

# **COMP5211: Machine Learning**

## **Lecture 5**

**Minhao Cheng**

# Adagrad

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

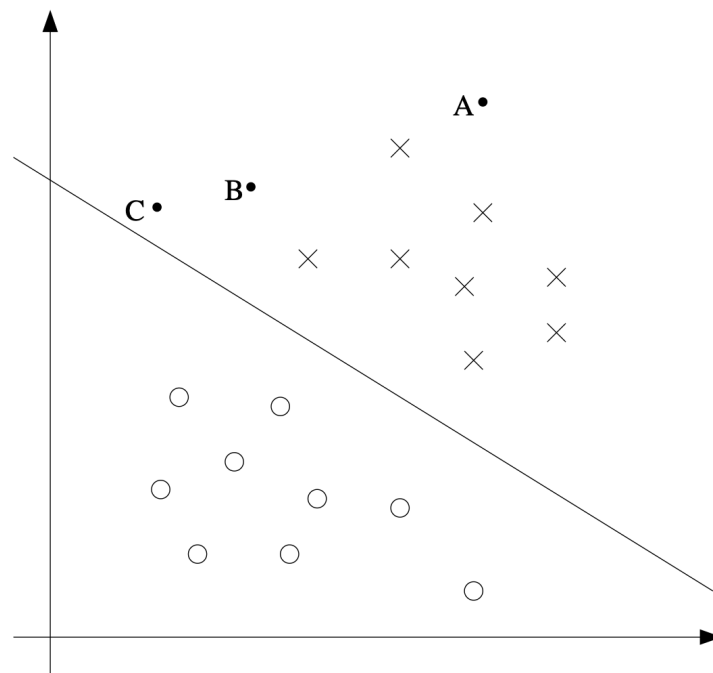
$$g_t = \frac{1}{n} \sum_{i=1}^n \nabla_{\theta} \mathcal{L}(x^{(i)}, y^{(i)}, \theta_t), \quad (2)$$

$$G_t = \sum_{\tau=1}^t g_{\tau} g_{\tau}^{\top}. \quad (3)$$

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

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



# Support Vector Machine

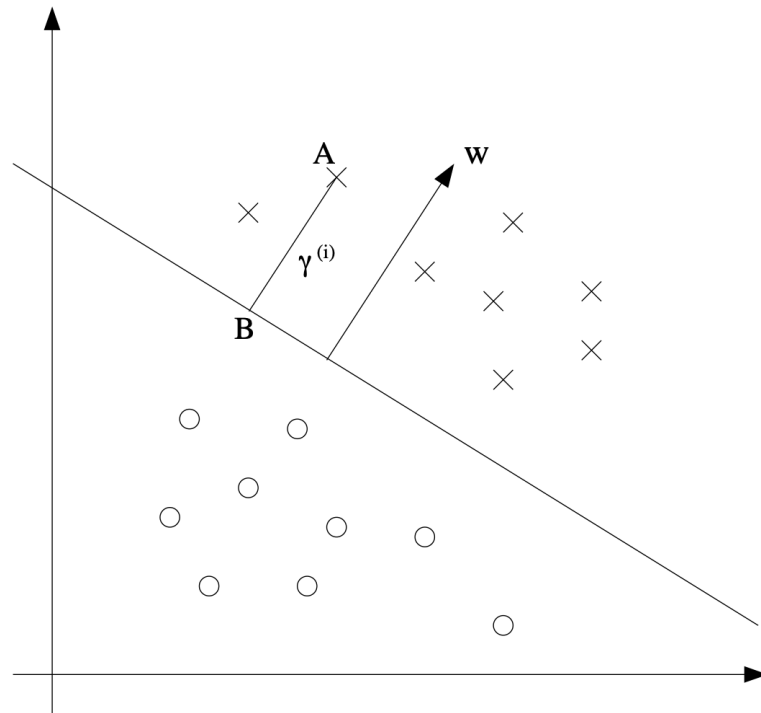
## Margin

- Find point B:

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

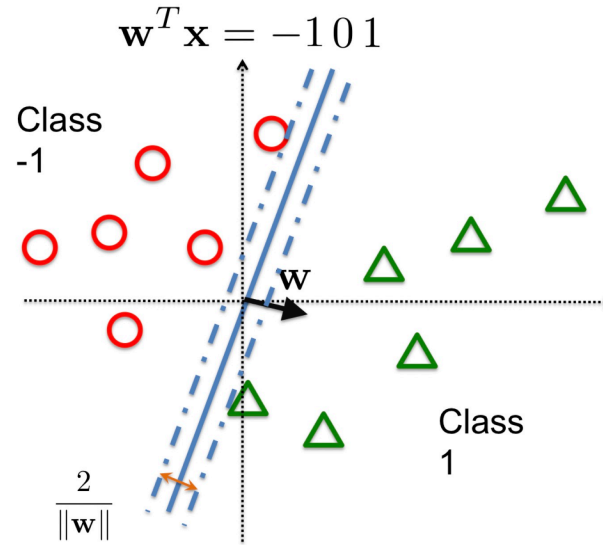
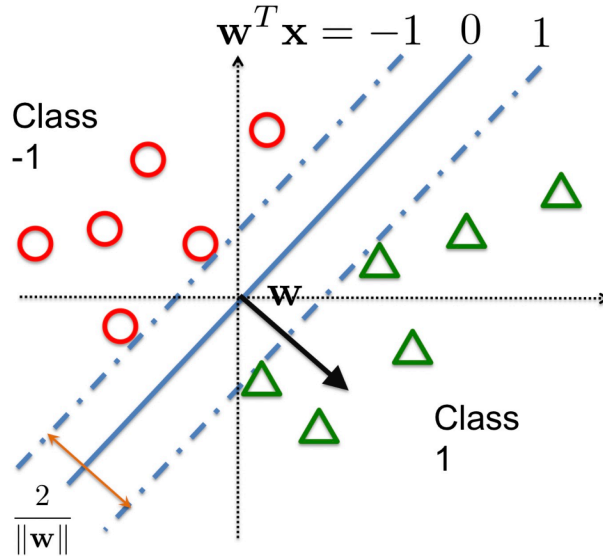
- Geometric margin:  $\gamma^{(i)} = \frac{w^T x^{(i)} + b}{\|w\|}$

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



# Support Vector Machine

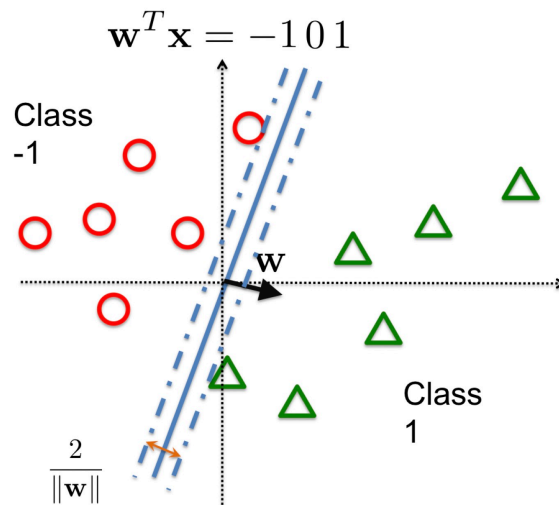
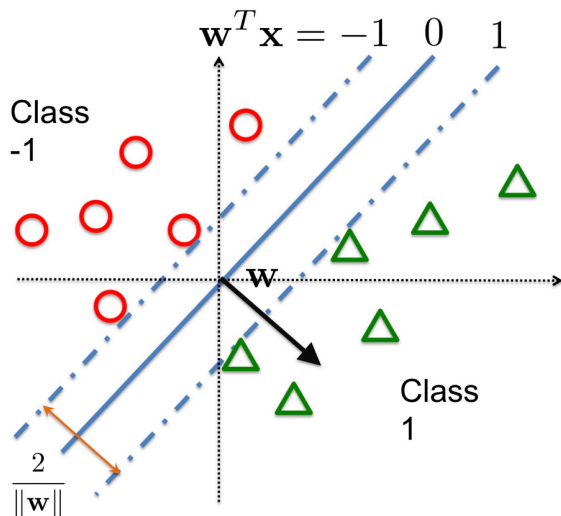
## Max margin



# Support Vector Machine

## Linear SVM

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



- Prefer a hyperplane with **maximum margin**

# Support Vector Machine

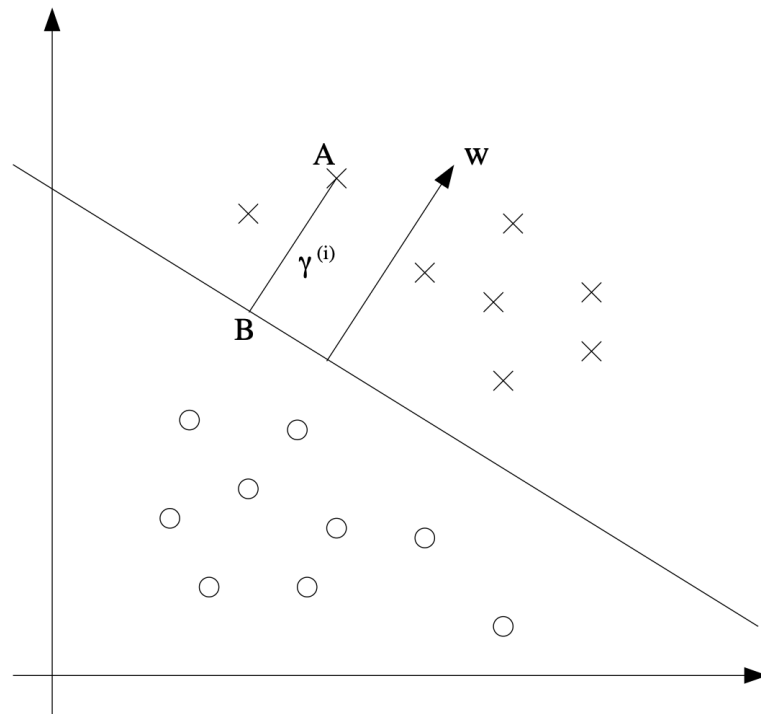
## Margin

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

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

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

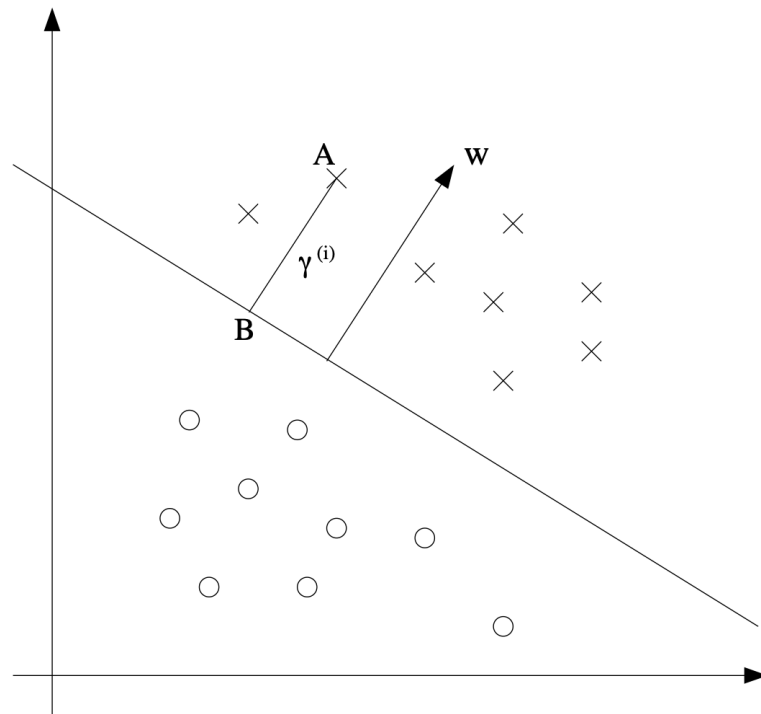
- s.t.  $y_i(w^T x_i + b) \geq \gamma, i = 1, \dots, n$



# Support Vector Machine

## Margin

- $$\max_{\gamma, w, b} \frac{\gamma}{\|w\|}$$
- s.t.  $y_i(w^T x_i + b) \geq \gamma, i = 1, \dots, n$
- $\gamma$  will increase linearly with  $w, b$
- Just set  $\gamma = 1$





# Support Vector Machine

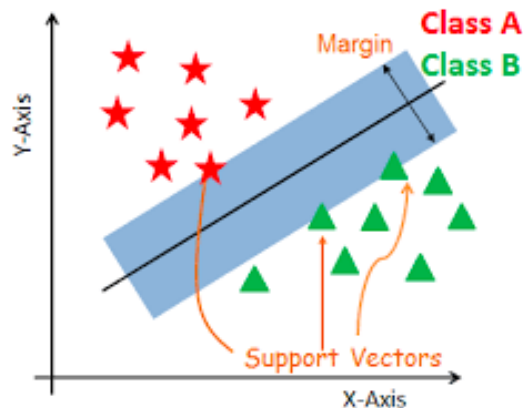
## Margin

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

- s.t.  $y_i(w^T x_i + b) \geq \gamma, i = 1, \dots, n$
- $\gamma$  will increase linearly with  $w, b$
- Just set  $\gamma = 1$

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

- s.t.  $y_i(w^T x_i + b) \geq 1, i = 1, \dots, n$



# Support Vector Machine

## Linear SVM (hard constraint)

- SVM primal problem (with hard constraints):

$$\begin{aligned} \min_w \quad & \frac{1}{2} w^T w \\ \text{s.t.} \quad & y_i(w^T x_i) \geq 1, i = 1, \dots, n \end{aligned}$$

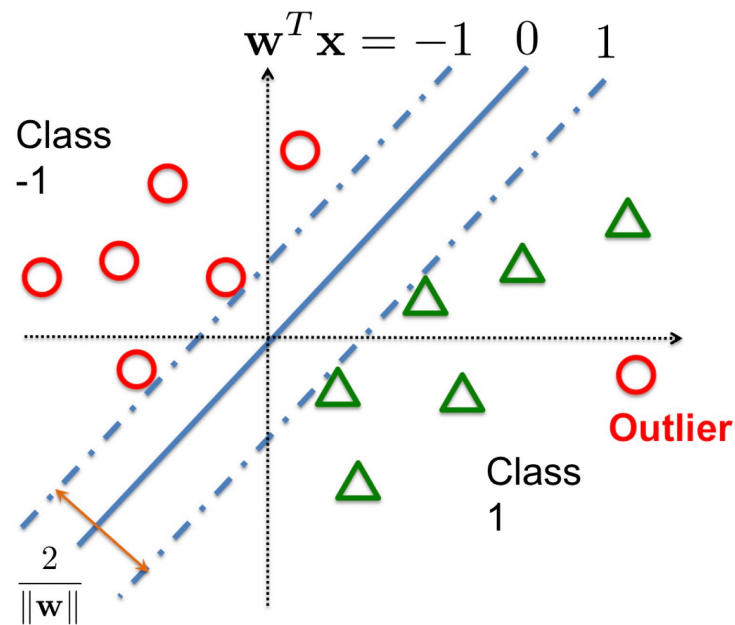
# Support Vector Machine

## Linear SVM (hard constraint)

- SVM primal problem (with hard constraints):

$$\min_w \quad \frac{1}{2} w^T w$$

- $\text{s.t. } y_i(w^T x_i) \geq 1, i = 1, \dots, n$
- What if there are outliers?



# Support Vector Machine

## Linear SVM

- Given training examples  $(x_1, y_1), \dots, (x_n, y_n)$

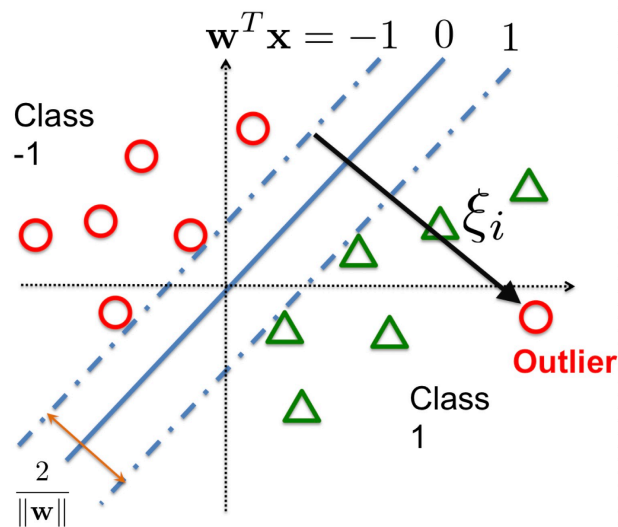
- Consider binary classification:

$$y_i \in \{+1, -1\}$$

- Linear Support Vector Machine (SVM):

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

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



# Support Vector Machine

## Linear SVM

- SVM primal problem:

$$\min_w \quad \frac{1}{2}w^Tw + C \sum_{i=1}^n \xi_i$$

- s.t.  $y_i(w^Tx_i) \geq 1 - \xi_i, i = 1, \dots, n$   
 $\xi_i \geq 0$

- Equivalent to

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

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

# Support Vector Machine

## Linear SVM

- Given training examples  $(x_1, y_1), \dots, (x_n, y_n)$

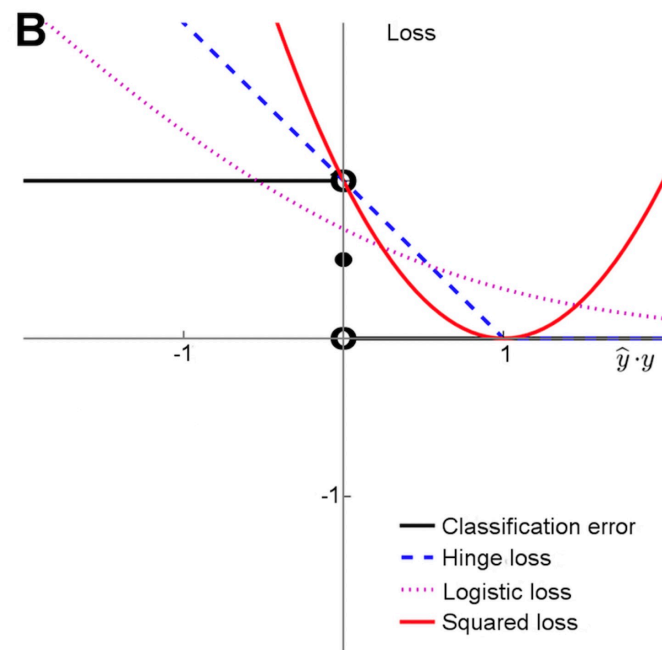
- Consider binary classification:

$$y_i \in \{+1, -1\}$$

- 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 l2 regularization)



# Support Vector Machine

## Stochastic subgradient method for SVM

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

$$\nabla_w \ell_i(w) = \begin{cases} -y_i x_i, & \text{if } 1 - y_i w^T x_i > 0 \\ 0, & \text{if } 1 - y_i w^T x_i < 0 \\ 0, & \text{if } 1 - y_i w^T x_i = 0 \end{cases}$$

- Stochastic subgradient descent for SVM:

For  $t = 1, 2, \dots$

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  $y_i \mathbf{w}^T \mathbf{x}_i \geq 1$ ):

$$\mathbf{w} \leftarrow (1 - \eta_t) \mathbf{w}$$

# Support Vector Machine

## Linear SVM

- SVM primal problem:

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

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

- Equivalent to

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

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



# Support Vector Machine

## Linear SVM dual

- SVM primal problem:

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

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

- Equivalent to: (using Lagrange multiplier):

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

# Support Vector Machine

## Linear SVM dual form

- SVM primal problem:

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

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

- Equivalent to: (using Lagrange multiplier):

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

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

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

# Support Vector Machine

## Linear SVM dual form

- Reorganize the equation:

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

- 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  $-\infty$

- Substitue these two equations back we get

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

# Support Vector Machine

## Linear SVM dual

- Therefore, we get the following dual problem

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

- 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

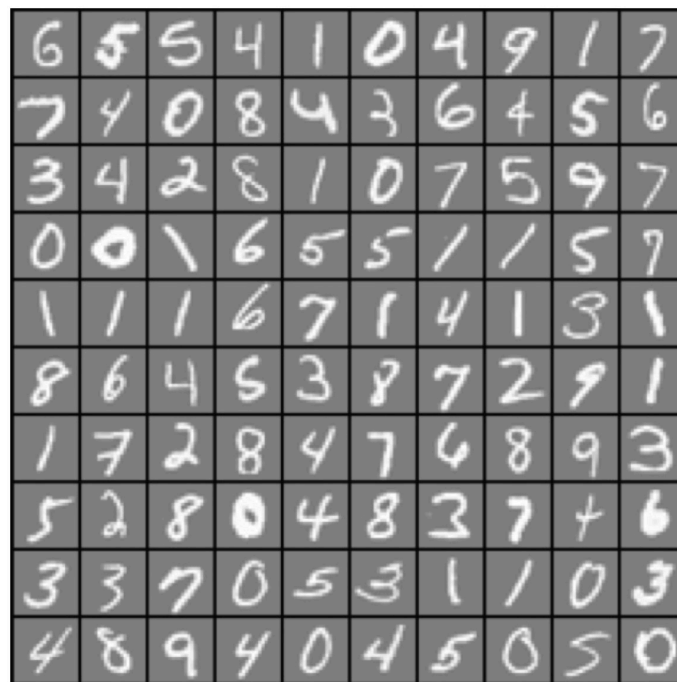
- $w^* = \sum_i y_i \alpha_i^* x_i$

- We can solve the dual problem instead of primal problem

# Multi 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
  - $f(x) \approx y$



# Multi problems

## 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
- 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)

- 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  $t$ )
    - $f_{t,s}(x) = -f_{s,t}(x)$
- Prediction:

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

- Example: using SVM to train each binary classifier



# Multi problems

## 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

# Multi problems

## 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:

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

# Multi problems

## Main idea

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

# Multi problems

## 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

- $-\log\left(\frac{e^{w_{y_i}^T x_i}}{\sum_j e^{w_j^T x_i}}\right)$  (probability of choosing the **correct label**)

- Solve a single optimization problem

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

# Multi problems

## Loss functions for multi-class classification

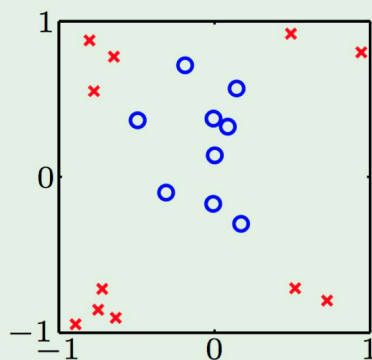
- Ranking based approaches: directly **minimizes the ranking loss**:
  - For multi-class classification, the score of  $y_i$  should be larger than other labels
- Soft-max loss:
  - Measure the **probability** of predicting correct class

# Nonlinear transformation

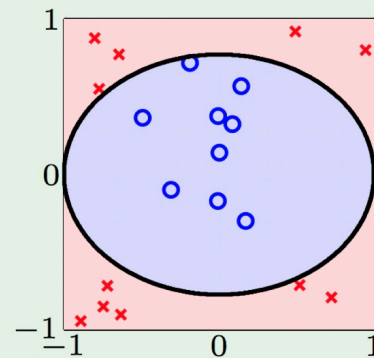
## Linear hypotheses

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

Data:



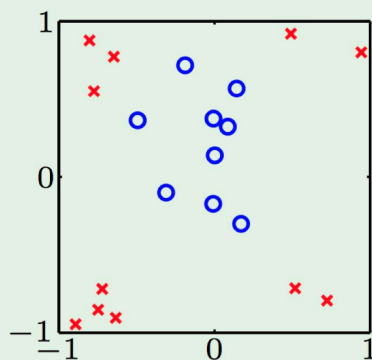
Hypothesis:



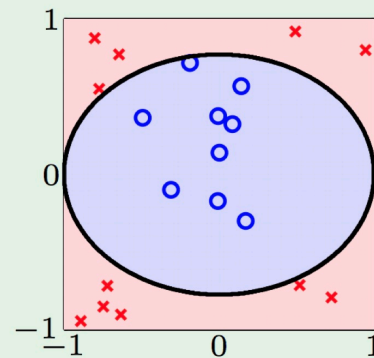
# Circular Separable

- Data is not linear separable

Data:



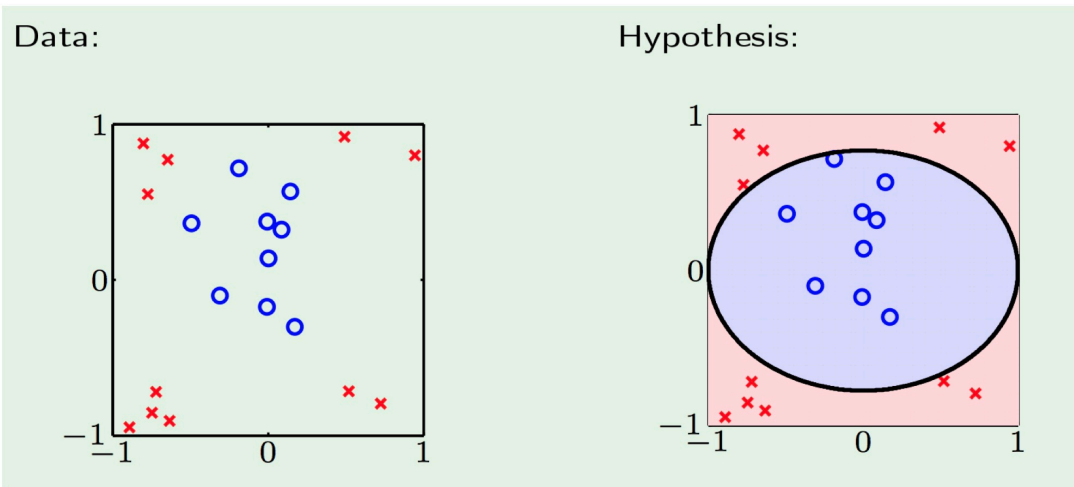
Hypothesis:



# Nonlinear transformation

## Circular Separable

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





# Nonlinear transformation

## Circular Separable and Linear Separable

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

# Nonlinear transformation

## Circular Separable and Linear Separable

$$h(x) = \text{sign}(\underbrace{0.6}_{\tilde{w}_0} \cdot \underbrace{1}_{\tilde{z}_0} + \underbrace{(-1)}_{\tilde{w}_1} \cdot \underbrace{x_1^2}_{\tilde{z}_1} + \underbrace{(-1)}_{\tilde{w}_2} \cdot \underbrace{x_2^2}_{\tilde{z}_2})$$

•

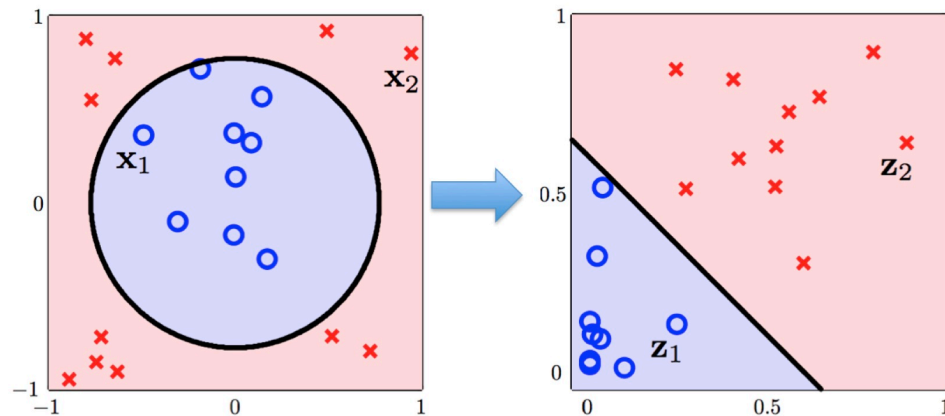
$$= \text{sign}(\tilde{w}^T z)$$

# Nonlinear transformation

## Circular Separable and Linear Separable

$$h(x) = \text{sign}(\underbrace{0.6}_{\tilde{w}_0} \cdot \underbrace{1}_{\tilde{z}_0} + \underbrace{(-1)}_{\tilde{w}_1} \cdot \underbrace{x_1^2}_{\tilde{z}_1} + \underbrace{(-1)}_{\tilde{w}_2} \cdot \underbrace{x_2^2}_{\tilde{z}_2})$$

- $= \text{sign}(\tilde{w}^T \tilde{z})$
- $\{(x_n, y_n)\}$  circular separable  $\Rightarrow$   
 $\{(z_n, y_n)\}$  linear separable

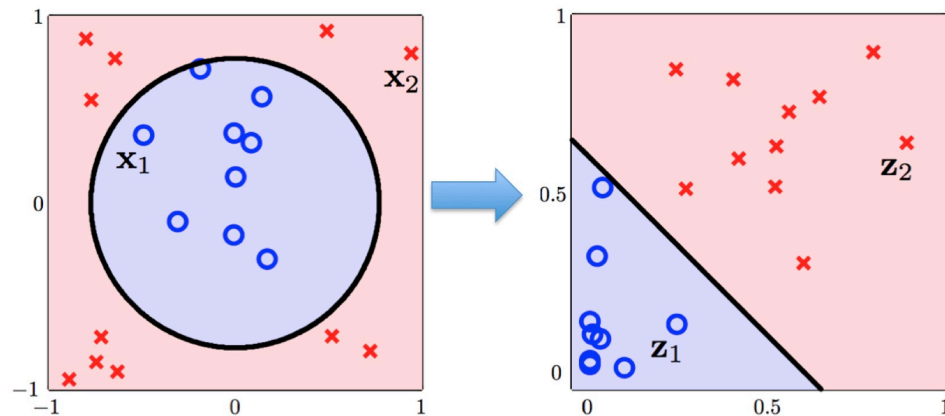


# Nonlinear transformation

## Circular Separable and Linear Separable

$$h(x) = \text{sign}(\underbrace{0.6 \cdot 1}_{\tilde{w}_0 \tilde{z}_0} + \underbrace{(-1) \cdot x_1^2}_{\tilde{w}_1 \tilde{z}_1} + \underbrace{(-1) \cdot x_2^2}_{\tilde{w}_2 \tilde{z}_2})$$

- $= \text{sign}(\tilde{w}^T z)$
- $\{(x_n, y_n)\}$  circular separable  $\Rightarrow$   
 $\{(z_n, y_n)\}$  linear separable
- $x \in \mathcal{X} \rightarrow x \in \mathcal{Z}$  (using a  
nonlinear transformation  $\phi$ )



# Nonlinear Transformation

## Definition

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

# Nonlinear Transformation

## Definition

- Define nonlinear transformation
  - $\phi(\mathbf{x}) = (1, x_1^2, x_2^2) = (z_0, z_1, z_2) = \mathbf{z}$
- Linear hypotheses in  $\mathcal{Z}$  space:
  - $\text{sign}(\tilde{h}(\mathbf{z})) = \text{sign}(\tilde{h}(\phi(\mathbf{x}))) = \text{sign}(w^T \phi(\mathbf{x}))$

# Nonlinear Transformation

## Definition

- Define nonlinear transformation
  - $\phi(\mathbf{x}) = (1, x_1^2, x_2^2) = (z_0, z_1, z_2) = \mathbf{z}$
- Linear hypotheses in  $\mathcal{Z}$ -space:
  - $\text{sign}(\tilde{h}(\mathbf{z})) = \text{sign}(\tilde{h}(\phi(\mathbf{x}))) = \text{sign}(w^T \phi(\mathbf{x}))$
- Line in  $\mathcal{Z}$ -space  $\Leftrightarrow$  some quadratic curves in  $\mathcal{X}$ -space

# Nonlinear Transformation

## General Quadratic Hypothesis Set

- A “bigger ”  $\mathcal{F}$  space:
  - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1x_2, x_2^2)$



# Nonlinear Transformation

## General Quadratic Hypothesis Set

- A “bigger ”  $\mathcal{Z}$ -space:
  - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1x_2, x_2^2)$
- Linear in  $\mathcal{Z}$ -space  $\Leftrightarrow$  quadratic hypotheses in  $\mathcal{X}$ -space

# Nonlinear Transformation

## General Quadratic Hypothesis Set

- A “bigger ”  $\mathcal{Z}$ -space:
  - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1x_2, x_2^2)$
- 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)

# Nonlinear Transformation

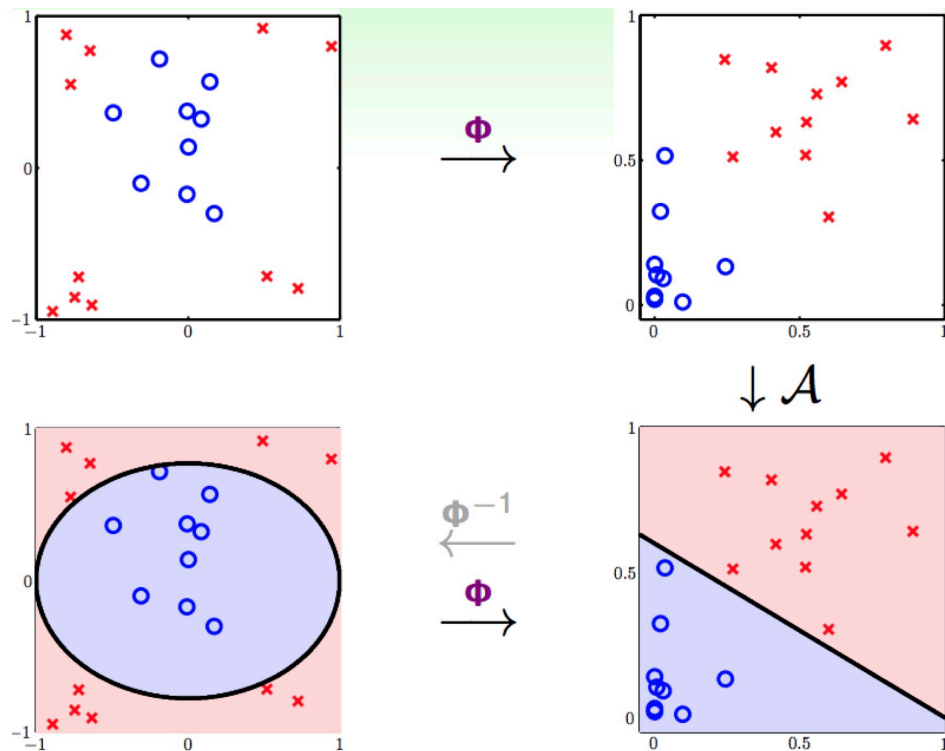
## General Quadratic Hypothesis Set

- A “bigger ”  $\mathcal{Z}$ -space:
  - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1x_2, x_2^2)$
- 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

# Nonlinear transformation

## 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  $\mathcal{A}$  to get a good model  $\tilde{w}$
- Return the model  $h(x) = \text{sign}(\tilde{w}^T \phi(x))$



# Nonlinear transformation

## Polynomial mappings

- Can now freely do quadratic classification, quadratic regression

# Nonlinear transformation

## Polynomial mappings

- Can now freely do quadratic classification, quadratic regression
- Can easily extend to any degree of polynomial mappings

- E.g.,

$$\phi(x) = (x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2^2, x_1x_3^2, x_1x_2^2, x_2^2x_3, x_2^2x_3, x_1^3, x_2^3, x_3^3)$$

# Support Vector Machine

## SVM with nonlinear mapping

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

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

- s.t.  $y_i(w^T \varphi(x_i)) \geq 1 - \xi_i, i = 1, \dots, n$

$$\xi_i \geq 0$$

- Hard to solve if  $\varphi(\cdot)$  maps to very high or infinite dimensional space

# Support Vector Machine

## SVM with nonlinear mapping

- Similarly, we could derive

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

- 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

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



# Nonlinear Transformation

The price we pay: computational complexity

- $Q$ -th order polynomial transform:

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

$$x_1^2, x_1x_2, \dots, x_d^2, \dots, x_d^2,$$

...

- $x_1^Q, x_1^{Q-1}x_2, \dots, x_d^Q)$

- $O(d^Q)$  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  $\alpha = [\alpha_1, \dots, \alpha_n]$  by solving the quadratic optimization problem:

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

- Where  $Q_{ij} = y_i y_j K(x_i, x_j)$

# Support Vector Machine

## SVM with kernel

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

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

- 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);
  - **Time:**  $O(n^3)$  for computing the exact solution

# 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);
  - **Time:**  $O(n^3)$  for computing the exact solution
- Good packages available:
  - LIBSVM ( can be called in scikit-learn)
  - LIBLINEAR ( for linear SVM, can be called in scikit-learn)