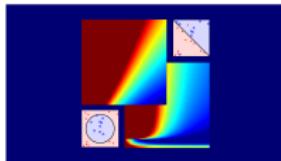


Machine Learning Foundations (機器學習基石)



Lecture 10: Logistic Regression

Hsuan-Tien Lin (林軒田)

htlin@csie.ntu.edu.tw

Department of Computer Science
& Information Engineering

National Taiwan University
(國立台灣大學資訊工程系)



Roadmap

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

Lecture 9: Linear Regression

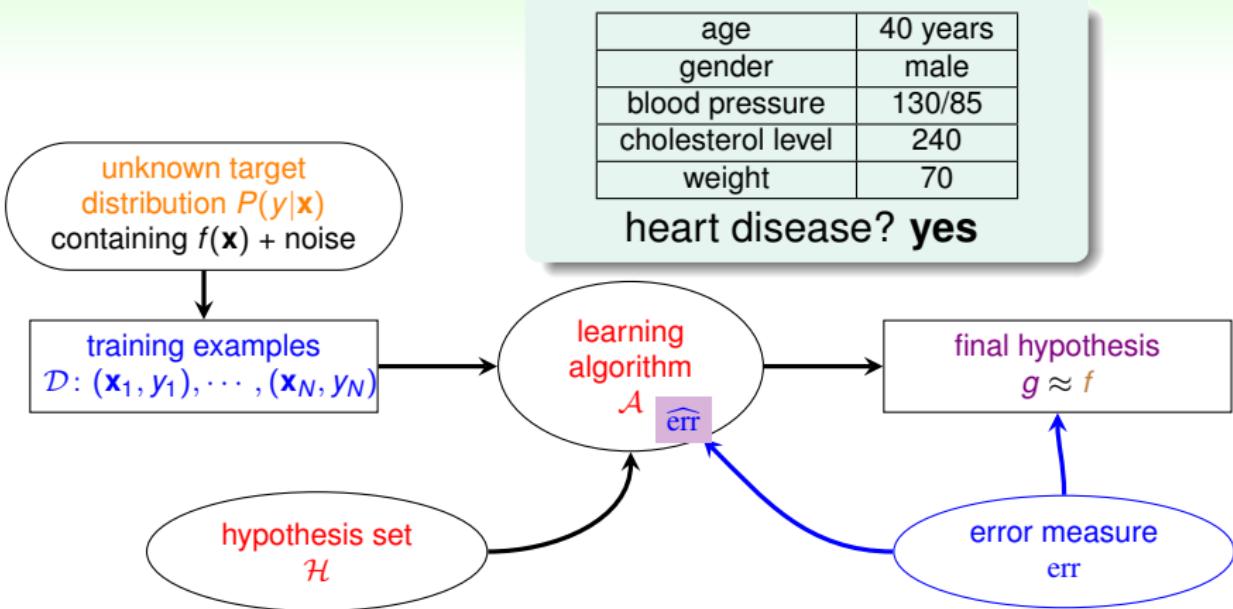
analytic solution $\mathbf{w}_{\text{LIN}} = \mathbf{X}^\dagger \mathbf{y}$ with
linear regression hypotheses and **squared error**

Lecture 10: Logistic Regression

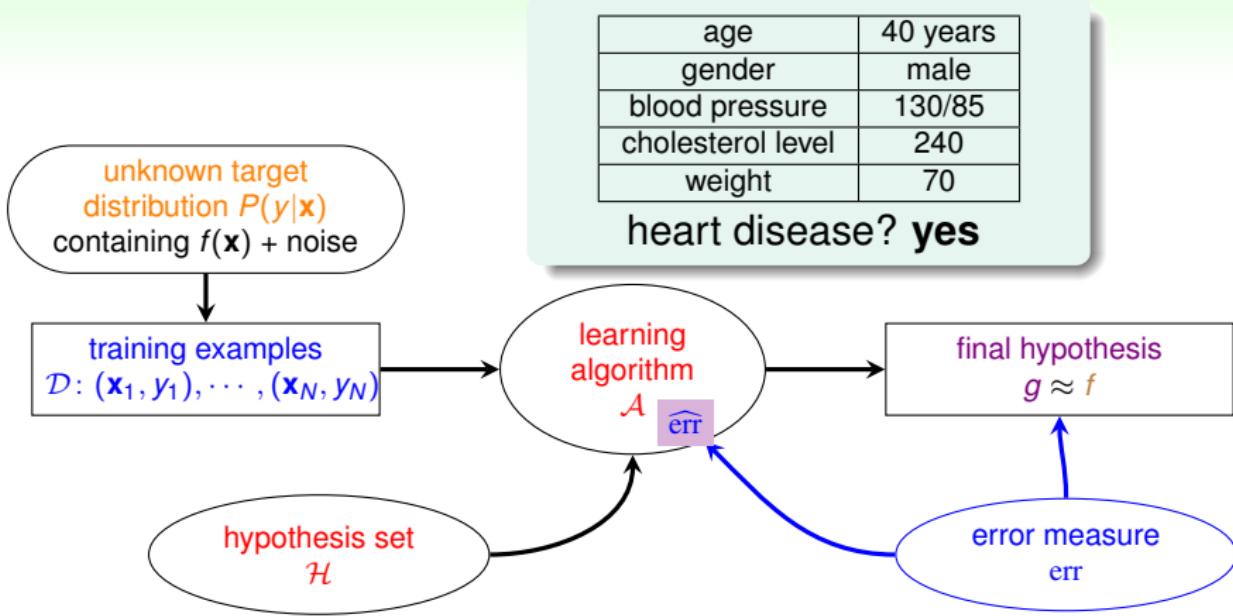
- Logistic Regression Problem
- Logistic Regression Error
- Gradient of Logistic Regression Error
- Gradient Descent

- ④ How Can Machines Learn Better?

Heart Attack Prediction Problem (1/2)



Heart Attack Prediction Problem (1/2)



age	40 years
gender	male
blood pressure	130/85
cholesterol level	240
weight	70

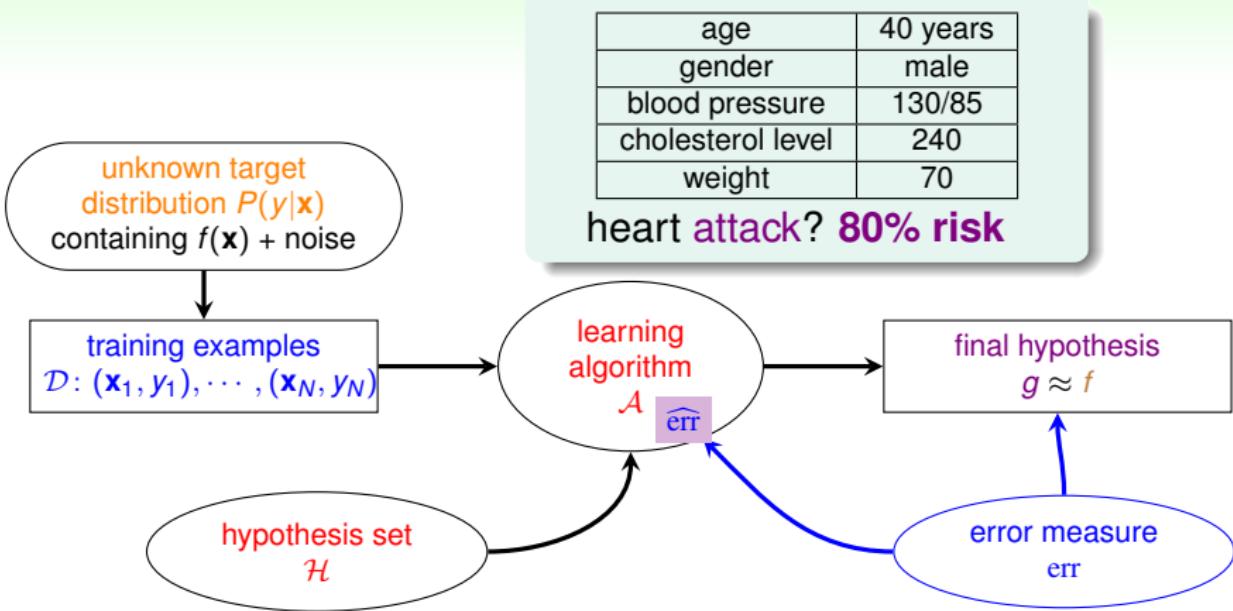
heart disease? **yes**

binary classification:

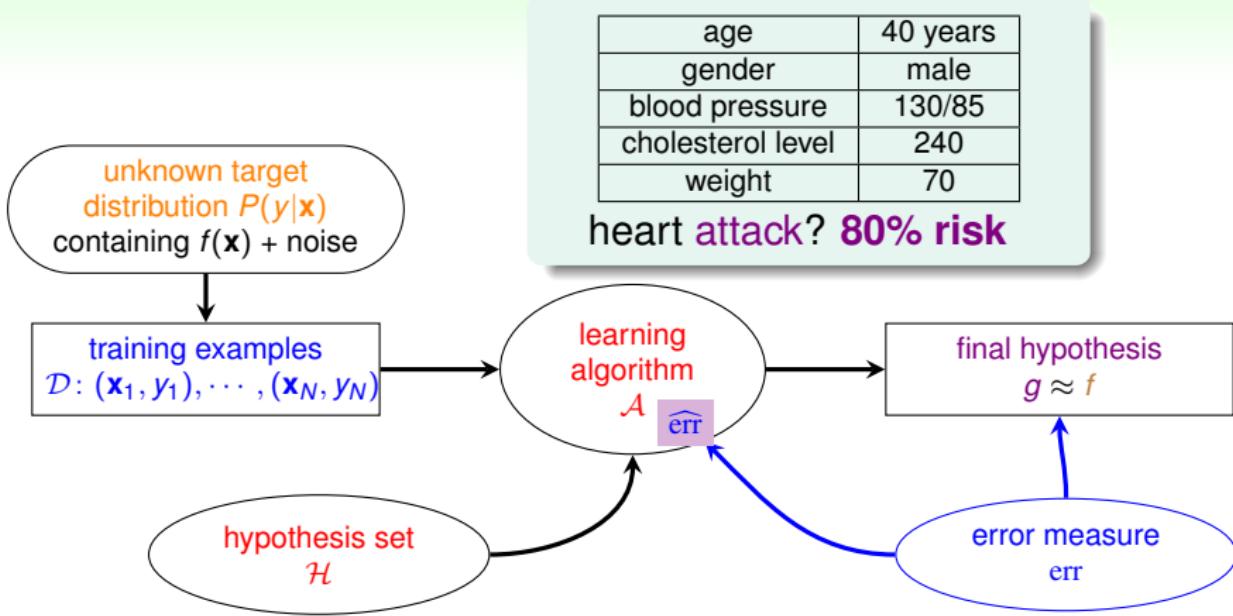
$$\text{ideal } f(\mathbf{x}) = \text{sign} (P(+1|\mathbf{x}) - \frac{1}{2}) \in \{-1, +1\}$$

because of **classification err**

Heart Attack Prediction Problem (2/2)



Heart Attack Prediction Problem (2/2)



‘soft’ binary classification:

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

Soft Binary Classification

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

ideal (noiseless) data

$$\left(\mathbf{x}_1, y'_1 = 0.9 = P(+1|\mathbf{x}_1) \right)$$

$$\left(\mathbf{x}_2, y'_2 = 0.2 = P(+1|\mathbf{x}_2) \right)$$

⋮

$$\left(\mathbf{x}_N, y'_N = 0.6 = P(+1|\mathbf{x}_N) \right)$$

Soft Binary Classification

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

ideal (noiseless) data

$$\begin{aligned} (\mathbf{x}_1, y'_1) &= 0.9 = P(+1|\mathbf{x}_1) \\ (\mathbf{x}_2, y'_2) &= 0.2 = P(+1|\mathbf{x}_2) \end{aligned}$$

⋮

$$(\mathbf{x}_N, y'_N) = 0.6 = P(+1|\mathbf{x}_N)$$

actual (noisy) data

$$\begin{aligned} (\mathbf{x}_1, y_1) &= \circ \sim P(y|\mathbf{x}_1) \\ (\mathbf{x}_2, y_2) &= \times \sim P(y|\mathbf{x}_2) \end{aligned}$$

⋮

$$(\mathbf{x}_N, y_N) = \times \sim P(y|\mathbf{x}_N)$$

Soft Binary Classification

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

ideal (noiseless) data

$$\left(\mathbf{x}_1, y'_1 = 0.9 = P(+1|\mathbf{x}_1) \right)$$

$$\left(\mathbf{x}_2, y'_2 = 0.2 = P(+1|\mathbf{x}_2) \right)$$

⋮

$$\left(\mathbf{x}_N, y'_N = 0.6 = P(+1|\mathbf{x}_N) \right)$$

actual (noisy) data

$$\left(\mathbf{x}_1, y'_1 = 1 = \left[\begin{array}{l} \circ \stackrel{?}{\sim} P(y|\mathbf{x}_1) \\ \circ \stackrel{?}{\sim} P(y|\mathbf{x}_2) \end{array} \right] \right)$$

$$\left(\mathbf{x}_N, y'_N = 0 = \left[\begin{array}{l} \circ \stackrel{?}{\sim} P(y|\mathbf{x}_N) \end{array} \right] \right)$$

Soft Binary Classification

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

ideal (noiseless) data

$$\begin{cases} \mathbf{x}_1, y'_1 = 0.9 = P(+1|\mathbf{x}_1) \\ \mathbf{x}_2, y'_2 = 0.2 = P(+1|\mathbf{x}_2) \end{cases}$$

⋮

$$\left(\mathbf{x}_N, y'_N = 0.6 = P(+1|\mathbf{x}_N) \right)$$

actual (noisy) data

$$\begin{cases} \mathbf{x}_1, y_1 = \circ \sim P(y|\mathbf{x}_1) \\ \mathbf{x}_2, y_2 = \times \sim P(y|\mathbf{x}_2) \end{cases}$$

⋮

$$\left(\mathbf{x}_N, y_N = \times \sim P(y|\mathbf{x}_N) \right)$$

same data as hard binary classification,
different **target function**

Logistic Hypothesis

age	40 years
gender	male
blood pressure	130/85
cholesterol level	240

- For $\mathbf{x} = (x_0, x_1, x_2, \dots, x_d)$ ‘features of patient’,

Logistic Hypothesis

age	40 years
gender	male
blood pressure	130/85
cholesterol level	240

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

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

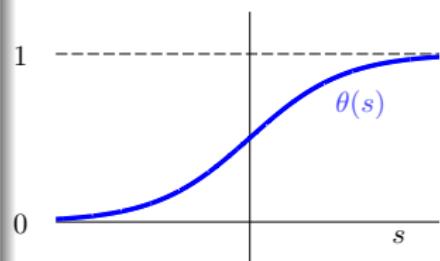
Logistic Hypothesis

age	40 years
gender	male
blood pressure	130/85
cholesterol level	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 $\theta(s)$



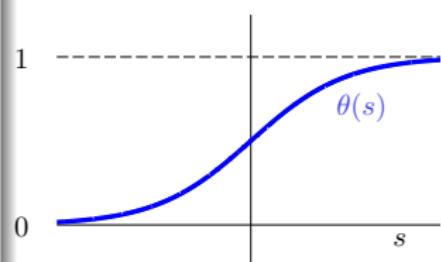
Logistic Hypothesis

age	40 years
gender	male
blood pressure	130/85
cholesterol level	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 $\theta(s)$



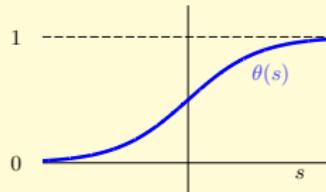
logistic hypothesis: $h(\mathbf{x}) = \theta(\mathbf{w}^T \mathbf{x})$

Logistic Function



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

Logistic Function



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

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

Logistic Function

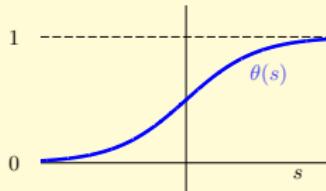


$$\theta(-\infty) = 0; \quad \theta(0) = \frac{1}{2}; \quad \theta(\infty) = 1$$

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

—smooth, monotonic, **sigmoid** function of s

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

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 $\text{sign}(h(\mathbf{x}) - \frac{1}{2})$. What is the equivalent formula for the binary classification prediction?

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

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?

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

Reference Answer: ②

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

Three Linear Models

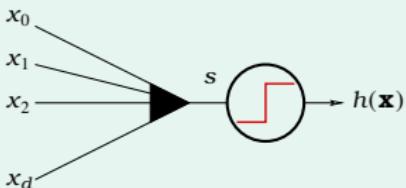
linear scoring function: $s = \mathbf{w}^T \mathbf{x}$

Three Linear Models

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

linear classification

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



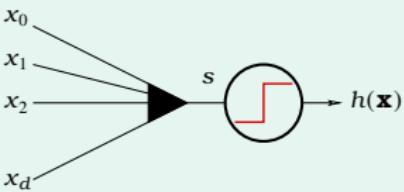
plausible err = 0/1
(small flipping noise)

Three Linear Models

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

linear classification

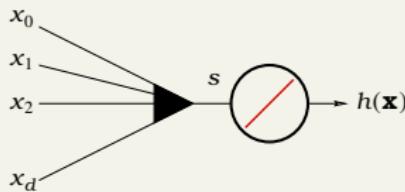
$$h(\mathbf{x}) = \text{sign}(s)$$



plausible err = 0/1
(small flipping noise)

linear regression

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



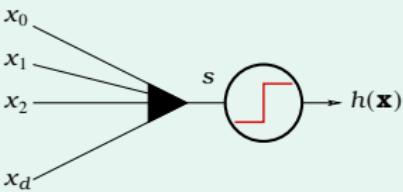
friendly err = squared
(easy to minimize)

Three Linear Models

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

linear classification

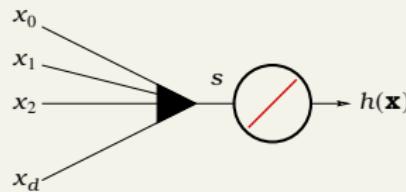
$$h(\mathbf{x}) = \text{sign}(s)$$



plausible err = 0/1
(small flipping noise)

linear regression

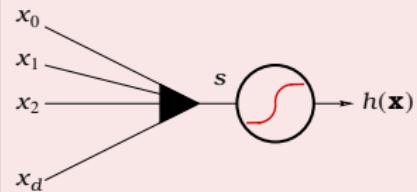
$$h(\mathbf{x}) = s$$



friendly err = squared
(easy to minimize)

logistic regression

$$h(\mathbf{x}) = \theta(s)$$



err = ?

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

Likelihood

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



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

Likelihood

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



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

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

Likelihood

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



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

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

probability that f generates \mathcal{D}

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

$$P(\mathbf{x}_2)P(\times|\mathbf{x}_2) \times$$

...

$$P(\mathbf{x}_N)P(\times|\mathbf{x}_N)$$

Likelihood

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



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

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

probability that f generates \mathcal{D}

$P(\mathbf{x}_1)f(\mathbf{x}_1) \times$

$P(\mathbf{x}_2)(1 - f(\mathbf{x}_2)) \times$

...

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

Likelihood

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



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

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

probability that f generates \mathcal{D}

$$\begin{aligned} P(\mathbf{x}_1)f(\mathbf{x}_1) \times \\ P(\mathbf{x}_2)(1 - f(\mathbf{x}_2)) \times \\ \dots \\ P(\mathbf{x}_N)(1 - f(\mathbf{x}_N)) \end{aligned}$$

likelihood that h generates \mathcal{D}

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

Likelihood

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



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

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

probability that f generates \mathcal{D}

$$\begin{aligned} P(\mathbf{x}_1)f(\mathbf{x}_1) \times \\ P(\mathbf{x}_2)(1 - f(\mathbf{x}_2)) \times \\ \dots \\ P(\mathbf{x}_N)(1 - f(\mathbf{x}_N)) \end{aligned}$$

likelihood that h generates \mathcal{D}

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

- if $h \approx f$,
then likelihood(h) \approx probability using f

Likelihood

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



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

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

probability that f generates \mathcal{D}

$$\begin{aligned} P(\mathbf{x}_1)f(\mathbf{x}_1) \times \\ P(\mathbf{x}_2)(1 - f(\mathbf{x}_2)) \times \\ \dots \\ P(\mathbf{x}_N)(1 - f(\mathbf{x}_N)) \end{aligned}$$

likelihood that h generates \mathcal{D}

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

- if $h \approx f$,
then likelihood(h) \approx probability using f
- probability using f usually **large**

Likelihood of Logistic Hypothesis

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

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

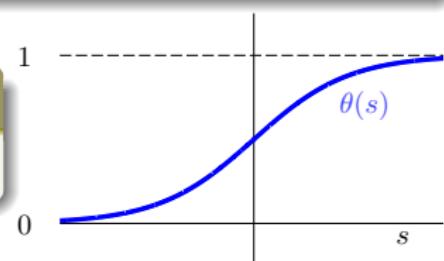
Likelihood of Logistic Hypothesis

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

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

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

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



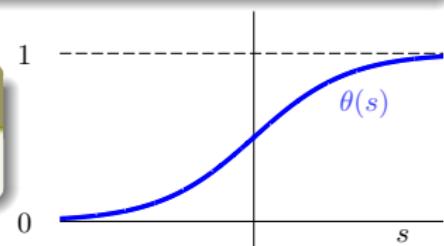
Likelihood of Logistic Hypothesis

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

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

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

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



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

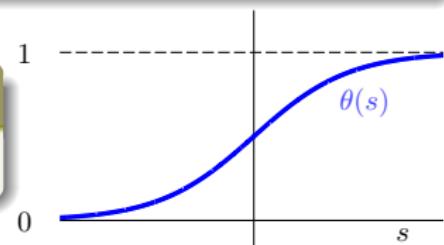
Likelihood of Logistic Hypothesis

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

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

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

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



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

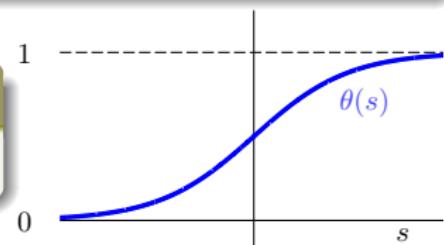
Likelihood of Logistic Hypothesis

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

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

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

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



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

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

Cross-Entropy Error

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

Cross-Entropy Error

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

Cross-Entropy Error

$$\max_{\mathbf{w}} \ln \prod_{n=1}^N \theta(y_n \mathbf{w}^T \mathbf{x}_n)$$

Cross-Entropy Error

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

Cross-Entropy Error

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

$$\theta(s) = \frac{1}{1 + \exp(-s)} \quad :$$

Cross-Entropy Error

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

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

Cross-Entropy Error

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

$$\begin{aligned}\theta(s) = \frac{1}{1 + \exp(-s)} \quad : \quad & \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^N \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)) \\ \implies \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^N & \underbrace{\text{err}(\mathbf{w}, \mathbf{x}_n, y_n)}_{E_{\text{in}}(\mathbf{w})}\end{aligned}$$

Cross-Entropy Error

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

$$\begin{aligned} \theta(s) = \frac{1}{1 + \exp(-s)} &: \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^N \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)) \\ \implies \min_{\mathbf{w}} & \underbrace{\frac{1}{N} \sum_{n=1}^N \text{err}(\mathbf{w}, \mathbf{x}_n, y_n)}_{E_{\text{in}}(\mathbf{w})} \end{aligned}$$

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

Fun Time

The four statements below help us understand more about the cross-entropy error $\text{err}(\mathbf{w}, \mathbf{x}, y) = \ln(1 + \exp(-y\mathbf{w}^T \mathbf{x}))$. Consider $\mathbf{w}^T \mathbf{x} \neq 0$. Which statement is not true?

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

Fun Time

The four statements below help us understand more about the cross-entropy error $\text{err}(\mathbf{w}, \mathbf{x}, y) = \ln(1 + \exp(-y\mathbf{w}^T \mathbf{x}))$. Consider $\mathbf{w}^T \mathbf{x} \neq 0$. Which statement is not true?

- 1 For any \mathbf{w} , \mathbf{x} , and y , $\text{err}(\mathbf{w}, \mathbf{x}, y) > 0$.
- 2 For any \mathbf{w} , \mathbf{x} , and y , $\text{err}(\mathbf{w}, \mathbf{x}, y) < 1126$.
- 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

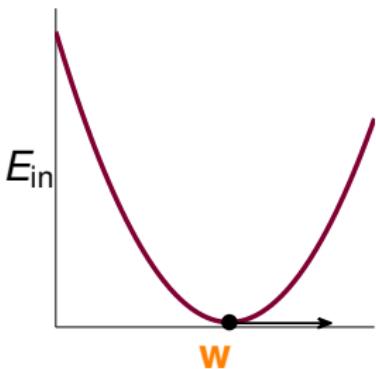
1126, really? :-) You are highly encouraged to plot the curve of err with respect to some fixed y and some varying score $s = \mathbf{w}^T \mathbf{x}$ to know more about the error measure. After plotting, it is easy to see that err is not bounded above, and the other three choices are correct.

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

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

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

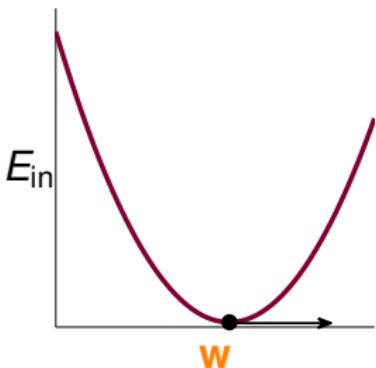
$$\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \ln \left(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n) \right)$$



- $E_{\text{in}}(\mathbf{w})$: continuous, differentiable, twice-differentiable, **convex**

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

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

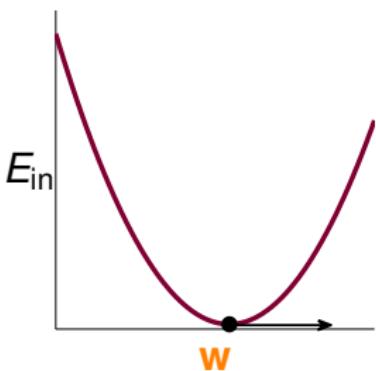


- $E_{\text{in}}(\mathbf{w})$: continuous, differentiable, twice-differentiable, **convex**
- how to minimize? locate **valley**

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

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

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



- $E_{\text{in}}(\mathbf{w})$: continuous, differentiable, twice-differentiable, **convex**
- how to minimize? locate **valley**

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

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

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

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

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

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

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

=

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

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

$$\begin{aligned} \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial w_i} &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\text{O}))}{\partial \text{O}} \right) \left(\frac{\partial -y_n \mathbf{w}^T \mathbf{x}_n}{\partial w_i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\quad \quad \right) \left(\quad \quad \right) \left(\quad \quad \right) \end{aligned}$$

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

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

$$\begin{aligned} \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial w_i} &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left(\frac{\partial -y_n \mathbf{w}^T \mathbf{x}_n}{\partial w_i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{1}{\square} \right) \left(\exp(\bigcirc) \right) \left(-y_n x_{n,i} \right) \end{aligned}$$

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

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

$$\begin{aligned} \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial w_i} &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left(\frac{\partial -y_n \mathbf{w}^T \mathbf{x}_n}{\partial w_i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{1}{\square} \right) \left(\exp(\bigcirc) \right) \left(-y_n x_{n,i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\quad \right) \left(-y_n x_{n,i} \right) \end{aligned}$$

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

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

$$\begin{aligned} \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial w_i} &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left(\frac{\partial -y_n \mathbf{w}^T \mathbf{x}_n}{\partial w_i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{1}{\square} \right) \left(\exp(\bigcirc) \right) \left(-y_n x_{n,i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\exp(\bigcirc)}{1 + \exp(\bigcirc)} \right) \left(-y_n x_{n,i} \right) \end{aligned}$$

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

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

$$\begin{aligned} \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial w_i} &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left(\frac{\partial -y_n \mathbf{w}^T \mathbf{x}_n}{\partial w_i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{1}{\square} \right) \left(\exp(\bigcirc) \right) \left(-y_n x_{n,i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\exp(\bigcirc)}{1 + \exp(\bigcirc)} \right) \left(-y_n x_{n,i} \right) = \frac{1}{N} \sum_{n=1}^N \theta(\bigcirc) (-y_n x_{n,i}) \end{aligned}$$

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

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

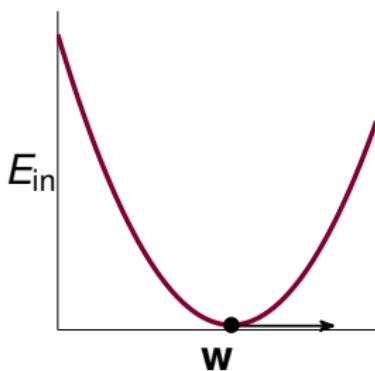
$$\begin{aligned} \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial w_i} &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\bigcirc))}{\partial \bigcirc} \right) \left(\frac{\partial -y_n \mathbf{w}^T \mathbf{x}_n}{\partial w_i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{1}{\square} \right) \left(\exp(\bigcirc) \right) \left(-y_n x_{n,i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\exp(\bigcirc)}{1 + \exp(\bigcirc)} \right) \left(-y_n x_{n,i} \right) = \frac{1}{N} \sum_{n=1}^N \theta(\bigcirc) (-y_n x_{n,i}) \end{aligned}$$

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

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

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

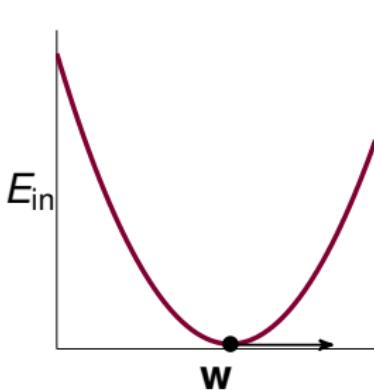
$$\text{want } \nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \theta \left(-y_n \mathbf{w}^T \mathbf{x}_n \right) (-y_n \mathbf{x}_n) = \mathbf{0}$$



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

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

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

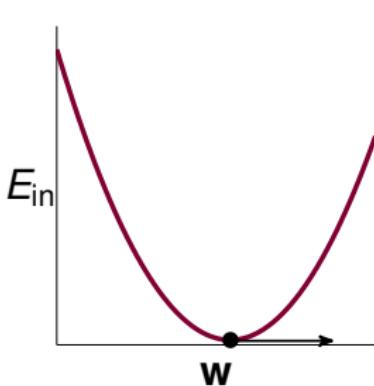


scaled θ -weighted sum of $-y_n \mathbf{x}_n$

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

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

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



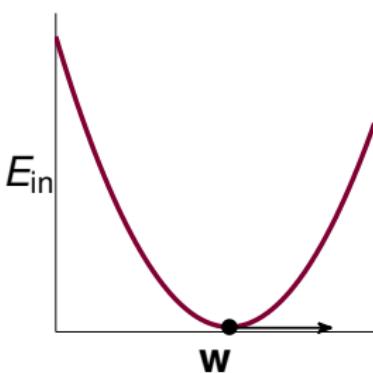
scaled θ -weighted sum of $-y_n \mathbf{x}_n$

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

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

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

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



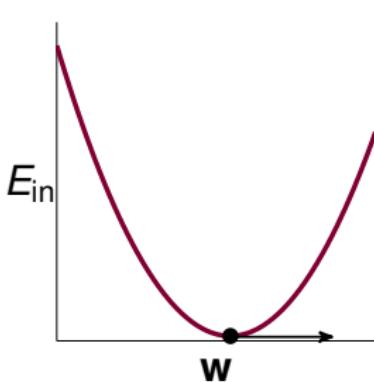
scaled θ -weighted sum of $-y_n \mathbf{x}_n$

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

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

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

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



scaled θ -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 = $\mathbf{0}$:
non-linear equation of \mathbf{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 $t = 0, 1, \dots$

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

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

- 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

PLA Revisited: Iterative Optimization

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

For $t = 0, 1, \dots$

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

$$\text{sign}(\mathbf{w}_t^T \mathbf{x}_{n(t)}) \neq y_{n(t)}$$

- ② (try to) correct the mistake by

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

- ① (equivalently) pick some n , and update \mathbf{w}_t by

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

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

PLA Revisited: Iterative Optimization

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

For $t = 0, 1, \dots$

- ① (equivalently) pick some n , and update \mathbf{w}_t by

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

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

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

Fun Time

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

Fun Time

Consider the gradient $\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \theta(-y_n \mathbf{w}^T \mathbf{x}_n) (-y_n \mathbf{x}_n)$. That is, each example (\mathbf{x}_n, y_n) contributes to the gradient by an amount of $\theta(-y_n \mathbf{w}^T \mathbf{x}_n)$. 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 θ 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 $t = 0, 1, \dots$

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

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

Iterative Optimization

For $t = 0, 1, \dots$

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

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

- PLA: \mathbf{v} comes from mistake correction

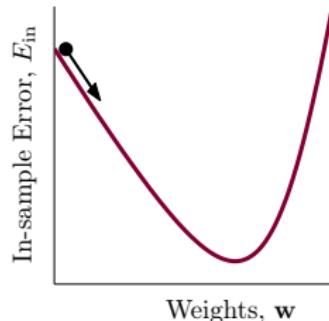
Iterative Optimization

For $t = 0, 1, \dots$

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

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

- PLA: \mathbf{v} comes from mistake correction
- smooth $E_{\text{in}}(\mathbf{w})$ for logistic regression:
choose \mathbf{v} to get the ball roll '**downhill**'?



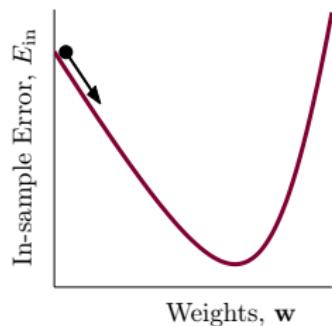
Iterative Optimization

For $t = 0, 1, \dots$

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

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

- PLA: \mathbf{v} comes from mistake correction
- smooth $E_{\text{in}}(\mathbf{w})$ for logistic regression:
choose \mathbf{v} to get the ball roll '**downhill**'?
 - direction \mathbf{v} :
(assumed) of unit length



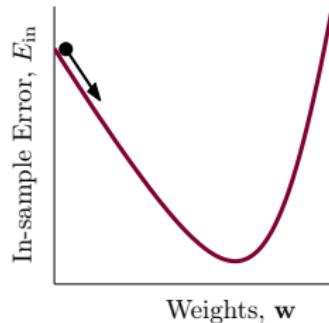
Iterative Optimization

For $t = 0, 1, \dots$

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

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

- PLA: \mathbf{v} comes from mistake correction
- smooth $E_{\text{in}}(\mathbf{w})$ for logistic regression:
choose \mathbf{v} to get the ball roll '**downhill**'?
 - direction \mathbf{v} :
(assumed) of unit length
 - step size η :
(assumed) positive



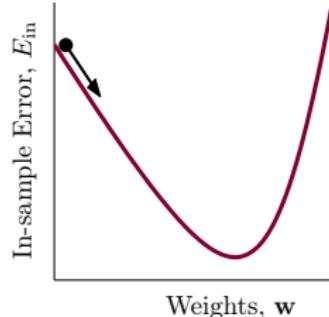
Iterative Optimization

For $t = 0, 1, \dots$

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

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

- PLA: \mathbf{v} comes from mistake correction
- smooth $E_{\text{in}}(\mathbf{w})$ for logistic regression:
choose \mathbf{v} to get the ball roll '**downhill**'?
 - direction \mathbf{v} :
(assumed) of unit length
 - step size η :
(assumed) positive



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

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

Linear Approximation

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

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

Linear Approximation

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

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

- still non-linear optimization, now **with constraints**
—not any easier than $\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w})$

Linear Approximation

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

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

- still non-linear optimization, now **with constraints**
—not any easier than $\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w})$
- local approximation by linear formula makes problem easier

$$E_{\text{in}}(\mathbf{w}_t + \eta \mathbf{v})$$

Linear Approximation

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

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

- still non-linear optimization, now **with constraints**
—not any easier than $\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w})$
- local approximation by linear formula makes problem easier

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

if η really small (Taylor expansion)

Linear Approximation

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

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

- still non-linear optimization, now **with constraints**
—not any easier than $\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w})$
- local approximation by linear formula makes problem easier

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

if η really small (Taylor expansion)

an **approximate** greedy approach for some given **small** η :

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

Gradient Descent

an **approximate** greedy approach for some given **small** η :

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

Gradient Descent

an **approximate** greedy approach for some given **small** η :

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

- optimal \mathbf{v} : opposite direction of $\nabla E_{\text{in}}(\mathbf{w}_t)$

$$\mathbf{v} =$$

Gradient Descent

an **approximate** greedy approach for some given **small** η :

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

- optimal \mathbf{v} : opposite direction of $\nabla E_{\text{in}}(\mathbf{w}_t)$

$$\mathbf{v} = - \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$$

Gradient Descent

an **approximate** greedy approach for some given **small** η :

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

- optimal \mathbf{v} : opposite direction of $\nabla E_{\text{in}}(\mathbf{w}_t)$

$$\mathbf{v} = - \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$$

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

Gradient Descent

an **approximate** greedy approach for some given **small** η :

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

- optimal \mathbf{v} : opposite direction of $\nabla E_{\text{in}}(\mathbf{w}_t)$

$$\mathbf{v} = - \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$$

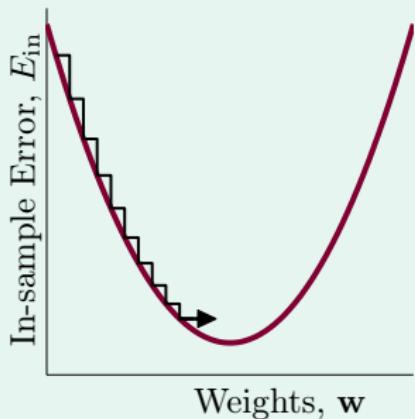
- gradient descent: for **small** η , $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$

gradient descent:
a simple & popular optimization tool

Choice of η

Choice of η

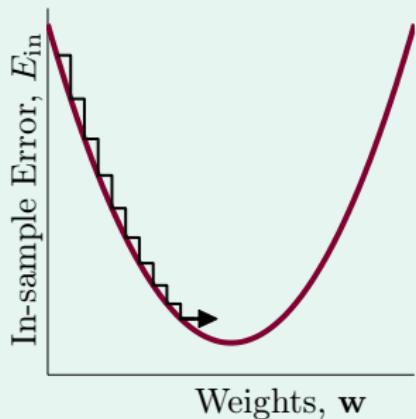
too small



too slow :-(

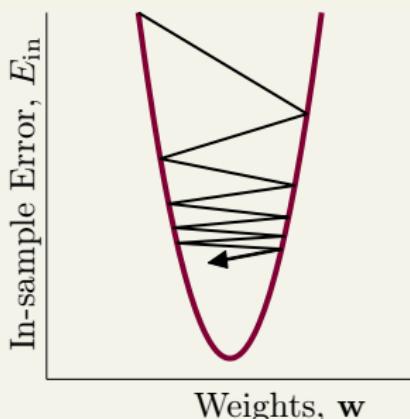
Choice of η

too small



too slow :-(

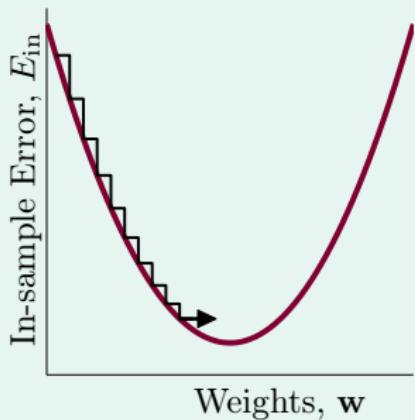
too large



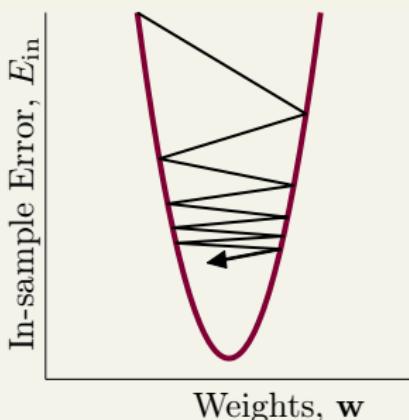
too unstable :-(

Choice of η

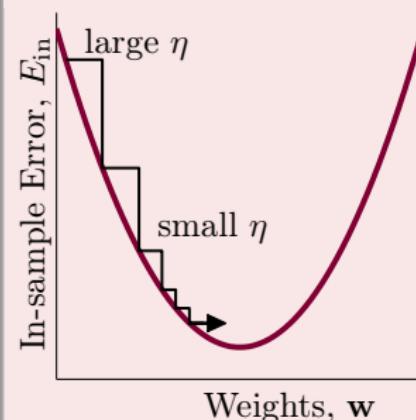
too small



too large

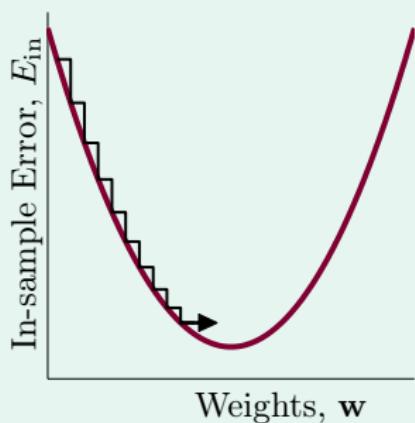


just right



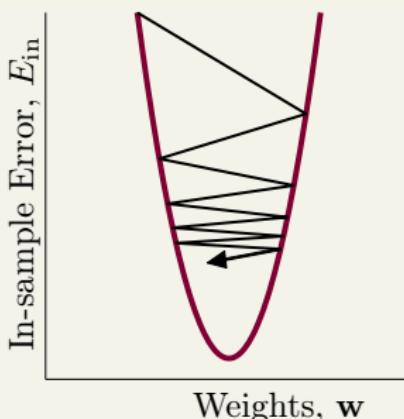
Choice of η

too small



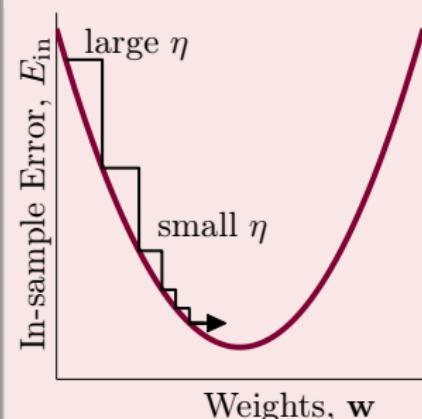
too slow :-)

too large



too unstable :-()

just right

use changing η

η better be **monotonic of $\|\nabla E_{in}(w_t)\|$**

Simple Heuristic for **Changing** η

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

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

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

Simple Heuristic for **Changing** η

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

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

$$\begin{aligned}\mathbf{w}_{t+1} &\leftarrow \mathbf{w}_t - \eta \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|} \\ &= \mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)\end{aligned}$$

Simple Heuristic for **Changing** η

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

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

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

- call purple η the **fixed learning rate**

Simple Heuristic for **Changing** η

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

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

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

$$\mathbf{w}_t - \eta \nabla E_{\text{in}}(\mathbf{w}_t)$$

- call purple η 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 \mathbf{w}_0

For $t = 0, 1, \dots$

Putting Everything Together

Logistic Regression Algorithm

initialize \mathbf{w}_0

For $t = 0, 1, \dots$

- ① compute

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

Putting Everything Together

Logistic Regression Algorithm

initialize \mathbf{w}_0

For $t = 0, 1, \dots$

- ① compute

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

- ② update by

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

Putting Everything Together

Logistic Regression Algorithm

initialize \mathbf{w}_0

For $t = 0, 1, \dots$

① compute

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

② update by

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

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

Putting Everything Together

Logistic Regression Algorithm

initialize \mathbf{w}_0

For $t = 0, 1, \dots$

① compute

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

② update by

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

...until $\nabla E_{\text{in}}(\mathbf{w}_{t+1}) \approx 0$ or enough iterations

Putting Everything Together

Logistic Regression Algorithm

initialize \mathbf{w}_0

For $t = 0, 1, \dots$

① compute

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

② update by

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

...until $\nabla E_{\text{in}}(\mathbf{w}_{t+1}) \approx 0$ or enough iterations

return last \mathbf{w}_{t+1} as g

Putting Everything Together

Logistic Regression Algorithm

initialize \mathbf{w}_0

For $t = 0, 1, \dots$

① compute

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

② update by

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

...until $\nabla E_{\text{in}}(\mathbf{w}_{t+1}) \approx 0$ 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?

- 1 $+0.1 \cdot \frac{1}{N} \sum_{n=1}^N y_n \mathbf{x}_n$
- 2 $-0.1 \cdot \frac{1}{N} \sum_{n=1}^N y_n \mathbf{x}_n$
- 3 $+0.05 \cdot \frac{1}{N} \sum_{n=1}^N y_n \mathbf{x}_n$
- 4 $-0.05 \cdot \frac{1}{N} \sum_{n=1}^N y_n \mathbf{x}_n$

Fun Time

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

- ① $+0.1 \cdot \frac{1}{N} \sum_{n=1}^N y_n \mathbf{x}_n$
- ② $-0.1 \cdot \frac{1}{N} \sum_{n=1}^N y_n \mathbf{x}_n$
- 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 $\theta(w^T x)$ 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 $-\nabla E_{\text{in}}(w)$

- next: linear model'S' for classification

- ④ How Can Machines Learn Better?