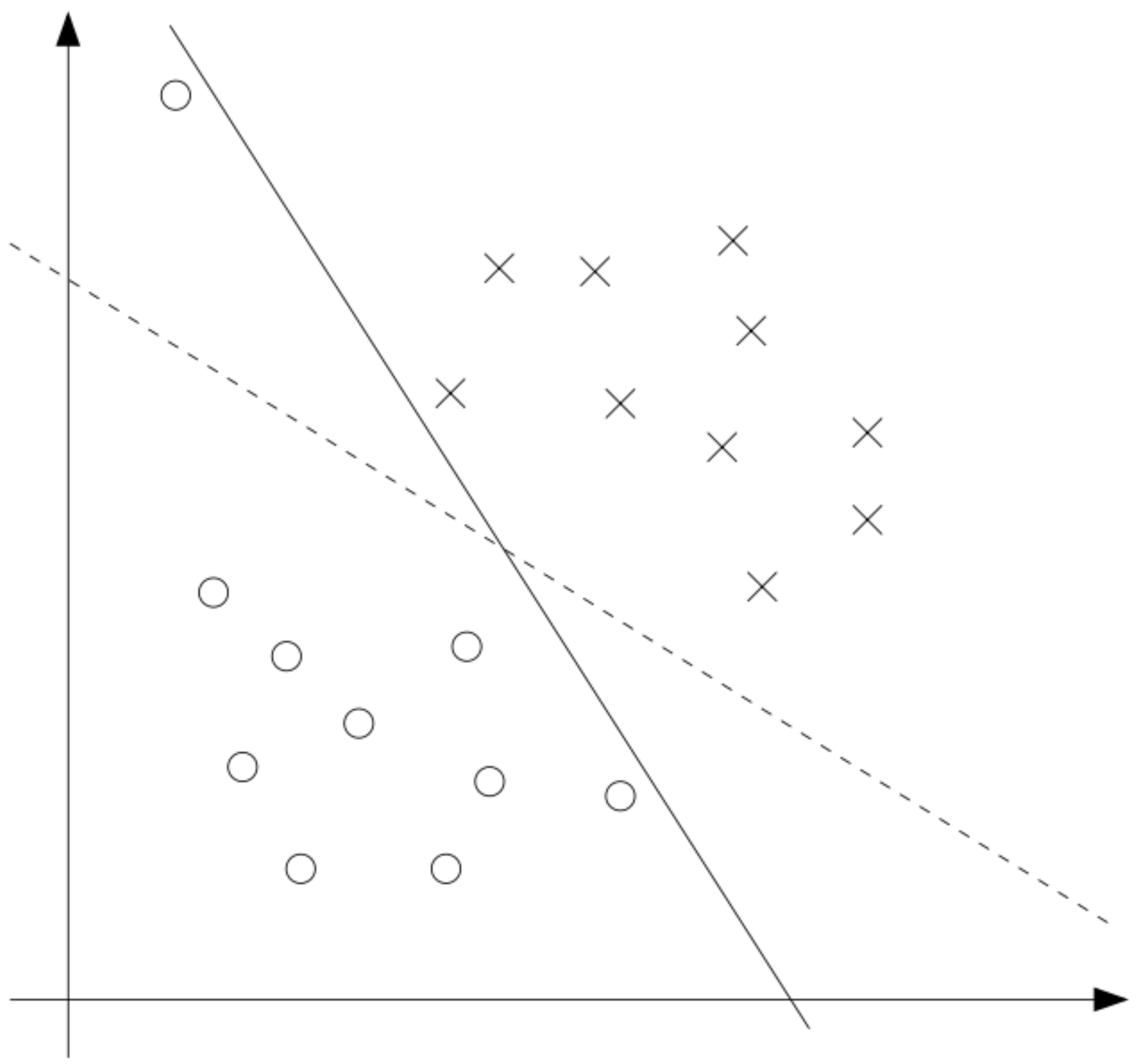
$$\begin{aligned} \max_\alpha \quad & W(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\ \text{s.t.} \quad & \alpha_i \geq 0, \quad i = 1, \ldots, n \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \end{aligned}$$

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