Machine Learning & Pattern Recognition

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Linear Regression

age	23 years
annual salary	NTD 1,000,000
year in job	0.5 year
current debt	200,000

Training dataset: $\mathcal{D} = \{(\boldsymbol{x_1}, y_1), (\boldsymbol{x_2}, y_2), \ldots, (\boldsymbol{x_m}, y_m)\}$;
Features of the i-th customer: $\boldsymbol{x_i} = (x_{i1}\ x_{i2}\ \ldots\ x_{id})^{\boldsymbol{T}}$; (Column vector)
The **ground truth** of the credit limit for the i-th customer: $y_i \in \mathbb{R}$ **.**

Linear regression: $f(\boldsymbol{x_i}) = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x_i} + b = \sum_{j=1}^{d} w_j x_{ij} + b$, where $\boldsymbol{w} = (w_1\ w_2\ \ldots\ w_d)^{\boldsymbol{T}} \in \mathbb{R}^{\boldsymbol{d}}$

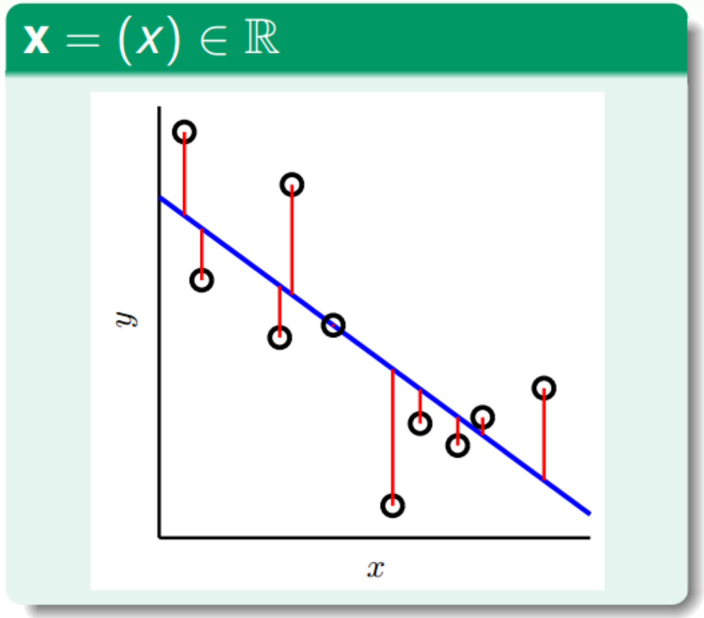
For simplicity, the bias b can be merged into the weight $\boldsymbol{w}$:

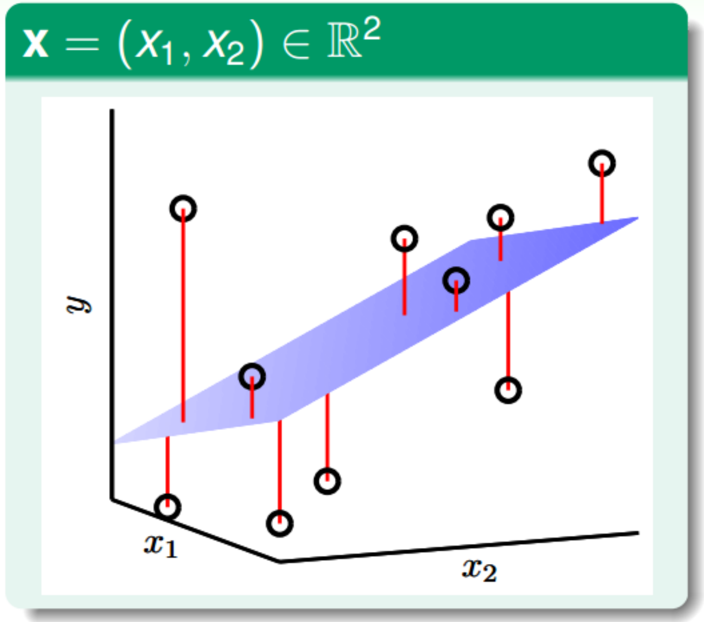
$$h(\boldsymbol{x_i}) = \widehat{\boldsymbol{w}}^{\boldsymbol{T}}\widehat{\boldsymbol{x}}_{\boldsymbol{i}}$$

$\widehat{\boldsymbol{w}} = (b; \boldsymbol{w}) = (b\ w_1\ w_2\ \ldots\ w_d) \in \mathbb{R}^{d+1}$
$\widehat{\boldsymbol{x}}_{\boldsymbol{i}} = (1;\ x_{i1}; x_{i2}; \ldots; x_{id}) \in \mathbb{R}^{d+1}$

Linear Regression

Linear regression hypothesis: $h(\boldsymbol{x_i}) = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x_i} = \sum_{j=0}^{d} w_j x_{ij}\,, x_{i0} = 1$





Linear regression: find lines/hyperplanes with small residuals

Empirical Error

We usually prefer to minimize the objective function where the expectation is taken across the data generating distribution p_{data} rather than just over the finite training set:

$$J^*(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x},y)\sim p_{data}} L(h(\boldsymbol{x}, \boldsymbol{\theta}), y)$$

However, in most cases, we do not know p_{data} but only have a training set of samples. One simplest way to convert the machine learning problem back into an optimization problem is to minimize the expected loss on the training set.

$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x},y)\sim \hat{P}_{data}} L(h(\boldsymbol{x}, \boldsymbol{\theta}), y)$$

Replacing the true distribution $p_{data}(\boldsymbol{x}, y)$ with the empirical distribution $\hat{P}_{data}(\boldsymbol{x}, y)$ defined by the training set.

Linear Regression

Popular/historical error measure:

squared error $err(\hat{y} - y) = (\hat{y} - y)^2$

$$E(\mathbf{w}) = \sum_{i=1}^{m} (\underbrace{h(\mathbf{x_i})}_{\mathbf{w}^T \mathbf{x_i}} - y_i)^2$$

Next: How to minimize $E(\mathbf{w})$?

Matrix Form of $E(\boldsymbol{w})$

$$E(\boldsymbol{w}) = \sum_{i=1}^{m} (h(\boldsymbol{x_i}) - y_i)^2 = \sum_{i=1}^{m} \left(\boldsymbol{w}^T \boldsymbol{x_i} - y_i\right)^2 = \sum_{i=1}^{m} \left(\boldsymbol{x_i}^T \boldsymbol{w} - y_i\right)^2$$

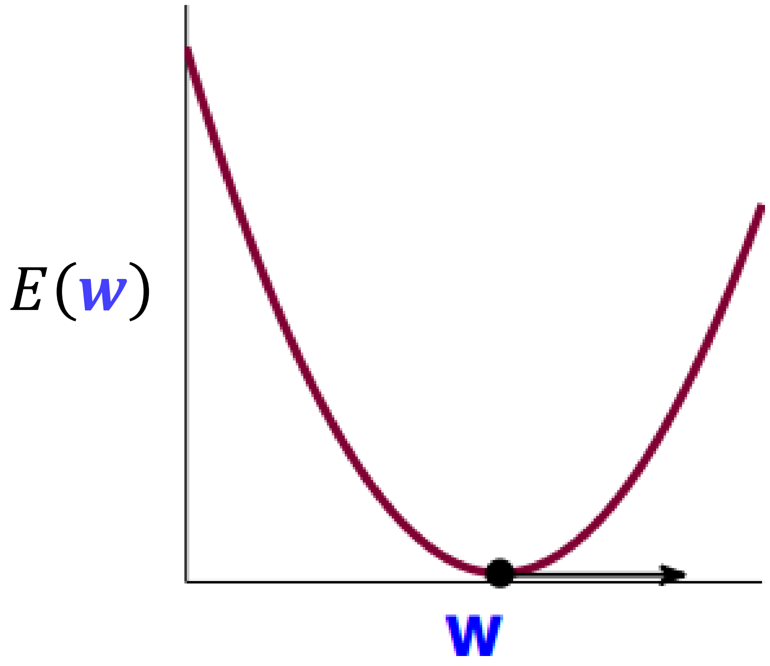
$$= \left\| \begin{matrix} \boldsymbol{x_1}^T \boldsymbol{w} - y_1 \\ \boldsymbol{x_2}^T \boldsymbol{w} - y_2 \\ \vdots \\ \boldsymbol{x_m}^T \boldsymbol{w} - y_m \end{matrix} \right\|^2 = \left\| \begin{bmatrix} - - \boldsymbol{x_1}^T - - \\ - - \boldsymbol{x_2}^T - - \\ \vdots \\ - - \boldsymbol{x_m}^T - - \end{bmatrix} \boldsymbol{w} - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \right\|^2$$

$$= \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2$$

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m1} & x_{m2} & \cdots & x_{md} \end{pmatrix} \in \mathbb{R}^{m \times (d+1)}, \boldsymbol{w} = \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{pmatrix} \in \mathbb{R}^{d+1}, \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} \in \mathbb{R}^m$$

Matrix Form of $E(\boldsymbol{w})$

$$\min E(\boldsymbol{w}) = \min \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2$$



- $E(\boldsymbol{w})$: continuous, differentiable, convex
- Necessary condition of 'best' $\boldsymbol{w}$.

$$\nabla E(\boldsymbol{w}) = \begin{bmatrix} \frac{\partial E}{\partial w_0}(\boldsymbol{w}) \\ \frac{\partial E}{\partial w_1}(\boldsymbol{w}) \\ \vdots \\ \frac{\partial E}{\partial w_d}(\boldsymbol{w}) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

✓ Not possible to 'roll down'

Task: find the $\boldsymbol{w}^*$ such that $\nabla E(\boldsymbol{w}^*) = 0$

The Gradient $\nabla E(\mathbf{w})$

$$\min_{\mathbf{w}} E(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y}) = \mathbf{w}^T \underbrace{\mathbf{X}^T\mathbf{X}}_{\boldsymbol{A}} \mathbf{w} - 2\mathbf{w}^T \underbrace{\mathbf{X}^T\mathbf{y}}_{\boldsymbol{b}} + \underbrace{\mathbf{y}^T\mathbf{y}}_{c}$$

One w only

$$E(w) = (aw^2 - 2bw + c)$$

$$\nabla E(w) = 2aw - 2b$$

Vector **w**

$$E(\mathbf{w}) = (\mathbf{w}^T \boldsymbol{A}\mathbf{w} - 2\mathbf{w}^T\boldsymbol{b} + c)$$

$$\nabla E(w) = 2\boldsymbol{A}\mathbf{w} - 2\boldsymbol{b}$$

$$\nabla E(w) = 2(\mathbf{X}^T\mathbf{X}\mathbf{w} - \mathbf{X}^T\mathbf{y})$$

Optimal Linear Regression Weights

Task: find $\boldsymbol{w}^*$ such that $\nabla E(\boldsymbol{w}^*) = 2(\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^T\boldsymbol{y}) = \mathbf{0}$

Invertible/positive definite $\boldsymbol{X}^T\boldsymbol{X}$

- Unique solution

$$w^* = \underbrace{(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T}_{\text{pseudo-inverse } \boldsymbol{X}^\dagger}\boldsymbol{y}$$

- Often the case because $N \gg d + 1$

Singular $\boldsymbol{X}^T\boldsymbol{X}$

- Many optimal solutions
- One of the solution
  - Define $\boldsymbol{X}^\dagger$ in other ways

Linear Regression Algorithm

1. From $\mathcal{D}$, construct input matrix $\boldsymbol{X}$ and output vector $\boldsymbol{y}$ by

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m1} & x_{m2} & \cdots & x_{md} \end{pmatrix} \in \mathbb{R}^{m\times(d+1)}, \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} \in \mathbb{R}^m$$

2. Calculate pseudo-inverse

$$\boldsymbol{X}^{\dagger} \in \mathbb{R}^{(d+1)\times m}$$

3. Return $\boldsymbol{w}^* = \boldsymbol{X}^{\dagger}\boldsymbol{y} \in \mathbb{R}^{(d+1)}$

Simple and efficient with **good $X^{\dagger}$ routine**

Exercise

After getting w^*, we can calculate the predictions $\hat{y}_n = (w^*)^T x_n$. If all $\hat{y}_n$ are collected in a vector $\hat{\mathbf{y}}$ similar to how we form $\mathbf{y}$, what is the matrix formula of $\hat{\mathbf{y}}$?

1. $\mathbf{y}$
2. $\mathrm{X}\mathrm{X}^T\mathbf{y}$
3. $\mathrm{X}\mathrm{X}^\dagger\mathbf{y}$
4. $\mathrm{X}\mathrm{X}^\dagger\mathrm{X}\mathrm{X}^T\mathbf{y}$

Exercise

After getting w^*, we can calculate the predictions $\hat{y}_n = (w^*)^T x_n$. If all $\hat{y}_n$ are collected in a vector $\hat{\mathbf{y}}$ similar to how we form $\mathbf{y}$, what is the matrix formula of $\hat{\mathbf{y}}$?

1. $\mathbf{y}$
2. $\mathrm{X}\mathrm{X}^T\mathbf{y}$
3. $\mathrm{X}\mathrm{X}^\dagger\mathbf{y}$
4. $\mathrm{X}\mathrm{X}^\dagger\mathrm{X}\mathrm{X}^T\mathbf{y}$

Reference Answer: 3

Note that $\hat{\mathbf{y}} = Xw^*$. Then, a simple substitution of w^* reveals the answer.

Heart Attack Prediction Problem

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

heart disease? **yes**

Binary classification:
Ideal $f(\boldsymbol{x}) = sign(p(+1|\boldsymbol{x}) - 0.5) \in \{-1, +1\}$

Heart Attack Prediction Problem

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

heart attack? **80% risk**

'Soft' Binary classification:

$$f(x) = p(+1|x) \in [0,1]$$

Soft Binary classification:

Target function $f(x) = p(+1|x) \in [0,1]$

Ideal data

$$
\begin{aligned}
&(\mathbf{x}_1, y_1' = 0.9 = P(+1|\mathbf{x}_1)) \\
&(\mathbf{x}_2, y_2' = 0.2 = P(+1|\mathbf{x}_2)) \\
&\qquad\vdots \\
&(\mathbf{x}_N, y_N' = 0.6 = P(+1|\mathbf{x}_N))
\end{aligned}
$$

Actual data

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

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

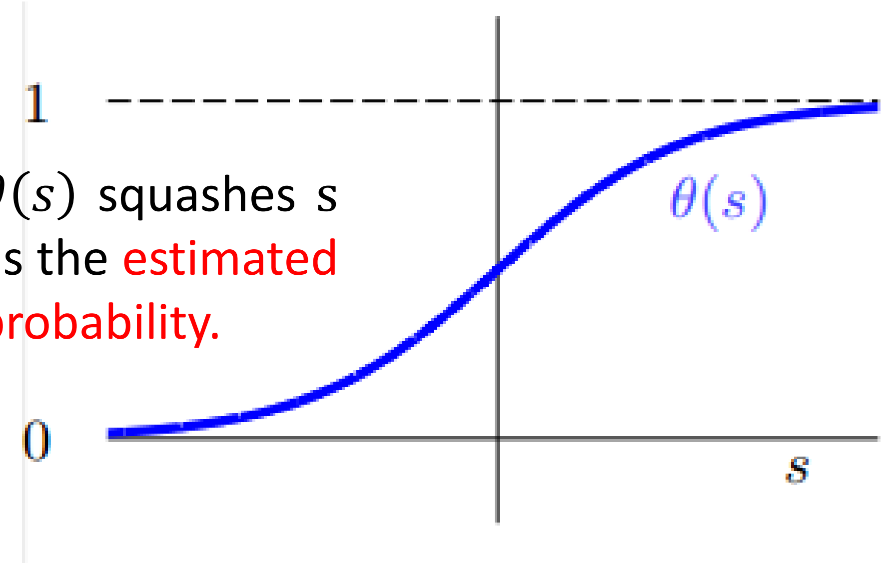
Logistic Hypothesis

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

Let $\boldsymbol{x_i} = (x_{i0}, x_{i1}, x_{i2},\ldots, x_{id})$ be the features of the patient, calculate a weighted 'risk score':

$$s = \sum_{j=0}^{d} w_j x_{ij} = \boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x_i},$$

Convert the score to estimated probability by logistic function $\theta(s)$.

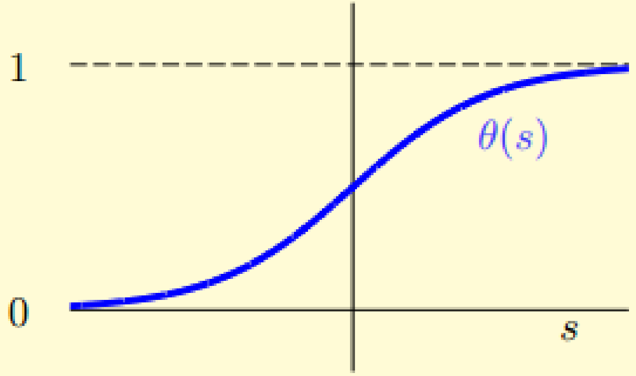


$\theta(s)$ squashes s as the estimated probability.

Logistic hypothesis: $h(\boldsymbol{x_i}) = \theta(\boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x_i})$

Logistic Function

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



smooth, monotonic, sigmoid function of s

Bound	$\theta(s) \in [0,1]$	$\theta(-\infty) = 0$	$\theta(0) = 0.5$	$\theta(\infty) = 1$
Symmetric	$1 - \theta(s) = \theta(-s)$			
Gradient	$\theta'(s) = \theta(s)(1-\theta(s))$			

Logistic regression use $h(\boldsymbol{x}) = \theta(\boldsymbol{w}^T\boldsymbol{x})$ to approximate the target $f(\boldsymbol{x}) = p(+1|\boldsymbol{x})$

Exercise

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

Exercise

Logistic Regression and Binary Classification

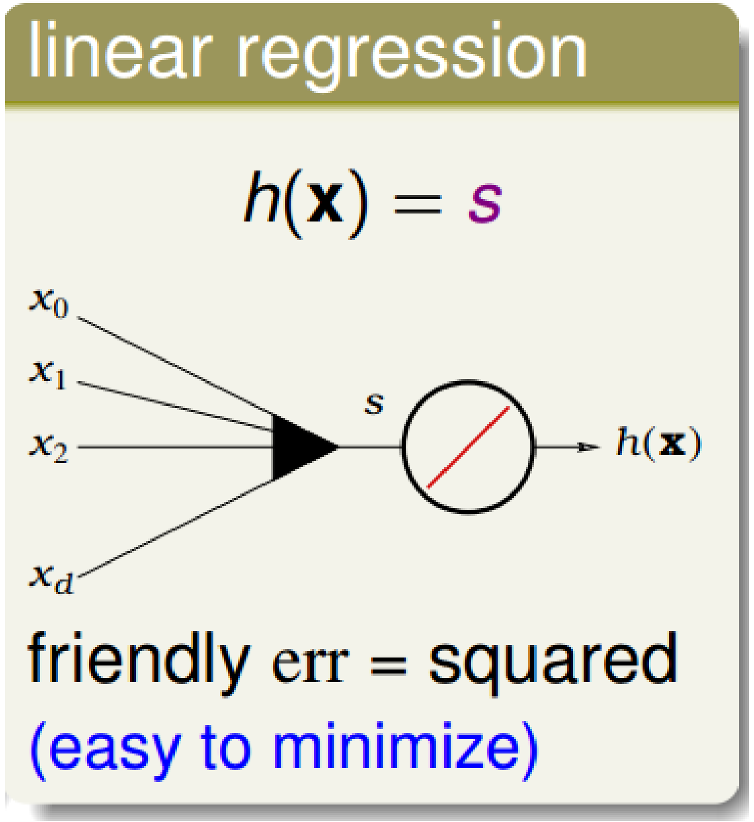
Consider any logistic hypothesis $h(\mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x})}$ that approximates $P(y|\mathbf{x})$. 'Convert' $h(\mathbf{x})$ to a binary classification prediction by taking $\text{sign}\left(h(\mathbf{x}) - \frac{1}{2}\right)$. What is the equivalent formula for the binary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

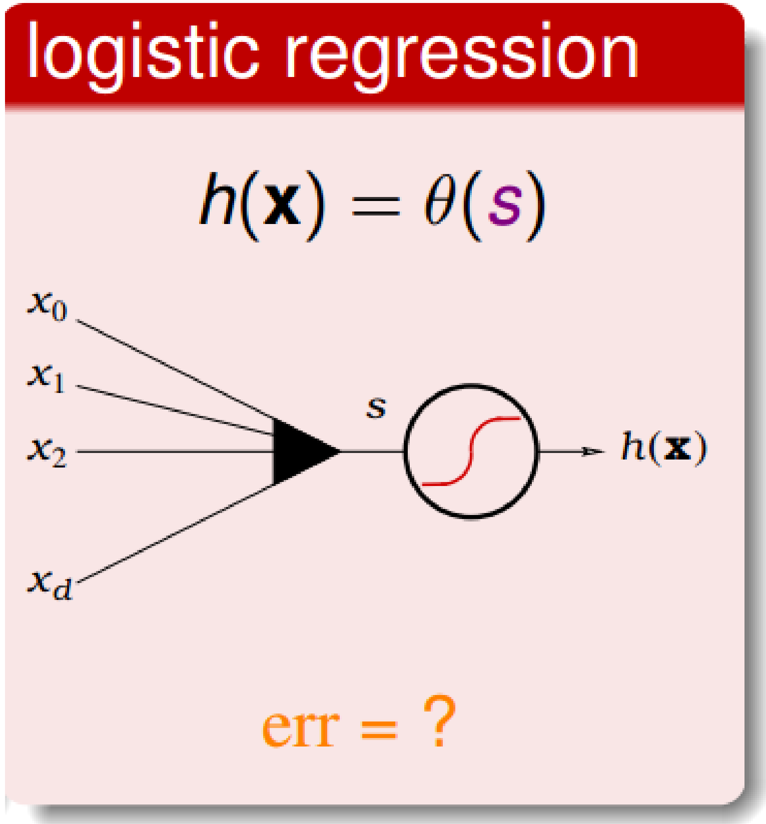
1. $\text{sign}\left(\mathbf{w}^T\mathbf{x} - \frac{1}{2}\right)$
2. $\text{sign}\left(\mathbf{w}^T\mathbf{x}\right)$
3. $\text{sign}\left(\mathbf{w}^T\mathbf{x} + \frac{1}{2}\right)$
4. none of the above

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.

Linear Models





How to define the cost (error) function for logistic regression?

Logistic Regression--$y \in \{0,1\}$

Target function:
$f(x) = p(+1|\boldsymbol{x})$

$\Longleftrightarrow$

$$p(y|\boldsymbol{x}) = \begin{cases} f(\boldsymbol{x}) & \text{for } y = 1 \\ 1 - f(\boldsymbol{x}) & \text{for } y = 0 \end{cases}$$

Consider $\mathcal{D} = \{(\boldsymbol{x}_1, +), (\boldsymbol{x}_2, -), \dots, (\boldsymbol{x}_m, -)\}$

Likelihood that h generates $\mathcal{D}$

Maximum-Likelihood Estimation

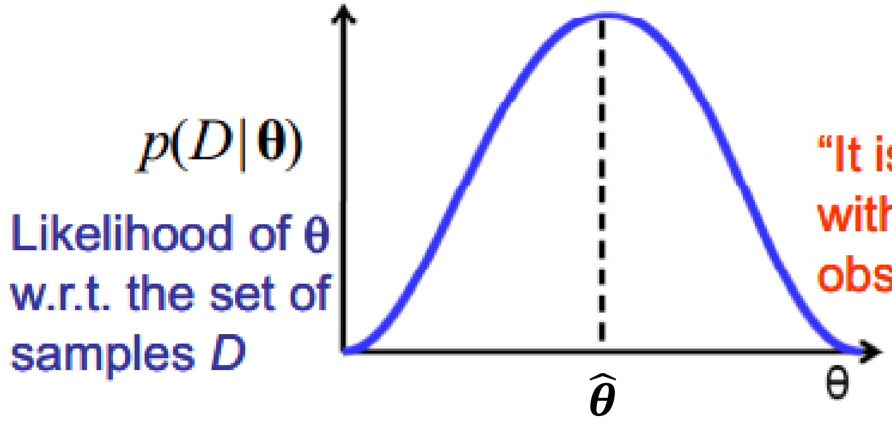
Given a dataset $\mathcal{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_n\}$, where the n samples are drawn independently from identical distribution $\mathrm{p}(\boldsymbol{x}|\boldsymbol{\theta})$, estimate parameters $\boldsymbol{\theta}$.

ML estimate parameters $\boldsymbol{\theta}$ maximizes $\mathrm{p}(\mathcal{D}|\boldsymbol{\theta})$

$\mathcal{D}$ is an i.i.d set

$$\widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \mathrm{p}(\mathcal{D}|\boldsymbol{\theta})$$

$$\mathrm{p}(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^{n} \mathrm{p}(\boldsymbol{x}_k|\boldsymbol{\theta})$$



"It is the value of θ that best agrees with or supports the actually observed training samples"

Logistic Regression--$y \in \{0,1\}$

Target function:
$f(x) = p(+1|\boldsymbol{x})$

$\Longleftrightarrow$

$$p(y|\boldsymbol{x}) = \begin{cases} f(\boldsymbol{x}) & \text{for } y = 1 \\ 1 - f(\boldsymbol{x}) & \text{for } y = 0 \end{cases}$$

Consider $\mathcal{D} = \{(\boldsymbol{x}_1, +), (\boldsymbol{x}_2, -), \ldots, (\boldsymbol{x}_m, -)\}$

Likelihood that h generates $\mathcal{D}$

$$p(\boldsymbol{x}_1)h(\boldsymbol{x}_1)$$
$$p(\boldsymbol{x}_2)(1 - h(\boldsymbol{x}_2))$$
$$\vdots$$
$$p(\boldsymbol{x}_m)(1 - h(\boldsymbol{x}_m))$$

- If $h \approx f$, then likelihood $(h) \approx$ that using (f)
- Probability using (f) is usually large

Likelihood of Logistic Regression

Goal: $\arg\max_{h} likelihood(h)$ $\quad$ $likelihood(h) = \prod_{i=1}^{m} p(\boldsymbol{x_i})p(y|\boldsymbol{x_i})$

Consider $\mathcal{D} = \{(\boldsymbol{x_1}, +), (\boldsymbol{x_2}, -), \dots, (\boldsymbol{x_m}, -)\}$

$$likelihood(h) = \prod_{i=1}^{m} p(\boldsymbol{x_i})p(y_i|\boldsymbol{x_i})$$

$$= p(x_1)h(\boldsymbol{x}_1)p(x_2)(1 - h(\boldsymbol{x}_2)) \cdots p(x_m)(1 - h(\boldsymbol{x}_m))$$

We remove all the $p(x_i)$ which remains the same for all the hypothesis h .

Likelihood of Logistic Regression

Goal: $\arg\max_{h} likelihood(h)$ $\quad likelihood(h) = \prod_{i=1}^{m} p(\boldsymbol{x_i}) p(y|\boldsymbol{x_i})$

Consider $\mathcal{D} = \{(\boldsymbol{x_1}, +), (\boldsymbol{x_2}, -), \dots, (\boldsymbol{x_m}, -)\}$

$$p(y_i|\boldsymbol{x_i}) = \begin{cases} h(\boldsymbol{x_i}) & \text{for } y_i = 1 \\ 1 - h(\boldsymbol{x_i}) & \text{for } y_i = 0 \end{cases} \Longleftrightarrow p(y_i|\boldsymbol{x_i}) = h(\boldsymbol{x_i})^{y_i}(1 - h(\boldsymbol{x_i}))^{(1-y_i)}$$

Bernoulli distribution

$$likelihood(h) \propto \prod_{i=1}^{m} p(y_i|\boldsymbol{x_i}) = \prod_{i=1}^{m} h(\boldsymbol{x_i})^{y_i}(1 - h(\boldsymbol{x_i}))^{(1-y_i)}$$

Log-Likelihood of Logistic Regression

Negative Log-likelihood

$$\min_{h} E(h) = \sum_{i=1}^{m} -(y_i ln\, h(\boldsymbol{x_i}) + (1 - y_i)\, ln(1 - h(\boldsymbol{x_i})))$$

Cross-entropy loss

Cross-entropy

$$H(p, q) = -\sum_{x} p(x) \log(q(x))$$

$$p \in \{y, 1 - y\}$$
$$q \in \{h(\boldsymbol{x}), 1 - h(\boldsymbol{x})\}$$

Negative Log-likelihood

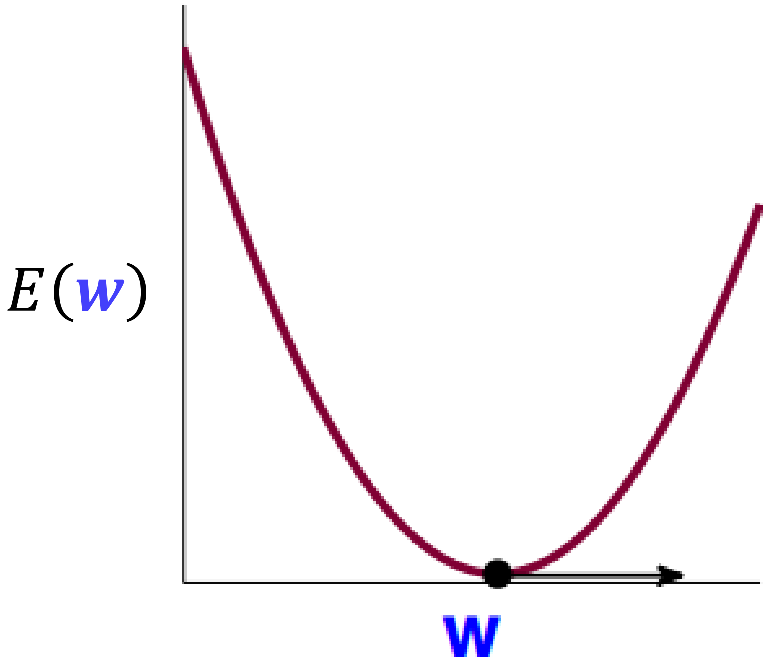
$$\min_{\boldsymbol{w}} \sum_{i=1}^{m} \left[-y_i ln\left(\frac{1}{1 + e^{-\boldsymbol{w}^T \boldsymbol{x}_i}}\right) - (1 - y_i) ln\left(\frac{1}{1 + e^{\boldsymbol{w}^T \boldsymbol{x}_i}}\right) \right]$$

$$\min_{\boldsymbol{w}} \sum_{i=1}^{m} \left[-y_i \boldsymbol{w}^T \boldsymbol{x_i} + ln(1 + e^{\boldsymbol{w}^T \boldsymbol{x}_i}) \right]$$

Minimize $E(w)$

$$\min_{\boldsymbol{w}} E(\boldsymbol{w}) = \sum_{i=1}^{m} \left[-y_i \boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x}_{\boldsymbol{i}} + ln(1 + e^{\boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x}_i}) \right]$$

Cross-entropy loss



$E(w)$: continuous, differentiable, twice-differentiable, **convex**

We want to find the valley

$$\nabla E(w) = 0$$

Gradient $\nabla E(w)$

$$\nabla E(\boldsymbol{w}) = \sum_{\mathrm{i}=1}^{m}\left[-y_i\boldsymbol{x_i} + \frac{e^{\boldsymbol{w}^T\boldsymbol{x}_i}}{1+e^{\boldsymbol{w}^T\boldsymbol{x}_i}}\boldsymbol{x_i}\right] = \sum_{\mathrm{i}=1}^{m}[\theta(\boldsymbol{w}^T\boldsymbol{x_i}) - y_i]\boldsymbol{x_i} = 0$$

- $\nabla E(\boldsymbol{w}) = 0 \;\Leftrightarrow\; \begin{cases}\theta(\boldsymbol{w}^T\boldsymbol{x_i}) = 1, \text{if } y_i = 1\\ \theta(\boldsymbol{w}^T\boldsymbol{x_i}) = 0, \text{if } y_i = 0\end{cases} \;\Leftrightarrow\; \begin{cases}\boldsymbol{w}^T\boldsymbol{x_i} \to \infty, \text{if } y_i = 1\\ \boldsymbol{w}^T\boldsymbol{x_i} \to -\infty, \text{if } y_i = 0\end{cases}$
  - ➢ The data must be linearly separable. :-(
- $\nabla E(\boldsymbol{w})$ is a non-linear equation of $\boldsymbol{w}$
  - ➢ It is hard to derive the closed form solution. :-(

Gradient $\nabla E(w)$

$$\nabla E(\boldsymbol{w}) = \sum_{i=1}^{m}\left[-y_i\boldsymbol{x}_i + \frac{e^{\boldsymbol{w}^T\boldsymbol{x}_i}}{1+e^{\boldsymbol{w}^T\boldsymbol{x}_i}}\boldsymbol{x}_i\right] = \sum_{i=1}^{m}[\theta(\boldsymbol{w}^T\boldsymbol{x}_i) - y_i]\boldsymbol{x}_i = \boldsymbol{X}^T(\hat{\boldsymbol{y}} - \boldsymbol{y})$$

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m1} & x_{m2} & \cdots & x_{md} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \vdots \\ \boldsymbol{x}_m^T \end{pmatrix} \in \mathbb{R}^{m\times(d+1)},\ \hat{\boldsymbol{y}} = \begin{pmatrix} \theta(\boldsymbol{w}^T\boldsymbol{x}_1) \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_2) \\ \vdots \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_m) \end{pmatrix} \in \mathbb{R}^m,\ \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} \in \mathbb{R}^m$$

- Apply the Newton's method to the logistic regression,

$$\boldsymbol{w} = \boldsymbol{w}_t - \boldsymbol{H}(\boldsymbol{w}_t)^{-1}\nabla E(\boldsymbol{w}_t)$$

- Need to solve,

$$\boldsymbol{H} = \nabla^2 E(\boldsymbol{w}) = \frac{\nabla E(\boldsymbol{w})}{\nabla \boldsymbol{w}} = ?$$

Gradient $\nabla E(w)$

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}\left[\theta\left(\mathbf{w}^T \mathbf{x}_i\right) - y_i\right]\mathbf{x}_i$$

$$\boldsymbol{H} = \nabla^2 E(\mathbf{w}) = \frac{\nabla E(\mathbf{w})}{\nabla \mathbf{w}}$$

$$\boldsymbol{H} = \sum_{i=1}^{m} \frac{\nabla\{\theta(\mathbf{w}^T \mathbf{x}_i)\mathbf{x}_i\}}{\nabla \mathbf{w}}$$

Identities: vector-by-vector $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$

Condition	Expression	Numerator layout, i.e. by $\mathbf{y}$ and $\mathbf{x}^T$	Denominator layout, i.e. by $\mathbf{y}^T$ and $\mathbf{x}$
$\mathbf{a}$ is not a function of $\mathbf{x}$	$\frac{\partial \mathbf{a}}{\partial \mathbf{x}} =$	$\mathbf{0}$	
	$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{I}$	
$\mathbf{A}$ is not a function of $\mathbf{x}$	$\frac{\partial \mathbf{A}\mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{A}$	$\mathbf{A}^\top$
$\mathbf{A}$ is not a function of $\mathbf{x}$	$\frac{\partial \mathbf{x}^\top \mathbf{A}}{\partial \mathbf{x}} =$	$\mathbf{A}^\top$	$\mathbf{A}$
a is not a function of $\mathbf{x}$, $\mathbf{u} = \mathbf{u}(\mathbf{x})$	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	
$a = a(\mathbf{x})$, $\mathbf{u} = \mathbf{u}(\mathbf{x})$	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{u}\frac{\partial a}{\partial \mathbf{x}}$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial a}{\partial \mathbf{x}}\mathbf{u}^\top$
$\mathbf{A}$ is not a function of $\mathbf{x}$, $\mathbf{u} = \mathbf{u}(\mathbf{x})$	$\frac{\partial \mathbf{A}\mathbf{u}}{\partial \mathbf{x}} =$	$\mathbf{A}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{A}^\top$
$\mathbf{u} = \mathbf{u}(\mathbf{x})$, $\mathbf{v} = \mathbf{v}(\mathbf{x})$	$\frac{\partial (\mathbf{u}+\mathbf{v})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$	
$\mathbf{u} = \mathbf{u}(\mathbf{x})$	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}$
$\mathbf{u} = \mathbf{u}(\mathbf{x})$	$\frac{\partial \mathbf{f}(\mathbf{g}(\mathbf{u}))}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}$

Gradient $\nabla E(w)$

$$\nabla E(\boldsymbol{w}) = \sum_{i=1}^{m}[\theta(\boldsymbol{w}^T\boldsymbol{x}_i) - y_i]\boldsymbol{x}_i$$

$$\boldsymbol{H} = \nabla^2 E(\boldsymbol{w}) = \frac{\nabla E(\boldsymbol{w})}{\nabla \boldsymbol{w}}$$

$$\boldsymbol{H} = \sum_{i=1}^{m}\frac{\nabla\{\theta(\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i\}}{\nabla \boldsymbol{w}}$$

a: $\theta(\boldsymbol{w}^T\boldsymbol{x}_i)$

$\boldsymbol{u}(\boldsymbol{w})$: $\boldsymbol{x}_i$

$\frac{\nabla\theta(\boldsymbol{w}^T\boldsymbol{x}_i)}{\nabla \boldsymbol{w}}$ is a scalar –by-vector problem.

Identities: vector-by-vector $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$

Condition	Expression	Numerator layout, i.e. by y and x^T	Denominator layout, i.e. by y^T and x
a is not a function of **x**	$\frac{\partial \mathbf{a}}{\partial \mathbf{x}} =$	$\mathbf{0}$	
	$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{I}$	
A is not a function of **x**	$\frac{\partial \mathbf{A}\mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{A}$	$\mathbf{A}^\top$
A is not a function of **x**	$\frac{\partial \mathbf{x}^\top \mathbf{A}}{\partial \mathbf{x}} =$	$\mathbf{A}^\top$	$\mathbf{A}$
a is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	
$a = a(\mathbf{x})$, **u** = **u**(**x**)	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{u}\frac{\partial a}{\partial \mathbf{x}}$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial a}{\partial \mathbf{x}}\mathbf{u}^\top$
A is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial \mathbf{A}\mathbf{u}}{\partial \mathbf{x}} =$	$\mathbf{A}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{A}^\top$
u = **u**(**x**), **v** = **v**(**x**)	$\frac{\partial(\mathbf{u}+\mathbf{v})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$	
u = **u**(**x**)	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}$
u = **u**(**x**)	$\frac{\partial \mathbf{f}(\mathbf{g}(\mathbf{u}))}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}$

Gradient $\nabla E(w)$

$\dfrac{\nabla \theta(w^T x_i)}{\nabla w}$ is a scalar –by-vector problem

Identities: scalar-by-vector $\dfrac{\partial y}{\partial \mathbf{x}} = \nabla_{\mathbf{x}} y$

Condition	Expression	Numerator layout, i.e. by $\mathbf{x}^T$; result is row vector	Denominator layout, i.e. by $\mathbf{x}$; result is column vector
a is not a function of $\mathbf{x}$	$\dfrac{\partial a}{\partial \mathbf{x}} =$	$\mathbf{0}^\top$ [4]	$\mathbf{0}$ [4]
a is not a function of $\mathbf{x}$, $u = u(\mathbf{x})$	$\dfrac{\partial au}{\partial \mathbf{x}} =$	$a\dfrac{\partial u}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$, $v = v(\mathbf{x})$	$\dfrac{\partial (u+v)}{\partial \mathbf{x}} =$	$\dfrac{\partial u}{\partial \mathbf{x}} + \dfrac{\partial v}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$, $v = v(\mathbf{x})$	$\dfrac{\partial uv}{\partial \mathbf{x}} =$	$u\dfrac{\partial v}{\partial \mathbf{x}} + v\dfrac{\partial u}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$	$\dfrac{\partial g(u)}{\partial \mathbf{x}} =$	$\dfrac{\partial g(u)}{\partial u}\dfrac{\partial u}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$	$\dfrac{\partial f(g(u))}{\partial \mathbf{x}} =$	$\dfrac{\partial f(g)}{\partial g}\dfrac{\partial g(u)}{\partial u}\dfrac{\partial u}{\partial \mathbf{x}}$	
$\mathbf{u} = \mathbf{u}(\mathbf{x})$, $\mathbf{v} = \mathbf{v}(\mathbf{x})$	$\dfrac{\partial (\mathbf{u}\cdot\mathbf{v})}{\partial \mathbf{x}} = \dfrac{\partial \mathbf{u}^\top \mathbf{v}}{\partial \mathbf{x}} =$	$\mathbf{u}^\top\dfrac{\partial \mathbf{v}}{\partial \mathbf{x}} + \mathbf{v}^\top\dfrac{\partial \mathbf{u}}{\partial \mathbf{x}}$ • assumes numerator layout of $\dfrac{\partial \mathbf{u}}{\partial \mathbf{x}}, \dfrac{\partial \mathbf{v}}{\partial \mathbf{x}}$	$\dfrac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{v} + \dfrac{\partial \mathbf{v}}{\partial \mathbf{x}}\mathbf{u}$ • assumes denominator layout of $\dfrac{\partial \mathbf{u}}{\partial \mathbf{x}}, \dfrac{\partial \mathbf{v}}{\partial \mathbf{x}}$

Gradient $\nabla E(w)$

$\frac{\nabla\theta(w^T x_i)}{\nabla w}$ is a scalar –by-vector problem $u: w^T x_i$ $\theta: g$ $\frac{\nabla\theta(w^T x_i)}{\nabla w} = \theta(w^T x_i)\theta(-w^T x_i)x_i$

Identities: scalar-by-vector $\frac{\partial y}{\partial \mathbf{x}} = \nabla_{\mathbf{x}} y$

Condition	Expression	Numerator layout, i.e. by $\mathbf{x}^T$; result is row vector	Denominator layout, i.e. by $\mathbf{x}$; result is column vector
a is not a function of $\mathbf{x}$	$\frac{\partial a}{\partial \mathbf{x}} =$	$\mathbf{0}^\top$ [4]	$\mathbf{0}$ [4]
a is not a function of $\mathbf{x}$, $u = u(\mathbf{x})$	$\frac{\partial au}{\partial \mathbf{x}} =$	$a\frac{\partial u}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$, $v = v(\mathbf{x})$	$\frac{\partial(u+v)}{\partial \mathbf{x}} =$	$\frac{\partial u}{\partial \mathbf{x}} + \frac{\partial v}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$, $v = v(\mathbf{x})$	$\frac{\partial uv}{\partial \mathbf{x}} =$	$u\frac{\partial v}{\partial \mathbf{x}} + v\frac{\partial u}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$	$\frac{\partial g(u)}{\partial \mathbf{x}} =$	$\frac{\partial g(u)}{\partial u}\frac{\partial u}{\partial \mathbf{x}}$	
$u = u(\mathbf{x})$	$\frac{\partial f(g(u))}{\partial \mathbf{x}} =$	$\frac{\partial f(g)}{\partial g}\frac{\partial g(u)}{\partial u}\frac{\partial u}{\partial \mathbf{x}}$	
$\mathbf{u} = \mathbf{u}(\mathbf{x})$, $\mathbf{v} = \mathbf{v}(\mathbf{x})$	$\frac{\partial(\mathbf{u}\cdot\mathbf{v})}{\partial \mathbf{x}} = \frac{\partial \mathbf{u}^\top\mathbf{v}}{\partial \mathbf{x}} =$	$\mathbf{u}^\top\frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \mathbf{v}^\top\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$ • assumes numerator layout of $\frac{\partial \mathbf{u}}{\partial \mathbf{x}}, \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{v} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\mathbf{u}$ • assumes denominator layout of $\frac{\partial \mathbf{u}}{\partial \mathbf{x}}, \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$

Gradient $\nabla E(w)$

$$\nabla E(\boldsymbol{w}) = \sum_{i=1}^{m}\left[\theta\left(\boldsymbol{w}^T\boldsymbol{x}_i\right) - y_i\right]\boldsymbol{x}_i$$

$$\boldsymbol{H} = \nabla^2 E(\boldsymbol{w}) = \frac{\nabla E(\boldsymbol{w})}{\nabla \boldsymbol{w}}$$

$$\boldsymbol{H} = \sum_{i=1}^{m} \frac{\nabla\{\theta(\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i\}}{\nabla \boldsymbol{w}}$$

$a:\ \theta(\boldsymbol{w}^T\boldsymbol{x}_i)$

$\boldsymbol{u}(\boldsymbol{w}):\boldsymbol{x}_i$

$$\frac{\nabla\theta(\boldsymbol{w}^T\boldsymbol{x}_i)}{\nabla \boldsymbol{w}} = \theta(\boldsymbol{w}^T\boldsymbol{x}_i)\theta(-\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i$$

$$\boldsymbol{H} = \sum_{i=1}^{m} \boldsymbol{x}_i\theta(\boldsymbol{w}^T\boldsymbol{x}_i)\theta(-\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i^T$$

Identities: vector-by-vector $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$

Condition	Expression	Numerator layout, i.e. by y and $\mathbf{x}^T$	Denominator layout, i.e. by $\mathbf{y}^T$ and x
a is not a function of **x**	$\frac{\partial \mathbf{a}}{\partial \mathbf{x}} =$	$\mathbf{0}$	
	$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{I}$	
A is not a function of **x**	$\frac{\partial \mathbf{A}\mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{A}$	$\mathbf{A}^\top$
A is not a function of **x**	$\frac{\partial \mathbf{x}^\top\mathbf{A}}{\partial \mathbf{x}} =$	$\mathbf{A}^\top$	$\mathbf{A}$
a is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	
a = *a*(**x**), **u** = **u**(**x**)	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{u}\frac{\partial a}{\partial \mathbf{x}}$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial a}{\partial \mathbf{x}}\mathbf{u}^\top$
A is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial \mathbf{A}\mathbf{u}}{\partial \mathbf{x}} =$	$\mathbf{A}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{A}^\top$
u = **u**(**x**), **v** = **v**(**x**)	$\frac{\partial(\mathbf{u}+\mathbf{v})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$	
u = **u**(**x**)	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}$
u = **u**(**x**)	$\frac{\partial \mathbf{f}(\mathbf{g}(\mathbf{u}))}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}$

Gradient $\nabla E(w)$

$$\nabla E(\boldsymbol{w}) = \sum_{i=1}^{m}\left[-y_i\boldsymbol{x}_i + \frac{e^{\boldsymbol{w}^T\boldsymbol{x}_i}}{1+e^{\boldsymbol{w}^T\boldsymbol{x}_i}}\boldsymbol{x}_i\right] = \sum_{i=1}^{m}[\theta(\boldsymbol{w}^T\boldsymbol{x}_i) - y_i]\boldsymbol{x}_i = \boldsymbol{X}^T(\hat{\boldsymbol{y}} - \boldsymbol{y})$$

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m1} & x_{m2} & \cdots & x_{md} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \vdots \\ \boldsymbol{x}_m^T \end{pmatrix} \in \mathbb{R}^{m\times(d+1)}, \hat{\boldsymbol{y}} = \begin{pmatrix} \theta(\boldsymbol{w}^T\boldsymbol{x}_1) \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_2) \\ \vdots \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_m) \end{pmatrix} \in \mathbb{R}^m, \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} \in \mathbb{R}^m$$

$$\boldsymbol{H} = \nabla^2 E(\boldsymbol{w}) = \frac{\nabla E(\boldsymbol{w})}{\nabla \boldsymbol{w}} = \sum_{i=1}^{m} \boldsymbol{x}_i\theta(\boldsymbol{w}^T\boldsymbol{x}_i)\theta(-\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i^T = \boldsymbol{X}^T\boldsymbol{R}\boldsymbol{X}$$

$\boldsymbol{R} \in \mathbb{R}^{m\times m}$ is a diagonal matrix with elements $R_{ii} = \theta(\boldsymbol{w}^T\boldsymbol{x}_i)\theta(-\boldsymbol{w}^T\boldsymbol{x}_i)$

- Is $\boldsymbol{H}$ invertible?

Gradient $\nabla E(w)$

$$\nabla E(\boldsymbol{w}) = \sum_{i=1}^{m}\left[-y_i\boldsymbol{x_i} + \frac{e^{\boldsymbol{w}^T\boldsymbol{x_i}}}{1+e^{\boldsymbol{w}^T\boldsymbol{x_i}}}\boldsymbol{x_i}\right] = \sum_{i=1}^{m}[\theta(\boldsymbol{w}^T\boldsymbol{x_i}) - y_i]\boldsymbol{x_i} = \boldsymbol{X}^T(\widehat{\boldsymbol{y}} - \boldsymbol{y})$$

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m1} & x_{m2} & \cdots & x_{md} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \vdots \\ \boldsymbol{x}_m^T \end{pmatrix} \in \mathbb{R}^{m\times(d+1)}, \widehat{\boldsymbol{y}} = \begin{pmatrix} \theta(\boldsymbol{w}^T\boldsymbol{x}_1) \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_2) \\ \vdots \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_m) \end{pmatrix} \in \mathbb{R}^m, \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} \in \mathbb{R}^m$$

$$\boldsymbol{H} = \nabla^2 E(\boldsymbol{w}) = \frac{\nabla E(\boldsymbol{w})}{\nabla \boldsymbol{w}} = \sum_{i=1}^{m}\boldsymbol{x_i}\theta(\boldsymbol{w}^T\boldsymbol{x_i})\theta(-\boldsymbol{w}^T\boldsymbol{x_i})\boldsymbol{x}_i^T = \boldsymbol{X}^T\boldsymbol{R}\boldsymbol{X}$$

$\boldsymbol{R} \in \mathbb{R}^{m\times m}$ is a diagonal matrix with elements $R_{ii} = \theta(\boldsymbol{w}^T\boldsymbol{x_i})\theta(-\boldsymbol{w}^T\boldsymbol{x_i})$

- Is $\boldsymbol{H}$ invertible?
  - Yes! $\boldsymbol{H}$ is positive definite.
  - Hint: prove $\boldsymbol{v}^T\boldsymbol{H}\boldsymbol{v}>0$ for any $\boldsymbol{v}$. Leave it as your homework.

Gradient $\nabla E(w)$

$$\nabla E(\boldsymbol{w}) = \sum_{i=1}^{m}\left[-y_i\boldsymbol{x}_i + \frac{e^{\boldsymbol{w}^T\boldsymbol{x}_i}}{1+e^{\boldsymbol{w}^T\boldsymbol{x}_i}}\boldsymbol{x}_i\right] = \sum_{i=1}^{m}[\theta(\boldsymbol{w}^T\boldsymbol{x}_i) - y_i]\boldsymbol{x}_i = \boldsymbol{X}^T(\hat{\boldsymbol{y}} - \boldsymbol{y})$$

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m1} & x_{m2} & \cdots & x_{md} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \vdots \\ \boldsymbol{x}_m^T \end{pmatrix} \in \mathbb{R}^{m\times(d+1)},\ \hat{\boldsymbol{y}} = \begin{pmatrix} \theta(\boldsymbol{w}^T\boldsymbol{x}_1) \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_2) \\ \vdots \\ \theta(\boldsymbol{w}^T\boldsymbol{x}_m) \end{pmatrix} \in \mathbb{R}^m,\ \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} \in \mathbb{R}^m$$

$$\boldsymbol{H} = \nabla^2 E(\boldsymbol{w}) = \frac{\nabla E(\boldsymbol{w})}{\nabla \boldsymbol{w}} = \sum_{i=1}^{m}\boldsymbol{x}_i\theta(\boldsymbol{w}^T\boldsymbol{x}_i)\theta(-\boldsymbol{w}^T\boldsymbol{x}_i)\boldsymbol{x}_i^T = \boldsymbol{X}^T\boldsymbol{R}\boldsymbol{X}$$

$\boldsymbol{R} \in \mathbb{R}^{m\times m}$ is a diagonal matrix with elements $R_{ii} = \theta(\boldsymbol{w}^T\boldsymbol{x}_i)\theta(-\boldsymbol{w}^T\boldsymbol{x}_i)$

- Apply the Newton's method to the logistic regression,

$$\boldsymbol{w} = \boldsymbol{w}_t - \boldsymbol{H}(\boldsymbol{w}_t)^{-1}\nabla E(\boldsymbol{w}_t)$$

Compare with Linear Regression

For the linear regression with the sum-of-squares error function, we have,

$$E(\boldsymbol{w}) = \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2 = (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})^T (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$$

$$\nabla E(\boldsymbol{w}) = \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^T\boldsymbol{y}$$

$$\boldsymbol{H} = \nabla^2 E(\boldsymbol{w}) = \frac{\nabla E(\boldsymbol{w})}{\nabla \boldsymbol{w}} = \boldsymbol{X}^T\boldsymbol{X}$$

$\boldsymbol{H}$ is a constant: the error function is quadratic.

Apply the Newton's method to the logistic regression,

$$\boldsymbol{w} = \boldsymbol{w}_t - \boldsymbol{H}(\boldsymbol{w}_t)^{-1}\nabla E(\boldsymbol{w}_t)$$

$$\boldsymbol{w} = \boldsymbol{w}_t - (\boldsymbol{X}^T\boldsymbol{X})^{-1}(\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}_t - \boldsymbol{X}^T\boldsymbol{y}) = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

Closed-form

The Newton method gives the exact solution in one step.

Summary

Linear Regression

- **Problem**
  - Use hyperplanes to approximate real values
- **Error (Cost) function**
  - Least square
  - $E(w)$: continuous, differentiable, **convex**
- **Algorithm**
  - Analytic solution with pseudo-inverse

Summary

Logistic Regression

- **Problem**
  - $P(+1|x)$ as target and $\theta(\boldsymbol{w}^T \boldsymbol{x_i})$ as hypotheses
- **Error (Cost) Function**
  - Negative log-likelihood (cross-entropy)
  - $E(w)$: continuous, differentiable, twice-differentiable, **convex**
- **Optimization**
  - Iterative methods, e.g., Gradient descent, newton method