01.112/50.007 Machine Learning

Lecture 7

Support Vector Machines (Part 1)

Recap

Linear Classifiers

- Given training data $\mathcal{S}_n = \left\{ \left(x^{(t)}, y^{(t)}\right) \,\middle|\, t = 1, \dots, n \right\}$, we define **linear classifier** as below:

$$h(x; \theta, \theta_0) = \mathrm{sign}(\theta^\top x + \theta_0)$$

- We estimate, model parameters, $\theta \in \mathbb{R}^d, \theta_0 \in \mathbb{R}$, by minimizing **empirical risk:**

$$\mathcal{R}(\theta, \theta_0) = \frac{1}{n} \sum_{t=1}^{n} Loss\left(y^{(t)} (\theta . x^{(t)} + \theta_0\right)$$

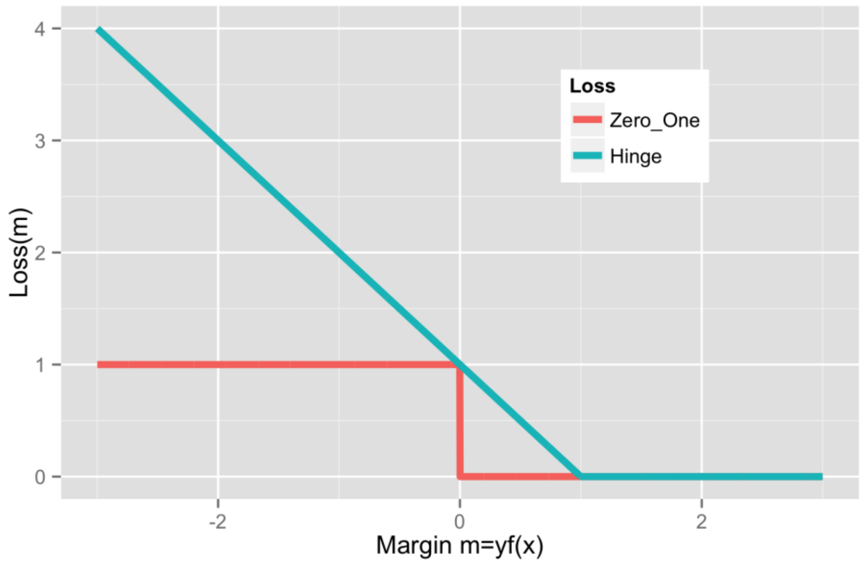
Loss Functions

- **Empirical risk:**

$$\mathcal{R}(\theta, \theta_0) = \frac{1}{n} \sum_{t=1}^{n} Loss\left(y^{(t)}(\theta . x^{(t)} + \theta_0\right)$$

- **Zero-one loss:** $\mathrm{Loss}_{0|1}(z) = [\![z \leq 0]\!]$

- **Hinge loss:** $\mathrm{Loss}_{\mathrm{h}}(z) = \max\{1 - z, 0\}$



CONVEX!
Penalize larger mistakes more.
Penalize near-mistakes, i.e. $0 \leq z \leq 1$.

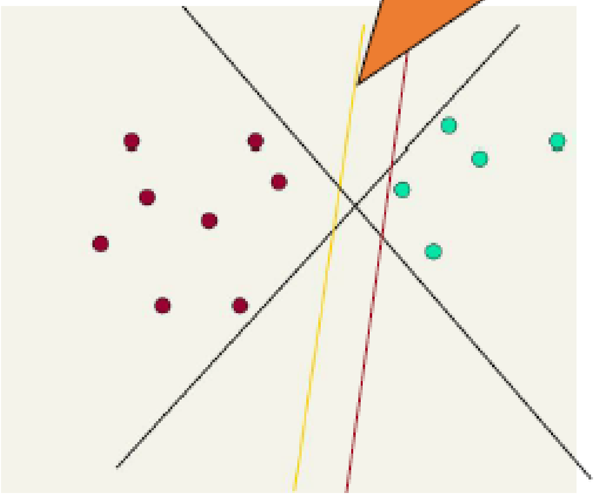
Linear Classifiers: Which Hyperplane?

- **Empirical risk does not constrain the parameters**. Lots of possible solutions for *a, b, c.*
- Constrain it using **regularization term** (similar to linear regression)

$$\frac{\lambda}{2}\|\theta\|^2 + \frac{1}{n}\sum_{t=1}^{n} \text{Loss}_h\left(y^{(t)}(\theta \cdot x^{(t)} + \theta_0)\right)$$

Using regularization term as part of the objective function.

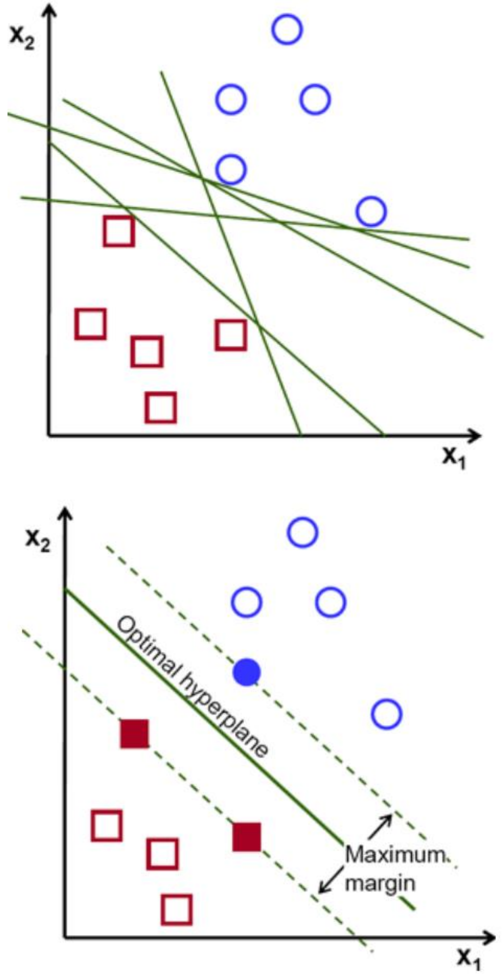
This line represents the decision boundary: $ax + by - c = 0$



Support Vector Machine

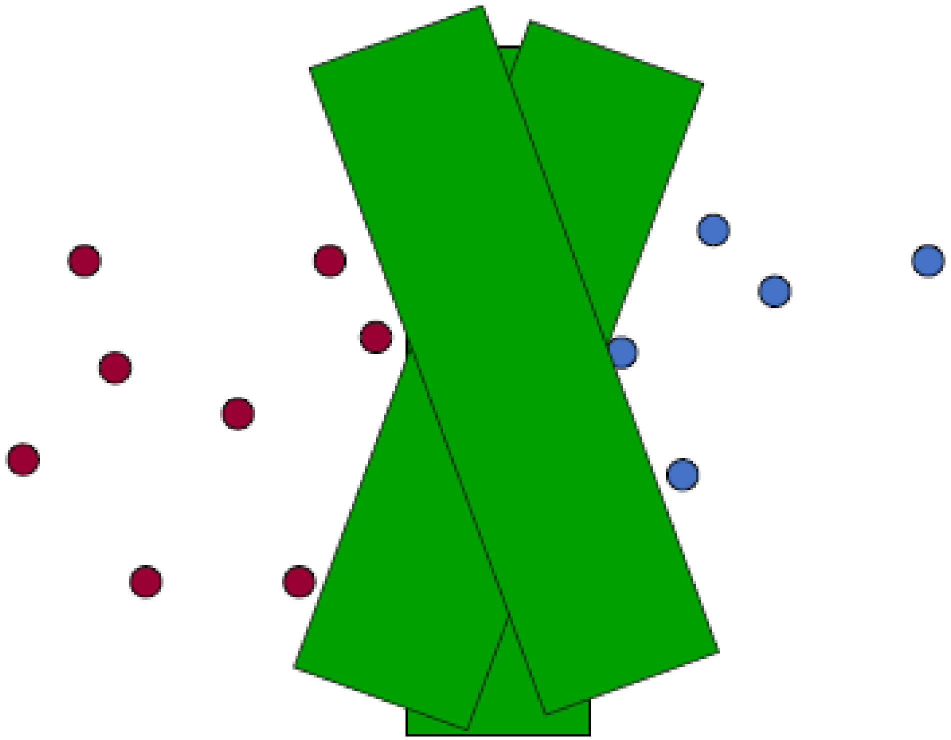
Support Vector Machine (SVM)

- **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 uncertain classification decisions.



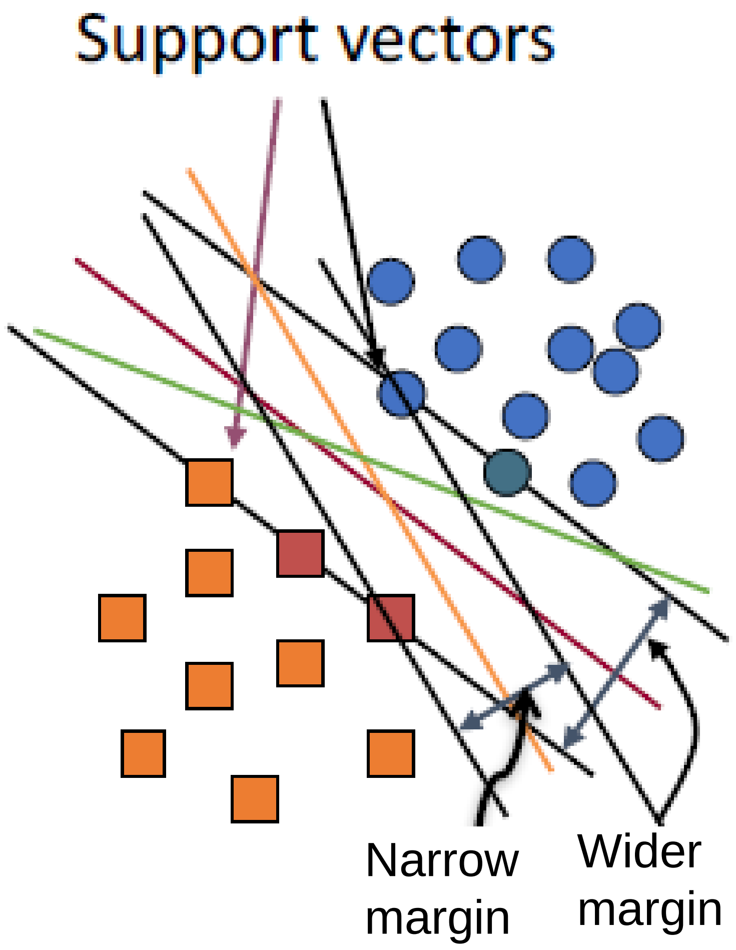
Another intuition

- If you have to place a fat separator between classes, you have fewer choices.



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*

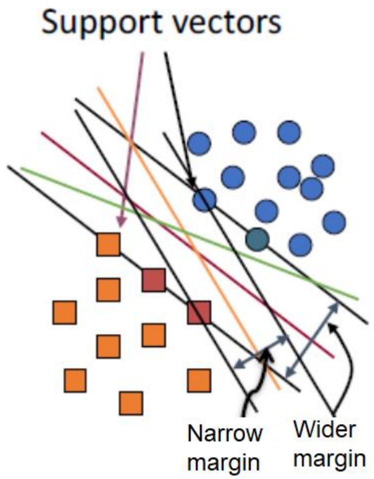


*but other discriminative methods often perform very similarly

Support Vector Machine (SVM)

- **Distance of each point from decision boundary**

$$\gamma^{(t)}(\theta, \theta_0) = \frac{y^{(t)}(\theta \cdot x^{(t)} + \theta_0)}{\|\theta\|}$$



- **Goal: Maximize minimum distance to the boundary**

$$\min_{t=1,\ldots,n} \gamma^{(t)}(\theta, \theta_0)$$

- Formulate the goal as **quadratic programming problem (SVM)**

$$\min \frac{1}{2}\|\theta\|^2 \text{ subject to } y^{(t)}(\theta \cdot x^{(t)} + \theta_0) \geq 1, t = 1, \ldots, n$$

Lagrange Multipliers

Background

Constrained Optimization

Want to minimize some function $f(x)$, but
there are some *constraints* on the values of x.

Method 1 (Dual Problem)

Solve a *dual optimization problem* where the constraints are nicer, and where it is easier to implement gradient descent.

Method 2 (Exact Solution)

Solve the *Lagrangian* system of equations.

Equality Constraints

Problem.

$$\begin{aligned} &\text{minimize} \quad f(x) \\ &\text{subject to} \quad h_1(x) = 0, \dots, h_l(x) = 0 \end{aligned}$$

Lagrangian.

$$L(x, \lambda) = f(x) + \lambda_1 h_1(x) + \cdots + \lambda_l h_l(x)$$

Example.

$$\begin{aligned} &\text{minimize} \quad f(x) = n_1 \log x_1 + \cdots + n_d \log x_d \\ &\text{subject to} \quad h(x) = x_1 + \cdots + x_d - 1 = 0 \end{aligned}$$

$$L(x, \lambda) = n_1 \log x_1 + \cdots + n_d \log x_d + \lambda(x_1 + \cdots + x_d - 1)$$

Two-Player Game

$$L(x, \lambda) = f(x) + \lambda_1 h_1(x) + \cdots + \lambda_l h_l(x)$$

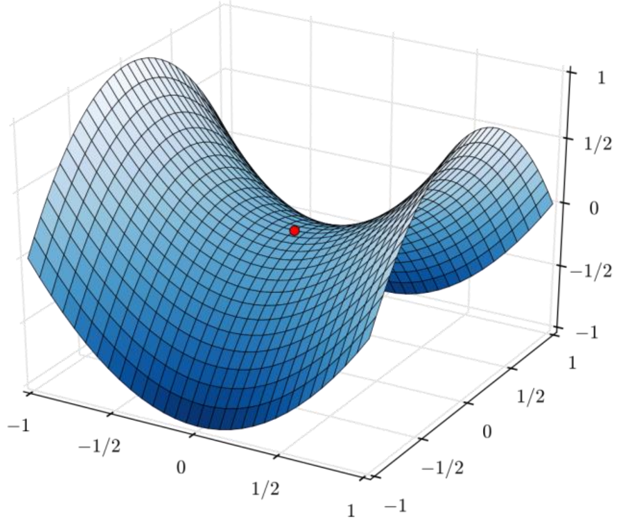
Rules.

- You get to choose the value of x.
  Your goal is to minimize $L(x, \lambda)$.
- Your adversary gets to choose the value of λ.
  His goal is to maximize $L(x, \lambda)$.

Primal Game

$$L(x, \lambda) = f(x) + \lambda_1 h_1(x) + \cdots + \lambda_l h_l(x)$$

Primal Game. You go first.



Your Strategy.

- Ensure that $h_1(x) = 0, \ldots, h_l(x) = 0$.
- Find x that minimizes $f(x)$.

Final Score. $p^* = \min_x \max_\lambda L(x, \lambda)$

The optimal x^*, λ^* are *saddle points* of $L(x, \lambda)$.

Dual Game

$$L(x,\lambda) = f(x) + \lambda_1 h_1(x) + \cdots + \lambda_l h_l(x)$$

Dual Game. You go second.

Adversary's Strategy.

- For each λ, compute $\ell(\lambda) = \min_x L(x,\lambda)$
- Find λ that maximizes $\ell(\lambda)$.

Final Score. $d^* = \max_\lambda \min_x L(x,\lambda)$

Max-Min Inequality

Primal. $p^* = \min_x \max_\lambda L(x, \lambda)$

Dual. $d^* = \max_\lambda \min_x L(x, \lambda)$

"you do better if you have the last say"

$$\boxed{\begin{aligned} p^* &= \min_x \max_\lambda L(x, \lambda) \\ &\geq \max_\lambda \min_x L(x, \lambda) = d^* \end{aligned}}$$

If $p^* = d^*$, we can solve the primal by solving the dual.

Max-Min Inequality

Example.

	$x = 1$	$x = 2$
$\lambda = 1$	1	4
$\lambda = 2$	3	2

Primal. $$p^* = \min_x \max_\lambda L(x, \lambda) = 3$$

Dual. $$d^* = \max_\lambda \min_x L(x, \lambda) = 2$$

Exact Solution

Problem.

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & h_1(x) = 0, \dots, h_l(x) = 0 \end{array}$$

Lagrange multipliers.

1. Write down the Lagrangian.

$$L(x, \lambda) = f(x) + \lambda_1 h_1(x) + \cdots + \lambda_l h_l(x)$$

2. Solve for critical points x, λ.

$$\nabla_x L(x, \lambda) = 0, \quad h_1(x) = 0, \dots, h_l(x) = 0$$

3. Pick critical point which gives global minimum.

Example

$$\begin{array}{ll} \text{minimize} & f(x) = n_1 \log x_1 + \cdots + n_d \log x_d \\ \text{subject to} & h(x) = x_1 + \cdots + x_d - 1 = 0 \end{array}$$

Lagrangian

$$L(x, \lambda) = n_1 \log x_1 + \cdots + n_d \log x_d + \lambda(x_1 + \cdots + x_d - 1)$$

Critical points

$$0 = n_i / x_i + \lambda \qquad\qquad x_i = n_i / (-\lambda)$$

$$0 = x_1 + \cdots + x_d - 1 \qquad\qquad (-\lambda) = n_1 + \cdots + n_d$$

Inequality Constraints (Primal-Dual)

Primal Problem.

$$\begin{aligned} &\text{minimize} \quad f(x) \\ &\text{subject to} \quad g_1(x) \leq 0, \ldots, g_m(x) \leq 0 \end{aligned}$$

Lagrangian.

$$L(x, \alpha) = f(x) + \alpha_1 g_1(x) + \cdots + \alpha_m g_m(x)$$

Dual Problem.

$$\begin{aligned} &\text{maximize} \quad \ell(\alpha) \\ &\text{subject to} \quad \alpha_1 \geq 0, \ldots, \alpha_m \geq 0 \end{aligned}$$

where $\ell(\alpha) = \min_{x \in \mathbb{R}^d} L(x, \alpha)$

Box constraints are easier to work with!

Inequality Constraints (Exact Solution)

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_1(x) \leq 0, \ldots, g_m(x) \leq 0 \end{array}$$

Lagrangian.

$$L(x, \alpha) = f(x) + \alpha_1 g_1(x) + \cdots + \alpha_m g_m(x)$$

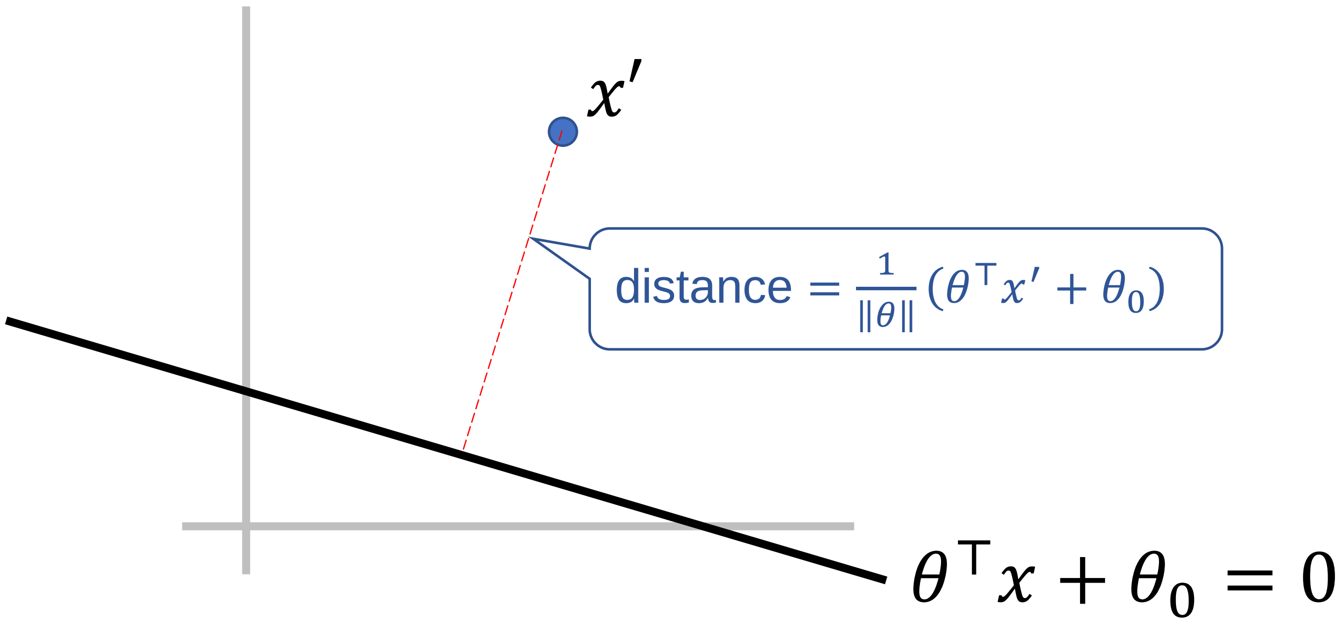
Solve for x, α satisfying

1. $\nabla_x L(x, \alpha) = 0$
2. $g_1(x) \leq 0, \ldots, g_m(x) \leq 0$
3. $\alpha_1 \geq 0, \ldots, \alpha_m \geq 0$
4. $\alpha_1 g_1(x) = 0, \ldots, \alpha_m g_m(x) = 0$

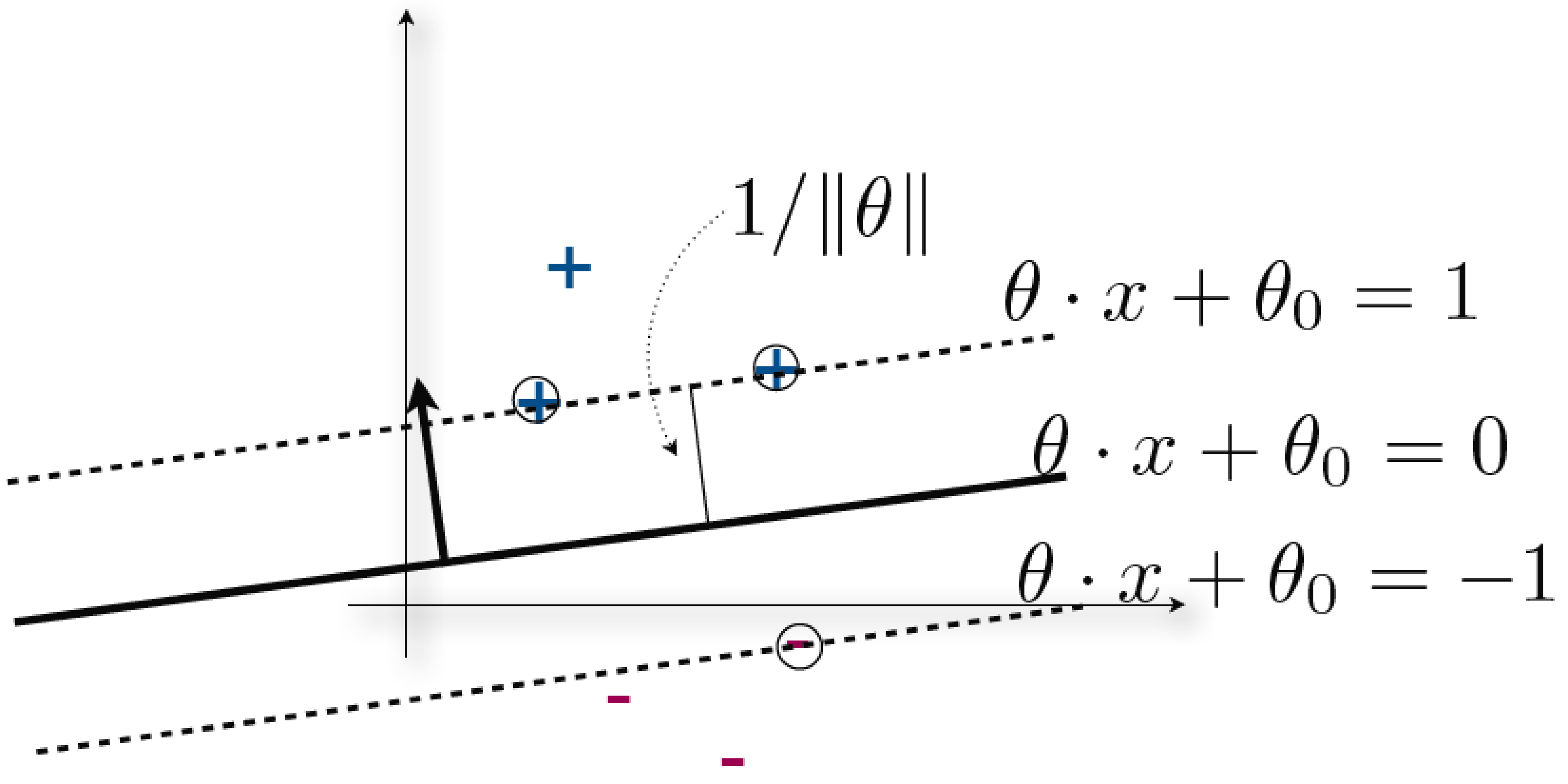
Complementary Slackness

SVM: Maximum Margins

Computing the margin



Computing the margin



Maximum Margin

Our goal is to

maximize $1/\|\theta\|$

subject to $y(\theta^\top x + \theta_0) \geq 1$ for all data (x, y)

Or equivalently,

minimize $\frac{1}{2}\|\theta\|^2$

subject to $y(\theta^\top x + \theta_0) \geq 1$ for all data (x, y)

Lagrangian

Primal. minimize $\frac{1}{2}\|\theta\|^2$

subject to $y(\theta^\top x) \geq 1$ for all data (x, y)

Lagrangian. $L(\theta, \alpha) = \frac{1}{2}\|\theta\|^2 + \sum_{(x,y)} \alpha_{x,y}\left(1 - y(\theta^\top x)\right)$

To find $\ell(\alpha) = \min_{\theta} L(\theta, \alpha)$, we solve

$$0 = \nabla_\theta L(\theta, \alpha) = \theta - \sum_{(x,y)} \alpha_{x,y}\, yx$$

to get $\theta = \sum_{(x,y)} \alpha_{x,y}\, yx$. Substituting into $L(\theta, \alpha)$ gives

$$\ell(\alpha) = \sum_{(x,y)} \alpha_{x,y} - \frac{1}{2}\sum_{(x,y)} \sum_{(x',y')} \alpha_{x,y}\, \alpha_{x',y'}\, yy'(x^\top x').$$

Primal-Dual

It can be shown that the primal and dual problems are equivalent (*strong duality*).

Primal.

minimize $\frac{1}{2}||\theta||^2$

subject to $y(\theta^\top x) \geq 1$ for all data (x, y)

Dual.

maximize $\sum_{(x,y)} \alpha_{x,y} - \frac{1}{2}\sum_{(x,y)} \sum_{(x',y')} \alpha_{x,y}\, \alpha_{x',y'} yy'(x^\top x')$

subject to $\alpha_{x,y} \geq 0$ for all (x, y)

After solving the dual to get the optimal $\alpha_{x,y}$'s,
we obtain the optimal θ using $\theta = \sum_{(x,y)} \alpha_{x,y}\, yx$.

Support Vectors

Complementary Slackness.

$$\hat{\alpha}_{x,y} > 0: \qquad y\left(\hat{\theta}^\top x\right) = 1$$

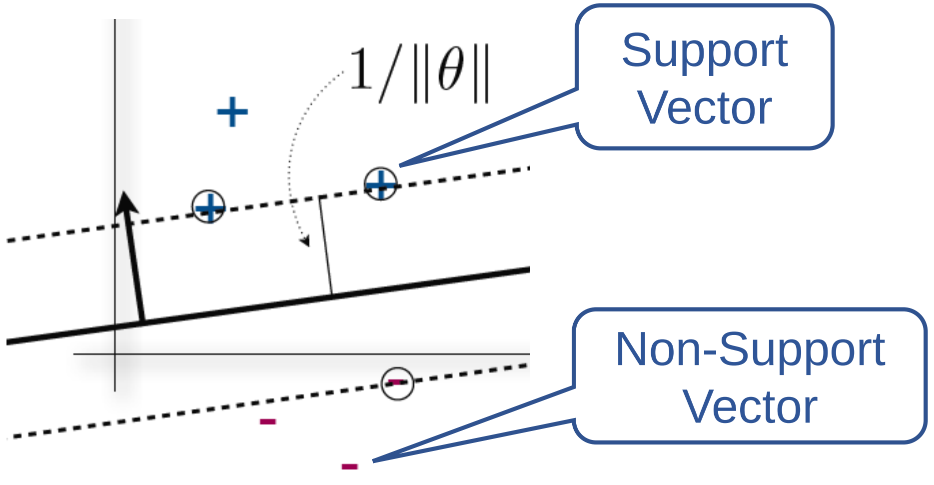
$$\hat{\alpha}_{x,y} = 0: \qquad y\left(\hat{\theta}^\top x\right) > 1$$

Support Vectors

Non-Support Vectors

Sparsity

Since very few data points are support vectors, most of the $\hat{\alpha}_{x,y}$ will be zero.



Summary

- **Lagrange Multipliers**
  - Lagrangian
  - Primal-Dual Problems
  - Inequality Constraints
  - Complementary Slackness

- **Support Vector Machines**
  - Maximum Margins
  - Dual Problem
  - Support Vectors

Intended Learning Outcomes

Support Vector Machines

- Write down the primal problem, and explain how it is derived from the maximum margin problem.
- Write down the dual problem.
  Describe how the optimal θ is derived from the $\alpha_{x,y}$'s.
  Describe in terms of the $\alpha_{x,y}$'s, how to do prediction.
- Define support vectors, both geometrically and in terms of the $\alpha_{x,y}$'s. Recognize that most of the $\alpha_{x,y}$'s are zero.