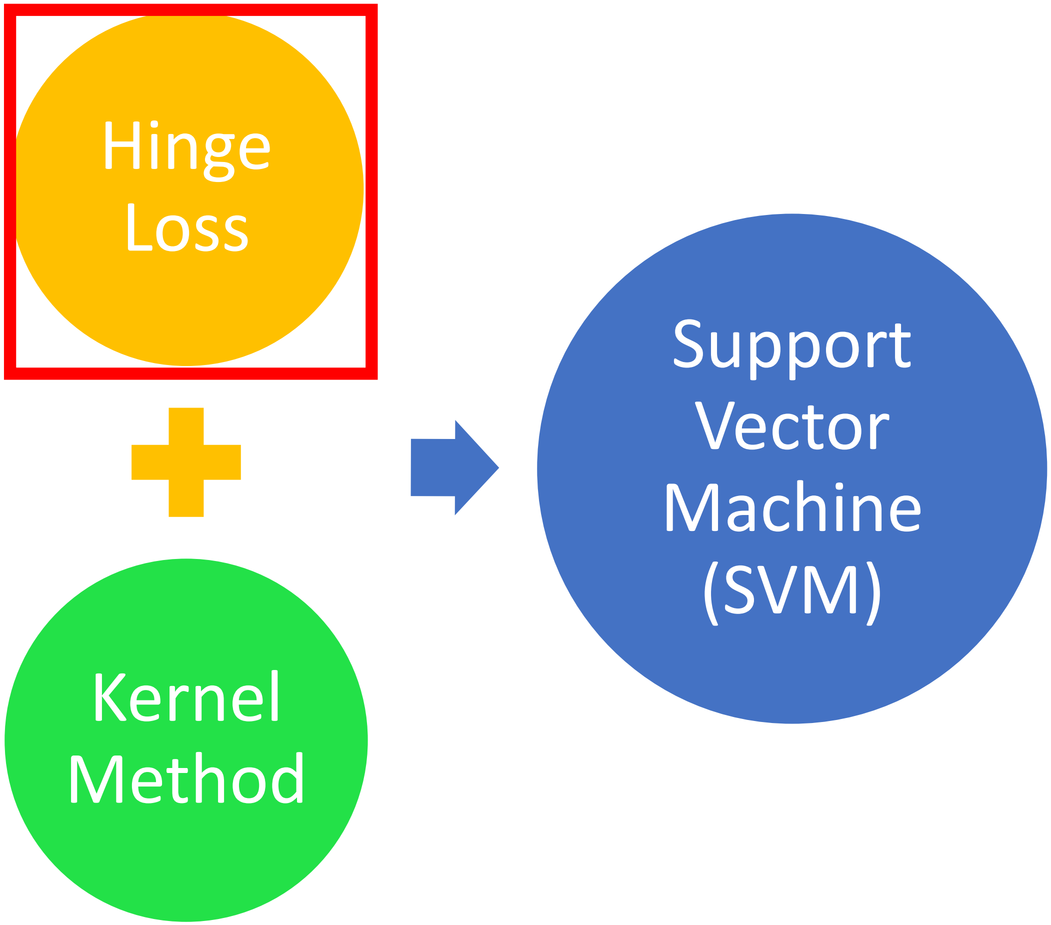
Support Vector Machine

Outline



Binary Classification

$$\begin{array}{cccc} x^1 & x^2 & x^3 & \\ \hat{y}^1 & \hat{y}^2 & \hat{y}^3 & \cdots\cdots \end{array}$$

$\hat{y}^n = +1, -1$

- Step 1: Function set (Model)

$$g(x) = \begin{cases} f(x) > 0 & \text{Output = +1} \\ f(x) < 0 & \text{Output = -1} \end{cases}$$

- Step 2: Loss function:

$$L(f) = \sum_n \cancel{\delta(g(x^n) \neq \hat{y}^n)}$$

$$l(f(x^n), \hat{y}^n)$$

The number of times g get incorrect results on training data.

- Step 3: Training by gradient descent is difficult

Gradient descent is possible if g$(*)$ and $\delta(*)$ is differentiable

Step 2: Loss function

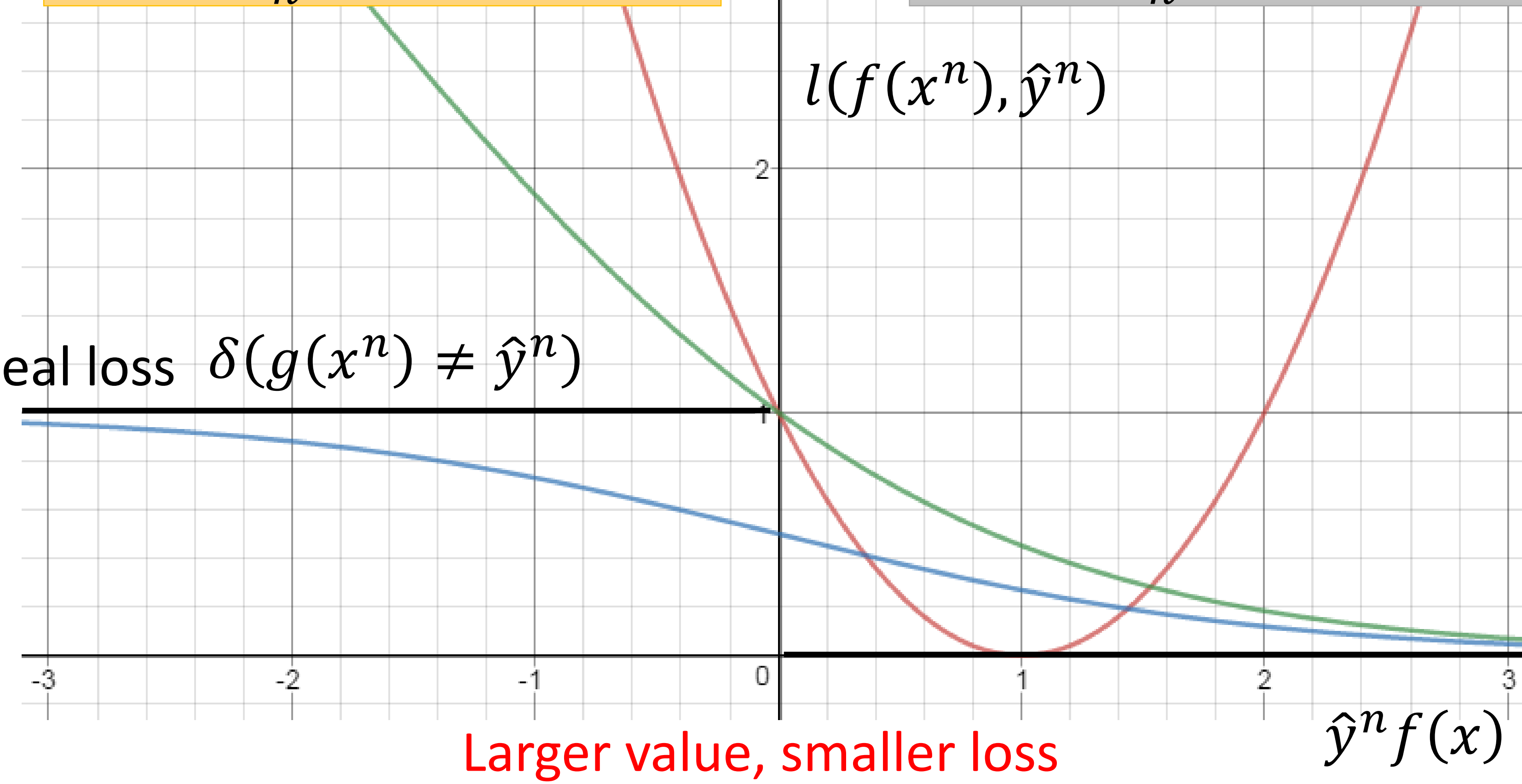
$$g(x) = \begin{cases} f(x) > 0 & \text{Output = +1} \\ f(x) < 0 & \text{Output = -1} \end{cases}$$

Ideal loss:

$$L(f) = \sum_n \delta(g(x^n) \neq \hat{y}^n)$$

Approximation:

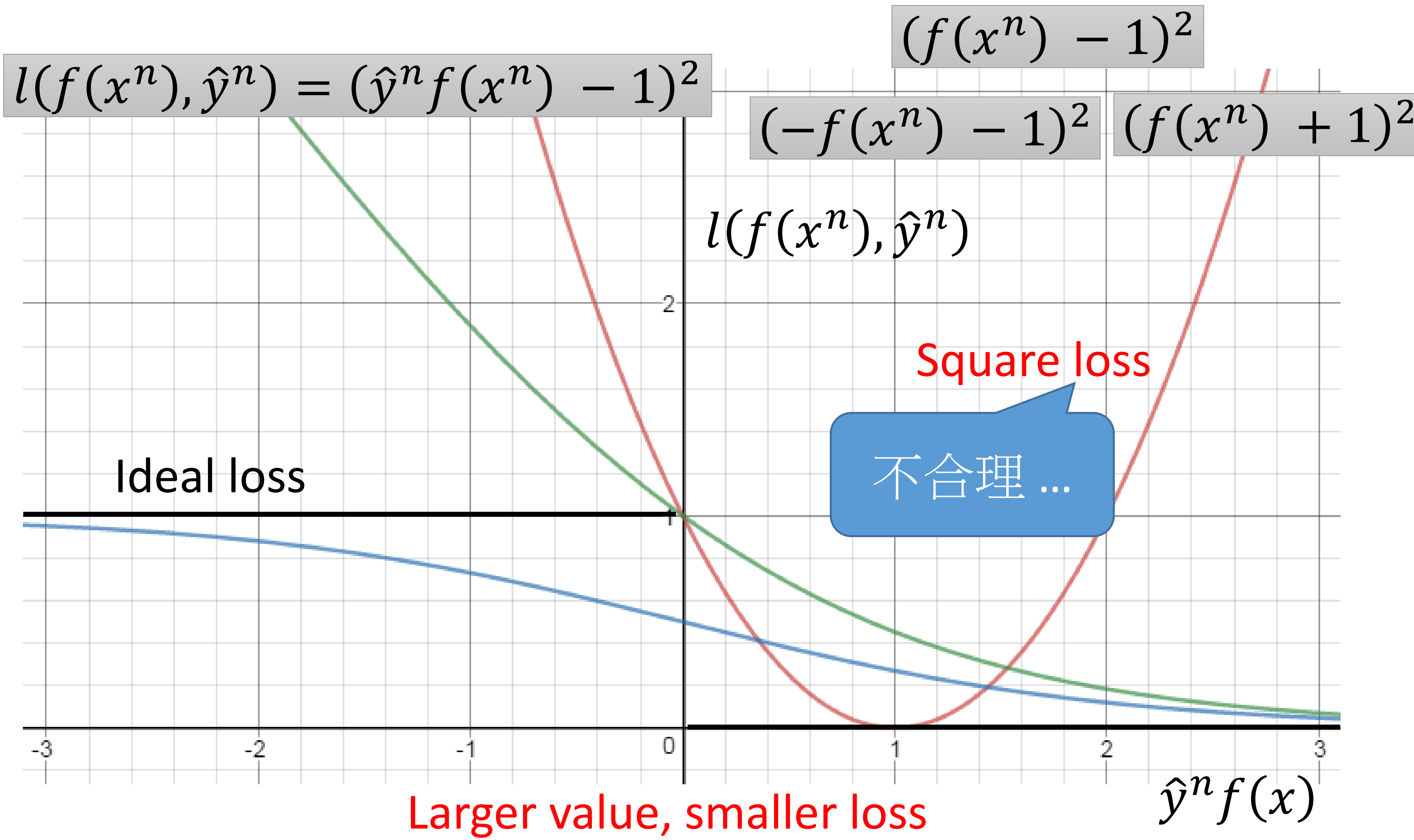
$$L(f) = \sum_n l(f(x^n), \hat{y}^n)$$



Step 2: Loss function

Square Loss: If $\hat{y}^n = 1$, $f(x)$ close to 1

If $\hat{y}^n = -1$, $f(x)$ close to -1

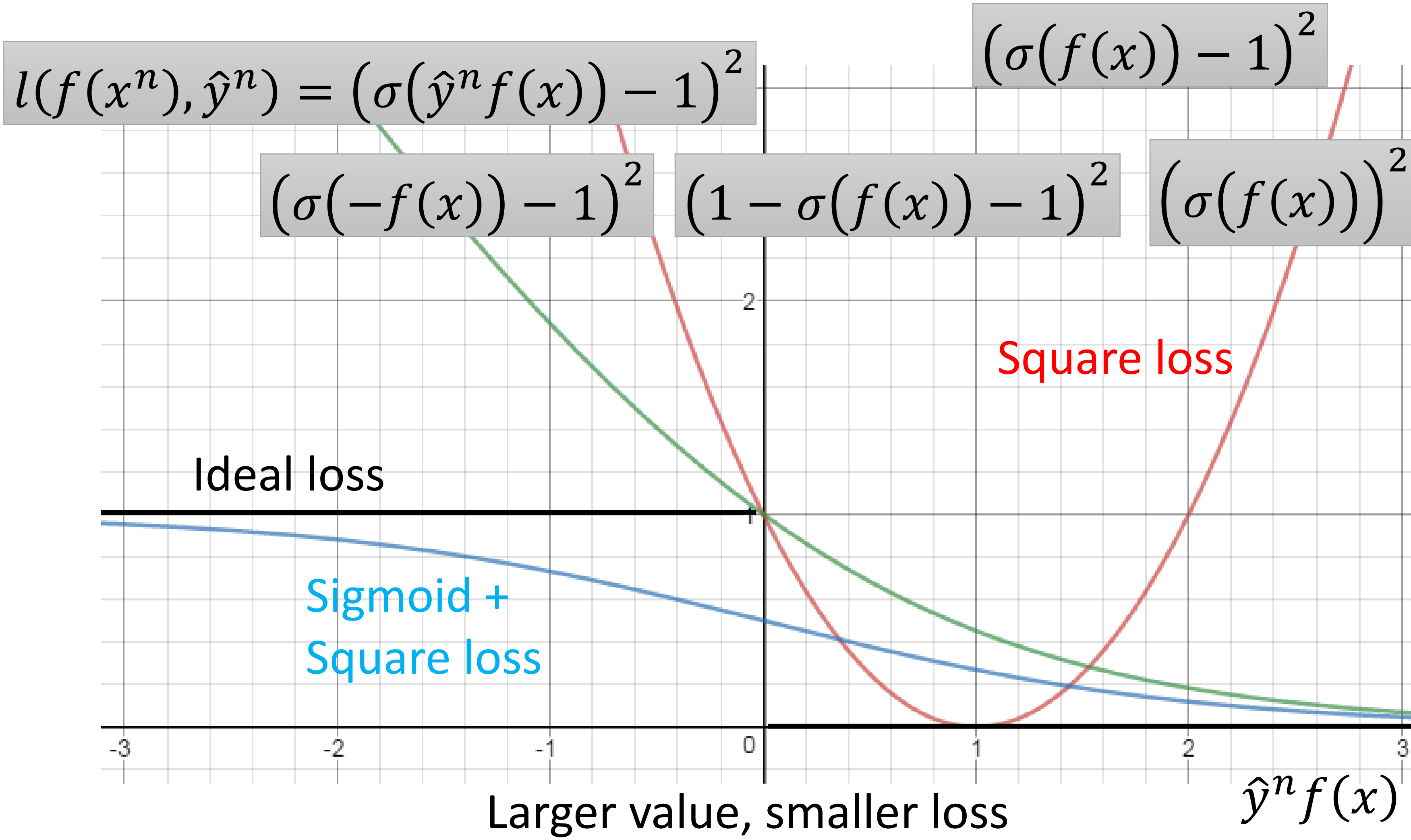


Step 2: Loss function

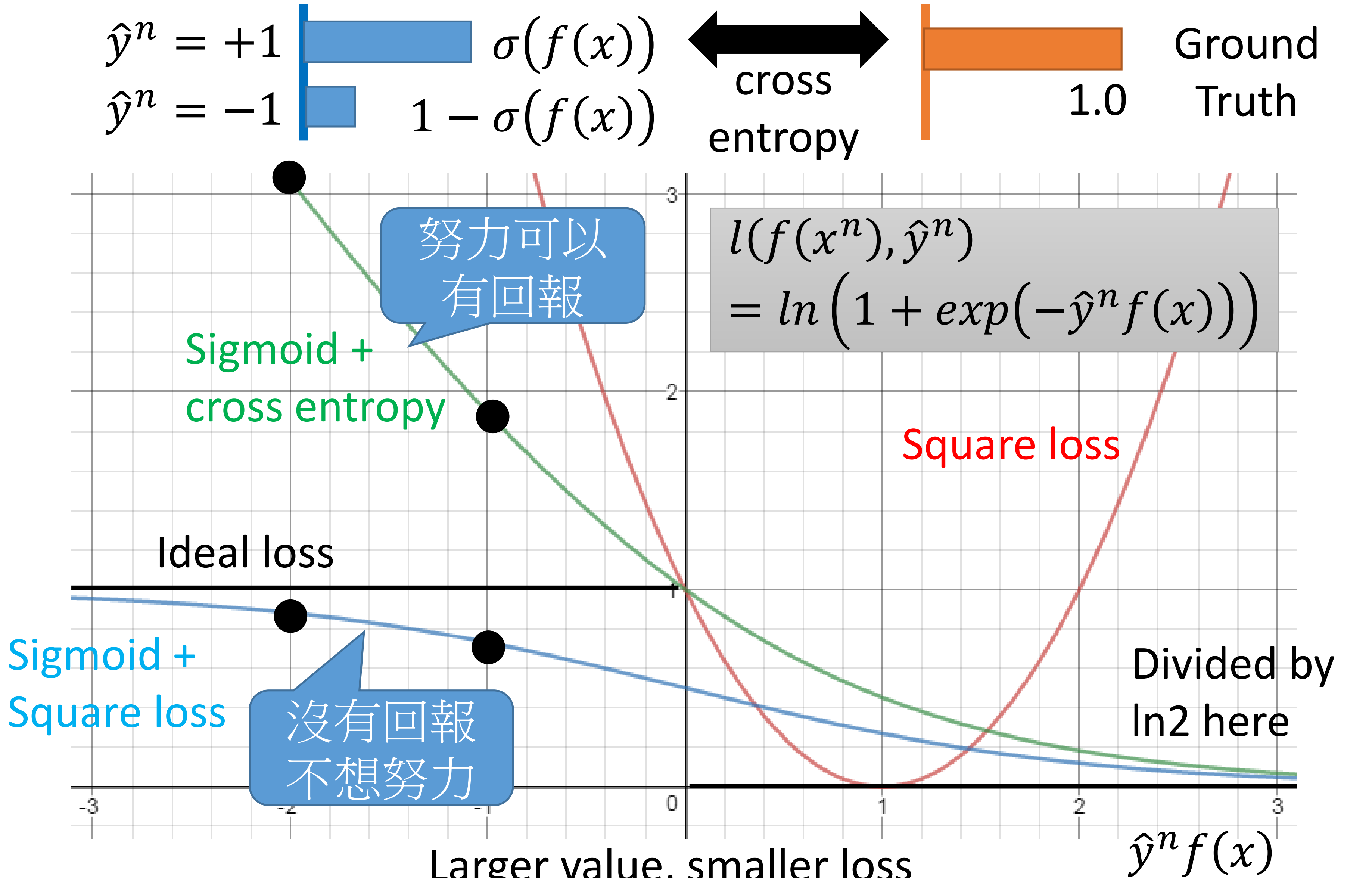
Sigmoid + Square Loss:

If $\hat{y}^n = 1$, $\sigma(f(x))$ close to 1

If $\hat{y}^n = -1$, $\sigma(f(x))$ close to 0



Step 2: Loss function Sigmoid + cross entropy (logistic regression)

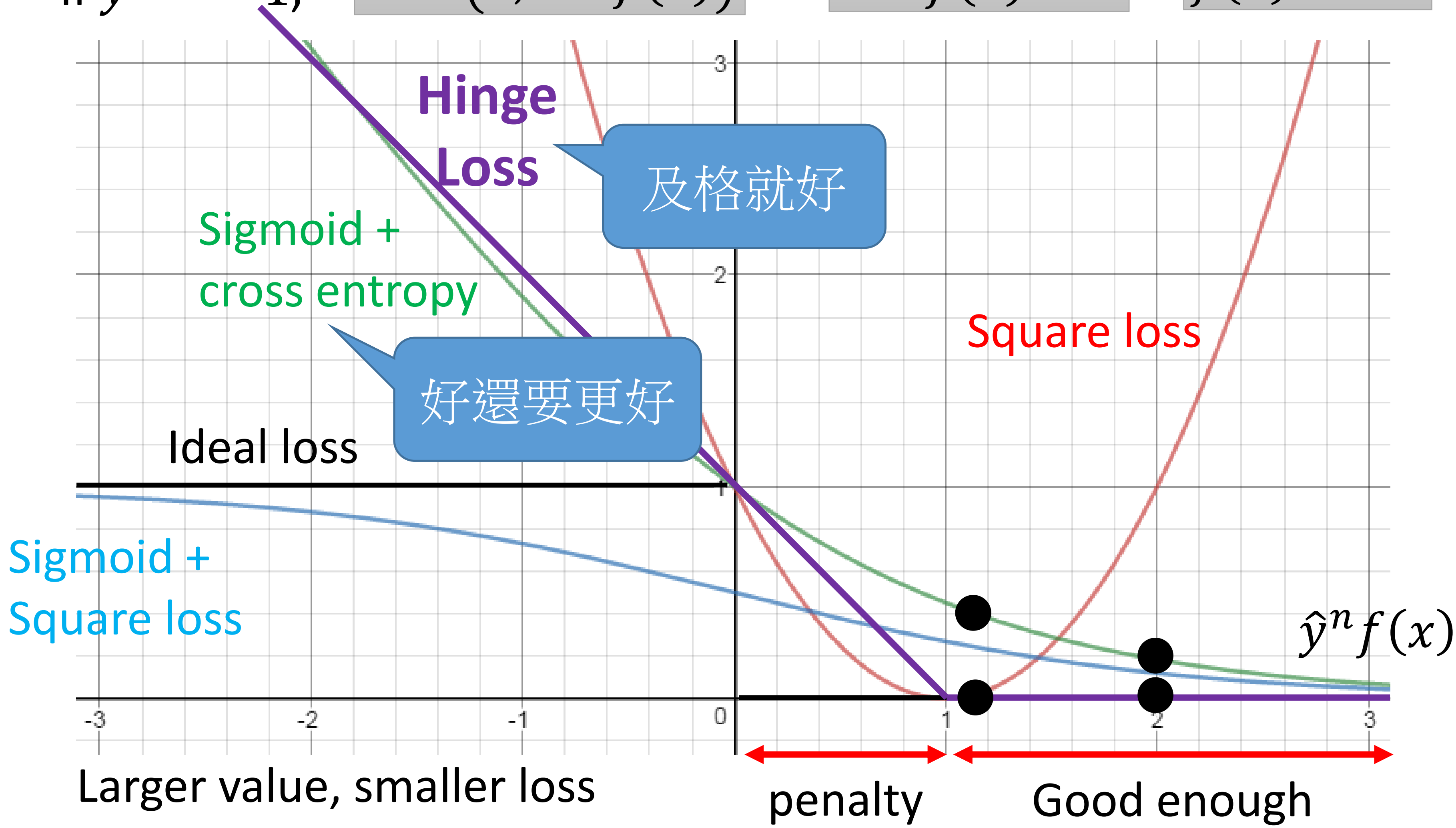


Step 2: Loss function

$$l(f(x^n), \hat{y}^n) = max\left(0, 1 - \hat{y}^n f(x)\right)$$

If $\hat{y}^n = 1$, $max\left(0, 1 - f(x)\right)$ $1 - f(x) < 0$ $f(x) > 1$

If $\hat{y}^n = -1$, $max\left(0, 1 + f(x)\right)$ $1 + f(x) < 0$ $f(x) < -1$



Linear SVM

Compared with logistic regression, linear SVM has different loss function

Deep version: Yichuan Tang , "Deep Learning using Linear Support Vector Machines", ICML 2013 Challenges in Representation Learning Workshop

- Step 1: Function (Model)

$$f(x) = \sum_i w_i x_i + b \quad = \overset{\text{New w}}{\boxed{\begin{bmatrix} w \\ b \end{bmatrix}}} \cdot \underset{\text{New x}}{\boxed{\begin{bmatrix} x \\ 1 \end{bmatrix}}} = w^T x$$

- Step 2: Loss function

$$L(f) = \sum_n l(f(x^n), \hat{y}^n) + \lambda \|w\|_2$$

$$l(f(x^n), \hat{y}^n) = max\left(0, 1 - \hat{y}^n f(x)\right)$$

- Step 3: gradient descent?

Recall relu, maxout network

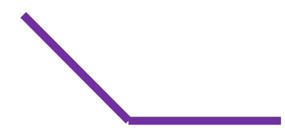
Linear SVM – gradient descent

Ignore regularization for simplicity

$$L(f) = \sum_n l(f(x^n), \hat{y}^n) \qquad l(f(x^n), \hat{y}^n) = max\left(0, 1 - \hat{y}^n f(x^n)\right)$$

$$\frac{\partial l(f(x^n), \hat{y}^n)}{\partial w_i} = \frac{\partial l(f(x^n), \hat{y}^n)}{\partial f(x^n)} \boxed{\frac{\partial f(x^n)}{\partial w_i}} \; x_i^n \qquad \boxed{\begin{array}{c} f(x^n) \\ = w^T \cdot x^n \end{array}}$$

$$\frac{\partial max\left(0, 1 - \hat{y}^n f(x^n)\right)}{\partial f(x^n)} = \begin{cases} -\hat{y}^n & \text{If } \hat{y}^n f(x^n) < 1 \\ 0 & \text{otherwise} \end{cases}$$



$$\frac{\partial L(f)}{\partial w_i} = \sum_n \underbrace{-\delta(\hat{y}^n f(x^n) < 1)\hat{y}^n}_{c^n(w)} x_i \qquad w_i \leftarrow w_i - \eta \sum_n c^n(w) x_i^n$$

Linear SVM – another formulation

Minimizing loss function L:

$$L(f) = \sum_n \varepsilon^n + \lambda \|w\|_2$$

$$\boxed{\varepsilon^n = max\big(0, 1 - \hat{y}^n f(x)\big)}$$

ε^n: slack variable

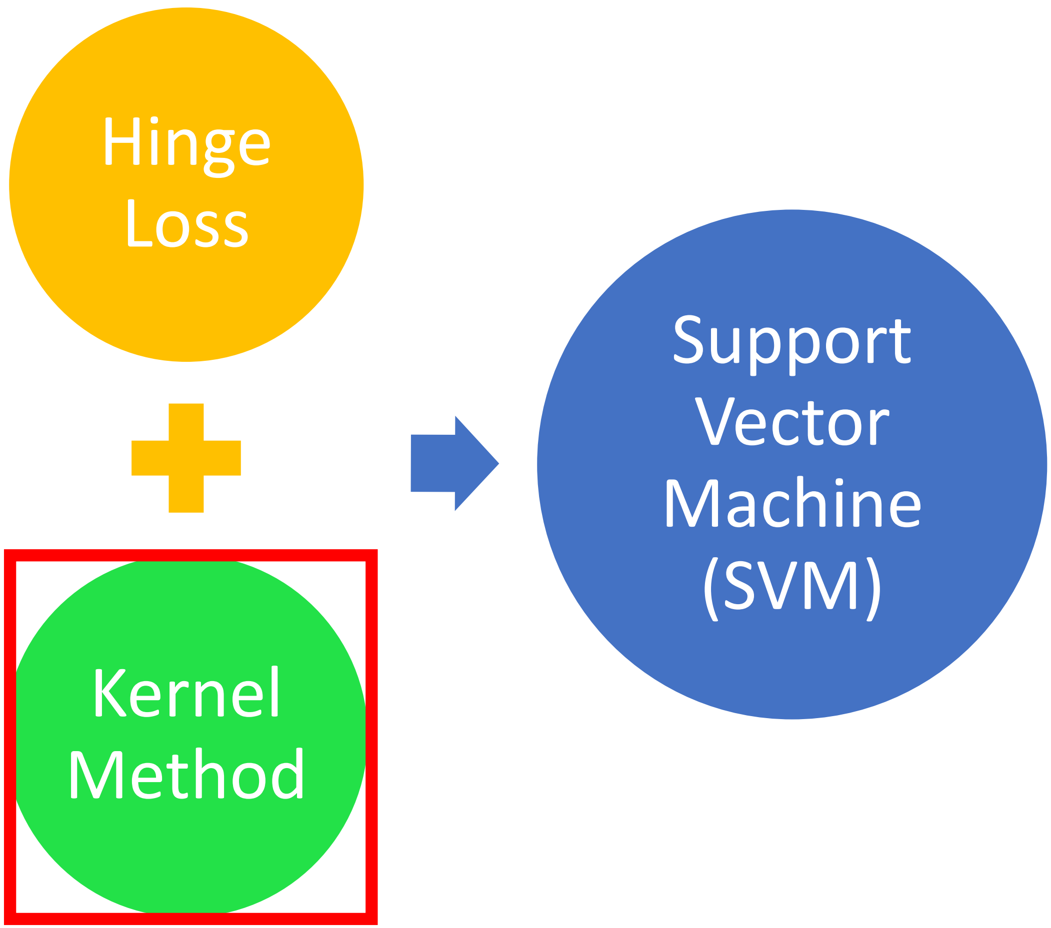
Quadradic programming problem

$$\shortparallel$$

$$\varepsilon^n \geq 0$$

$$\varepsilon^n \geq 1 - \hat{y}^n f(x) \Rightarrow \hat{y}^n f(x) \geq 1 - \varepsilon^n$$

Outline



Dual Representation

$$w^* = \sum_n \alpha_n^* x^n$$ Linear combination of data points

α_n^* may be sparse $\Rightarrow$ x^n with non-zero α_n^* are support vectors

$$\left.\begin{aligned} w_1 &\leftarrow w_1 - \eta \sum_n c^n(w) x_1^n \\ &\vdots \\ w_i &\leftarrow w_i - \eta \sum_n c^n(w) x_i^n \\ &\vdots \\ w_k &\leftarrow w_k - \eta \sum_n c^n(w) x_k^n \end{aligned}\right\}$$

If w initialized as **0**

$$w \leftarrow w - \eta \sum_n c^n(w) x^n$$

$$c^n(w) = \frac{\partial l(f(x^n), \hat{y}^n)}{\partial f(x^n)}$$

Hinge loss: usually zero

c.f. for logistic regression, it is always non-zero

Dual Representation

$$w = \sum_n \alpha_n x^n = X\boldsymbol{\alpha} \qquad X = \boxed{\begin{matrix} x^1 & x^2 & \cdots\cdots & x^N \end{matrix}} \qquad \boldsymbol{\alpha} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix}$$

Step 1: $f(x) = w^T x \xrightarrow{w = X\boldsymbol{\alpha}} f(x) = \boldsymbol{\alpha}^T X^T x$

$$\begin{bmatrix} \alpha_1 & \cdots & \alpha_N \end{bmatrix} \qquad \boxed{\begin{matrix} x^1 \\ x^2 \\ \vdots \\ x^N \end{matrix}} \qquad x$$

$$f(x) = \sum_n \alpha_n (x^n \cdot x)$$

$$= \sum_n \alpha_n K(x^n, x)$$

$$\begin{bmatrix} x^1 \cdot x \\ x^2 \cdot x \\ \vdots \\ x^N \cdot x \end{bmatrix}$$

Dual Representation

Step 1: $f(x) = \sum_n \alpha_n K(x^n, x)$

Step 2, 3: Find $\{\alpha_1^*, \cdots, \alpha_n^*, \cdots, \alpha_N^*\}$, minimizing loss function L

$$L(f) = \sum_n l(\underline{f(x^n)}, \hat{y}^n)$$

$$= \sum_n l\left(\underline{\sum_{n'} \alpha_{n'} K\left(x^{n'}, x^n\right)}, \hat{y}^n\right)$$

We don't really need to know vector x

We only need to know the inner project between a pair of vectors x and z

$K(x, z)$

Kernel Trick

Kernel Trick

Directly computing $K(x, z)$ can be faster than "feature transformation + inner product" sometimes.

Kernel trick is useful when we transform all x to $\phi(x)$

$$K(x, z) = \phi(x) \cdot \phi(z) = \begin{bmatrix} {x_1}^2 \\ \sqrt{2}x_1x_2 \\ {x_2}^2 \end{bmatrix} \cdot \begin{bmatrix} {z_1}^2 \\ \sqrt{2}z_1z_2 \\ {z_2}^2 \end{bmatrix}$$

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$= {x_1}^2{z_1}^2 + 2x_1x_2z_1z_2 + {x_2}^2{z_2}^2$$

$$\phi(x) = \begin{bmatrix} {x_1}^2 \\ \sqrt{2}x_1x_2 \\ {x_2}^2 \end{bmatrix}$$

$$= (x_1z_1 + x_2z_2)^2 = \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \cdot \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}\right)^2$$

$$= (x \cdot z)^2$$

Kernel Trick

Directly computing $K(x,z)$ can be faster than "feature transformation + inner product" sometimes.

$$K(x,z) = (x \cdot z)^2$$

$$= (x_1 z_1 + x_2 z_2 + \cdots + x_k z_k)^2$$

$$= \underline{x_1{}^2}\,\underline{z_1{}^2} + \underline{x_2{}^2}\,\underline{z_2{}^2} + \cdots + \underline{x_k{}^2}\,\underline{z_k{}^2}$$

$$+2\underline{x_1 x_2}\,\underline{z_1 z_2} + 2\underline{x_1 x_3}\,\underline{z_1 z_3} + \cdots$$

$$+2\underline{x_2 x_3}\,\underline{z_2 z_3} + 2\underline{x_2 x_4}\,\underline{z_2 z_4} + \cdots$$

$$= \phi(x) \cdot \phi(z)$$

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_k \end{bmatrix} \quad z = \begin{bmatrix} z_1 \\ \vdots \\ z_k \end{bmatrix}$$

$$\phi(x) = \begin{bmatrix} x_1{}^2 \\ \vdots \\ x_k{}^2 \\ \sqrt{2}x_1 x_2 \\ \sqrt{2}x_1 x_3 \\ \vdots \\ \sqrt{2}x_2 x_3 \\ \vdots \end{bmatrix}$$

Radial Basis Function Kernel

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \end{bmatrix} \quad z = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \end{bmatrix}$$

$$K(x,z) = exp\left(-\frac{1}{2}\|x-z\|_2\right) = \phi(x)\cdot\phi(z)?$$

$\phi(*)$ has inf dim!!!

$$= exp\left(-\frac{1}{2}\|x\|_2 - \frac{1}{2}\|z\|_2 + x\cdot z\right)$$

$$= exp\left(-\frac{1}{2}\|x\|_2\right) exp\left(-\frac{1}{2}\|z\|_2\right) exp(x\cdot z) \quad = C_x C_z exp(x\cdot z)$$

$$= C_x C_z \sum_{i=0}^{\infty} \frac{(x\cdot z)^i}{i!} = C_x C_z + C_x C_z (x\cdot z) + C_x C_z \frac{1}{2}(x\cdot z)^2 \cdots$$

$$[C_x]\cdot[C_z] \quad \begin{bmatrix} C_x x_1 \\ C_x x_2 \\ \vdots \end{bmatrix}\cdot\begin{bmatrix} C_z z_1 \\ C_z z_2 \\ \vdots \end{bmatrix} \quad \frac{1}{\sqrt{2}}\begin{bmatrix} C_x {x_1}^2 \\ \vdots \\ \sqrt{2} C_x x_1 x_2 \\ \vdots \end{bmatrix}\cdot\frac{1}{\sqrt{2}}\begin{bmatrix} C_z {z_1}^2 \\ \vdots \\ \sqrt{2} C_z z_1 z_2 \\ \vdots \end{bmatrix}$$

Sigmoid Kernel

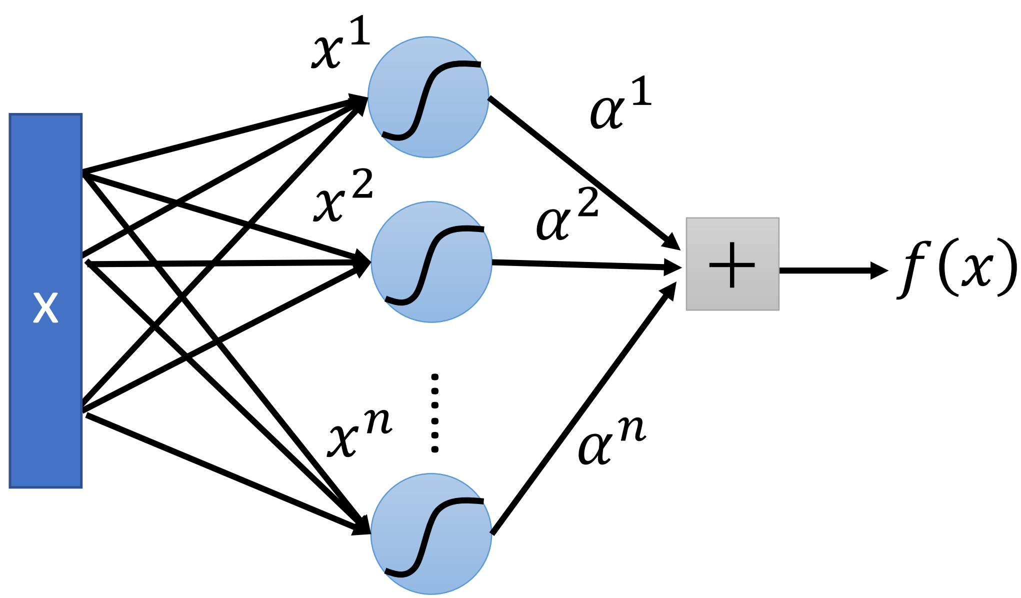
$$K(x,z) = tanh(x \cdot z)$$

- When using sigmoid kernel, we have a 1 hidden layer network.

$$f(x) = \sum_n \alpha_n K(x^n, x) = \sum_n \alpha^n tanh(x^n \cdot x)$$

The weight of each neuron is a data point

The number of support vectors is the number of neurons.

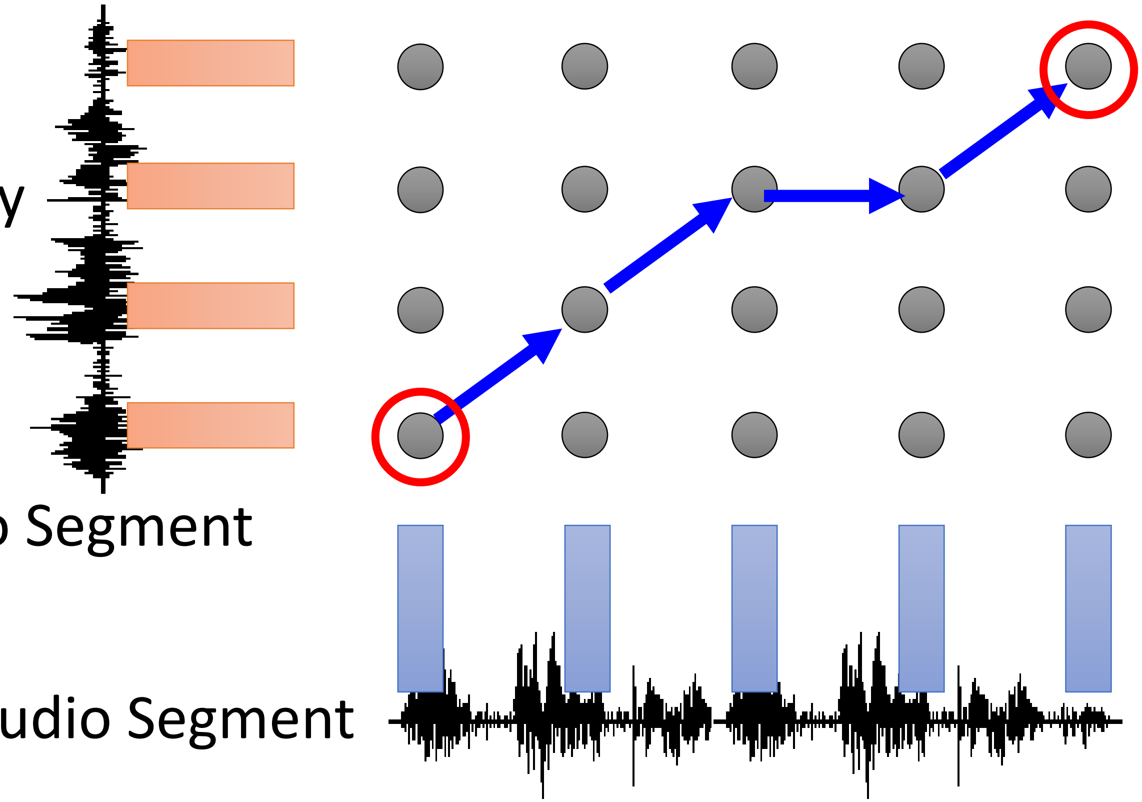


You can directly design $K(x,z)$ instead of considering $\phi(x), \phi(z)$

When x is structured object like sequence, hard to design $\phi(x)$

$K(x,z)$ is something like similarity (Mercer's theory to check)

Evaluate the similarity between sequences as $K(x,z)$



More about kernel design in [Bishop chapter 6.2]

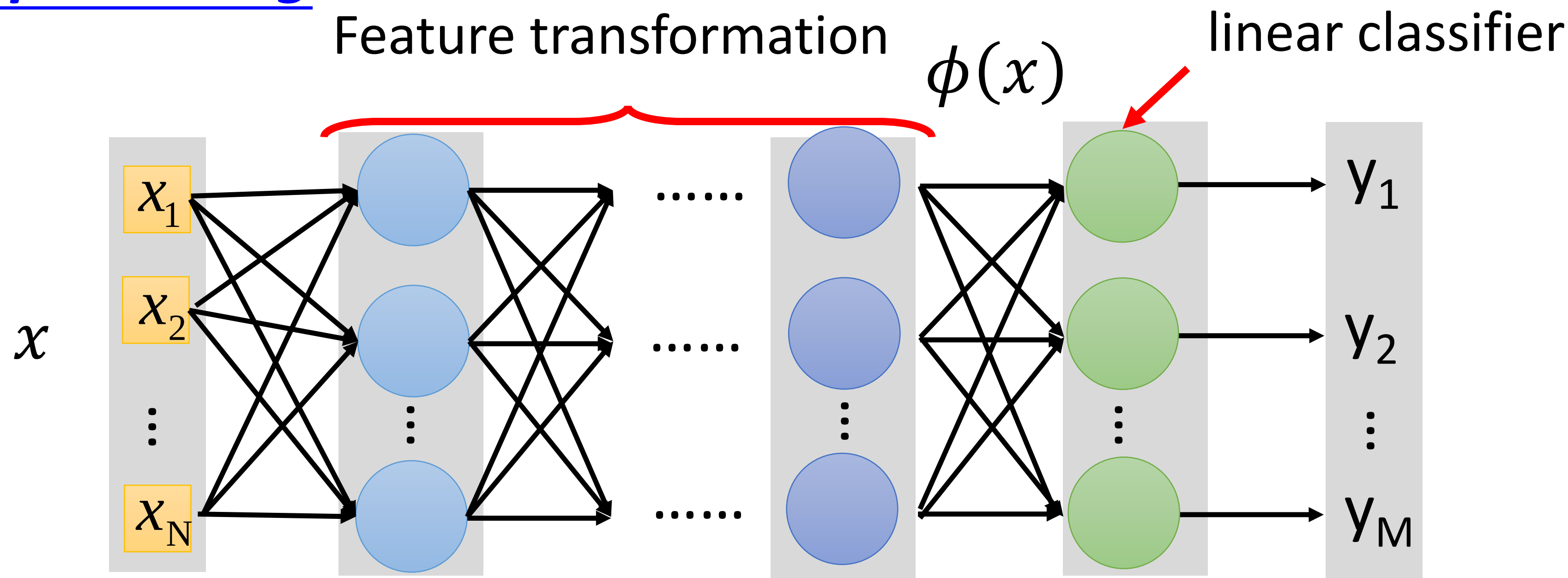
Hiroshi Shimodaira, Ken-ichi Noma, Mitsuru Nakai, Shigeki Sagayama, "Dynamic Time-Alignment Kernel in Support Vector Machine", NIPS, 2002

Marco Cuturi, Jean-Philippe Vert, Oystein Birkenes, Tomoko Matsui, A kernel for time series based on global alignments, ICASSP, 2007

SVM related methods

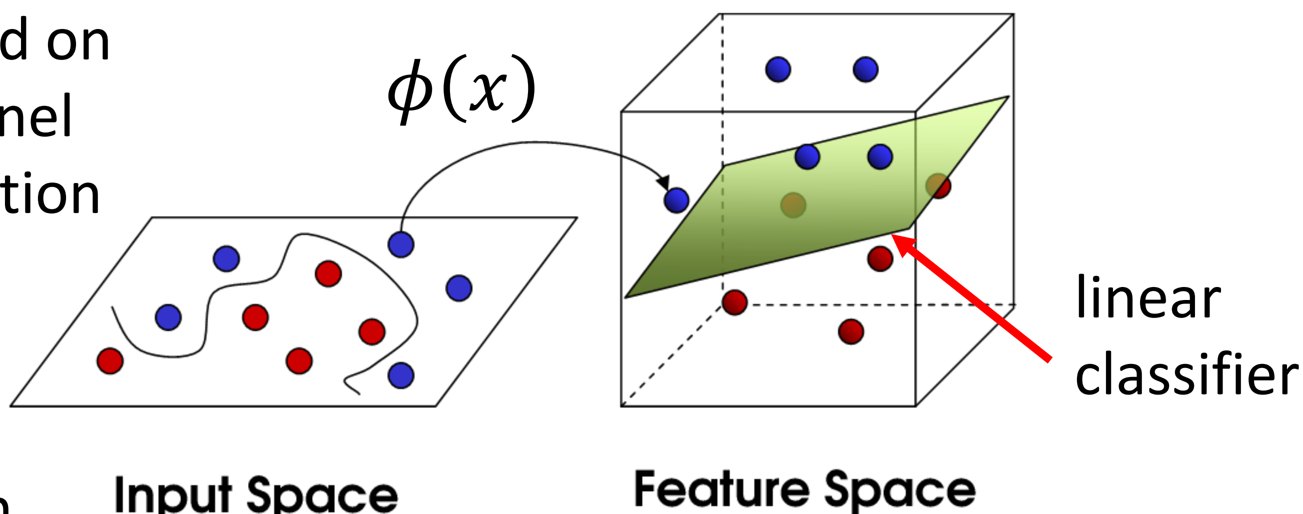
- Support Vector Regression (SVR)
  - [Bishop chapter 7.1.4]
- Ranking SVM
  - [Alpaydin, Chapter 13.11]
- One-class SVM
  - [Alpaydin, Chapter 13.11]

Deep Learning



SVM

Based on kernel function



Multiple Kernel learning [Alpaydin, Chapter 13.8]