

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

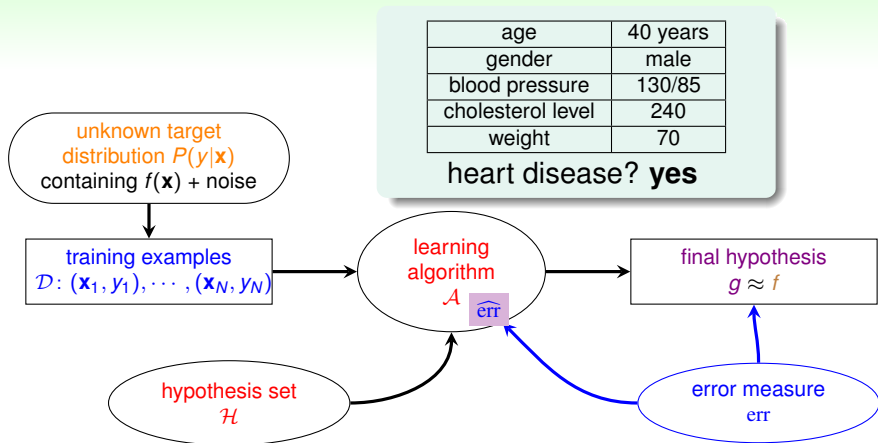
analytic solution $\mathbf{w}_{\text{LIN}} = \mathbf{X}^\dagger \mathbf{y}$ with
linear regression hypotheses and **squared error**

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)

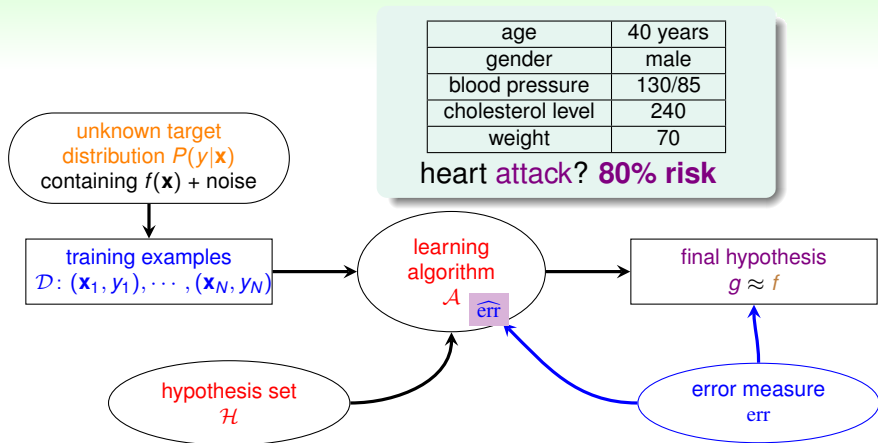


binary classification:

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

because of classification err

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

$$\left\{ \begin{array}{l} (\mathbf{x}_1, y'_1 = 0.9 = P(+1|\mathbf{x}_1)) \\ (\mathbf{x}_2, y'_2 = 0.2 = P(+1|\mathbf{x}_2)) \\ \vdots \\ (\mathbf{x}_N, y'_N = 0.6 = P(+1|\mathbf{x}_N)) \end{array} \right\}$$

actual (noisy) data

$$\left\{ \begin{array}{l} (\mathbf{x}_1, y_1 = \circ \sim P(y|\mathbf{x}_1)) \\ (\mathbf{x}_2, y_2 = \times \sim P(y|\mathbf{x}_2)) \\ \vdots \\ (\mathbf{x}_N, y_N = \times \sim P(y|\mathbf{x}_N)) \end{array} \right\}$$

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

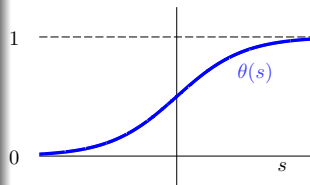
Logistic Hypothesis

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', calculate a **weighted** 'risk score':

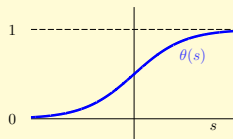
$$s = \sum_{i=0}^d w_i x_i$$

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



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

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

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

Reference Answer: ②

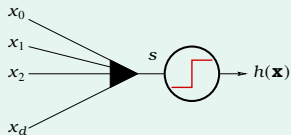
When $\mathbf{w}^T \mathbf{x} = 0$, $h(\mathbf{x})$ is exactly $\frac{1}{2}$. So thresholding $h(\mathbf{x})$ at $\frac{1}{2}$ is the same as thresholding $(\mathbf{w}^T \mathbf{x})$ at 0.

Three Linear Models

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

linear classification

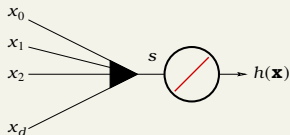
$$h(\mathbf{x}) = \text{sign}(\mathbf{s})$$



plausible err = 0/1
(small flipping noise)

linear regression

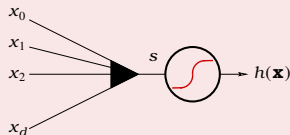
$$h(\mathbf{x}) = \mathbf{s}$$



friendly err = squared
(easy to minimize)

logistic regression

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



err = ?

how to define

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

Likelihood

target function

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



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

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

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

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

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}

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likelihood that h generates \mathcal{D}

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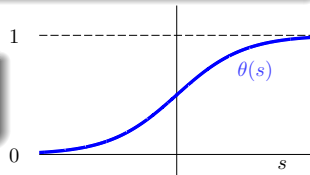
Likelihood of Logistic Hypothesis

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

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

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

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



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

$p(\mathbf{x}_n)$ 是固定的

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

Cross-Entropy Error

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

Cross-Entropy Error

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

Cross-Entropy Error

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

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

$$\Rightarrow \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^N \underbrace{\text{err}(\mathbf{w}, \mathbf{x}_n, y_n)}_{E_{\text{in}}(\mathbf{w})}$$

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

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 $y \neq \text{sign}(\mathbf{w}^T \mathbf{x})$, $\text{err}(\mathbf{w}, \mathbf{x}, y) \geq \ln 2$.

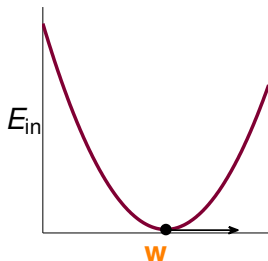
Reference Answer: ②

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

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

此函数也为凸函数



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

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

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

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

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

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

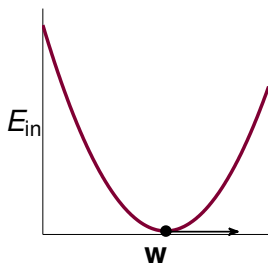
$$\begin{aligned} \frac{\partial E_{\text{in}}(\mathbf{w})}{\partial w_i} &= \frac{1}{N} \sum_{n=1}^N \left(\frac{\partial \ln(\square)}{\partial \square} \right) \left(\frac{\partial (1 + \exp(\circ))}{\partial \circ} \right) \left(\frac{\partial -y_n \mathbf{w}^T \mathbf{x}_n}{\partial w_i} \right)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

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

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

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

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



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

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

- 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

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

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

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

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

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.

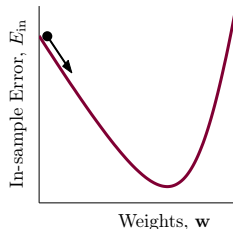
Iterative Optimization

For $t = 0, 1, \dots$

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

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

- 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 $\eta > 0$:

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

- 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 :

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

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

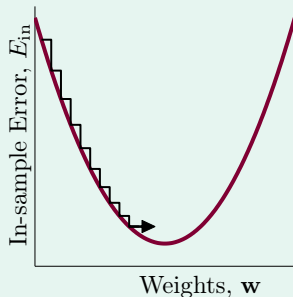
$$\mathbf{v} = - \frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$$

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

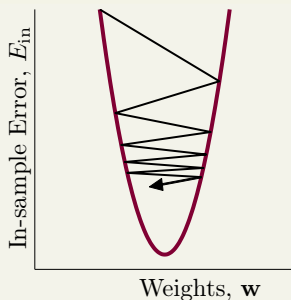
gradient descent:
a simple & popular optimization tool

Choice of η

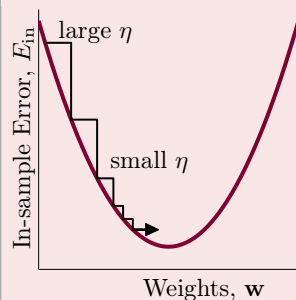
too small

too slow :-(

too large

too unstable :-(

just right

use changing η

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

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

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

$$\parallel$$

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

- call **purple** 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 $t = 0, 1, \dots$

1 compute

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

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

return last \mathbf{w}_{t+1} as \mathbf{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 $-0.05 \cdot \frac{1}{N} \sum_{n=1}^N y_n \mathbf{x}_n$

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
 $P(+1|\mathbf{x})$ as target and $\theta(\mathbf{w}^T \mathbf{x})$ 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 $-\nabla E_{\text{in}}(\mathbf{w})$

- **next: linear model 'S' for classification**

- 4 How Can Machines Learn Better?