Linear Models - Classification and Regression

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Outline

- Introduction
- Linear Classification
- Linear Regression

Introduction (1/2)

- Supervised learning 監督式學習
 - The most popular paradigm for machine learning
 - Given a dataset with input attribute(s) and output label(s), discovering a relationship between the input and the output
 - Can be divided into classification and regression problems
 - Classification(分類): with nominal (名目式) output label(s)
 - Regression(迴歸): with numeric (數值式) output label(s)

Introduction (2/2)

Linear models

Algorithms searching a hypothesis over the hyperplane(超平面)
hypothesis space

Hyperplane

- The set of all points that are in R^M and satisfy a linear equation
- In R², the hyperplanes are straight lines (直線,一維(2-1))
- In R³, hyperplanes are planes (平面,二維(3-1))
- More generally, if the input instance space is M-dimensional then its hyperplanes are (M-1)-dimensional
- 超過三度空間之後我們就沒有辦法畫了,所以超過三度空間的我們叫做超平面
- 狹義的說法:在R4、R5、R6
- 廣義的說法:在R2、R3、R4 、R5、R6

Outline

- Introduction
- Linear Classification
- Linear Regression

Illustrative Example for Linear Classification

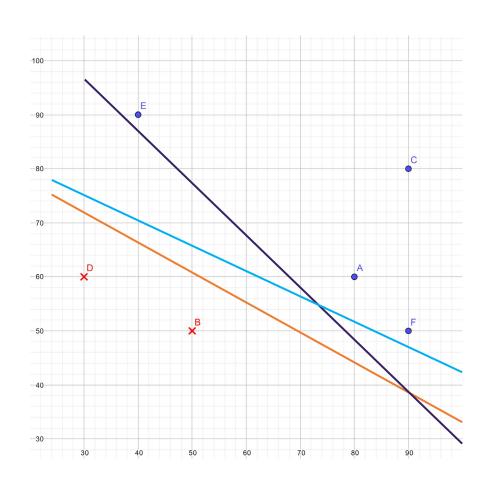
- Dataset D
 - Students take a class on a Pass/Fail basis

Student	x_1 (Midterm)	X_2 (Final)	y (Pass/Fail)
S			
A	80	60	+1 (Pass)
В	50	50	–1 (Fail)
C	90	80	+1 (Pass)
D	30	60	–1 (Fail)
E	40	90	+1 (Pass)
F	90	50	+1 (Pass)

Data Representation

- The dataset D
 - Training Examples: $(\mathbf{x}_A, y_A), (\mathbf{x}_B, y_B), \dots, (\mathbf{x}_F, y_F)$
 - 註:粗體表示向量 ex: **X**A(第一個同學的兩個分量)
 - **x**_A, **x**_B, ..., **x**_F: input
 - Each x is a vector with two attributes
 - **x** = (Midterm, Final) = $(x_1, x_2) = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$
 - y_A , y_B , ..., y_F : output (+1 or -1)

Hypothesis Space and Version Space



Hypothesis Space (假說空間) H = The set of straight lines

<註>所有的假說形成的集合。是我認為一條直線可以把它分開,但是這條直線可能可以分開,可能不能分開,對於那些可以分開的我們叫它Version Space

Version Space $VS_{H,D}$ = {All straight lines that separate positive and negative examples.}

註記: Version Space並不唯一

->如果點(data)越多,能找到正確的直線的可能性就變高了

We can apply the Perceptron Learning Algorithm (PLA) to find a consistent hypothesis(一致假設)

Perceptron Learning Algorithm (PLA) (1/2)

透過不斷的內積、修正錯誤,進而找到一條可以將資料分成兩類的演算法

- For input $\mathbf{x} = (x_1, x_2)$ //grades of a students
- Pass if $w_1 x_1 + w_2 x_2 >$ threshold $((w_1 x_1 + w_2 x_2) -$ threshold) > 0
- Fail if $w_1 x_1 + w_2 x_2 < \text{threshold}$ $((w_1 x_1 + w_2 x_2) - \text{threshold}) < 0$
- This linear formula $h \in H$ can be written as
- $h(\mathbf{x}) = \text{sign}((w_1 x_1 + w_2 x_2) \text{threshold})$

Perceptron Learning Algorithm (PLA) (2/2)

```
• h(\mathbf{x}) = \text{sign } ((w_1 x_1 + w_2 x_2) - \text{threshold})
Let w_0 = -\text{threshold}
\Rightarrow h(\mathbf{x}) = \text{sign } ((w_1 x_1 + w_2 x_2) + w_0)
Introduce an artificial coordinate x_0 = 1 (\text{Atgh. A}) \text{BYA - OUR CPS ALTHOUSE} \text{ATGH.}
\Rightarrow h(\mathbf{x}) = \text{sign } (w_0 x_0 + w_1 x_1 + w_2 x_2)
```

• We can write h(x) in vector form:

```
h (x) = sign (w•x) // • inner product
where w = (w_0, w_1, w_2) and x = (x_0, x_1, x_2) // x_0 = 1
```

What PLA Does? (1/4)

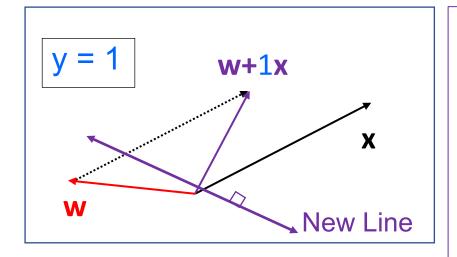
```
Given the training examples: (\mathbf{x}_A, y_A), (\mathbf{x}_B, y_B), ..., (\mathbf{x}_F, y_F) if an input example, \mathbf{x}_k, is misclassified (它該+1時,你算出來是-1,它該是-1時,你算出來是+1) (i.e., sign (\mathbf{w} \bullet \mathbf{x}_k) \neq y_k, k \in \{A, B, ..., F\}) then update the weight vector \mathbf{w} \mathbf{w} \leftarrow \mathbf{w} + y_k \mathbf{x}_k // Note that y_k is +1 or -1
```

What PLA Does? (2/4)

- Two misclassified types for a training example (x, y)
- Type 1: (答案應是1,我算出來的卻是-1)

```
y = 1 (正解) but h(\mathbf{x}) = \text{sign} (w_0 x_0 + w_1 x_1 + w_2 x_2) = -1 (x_0 \setminus x_1 \setminus x_{2\pi} w_0 \setminus w_1 \setminus w_2在平面的兩側) \Rightarrow PLA: \mathbf{w} \leftarrow \mathbf{w} + y\mathbf{x} \Rightarrow PLA: \mathbf{w} \leftarrow \mathbf{w} + 1\mathbf{x} // make \mathbf{w} close to \mathbf{x}
```

• W想成是法向量



$$y = 1$$

我希望 $X_0 \ X_1 \ X_{2\pi} W_0 \ W_1 \ W_2$ 在同一面

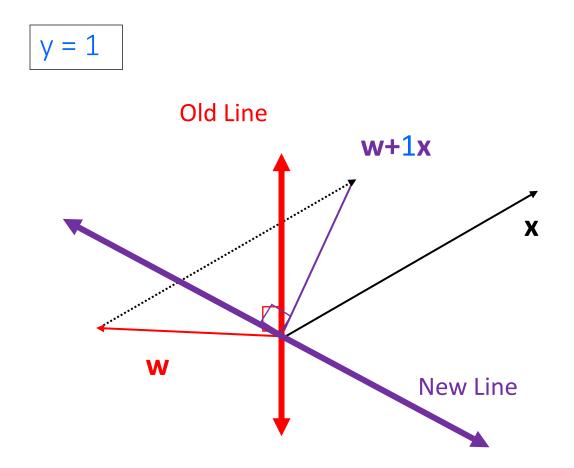
w : Normal vector of the line

x: The training example

w+1x: Normal vector of the new line

- w_0 、 w_1 、 w_{2} 代表 R_3 空間的平面的法向量
- x_0 、 x_1 、 x_2 代表 R_3 空間的任何一個點,只是有一個虛擬的 x_0 的x軸=1,所以我所有的 x_0 都是在1這個地方,但可以假想成自從引入了這個虛擬的x軸以後,好像 x_0
- $^{\bullet}$ 請問 $^{\bullet}X_0$ 、 $^{\bullet}X_1$ 、 $^{\bullet}X_2$ 和 $^{\bullet}W_0$ 、 $^{\bullet}W_1$ 、 $^{\bullet}W_2$ 的內積是多少?
- * 若>0,表示W跟X是在同一個法向量的平面上
- 若<0,表示W跟X是在法向量的另外兩側</p>

What PLA Does? (3/4)



PLA:

 $w \leftarrow w + 1x$ // make w close to x

w: Normal vector of the line

x: The training example

w+1x: Normal vector of the new line

(怎麼加? Ans:平行四邊形的對角線)

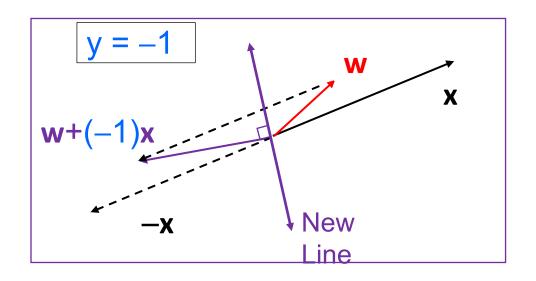
What PLA Does? (4/4)

• Type 2: (答案是-1,你卻算出來是+1,表示其實你的X應該要跟法向量是另外一邊)

```
y = -1 but h(x) = sign (w_0 x_0 + w_1 x_1 + w_2 x_2) = 1

\Rightarrow PLA: w \leftarrow w + yx
```

 \Rightarrow PLA: w \leftarrow w + (-1)x // move w away from x



w : Normal vector of the line

x: The training example

 $\mathbf{w}+(-1)\mathbf{x}$: Normal vector of the new line

The PLA Algorithm

Epoch: scan所有的data一次

Given training dataset:

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\} // N \text{ training examples}$$

Initialize all weights w_i to random values

// **w** =
$$(w_0, w_1, ..., w_M)$$
; M+1 attributes

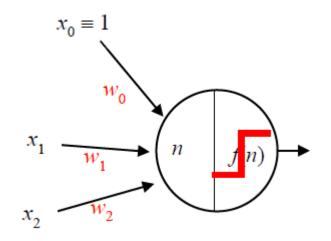
WHILE not all examples correctly predicted DO

FOR each training example $\mathbf{x}_k \in D$

If sign $(\mathbf{w} \bullet \mathbf{x}_k) \neq y_k$ then $\mathbf{w} \leftarrow \mathbf{w} + y_k \mathbf{x}_k$

Note: The PLA is guaranteed to converge if the training set is linearly separable.

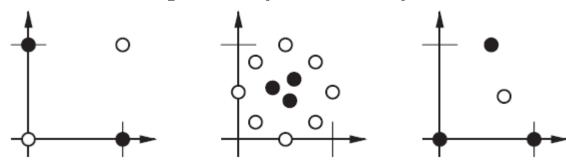
Perceptron Architecture



- Net input: $n = w_0 x_0 + w_1 x_1 + w_2 x_2$
- Activation Function:
 - f(n) = sign(n)
 - Two different outputs
 - Binary Classification

Remarks on PLA (1/2)

- The decision boundary is always orthogonal (正交的) to the weight vector.
- Single-layer perceptrons can only classify linearly separable inputs(只能分類可線性分離的資料們).
- The PLA cannot solve linearly inseparable problems.
- Examples of linearly inseparable problems:



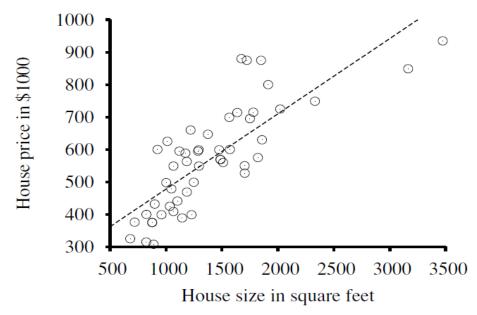
Remarks on PLA (2/2)

- Variants of PLA:
 - Activation Function: $a = f(n) = \begin{cases} 0 & \text{if } n < 0 \\ 1 & \text{if } n \ge 0 \end{cases}$
 - $\mathbf{w} \leftarrow \mathbf{w} + e \mathbf{x}$; e = (y a)

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Illustrative Example for Linear Regression



Simple Linear Regression:

Finding a relationship between two continuous variables; x and y = f(x)

Data points of Price (= y) vs. House size (= x) for sale in Berkeley, CA, in July 2009, along with the linear regression that minimizes squared error: $\hat{y} = 0.232x + 246$.

Data Representation

In general, a dataset has N examples with M input attributes

N Training Examples: (\mathbf{x}_1, y_1) , (\mathbf{x}_2, y_2) , ..., (\mathbf{x}_N, y_N)

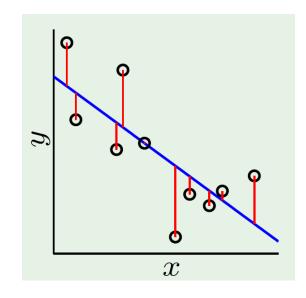
x₁, **x**₂, ..., **x**_N: input

Each x is a vector with M attributes

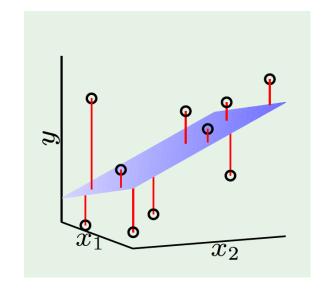
$$\mathbf{x} = (x_1, x_2, ..., x_M) = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_M \end{bmatrix} : M \text{ input attributes}$$

 $y_1, y_2, ..., y_N$: output; each y is a real number

Illustration of Linear Regression



10 (= N) training examples 1 (= M) attribute; *x*



10 (= N) training examples 2 (= M) attributes; x_1, x_2

How to Measure the Error? (1/2)

- How well does a hypothesis function
 h(x) approximate the target function f(x)?
- In linear regression, we can measure the accuracy of our hypothesis function using an error function (又稱 cost function or loss function).
- One common measure:

the squared error $(h(\mathbf{x}) - f(\mathbf{x}))^2$

How to Measure the Error? (2/2)

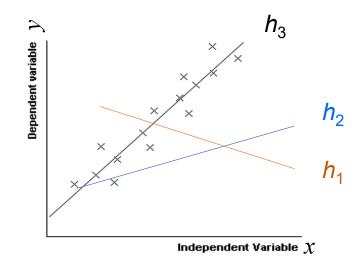
Error of the training examples

:
$$E(h) = \frac{1}{2} \frac{1}{N} \sum_{k=1}^{N} (h(\mathbf{x}_k) - y_k)^2$$
 // Replace $f(\mathbf{x})$ by y_k

- $\frac{1}{N}\sum_{k=1}^{N}(h(\mathbf{x}_k)-y_k)^2$: Mean of the squares of $(h(\mathbf{x}_k)-y_k)$, k=1,...,N
- Half the mean (½) as a convenience (1/2是為了之後方便計算) for the later computation of the gradient descent

Minimizing Error Function

- Each *h* represents a line, $h(x) = w_0 + w_1 x$ if training examples have only one attribute *x*
 - Minimize $E(h) = E(w_0, w_1) = \frac{1}{2} \frac{1}{N} \sum_{k=1}^{N} (h(x_k) y_k)^2$



Note: $h(x) = w_0 + w_1 x$

 w_0 : y-intercept

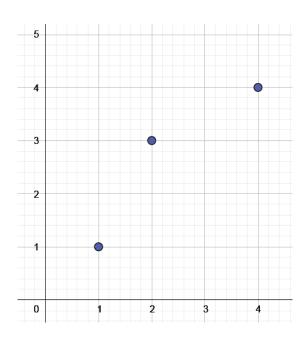
 w_1 : the slope of line

Error Function – one weight (1/5)

Assume that $w_0 = 0$ 通過原點

// A line pass through the origin $h(x) = w_0 + w_1 x = w_1 x$

$$\Rightarrow h(x) = wx$$
 // Let $w_1 = w$ for the sake of simplicity(為了簡單)



Training examples (x, y): (1, 1), (2, 3), (4, 4)

$$E(h) = E(w) = \frac{1}{2} \frac{1}{3} \sum_{k=1}^{3} (h(x_k) - y_k)^2$$

Error Function – one weight (2/5)

Training examples:
$$(x_1, y_1) = (1, 1)$$
; $(x_2, y_2) = (2, 3)$; $(x_3, y_3) = (4, 4)$

$$E(h) = E(w) = \frac{1}{2} \frac{1}{3} \sum_{k=1}^{3} (h(x_k) - y_k)^2$$
If $w = \frac{1}{2}$ then $h1(x_1) = wx_1 = \frac{1}{2} * 1 = \frac{1}{2}$

$$h1(x_2) = wx_2 = \frac{1}{2} * 2 = 1$$

$$h1(x_3) = wx_3 = \frac{1}{2} * 4 = 2$$

$$\Rightarrow E(w) = \frac{1}{2} \frac{1}{3} \sum_{k=1}^{3} (h1(x_k) - y_k)^2$$

$$= \frac{1}{2} \frac{1}{3} \{(\frac{1}{2} - 1)^2 + (1 - 3)^2 + (2 - 4)^2\} = \frac{33}{24}$$

Error Function – one weight (3/5)

If
$$w = 1$$
 then $h2(x_1) = wx_1 = 1^* \ 1 = 1$
 $h2(x_2) = wx_2 = 1^* \ 2 = 2$
 $h2(x_3) = wx_3 = 1^* \ 4 = 4$

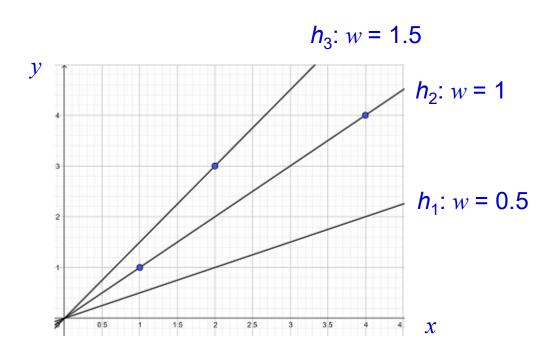
$$\Rightarrow E(w) = \frac{1}{2} \frac{1}{3} \sum_{k=1}^{3} (h2(x_k) - y_k)^2$$

$$= \frac{1}{2} \frac{1}{3} \{ (1-1)^2 + (2-3)^2 + (4-4)^2 \} = \frac{1}{6}$$
If $w = \frac{3}{2}$ then $h3(x_1) = wx_1 = \frac{3}{2} * 1 = \frac{3}{2}$
 $h3(x_2) = wx_2 = \frac{3}{2} * 2 = 3$
 $h3(x_3) = wx_3 = \frac{3}{2} * 4 = 6$

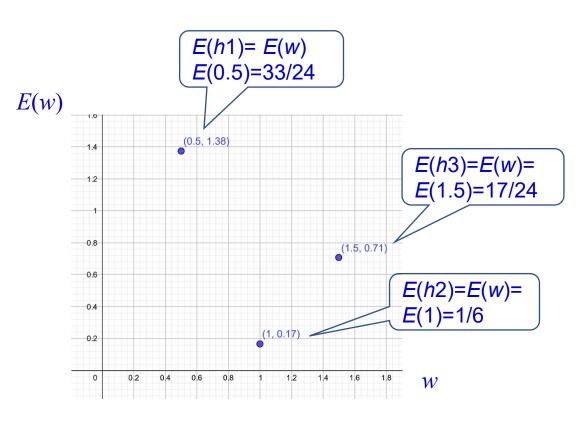
$$\Rightarrow E(w) = \frac{1}{2} \frac{1}{3} \sum_{k=1}^{3} (h3(x_k) - y_k)^2$$

$$= \frac{1}{2} \frac{1}{3} \{ (\frac{3}{2} - 1)^2 + (3-3)^2 + (6-4)^2 \} = \frac{17}{24}$$

Error Function – one weight (4/5)

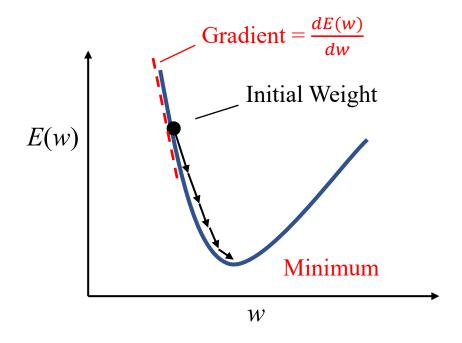


Data points and different hypotheses



Error Function: E(w)

Error Function – one weight (5/5)



Note: When w is a scalar, the gradient(梯度) is the tangent line.

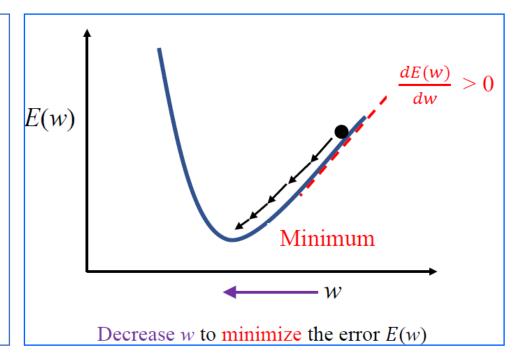
Gradient Descent – one weight (1/5)

Update the current weight w using the gradient descent $(-\frac{dE(w)}{dw})$ multiplied by some factor called the learning rate, η

Case 1: slope $\geq 0 \ (\frac{dE(w)}{dw} \geq 0)$

$$W \leftarrow W - \boxed{\eta \frac{dE(w)}{dw}}$$
 Positive

// Decrease w to minimize the error E(w)



Gradient Descent – one weight (2/5)

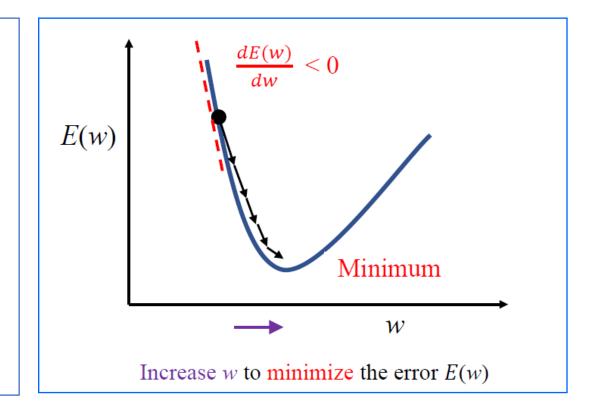
這個error function要往Minimum的方向走的話, 一定都是跟它的微分的負方向有關

Case 2: slope
$$\leq 0$$
 $\left(\frac{dE(w)}{dw} \leq 0\right)$
 $W \leftarrow W - \eta \frac{dE(w)}{dw}$

Negative

 e

// Increase w to minimize the error $E(w)$



Gradient Descent – one weight (3/5)

Training rule for gradient descent:

$$W \leftarrow W + \eta \left(-\frac{dE(w)}{dw}\right)$$

- We make steps down the error function in the direction with the steepest descent(下降最陡的方向).
- The size of each step is determined by the parameter η , which is called the learning rate.
 - If η is too small, gradient descent can be slow.
 - If η is too large(一次走太大步), gradient descent can overshoot the minimum of E. It may fail to converge, or even diverge(發散).

Gradient Descent – one weight (4/5)

• What is $\frac{dE(w)}{dw}$?

If we assume one single training example only (x, y)

then
$$E(h) = E(w) = \frac{1}{2}(h(x) - y)^2 = \frac{1}{2}(wx - y)^2$$

 \Rightarrow The gradient of E (= the slope of E)

$$\frac{dE(w)}{dw} = \frac{d(\frac{1}{2}(wx - y)^2)}{dw} = \frac{1}{2}(2)(wx - y)\frac{d(wx - y)}{dw} = (wx - y)x$$
 $\frac{dE(w)}{dw} = \frac{d(\frac{1}{2}(wx - y)^2)}{dw} = \frac{1}{2}(2)(wx - y)\frac{d(wx - y)}{dw} = (wx - y)x$

Gradient Descent – one weight (5/5)

Training rule for gradient descent:

$$w \leftarrow w + \eta \left(-\frac{dE(w)}{dw}\right)$$

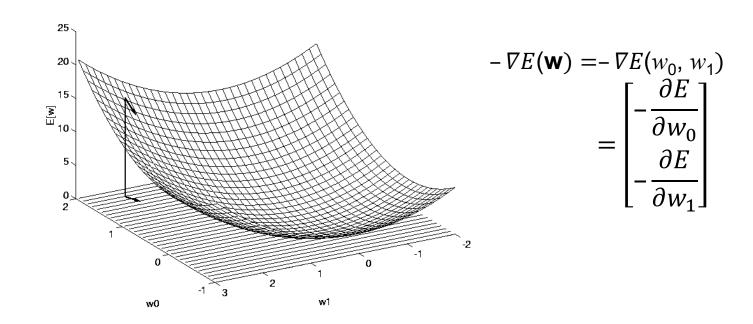
$$\Rightarrow w \leftarrow w + \eta \left(-(wx - y)x\right)$$

$$\Rightarrow w \leftarrow w + \eta \left(y - wx\right)x$$
Learning Rate Input

(Output Label – Estimated Output)

Error Function - two weights

- Example: two weights: $\mathbf{w} = (w_0, w_1)$
 - Arrow: negated gradient at one point
 - Steepest descent along the surface: $-\nabla E(\mathbf{w})$



Gradient Descent – two weights (1/2)

• If $w_0 \neq 0$ and one single training example only: (x, y), then

$$E(h) = E(w_0, w_1) = \frac{1}{2} (h(x) - y)^2$$
$$= \frac{1}{2} (w_0 x_0 + w_1 x_1 - y)^2 // x_0 = 1, x_1 = x$$

The gradient of E

•
$$\nabla E(\mathbf{w}) = \nabla E(w_0, w_1) = \begin{bmatrix} \frac{\partial E}{\partial w_0} \\ \frac{\partial E}{\partial w_1} \end{bmatrix} = \begin{bmatrix} (w_0 x_0 + w_1 x_1 - y) x_0 \\ (w_0 x_0 + w_1 x_1 - y) x_1 \end{bmatrix}$$

Gradient Descent – two weights (2/2)

Training rule for gradient descent:

$$w_0 \leftarrow w_0 + \eta \left(y - \left(w_0 x_0 + w_1 x_1 \right) x_0 \right)$$

$$w_1 \leftarrow w_1 + \eta \left(y - \left(w_0 x_0 + w_1 x_1 \right) x_1 \right)$$

Vector form

Let
$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$
, and $\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix}$, then
$$\mathbf{w} \leftarrow \mathbf{w} + \eta (\mathbf{y} - \mathbf{w}^\mathsf{T} \mathbf{x}) \mathbf{x}$$
Learning Rate Input (Output Label – Estimated Output)

Error Function – (M+1) weights (1/2)

Now, consider a single example with M attributes:

•
$$E(h) = \frac{1}{2}(h(\mathbf{x}) - y)^2$$

where $\mathbf{x} = (x_0, x_1, x_2, ..., x_M) = \begin{bmatrix} x_0 \equiv 1 \\ x_1 \\ x_2 \\ \vdots \\ x_M \end{bmatrix}$, and

$$h(\mathbf{x}) = w_0 x_0 + w_1 x_1 + w_2 x_2 + \dots + w_M x_M$$

- = w·x // inner product of two column vectors
- = $\mathbf{w}^{\mathsf{T}}\mathbf{x}$ // row vector \mathbf{w}^{T} times column vector \mathbf{x}

Error Function— (M+1) weights (2/2)

- $\mathbf{w} = (w_0, w_1, w_2, w_3, ..., w_M)$ is to be determined and to be fit in the learning problem.
- The space *H* of candidate hypothesis is the set of all possible real-valued weight vectors:

```
H = \{\mathbf{w} | \mathbf{w} \in \mathbb{R}^{M+1}\}
```

Gradient Descent – (M+1) weights (1/2)

• Gradient of E with respect to $\mathbf{w} = (w_0, w_1, ..., w_M)$:

$$\nabla E(\mathbf{w}) = \nabla E(w_0, w_1, \dots, w_M) = \begin{bmatrix} \frac{\partial E}{\partial w_0} \\ \frac{\partial E}{\partial w_1} \\ \vdots \\ \frac{\partial E}{\partial w_M} \end{bmatrix} = \begin{bmatrix} (w_0 x_0 + w_1 x_1 + \dots + w_M x_M - y) x_0 \\ (w_0 x_0 + w_1 x_1 + \dots + w_M x_M - y) x_1 \\ \vdots \\ (w_0 x_0 + w_1 x_1 + \dots + w_M x_M - y) x_M \end{bmatrix}$$

$$= \begin{bmatrix} (h(\mathbf{x}) - y)x_0 \\ (h(\mathbf{x}) - y)x_1 \\ \vdots \\ (h(\mathbf{x}) - y)x_M \end{bmatrix} = (h(\mathbf{x}) - y) \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_M \end{bmatrix} = (\mathbf{w}^\mathsf{T}\mathbf{x} - y) \mathbf{x}$$

Gradient Descent – (M+1) weights (2/2)

Training rule for gradient descent:

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \left(-\nabla E(\mathbf{w}) \right)$$

$$\Rightarrow \mathbf{w} \leftarrow \mathbf{w} + \eta \left(-(\mathbf{w}^{\mathsf{T}} \mathbf{x} - y) \mathbf{x} \right)$$

$$\Rightarrow \mathbf{w} \leftarrow \mathbf{w} + \eta \left(y - \mathbf{w}^{\mathsf{T}} \mathbf{x} \right) \mathbf{x} // \text{ Vector form}$$

We may write the rule in its component form

$$w_i \leftarrow w_i + \eta (y - \mathbf{w}^\mathsf{T} \mathbf{x}) x_i$$

// Component form; $i = 0, 1, ..., M$

The Gradient Descent Algorithm

Given training data set:

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\} // N \text{ training examples}$$

Initialize all weights w_i to random values

// **w** =
$$(w_0, w_1, ..., w_M)$$
; M+1 attributes

UNTIL the termination condition is met, DO

FOR each training example $\mathbf{x}_k \in D$

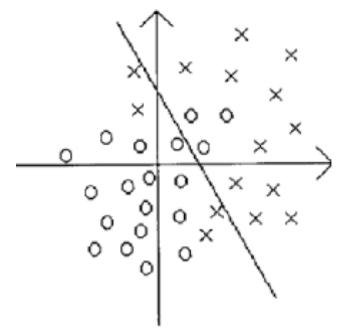
$$\mathbf{w} \leftarrow \mathbf{w} + \eta (y_k - \mathbf{w}^\mathsf{T} \mathbf{x}_k) \mathbf{x}_k$$

Remarks on the Gradient Descent Algorithm (1/2)

- The gradient descent algorithm is also known as 又稱為
 - Delta rule
 - ADALINE rule
 - Widrow-Hoff rule
- The gradient descent algorithm is used in regression(迴歸) problems whose training data have an infinite(無限) number of outputs.
 - Regression: with numeric output label(s) ⇒ an infinite number of values
- However, it can also be used in classification(分類) problems whose training data have a finite(有限) number of outputs.
 - Classification: with nominal output label(s) ⇒ a finite number of values

Remarks on the Gradient Descent Algorithm (2/2)

• When we use the gradient descent algorithm to solve a classification problem, it converges toward a best-fit(最適合的) approximation to the target concept If the training examples are not linearly separable(不可線性分離).



Summary

- Linear Classification(分類)
 - Perceptron Learning Algorithm
 - If sign $(\mathbf{w} \bullet \mathbf{x}) \neq y$ then $\mathbf{w} \leftarrow \mathbf{w} + y \mathbf{x}$
 - w: Normal vector of the decision boundary
 - (\mathbf{x} , \mathbf{y}): Training example with nominal output \mathbf{y} (= ± 1)
- Linear Regression(迴歸)
 - The Gradient Descent Algorithm
 - w \leftarrow w + $\eta (y \mathbf{w}^\mathsf{T} \mathbf{x}) \mathbf{x}$
 - w: Normal vector of the linear function
 - (x, y): Training example with numeric output y
 - η : Learning rate

Kahoot

- (T)1. A one-neuron perceptron can classify two classes of objects.
- (F) 2. The average squared difference between classifier predicted output and actual output is the Mean Absolute Error.
- (T) 3. The goal of the gradient descent is to minimize a given loss function of the neural network.
- (F) 4. Gradient descent always converges to some global minimum.
- (T) 5. The "learning rate" is the step size that is the amount the weights are updated during training.

- (F) 6. In batch gradient descent, we consider one example at a time to update the current weight and bias values.
- (F) 7. Logistic regression is mainly used for regression. (It is popularly used for classification.)
- (T) 8. The cost function for logistic regression is the Cross-Entropy.
- (T) 9. Logistic regression predicts the probability of the occurrence of a binary outcome.
- (F) 10. Logistic regression transforms its output using the tanh function to return a probability value.(tanh function(+1~-1)只能視為是Logistic regression的變形

References

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