# COMP5211: Machine Learning

Lecture 5

# Adagrad

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\varepsilon I + diag(G_t)}} \cdot g_t, \tag{1}$$

$$g_t = \frac{1}{n} \sum_{i=1}^n \nabla_{\theta} \mathcal{L}(x^{(i)}, y^{(i)}, \theta_t), \tag{2}$$

$$G_t = \sum_{\tau=1}^t g_{\tau} g_{\tau}^{\top}. \tag{3}$$

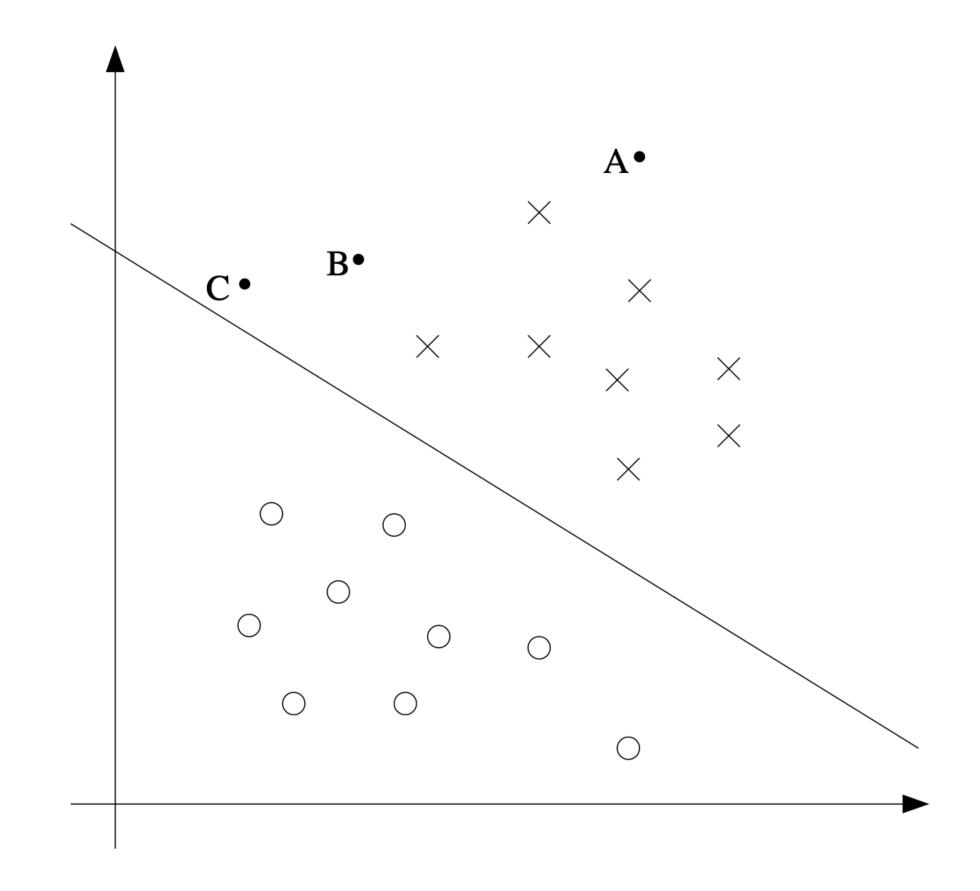
$$\begin{bmatrix} \theta_{t+1}^{(1)} \\ \theta_{t+1}^{(2)} \\ \vdots \\ \theta_{t+1}^{(m)} \end{bmatrix} = \begin{bmatrix} \theta_{t}^{(1)} \\ \theta_{t}^{(2)} \\ \vdots \\ \theta_{t}^{(m)} \end{bmatrix} - \begin{bmatrix} \frac{\eta}{\sqrt{\varepsilon + G_{t}^{(1,1)}}} & 0 & \cdots & 0 \\ 0 & \frac{\eta}{\sqrt{\varepsilon + G_{t}^{(2,2)}}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{\eta}{\sqrt{\varepsilon + G_{t}^{(m,m)}}} \end{bmatrix} \cdot \begin{bmatrix} g_{t}^{(1)} \\ g_{t}^{(2)} \\ \vdots \\ g_{t}^{(m)} \end{bmatrix}$$
(5)

# Support Vector Machine Margin

- Intuition
  - Confidence of A,B,C
- Let our decision function as

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

- g(z) = 1 if  $z \ge 0$ , g(z) = -1 otherwise
- Function margins:  $\hat{\gamma}^{(i)} = y^{(i)}(w^Tx + b)$
- However, it will double just replace w with 2w, b with 2b



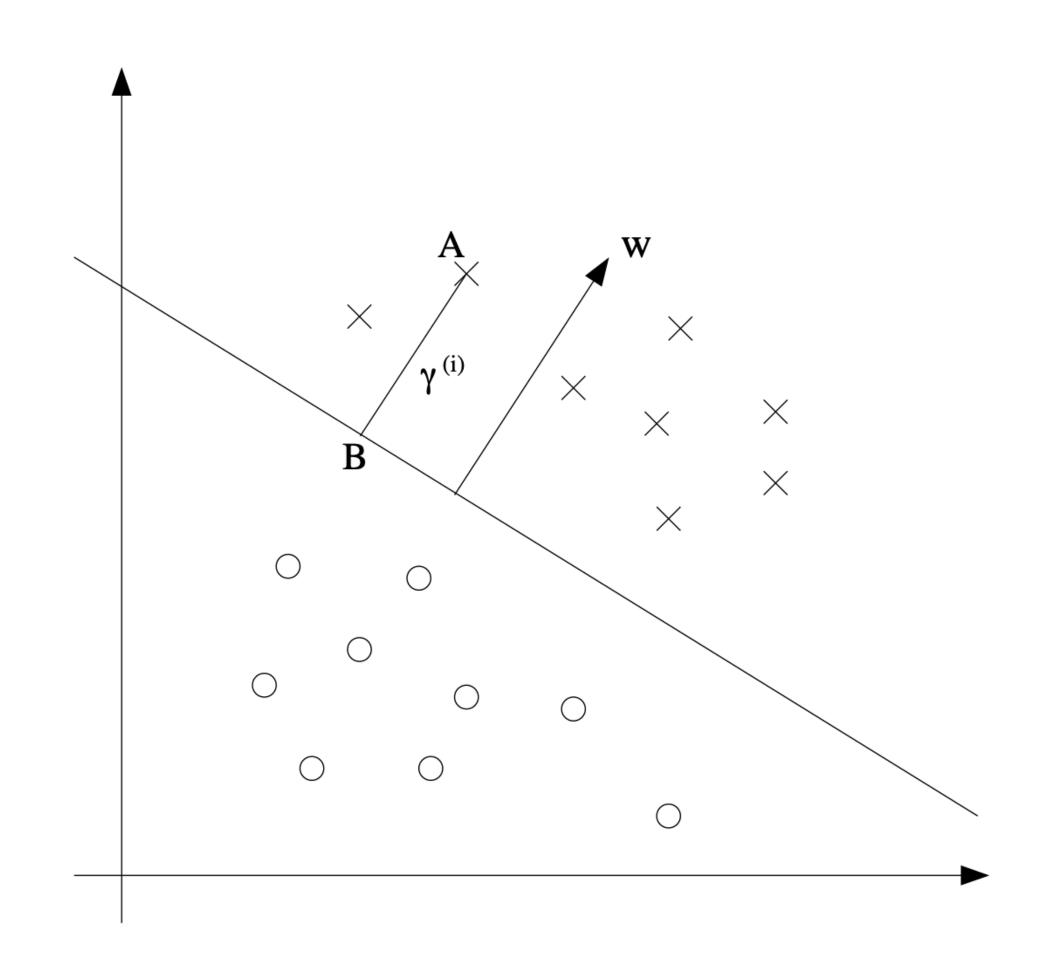
## Margin

• Find point B:

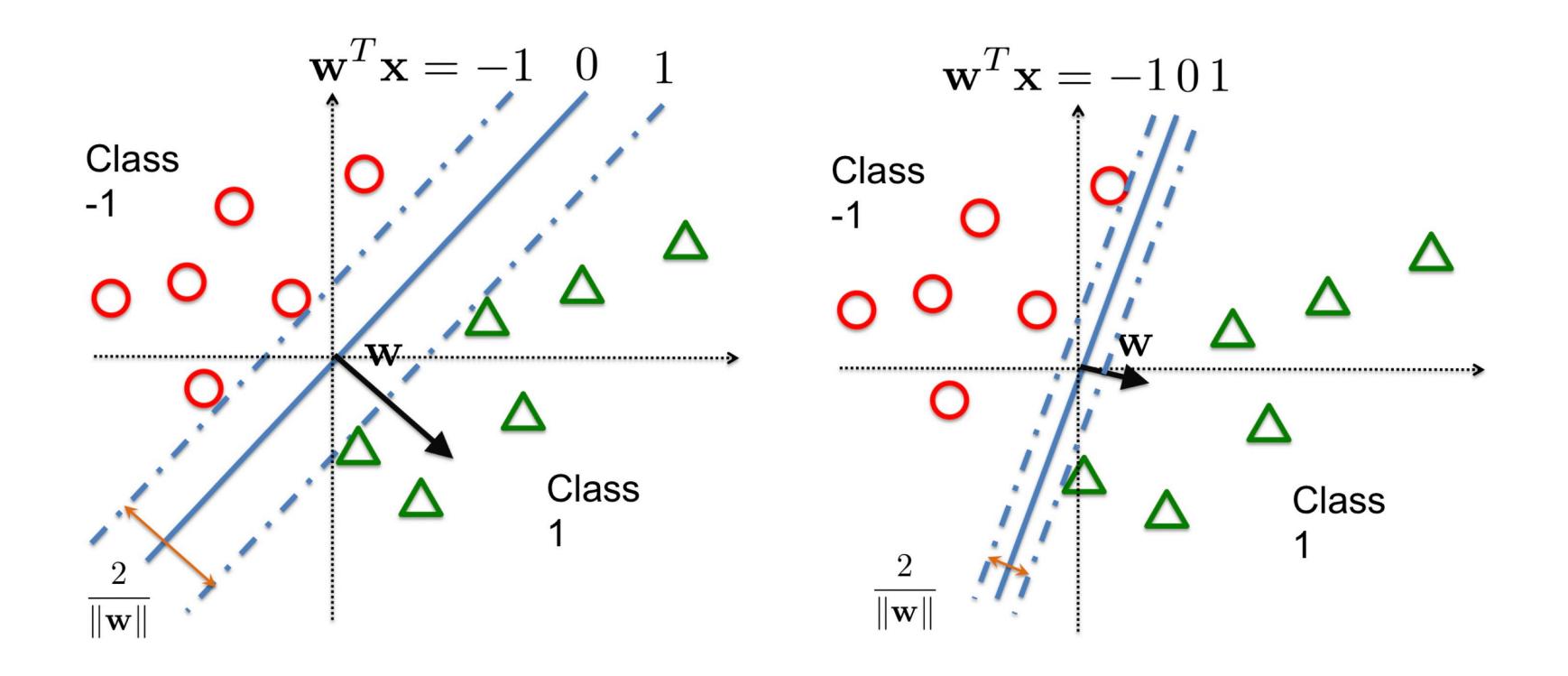
$$w^{T}(x^{(i)} - \gamma^{(i)} \frac{w}{\|w\|}) + b = 0$$

. Geometric margin:  $\gamma^{(i)} = \frac{w^T x^{(i)} + b}{\|w\|}$ 

$$\gamma = \min_{i=1,...,N} \gamma^{(i)}$$

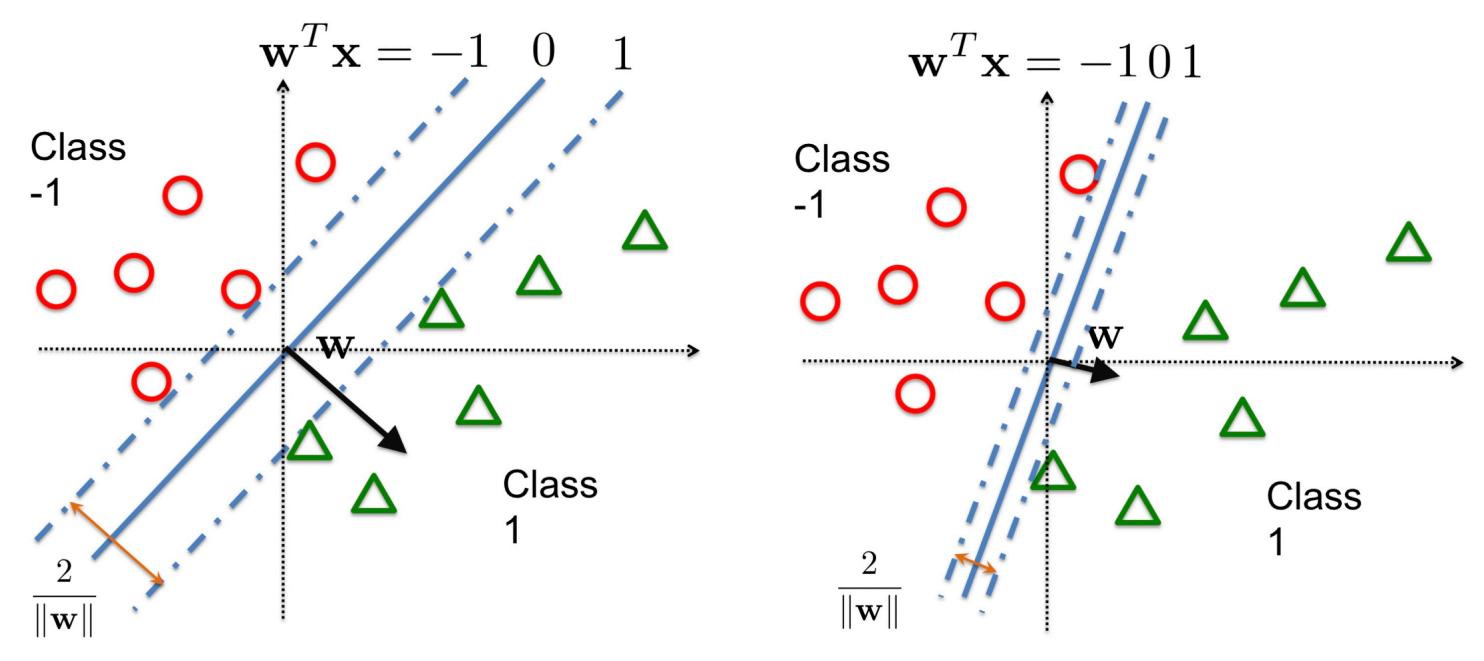


## Max margin



#### **Linear SVM**

• Goal: Find a hyperplane to separate these two classes of data: if  $y_i = 1, w^T x_i \ge 1$ ; if  $y_i = -1, w^T x_i \ge -1$ 



• Prefer a hyperplane with maximum margin

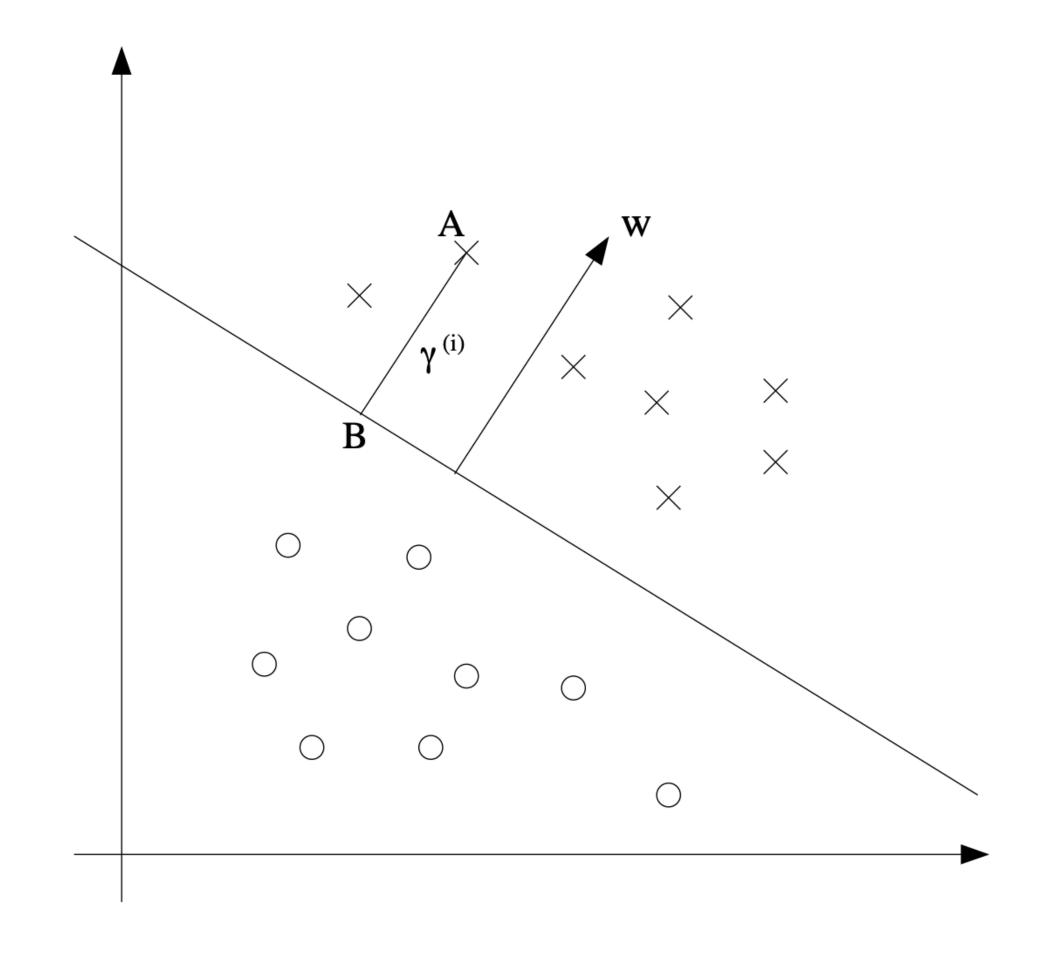
## Margin

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

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

$$\max_{\gamma,w,b} \frac{\gamma}{\|w\|}$$

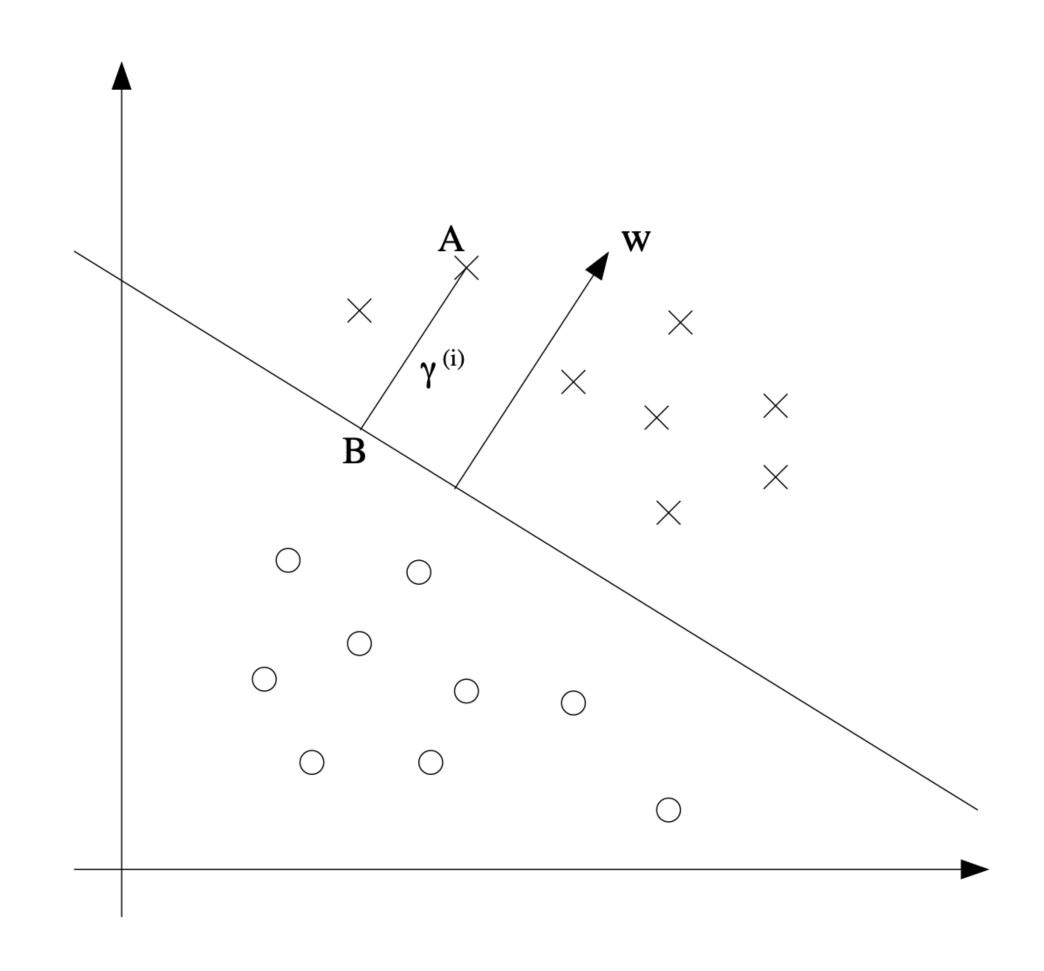
• s.t.  $y_i(w^Tx_i + b) \ge \gamma, i = 1,...,n$ 



## Margin

$$\max_{\gamma,w,b} \frac{\gamma}{\|w\|}$$

- s.t.  $\overline{\|w\|}$   $y_i(w^Tx_i + b) \ge \gamma, i = 1,..., n$
- $\gamma$  will increase linearly with w, b
- Just set  $\gamma = 1$



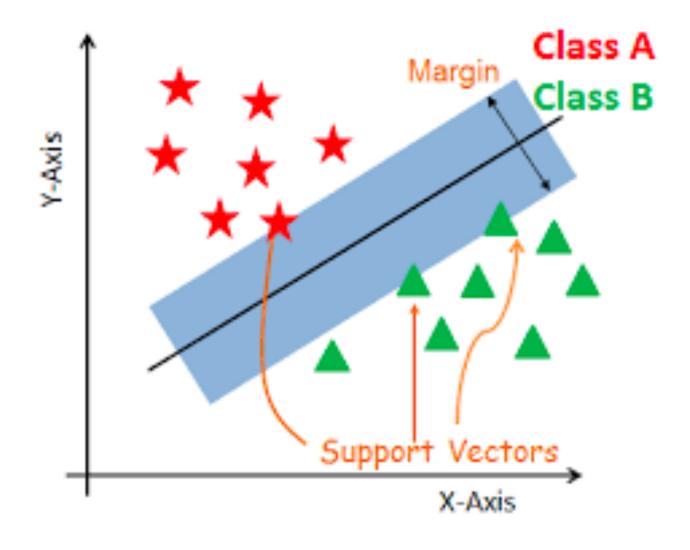
# Support Vector Machine Margin

$$\max_{\gamma,w,b} \frac{\gamma}{\|w\|}$$

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- $\gamma$  will increase linearly with w, b
- Just set  $\gamma = 1$

$$\max_{w,b} \frac{1}{\|w\|}$$

• s.t.  $y_i(w^T x_i + b) \ge 1, i = 1, ..., n$ 



### Linear SVM (hard constraint)

• SVM primal problem (with hard constraints):

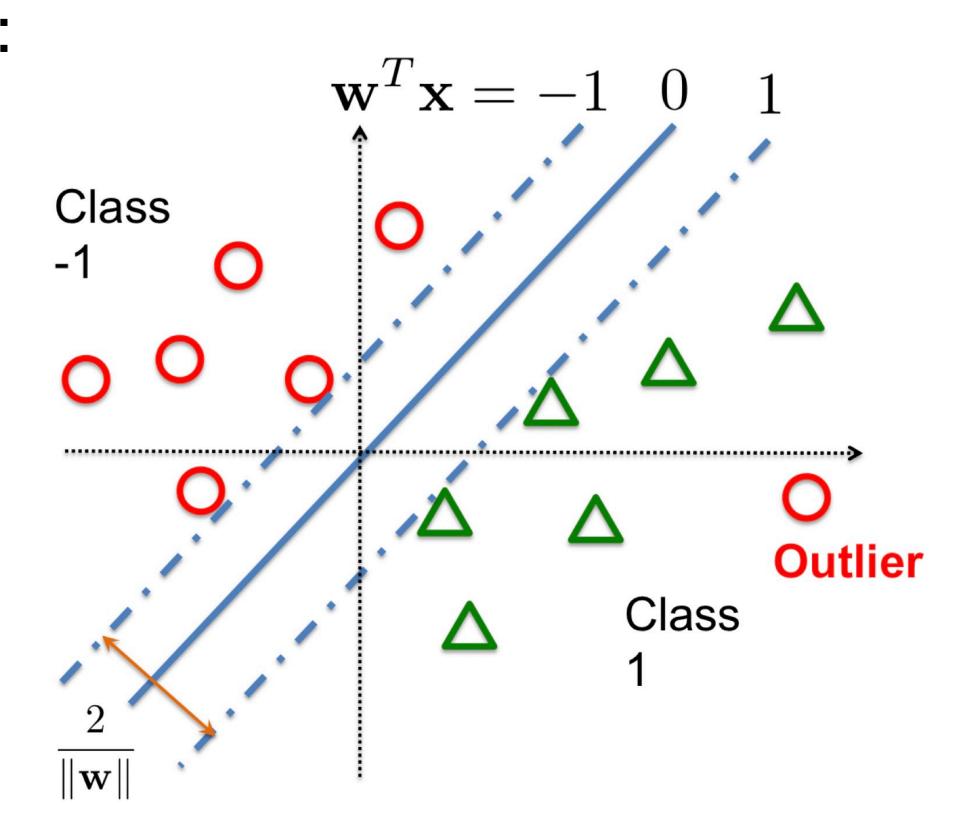
$$\min_{w} \frac{1}{2} w^{T} w$$
s.t.  $y_{i}(w^{T} x_{i}) \geq 1, i = 1,...,n$ 

### Linear SVM (hard constraint)

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s.t.  $y_i(w^T x_i) \ge 1, i = 1, ..., n$ 

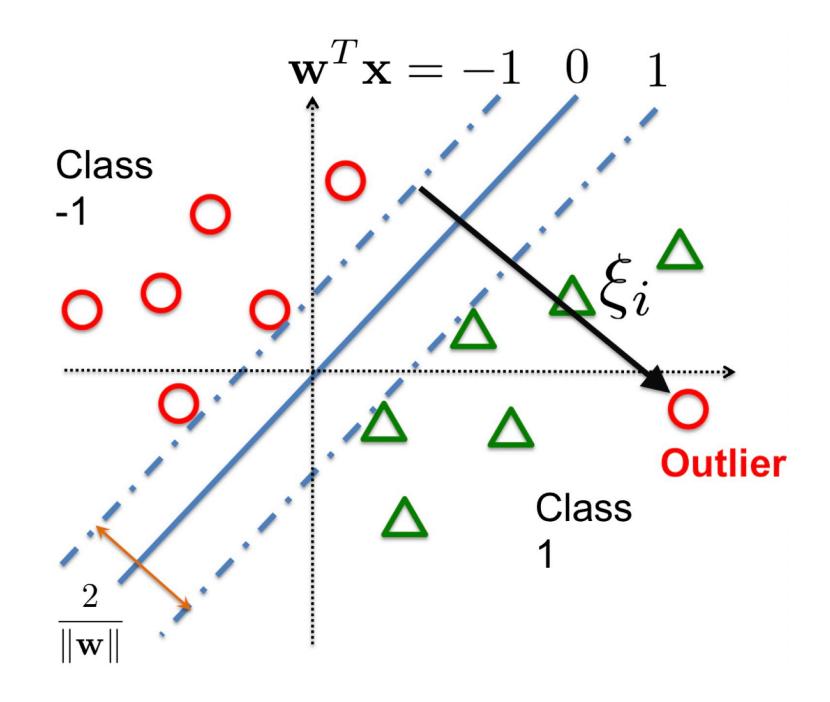
What if there are outliers?



- Given training examples  $(x_1, y_1), \ldots, (x_n, y_n)$ 
  - Consider binary classification:  $y_i \in \{+1, -1\}$
- Linear Support Vector Machine (SVM):

$$\min_{w} \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i$$

• s.t.  $y_i(w^T x_i) \ge 1 - \xi_i, i = 1, ..., n$  $\xi_i \ge 0$ 



• SVM primal problem:

 $\xi_i \geq 0$ 

$$\min_{w} \frac{1}{2} w^{T} w + C \sum_{i=1}^{n} \xi_{i}$$
s.t.  $y_{i}(w^{T} x_{i}) \geq 1 - \xi_{i}, i = 1, ..., n$ 

Equivalent to

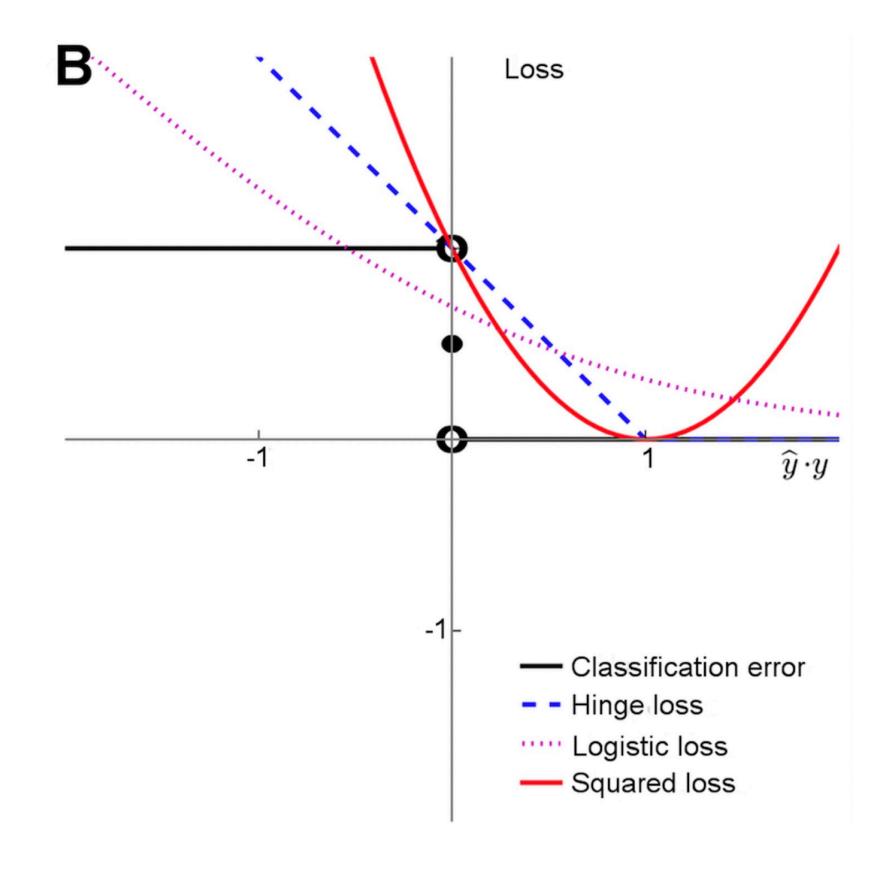
$$\underbrace{ \underset{w}{\operatorname{arg\,min}} \, C \sum_{i=1}^{n} \max(1 - y_i w^T x_i, 0) + \underbrace{\frac{1}{2} w^T w}_{\text{hinge loss}} } + \underbrace{\frac{1}{2} w^T w}_{\text{L2 regularization}}$$

• None-differentiable when  $y_i w^T x_i = 1$  for some i

- Given training examples  $(x_1, y_1), \ldots, (x_n, y_n)$ 
  - Consider binary classification:  $y_i \in \{+1, -1\}$
- Linear Support Vector Machine (SVM):

• 
$$\arg\min_{w} C \sum_{i=1}^{n} \max(1 - y_i w^T x_i, 0) + \frac{1}{2} w^T w$$

• (Hinge loss with I2 regularization)



### Stochastic subgradient method for SVM

• A sub gradient of  $\ell_i(w) = \max(0, 1 - y_i w^T x_i)$ :

$$\nabla_{w} \mathcal{E}_{i}(w) = \begin{cases} -y_{i} x_{i}, & \text{if } 1 - y_{i} w^{T} x_{i} > 0 \\ 0, & \text{if } 1 - y_{i} w^{t} x_{i} < 0 \\ 0, & \text{if } 1 - y_{i} w^{T} x_{i} = 0 \end{cases}$$

Stochastic subgradient descent for SVM:

For 
$$t = 1, 2, ...$$
Randomly pick an index  $i$ 
If  $y_i \mathbf{w}^T \mathbf{x}_i < 1$ , then
$$\mathbf{w} \leftarrow (1 - \eta_t) \mathbf{w} + \eta_t n C y_i \mathbf{x}_i$$
Else (if  $y_i \mathbf{w}^T \mathbf{x}_i \geq 1$ ):
$$\mathbf{w} \leftarrow (1 - \eta_t) \mathbf{w}$$

• SVM primal problem:

$$\min_{w} \frac{1}{2} w^{T} w + C \sum_{i=1}^{n} \xi_{i}$$
s.t.  $y_{i}(w^{T} x_{i}) \ge 1 - \xi_{i}, i = 1, ..., n$ 

$$\xi_{i} \ge 0$$

Equivalent to

$$\underbrace{\arg\min_{w} C \sum_{i=1}^{n} \max(1 - y_{i}w^{T}x_{i}, 0)}_{\text{w}} + \underbrace{\frac{1}{2}w^{T}w}_{\text{binge loss}} + \underbrace{\frac{1}{2}w^{T}w}_{\text{L2 regularization}}$$

- None-differentiable when  $y_i w^T x_i = 1$  for some i
- Alternatively, we show how to derive the dual form of SVM

#### Linear SVM dual

• SVM primal problem:

$$\min_{w} \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i$$

- s.t.  $y_i(w^T x_i) \ge 1 \xi_i, i = 1, ..., n$  $\xi_i \ge 0$
- Equivalent to: (using Lagrange multiplier):

$$\min_{w,\xi} \max_{\alpha \ge 0, \beta \ge 0} \frac{1}{2} \|w\|^2 + C \sum_{i} \xi_i - \sum_{i} \alpha_i (y_i w^T x_i - 1 + \xi_i) - \sum_{i} \beta_i \xi_i$$

#### Linear SVM dual form

• SVM primal problem:

$$\min_{w} \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i$$

- s.t.  $y_i(w^T x_i) \ge 1 \xi_i, i = 1, ..., n$  $\xi_i \ge 0$
- Equivalent to: (using Lagrange multiplier):

$$\min_{w,\xi} \max_{\alpha \ge 0, \beta \ge 0} \frac{1}{2} ||w||^2 + C \sum_{i} \xi_i - \sum_{i} \alpha_i (y_i w^T x_i - 1 + \xi_i) - \sum_{i} \beta_i \xi_i$$

• Under certain condition (e.g., Slater's condition), exchanging min, max will not change the optimal solution:

• 
$$\max_{\alpha \ge 0, \beta \ge 0} \min_{w, \xi} \frac{1}{2} ||w||^2 + C \sum_{i} \xi_i - \sum_{i} \alpha_i (y_i w^T x_i - 1 + \xi_i) - \sum_{i} \beta_i \xi_i$$

#### Linear SVM dual form

• Reorganize the equation:

$$\max_{\alpha \ge 0, \beta \ge 0} \min_{w, \xi} \frac{1}{2} ||w||^2 - \sum_{i} \alpha_i y_i w^T x_i + \sum_{i} \xi_i (C - \alpha_i - \beta_i) + \sum_{i} \alpha_i$$

• Now, for any given  $\alpha, \beta$ , the minimizer of w will satisfy

$$\frac{\partial L}{\partial w} = w - \sum_{i} \alpha_{i} y_{i} x_{i} = 0 \Rightarrow w^{*} = \sum_{i} y_{i} \alpha_{i} x_{i}$$

- Also, we have  $C = \alpha_i + \beta_i$ , otherwise  $\xi_i$  can make the objective function  $-\infty$
- Substitute these two equations back we get

$$\max_{\alpha \ge 0, \beta \ge 0, C = \alpha + \beta} - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_i \alpha_i$$

#### • Therefore, we get the following dual problem

$$\max_{C \ge \alpha \ge 0} \left\{ -\frac{1}{2} \alpha^T Q \alpha + e^T \alpha \right\} := D(\alpha),$$

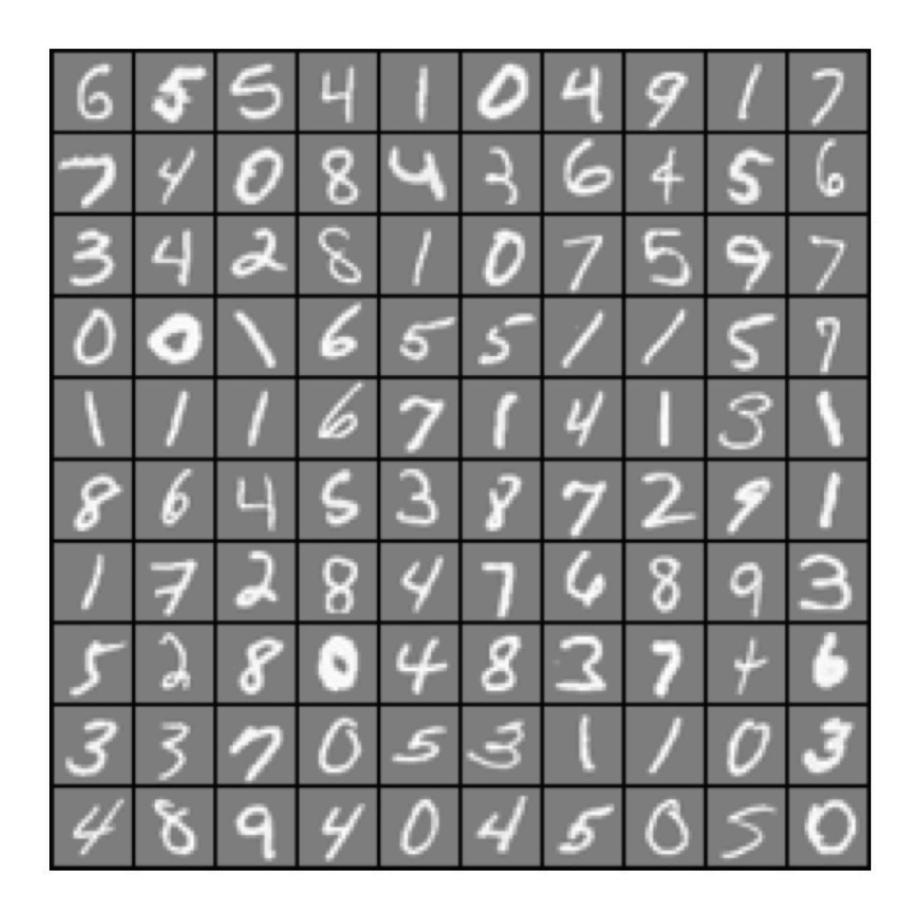
- Where Q is an  $n \times n$  matrix with  $Q_{ij} = y_i y_j x_i^T x_j$
- · Based on the derivations, we know
  - Primal minimum = dual maximum (under Slater's condition)
  - Let  $\alpha^*$  be the dual solution and  $w^*$  be the primal solution, we have

$$w^* = \sum_i y_i \alpha_i^* x_i$$

• We can solve the dual problem instead of primal problem

#### Multi-class

- n data points, L labels, d features
- Input: training data  $\{x_i, y_i\}_{i=1}^n$ :
  - Each  $x_i$  is a d dimensional feature vector
  - Each  $y_i \in \{1, \dots, L\}$  is the corresponding label
  - Each training data belongs to one category
- Goal: find a function to predict the correct label
  - $f(x) \approx y$



### Reduction to binary classification

- Many algorithms for binary classification
- Idea: transform multi-class or multi-label problems to multiple binary classification problems
- Two approaches:
  - One versus All (OVA)
  - One versus One (OVO)

# Multi problems One Versus All (OVA)

- Multi-class/multi-label problems with L categories
- ullet Build L different binary classifiers
- For the *t*-th classifier:
  - Positive samples: all the points in class  $t (\{x_i : t \in y_i\})$
  - Negative samples: all the points not in class t  $(\{x_i : t \notin y_i\})$
  - $f_t(x)$ : the decision value for the *t*-th classifier
    - (Larger  $f_t \Rightarrow$  higher probability that x in class t)
- Prediction:
  - $f(x) = \arg \max_{t} f_t(x)$
- Example: using SVM to train each binary classifier

# Multi problems One Versus One (OVO)

- ullet Multi-class/multi-label problems with L categories
- Build L(L-1) different binary classifiers
- For the (s, t)-th classifier:
  - Positive samples: all the points in class s ( $\{x_i : s \in y_i\}$ )
  - Negative samples: all the points in class t ( $\{x_i : t \notin y_i\}$ )
  - $f_{s,t}(x)$ : the decision value for the *t*-th classifier
    - (Larger  $f_{s,t}(x) \Rightarrow$  label s has higher probability than label t)
    - $\bullet \ f_{t,s}(x) = -f_{s,t}(x)$
- Prediction:

$$f(x) = \arg\max_{s} \left( \sum_{t} f_{s,t}(x) \right)$$

• Example: using SVM to train each binary classifier

### Another approach for multi-class classification

- OVA and OVO: decompose the problem by labels
  - But good binary classifiers may not imply good multi-class prediction
- Design a multi-class loss function and solve a single optimization problem

### Another approach for multi-class classification

- OVA and OVO: decompose the problem by labels
  - But good binary classifiers may not imply good multi-class prediction
- Design a multi-class loss function and solve a single optimization problem
- Minimize the regularized training error:

$$\min_{w_1, ..., w_L} \sum_{i=1}^n loss(x_i, y_i) + \lambda \sum_{j=1, ..., L} w_j^T w_j$$

#### Main idea

- For simplicity, we assume a linear model
- Model parameters:  $w_1, ..., w_L$
- For each data point *x*, compute the decision value for each label:
  - $w_1^T x, w_2^T x, ..., w_L^T x$
- Prediction:
  - $y = \arg \max_{t} w_t^T x$
- For training data  $x_i$ ,  $y_i$  is the true label, so we want
  - $y_i \approx \arg\max_t w_t^T x_i$ ,  $\forall i$

#### Softmax

- The predicted score for each class:
  - $w_1^T x_i, w_2^T x_i, \dots$
- Loss for the i-th data is defined by
  - $-\log(\frac{e^{w_{y_i}^Tx_i}}{\sum_{j}e^{w_j^Tx_i}}) \text{ (probability of choosing the correct label)}$
- Solve a single optimization problem

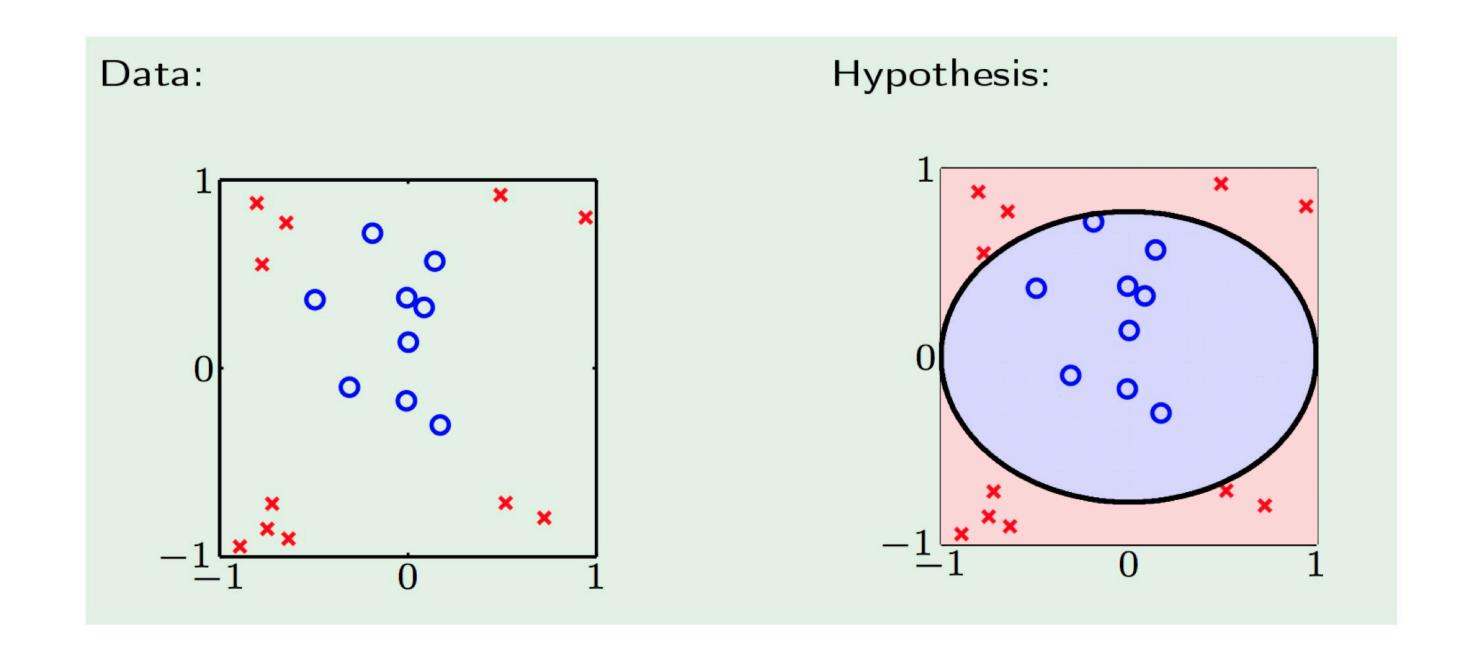
$$\min_{w_1, \dots, w_L} \sum_{i=1}^n -\log(\frac{e^{w_{y_i}^T x_i}}{\sum_j e^{w_j^T x_i}}) + \lambda \sum_j w_j^T w_j$$

#### Loss functions for multi-class classification

- Ranking based approaches: directly minimizes the ranking loss:
  - For multi-class classification, the score of  $y_i$  should be larger than other labels
- Soft-max loss:
  - Measure the probability of predicting correct class

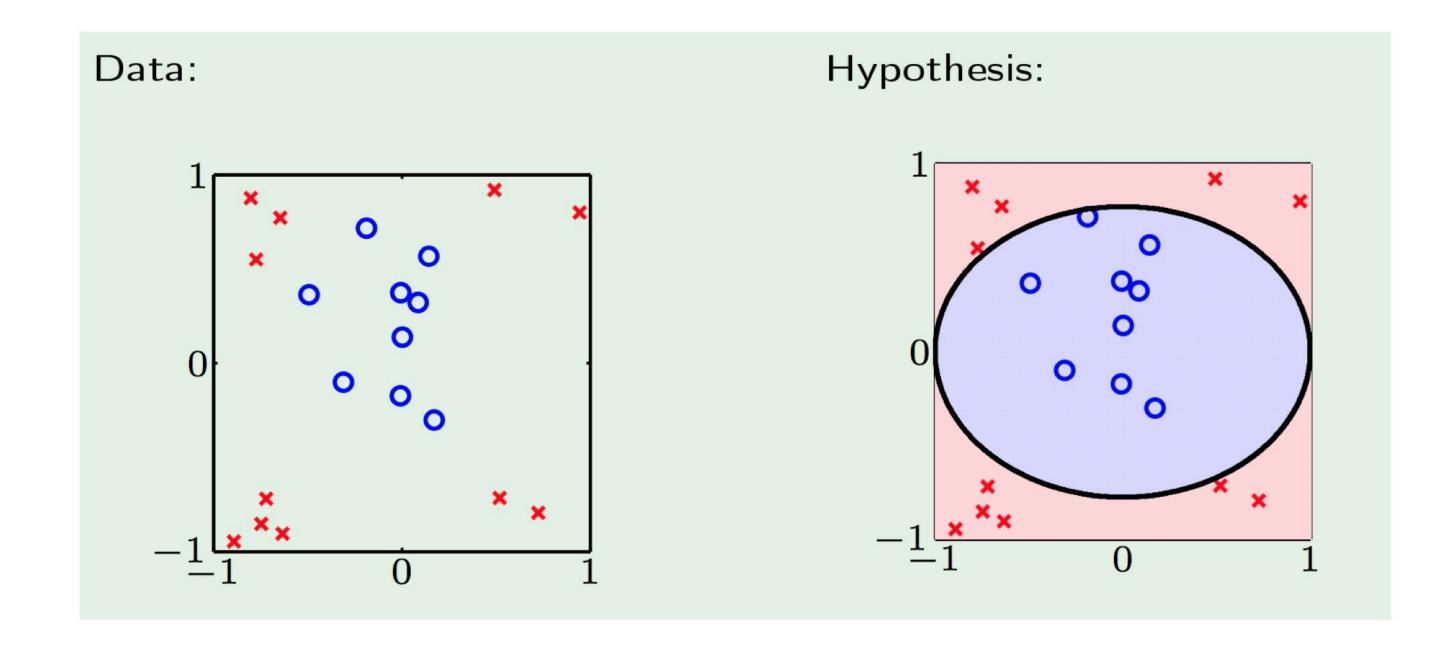
### Linear hypotheses

- Up to now: linear hypotheses
  - Perception, Linear regression, Logistic regression, ...
- Many problems are not linearly separable



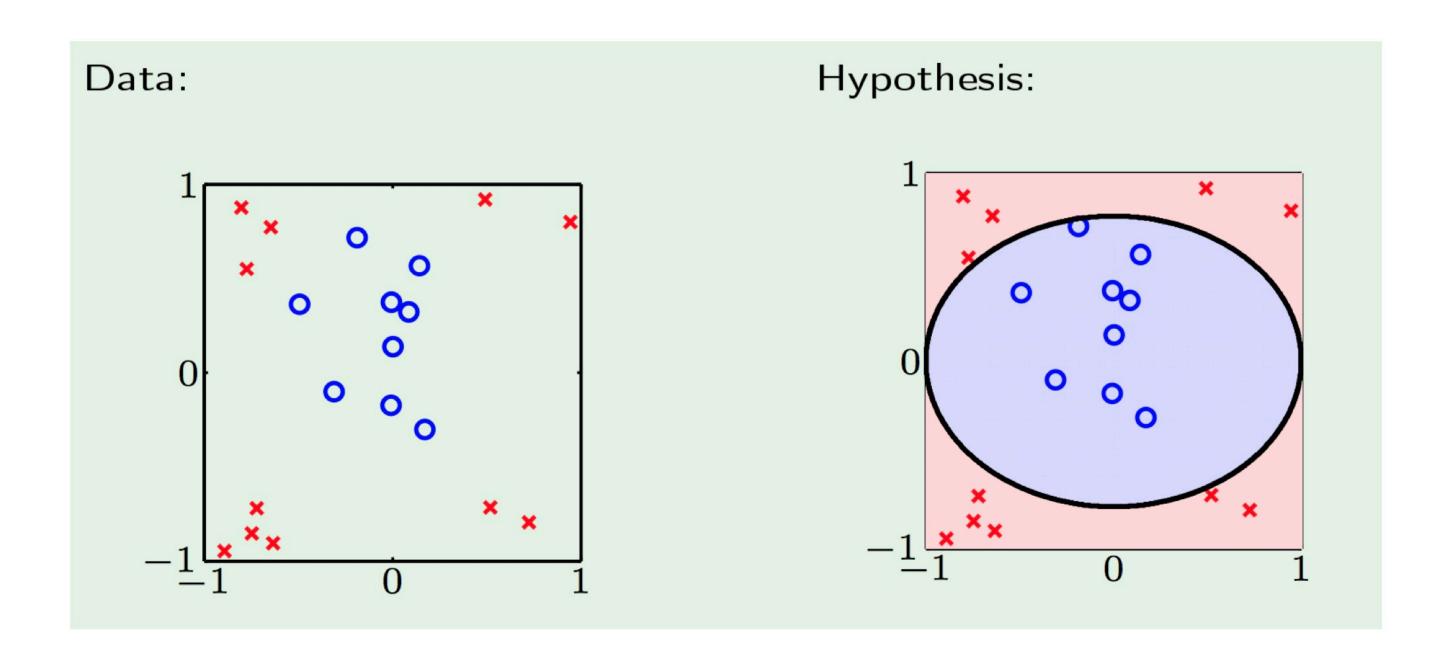
## Circular Separable

Data is not linear separable



### Circular Separable

- Data is not linear separable
- But circular separable by a circle of radius  $\sqrt{0.6}$  centered at origin:
  - $h_{SEP}(x) = sign(-x_1^2 x_2^2 + 0.6)$



Circular Separable and Linear Separable

• 
$$h(x) = sign(0.6 \cdot 1 + (-1) \cdot x_1^2 + (-1) \cdot x_2^2)$$

### Circular Separable and Linear Separable

$$h(x) = \operatorname{sign}(\underbrace{0.6} \cdot \underbrace{1} + \underbrace{(-1)} \cdot \underbrace{x_1^2} + \underbrace{(-1)} \cdot \underbrace{x_2^2})$$

$$\overset{\tilde{w}_0}{=} z_0 \qquad \overset{\tilde{v}_0}{=} z_1 \qquad \overset{\tilde{w}_2}{=} z_2$$

$$= \operatorname{sign}(\tilde{w}^T z)$$

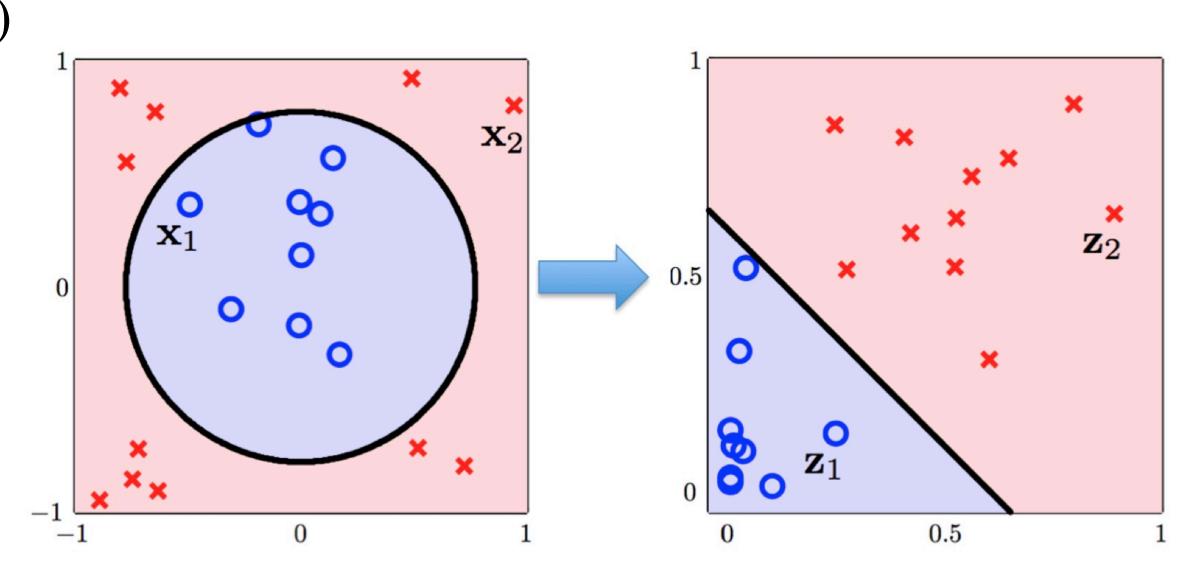
### Circular Separable and Linear Separable

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•  $\{(x_n, y_n)\}$  circular separable  $\Rightarrow$   $\{(z_n, y_n)\}$  linear separable



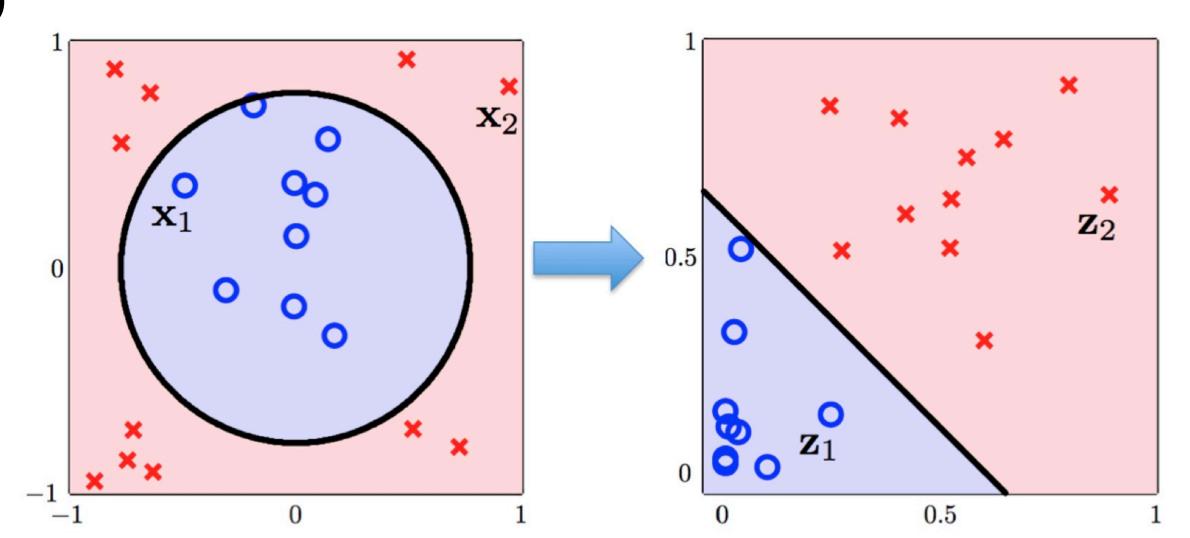
## Circular Separable and Linear Separable

$$h(x) = \operatorname{sign}(\underbrace{0.6} \cdot \underbrace{1} + \underbrace{(-1)} \cdot \underbrace{x_1^2} + \underbrace{(-1)} \cdot \underbrace{x_2^2})$$

$$\overset{\tilde{w_0}}{\sim} \overset{\tilde{z_0}}{\sim} \overset{\tilde{w_1}}{\sim} \overset{\tilde{z_1}}{\sim} \overset{\tilde{w_2}}{\sim} \overset{\tilde{z_2}}{\sim}$$

$$= \operatorname{sign}(\tilde{w}^T z)$$

- $\{(x_n, y_n)\}$  circular separable  $\Rightarrow$   $\{(z_n, y_n)\}$  linear separable
- $x \in \mathcal{X} \to x \in \mathcal{Z}$  (using a nonlinear transformation  $\phi$ )



#### **Definition**

- Define nonlinear transformation
  - $\phi(\mathbf{x}) = (1, x_1^2, x_2^2) = (z_0, z_1, z_2) = \mathbf{z}$

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  - $\operatorname{sign}(\tilde{h}(\mathbf{z})) = \operatorname{sign}(\tilde{h}(\phi(\mathbf{x}))) = \operatorname{sign}(w^T \phi(\mathbf{x}))$

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- Line in  ${\mathcal Z}$ -space  $\Leftrightarrow$  some quadratic curves in  ${\mathcal X}$ -space

#### **General Quadratic Hypothesis Set**

- A "bigger"  $\mathcal{Z}$  space:
  - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$

#### General Quadratic Hypothesis Set

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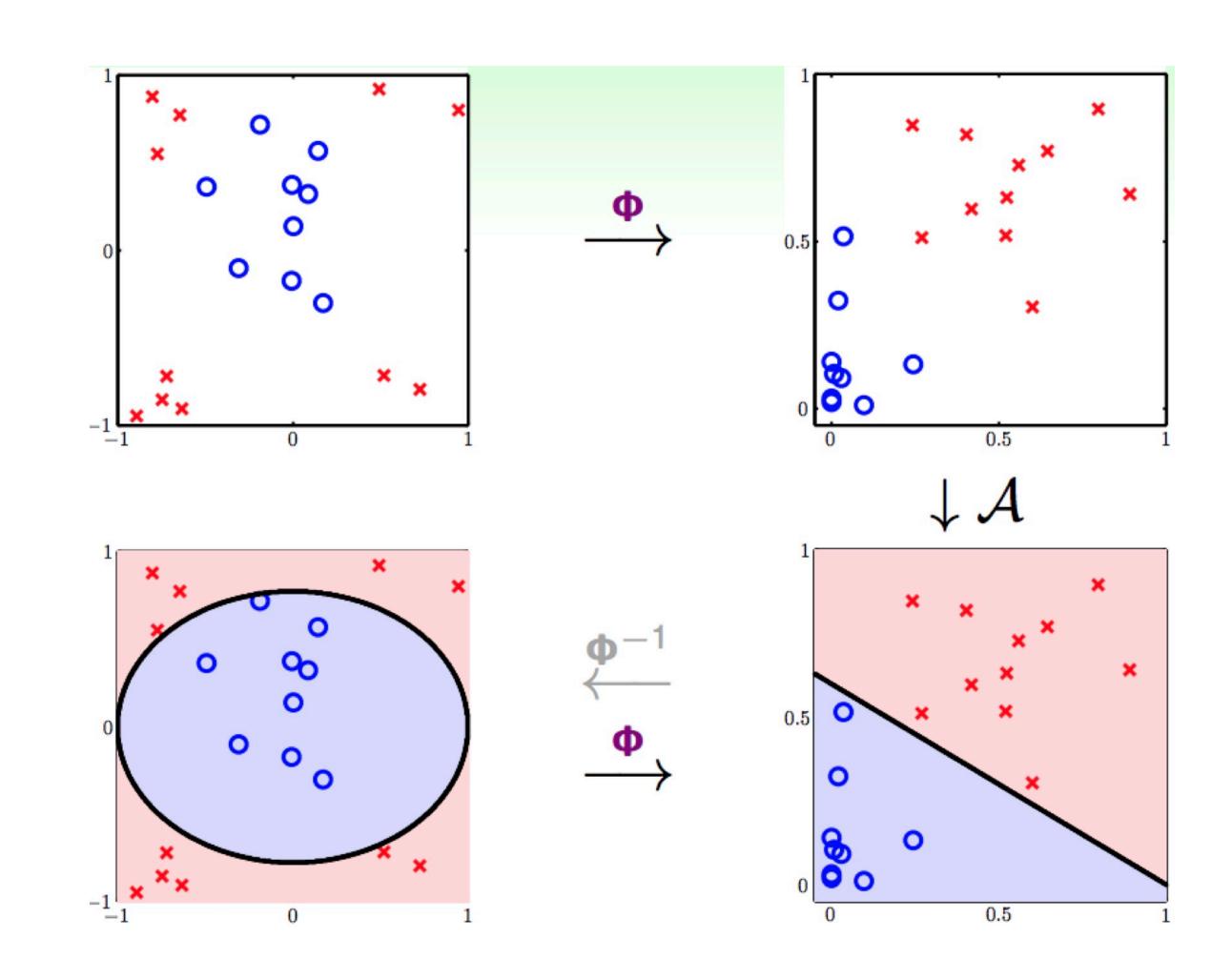
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- Linear in  ${\mathcal Z}$ -space  $\Leftrightarrow$  quadratic hypotheses in  ${\mathcal X}$ -space
- The hypotheses space:
  - $\mathcal{H}_{\phi_2} = \{h(x) : h(x) = \tilde{w}^T \phi_2(x) \text{ for some } \tilde{w}\}$  (quadratic hypotheses)

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- Linear in  ${\mathcal Z}$ -space  $\Leftrightarrow$  quadratic hypotheses in  ${\mathcal X}$ -space
- The hypotheses space:
  - $\mathcal{H}_{\phi_2} = \{h(x) : h(x) = \tilde{w}^T \phi_2(x) \text{ for some } \tilde{w}\}$  (quadratic hypotheses)
- Also include linear model as a degenerate case

#### Learning a good quadratic function

- Transform original data  $\{x_n, y_n\}$  to  $\{z_n = \phi(x_n), y_n\}$
- Solve a linear problem on  $\{z_n, y_n\}$  using your favorite algorithm  $\mathscr{A}$  to get a good model  $\tilde{w}$
- Return the model  $h(x) = \operatorname{sign}(\tilde{w}^T \phi(x))$



#### Polynomial mappings

Can now freely do quadratic classification, quadratic regression

#### Polynomial mappings

- Can now freely do quadratic classification, quadratic regression
- Can easily extend to any degree of polynomial mappings
  - E.g.,  $\phi(x) = (x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2^2, x_1x_3^2, x_1x_2^2, x_2^2x_3, x_2^2x_3, x_2^2x_3, x_1^3, x_2^3, x_3^3)$

# Support Vector Machine

#### SVM with nonlinear mapping

• SVM with nonlinear mapping  $\varphi(\cdot)$ :

$$\min_{w} \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i$$

- s.t.  $y_i(w^T \varphi(x_i)) \ge 1 \xi_i, i = 1, ..., n$  $\xi_i \ge 0$
- Hard to solve if  $oldsymbol{arphi}(\,\cdot\,)$  maps to very high or infinite dimensional space

# Support Vector Machine SVM with nonlinear mapping

- Similarly, we could derive
  - $\max_{C \ge \alpha \ge 0} \left\{ -\frac{1}{2} \alpha^T Q \alpha + e^T \alpha \right\} := D(\alpha),$
  - Where Q is an  $n \times n$  matrix with  $Q_{ij} = y_i y_j \varphi(x_i)^T \varphi(x_j)$
- Based on the derivations, we know
  - Primal minimum = dual maximum (under Slater's condition)
  - Let  $\alpha^*$  be the dual solution and  $w^*$  be the primal solution, we have

$$w^* = \sum_i y_i \alpha_i^* \varphi(x_i)$$

#### The price we pay: computational complexity

• Q-th oder polynomial transform:

$$\phi(x) = (1, x_1, x_2, \dots, x_d, x_d, x_1^2, x_1 x_2, \dots, x_d^2, \dots, x$$

•  $O(d^Q)$  dimensional vector  $\Rightarrow$  High computational cost

# Support Vector Machine

#### Kernel trick

- Do not directly define  $\varphi(\,\cdot\,)$
- Instead, define "kernel"
  - $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$

# Support Vector Machine

#### **Kernel trick**

- Do not directly define  $\varphi(\cdot)$
- Instead, define "kernel"
  - $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$
- Examples:
  - Gaussian kernel:  $K(x_i, x_j) = e^{-\gamma ||x_i x_j||^2}$
  - Polynomial kernel:  $K(x_i, x_j) = (\gamma x_i^T x_j + c)^d$
  - Other kernels for specific problems:
    - Graph kernels (Vishwanathan et al., "Graph Kernels", JMLR, 2010)
    - Pyramid kernel for image matching (Grauman and Darrell, "The Pyramid Match Kernel: Discriminative Classification with Sets of Image Features". In ICCV, 2005)
    - String kernel (Lodhi et al., "Text classification using string kernels". JMLR, 2002)

# Support Vector Machine SVM with kernel

• Training: compute  $\alpha = [\alpha_1, ..., \alpha_n]$  by solving the quadratic optimization problem:

$$\min_{0 \le \alpha \le C} \frac{1}{2} \alpha^T Q \alpha - e^T \alpha$$

• Where  $Q_{ij} = K(x_i, x_j)$ 

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  - Where  $Q_{ij} = y_i y_j K(x_i, x_j)$
- Prediction: for a test data x,

• 
$$w^{T}\varphi(x) = \sum_{i=1}^{n} y_{i}\alpha_{i}\varphi(x_{i})^{T}\varphi(x) = \sum_{i=1}^{n} y_{i}\alpha_{i}K(x_{i}, x)$$

# Kernel trick

#### Kernel Ridge Regression

- Actually, this "kernel method" works for many different losses
- Example: ridge regression

• 
$$\min_{w} \frac{1}{2} ||w||^2 + \frac{1}{2} \sum_{i=1}^{n} (w^T \varphi(x_i) - y_i)^2$$

Dual problem:

$$\min_{\alpha} \alpha^T Q \alpha + \|\alpha\|^2 - 2\alpha^T y$$

# Kernel trick Scalability

- Challenge for solving kernel SVMs (for dataset with n samples):
  - Space:  $O(n^2)$  for storing the  $n \times n$  kernel matrix (can be reduced in some cases);
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- Good packages available:
  - LIBSVM (can be called in scikit-learn)
  - LIBLINEAR (for linear SVM, can be called in scikit-learn)