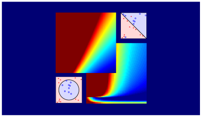
Machine Learning Foundations
(機器學習基石)



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

Lecture 10: Logistic Regression

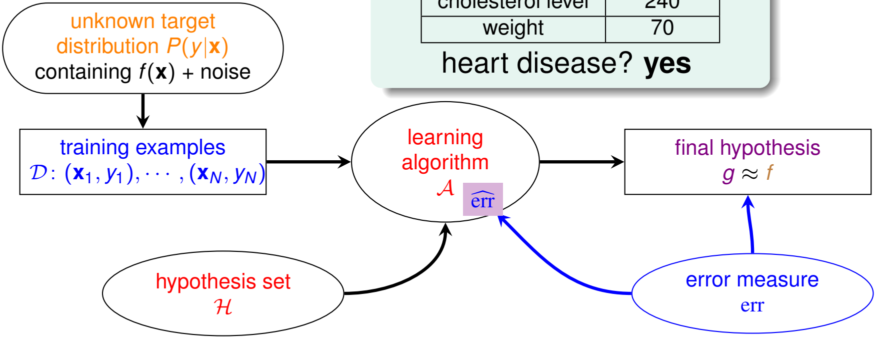
- Logistic Regression Problem
- Logistic Regression Error
- Gradient of Logistic Regression Error
- Gradient Descent

4. How Can Machines Learn Better?

Heart Attack Prediction Problem (1/2)

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

heart disease? **yes**



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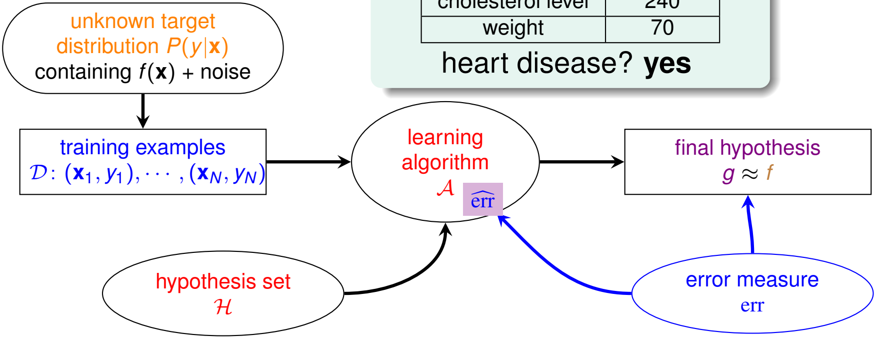


binary classification:

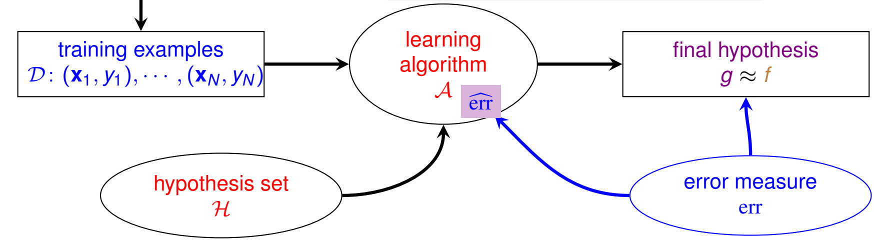
$$\text{ideal } f(\mathbf{x}) = \text{sign}\left(P(+1|\mathbf{x}) - \tfrac{1}{2}\right) \in \{-1, +1\}$$

because of classification err

Heart Attack Prediction Problem (2/2)

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

heart attack? **80% risk**



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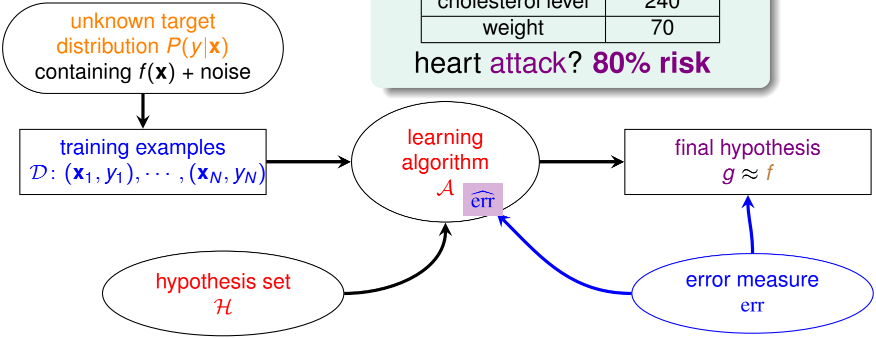

'soft' binary classification:

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

Soft Binary Classification

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

ideal (noiseless) data

$$\left(\mathbf{x}_1, y_1' = 0.9 = P(+1|\mathbf{x}_1)\right)$$
$$\left(\mathbf{x}_2, y_2' = 0.2 = P(+1|\mathbf{x}_2)\right)$$
$$\vdots$$
$$\left(\mathbf{x}_N, y_N' = 0.6 = P(+1|\mathbf{x}_N)\right)$$

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\end{array}$$

actual (noisy) data

$$\begin{array}{lll}
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\end{aligned}
$$

actual (noisy) data

$$
\begin{aligned}
&\left(\mathbf{x}_1, y'_1 = 1 = \left[\!\left[\circ \overset{?}{\sim} P(y|\mathbf{x}_1) \right]\!\right]\right)\\
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$$

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

Logistic Hypothesis

age	40 years
gender	male
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cholesterol level	240

- For $\mathbf{x} = (x_0, x_1, x_2, \cdots, x_d)$ 'features of patient',

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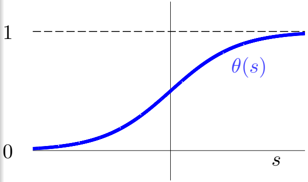
- convert the score to estimated probability by logistic function $\theta(s)$



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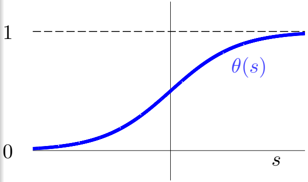
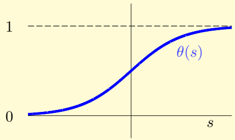


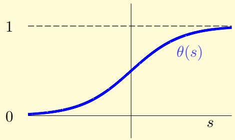
logistic hypothesis: $h(\mathbf{x}) = \theta(\mathbf{w}^T\mathbf{x})$

Logistic Function



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

Logistic Function



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

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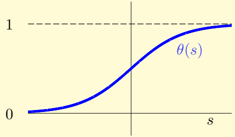

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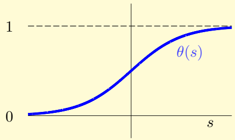
Logistic Function



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

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

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

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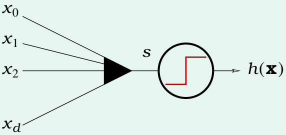
linear classification

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



plausible err = 0/1

(small flipping noise)

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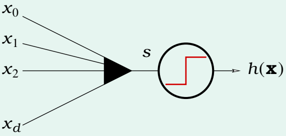

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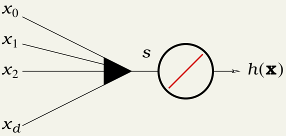
linear regression

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



friendly err = squared

(easy to minimize)

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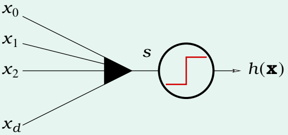

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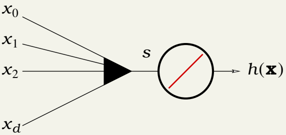
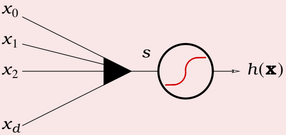


friendly err = squared
(easy to minimize)

logistic regression

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



err = ?

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

Likelihood

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

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probability that f generates $\mathcal{D}$

$$P(\mathbf{x}_1)P(\circ|\mathbf{x}_1) \times$$
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likelihood that h generates $\mathcal{D}$

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- 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

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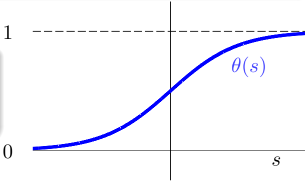

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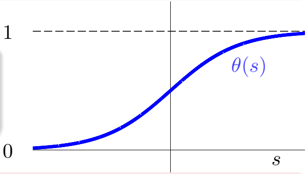

$$\text{likelihood}(h) = P(\mathbf{x}_1)h(\mathbf{x}_1) \times P(\mathbf{x}_2)(1 - h(\mathbf{x}_2)) \times \ldots P(\mathbf{x}_N)(1 - h(\mathbf{x}_N))$$

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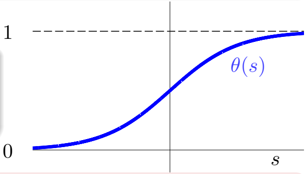

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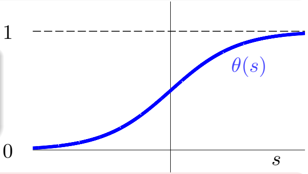

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$$\text{likelihood}(\text{logistic } h) \propto \prod_{n=1}^{N} h(y_n \mathbf{x}_n)$$

Cross-Entropy Error

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

Cross-Entropy Error

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

Cross-Entropy Error

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

Cross-Entropy Error

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

Cross-Entropy Error

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

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

Cross-Entropy Error

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

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

Cross-Entropy Error

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

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

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

Cross-Entropy Error

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

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

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

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

cross-entropy error

Fun Time

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

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

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

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

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

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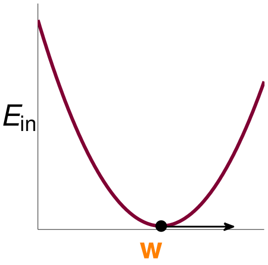

- $E_{\text{in}}(\mathbf{w})$: continuous, differentiable, twice-differentiable, **convex**

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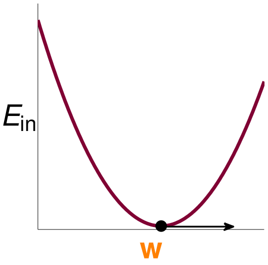

- $E_{\text{in}}(\mathbf{w})$: continuous, differentiable, twice-differentiable, **convex**
- how to minimize? locate **valley**

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

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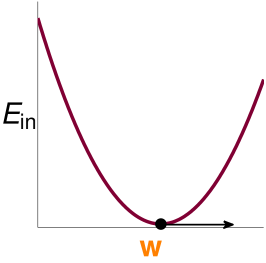

- $E_{in}(\mathbf{w})$: continuous, differentiable, twice-differentiable, **convex**
- how to minimize? locate **valley**

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

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

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

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

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

$$=$$

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$$= \frac{1}{N}\sum_{n=1}^{N}\left(\qquad\right)\left(\qquad\right)\left(\qquad\right)$$

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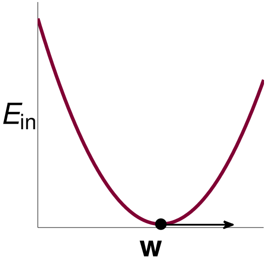

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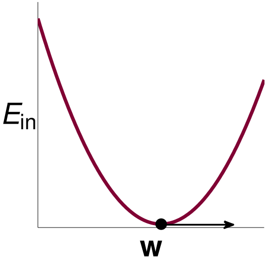

scaled θ-weighted sum of $-y_n\mathbf{x}_n$

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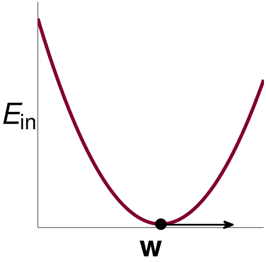

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- all $\theta(\cdot) = 0$: only if $y_n\mathbf{w}^T\mathbf{x}_n \gg 0$
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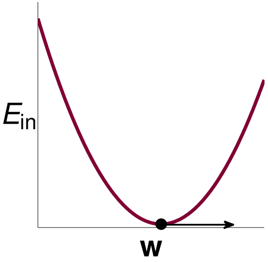

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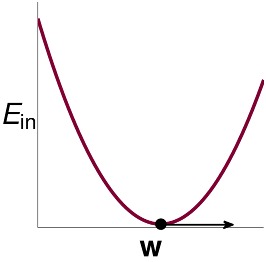

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closed-form solution? no :-(

PLA Revisited: Iterative Optimization

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

For $t = 0, 1, \ldots$

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

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

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

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

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

when stop, return last $\mathbf{w}$ 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
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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 $t = 0, 1, \ldots$

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

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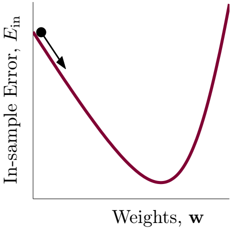
- smooth $E_{\text{in}}(\mathbf{w})$ for logistic regression: choose $\mathbf{v}$ to get the ball roll '**downhill**'?



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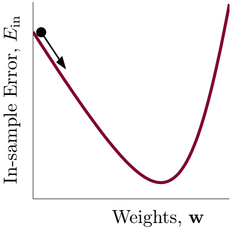
  - direction $\mathbf{v}$: (assumed) of unit length



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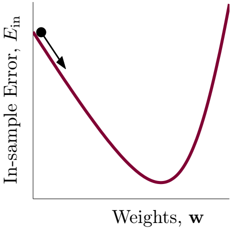
  - step size η: (assumed) positive



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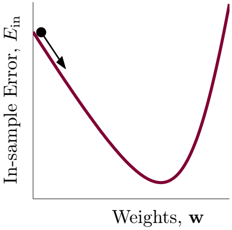

a greedy approach for some given $\eta > 0$:

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

Linear Approximation

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

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

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

- 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 $\eta > 0$:

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

- 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 $\eta > 0$:

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

- 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 $\eta > 0$:

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

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if η really small (Taylor expansion)

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

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

Gradient Descent

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

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

$$\mathbf{v} =$$

Gradient Descent

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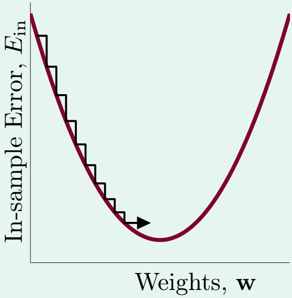
gradient descent:
a simple & popular optimization tool

Choice of η

Choice of η

too small



too slow :-(

Choice of η

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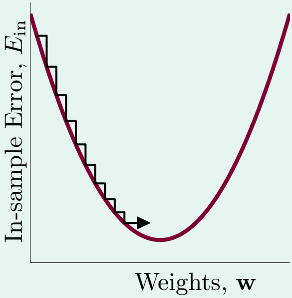

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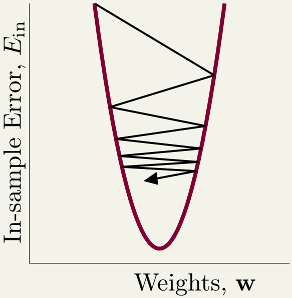

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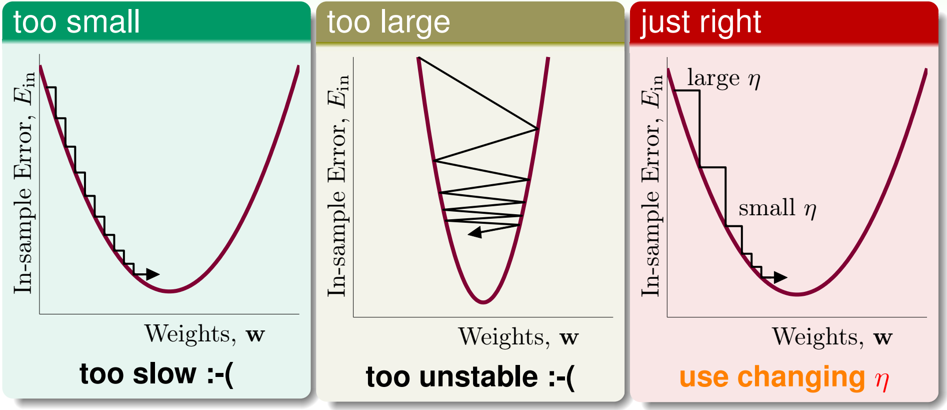
Choice of η



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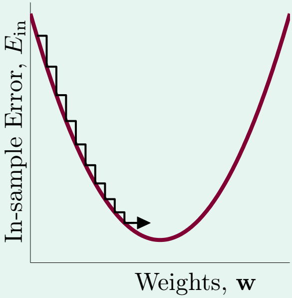

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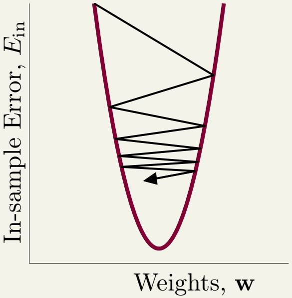
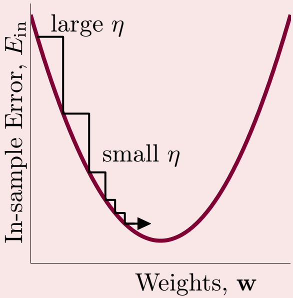


too unstable :-(

just right



use changing η

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

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

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

$$||$$

Simple Heuristic for **Changing** η

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

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

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$$||$$

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

- call purple η the fixed learning rate

Simple Heuristic for **Changing** η

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

- 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 $t = 0, 1, \cdots$

Putting Everything Together

Logistic Regression Algorithm

initialize $\mathbf{w}_0$

For $t = 0, 1, \cdots$

1. compute

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

Putting Everything Together

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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

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Putting Everything Together

Logistic Regression Algorithm

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For $t = 0, 1, \cdots$

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

Putting Everything Together

Logistic Regression Algorithm

initialize $\mathbf{w}_0$

For $t = 0, 1, \cdots$

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

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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?