UVA CS 4774: Machine Learning

S4: Lecture 21: Support Vector Machine (nonlinear) Kernel Trick and in Practice

Module I

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What Left in SVM?

❑ Support Vector Machine (SVM)

- ✓ History of SVM
- ✓ Large Margin Linear Classifier
- ✓ Define Margin (M) in terms of model parameter
- ✓ Optimization to learn model parameters (w, b)
- ✓ Linearly Non-separable case (soft SVM)
- ✓ Optimization with dual form
- ✓ Nonlinear decision boundary
- ✓ Practical Guide

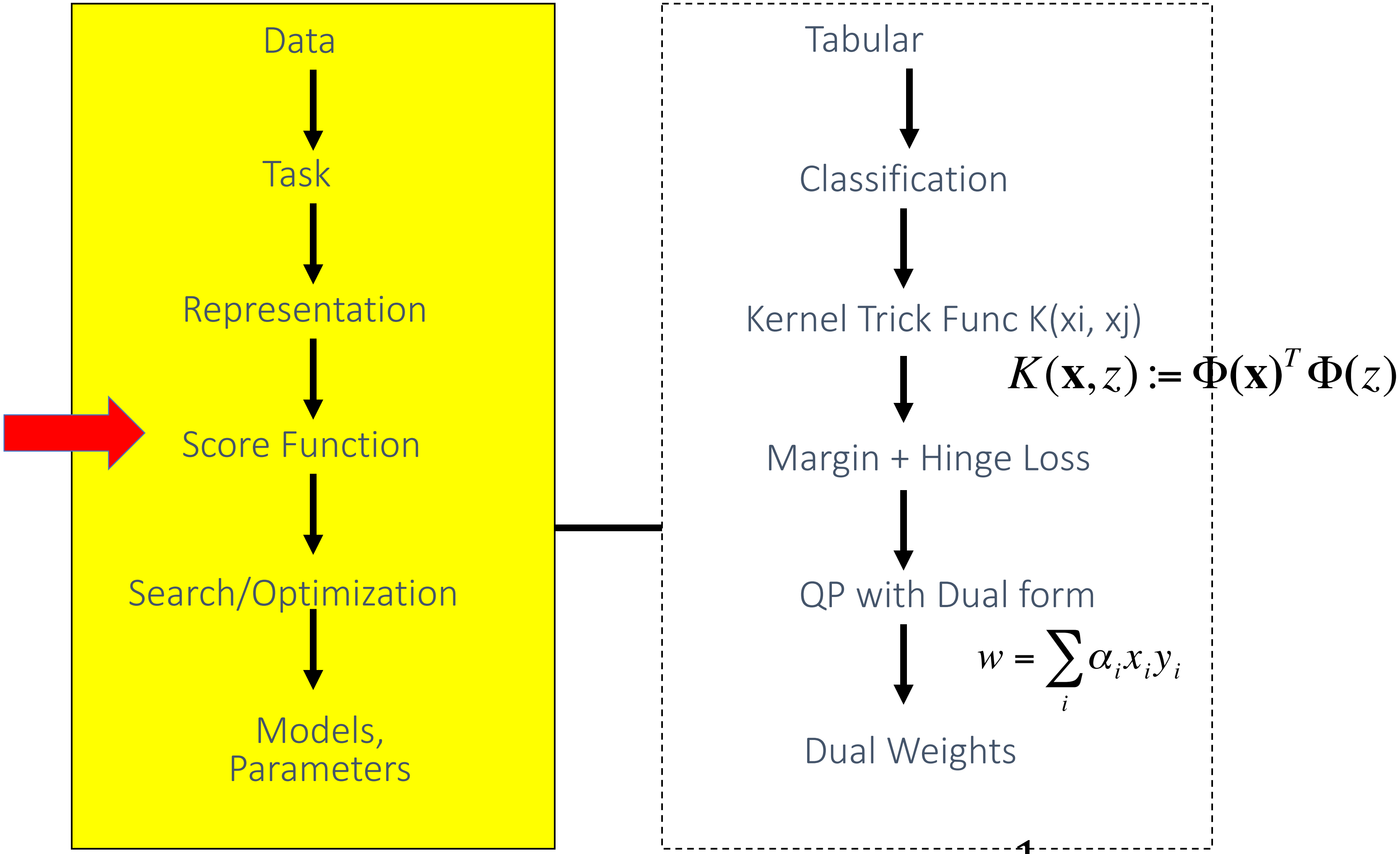
Today

- ❑ Support Vector Machine (SVM)
  - ✓ History of SVM
  - ✓ Large Margin Linear Classifier
  - ✓ Define Margin (M) in terms of model parameter
  - ✓ Optimization to learn model parameters (w, b)
  - ✓ Non linearly separable case (Extra)
  - ✓ Optimization with dual form (Extra)
  - ✓ Nonlinear decision boundary
  - ✓ Practical Guide

Extra

Today

Last: Basic Support Vector Machine



Data

Task

Representation

Score Function

Search/Optimization

Models, Parameters

Tabular

Classification

Kernel Trick Func K(xi, xj)

$$K(\mathbf{x}, z) := \Phi(\mathbf{x})^T \Phi(z)$$

Margin + Hinge Loss

QP with Dual form

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

Dual Weights

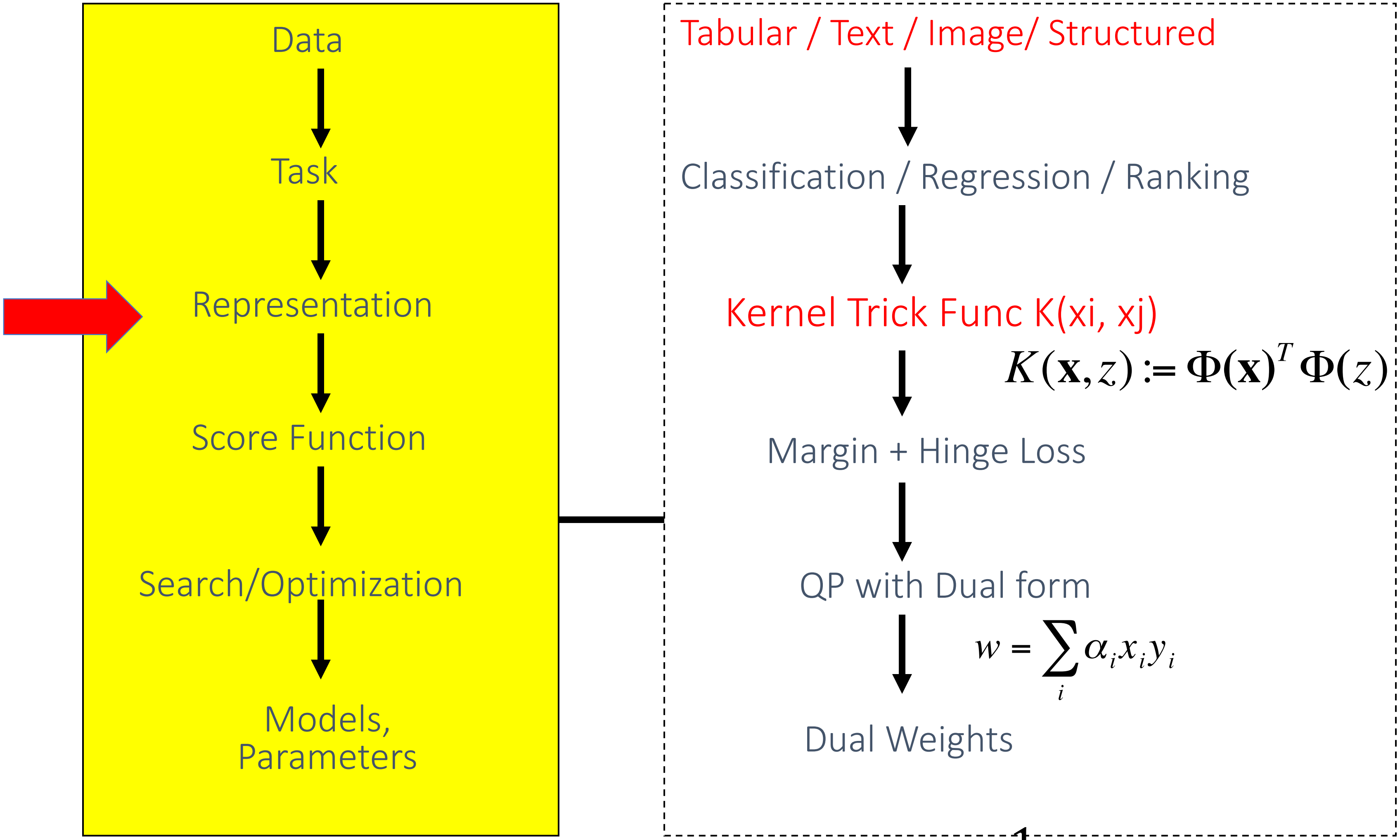
$$\underset{\mathbf{w},b}{\operatorname{argmin}} \sum_{i=1}^{p} w_i^2 + \mathrm{C}\sum_{\mathrm{i}=1}^{\mathrm{n}} \varepsilon_{\mathrm{i}}$$

subject to $\forall \mathbf{x}_i \in Dtrain : y_i\left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq 1 - \varepsilon_{\mathrm{i}}$

$$\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_{\mathrm{i}} y_j \mathbf{x}_{\mathbf{i}}^T \mathbf{x}_{\mathbf{j}}$$

$$\sum_i \alpha_i \mathrm{y}_{\mathrm{i}} = 0, \qquad \alpha_i \geq 0 \qquad \forall i$$

This: Kernel Support Vector Machine



Data → Task → Representation → Score Function → Search/Optimization → Models, Parameters

Tabular / Text / Image/ Structured

Classification / Regression / Ranking

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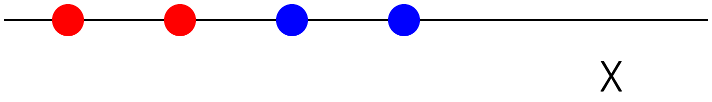
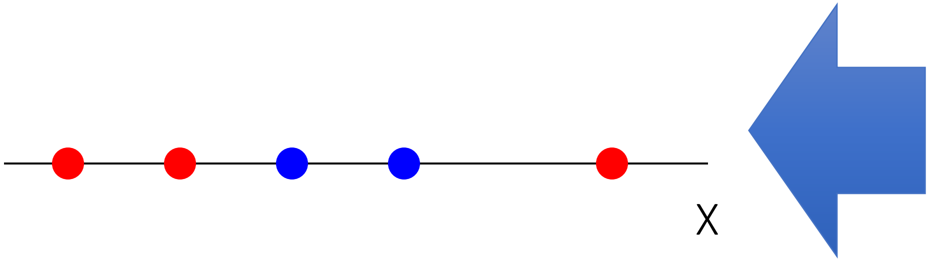
Classifying in 1-d

Can an SVM correctly classify this data?

What about this?





Classifying in 1-d

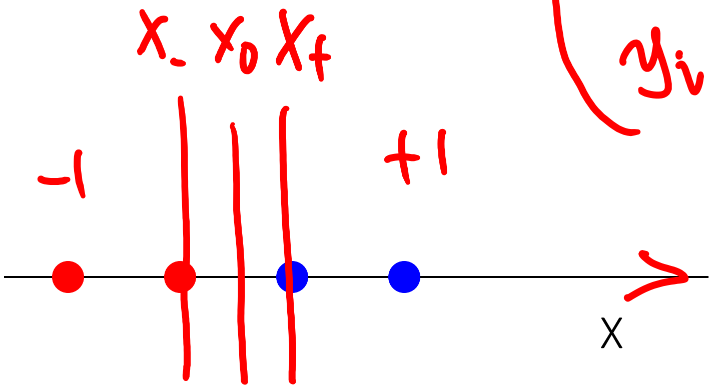
Can an SVM correctly classify this data?

$$M = \frac{2}{\sqrt{w^T w}} \Rightarrow \max M \Downarrow \min w^T w$$

s.t.

$\forall i \in \text{train}$

$y_i(w^T x_i + b) \geq 1$



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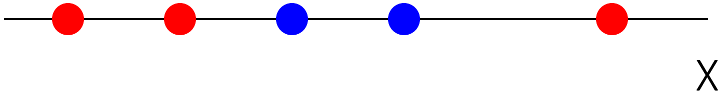


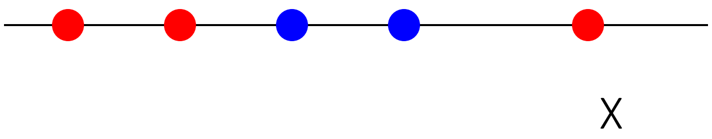
Classifying in 1-d

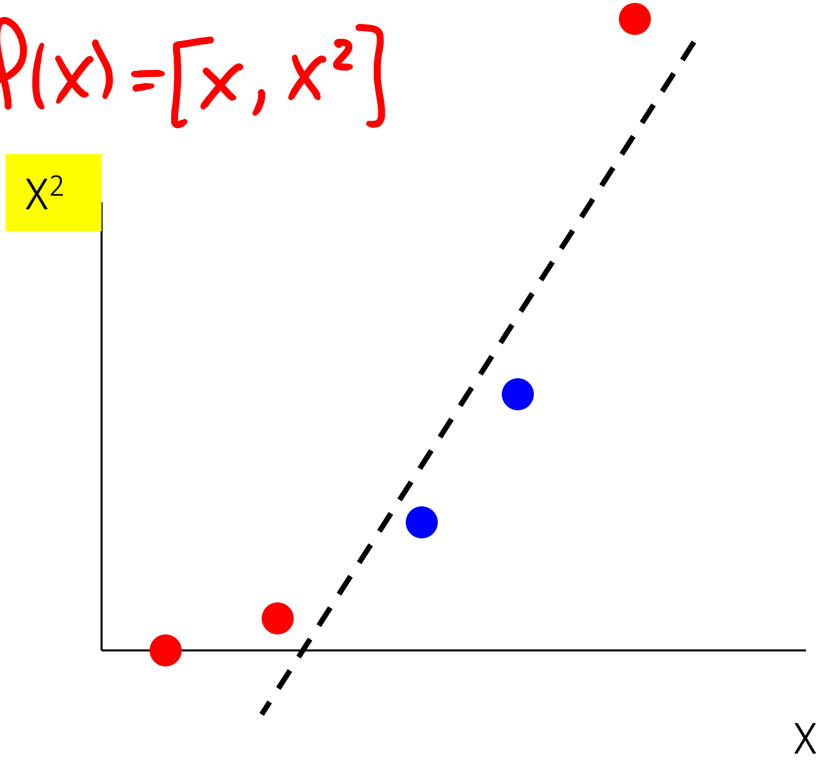
→ separable
→ nonlinear

Can an SVM correctly classify this data?

And now? (extend with polynomial basis)

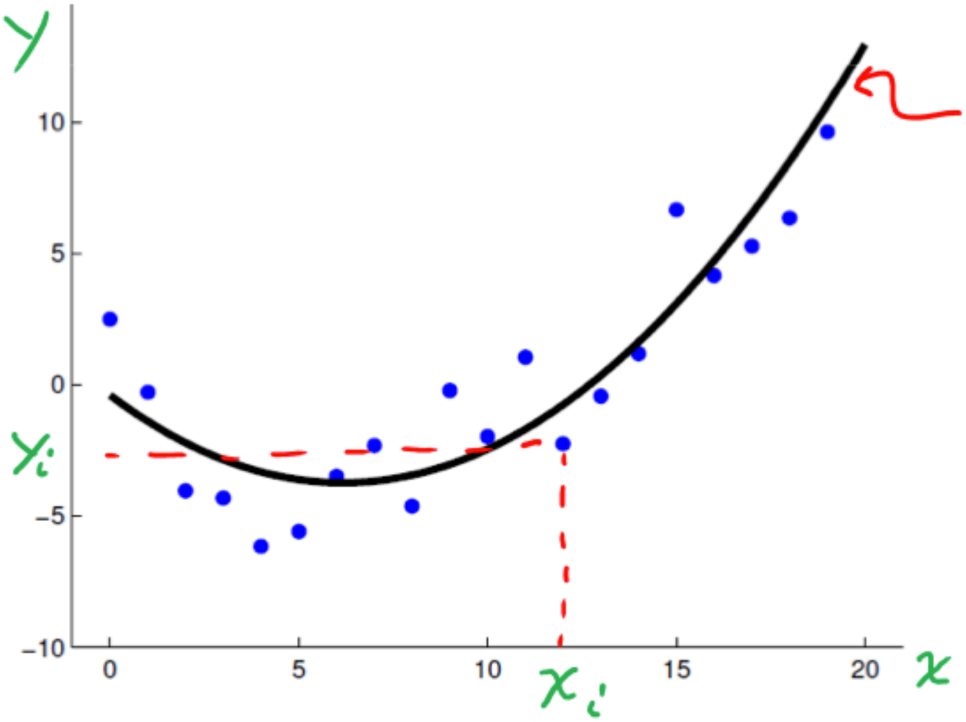
$(x) \longrightarrow \phi(x) = [x, x^2]$





RECAP: Polynomial regression

For example, $\phi(x) = [1, x, x^2]$

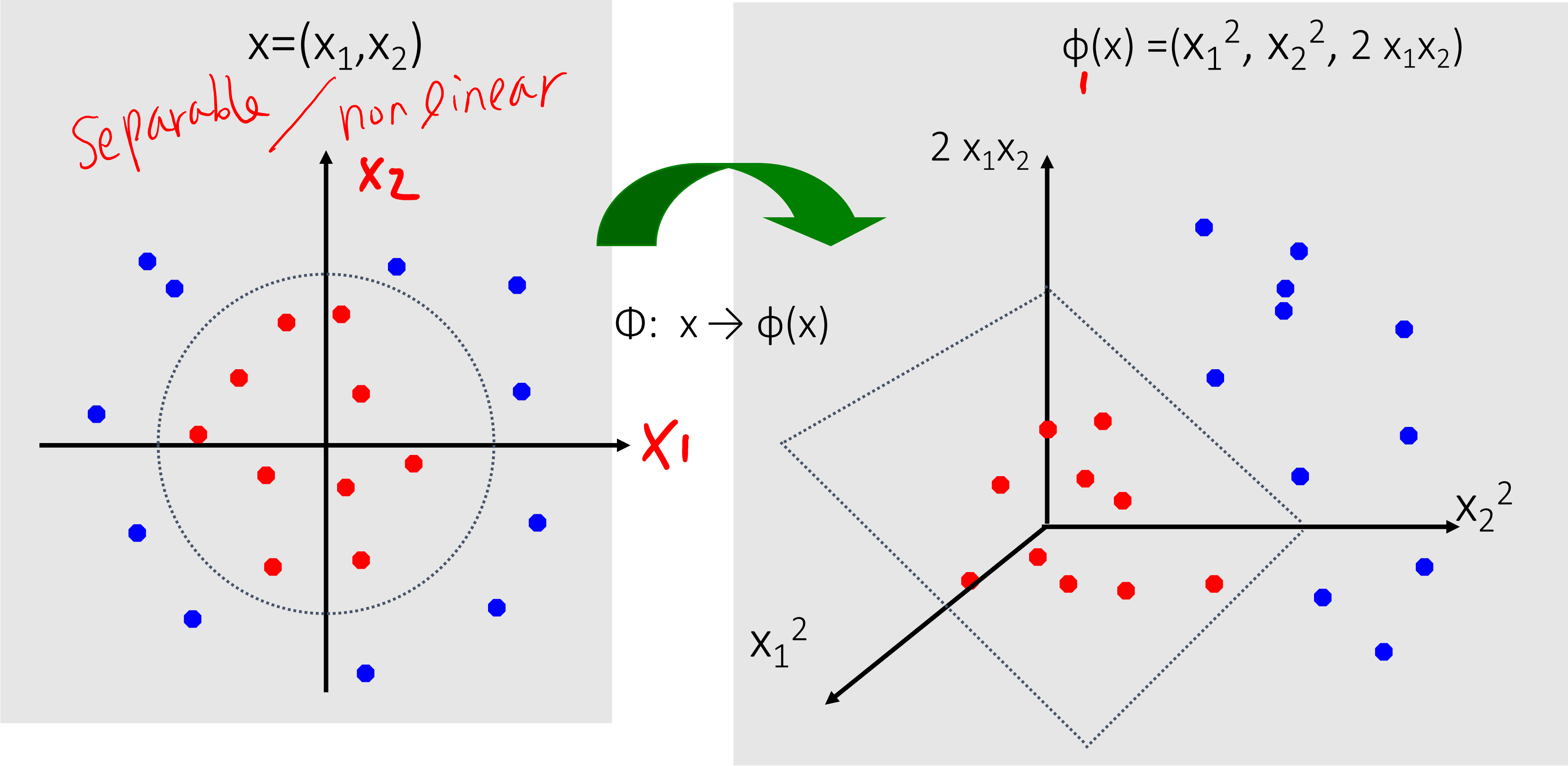


$$\hat{y} = \phi(x)\,\theta$$
$$= \theta_0 + x\theta_1 + x^2\theta_2$$

Dr. Nando de Freitas's tutorial slide

Non-linear SVMs: 2D

- The original input space (x) can be mapped to some higher-dimensional feature space ($\phi(x)$)where the training set is separable:



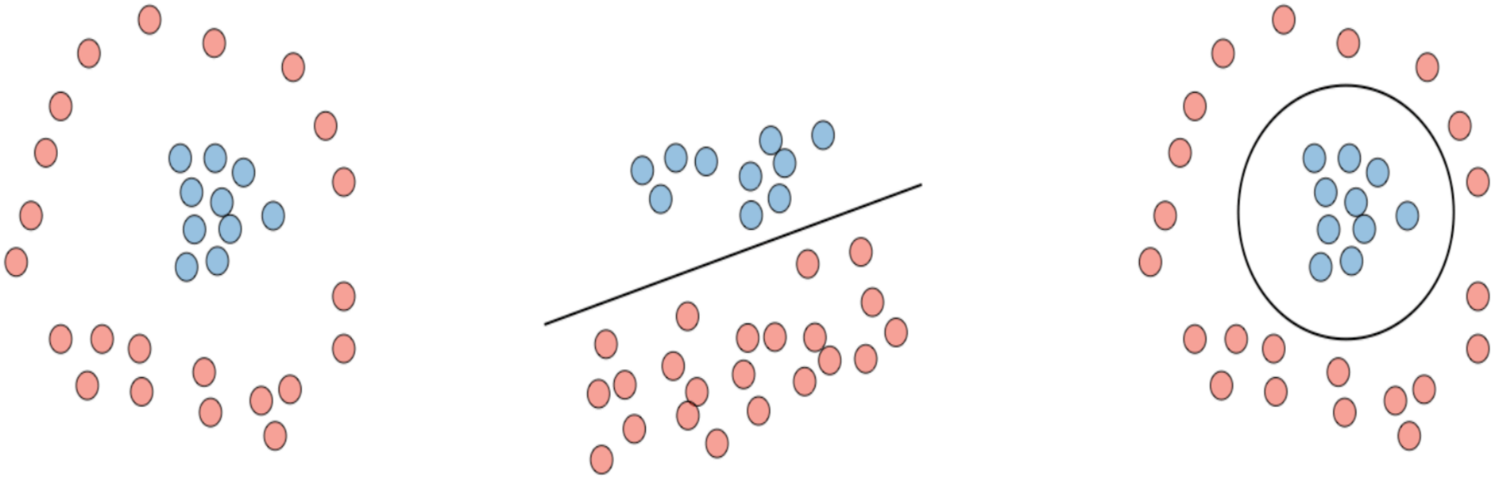
This slide is courtesy of www.iro.umontreal.ca/~pift6080/documents/papers/svm_tutorial.ppt

❒ **Kernel** – Given a feature mapping ϕ, we define the kernel K to be defined as:

$$\boxed{K(x,z)=\phi(x)^T\phi(z)}$$

In practice, the kernel K defined by $K(x,z) = \underbrace{\exp\left(-\frac{||x-z||^2}{2\sigma^2}\right)}_{\text{RBF}}$ is called the Gaussian kernel and is commonly used.

$\phi_2(x)^T\phi_2(z)$



Non-linear separability ➡ Use of a kernel mapping ϕ ➡ Decision boundary in the original space

~~Remark:~~ When *we say that we use the "kernel trick" to compute the cost function using the kernel ~~because~~ we actually don't need to know the explicit mapping ϕ, which is often very complicated. Instead, only the values $K(x,z)$ are needed.*

Credit: Stanford ML course

A little bit theory:

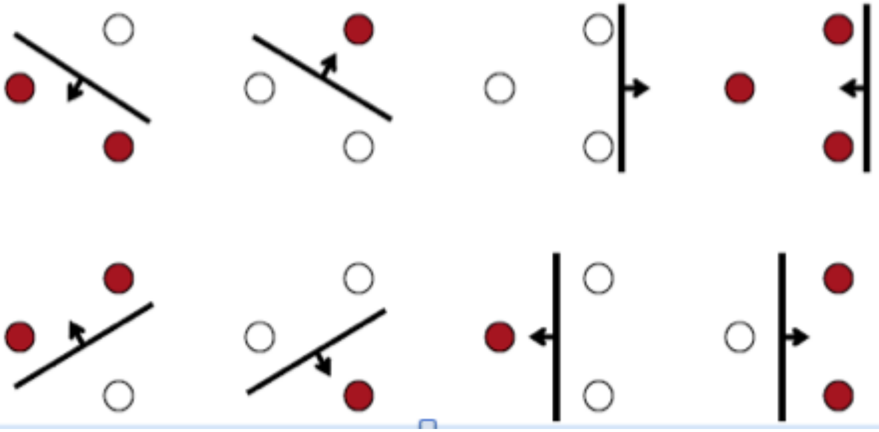
Vapnik-Chervonenkis (VC) dimension

$X \longrightarrow \phi(x)$

$\geq N-1$

If data is mapped into sufficiently high dimension, then samples will in general be linearly separable;
N data points are in general separable in a space of N-1 dimensions or more!!!

- VC dimension of the set of oriented lines in R^2 is 3
  - It can be shown that the VC dimension of the family of oriented separating hyperplanes in R^N is at least N+1



If data is mapped into sufficiently high dimension, then samples will in general be linearly separable;

N data points are in general separable in a space of N-1 dimensions or more!!!

$$X \longrightarrow \Phi(X)$$

linearly separated into two classes $\{+1, -1\}$

Thank You

Thank you

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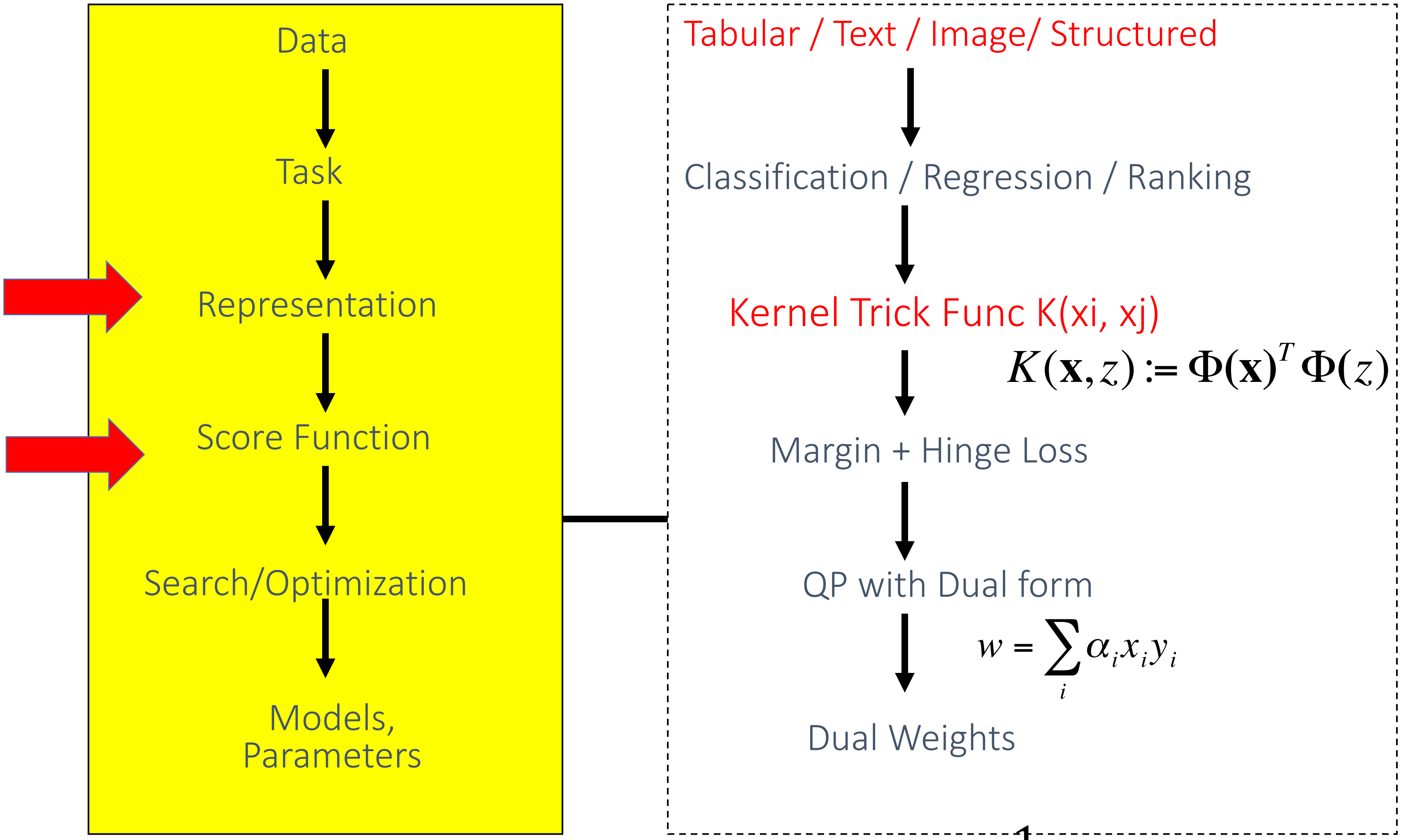
Module II

Kernel Support Vector Machine



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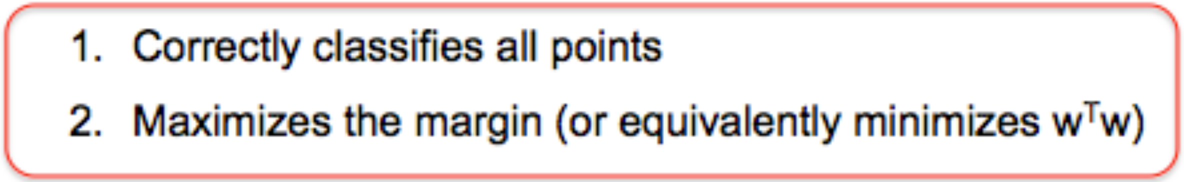
$$\max_\alpha \sum_i \alpha_i - \frac{1}{2}\sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_{\mathrm{i}} y_j \mathbf{x}_{\mathbf{i}}^T \mathbf{x}_{\mathbf{j}}$$

$$\sum_i \alpha_i \mathrm{y}_{\mathrm{i}} = 0, \qquad \alpha_i \geq 0 \qquad \forall i$$

Optimization Reformulation (for linearly separable case)

$x_i \rightarrow \phi(x_i)$

f(x,w,b) = sign(w^{T}x + b)



1. Correctly classifies all points
2. Maximizes the margin (or equivalently minimizes w^{T}w)

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

Min (w^{T}w)/2

subject to the following constraints:

For all x in class + 1

w^{T}x+b >= 1

For all x in class - 1

w^{T}x+b <= -1

A total of n constraints if we have n input samples

Quadratic Objective

$$\underset{\boxed{\mathbf{w},b}}{\operatorname{argmin}} \sum_{i=1}^{p} w_i^2 = \frac{1}{2} w^T W$$

$$\text{subject to } \forall \mathbf{x}_i \in Dtrain : \underbrace{y_i}_{1\times1}\left(\underbrace{\underbrace{\mathbf{w}^T}_{1\times P}\underbrace{\mathbf{x}_i}_{P\times1}}_{1\times1} + \underbrace{b}_{1\times1}\right) \geq 1$$

Quadratic programming i.e.,
- Quadratic objective
- Linear constraints

An alternative representation of the SVM QP

- Instead of encoding the correct classification rule and constraint we will use Lagrange multiplies to encode it as part of the our minimization problem

Min $(w^T w)/2$

s.t.

$(w^T x_i + b) y_i >= 1$

Recall that Lagrange multipliers can be applied to turn the following problem:

$\forall i, \alpha_i \geq 0$ every training

$$L_{primal}(w,b,\alpha)=\frac{1}{2}\mathbf{w}^{T}\cdot\mathbf{w}-\sum_{i=1}^{N}\underset{m}{\alpha_i}\left(\underbrace{y_i(\mathbf{w}^{T}\cdot\mathbf{x}_i+b)}_{\geq 1}-1\right)$$

The Dual Problem (Extra)

$$\max_{\alpha_i \geq 0} \underline{\min_{w,b} L(w,b,\alpha)}$$

Dual formulation

- We minimize L with respect to w and b first:

$$\nabla_w L(w,b,\alpha) = w - \sum_{i=1}^{train} \alpha_i y_i x_i = 0, \qquad (*)$$

$$\nabla_b L(w,b,\alpha) = \sum_{i=1}^{train} \alpha_i y_i = 0, \qquad (**)$$

$$f(x_t) = \text{sign}(\vec{w}^T \vec{x}_t + b)$$

Note that **(*)** implies:

$$\underline{w = \sum_{i=1}^{train} \alpha_i y_i x_i} \qquad (***)$$

- Plus (***) back to L , and using (**), we have:

$$L(w,b,\alpha) = \sum_{i=1} \alpha_i - \frac{1}{2} \sum_{i,j=1} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

SVM goal

Summary: Dual SVM for linearly separable case

Dual formulation

$$\max_\alpha \sum_i \alpha_i - \frac{1}{2}\sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_\mathrm{i} y_j \mathbf{x}_\mathbf{i}^T \mathbf{x}_\mathbf{j}$$

$$\sum_i \alpha_i \mathrm{y}_\mathrm{i} = 0$$

$$\alpha_i \geq 0 \qquad \forall i$$

n α_i

Min $(w^Tw)/2$

subject to the following inequality constraints:

For all x in class + 1

$w^Tx+b >= 1$

For all x in class - 1

$w^Tx+b <= -1$

A total of n constraints if we have n input samples

Easier than original QP, more efficient algorithms exist to find $a_{i;}$ e.g. SMO (see extra slides)

Dual SVM for linearly separable case – Training / Testing

$$\{\alpha_1, \alpha_2, \ldots\ldots, \alpha_n\}$$

Our dual target function:

$$\max_{\alpha} \sum_{i} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \mathrm{y}_i y_j \mathbf{x}_{\mathbf{i}}^{T} \mathbf{x}_{\mathbf{j}}$$

$$\sum_{i} \alpha_i \mathrm{y}_{\mathrm{i}} = 0$$

$$\alpha_i \geq 0 \qquad \forall i$$

Dot product for all training samples

$$\begin{cases} \text{most } \alpha_i = 0 \\ \text{only support vectors } \alpha_i > 0 \end{cases}$$

Dual SVM for linearly separable case – Training / Testing

Our dual target function:

$$\max_{\alpha} \sum_{i} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1} \alpha_i \alpha_j \mathrm{y}_{\mathrm{i}} y_j \mathbf{x_i}^T \mathbf{x_j}$$

$$\sum_{i} \alpha_i \mathrm{y}_{\mathrm{i}} = 0$$

$$\alpha_i \geq 0 \qquad \forall i$$

Dot product for all training samples

Dot product with ("all" ??) training samples

To evaluate a new sample x_{ts} we need to compute:

$$\mathrm{w}^{\mathrm{T}} x_{ts} + b = \sum_{\mathrm{i}} \alpha_i \mathrm{y}_{\mathrm{i}} \mathbf{x_i}^T \mathbf{x}_{ts} + b$$

$$\xrightarrow{} K(x_i, x_{ts}) = \phi(x_i)^T \phi(x_{ts})$$

$$\widehat{y_{ts}} = \mathrm{sign}\left(\sum_{i \in SupportVectors} \alpha_i y_i \left(\mathbf{x}_i^T \mathbf{x}_{ts} \right) + b \right)$$

$$\max_\alpha \sum_i \alpha_i - \frac{1}{2}\sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_\mathrm{i} y_j \mathbf{x}_\mathbf{i}{}^T \mathbf{x}_\mathbf{j}$$

$$\sum_i \alpha_i \mathrm{y}_\mathrm{i} = 0$$

$$C > \alpha_i \geq 0, \forall i$$

$x_i^T x_j = x_j^T x_i$

nonlinear $\Longrightarrow$

$$\max_\alpha \sum_i \alpha_i - \sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_\mathrm{i} y_j \mathbf{\Phi}(\mathbf{x}_\mathbf{i})^T \mathbf{\Phi}(\mathbf{x}_\mathbf{j})$$

$$\sum_i \alpha_i \mathrm{y}_\mathrm{i} = 0$$

$$C > \alpha_i \geq 0, \forall i$$

$K(x_i, x_j)$

$$\begin{array}{c|ccccc} & 1 & 2 & \cdots & j & n \\ \hline 1 & & & & & \\ 2 & & & & & \\ i & & & & x_i^T x_j & \\ n & & & & & \end{array}$$

n×n

$O(p \cdot n^2/2)$

$$\begin{array}{c|ccccc} & 1 & 2 & \cdots & j & n \\ \hline 1 & & & & & \\ 2 & & & & & \\ i & & & & \Phi(x_i)^T \Phi(x_j) \rightarrow K(x_i, x_j) & \\ n & & & & & \end{array}$$

n×n

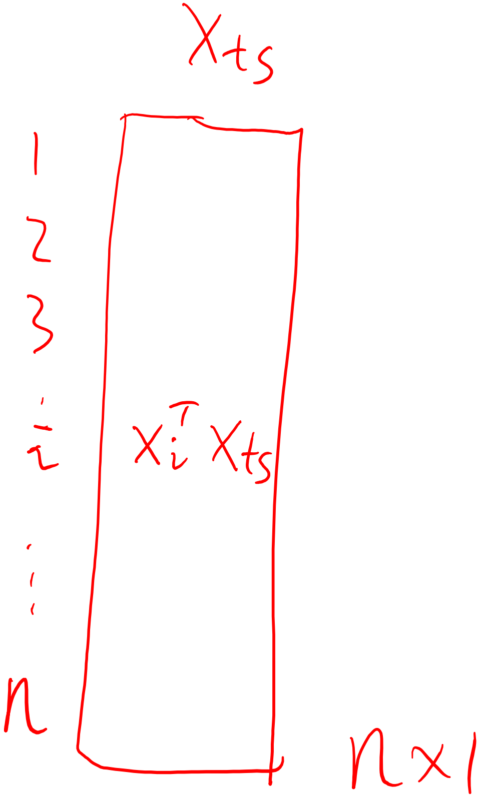
$O(p \cdot n^2/2)$

Training

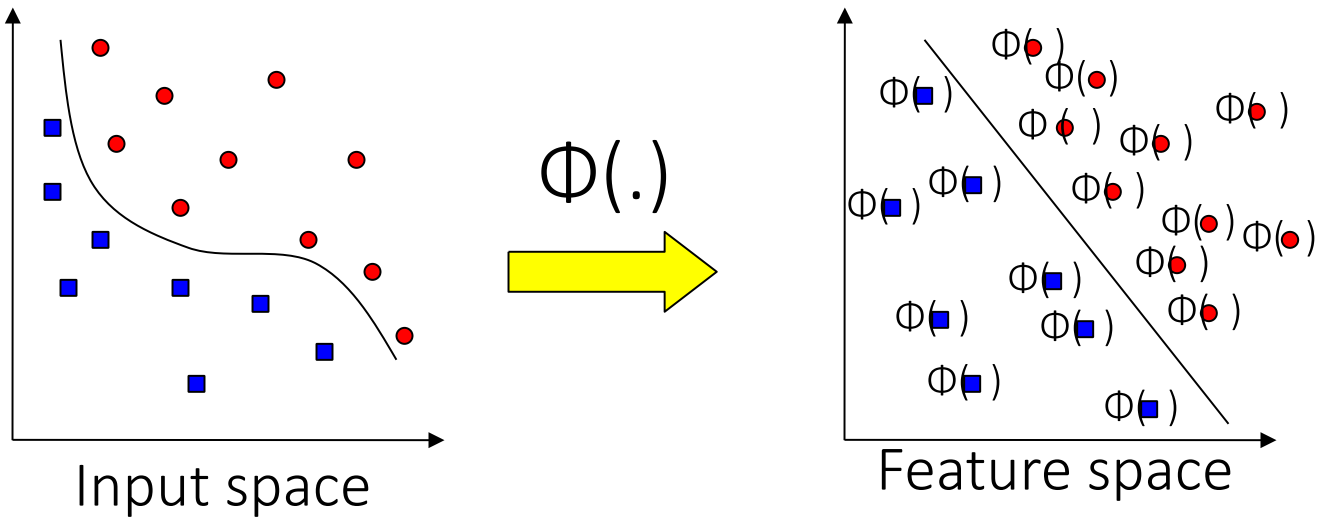
$$\mathrm{w}^{\mathrm{T}} x_{ts} + b = \sum_{\mathrm{i}} \alpha_i \mathrm{y}_{\mathrm{i}} \mathbf{x}_{\mathbf{i}}^{T} \mathbf{x}_{ts} + b$$

$$\widehat{y_{ts}} = \mathrm{sign}\left(\sum_{i \in SupportVectors} \alpha_i y_i \left(\mathbf{x}_i^T \mathbf{x}_{ts} \right) + b \right)$$

$$\Rightarrow \sum_{SV} \alpha_i y_i \underbrace{\Phi(x_i)\Phi(x_{ts})}_{} + b$$



Testing



SVM solves these two issues simultaneously

- “Kernel tricks” for efficient computation
- Dual formulation only assigns parameters to samples, not to features

- SVM solves these two issues simultaneously
  - “Kernel tricks” for efficient computation
  - Dual formulation only assigns parameters to samples, not features

(1). “Kernel tricks” for efficient computation

Never represent features explicitly
⍰ Compute dot products in closed form
Very interesting theory – Reproducing Kernel Hilbert Spaces
⍰ Not covered in detail here

$k(x, z)$

- SVM solves these two issues simultaneously
  - “Kernel tricks” for efficient computation
  - Dual formulation only assigns parameters to samples, not features

(1). “Kernel tricks” for efficient computation

~~$\Phi(x)$~~

Never represent features explicitly
⍰ Compute dot products in closed form
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⍰ Not covered in detail here

$k(x, z)$

$K(\mathbf{x}_i,\mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)$ is called the kernel function.

- Linear kernel (we've seen it)

$$K(\mathbf{x},z)=\mathbf{x}^T z \qquad \begin{cases} x \in R^p \\ z \in R^p \end{cases}$$

- Polynomial kernel (we will see an example)

$$K(\mathbf{x},z)=\underbrace{\left(1+\mathbf{x}^T z\right)}_{O(p)}^d = \Phi_p(x)^T \underbrace{\Phi_p(z)}_{p_\Phi \to O(p^d)}$$

where d = 2, 3, … To get the feature vectors we concatenate all dth order polynomial terms of the components of x (weighted appropriately)

- Radial basis kernel

$$K(\mathbf{x},z)=\exp\left(-r\underbrace{\left\|\mathbf{x}-z\right\|^2}_{O(p)}\right) = \underbrace{\Phi_r(x)^T}_{} \Phi_r(z) \qquad p_\Phi = \infty$$

In this case., r is hyperpara. The feature space of the RBF kernel has an infinite number of dimensions

Never represent features explicitly
 Compute dot products with a closed form
Very interesting theory – Reproducing Kernel Hilbert Spaces
 Not covered in detail here

Example: Quadratic kernels

$$K(\mathbf{x},z)=\left(1+\mathbf{x}^{T}z\right)^{d}$$ ⇨ $(1+x^{T}z)^{2}$

$$\boxed{K(\mathbf{x},z) := \Phi(\mathbf{x})^{T}\Phi(z)}$$

- Consider all quadratic terms for x_1, x_2 … x_p

⇨ $$\Phi(x) = \begin{bmatrix} 1 \\ \sqrt{2}x_1 \\ \vdots \\ \sqrt{2}x_p \\ x_1^2 \\ \vdots \\ x_p^2 \\ \sqrt{2}x_1x_2 \\ \vdots \\ \sqrt{2}x_{p-1}x_p \end{bmatrix}$$

$$\max_{\alpha} \sum_{i} \alpha_i - \sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_{\mathrm{i}} y_j \Phi(\mathbf{x_i})^{T}\Phi(\mathbf{x_j})$$

$$\sum_{i} \alpha_i \mathrm{y}_{\mathrm{i}} = 0$$

$$\alpha_i \geq 0 \qquad \forall i$$

$$K(\mathbf{x},z)=\left(1+\mathbf{x}^T z\right)^{\cancel{d}\,2} \quad [d=2], \quad [p=2] \quad \left(\begin{array}{l} x=(x_1,x_2) \\ z=(z_1,z_2) \end{array}\right)$$

$$\underbrace{K(x,z)} = \left(1+x_1 z_1 + x_2 z_2\right)^2 \Rightarrow \boxed{O(p)}$$

$$\boxed{O(p^2)} \left\{ \begin{array}{l} = \left(1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1 x_2\right)^T \\ \left(1, \sqrt{2}z_1, \sqrt{2}z_2, z_1^2, z_2^2, \sqrt{2}z_1 z_2\right) \end{array} \right.$$

$$= \underbrace{\Phi(x)^T \Phi(z)}$$

The kernel trick

$$\Phi(\mathbf{x})^T\Phi(z)$$

O(p^d) operations if using the basis function representations in building a poly-kernel matrix

So, if we define the kernel function as follows, there is no need to carry out basis function explicitly

$$K(\mathbf{x},z)=(1+x^Tz)^d$$

O(p) operations if building a poly-kernel matrix directly through the K(x,z) function ➔

This is because x^Tz gives a scalar, then its power of d only costs constant FLOPS.

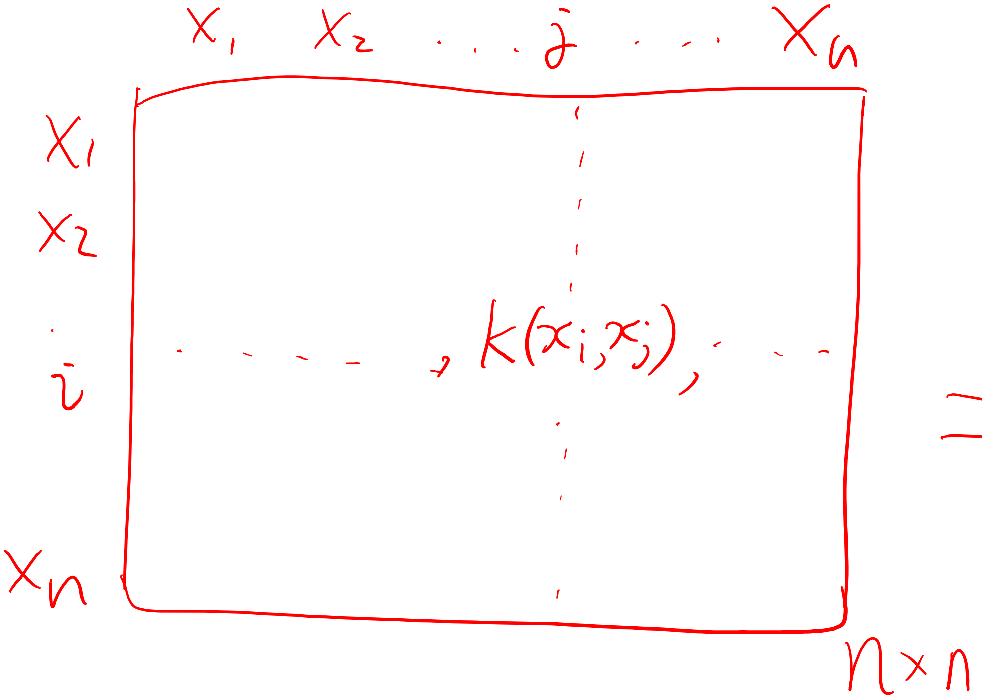
$$\max_\alpha \sum_i \alpha_i - \frac{1}{2}\sum_{\mathrm{i,j}} \alpha_i\alpha_j \mathrm{y}_\mathrm{i} y_j K(\mathbf{x_i},\mathbf{x_j})$$

$$\sum_i \alpha_i \mathrm{y}_\mathrm{i} = 0$$

$$C > \alpha_i \geq 0, \forall i \in train$$

Kernel Matrix

- Kernel function creates the kernel matrix, which summarize all the (train) data



$\Rightarrow K_{n \times n}$

[kernel matrix]

positive-semi-definite

Summary:
Modification Due to Kernel Trick

- Change all inner products to kernel functions
- For training,

Original Linear

$$\max_{\alpha} \sum_i \alpha_i - \frac{1}{2}\sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_{\mathrm{i}} y_j \mathbf{x}_{\mathbf{i}}{}^T \mathbf{x}_{\mathbf{j}}$$

$$\sum_i \alpha_i \mathrm{y}_{\mathrm{i}} = 0$$

$$C > \alpha_i \geq 0, \forall i \in train$$

With kernel function - nonlinear

$$\max_{\alpha} \sum_i \alpha_i - \frac{1}{2}\sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_{\mathrm{i}} y_j \underline{K(\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}})}$$

VC: $\underline{\Phi(x)}$ large

$$\sum_i \alpha_i \mathrm{y}_{\mathrm{i}} = 0$$

$$C > \alpha_i \geq 0, \forall i \in train$$

Summary:
Modification Due to Kernel Trick

- For testing, the new data **x_ts**

Original Linear

$$\widehat{y_{ts}} = \text{sign}\left(\sum_{\mathrm{i} \in \mathrm{supportVectorn}} \alpha_i \mathrm{y}_\mathrm{i} \mathbf{x}_\mathbf{i}^T \mathbf{x}_{ts} + b \right)$$

With kernel function - nonlinear

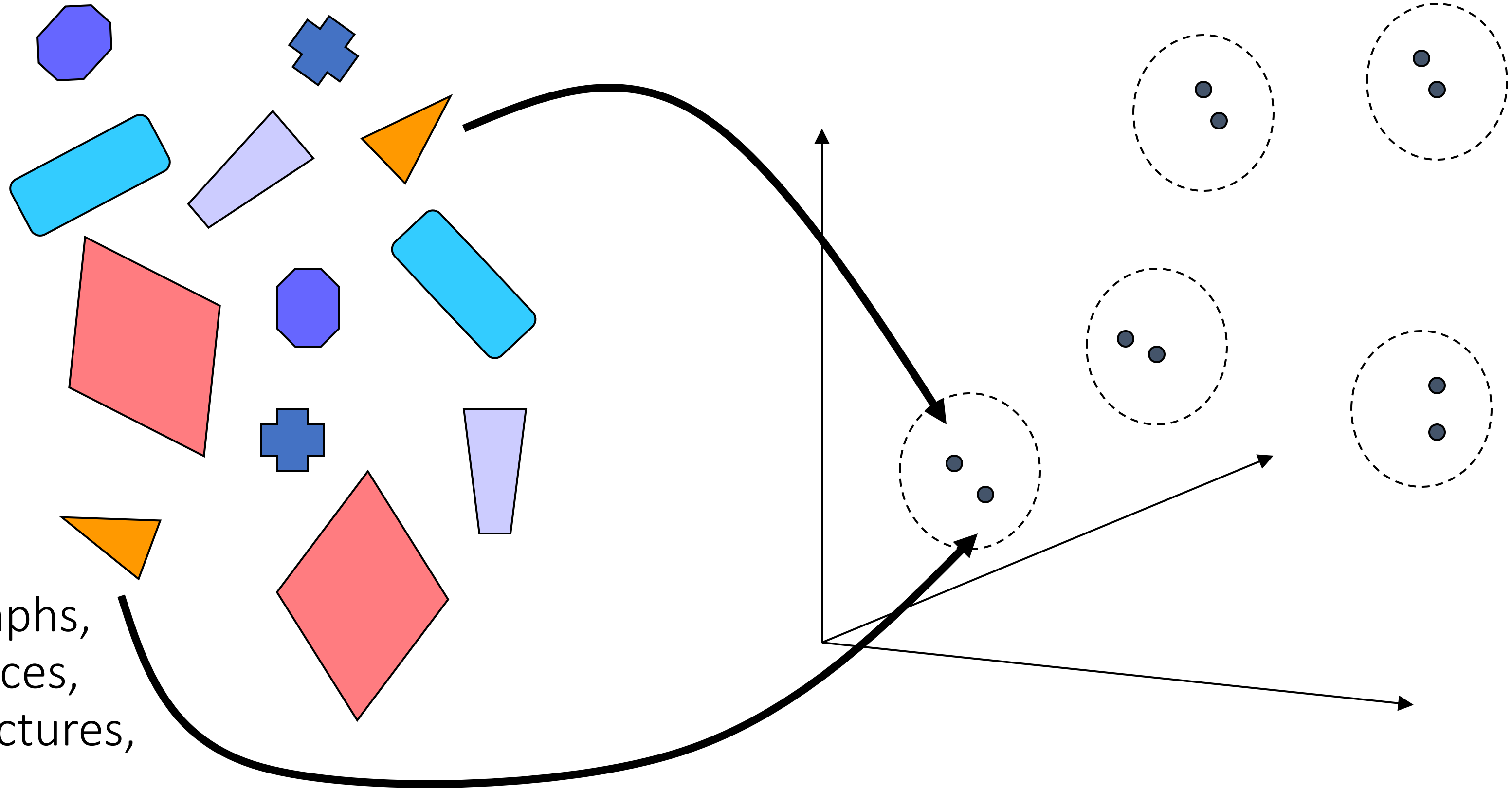
$$\widehat{y_{ts}} = \text{sign}\left(\sum_{\mathrm{i} \in \mathrm{supportVectors}} \alpha_i \mathrm{y}_\mathrm{i} K(\mathbf{x}_\mathbf{i}, \mathbf{x}_{ts}) + b \right)$$

Kernel trick has helped Non-traditional data like strings and trees able to be used as input to SVM, instead of feature vectors

When numerical x and z do not exist, we can calculate

$K(x,z)$

Vector vs. Relational data



e.g. Graphs,
Sequences,
3D structures,

Original Space

Feature Space

Thank You

Thank you

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Module III

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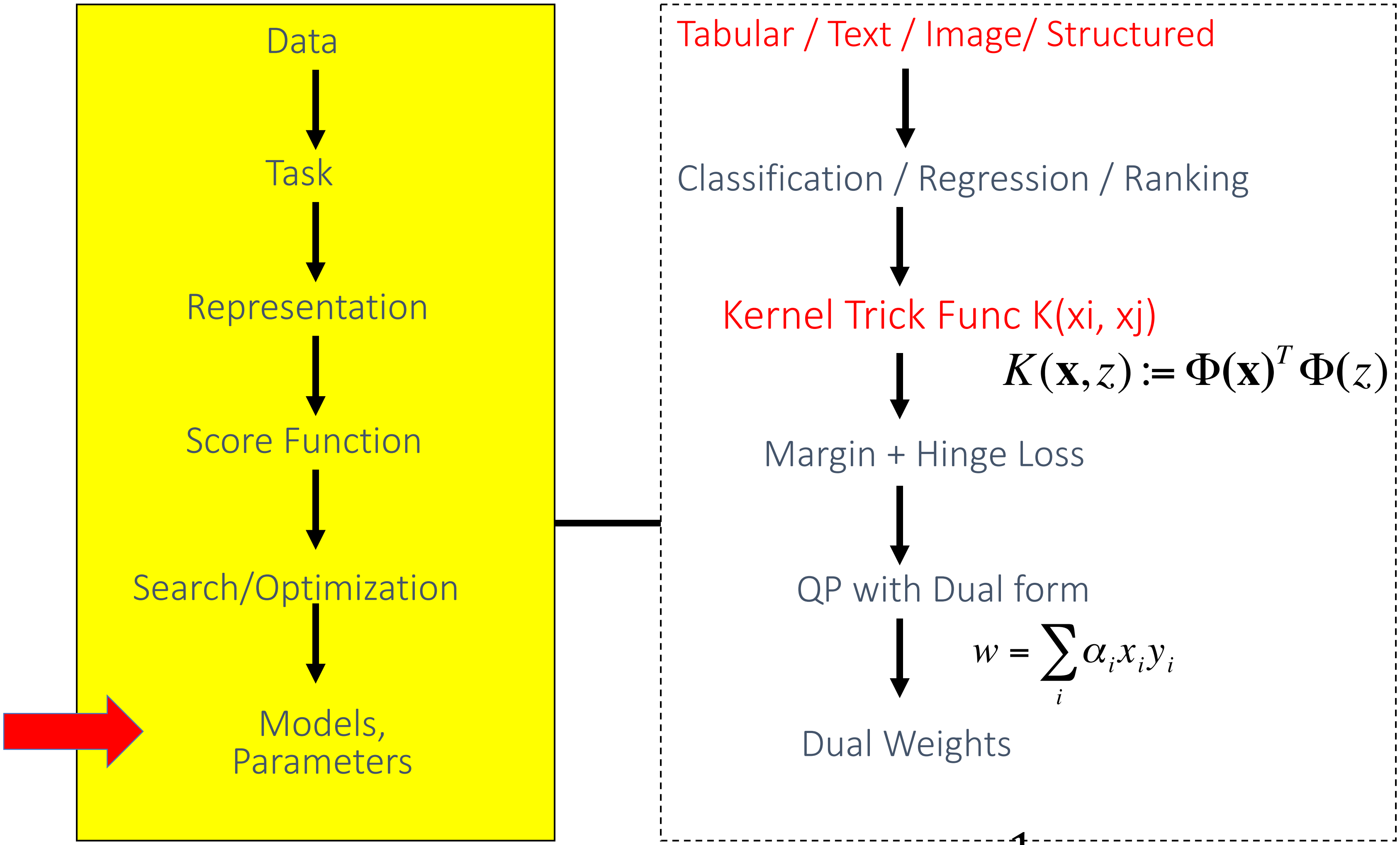
Today

- ❑ Support Vector Machine (SVM)
  - ✓ History of SVM
  - ✓ Large Margin Linear Classifier
  - ✓ Define Margin (M) in terms of model parameter
  - ✓ Optimization to learn model parameters (w, b)
  - ✓ Non linearly separable case
  - ✓ Optimization with dual form
  - ✓ Nonlinear decision boundary
  - ✓ Practical Guide

This: Kernel Support Vector Machine



Data

Task

Representation

Score Function

Search/Optimization

Models, Parameters

Tabular / Text / Image/ Structured

Classification / Regression / Ranking

Kernel Trick Func K(xi, xj)

$$K(\mathbf{x},z) := \Phi(\mathbf{x})^T \Phi(z)$$

Margin + Hinge Loss

QP with Dual form

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

Dual Weights

$$\underset{\mathbf{w},b}{\text{argmin}} \sum_{i=1}^{p} w_i^2 + \mathrm{C}\sum_{\mathrm{i}=1}^{\mathrm{n}} \varepsilon_{\mathrm{i}}$$

subject to $\forall \mathbf{x}_i \in Dtrain : y_i\left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq 1 - \varepsilon_{\mathrm{i}}$

$$\max_\alpha \sum_i \alpha_i - \frac{1}{2}\sum_{\mathrm{i,j}} \alpha_i \alpha_j \mathrm{y}_{\mathrm{i}} y_j \mathbf{x}_{\mathbf{i}}^T \mathbf{x}_{\mathbf{j}}$$

$$\sum_i \alpha_i \mathrm{y}_{\mathrm{i}} = 0, \qquad \alpha_i \geq 0 \qquad \forall i$$

Software

- A list of SVM implementation can be found at
  - http://www.kernel-machines.org/software.html

- Some implementation (such as LIBSVM) can handle multi-class classification
- SVMLight is among one of the earliest implementation of SVM
- Several Matlab toolboxes for SVM are also available

Summary: Steps for Using SVM in HW

- Prepare the feature-data matrix
- Select the kernel function to use
- Select the parameter of the kernel function and the value of *C*
- Execute the training algorithm and obtain the \a$_i$
- Unseen data can be classified using the a_i and the support vectors

Practical Guide to SVM

- From authors of as LIBSVM:
  - A Practical Guide to Support Vector Classification Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin, 2003-2010
  - http://www.csie.ntu.edu.tw/~cjlin/papers/guide/guide.pdf

LIBSVM

- http://www.csie.ntu.edu.tw/~cjlin/libsvm/
    - ✓Developed by Chih-Jen Lin etc.
    - ✓Tools for Support Vector classification
    - ✓Also support multi-class classification
    - ✓C++/Java/Python/Matlab/Perl wrappers
    - ✓Linux/UNIX/Windows
    - ✓SMO implementation, fast!!!

A Practical Guide to Support Vector Classification

(a) Data file formats for LIBSVM

- Training.dat

```
+1 1:0.708333 2:1 3:1 4:-0.320755
-1 1:0.583333 2:-1  4:-0.603774 5:1
+1 1:0.166667 2:1 3:-0.333333 4:-0.433962
-1 1:0.458333 2:1 3:1 4:-0.358491 5:0.374429
…
```

- Testing.dat

(b) Feature Preprocessing

- (1) Categorical Feature
  - Recommend using m numbers to represent an m-category attribute.
  - Only one of the m numbers is one, and others are zero.

  - For example, a three-category attribute such as {red, green, blue} can be represented as (0,0,1), (0,1,0), and (1,0,0)

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(b) Feature Preprocessing

- (2) Scaling before applying SVM is very important
  - to avoid attributes in greater numeric ranges dominating those in smaller numeric ranges.
  - to avoid numerical difficulties during the calculation
  - Recommend linearly scaling each attribute to the range [1, +1] or [0, 1].

① Normalization → $\begin{cases} \text{mean} & 0 \\ \text{std} & 1 \end{cases}$

② Scalig → linear ⇒ $[ax+b]$

e.g. $\left[\dfrac{X - X_{min}}{max - X_{min}}\right] \Leftarrow$

For i-th feature $\Rightarrow$ [Column operation on $X_{n \times p}$]

Centering : $X_i - \bar{X}_i \Rightarrow E(X_i) = 0$

Scaling : $aX_i + b \Rightarrow$ e.g. $\dfrac{X_i - \min(X_i)}{\max(X_i) - \min(X_i)}$

Normalization : $\Rightarrow \begin{cases} E(X_i) = 0 \\ var(X_i) = 1 \end{cases}$

[good practice : never touch test samples in any stage before testing]

Of course we have to use the same method to scale both training and testing data. For example, suppose that we scaled the first attribute of training data from $[-10, +10]$ to $[-1, +1]$. If the first attribute of testing data lies in the range $[-11, +8]$, we must scale the testing data to $[-1.1, +0.8]$. See Appendix B for some real examples.

If training and testing sets are separately scaled to $[0, 1]$, the resulting accuracy is lower than 70%.

```
$ ../svm-scale -l 0 svmguide4 > svmguide4.scale
$ ../svm-scale -l 0 svmguide4.t > svmguide4.t.scale
$ python easy.py svmguide4.scale svmguide4.t.scale
Accuracy = 69.2308% (216/312) (classification)
```

Using the same scaling factors for training and testing sets, we obtain much better accuracy.

```
$ ../svm-scale -l 0 -s range4 svmguide4 > svmguide4.scale
$ ../svm-scale -r range4 svmguide4.t > svmguide4.t.scale
$ python easy.py svmguide4.scale svmguide4.t.scale
Accuracy = 89.4231% (279/312) (classification)
```

(b) Feature Preprocessing

- (3) missing value
  - Very very tricky !
  - Easy way: to substitute the missing values by the mean value of the variable
  - A little bit harder way: imputation using nearest neighbors
  - Even more complex: e.g. EM based (beyond the scope)

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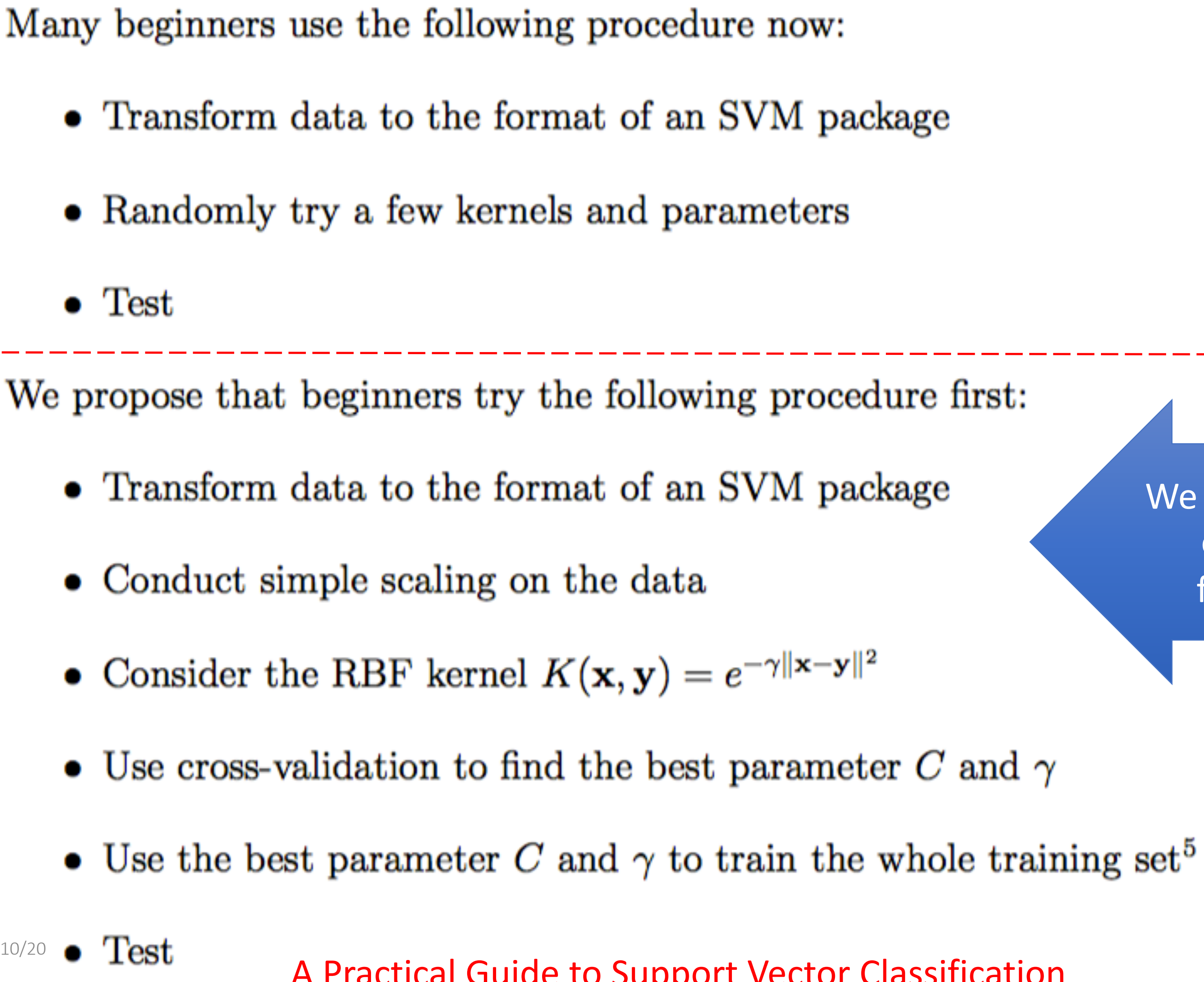
(b) Feature Preprocessing

- (4) out of dictionary token issue
  - For discrete feature variable, very trick to handle
  - Easy way: to substitute the values by the most likely value (in train) of the variable
  - Easy way: to substitute the values by a random value (in train) of the variable
  - More solutions later in the NaiveBayes slides!

(C) Pipeline Procedures for model selection

- (I) train / test
- (II) k-folds cross validation
- (III) k-CV on train to choose hyperparameter / then test



Many beginners use the following procedure now:

- Transform data to the format of an SVM package
- Randomly try a few kernels and parameters
- Test

We propose that beginners try the following procedure first:

- Transform data to the format of an SVM package
- Conduct simple scaling on the data
- Consider the RBF kernel $K(\mathbf{x}, \mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|^2}$
- Use cross-validation to find the best parameter C and γ
- Use the best parameter C and γ to train the whole training set[5]
- Test

We use lower option for HW

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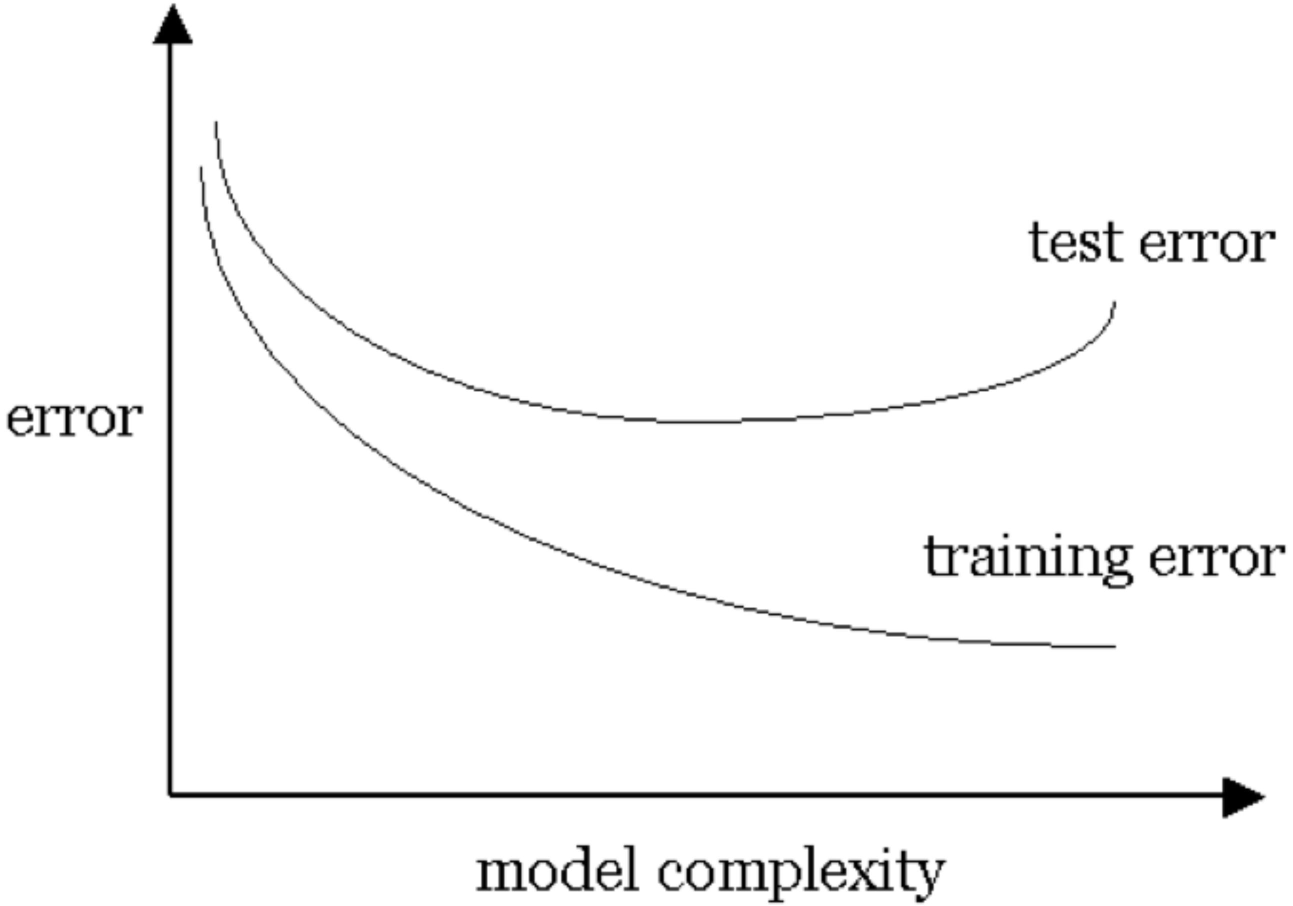
(c) Model Selection

Our goal: find the model M which minimizes the test error:

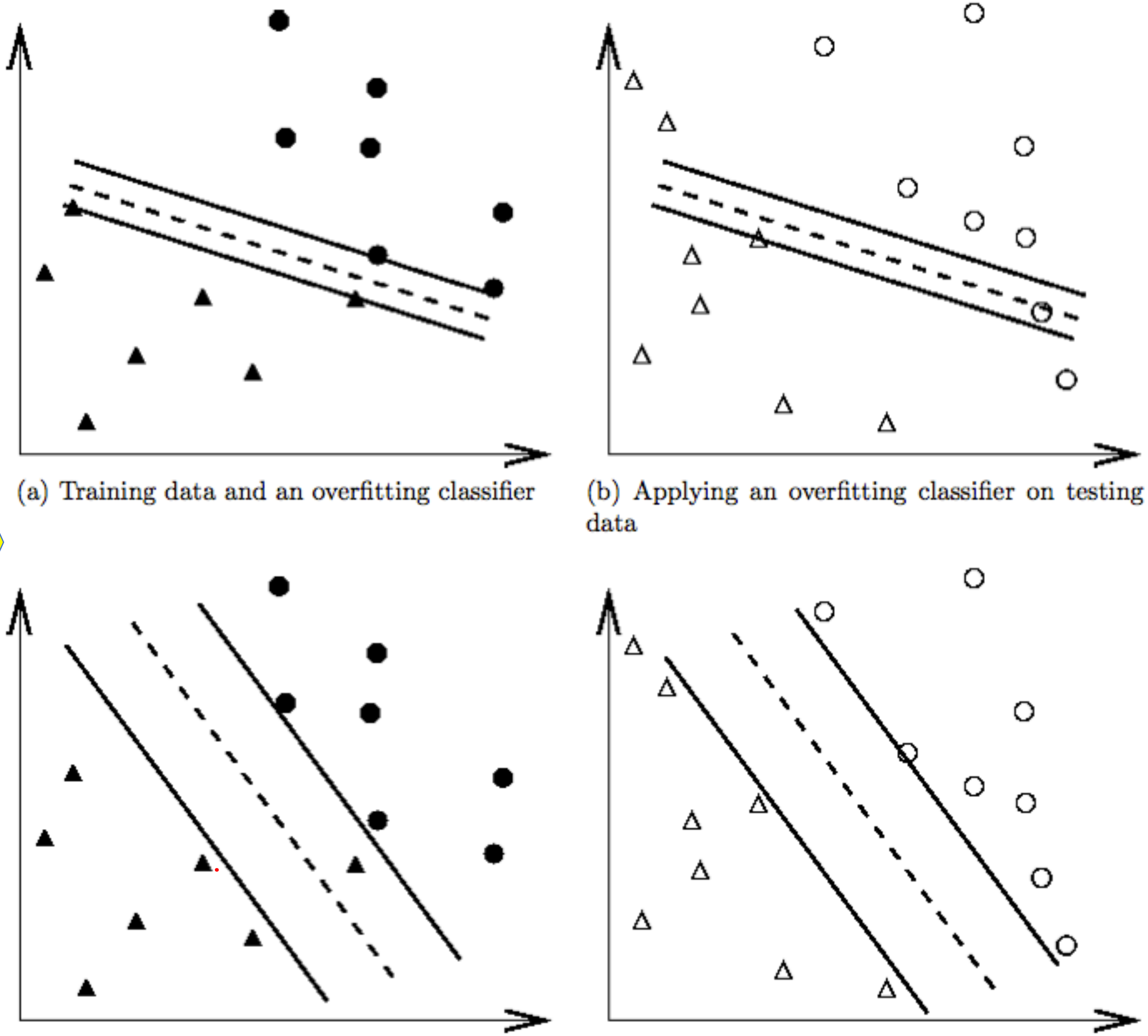


Model Selection, find right C

large C

Select the right penalty parameter C

small C



(a) Training data and an overfitting classifier

(b) Applying an overfitting classifier on testing data

(c) Training data and a better classifier

(d) Applying a better classifier on testing data

Model Selection, find right C

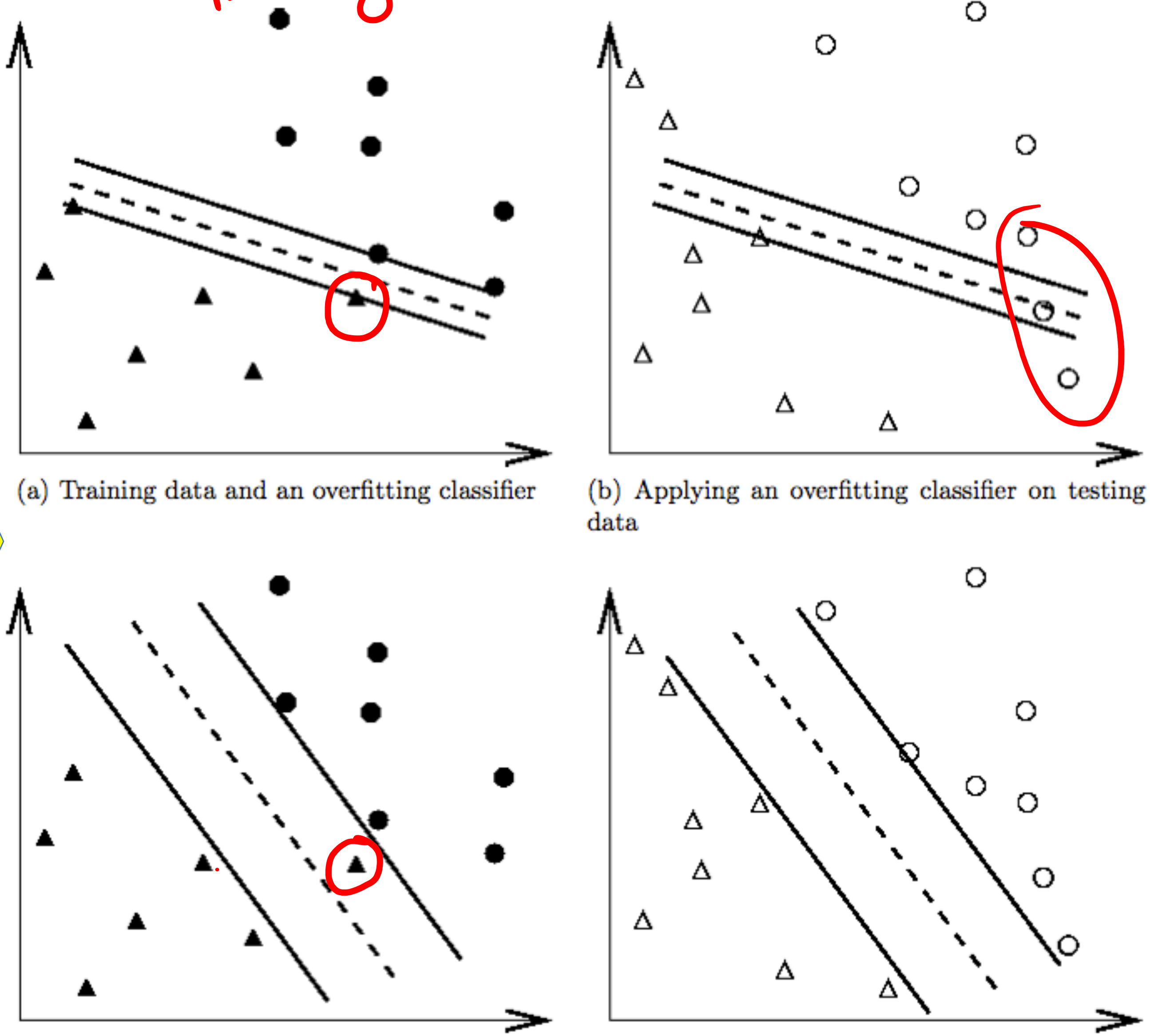
Training

Test

large C

Select the right penalty parameter C

small C



(a) Training data and an overfitting classifier

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Model Selection, find right C

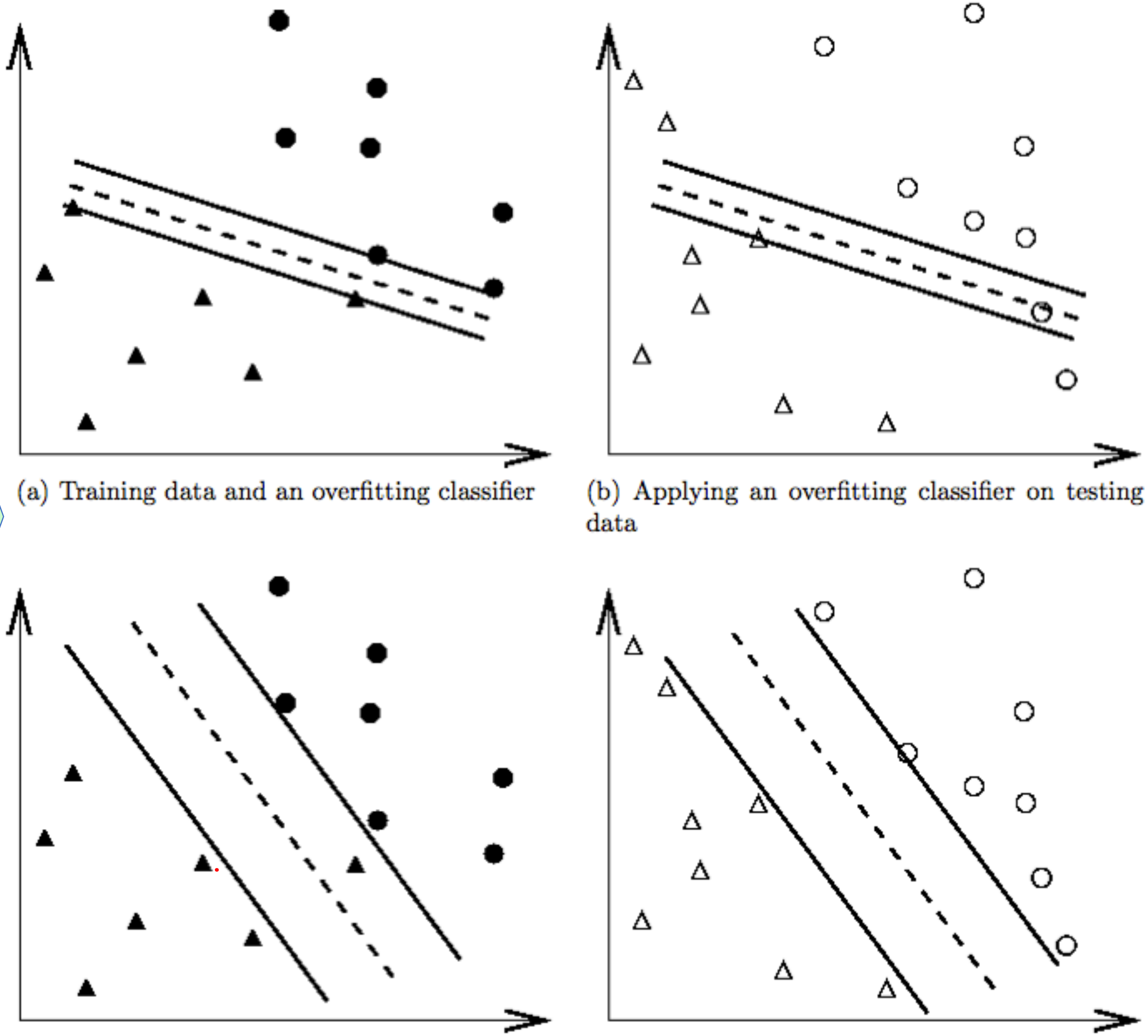
large C

A large value of C means that misclassifications are bad - resulting in smaller margins and less training error (but more expected true error).

may lead

A small C results in more training error, hopefully better true error.

small C



(a) Training data and an overfitting classifier

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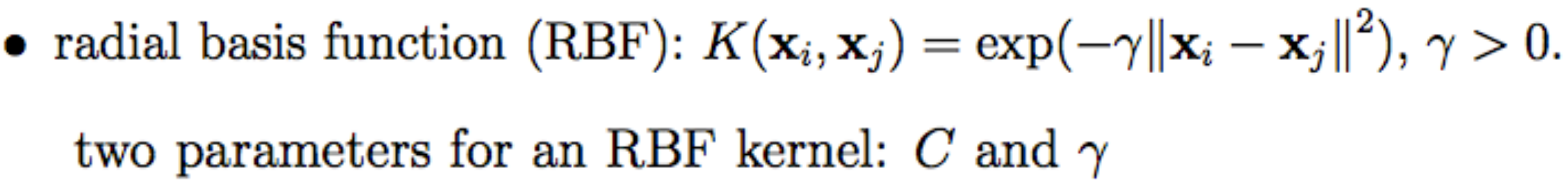
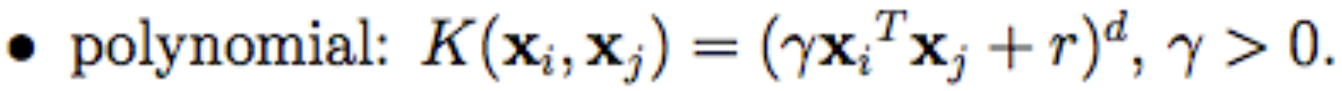
(c) Model Selection



- radial basis function (RBF): $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2)$, $\gamma > 0$.

  two parameters for an RBF kernel: C and γ



- polynomial: $K(\mathbf{x}_i, \mathbf{x}_j) = (\gamma \mathbf{x}_i{}^T \mathbf{x}_j + r)^d$, $\gamma > 0$.

  Three parameters for a polynomial kernel

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Choosing the Kernel Function

- Probably the most tricky part of using SVM.
- The kernel function is important because it creates the kernel matrix, which summarize all the data
- Many principles have been proposed (diffusion kernel, Fisher kernel, string kernel, tree kernel, graph kernel, ...)
  - Kernel trick has helped Non-traditional data like strings and trees able to be used as input to SVM, instead of feature vectors
- In practice, a low degree polynomial kernel or RBF kernel with a reasonable width is a good initial try for most applications.

Kernel Trick: Implicit Basis Representation

- For some kernels (e.g. RBF) the implicit transform basis form \phi(**x**) is infinite-dimensional!
  - But calculations with kernel are done in original space, so computational burden and curse of dimensionality aren't a problem.

$$\overset{O(p)}{\underline{K(\mathbf{x},z)}}=\exp\left(-r\left\|\mathbf{x}-z\right\|^{2}\right)$$

⇓

*O(p*n^2)* operations in building a RBF-kernel matrix for training

➔ Gaussian RBF Kernel corresponds to an infinite-dimensional vector space.

YouTube video of Caltech: Abu-Mostafa explaining this in more detailhttps://www.youtube.com/watch?v=XUj5JbQihlU&t=25m53s

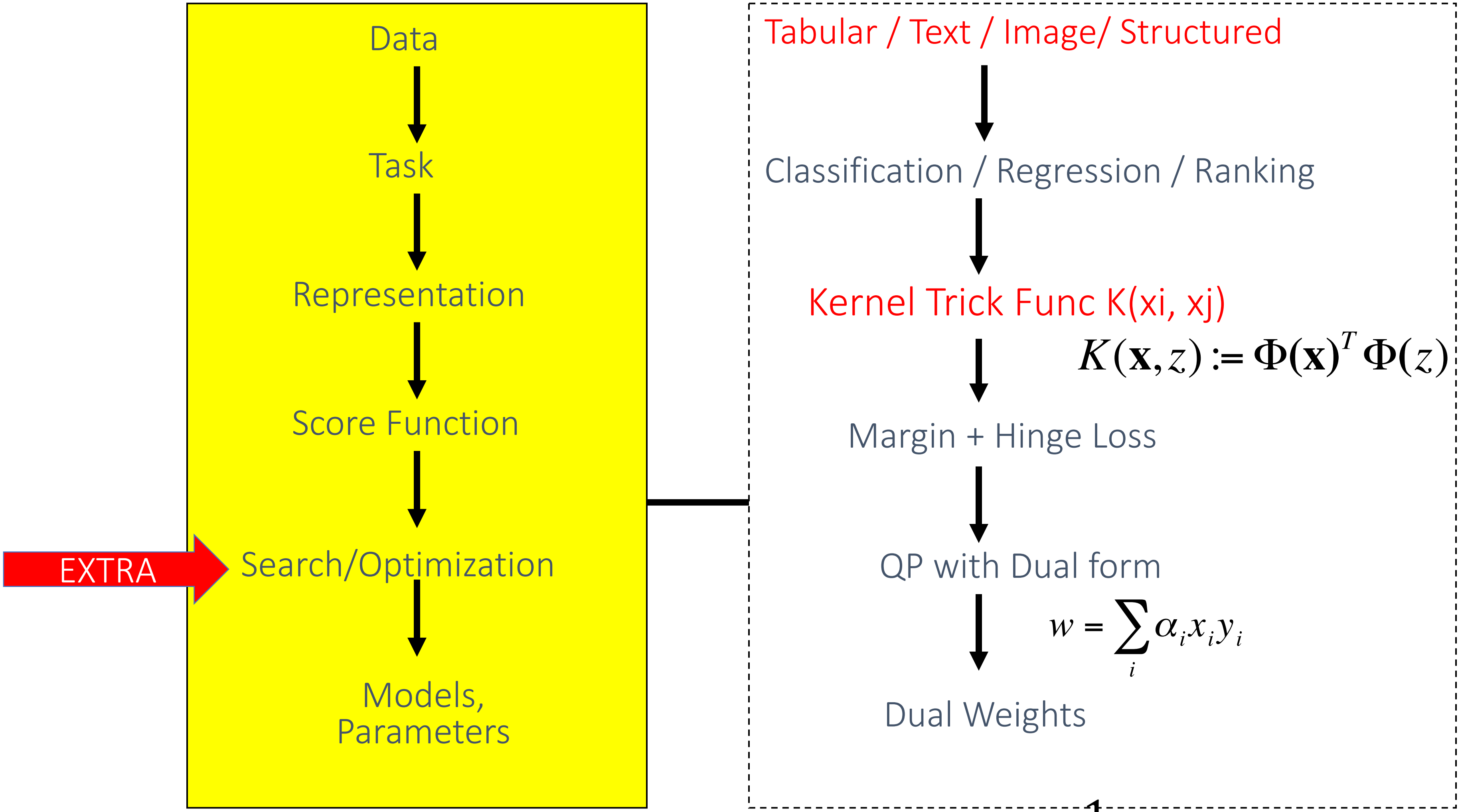
Kernel Functions (Extra)

- In practical use of SVM, only the kernel function (and not basis function) is specified
- Kernel function can be thought of as a similarity measure between the input objects
- Not all similarity measure can be used as kernel function, however Mercer's condition states that any positive semi-definite kernel *K*(*x*, *y*), i.e.

$$\sum_{i,j} K(x_i, x_j)c_i c_j \geq 0$$

can be expressed as a dot product in a high dimensional space.

This: Kernel Support Vector Machine



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EXTRA

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$$\text{subject to } \forall \mathbf{x}_i \in Dtrain : y_i\left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq 1 - \varepsilon_i$$

$$\max_\alpha \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\sum_i \alpha_i y_i = 0, \qquad \alpha_i \geq 0 \qquad \forall i$$

Why SVM Works? (Extra)

- Vapnik argues that the fundamental problem is not the number of parameters to be estimated. Rather, the problem is about the flexibility of a classifier

- Vapnik argues that the flexibility of a classifier should not be characterized by the number of parameters, but by the capacity of a classifier
  - This is formalized by the "VC-dimension" of a classifier

- The SVM objective can also be justified by structural risk minimization: the empirical risk (training error), plus a term related to the generalization ability of the classifier, is minimized

- Another view: the SVM loss function is analogous to ridge regression. The term $½||w||^2$ "shrinks" the parameters towards zero to avoid overfitting

Thank You

Thank you

References

- Big thanks to Prof. Ziv Bar-Joseph and Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- Elements of Statistical Learning, by Hastie, Tibshirani and Friedman
- Prof. Andrew Moore @ CMU's slides
- Tutorial slides from Dr. Tie-Yan Liu, MSR Asi
- A Practical Guide to Support Vector Classification Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin, 2003-2010
- Tutorial slides from Stanford "Convex Optimization I — Boyd & Vandenberghe

Mercer Kernel vs. Smoothing Kernel (Extra)

- The Kernels used in Support Vector Machines are different from the Kernels used in LocalWeighted /Kernel Regression.

- We can think
  - Support Vector Machines' kernels as **Mercer Kernels**
  - Local Weighted / Kernel Regression's kernels as **Smoothing Kernels**

KNN : $\hat{y}_{ts} = \frac{1}{k} \sum_{i \in kNeighbors\text{-}of\ X_{ts}} y_i$

find k neighbor of $X_{ts} \sim O(n\times)$

SVM : $\hat{y}_{ts} = \sum_{i \in SV} \alpha_i y_i K(\vec{X}_i, \vec{X}_{ts}) + b$

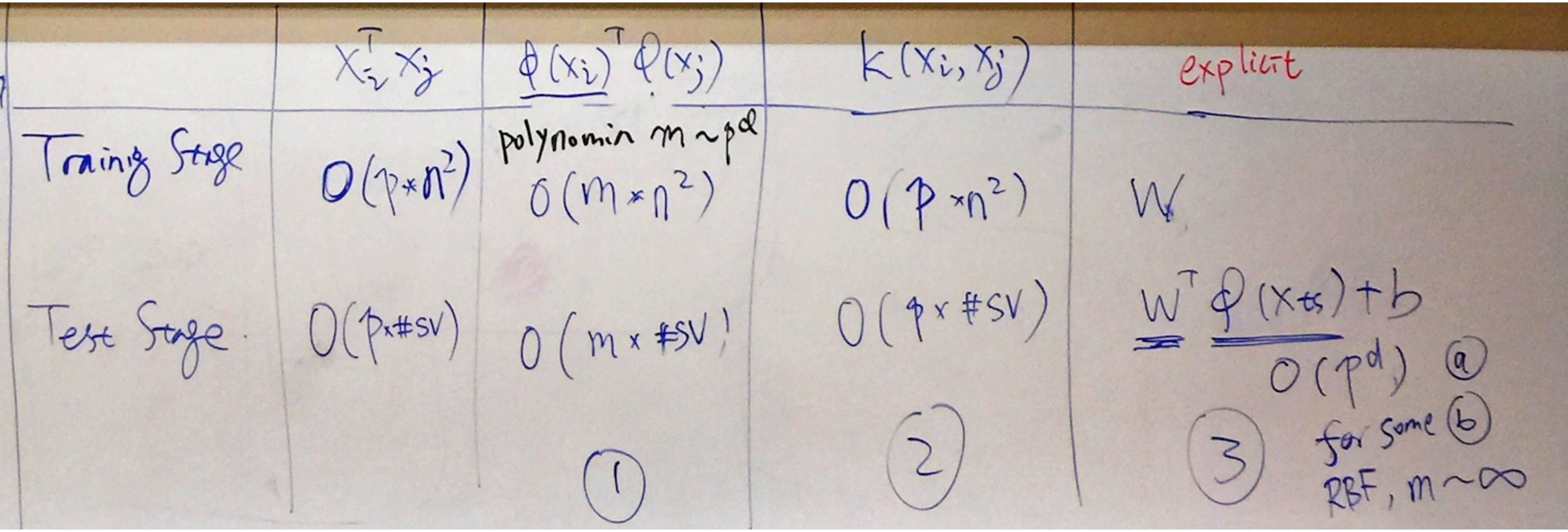
para $\sim O(n)$

Logistic Regression/ Linear Classifier

$\hat{y}_{ts} = \sigma(W^T X_{ts} + b)$

para $\sim O(p)$

Time Cost Comparisons



	$X_i^T X_j$	$\phi(x_i)^T \phi(x_j)$	$K(x_i, x_j)$	explicit
Training Stage	$O(p * n^2)$	polynomin $m \sim p^d$ $O(m * n^2)$	$O(p \times n^2)$	W
Test Stage	$O(p \times \#SV)$	$O(m \times \#SV)$	$O(p \times \#SV)$	$\underline{W}^T \underline{\phi(x_{ts})} + b$ $O(p^d)$ ⓐ for some ⓑ RBF, $m \sim \infty$
		①	②	③

Why do SVMs work?

$x \rightarrow \phi(x)$ e.g. RBF

- ❑ If we are using huge features spaces (e.g., with kernels), how come we are not overfitting the data?
  - ✓ Number of parameters remains the same (and most are set to 0) $O(n)$, α_i $i=1, \cdots, n$
  - ✓ While we have a lot of inputs, at the end we only care about the support vectors and these are usually a small group of samples
  - ✓ The maximizing of the margin acts as a sort of regularization term leading to reduced overfitting