香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
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COMP 5212

Machine Learning

Lecture 7

Support Vector Machines

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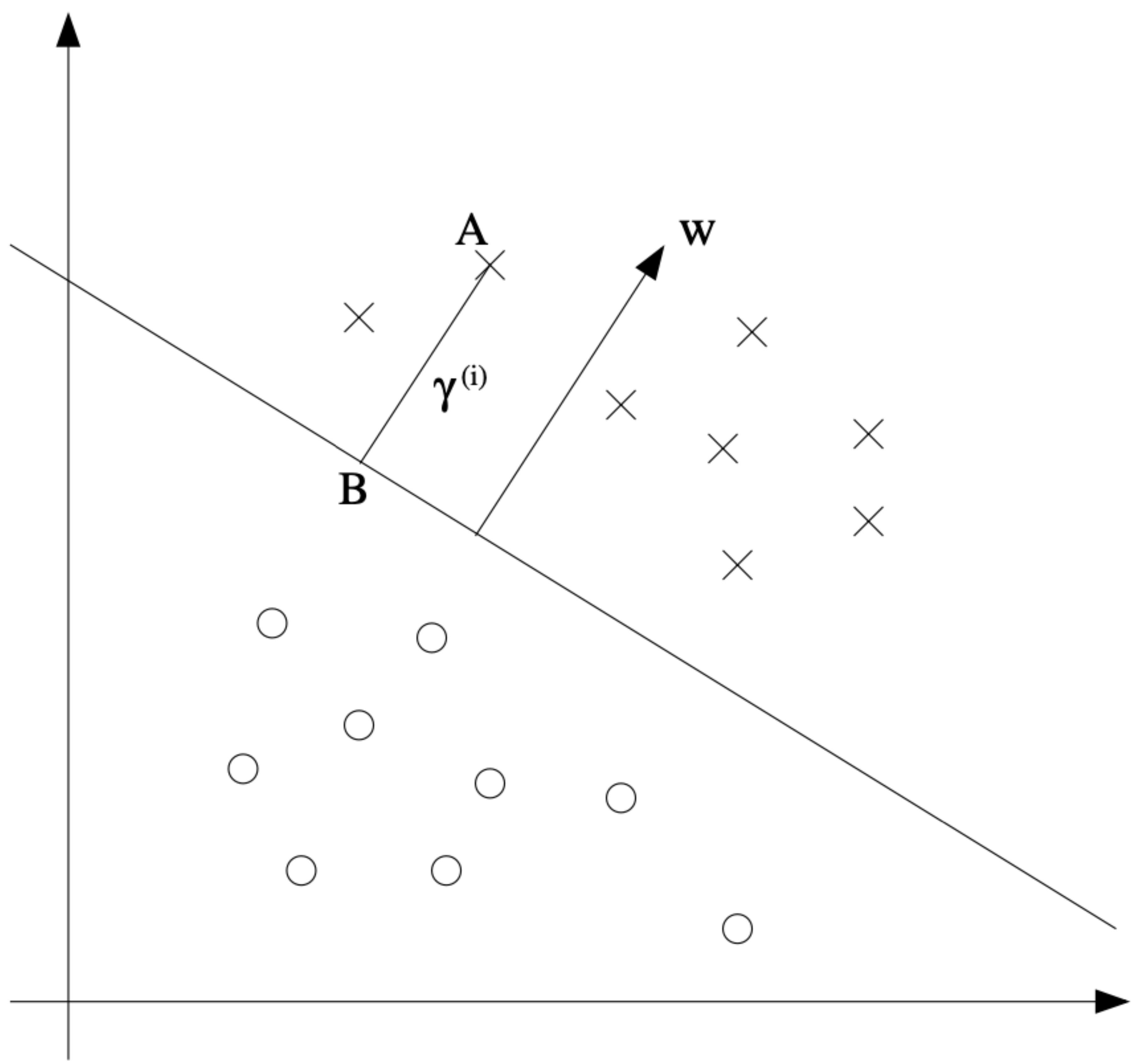
Recap: Support Vector Machines



Recap: The Optimization Problem

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

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

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

Recap: 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?

Recap: 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

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

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

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

Recap: 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 (Strong Duality)

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:

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

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

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

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

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

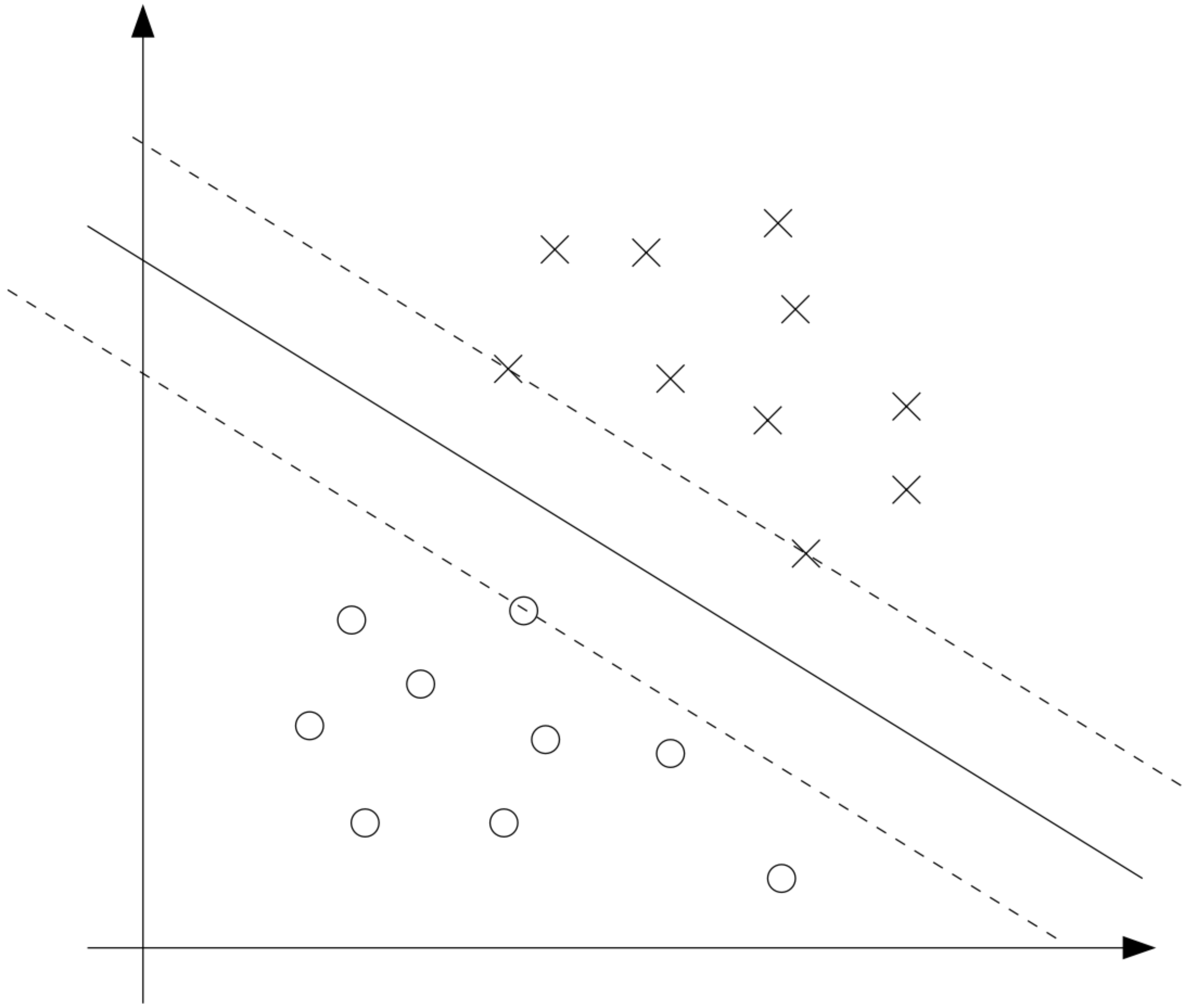
$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

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

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 α_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

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

Kernel is all we need!

After solving α (coordinate ascent with clipping, 6.8.2 of the CS229 Notes)

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

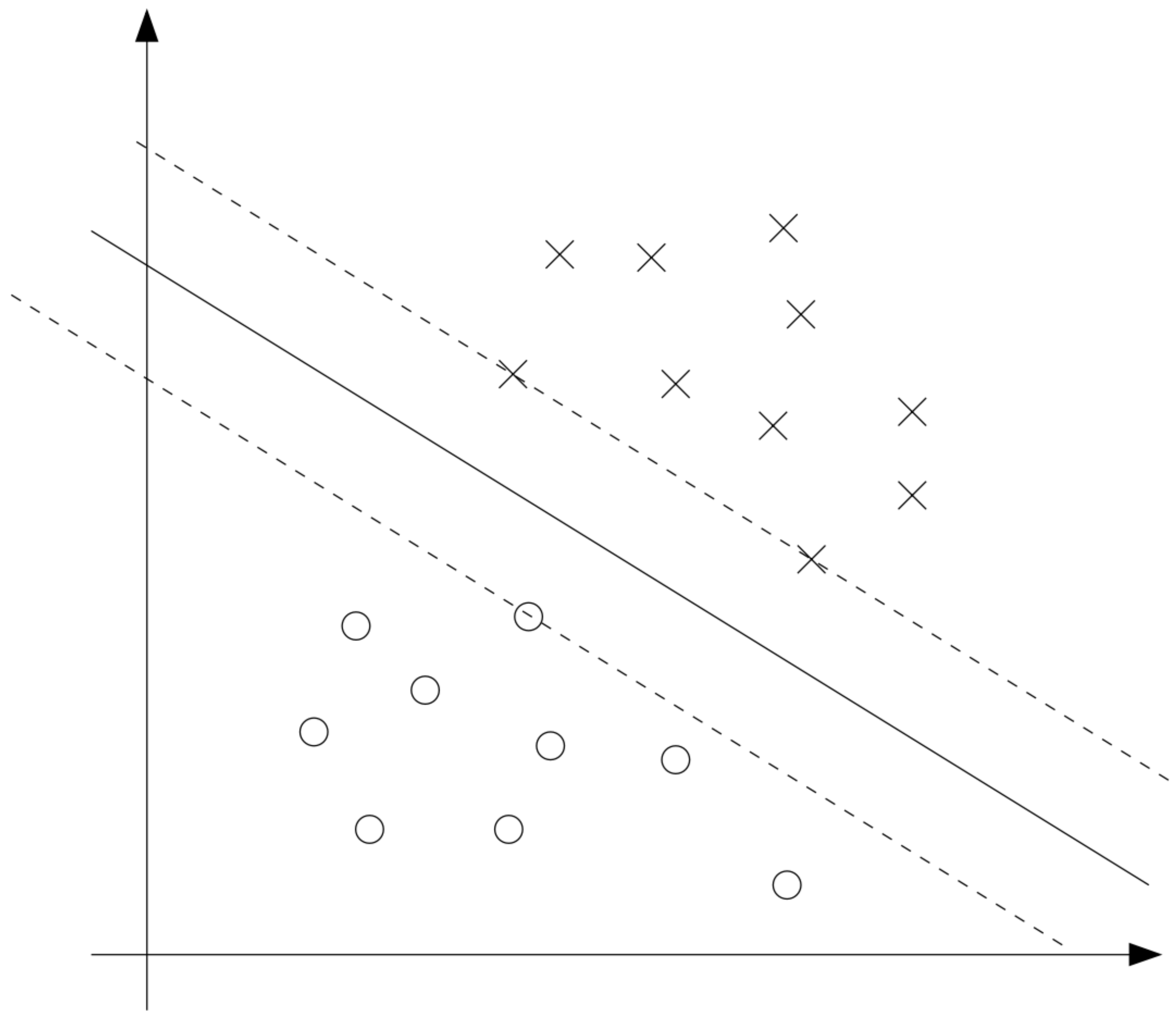
From KKT Conditions

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

From the original constraints

Inference

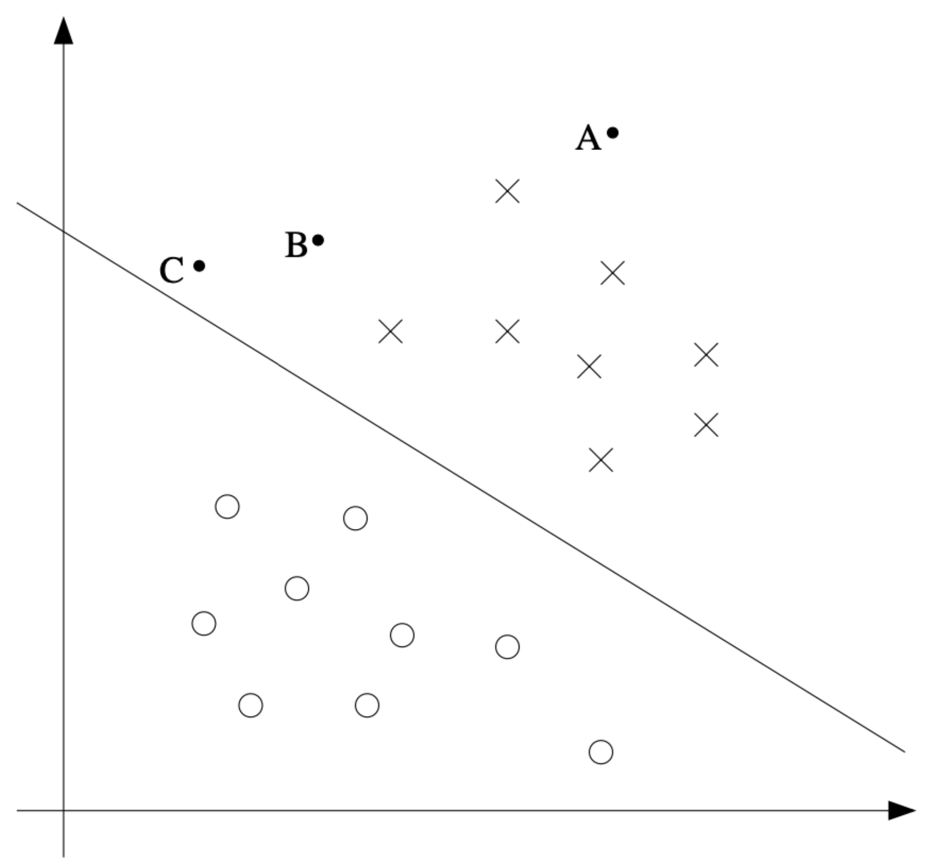
$$
\begin{aligned}
w^T x + b &= \left(\sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)}\right)^T x + b \\
&= \sum_{i=1}^{n} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b.
\end{aligned}
$$



We never need to really compute w

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

Most 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**

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

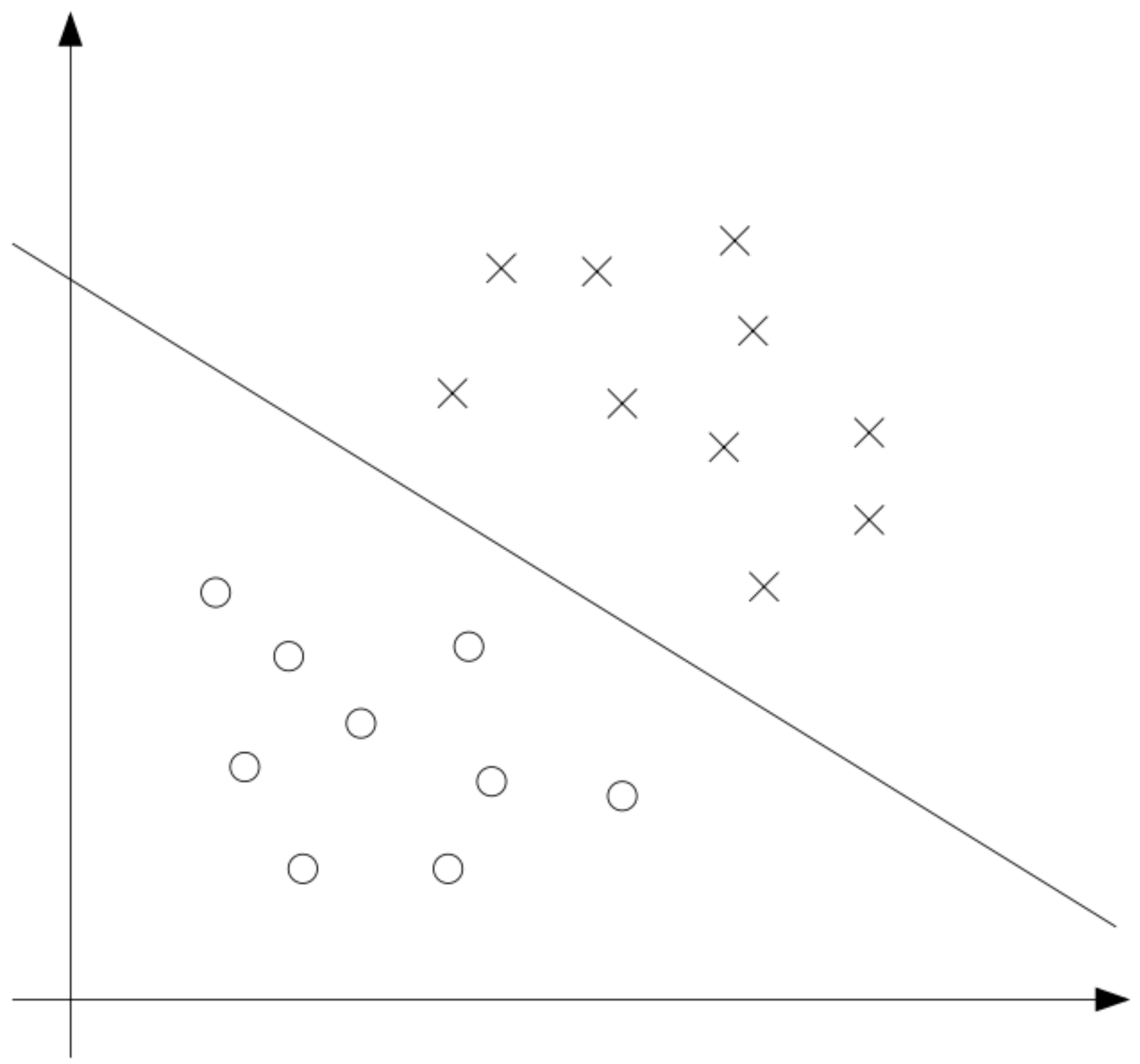
$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}||w||^2 \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad i = 1, \ldots, n \end{aligned}$$

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

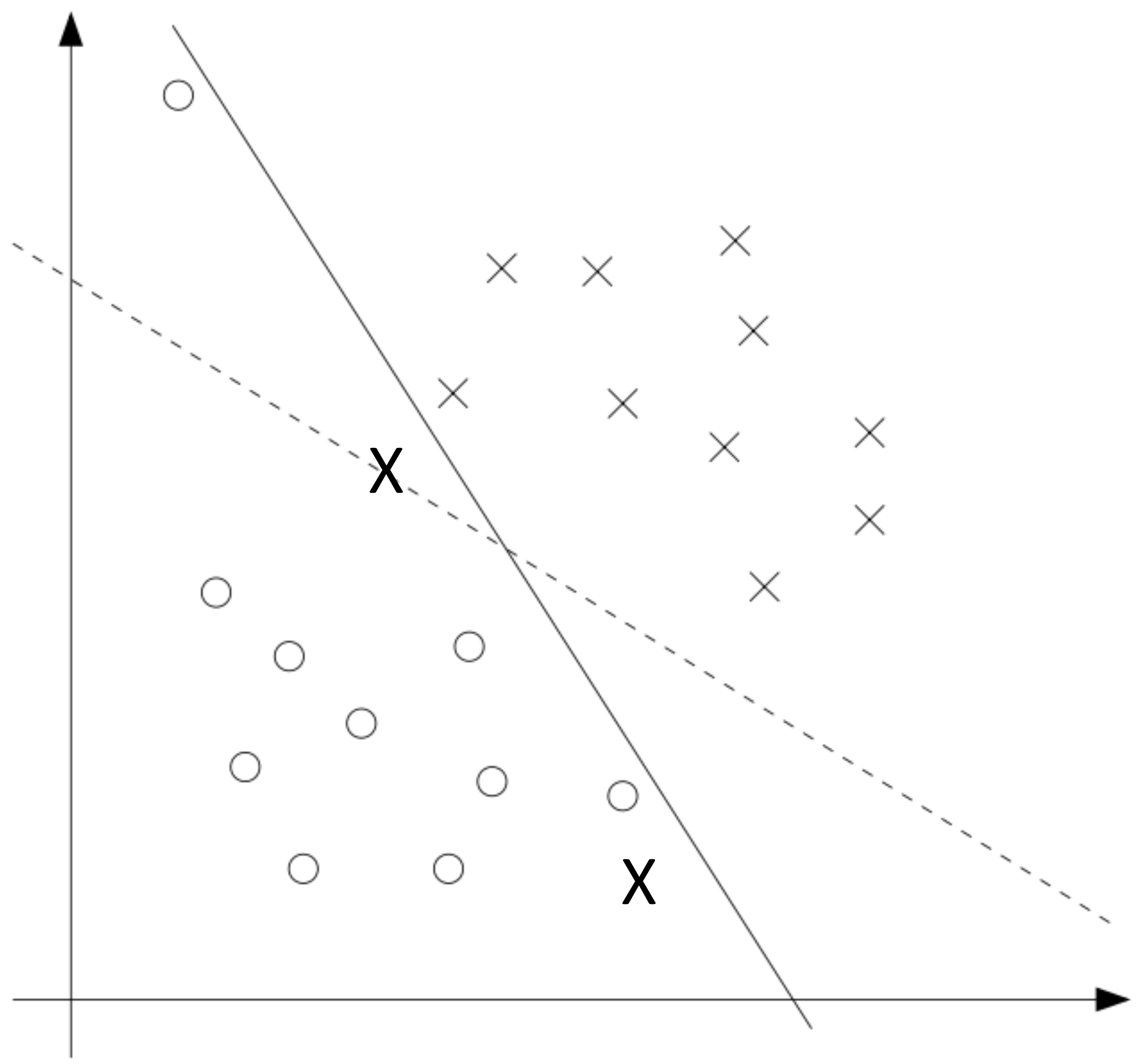
$$\begin{aligned} \max_\alpha \quad & W(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\ \text{s.t.} \quad & \alpha_i \geq 0, \quad i = 1, \ldots, n \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \end{aligned}$$

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

You will prove this in your hw

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

Thank You!
Q & A