

Lecture 5: Linear Models and Kernel Trick

http://cs.nju.edu.cn/yuy/course_dm12.ashx



Linear model



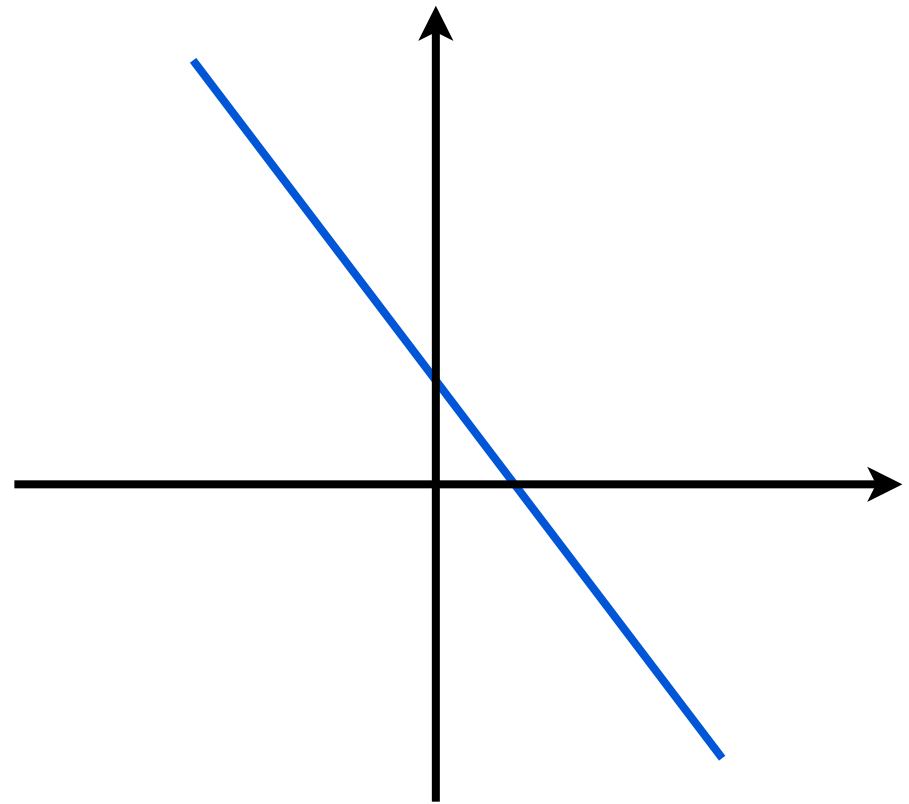
model space: \mathbb{R}^{n+1}

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

we sometimes omit the bias

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$$

1. w with a constant element
2. practically as good as with bias (centered data)



Least square regression



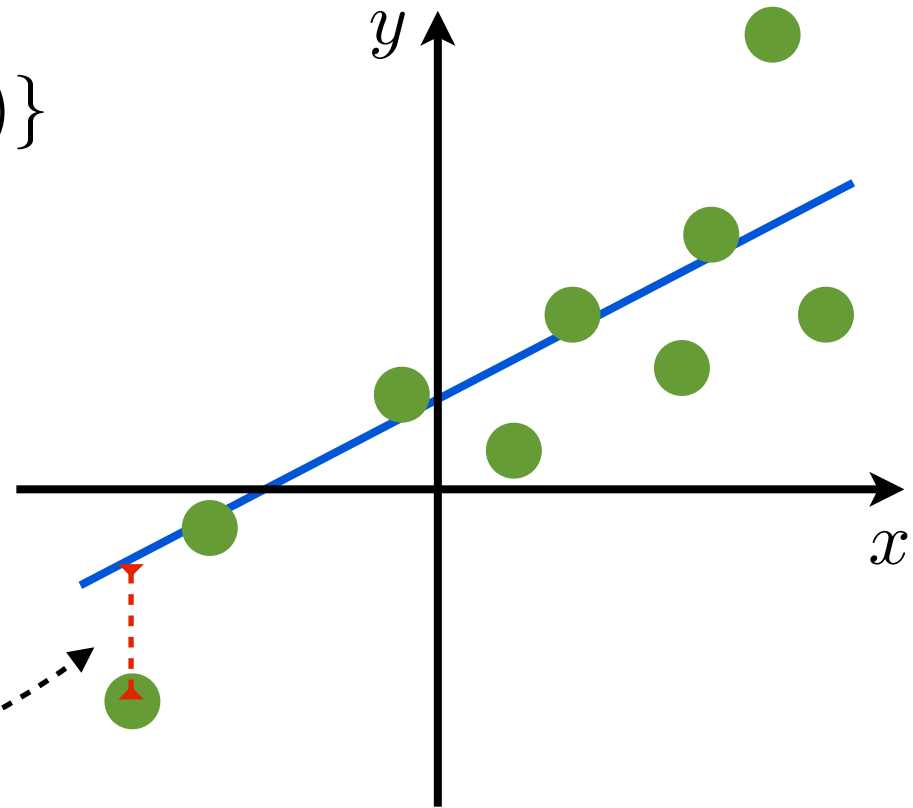
Regression: $y \in \mathbb{R}$

Training data:

$$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), (\mathbf{x}_m, y_m)\}$$

Least square loss:

$$\frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2$$





Least square regression

$$L(\mathbf{w}, b) = \frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2$$

$$\frac{\partial L(\mathbf{w}, b)}{\partial b} = \frac{1}{m} \sum_{i=1}^m 2(\mathbf{w}^\top \mathbf{x}_i + b - y_i) = 0$$

$$\frac{\partial L(\mathbf{w}, b)}{\partial \mathbf{w}} = \frac{1}{m} \sum_{i=1}^m 2(\mathbf{w}^\top \mathbf{x}_i + b - y_i) \mathbf{x}_i = 0$$

$$b = \frac{1}{m} \sum_{i=1}^m (y_i - \mathbf{w}^\top \mathbf{x}_i) = \bar{y} - \mathbf{w}^\top \bar{\mathbf{x}}$$

$$\mathbf{w} = \left(\frac{1}{m} \sum_{i=1}^m \mathbf{x}_i \mathbf{x}_i^\top - \bar{\mathbf{x}} \bar{\mathbf{x}}^\top \right)^{-1} \left(\frac{1}{m} \sum_{i=1}^m (y_i \mathbf{x}_i) - \bar{y} \bar{\mathbf{x}} \right)$$

$$= \text{var}(\mathbf{x})^{-1} \text{cov}(\mathbf{x}, y) = (X^\top X)^{-1} X^\top Y$$

closed
form
solution

Least absolute deviation regression



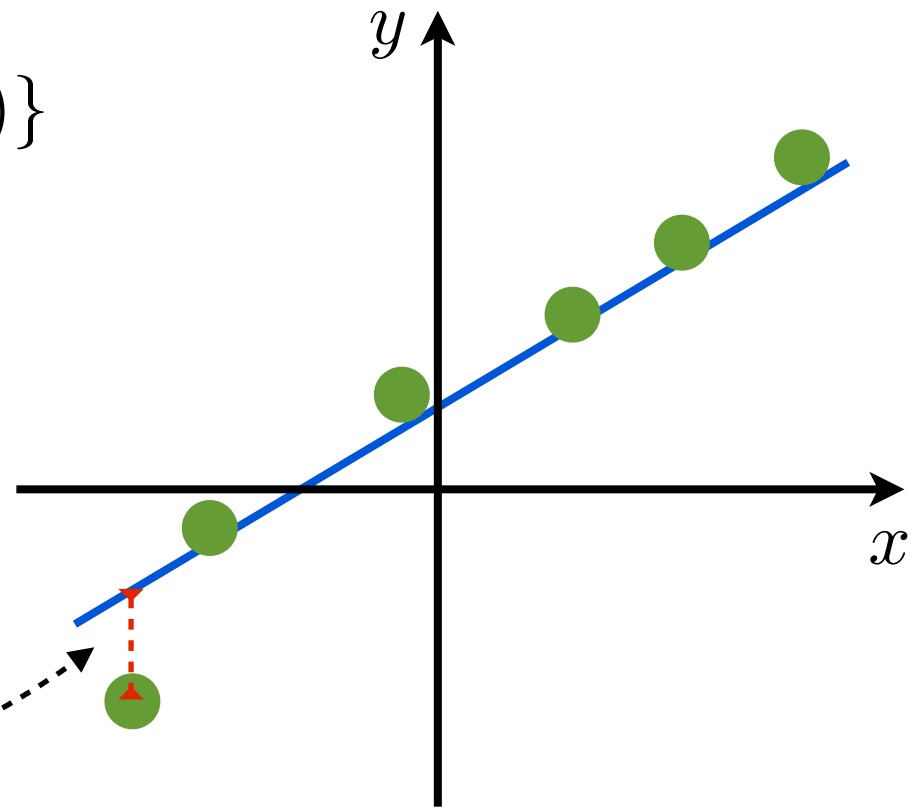
Regression: $y \in \mathbb{R}$

Training data:

$$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), (\mathbf{x}_m, y_m)\}$$

LAD loss:

$$\frac{1}{m} \sum_{i=1}^m |\mathbf{w}^\top \mathbf{x}_i + b - y_i|$$



compare with least square regression:
robust to noise
unstable solution

Regularization



make hypothesis space small

→ better generalization ability

make numerical analysis stable

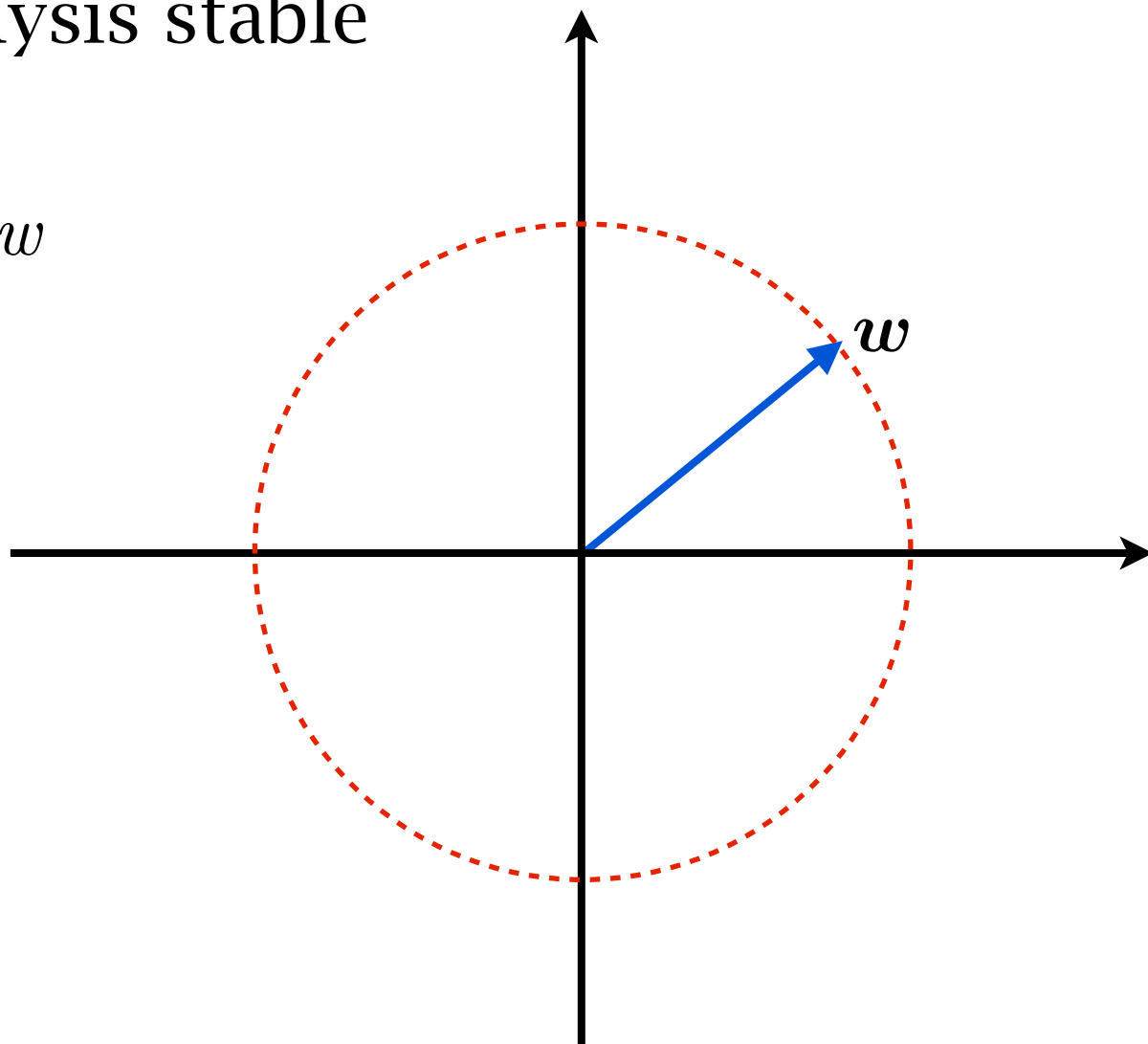
restrict the norm of w

$$\|w\|_p = \left(\sum_{i=1}^n |w_i|^p \right)^{1/p}$$

$$\|w\|_2 = \sqrt{\sum_{i=1}^n w_i^2}$$

$$\|w\|_1 = \sum_{i=1}^n |w_i|$$

$$\|w\|_\infty = \max_{i=1, \dots, n} |w_i|$$



Ridge regression



Regression: $y \in \mathbb{R}$

Training data:

$$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), (\mathbf{x}_m, y_m)\}$$

objective:

$$\arg \min_{\mathbf{w}, b} \frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2 + \lambda \|\mathbf{w}\|_2$$

or:

$$\arg \min_{\mathbf{w}, b} \frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2$$

$$s.t. \quad \|\mathbf{w}\|_2 \leq \theta$$

Ridge regression



centered data, no bias:

$$\arg \min_{\mathbf{w}} \frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i - y_i)^2 + \lambda \|\mathbf{w}\|_2$$

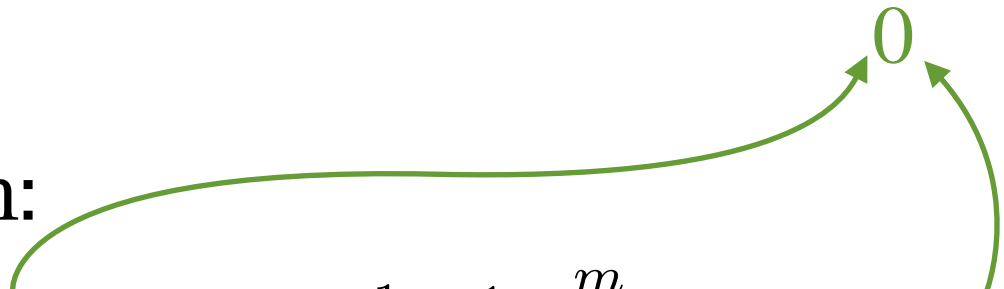
closed form solution:

$$\mathbf{w} = \left(\frac{1}{m} \sum_{i=1}^m \mathbf{x}_i \mathbf{x}_i^\top - \bar{\mathbf{x}} \bar{\mathbf{x}}^\top + \lambda \mathbf{I} \right)^{-1} \left(\frac{1}{m} \sum_{i=1}^m (y_i \mathbf{x}_i) - \bar{y} \bar{\mathbf{x}} \right)$$

$$= (\text{var}(\mathbf{x}) + \lambda \mathbf{I})^{-1} \text{cov}(\mathbf{x}, y)$$

$$= (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{Y}$$

\mathbf{I} is the identity matrix



Least absolute shrinkage and selection operator (LASSO)



Regression: $y \in \mathbb{R}$

Training data:

$$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), (\mathbf{x}_m, y_m)\}$$

objective:

$$\arg \min_{\mathbf{w}, b} \frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2 + \lambda \|\mathbf{w}\|_1$$

or:

$$\arg \min_{\mathbf{w}, b} \frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2$$

$$s.t. \quad \|\mathbf{w}\|_1 \leq \theta$$

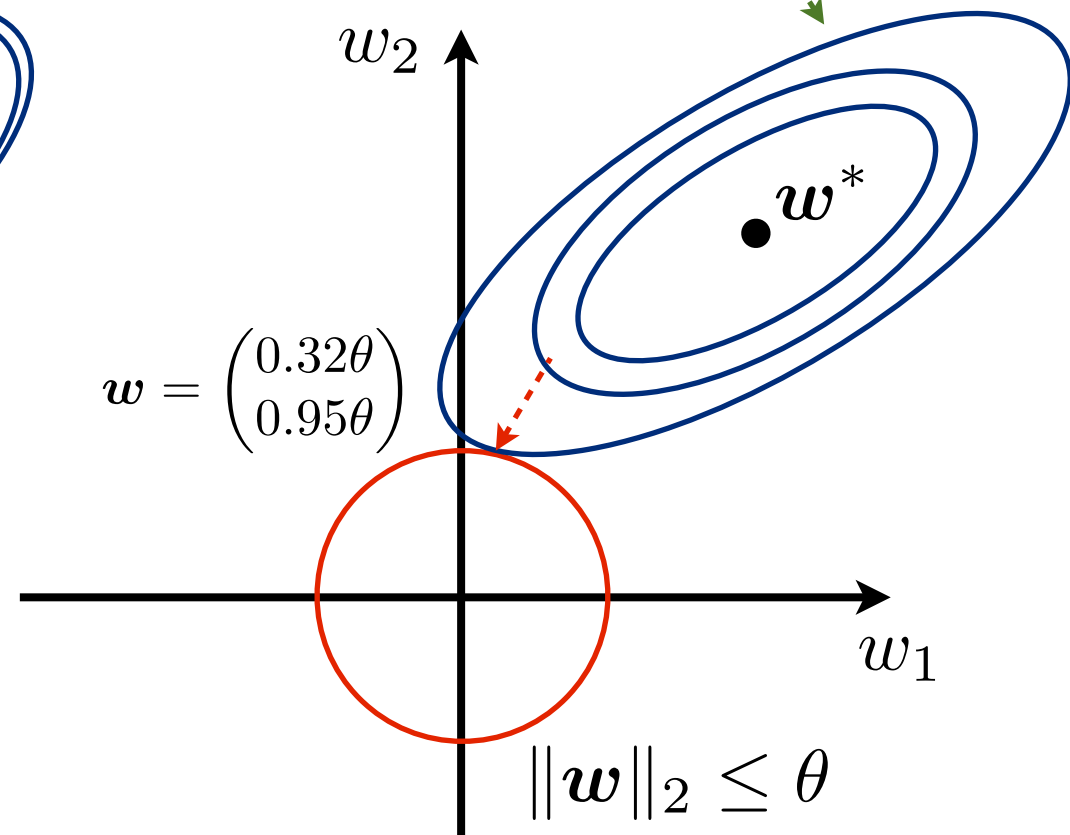
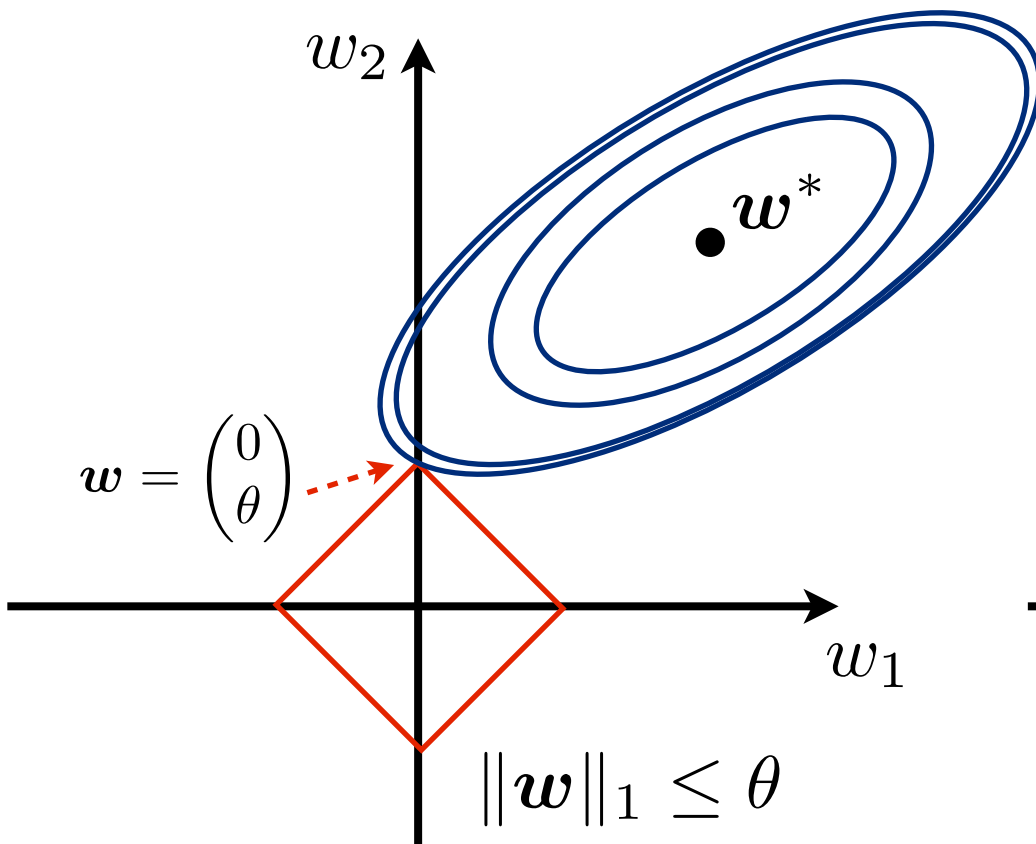
Comparing ridge regression with lasso



L1-norm leads to sparser solution, but worse empirical loss

spare: many zero elements

$$\frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2$$



A general framework



objective function:

$$\arg \min_{\mathbf{w}, b} L(\mathbf{w}, b) + \|\mathbf{w}\|_p$$

general optimization: gradient descent

$$(\mathbf{w}, b)_- = \eta \frac{\partial(L(\mathbf{w}, b) + \|\mathbf{w}\|_p)}{\partial(\mathbf{w}, b)}$$

good for convex objective functions

$$f(\alpha \mathbf{w}_1 + (1 - \alpha) \mathbf{w}_2) \geq \alpha f(\mathbf{w}_1) + (1 - \alpha) f(\mathbf{w}_2)$$

linear, quadratic

convex + convex \rightarrow convex

Linear classifier



model space: \mathbb{R}^{n+1}

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

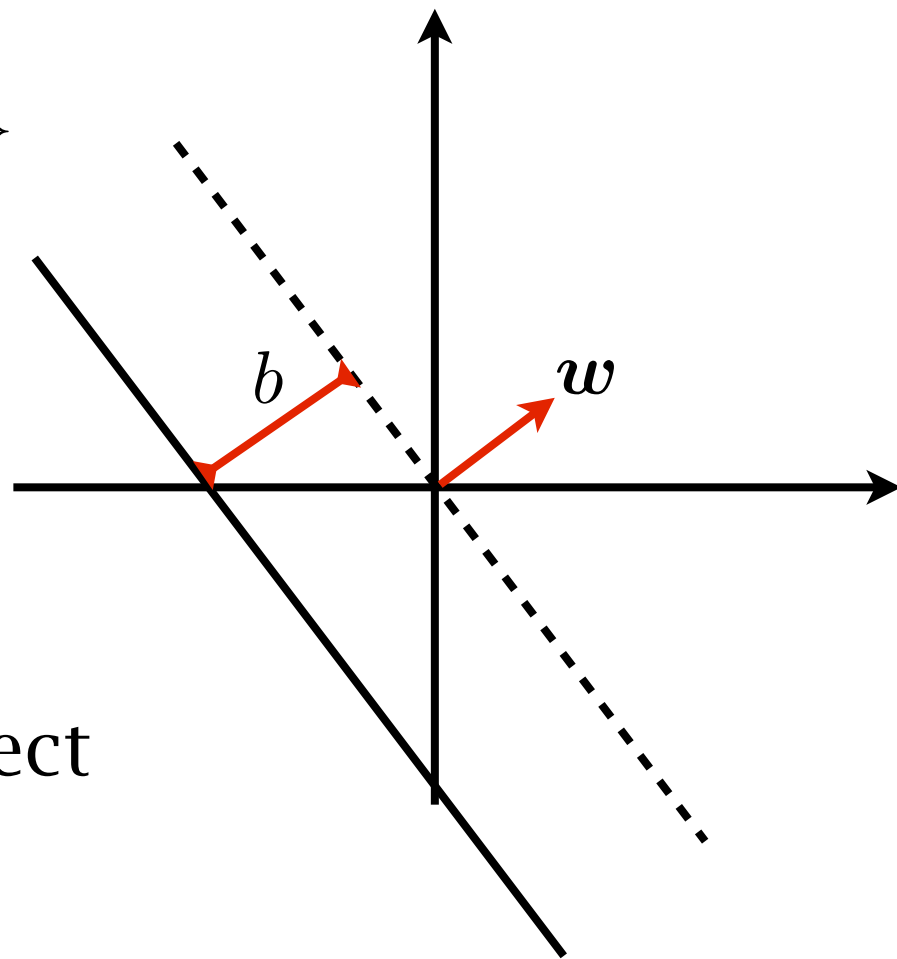
for classification $y \in \{-1, +1\}$

we predict an instance by

$$\text{sign}(\mathbf{w}^\top \mathbf{x} + b) = \begin{cases} +1, & \mathbf{w}^\top \mathbf{x} + b > 0 \\ -1, & \mathbf{w}^\top \mathbf{x} + b < 0 \\ \text{random,} & \text{otherwise} \end{cases}$$

for an example (\mathbf{x}, y) , a correct prediction means

$$y(\mathbf{w}^\top \mathbf{x} + b) > 0$$



Prototype

simple, but too many assumptions

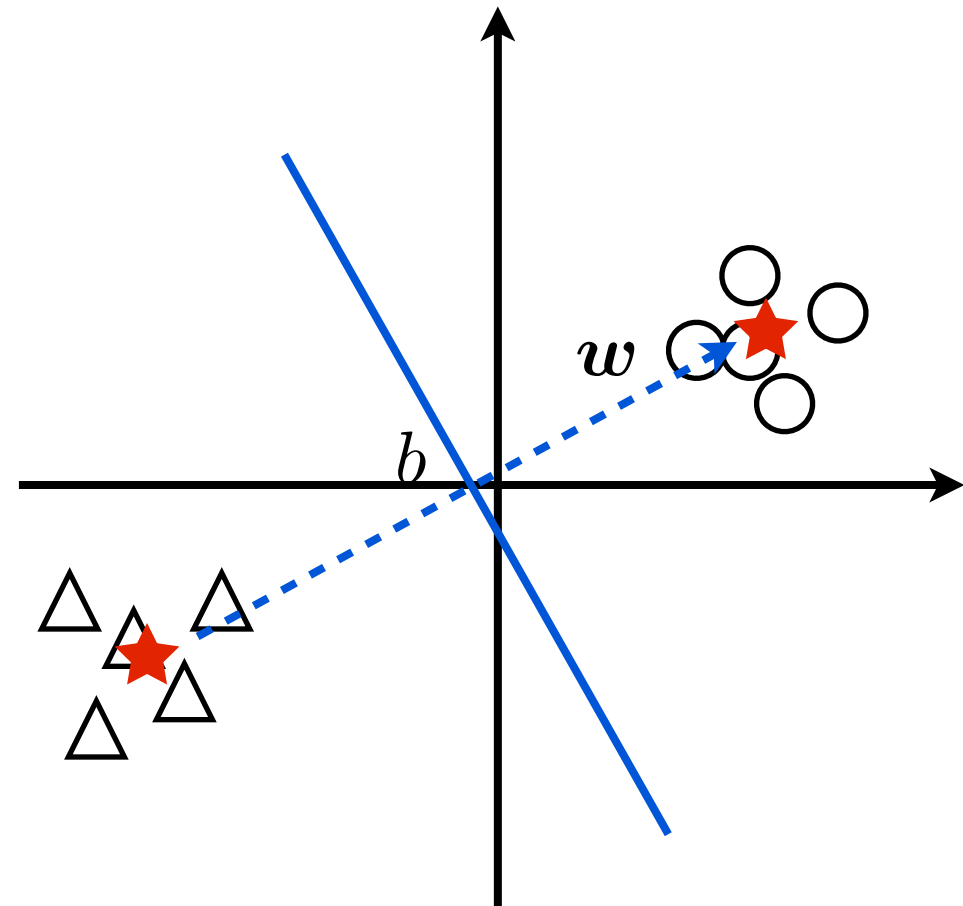


$$\bar{\mathbf{x}}^+ = \frac{1}{\sum_{i:y_i=+1} 1} \sum_{i:y_i=+1} \mathbf{x}_i$$

$$\bar{\mathbf{x}}^- = \frac{1}{\sum_{i:y_i=-1} 1} \sum_{i:y_i=-1} \mathbf{x}_i$$

$$\mathbf{w} = \bar{\mathbf{x}}^+ - \bar{\mathbf{x}}^-$$

$$b = \frac{1}{2} \|\mathbf{w}\|_2$$



Perceptron

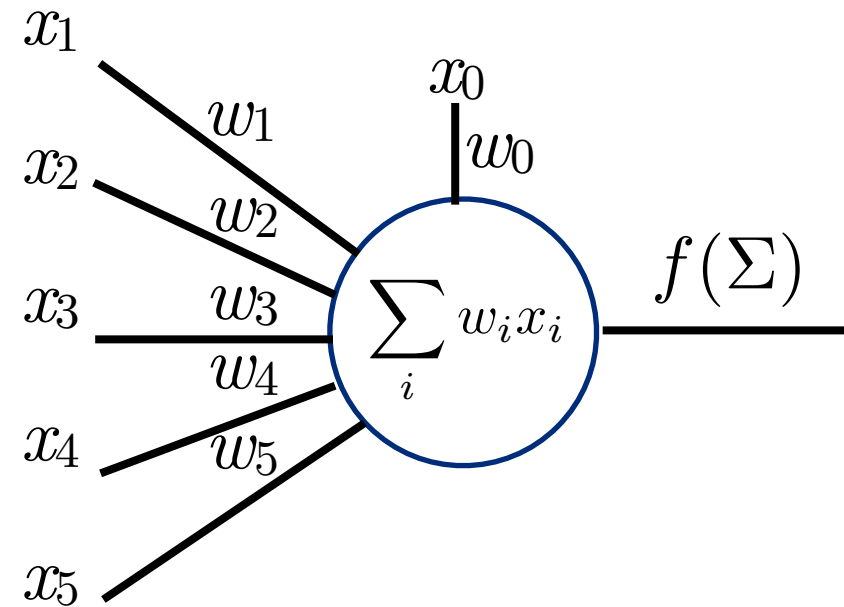


feed training examples one by one

1. $\mathbf{w} = 0$

2. for each example (\mathbf{x}, y)
if $\text{sign}(y\mathbf{w}^\top \mathbf{x}) < 0$

$$\mathbf{w} = \mathbf{w} + y\mathbf{x}$$



$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

Perceptron



feed training examples one by one

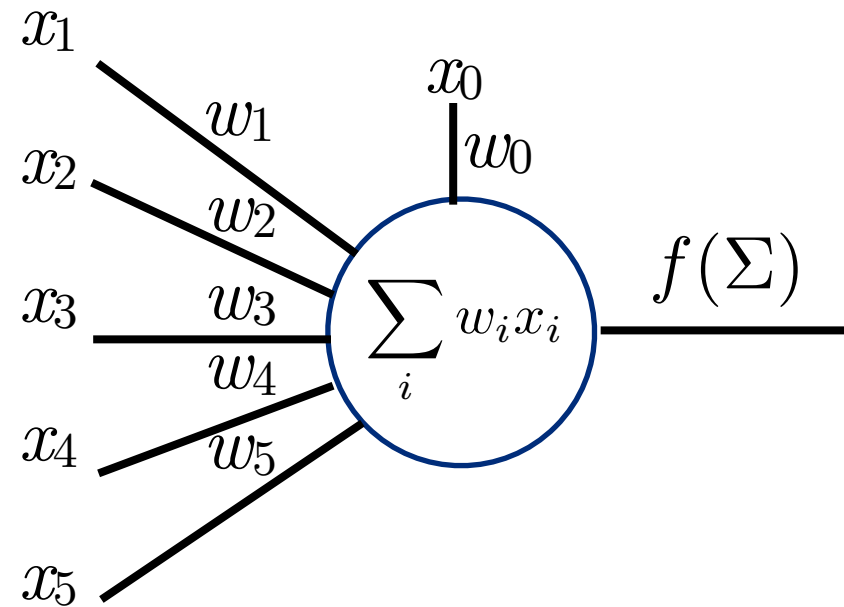
1. $w = 0$

2. for each example (x, y)
if $\text{sign}(y w^\top x) < 0$

$$w = w + yx$$

gradient ascent

$$\frac{\partial y w^\top x}{\partial w} = yx$$



$$f(x) = w^\top x + b$$

Perceptron



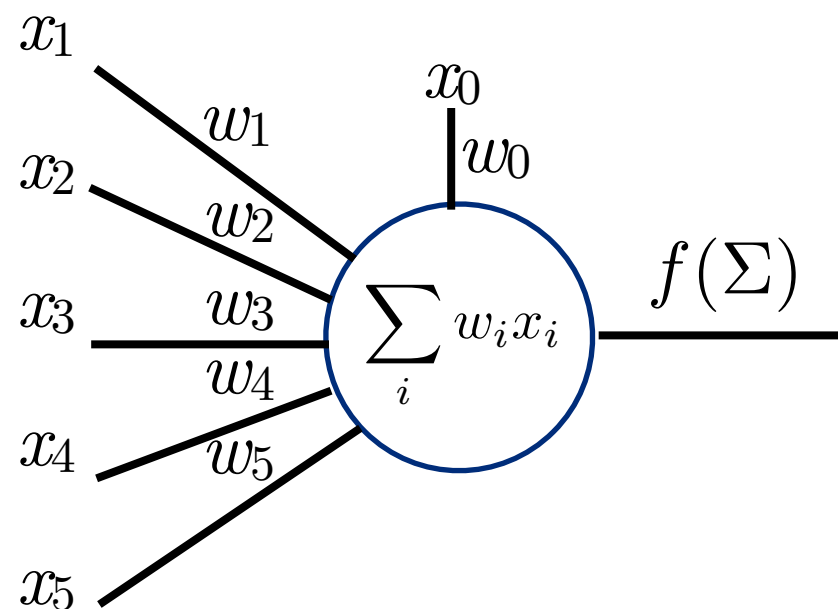
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1. $\mathbf{w} = 0$
2. for each example (\mathbf{x}, y)
if $\text{sign}(y\mathbf{w}^\top \mathbf{x}) < 0$

$$\mathbf{w} = \mathbf{w} + y\mathbf{x}$$

gradient ascent

$$\frac{\partial y\mathbf{w}^\top \mathbf{x}}{\partial \mathbf{w}} = y\mathbf{x}$$



$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

when all examples are with length 1 and are linearly separable by \mathbf{w}^* , perceptron algorithm makes at most $\left(1 / \min_{\mathbf{x}} \frac{|\mathbf{w}^{*\top} \mathbf{x}|}{\|\mathbf{x}\|_2}\right)^2$ mistakes

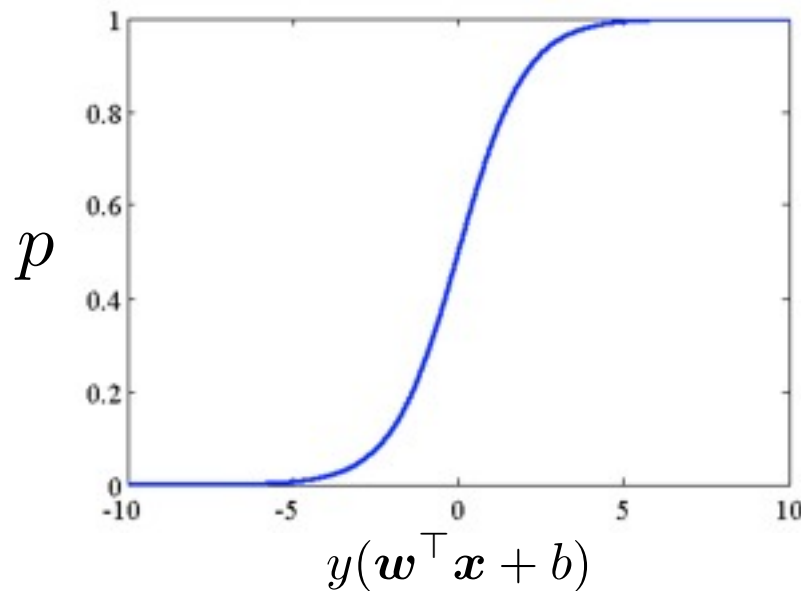
Logistic regression



assume logit model: for a positive example

$$\mathbf{w}^\top \mathbf{x} = \log \frac{p(+1 | \mathbf{x})}{1 - p(+1 | \mathbf{x})}$$

so that $p(y | \mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-y(\mathbf{w}^\top \mathbf{x})}}$



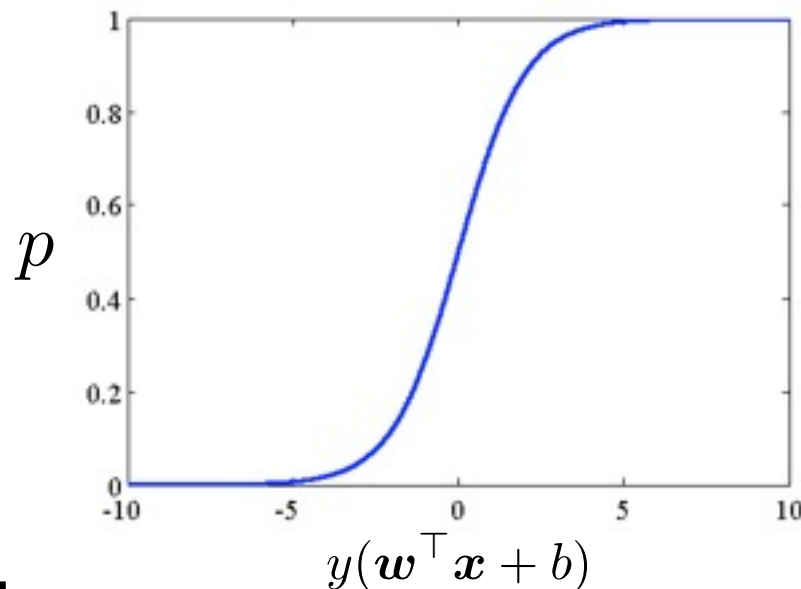
Logistic regression



assume logit model: for a positive example

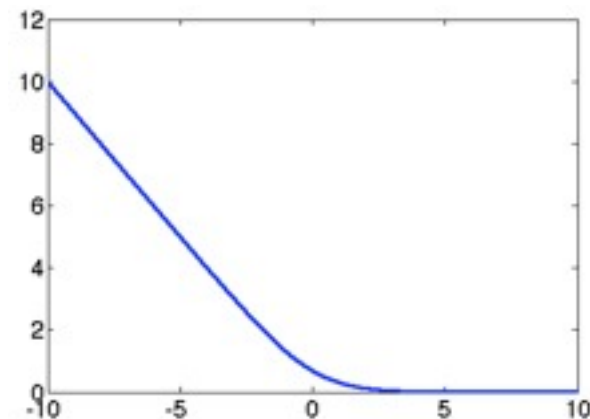
$$\mathbf{w}^\top \mathbf{x} = \log \frac{p(+1 | \mathbf{x})}{1 - p(+1 | \mathbf{x})}$$

$$\text{so that } p(y | \mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-y(\mathbf{w}^\top \mathbf{x})}}$$



minimize negative log-likelihood:

$$\begin{aligned} \arg \min_{\mathbf{w}, b} -\log \prod_{i=1}^m p(y_i | \mathbf{x}_i, \mathbf{w}) &= -\sum_i \log p(y_i | \mathbf{x}_i, \mathbf{w}) \\ &= \sum_i \log \left(1 + e^{-y_i(\mathbf{w}^\top \mathbf{x}_i)} \right) \end{aligned}$$



Logistic regression



Maximize a posterior (minimize negative a posterior)

$$\arg \min_{\mathbf{w}, b} - \log \left(\prod_{i=1}^m p(y_i | \mathbf{x}_i, \mathbf{w}) \right) p(\mathbf{w})$$

a prior: $\mathbf{w} \sim \mathcal{N}(0, \delta \mathbf{I})$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; 0, \delta \mathbf{I}) = \frac{1}{\delta \sqrt{2\pi}} e^{-\frac{\|\mathbf{w}-0\|_2^2}{2\delta^2}}$$

$$= - \sum_i \log p(y_i | \mathbf{x}_i, \mathbf{w}) - \log p(\mathbf{w})$$

$$= \sum_i \log \left(1 + e^{-y_i (\mathbf{w}^\top \mathbf{x}_i)} \right) + \frac{1}{2\delta^2} \|\mathbf{w}\|_2^2 + \text{const}$$

Logistic regression



Maximize a posterior (minimize negative a posterior)

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convex

regularized logistic regression

Linear classifier revisit



model space: \mathbb{R}^{n+1}

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

for classification $y \in \{-1, +1\}$

Original objective:

$$\arg \min_{\mathbf{w}, b} \sum_i I(y(\mathbf{w}^\top \mathbf{x}_i + b) \leq 0)$$

0-1 loss
hard to optimize

Surrogate objective:

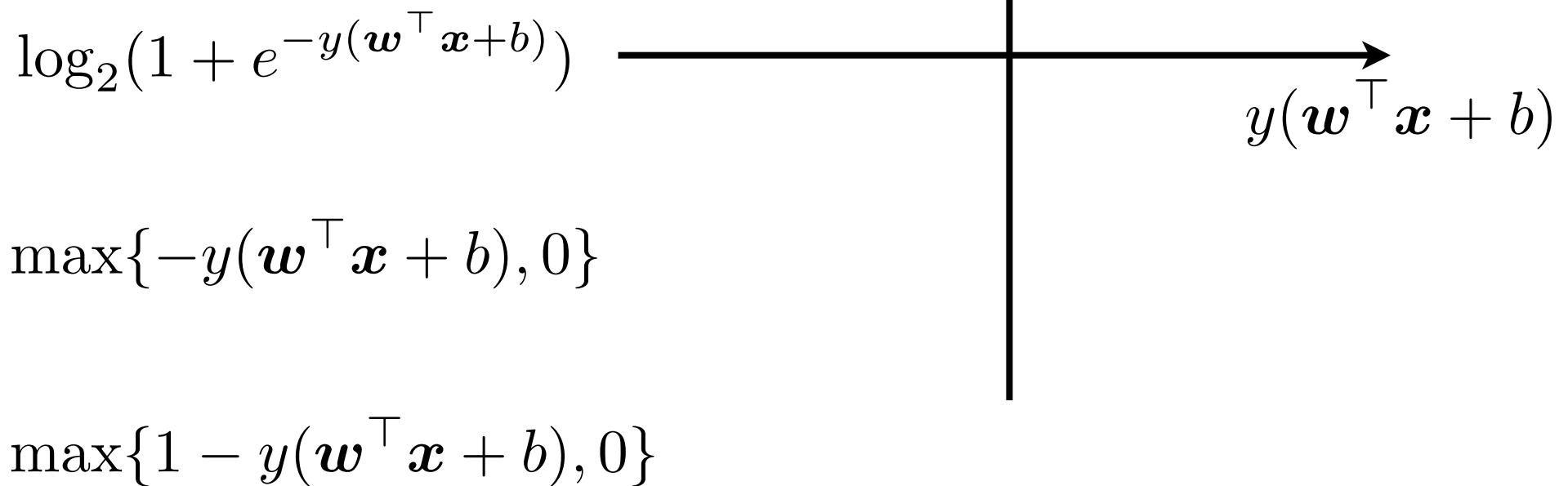
$$\arg \min_{\mathbf{w}, b} \sum_i \log \left(1 + e^{-y_i(\mathbf{w}^\top \mathbf{x}_i + b)} \right)$$

logistic regression

$$\arg \min_{\mathbf{w}, b} \sum_i \max\{-y_i(\mathbf{w}^\top \mathbf{x}_i + b), 0\}$$

perceptron

Linear classifier revisit



Linear classifier revisit



0-1 loss

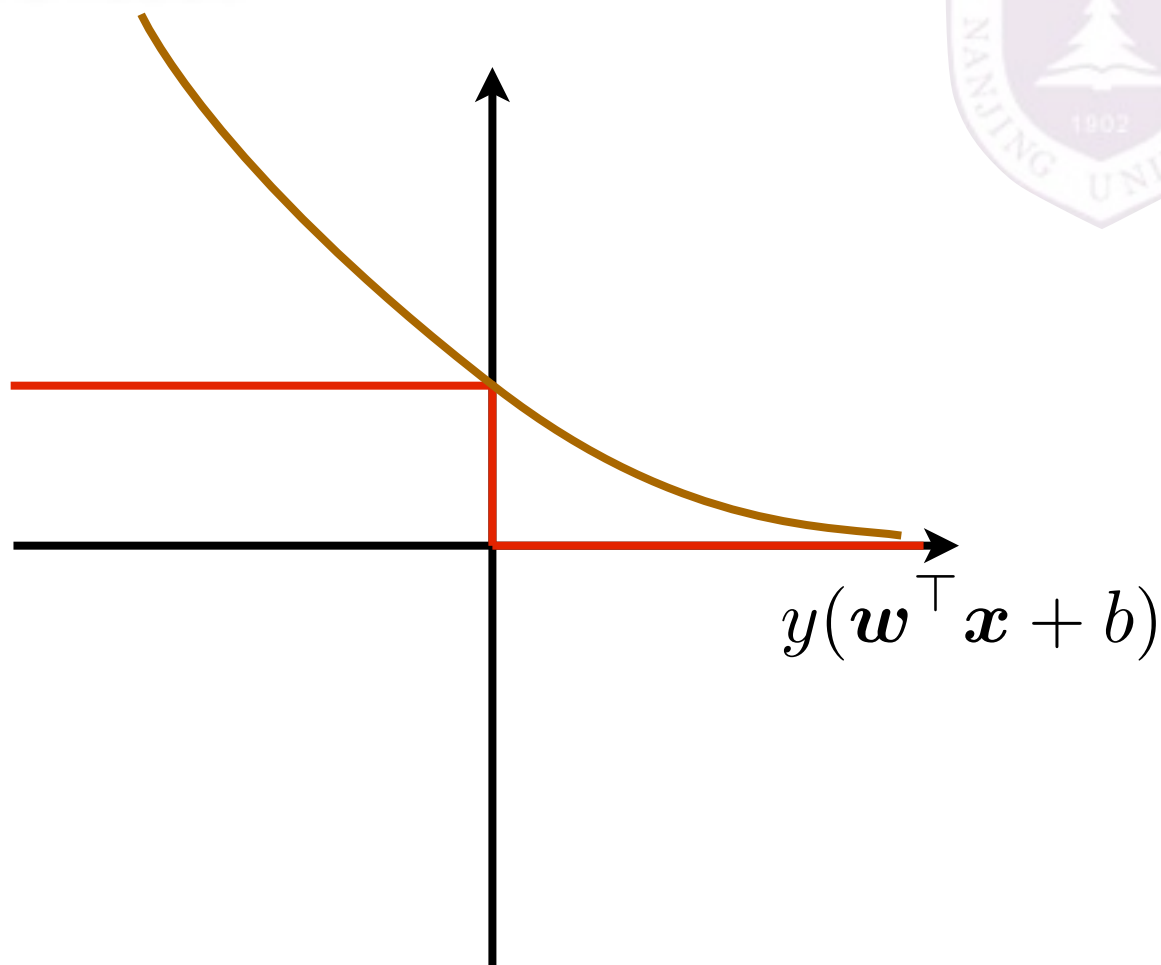
$$I(y(\mathbf{w}^\top \mathbf{x} + b) \leq 0)$$

logistic regression

$$\log_2(1 + e^{-y(\mathbf{w}^\top \mathbf{x} + b)})$$

$$\max\{-y(\mathbf{w}^\top \mathbf{x} + b), 0\}$$

$$\max\{1 - y(\mathbf{w}^\top \mathbf{x} + b), 0\}$$



Linear classifier revisit



0-1 loss

$$I(y(\mathbf{w}^\top \mathbf{x} + b) \leq 0)$$

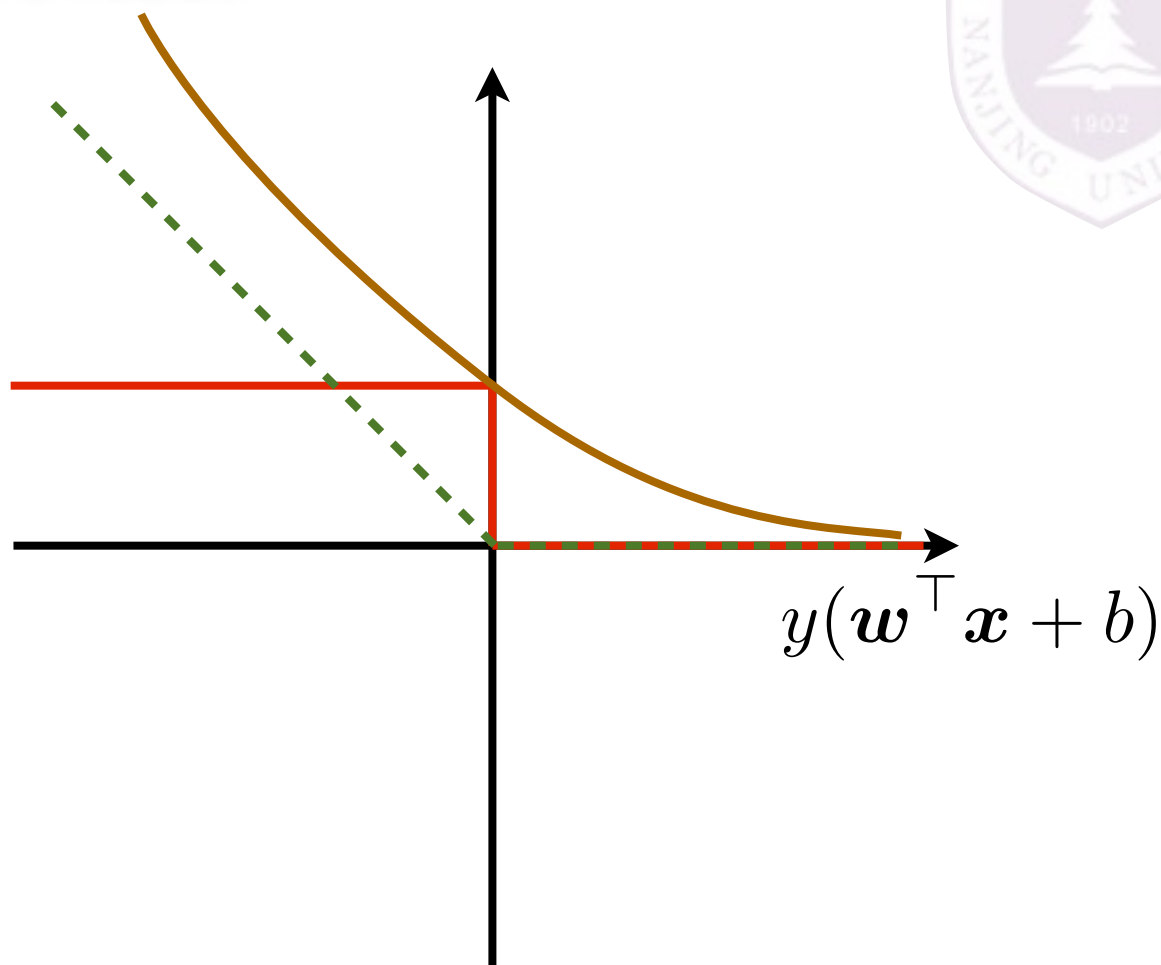
logistic regression

$$\log_2(1 + e^{-y(\mathbf{w}^\top \mathbf{x} + b)})$$

perceptron

$$\max\{-y(\mathbf{w}^\top \mathbf{x} + b), 0\}$$

$$\max\{1 - y(\mathbf{w}^\top \mathbf{x} + b), 0\}$$



Linear classifier revisit



0-1 loss

$$I(y(\mathbf{w}^\top \mathbf{x} + b) \leq 0)$$

logistic regression

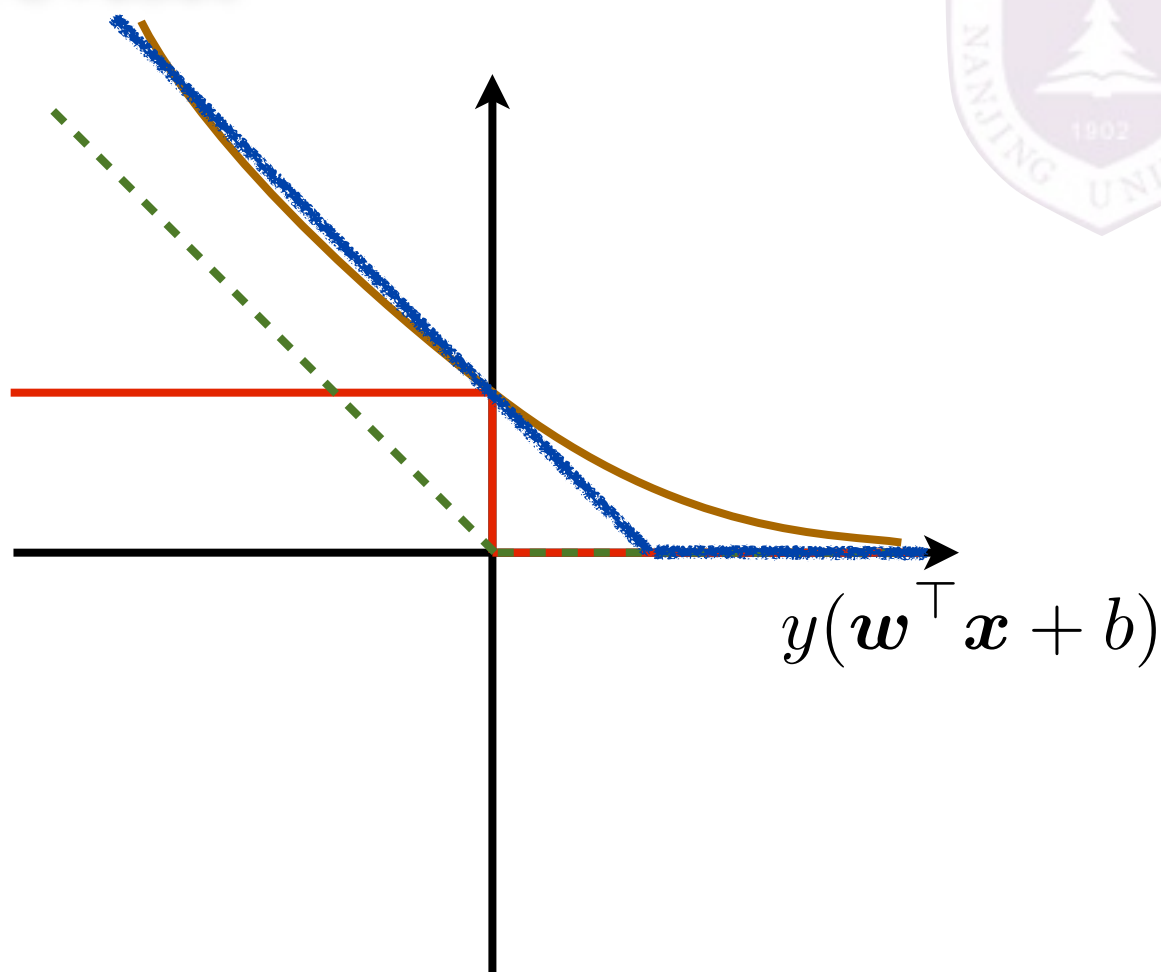
$$\log_2(1 + e^{-y(\mathbf{w}^\top \mathbf{x} + b)})$$

perceptron

$$\max\{-y(\mathbf{w}^\top \mathbf{x} + b), 0\}$$

hinge loss

$$\max\{1 - y(\mathbf{w}^\top \mathbf{x} + b), 0\}$$



Support vector machines (SVM)



hinge loss + L2-norm

$$\arg \min_{\mathbf{w}, b} \sum_i \max(1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b), 0) + \lambda \|\mathbf{w}\|_2$$

Support vector machines (SVM)



hinge loss + L2-norm

$$\arg \min_{\mathbf{w}, b} \sum_i \max(1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b), 0) + \lambda \|\mathbf{w}\|_2$$

$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2 + C \sum_i \xi_i$$

$$\begin{aligned} s.t. \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \\ & \xi_i \geq 0 \end{aligned}$$

$$\begin{aligned} \max(1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b), 0) &= \xi_i \\ \xi_i &\geq 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b) \\ \xi_i &\geq 0 \end{aligned}$$

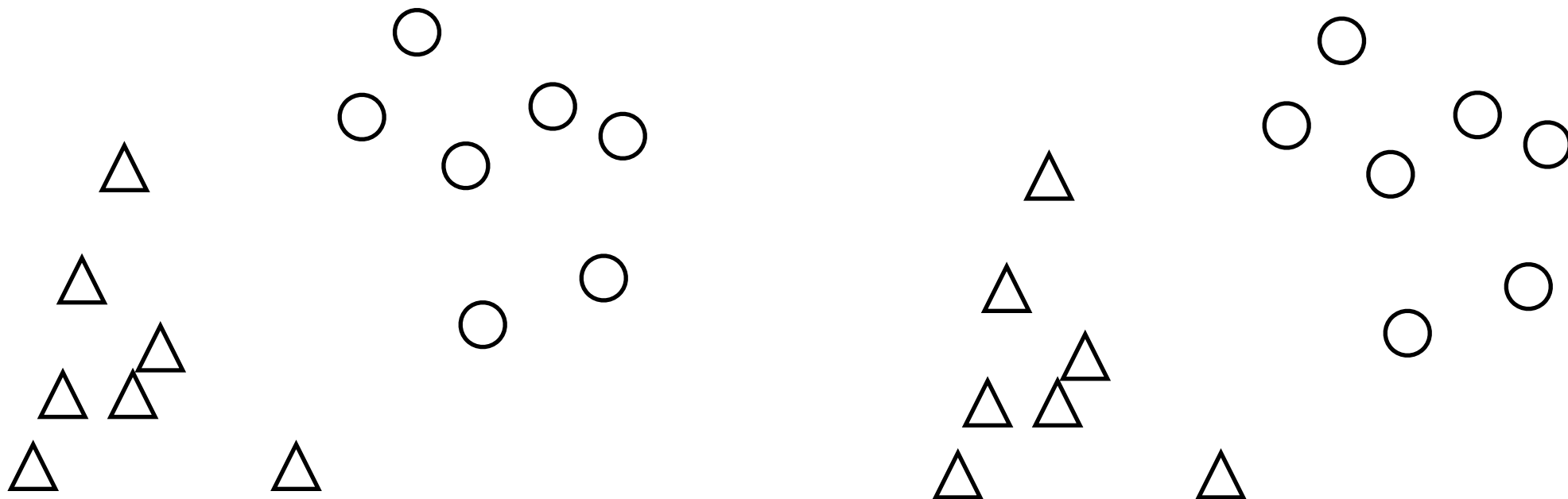
quadratic

Support vector machines (SVM)



$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2 + C \sum_i \xi_i$$

$$s.t. \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \\ \xi_i \geq 0$$

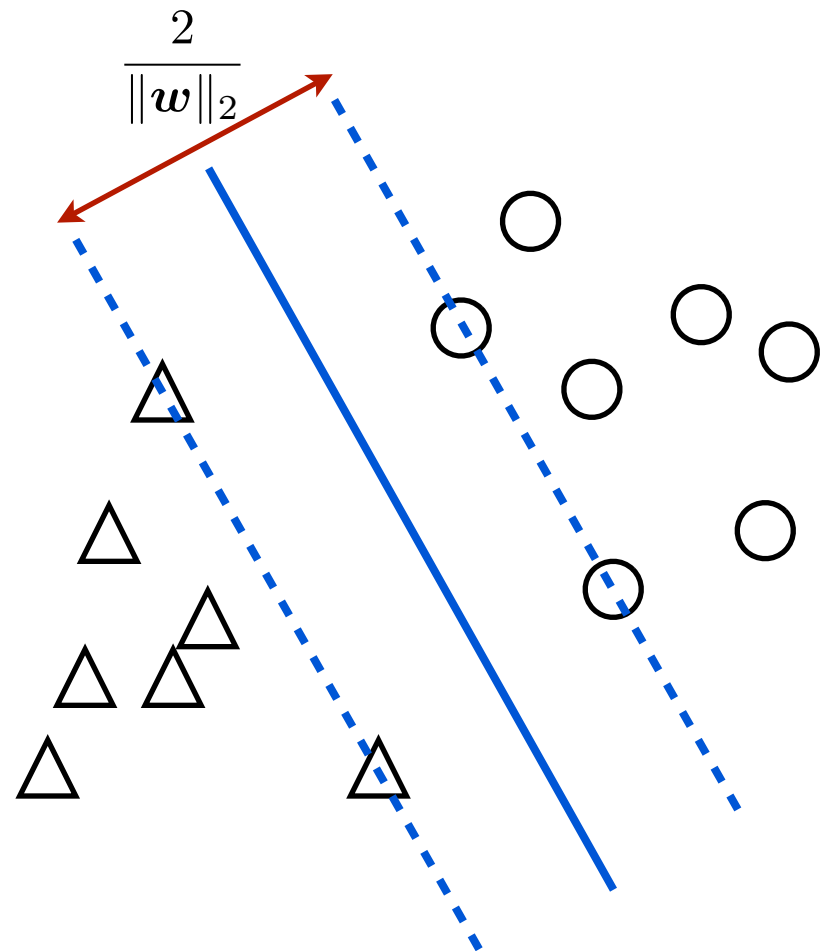
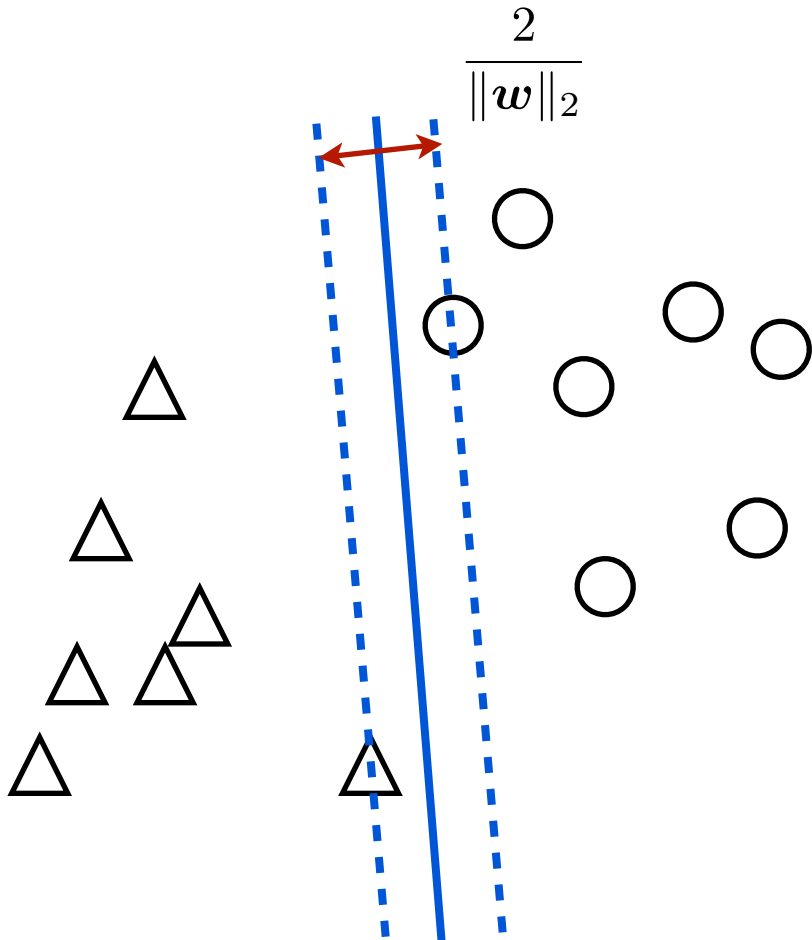


Support vector machines (SVM)



$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2 + C \sum_i \xi_i$$

$$\begin{aligned} \text{s.t.} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \\ & \xi_i \geq 0 \end{aligned}$$

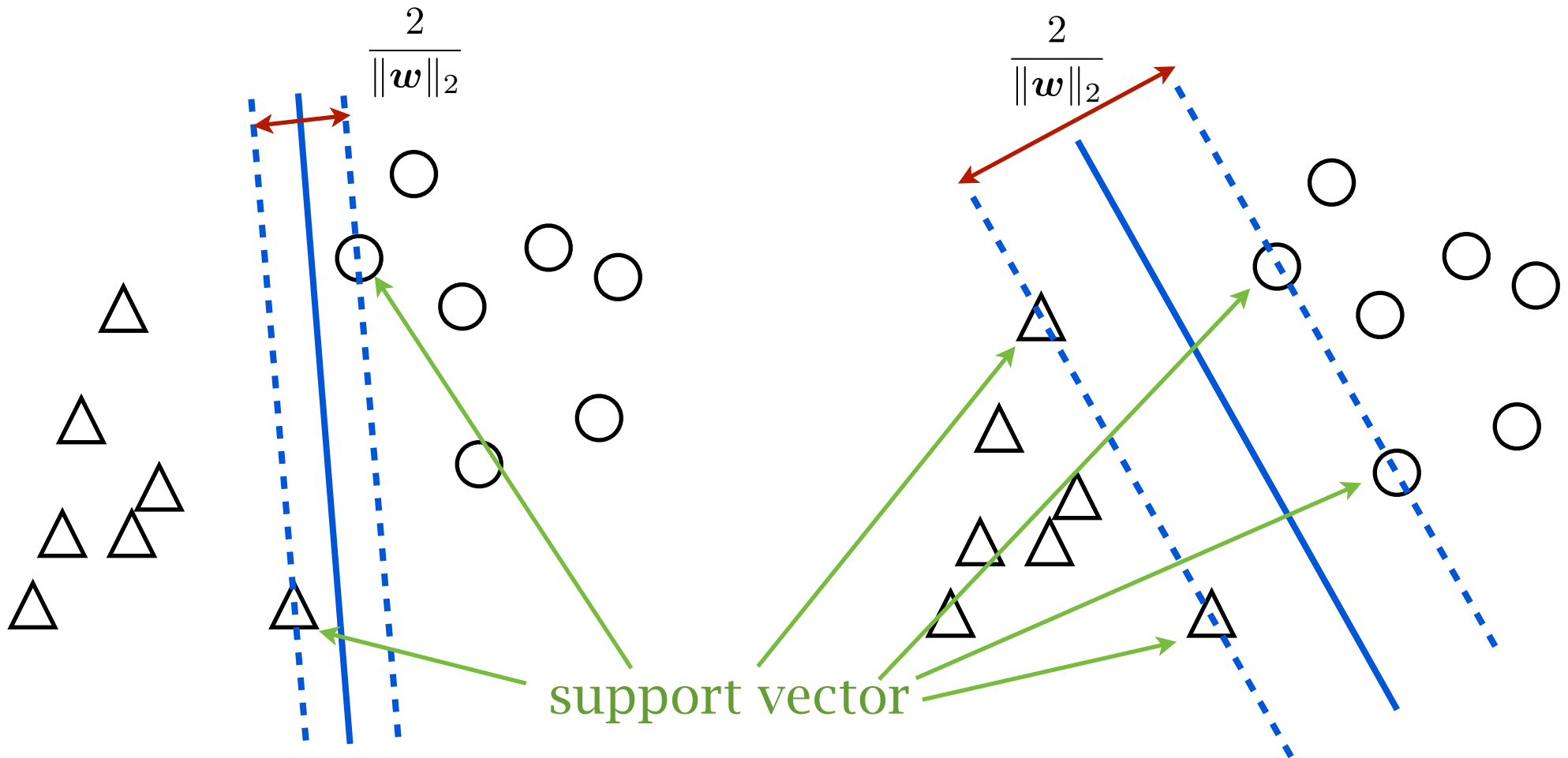


Support vector machines (SVM)



$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2 + C \sum_i \xi_i$$

$$s.t. \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \\ \xi_i \geq 0$$

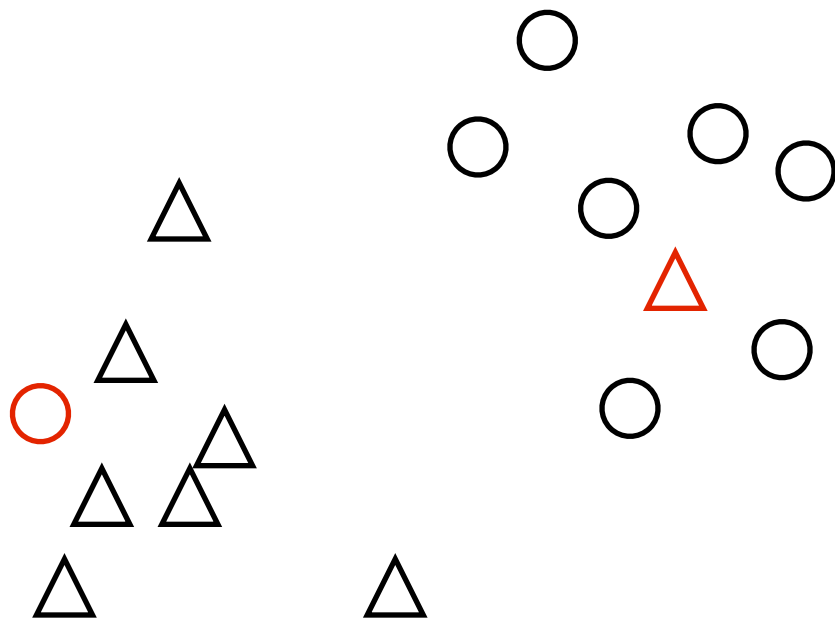


Support vector machines (SVM)



$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2 + C \sum_i \xi_i$$

$$s.t. \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \\ \xi_i \geq 0$$

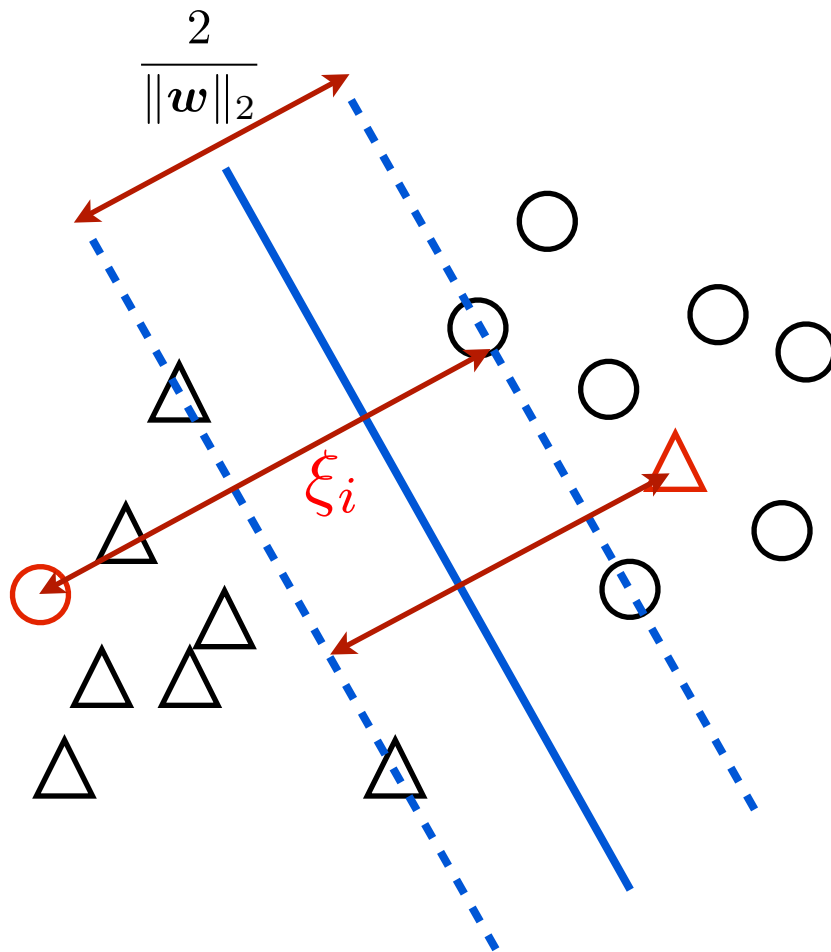


Support vector machines (SVM)



$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2 + C \sum_i \xi_i$$

$$s.t. \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \\ \xi_i \geq 0$$



slack variables

Scoring functions



$$\frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2 \quad \text{least square regression}$$

$$\frac{1}{m} \sum_{i=1}^m |\mathbf{w}^\top \mathbf{x}_i + b - y_i| \quad \text{LAD regression}$$

$$\frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2 + \lambda \|\mathbf{w}\|_2 \quad \text{ridge regression}$$

$$\frac{1}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i + b - y_i)^2 + \lambda \|\mathbf{w}\|_1 \quad \text{LASSO}$$

Scoring functions



$$\sum_i I(y(\mathbf{w}^\top \mathbf{x} + b) > 0)$$

0-1 loss

$$\sum_i \max\{-y_i(\mathbf{w}^\top \mathbf{x}_i + b), 0\}$$

perceptron

$$\sum_i \log\left(1 + e^{-y_i(\mathbf{w}^\top \mathbf{x}_i + b)}\right)$$

logistic regression

$$\sum_i \log\left(1 + e^{-y_i(\mathbf{w}^\top \mathbf{x}_i + b)}\right) + \lambda \|\mathbf{w}\|_2$$

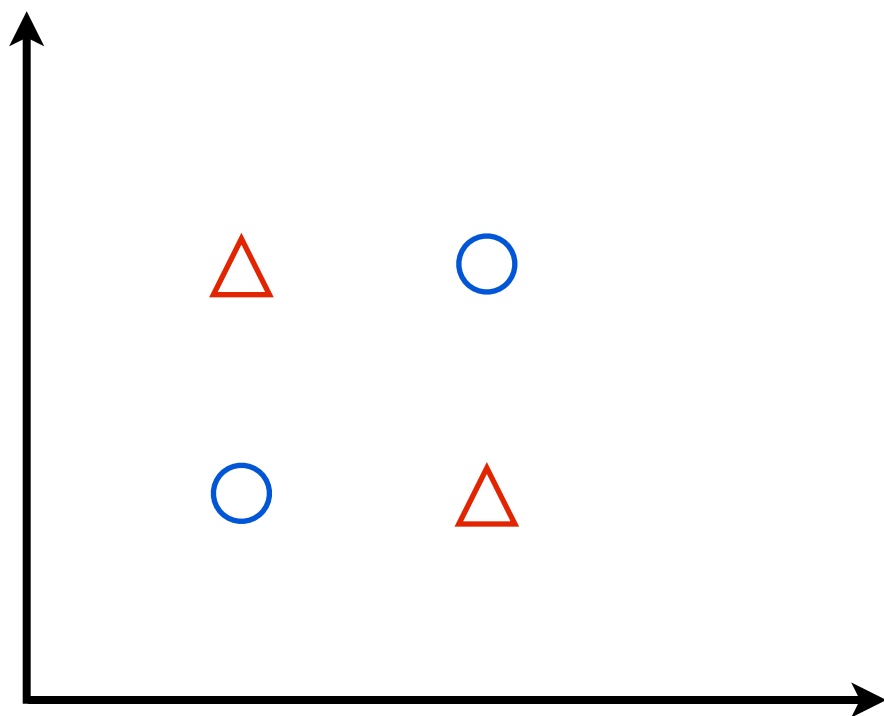
regularized LR

$$\sum_i \max(1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b), 0) + \lambda \|\mathbf{w}\|_2$$

SVM

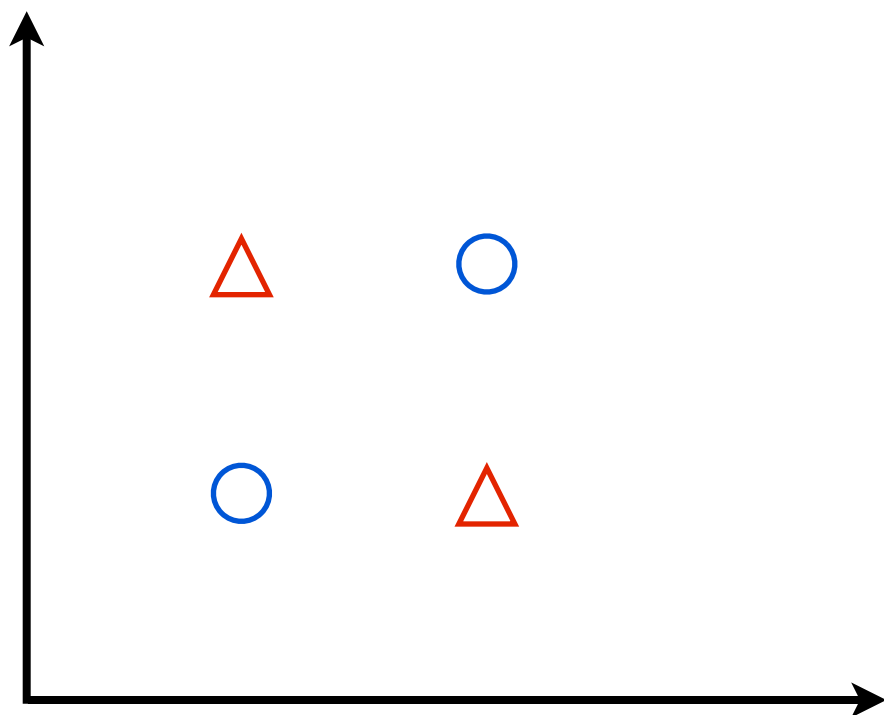
minimize loss + regularization

Linearity v.s. dimensionality

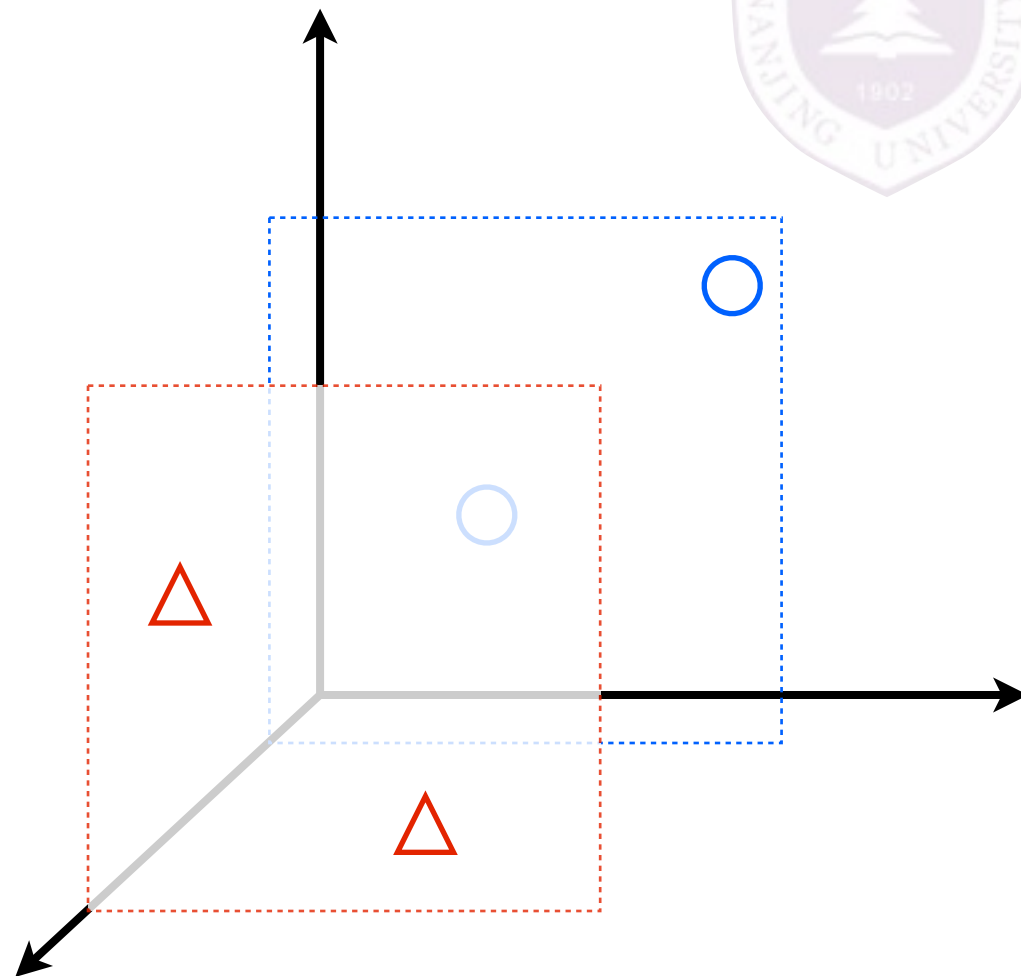


XOR in 2D

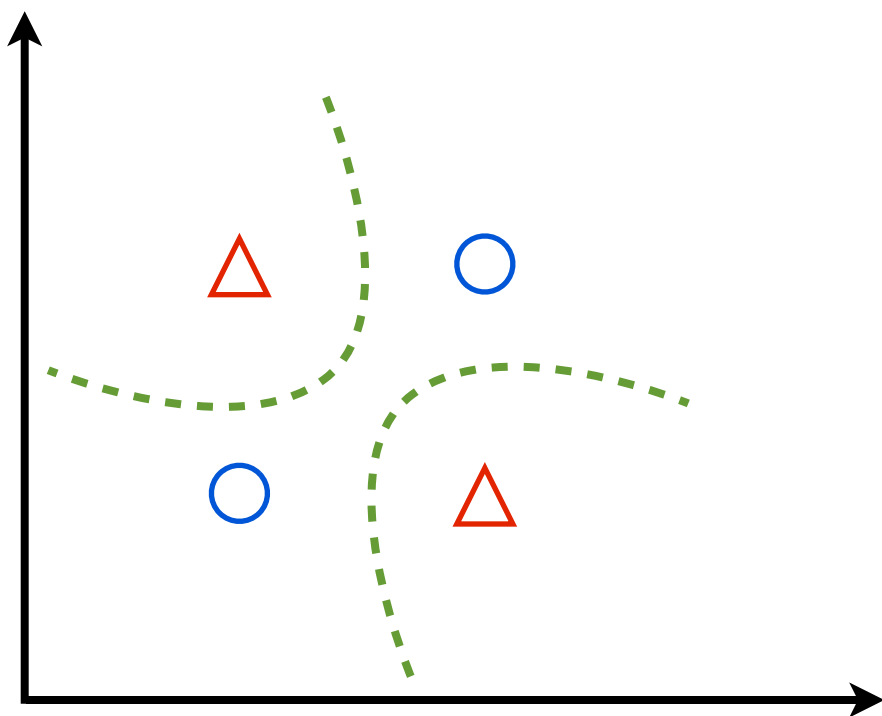
Linearity v.s. dimensionality



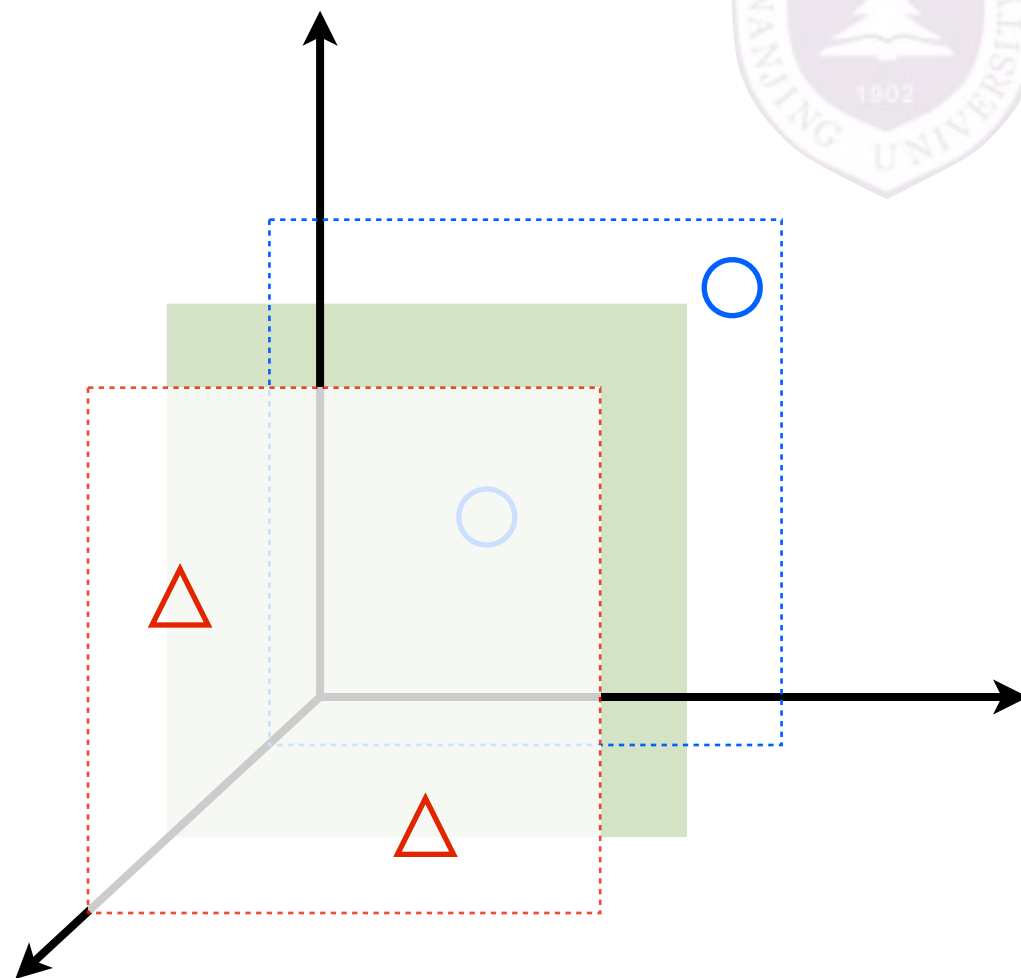
XOR in 2D



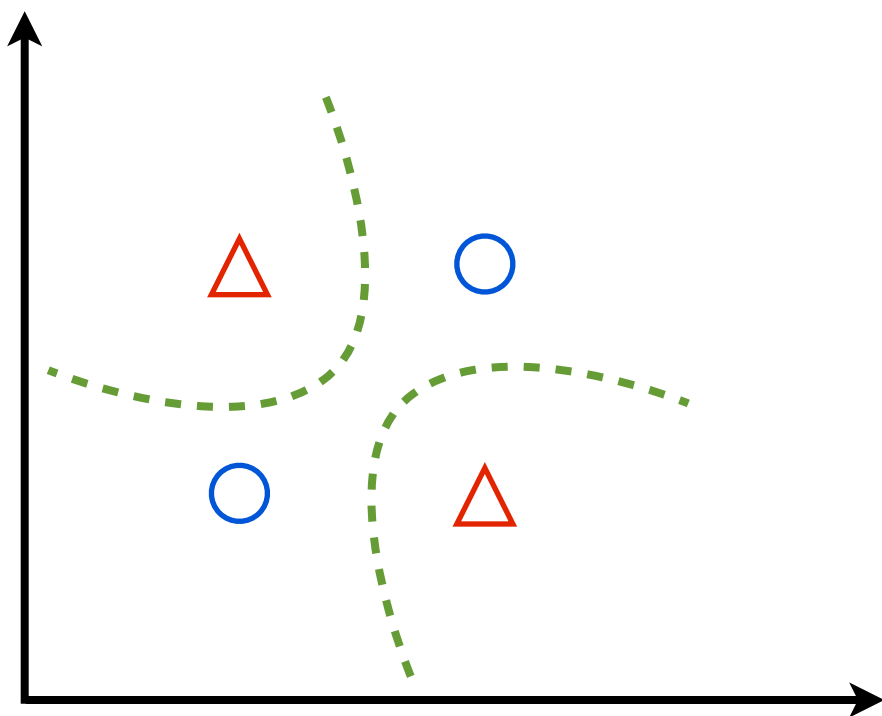
Linearity v.s. dimensionality



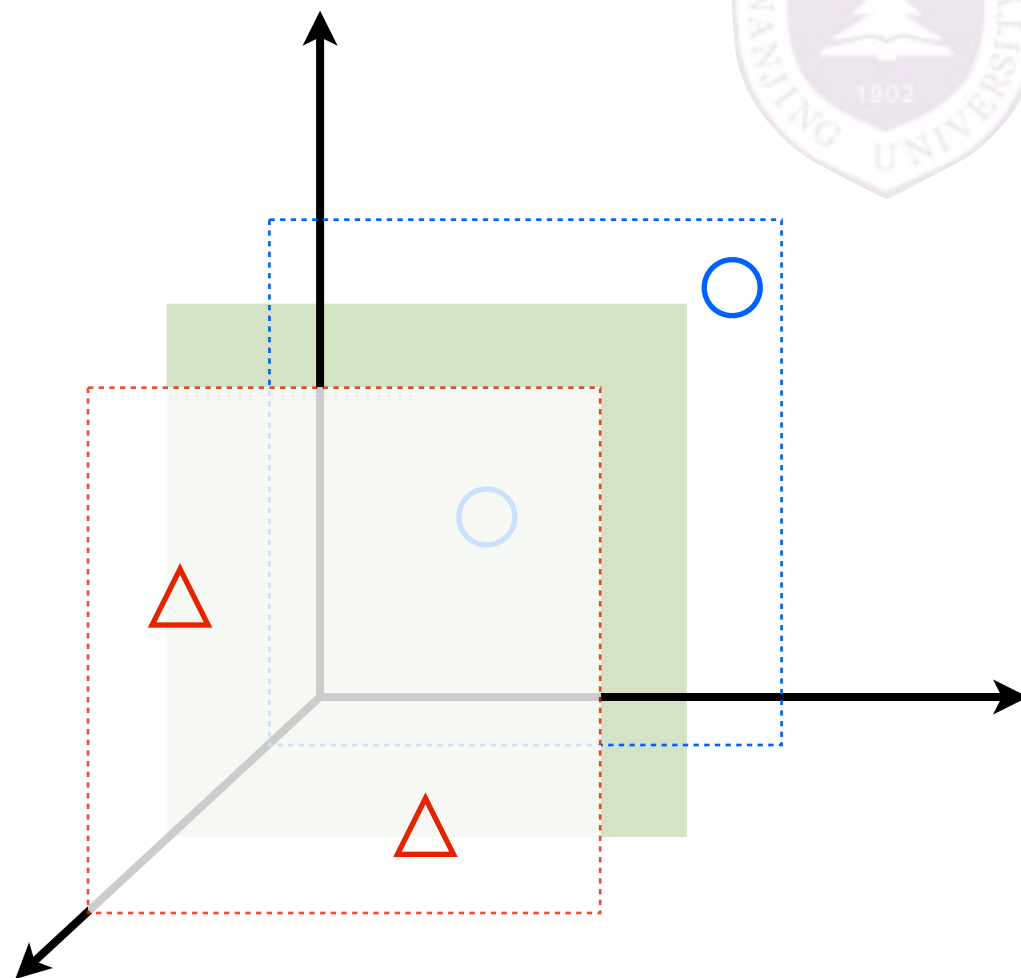
XOR in 2D



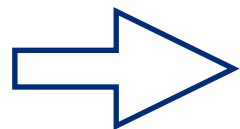
Linearity v.s. dimensionality



XOR in 2D



| x_1 | x_2 | y |
|-------|-------|-----|
| 0 | 0 | +1 |
| 0 | 1 | -1 |
| 1 | 0 | -1 |
| 1 | 1 | +1 |



| x_1 | x_2 | x_1x_2 | y |
|-------|-------|----------|-----|
| 0 | 0 | 0 | +1 |
| 0 | 1 | 0 | -1 |
| 1 | 0 | 0 | -1 |
| 1 | 1 | 1 | +1 |

$$w = \begin{pmatrix} -1 \\ -1 \\ 2 \end{pmatrix}, b = -0.5$$

Representer theorem



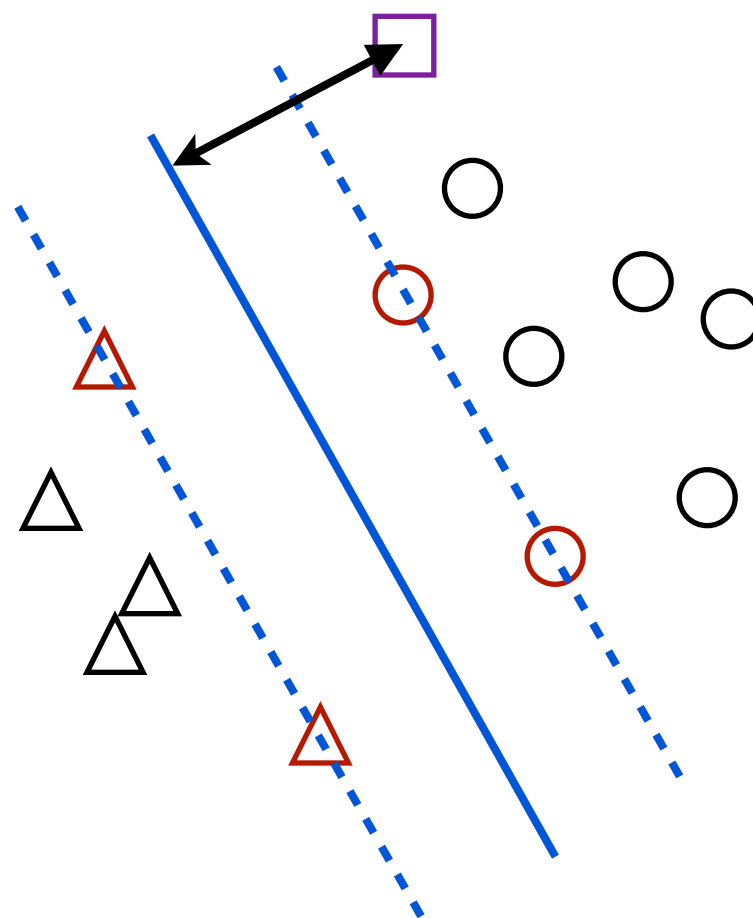
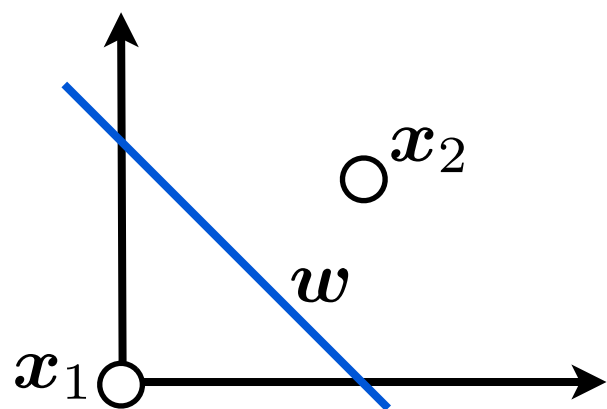
$$w = \sum_i \alpha_i x_i$$

$$w^\top z = \sum_i \alpha_i x_i^\top z$$

e.g.:

$$w = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad x_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad x_2 = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$$

$$w = 0.5x_1 + 0.5x_2$$



Representer theorem



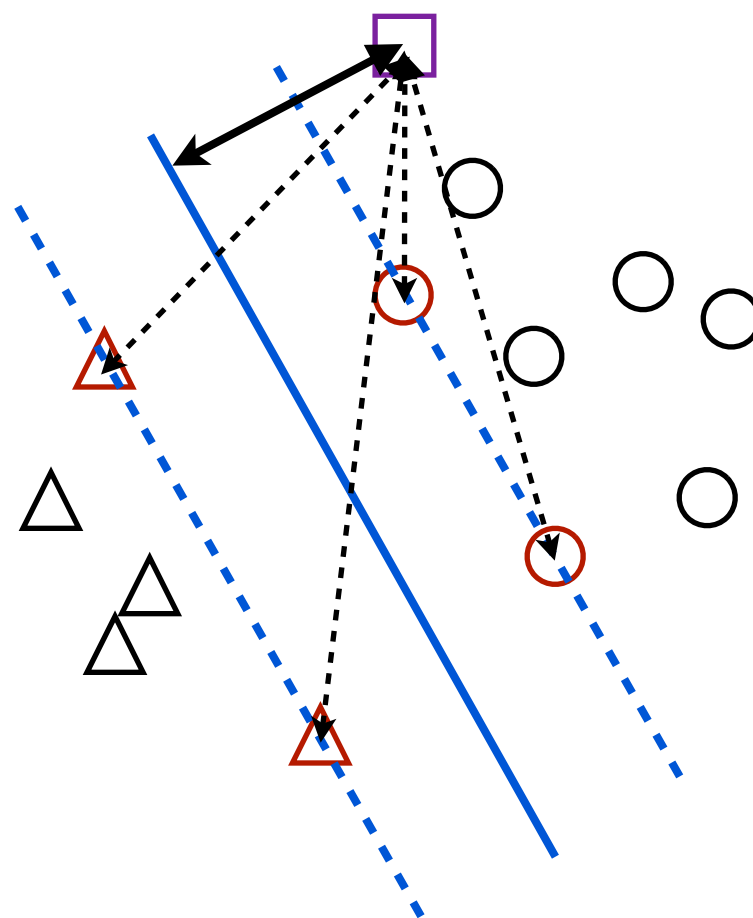
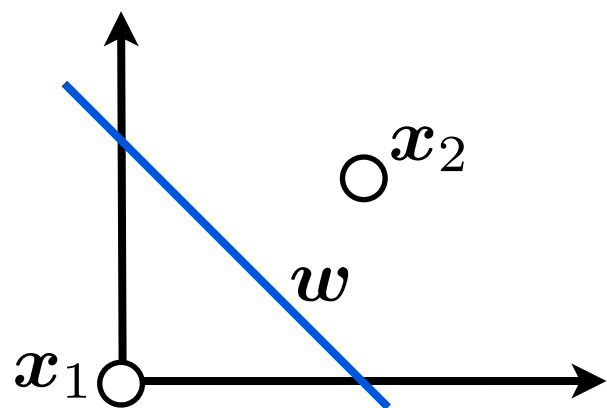
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support vectors



Kernelization

inner product by kernel distance

$$K(\mathbf{x}_1, \mathbf{x}_2) = \langle \phi(\mathbf{x}_1), \phi(\mathbf{x}_2) \rangle$$

polynomial $K(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1^\top \mathbf{x}_2)^n$

Gaussian radial basis $K(\mathbf{x}_1, \mathbf{x}_2) = e^{-\frac{\|\mathbf{x}_1 - \mathbf{x}_2\|_2^2}{\delta^2}}$

e.g. $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ $\mathbf{x}' = \begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix}$ $\phi(\mathbf{x}) = \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix}$

explicit inner product in higher dimension space:

$$\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle = x_1^2x'^2_1 + x_2^2x'^2_2 + 2x_1x_2x'_1x'_2$$

kernel function of the inner product in original space:

$$K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}')^2 = (x_1x'_1 + x_2x'_2)^2$$

$$= x_1^2x'^2_1 + x_2^2x'^2_2 + 2x_1x_2x'_1x'_2$$

equal

this is easier to calculate

Kernelization



inner product by kernel distance

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Kernelization



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linear model in mapped feature space

$$\begin{aligned} f(\mathbf{x}) &= \mathbf{w}^\top \phi(\mathbf{x}) = \sum_i \alpha_i \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}) \rangle \\ &= \sum_i \alpha_i K(\mathbf{x}_i, \mathbf{x}) \end{aligned}$$

Kernelization



inner product by kernel distance

$$K(\mathbf{x}_1, \mathbf{x}_2) = \langle \phi(\mathbf{x}_1), \phi(\mathbf{x}_2) \rangle$$

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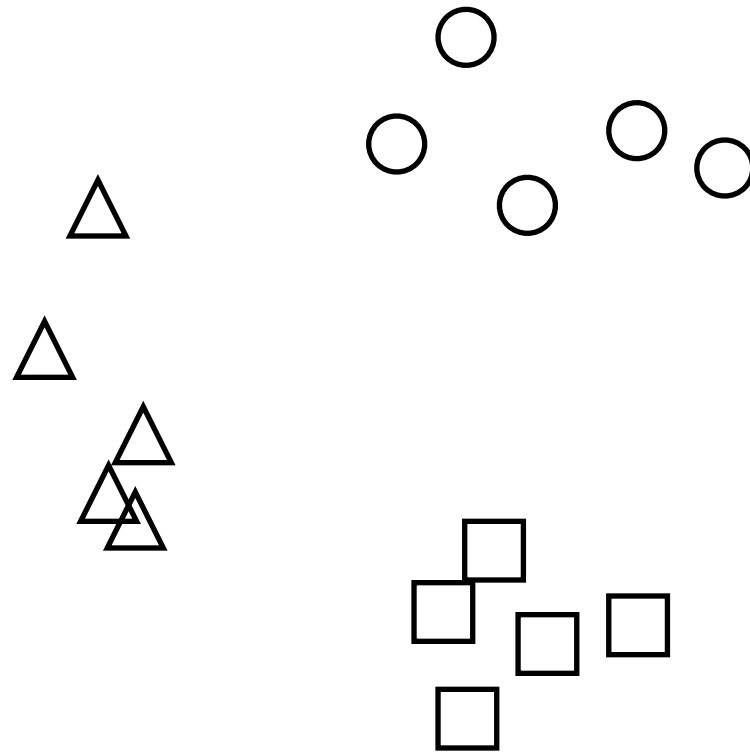
kernel ridge regression:

$$f(\mathbf{x}) = \mathbf{w}^\top \phi(\mathbf{x}) = Y(K + \lambda I)^{-1} \begin{pmatrix} K(\mathbf{x}_1, \mathbf{x}) \\ \dots \\ K(\mathbf{x}_m, \mathbf{x}) \end{pmatrix}$$

Multi-class classification



one-vs-rest

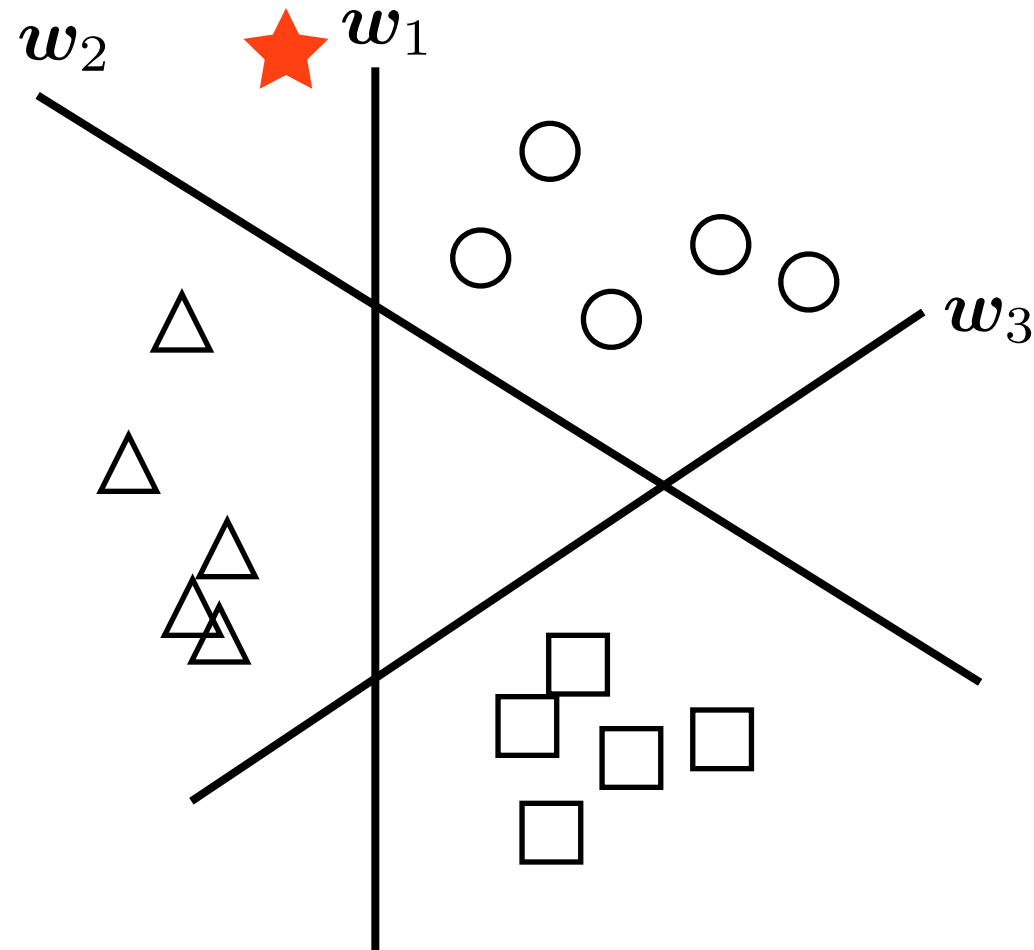


for C classes, need to train C binary classifiers

Multi-class classification



one-vs-rest

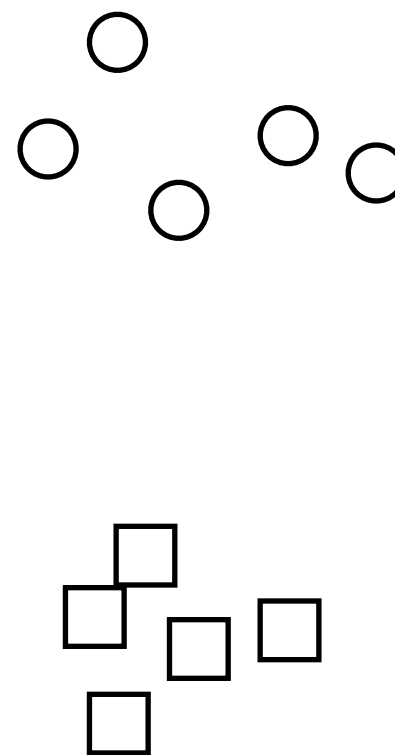
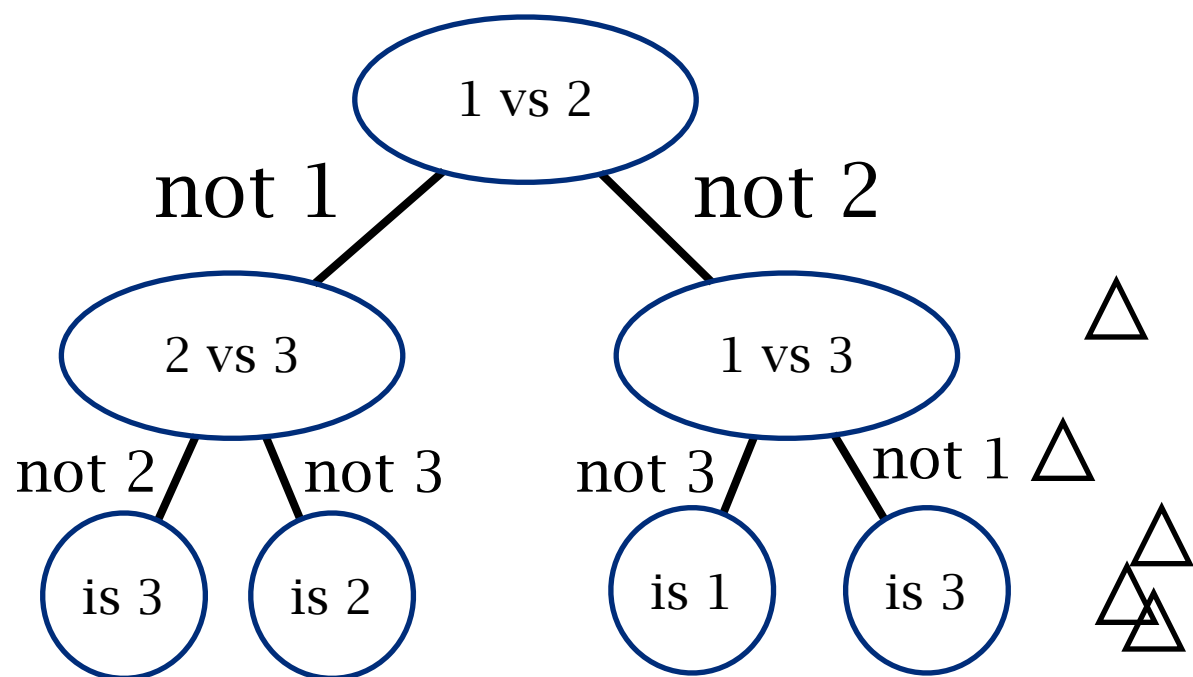


for C classes, need to train C binary classifiers

Multi-class classification



one-vs-one

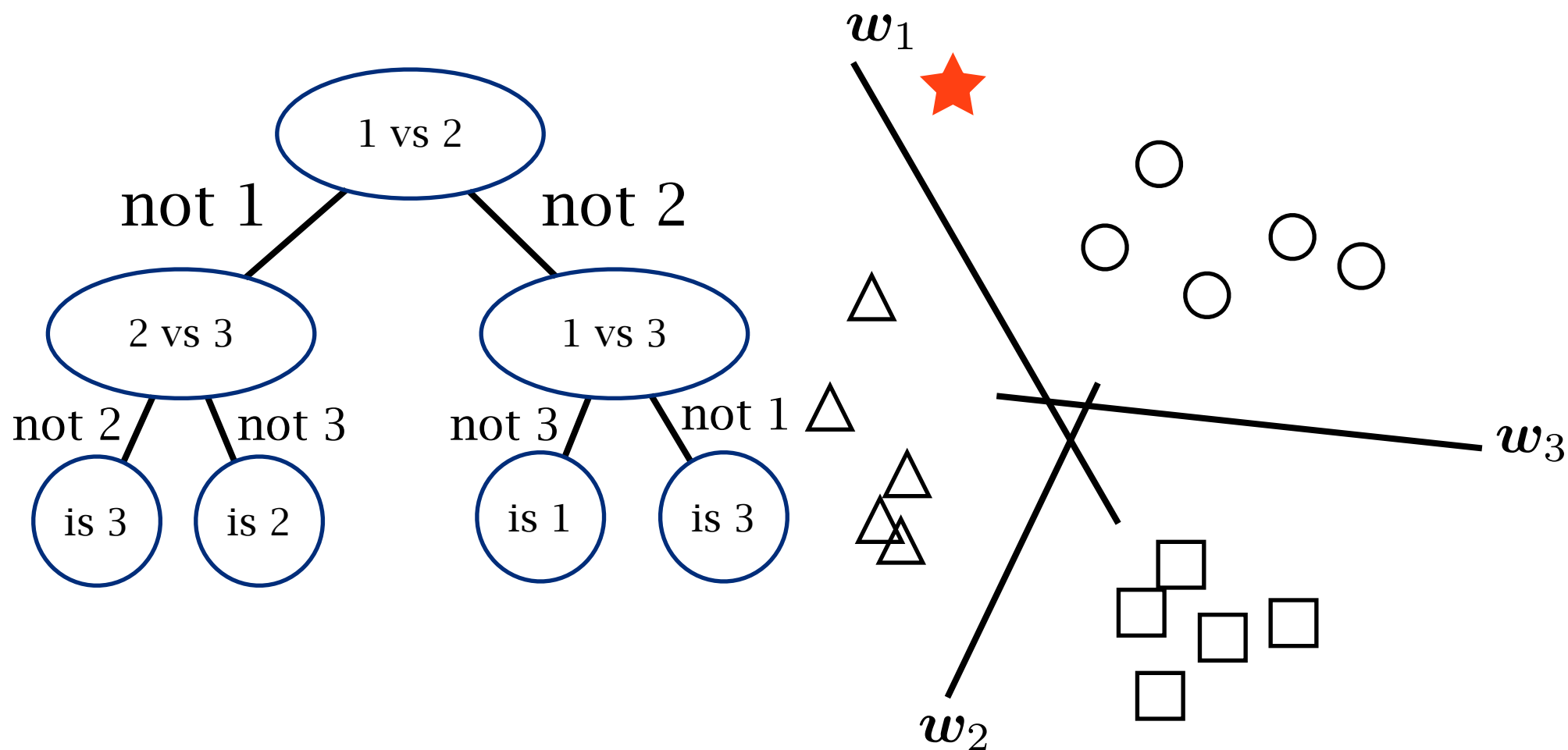


for C classes, need to train $C(C-1)$ binary classifiers

Multi-class classification



one-vs-one



for C classes, need to train $C(C-1)$ binary classifiers

习题



L1-norm作为正则化项(regularization)时为何会获得更稀疏(sparse)的解?

Logistic regression是用于回归还是分类?

在低维空间线性不可分的样本是否可以在高维空间线性可分?