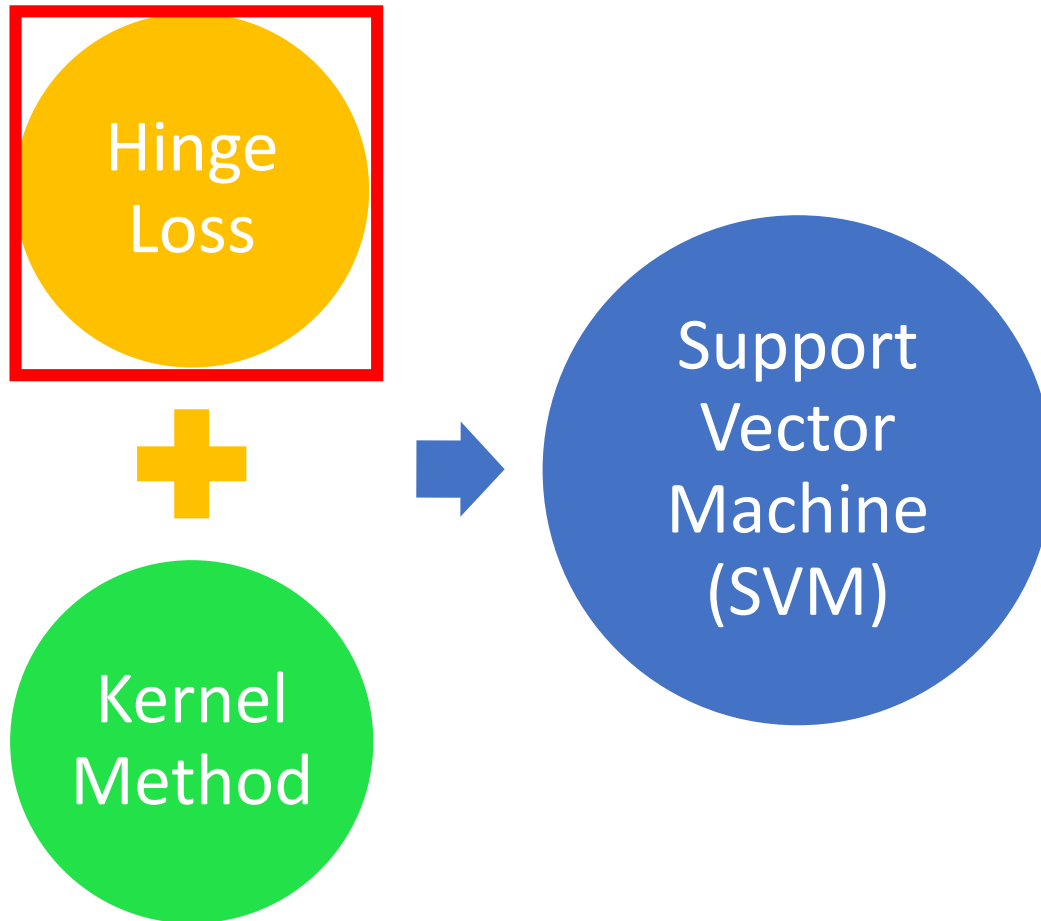


Support Vector Machine

Outline



Binary Classification

x^1	x^2	x^3	...
\hat{y}^1	\hat{y}^2	\hat{y}^3	...

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

- 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:

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

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

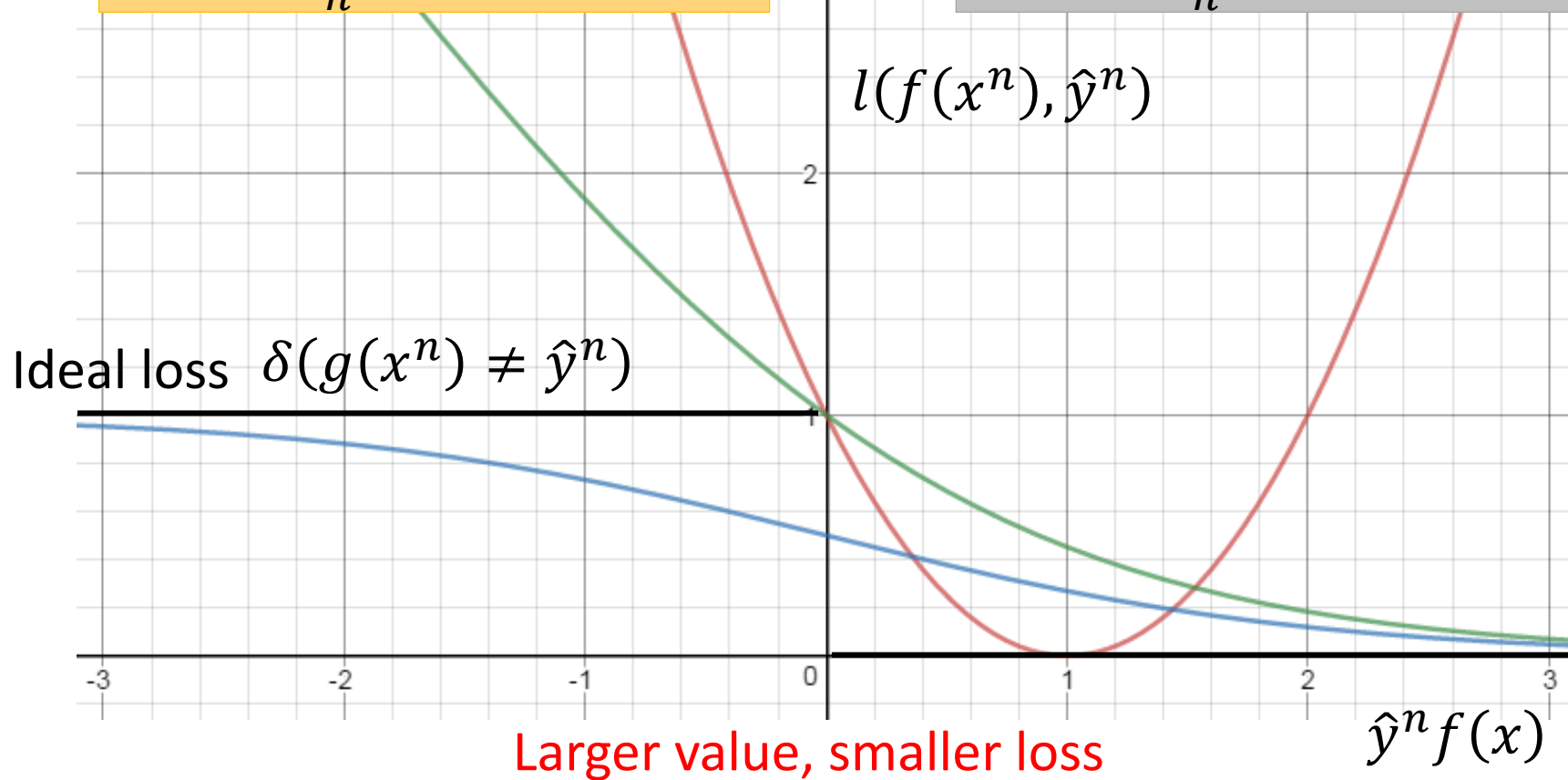
$$g(x) = \begin{cases} f(x) > 0 & \text{Output} = +1 \\ f(x) < 0 & \text{Output} = -1 \end{cases}$$

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

$$(f(x^n) - 1)^2$$

$$l(f(x^n), \hat{y}^n) = (\hat{y}^n f(x^n) - 1)^2$$

$$(-f(x^n) - 1)^2$$

$$(f(x^n) + 1)^2$$

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

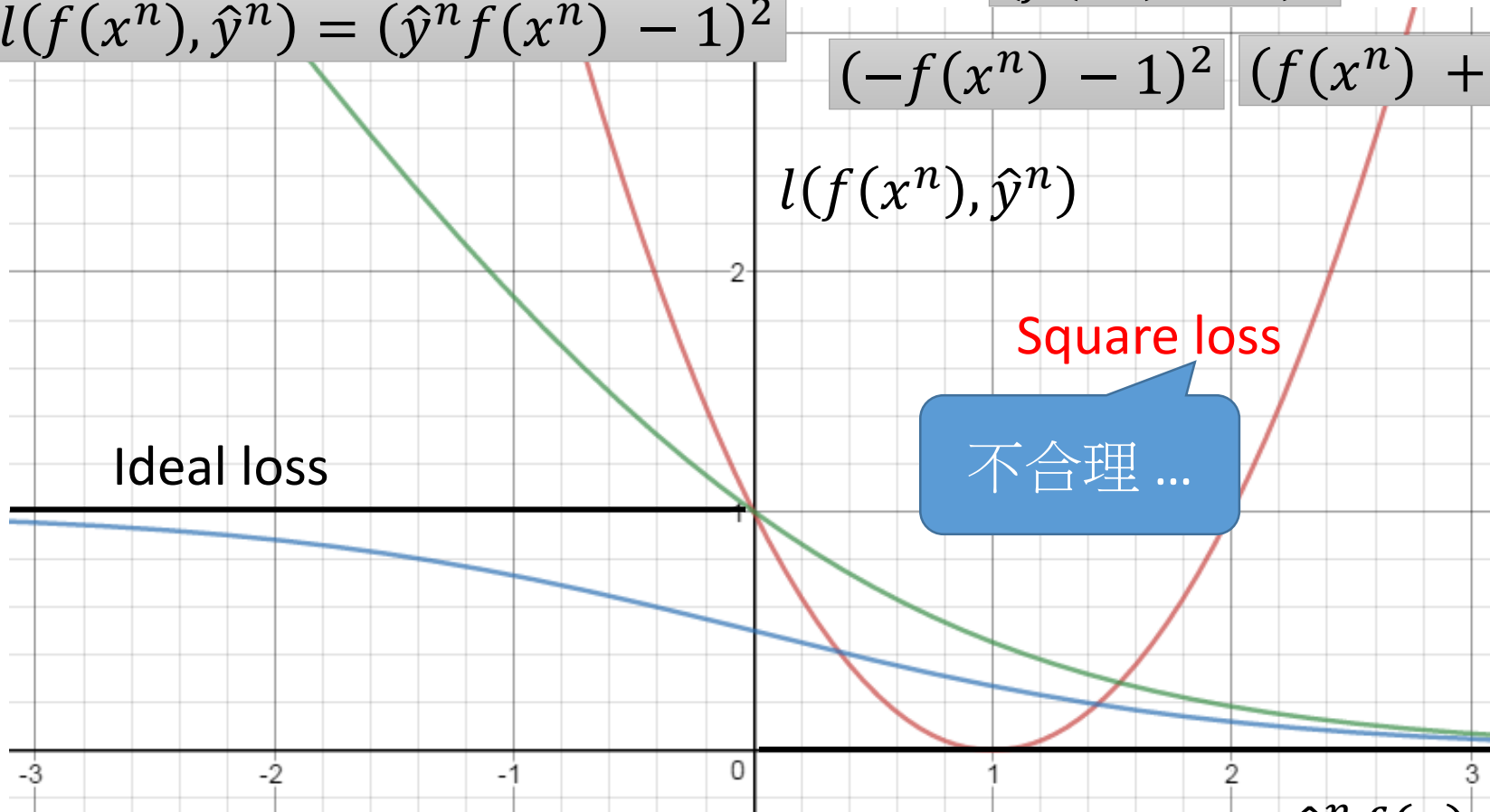
Square loss

不合理 ...

Ideal loss

Larger value, smaller loss

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

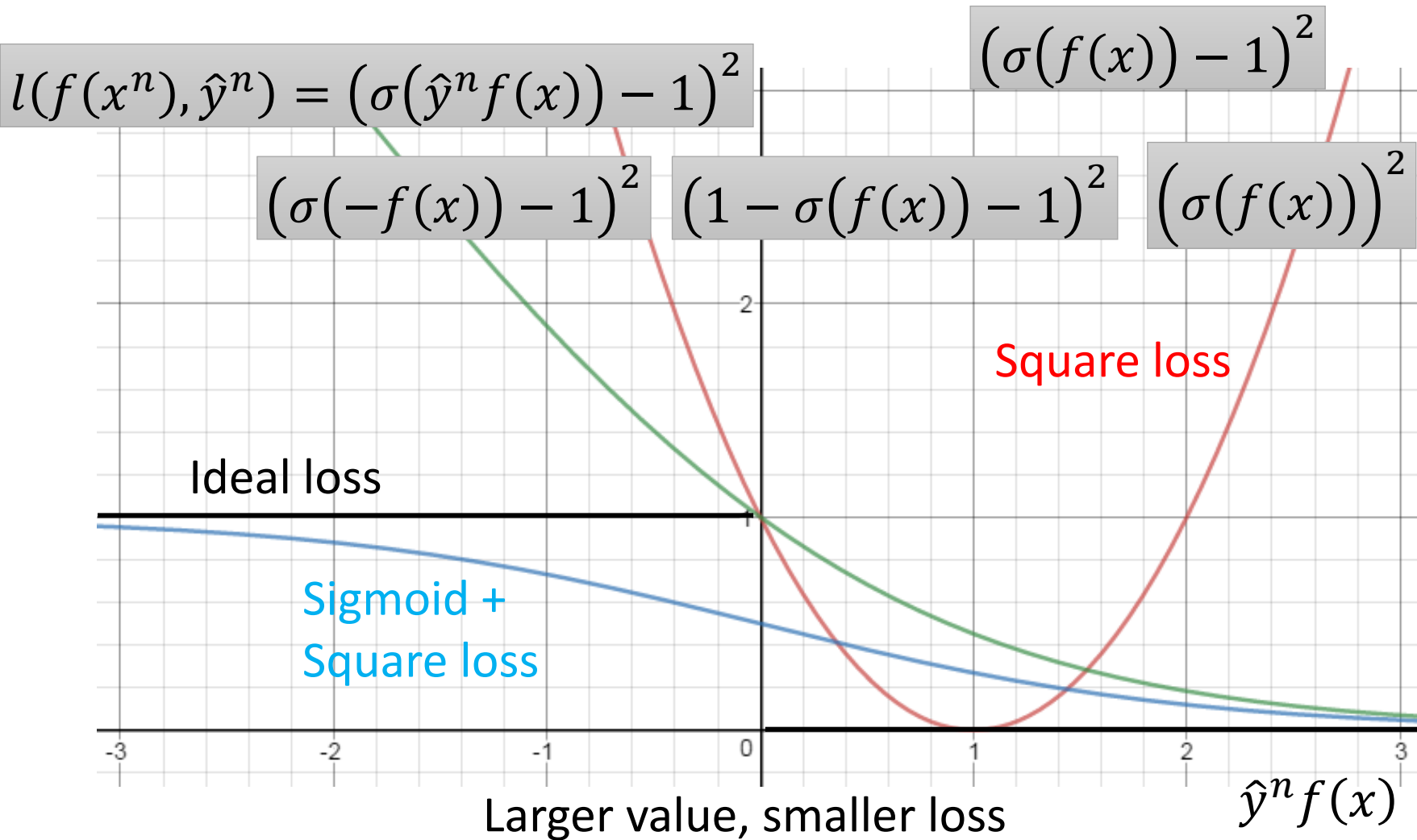


Step 2: Loss function

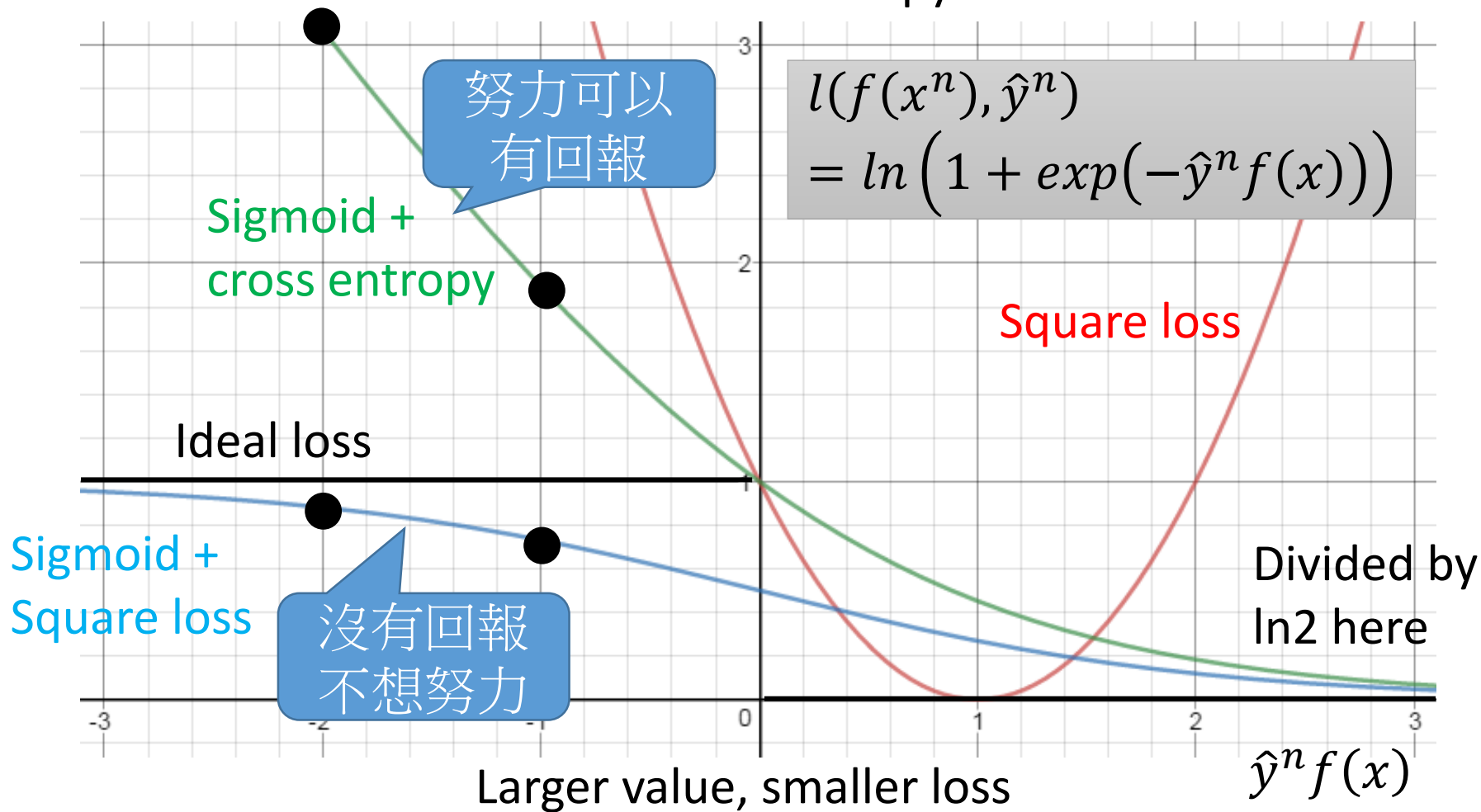
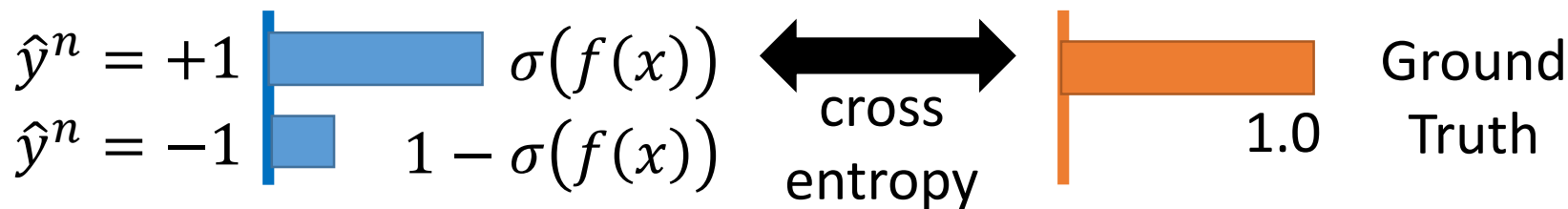
Sigmoid + Square Loss:

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

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

If $\hat{y}^n = 1$,

$$\max(0, 1 - f(x))$$

$$1 - f(x) < 0$$

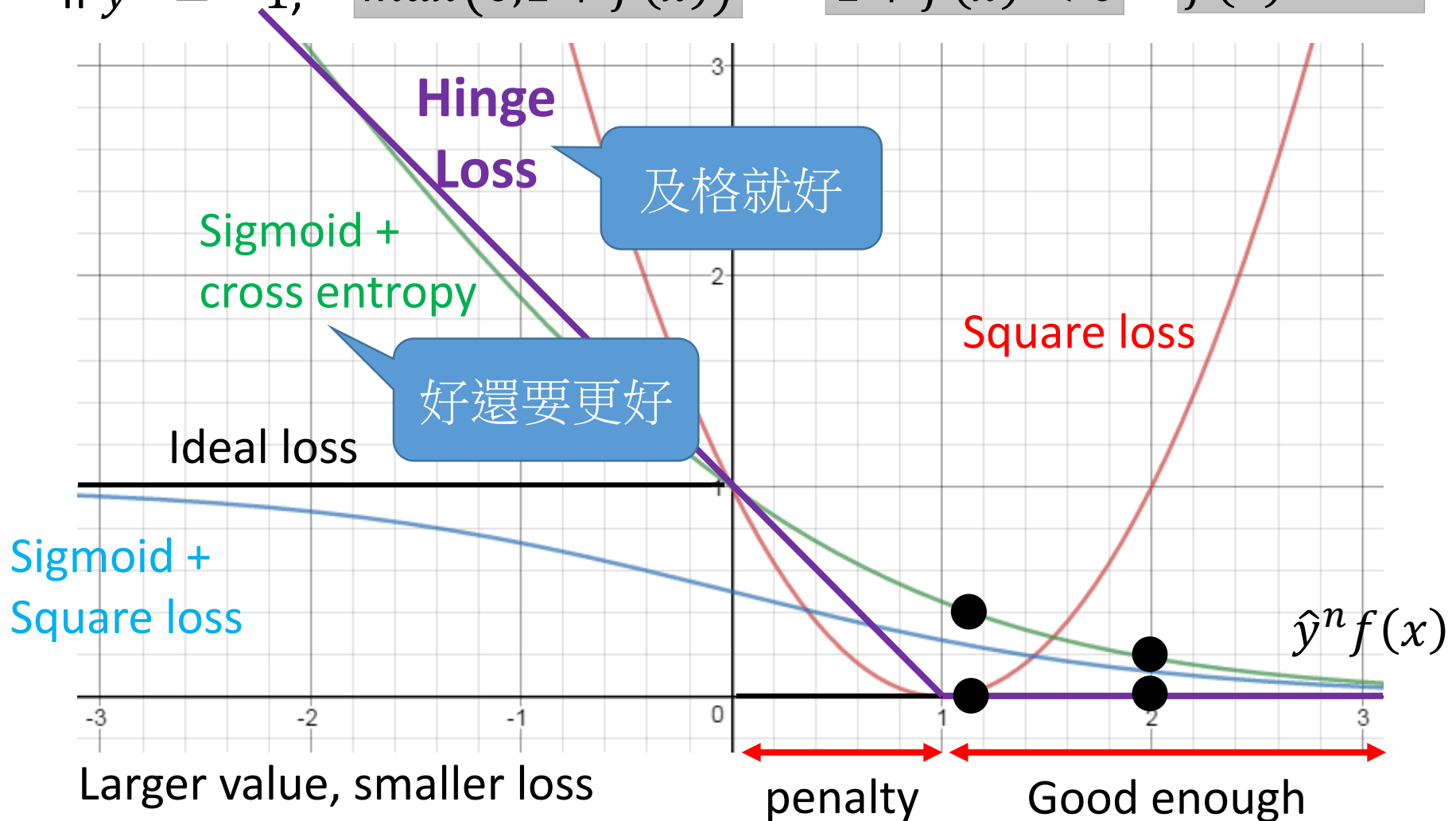
$$f(x) > 1$$

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

$$\max(0, 1 + f(x))$$

$$1 + f(x) < 0$$

$$f(x) < -1$$



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)

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

- Step 2: Loss function



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

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

- Step 3: gradient descent?

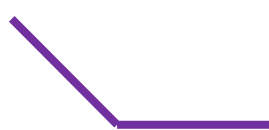
Recall relu, maxout network

Linear SVM – gradient descent

Ignore regularization for simplicity

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

$$\frac{\partial l(f(x^n), \hat{y}^n)}{\partial w_i} = \frac{\partial l(f(x^n), \hat{y}^n)}{\partial f(x^n)} \frac{\partial f(x^n)}{\partial w_i} x_i^n \quad \boxed{f(x^n) = w^T \cdot x^n}$$

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


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

Linear SVM – another formulation

Minimizing loss function L:

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

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

||

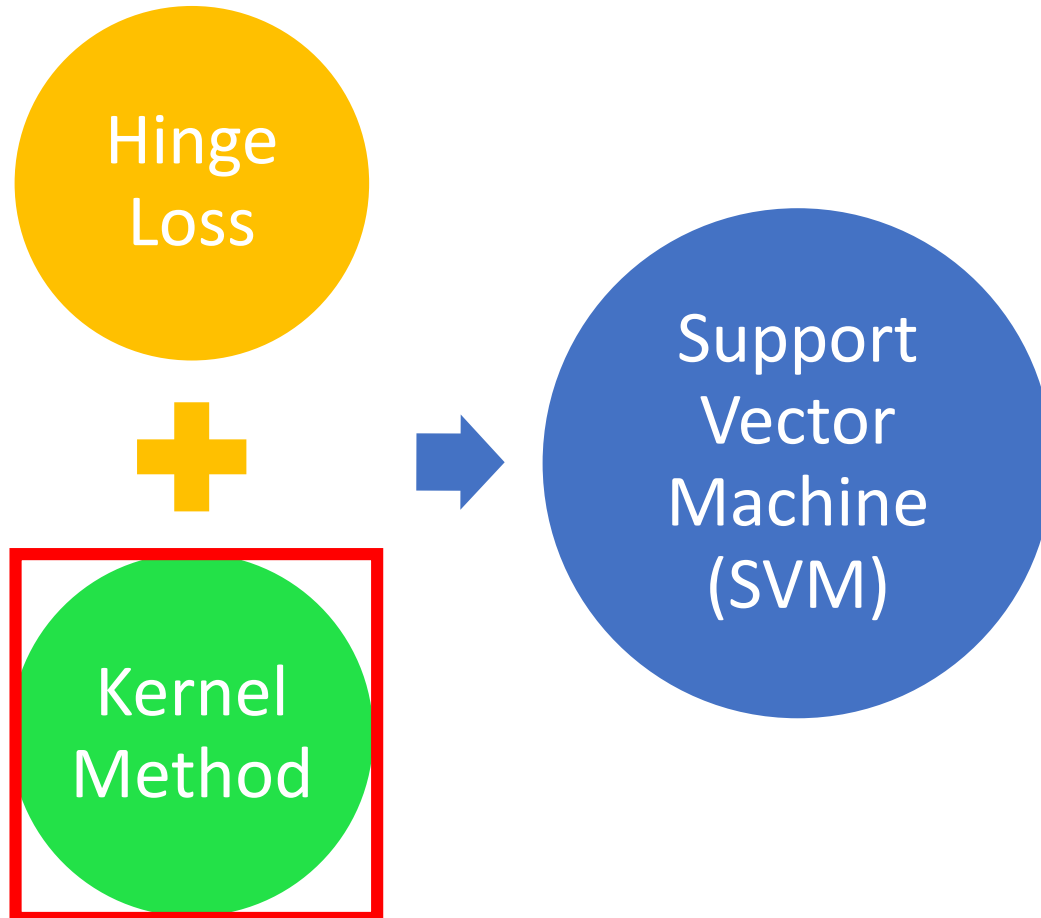
ε^n : slack variable

Quadratic programming
problem

$$\varepsilon^n \geq 0$$

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

Outline



Dual Representation

$$w^* = \sum_n \alpha_n^* x^n \quad \text{Linear combination of data points}$$

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 $\mathbf{0}$

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

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

Hinge loss:
usually zero

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

Dual Representation

$$w = \sum_n \alpha_n x^n = X\alpha \quad X = \begin{bmatrix} x^1 & x^2 & \dots & x^N \end{bmatrix} \quad \alpha = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix}$$

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

Diagram illustrating the matrix multiplication $\alpha^T X^T x$:

- α^T is represented as the row vector $[\alpha_1 \quad \dots \quad \alpha_N]$.
- X^T is represented as a column of inner products: $\begin{bmatrix} x^1 \cdot x \\ x^2 \cdot x \\ \vdots \\ x^N \cdot x \end{bmatrix}$.
- The input x is shown as a green box.
- A blue box contains the individual input vectors x^1, x^2, \dots, x^N .
- Arrows indicate that α^T multiplies the column of inner products, and X^T is formed by computing the inner products of each x^n with x .

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

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

Dual Representation

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

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

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

We don't really need to know vector x

We only need to know the inner product 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 $\phi(x)$

$$\begin{aligned} x &= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ K(x, z) &= \phi(x) \cdot \phi(z) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \cdot \begin{bmatrix} z_1^2 \\ \sqrt{2}z_1z_2 \\ z_2^2 \end{bmatrix} \\ &= x_1^2z_1^2 + 2x_1x_2z_1z_2 + x_2^2z_2^2 \\ \phi(x) &= \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix} \\ &= (x_1z_1 + x_2z_2)^2 = \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \cdot \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \right)^2 \\ &= (x \cdot z)^2 \end{aligned}$$

Kernel Trick

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

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

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

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

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

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

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

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

$$\phi(x) = \begin{bmatrix} x_1^2 \\ \vdots \\ x_k^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ \vdots \\ \sqrt{2}x_2x_3 \\ \vdots \end{bmatrix}$$

Radial Basis Function Kernel

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

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

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

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

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

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

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

Sigmoid Kernel

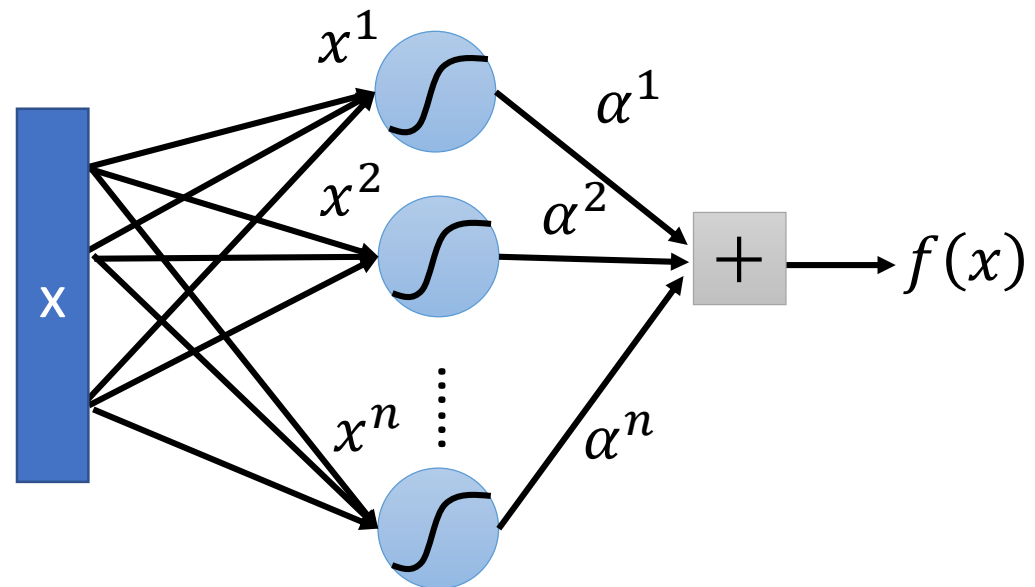
$$K(x, z) = \tanh(x \cdot z)$$

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

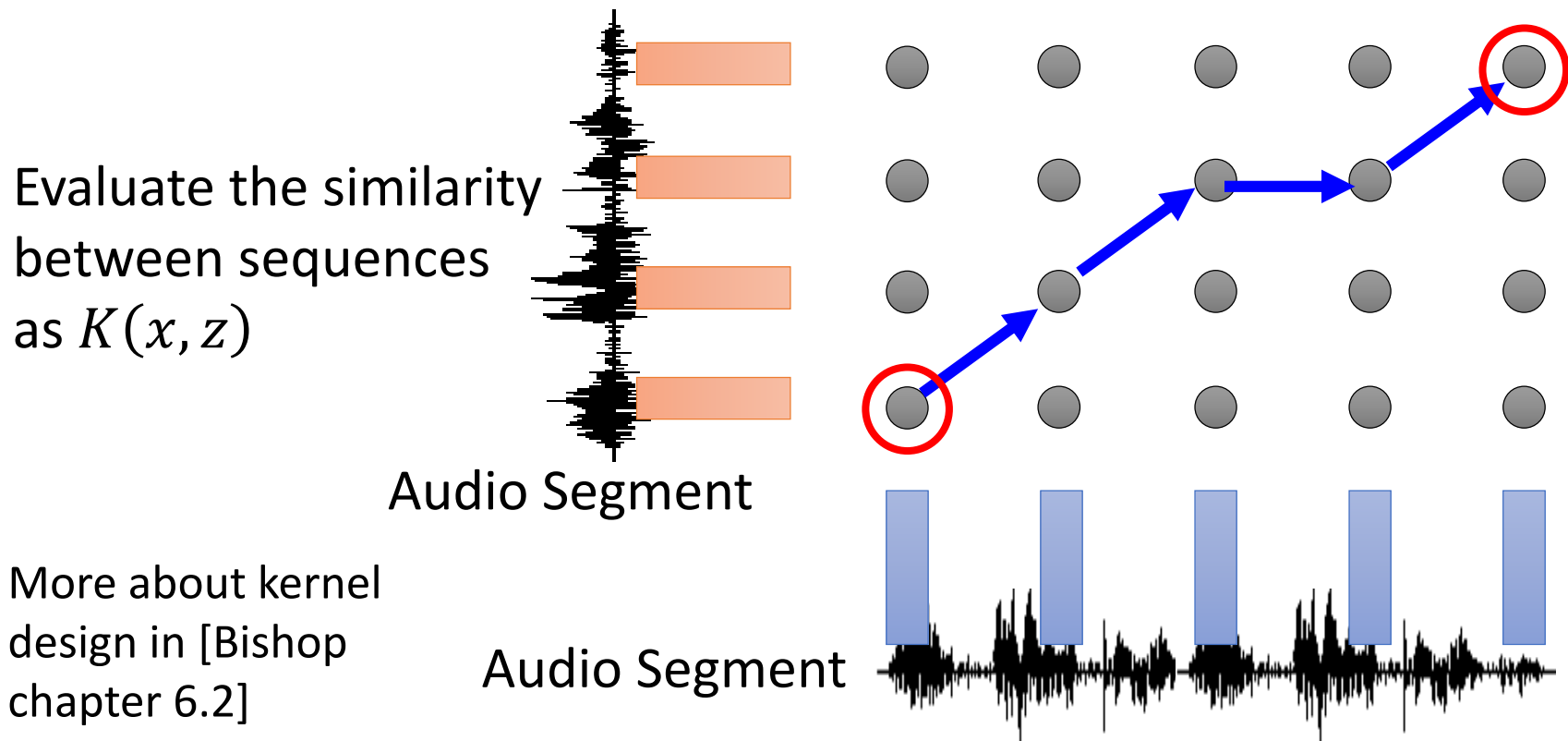
$$f(x) = \sum_n \alpha_n K(x^n, x) = \sum_n \alpha^n \tanh(x^n \cdot x)$$

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)



More about kernel design in [Bishop chapter 6.2]

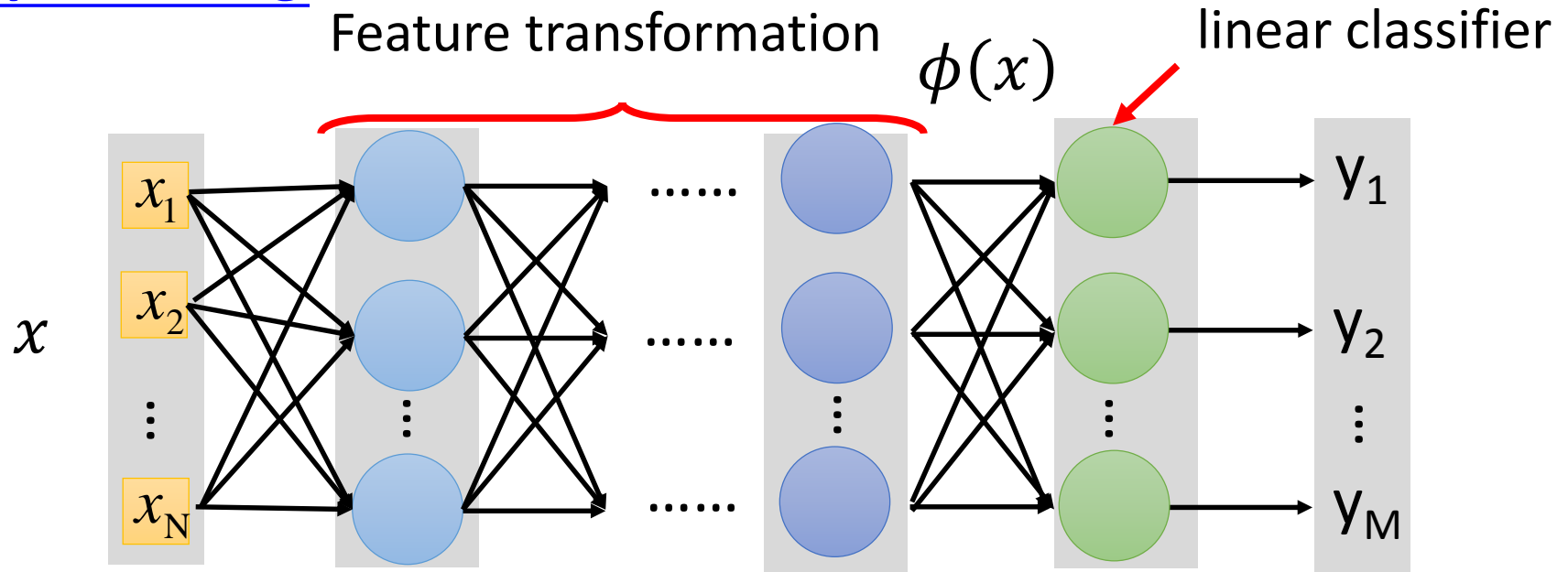
Hiroshi Shimodaira, Ken-ichi Noma, Mitsuru Nakai, Shigeki Sagayama, "Dynamic Time-Alignment Kernel in Support Vector Machine", NIPS, 2002

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

