#### Machine Learning Foundations

(機器學習基石)



Lecture 10: Logistic Regression

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## Roadmap

- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- **3 How Can Machines Learn?**

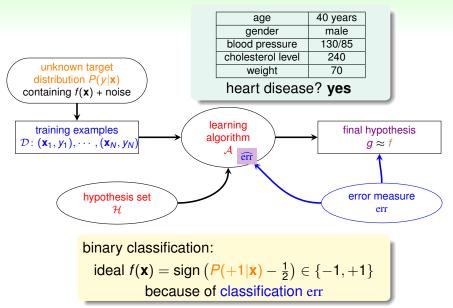
#### Lecture 9: Linear Regression

analytic solution  $\mathbf{w}_{\text{LIN}} = X^{\dagger} \mathbf{y}$  with linear regression hypotheses and squared error

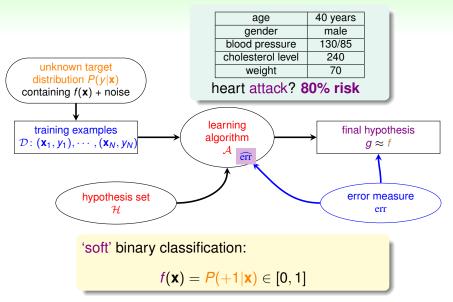
#### Lecture 10: Logistic Regression

- Logistic Regression Problem
- Logistic Regression Error
- Gradient of Logistic Regression Error
- Gradient Descent
- 4 How Can Machines Learn Better?

## Heart Attack Prediction Problem (1/2)



## Heart Attack Prediction Problem (2/2)



# Soft Binary Classification

target function 
$$f(\mathbf{x}) = P(+1|\mathbf{x}) \in [0,1]$$

#### ideal (noiseless) data

$$\begin{pmatrix} \mathbf{x}_{1}, y'_{1} &= 0.9 &= P(+1|\mathbf{x}_{1}) \\ (\mathbf{x}_{2}, y'_{2} &= 0.2 &= P(+1|\mathbf{x}_{2}) \\ \vdots \\ (\mathbf{x}_{N}, y'_{N} &= 0.6 &= P(+1|\mathbf{x}_{N}) \end{pmatrix}$$

#### actual (noisy) data

$$\begin{pmatrix} \mathbf{x}_{1}, y_{1} &= \circ & \sim P(y|\mathbf{x}_{1}) \\ (\mathbf{x}_{2}, y_{2} &= \times & \sim P(y|\mathbf{x}_{2}) \end{pmatrix}$$

$$\vdots$$

$$\begin{pmatrix} \mathbf{x}_{N}, y_{N} &= \times & \sim P(y|\mathbf{x}_{N}) \end{pmatrix}$$

same data as hard binary classification, different target function

# Soft Binary Classification

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#### actual (noisy) data

$$\begin{pmatrix} \mathbf{x}_{1}, y'_{1} &= 1 &= \left[ \circ \stackrel{?}{\sim} P(y|\mathbf{x}_{1}) \right] \\ \left( \mathbf{x}_{2}, y'_{2} &= 0 &= \left[ \circ \stackrel{?}{\sim} P(y|\mathbf{x}_{2}) \right] \right) \\ &\vdots \\ \left( \mathbf{x}_{N}, y'_{N} &= 0 &= \left[ \circ \stackrel{?}{\sim} P(y|\mathbf{x}_{N}) \right] \right)$$

same data as hard binary classification, different target function

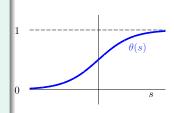
# Logistic Hypothesis

40 years
male
130/85
240

• For  $\mathbf{x} = (x_0, x_1, x_2, \dots, x_d)$  'features of patient', calculate a weighted 'risk score':

$$s = \sum_{i=0}^{d} w_i x_i$$

• convert the score to estimated probability by logistic function  $\theta(s)$ 



logistic hypothesis:  $h(\mathbf{x}) = \theta(\mathbf{w}^T\mathbf{x})$ 

# Logistic Function



$$\theta(-\infty)=0$$
;

$$\theta(0)=\frac{1}{2};$$

$$\theta(\infty)=1$$

$$\theta(s) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$$

—smooth, monotonic, sigmoid function of s

logistic regression: use

$$h(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$$

to approximate target function  $f(\mathbf{x}) = P(y|\mathbf{x})$ 

#### Fun Time

#### Logistic Regression and Binary Classification

Consider any logistic hypothesis  $h(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$  that approximates  $P(y|\mathbf{x})$ . 'Convert'  $h(\mathbf{x})$  to a binary classification prediction by taking sign  $(h(\mathbf{x}) - \frac{1}{2})$ . What is the equivalent formula for the binary classification prediction?

- 2 sign  $(\mathbf{w}^T \mathbf{x})$
- 3 sign  $\left(\mathbf{w}^{\mathsf{T}}\mathbf{x} + \frac{1}{2}\right)$
- 4 none of the above

# Reference Answer: (2)

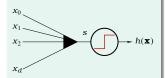
When  $\mathbf{w}^{\mathsf{T}}\mathbf{x} = 0$ ,  $h(\mathbf{x})$  is exactly  $\frac{1}{2}$ . So thresholding  $h(\mathbf{x})$  at  $\frac{1}{2}$  is the same as thresholding  $(\mathbf{w}^{\mathsf{T}}\mathbf{x})$  at 0.

#### Three Linear Models

linear scoring function:  $s = \mathbf{w}^T \mathbf{x}$ 

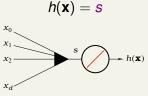
#### linear classification

$$h(\mathbf{x}) = \operatorname{sign}(\mathbf{s})$$



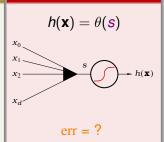
plausible err = 0/1 (small flipping noise)

#### linear regression



friendly err = squared (easy to minimize)

#### logistic regression



how to define  $E_{in}(\mathbf{w})$  for logistic regression?

#### Likelihood

target function 
$$f(\mathbf{x}) = P(+1|\mathbf{x})$$

$$\Leftrightarrow$$

$$P(y|\mathbf{x}) = \begin{cases} f(\mathbf{x}) & \text{for } y = +1\\ 1 - f(\mathbf{x}) & \text{for } y = -1 \end{cases}$$

consider 
$$\mathcal{D} = \{(\mathbf{x}_1, \circ), (\mathbf{x}_2, \times), \dots, (\mathbf{x}_N, \times)\}$$

#### probability that f generates $\mathcal{D}$

$$P(\mathbf{x}_1)P(\circ|\mathbf{x}_1) \times P(\mathbf{x}_2)P(\times|\mathbf{x}_2) \times \dots P(\mathbf{x}_N)P(\times|\mathbf{x}_N)$$

# likelihood that h generates $\mathcal{D}$

$$P(\mathbf{x}_1)h(\mathbf{x}_1) \times P(\mathbf{x}_2)(1 - h(\mathbf{x}_2)) \times \dots$$

$$P(\mathbf{x}_N)(1 - h(\mathbf{x}_N))$$

- if *h* ≈ *f*,
   then likelihood(*h*) ≈ probability using *f*
- probability using f usually large

#### Likelihood

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 $P(\mathbf{x}_N)(1-f(\mathbf{x}_N))$ 

# likelihood that h generates $\mathcal{D}$

$$P(\mathbf{x}_1)h(\mathbf{x}_1) \times P(\mathbf{x}_2)(1-h(\mathbf{x}_2)) \times \dots P(\mathbf{x}_N)(1-h(\mathbf{x}_N))$$

- if *h* ≈ *f*,
   then likelihood(*h*) ≈ probability using *f*
- probability using f usually large

## Likelihood of Logistic Hypothesis

likelihood(h)  $\approx$  (probability using f)  $\approx$  large

$$g = \underset{h}{\operatorname{argmax}} \operatorname{likelihood}(h)$$

# when logistic: $h(\mathbf{x}) = \theta(\mathbf{w}^T \mathbf{x})$

$$1 - h(\mathbf{x}) = h(-\mathbf{x})$$



likelihood(h) =  $P(\mathbf{x}_1)h(\mathbf{x}_1) \times P(\mathbf{x}_2)(1 - h(\mathbf{x}_2)) \times \dots P(\mathbf{x}_N)(1 - h(\mathbf{x}_N))$ 

likelihood(logistic 
$$h$$
)  $\propto \prod_{n=1}^{N} h(y_n \mathbf{x}_n)$ 

# Likelihood of Logistic Hypothesis

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$$1 - h(\mathbf{x}) = h(-\mathbf{x})$$



likelihood(
$$h$$
) =  $P(\mathbf{x}_1)h(+\mathbf{x}_1) \times P(\mathbf{x}_2)h(-\mathbf{x}_2) \times \dots P(\mathbf{x}_N)h(-\mathbf{x}_N)$ 

likelihood(logistic 
$$h$$
)  $\propto \prod_{n=1}^{N} h(y_n \mathbf{x}_n)$ 

$$\max_{h} \quad \text{likelihood(logistic } h) \propto \prod_{n=1}^{N} h(y_n \mathbf{x}_n)$$

$$\max_{\mathbf{w}} \quad likelihood(\mathbf{w}) \propto \prod_{n=1}^{N} \theta \left( y_n \mathbf{w}^T \mathbf{x}_n \right)$$

$$\max_{\mathbf{w}} \quad \ln \prod_{n=1}^{N} \theta \left( y_{n} \mathbf{w}^{T} \mathbf{x}_{n} \right)$$

$$\frac{1}{N} \sum_{n=1}^{N} - \ln \theta \left( y_n \mathbf{w}^T \mathbf{x}_n \right)$$

$$\theta(s) = \frac{1}{1 + \exp(-s)} : \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^{N} \ln\left(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)\right)$$

$$\implies \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^{N} \frac{1}{\exp(\mathbf{w}, \mathbf{x}_n, \mathbf{y}_n)}$$

$$E_{\text{in}}(\mathbf{w})$$

$$err(\mathbf{w}, \mathbf{x}, y) = ln(1 + exp(-y\mathbf{w}\mathbf{x})):$$
 cross-entropy error

#### Fun Time

The four statements below help us understand more about the cross-entropy error  $\operatorname{err}(\mathbf{w}, \mathbf{x}, y) = \ln (1 + \exp(-y\mathbf{w}^T\mathbf{x}))$ . Which statement is not true?

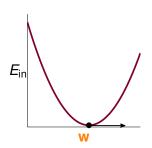
- 1 For any  $\mathbf{w}, \mathbf{x}$ , and y,  $err(\mathbf{w}, \mathbf{x}, y) > 0$ .
- ② For any w, x, and y, err(w, x, y) < 1126.
- 3 When  $y = \text{sign}(\mathbf{w}^T \mathbf{x}), \text{err}(\mathbf{w}, \mathbf{x}, y) < \ln 2$ .
- 4 When  $y \neq \text{sign}(\mathbf{w}^T\mathbf{x})$ ,  $\text{err}(\mathbf{w}, \mathbf{x}, y) \geq \ln 2$ .

# Reference Answer: 2

**1126, really? :-)** You are highly encouraged to plot the curve of err with respect to some fixed y and some varying score  $s = \mathbf{w}^T \mathbf{x}$  to know more about the error measure. After plotting, it is easy to see that err is not bounded above, and the other three choices are correct.

# Minimizing $E_{in}(\mathbf{w})$

$$\min_{\mathbf{w}} \quad E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln \left( 1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n) \right)$$



- E<sub>in</sub>(w): continuous, differentiable, twice-differentiable, convex
- how to minimize? locate valley

want 
$$\nabla E_{in}(\mathbf{w}) = \mathbf{0}$$

first: derive  $\nabla E_{in}(\mathbf{w})$ 

#### The Gradient $\nabla E_{in}(\mathbf{w})$

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln \left( \underbrace{1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)}_{\square} \right)$$

$$\frac{\partial E_{in}(\mathbf{w})}{\partial w_{i}} = \frac{1}{N} \sum_{n=1}^{N} \left( \frac{\partial \ln(\square)}{\partial \square} \right) \left( \frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left( \frac{\partial - y_{n} \mathbf{w}^{T} \mathbf{x}_{n}}{\partial w_{i}} \right) \\
= \frac{1}{N} \sum_{n=1}^{N} \left( \frac{\exp(\bigcirc)}{1 + \exp(\bigcirc)} \right) \left( -y_{n} \mathbf{x}_{n,i} \right) = \frac{1}{N} \sum_{n=1}^{N} \theta(\bigcirc) \left( -y_{n} \mathbf{x}_{n,i} \right)$$

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left( -y_n \mathbf{w}^T \mathbf{x}_n \right) \left( -y_n \mathbf{x}_n \right)$$

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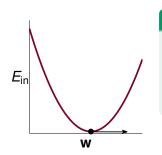
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= \frac{1}{N} \sum_{n=1}^{N} \left( \frac{\exp(\bigcirc)}{1 + \exp(\bigcirc)} \right) \left( -y_{n} x_{n,i} \right) = \frac{1}{N} \sum_{n=1}^{N} \theta(\bigcirc) \left( -y_{n} x_{n,i} \right)$$

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left( -y_n \mathbf{w}^T \mathbf{x}_n \right) \left( -y_n \mathbf{x}_n \right)$$

# Minimizing $E_{in}(\mathbf{w})$

$$\min_{\mathbf{w}} E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln \left( 1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n) \right)$$

$$\text{want } \nabla E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left( -y_n \mathbf{w}^T \mathbf{x}_n \right) \left( -y_n \mathbf{x}_n \right) = \mathbf{0}$$



#### scaled $\theta$ -weighted sum of $-y_n \mathbf{x}_n$

- all  $\theta(\cdot) = 0$ : only if  $y_n \mathbf{w}^T \mathbf{x}_n \gg 0$ —linear separable  $\mathcal{D}$
- weighted sum = 0: non-linear equation of w

closed-form solution? no :-(

## PLA Revisited: Iterative Optimization

PLA: start from some  $\mathbf{w}_0$  (say,  $\mathbf{0}$ ), and 'correct' its mistakes on  $\mathcal{D}$ 

For t = 0, 1, ...

1 find a mistake of  $\mathbf{w}_t$  called  $(\mathbf{x}_{n(t)}, y_{n(t)})$ 

$$sign\left(\mathbf{w}_{t}^{\mathsf{T}}\mathbf{x}_{n(t)}\right) \neq y_{n(t)}$$

2 (try to) correct the mistake by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + y_{n(t)} \mathbf{x}_{n(t)}$$

when stop, return last  $\mathbf{w}$  as g

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2 (try to) correct the mistake by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + y_{n(t)} \mathbf{x}_{n(t)}$$

 $\bullet$  (equivalently) pick some n, and update  $\mathbf{w}_t$  by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \left[ \operatorname{sign} \left( \mathbf{w}_t^\mathsf{T} \mathbf{x}_n \right) \neq y_n \right] y_n \mathbf{x}_n$$

when stop, return last w as q

# PLA Revisited: Iterative Optimization

PLA: start from some  $\mathbf{w}_0$  (say,  $\mathbf{0}$ ), and 'correct' its mistakes on  $\mathcal{D}$ 

For t = 0, 1, ...

(equivalently) pick some n, and update  $\mathbf{w}_t$  by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \underbrace{\mathbf{1}}_{\eta} \cdot \underbrace{\left( \left[ \operatorname{sign}\left( \mathbf{w}_t^\mathsf{T} \mathbf{x}_n \right) \neq y_n \right] \cdot y_n \mathbf{x}_n \right)}_{\mathbf{v}}$$

when stop, return last w as g

choice of  $(\eta, \mathbf{v})$  and stopping condition defines iterative optimization approach

#### Fun Time

Consider the gradient  $\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \theta \left( -y_n \mathbf{w}^T \mathbf{x}_n \right) \left( -y_n \mathbf{x}_n \right)$ . That is, each example  $(\mathbf{x}_n, y_n)$  contributes to the gradient by an amount of  $\theta \left( -y_n \mathbf{w}^T \mathbf{x}_n \right)$ . For any given  $\mathbf{w}$ , which example contributes the most amount to the gradient?

- 1 the example with the smallest  $y_n \mathbf{w}^T \mathbf{x}_n$  value
- 2 the example with the largest  $y_n \mathbf{w}^T \mathbf{x}_n$  value
- 3 the example with the smallest  $\mathbf{w}^T \mathbf{x}_n$  value
- 4 the example with the largest  $\mathbf{w}^T \mathbf{x}_n$  value

# Reference Answer: 1

Using the fact that  $\theta$  is a monotonic function, we see that the example with the smallest  $y_n \mathbf{w}^T \mathbf{x}_n$  value contributes to the gradient the most.

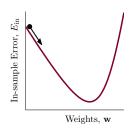
# **Iterative Optimization**

For t = 0, 1, ...

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \eta \mathbf{v}$$

when stop, return last w as g

- PLA: v comes from mistake correction
- smooth E<sub>in</sub>(w) for logistic regression: choose v to get the ball roll 'downhill'?
  - direction v: (assumed) of unit length
  - step size η:
     (assumed) positive



a greedy approach for some given  $\eta > 0$ :

$$\min_{\|\mathbf{v}\|=1} E_{\text{in}}(\underbrace{\mathbf{w}_t + \frac{\eta \mathbf{v}}{\mathbf{w}_{t+1}}})$$

## Linear Approximation

a greedy approach for some given  $\eta > 0$ :

$$\min_{\|\mathbf{v}\|=1} \quad E_{in}(\mathbf{w}_t + \frac{\eta \mathbf{v}}{\mathbf{v}})$$

- still non-linear optimization, now with constraints
   —not any easier than min<sub>w</sub> E<sub>in</sub>(w)
- · local approximation by linear formula makes problem easier

$$E_{\text{in}}(\mathbf{w}_t + \mathbf{\eta v}) \approx E_{\text{in}}(\mathbf{w}_t) + \mathbf{\eta v}^T \nabla E_{\text{in}}(\mathbf{w}_t)$$

if  $\eta$  really small (Taylor expansion)

an approximate greedy approach for some given small  $\eta$ :

$$\min_{\|\mathbf{v}\|=1} \quad \underbrace{E_{\text{in}}(\mathbf{w}_t)}_{\text{known}} + \underbrace{\eta}_{\text{given positive}} \mathbf{v}^T \underbrace{\nabla E_{\text{in}}(\mathbf{w}_t)}_{\text{known}}$$

#### **Gradient Descent**

an approximate greedy approach for some given small  $\eta$ :

$$\min_{\|\mathbf{v}\|=1} \quad \underbrace{E_{\text{in}}(\mathbf{w}_t)}_{\text{known}} + \underbrace{\eta}_{\text{given positive}} \mathbf{v}^T \underbrace{\nabla E_{\text{in}}(\mathbf{w}_t)}_{\text{known}}$$

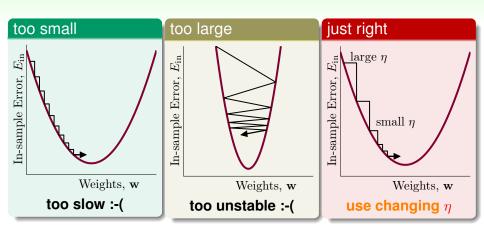
optimal v: opposite direction of ∇E<sub>in</sub>(v<sub>t</sub>)

$$\mathbf{v} = -rac{
abla E_{\mathsf{in}}(\mathbf{w}_t)}{\|
abla E_{\mathsf{in}}(\mathbf{w}_t)\|}$$

• gradient descent: for small  $\eta$ ,  $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$ 

gradient descent: a simple & popular optimization tool

## Choice of $\eta$



 $\eta$  better be monotonic of  $\|\nabla E_{in}(\mathbf{w}_t)\|$ 

# Simple Heuristic for Changing $\eta$ better be monotonic of $\|\nabla E_{in}(\mathbf{w}_t)\|$

• if red  $\eta \propto \|\nabla E_{\text{in}}(\mathbf{w}_t)\|$  by ratio purple  $\eta$ 

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$$
 $\parallel$ 
 $\mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)$ 

• call purple  $\eta$  the fixed learning rate

fixed learning rate gradient descent:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)$$

## **Putting Everything Together**

#### Logistic Regression Algorithm

initialize wo

For 
$$t = 0, 1, \dots$$

1 compute

$$\nabla E_{\text{in}}(\mathbf{w}_t) = \frac{1}{N} \sum_{n=1}^{N} \theta \left( -y_n \mathbf{w}_t^T \mathbf{x}_n \right) \left( -y_n \mathbf{x}_n \right)$$

update by

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)$$

...until  $\nabla E_{in}(\mathbf{w}_{t+1}) = 0$  or enough iterations return last  $\mathbf{w}_{t+1}$  as g

similar time complexity to **pocket** per iteration

#### Fun Time

If  $\mathbf{w}_0 = \mathbf{0}$ , and take  $\eta = 0.1$ . What is  $\mathbf{w}_1$  in the logistic regression algorithm?

$$\mathbf{1} + 0.1 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

$$2 -0.1 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

$$\mathbf{3} + 0.05 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

**4** 
$$-0.05 \cdot \frac{1}{N} \sum_{n=1}^{N} y_n \mathbf{x}_n$$

# Reference Answer: (3)

You can do a simple substitution using the fact that  $\theta(0) = \frac{1}{2}$ . This result shows that a scaled average of  $y_n \mathbf{x}_n$  is somewhat 'one-step' better than the zero vector.

#### Summary

- 1 When Can Machines Learn?
- 2 Why Can Machines Learn?
- **3 How Can Machines Learn?**

#### Lecture 9: Linear Regression

#### Lecture 10: Logistic Regression

- Logistic Regression Problem
   P(+1|x) as target and θ(w<sup>T</sup>x) as hypotheses
- Logistic Regression Error cross-entropy (negative log likelihood)
- Gradient of Logistic Regression Error
   θ-weighted sum of data vectors
- Gradient Descent

roll downhill by  $-\nabla E_{in}(\mathbf{w})$ 

- next: linear model'S' for classification
- 4 How Can Machines Learn Better?