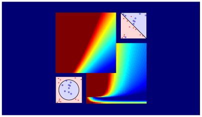
Machine Learning Foundations
(機器學習基石)



Lecture 10: Logistic Regression

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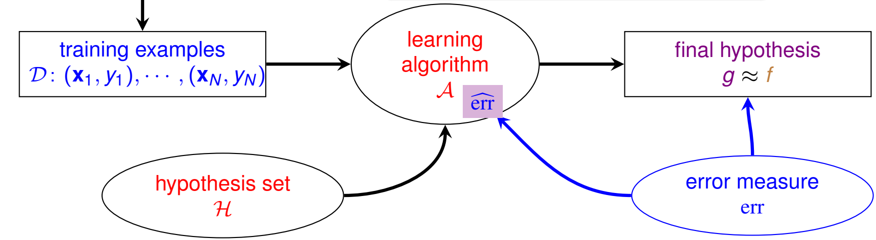
Heart Attack Prediction Problem (1/2)

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

heart disease? **yes**



binary classification:

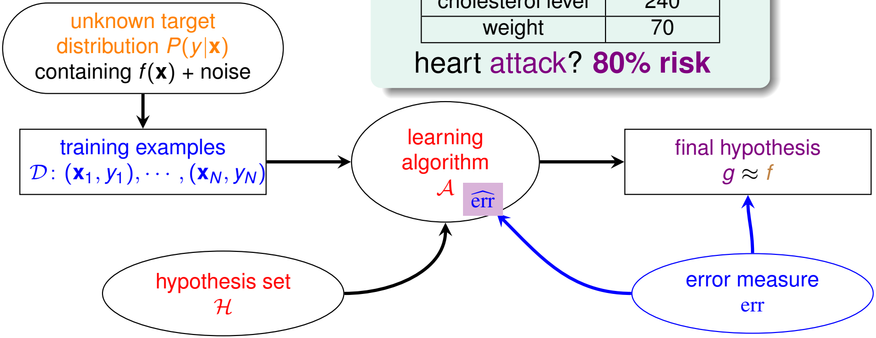
$$\text{ideal } f(\mathbf{x}) = \text{sign}\left(P(+1|\mathbf{x}) - \tfrac{1}{2}\right) \in \{-1, +1\}$$

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**



'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

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

actual (noisy) data

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

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

Soft Binary Classification

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

ideal (noiseless) data

$$\begin{array}{lll} \big(\mathbf{x}_1, y'_1 & = 0.9 & = P(+1|\mathbf{x}_1)\big) \\ \big(\mathbf{x}_2, y'_2 & = 0.2 & = P(+1|\mathbf{x}_2)\big) \\ \quad\vdots & & \\ \big(\mathbf{x}_N, y'_N & = 0.6 & = P(+1|\mathbf{x}_N)\big) \end{array}$$

actual (noisy) data

$$\begin{array}{lll} \big(\mathbf{x}_1, y'_1 & = 1 & = [\![\circ \overset{?}{\sim} P(y|\mathbf{x}_1)]\!]\big) \\ \big(\mathbf{x}_2, y'_2 & = 0 & = [\![\circ \overset{?}{\sim} P(y|\mathbf{x}_2)]\!]\big) \\ \quad\vdots & & \\ \big(\mathbf{x}_N, y'_N & = 0 & = [\![\circ \overset{?}{\sim} P(y|\mathbf{x}_N)]\!]\big) \end{array}$$

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

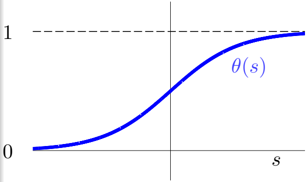
Logistic Hypothesis

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

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

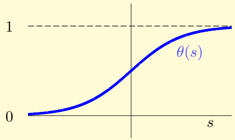
$$s = \sum_{i=0}^{d} w_i x_i$$

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



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

Logistic Function



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

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

—smooth, monotonic, sigmoid function of s

logistic regression: use

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

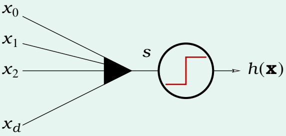
to approximate target function $f(\mathbf{x}) = P(+1|\mathbf{x})$

Three Linear Models

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

linear classification

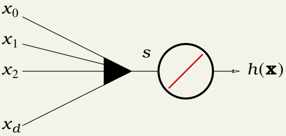
$h(\mathbf{x}) = \text{sign}(s)$



plausible err = 0/1
(small flipping noise)

linear regression

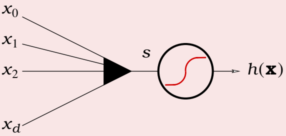
$h(\mathbf{x}) = s$



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

$\Leftrightarrow$

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

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

probability that f generates $\mathcal{D}$

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

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

$\ldots$

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

likelihood that h generates $\mathcal{D}$

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

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

$\ldots$

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

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

Likelihood

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

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

probability that f generates $\mathcal{D}$

$$P(\mathbf{x}_1)f(\mathbf{x}_1) \times$$
$$P(\mathbf{x}_2)(1 - f(\mathbf{x}_2)) \times$$
$$\ldots$$
$$P(\mathbf{x}_N)(1 - f(\mathbf{x}_N))$$

likelihood that h generates $\mathcal{D}$

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

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

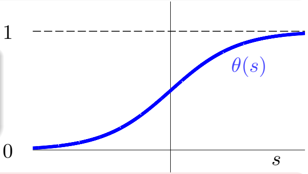
Likelihood of Logistic Hypothesis

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

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

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

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



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

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

Likelihood of Logistic Hypothesis

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

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

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

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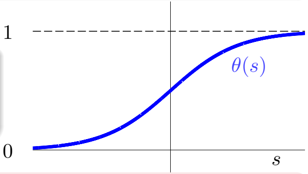


$$\text{likelihood}(h) = P(\mathbf{x}_1)h(+\mathbf{x}_1) \times P(\mathbf{x}_2)h(-\mathbf{x}_2) \times \ldots P(\mathbf{x}_N)h(-\mathbf{x}_N)$$

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

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

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

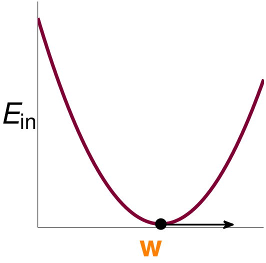
$$\theta(s) = \frac{1}{1+\exp(-s)} \quad : \quad \min_{\mathbf{w}} \quad \frac{1}{N}\sum_{n=1}^{N} \ln\left(1+\exp(-y_n \mathbf{w}^T \mathbf{x}_n)\right)$$

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

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

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

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



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

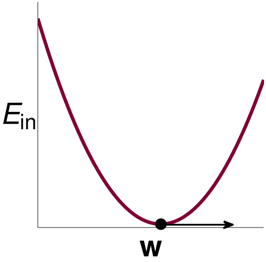
$$\text{want } \nabla E_{\text{in}}(\mathbf{w}) = \mathbf{0}$$

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

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

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

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



scaled 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 :-(

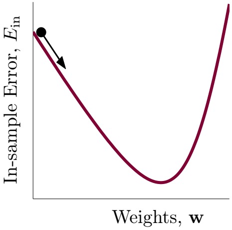
Iterative Optimization

For $t = 0, 1, \ldots$

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

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 $\eta > 0$:

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

- 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)

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

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

Gradient Descent

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

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

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

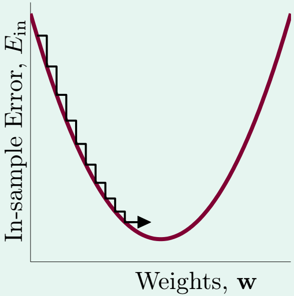
$$\mathbf{v} = -\frac{\nabla E_{\text{in}}(\mathbf{w}_t)}{\|\nabla E_{\text{in}}(\mathbf{w}_t)\|}$$

- 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

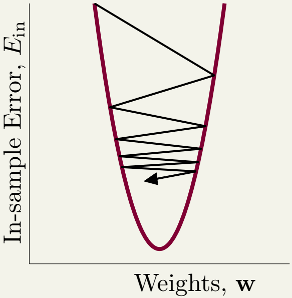
Choice of η

too small



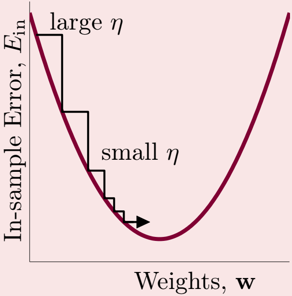
too slow :-(

too large



too unstable :-(

just right



use changing η

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

Putting Everything Together

Logistic Regression Algorithm

initialize $\mathbf{w}_0$

For $t = 0, 1, \cdots$

1. compute

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

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 g

similar time complexity to **pocket** per iteration