



### **Generalized linear model**

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#### ≻Linear regression

#### ➤Classification and logistic regression

#### ➤Generalized linear model



## Part I. Linear regression

#### Linear regression





hypothesis function:  $h_{\theta}(x) = \theta_0 + \theta_1 x$ 



What if we have more features?

$$h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x, \qquad \text{let } x_0 = 1$$

How to learn this model?

Find a set of  $\theta$  so that h(x) is close to given examples.



So we define the cost function:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2.$$

We want to choose  $\theta$  so as to minimize  $J(\theta)$ .

Question 1. Why we choose the ordinary least squares method? Question 2. Where does the  $\frac{1}{2}$  come from?



## Gradient descent can converge to a local minimum, even with the learning rate $\alpha$ fixed.



#### Gradient descent



**Data Mining Lab** 



Andrew Ng

#### Gradient descent





#### Gradient descent





 $J(\theta)$  is a quadratic function—global optimum

Different alpha

## Batch gradient descent 数据挖掘实验室 **Data Mining Lab** $\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2} \left( h_{\theta}(x) - y \right)^2$ $= 2 \cdot \frac{1}{2} \left( h_{\theta}(x) - y \right) \cdot \frac{\partial}{\partial \theta_j} \left( h_{\theta}(x) - y \right)$ $J(\theta) = \frac{1}{2} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2.$ $= (h_{\theta}(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left( \sum_{i=0}^n \theta_i x_i - y \right)$ $= (h_{\theta}(x) - y) x_i$ $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_i} J(\theta).$ Repeat until convergence { $\theta_j := \theta_j + \alpha \sum_{i=1}^m \left( y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)} \qquad \text{(for every } j\text{)}.$ } Batch gradient descent

Stochastic gradient descent

Stochastic gradient descent Loop { for i=1 to m, {  $\theta_{i} := \theta_{i} + \alpha_{i} (u^{(i)} - h_{i}(x^{(i)}))$ 

for i=1 to m, {  $\theta_j := \theta_j + \alpha \left( y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)} \quad \text{(for every } j\text{)}.$ }

- }
- Batch gradient descent has to scan through the entire training set before taking a single step—a costly operation if m is large;
- 2. Stochastic gradient descent gets  $\theta$  "close" to the minimum much faster than batch gradient descent;
- 3. The parameters  $\theta$  will keep oscillating around the minimum of J( $\theta$ );
- 4. Particularly when the training set is large, stochastic gradient descent is often preferred over batch gradient descent.

#### Stochastic gradient descent



2000



BGD

SGD

#### Probabilistic interpretation



- Why might the least-squares cost function J, be a reasonable choice?
- Let us assume that the target variables and the inputs are related via the equation:

$$y^{(i)} = \theta^T x^{(i)} + \epsilon^{(i)},$$

assume that  $\epsilon^{(i)} \sim N(0, \sigma^2).$ 

 According to *central limit theorem*, for the most commonly studied scenarios, when independent random variables are added, their sum tends toward a normal distribution. Probabilistic interpretation



The density of  $\epsilon^{(i)}$  is given by

$$p(\epsilon^{(i)}) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(\epsilon^{(i)})^2}{2\sigma^2}\right).$$

This implies that

$$p(y^{(i)}|x^{(i)};\theta) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right).$$



#### likelihood function:

$$L(\theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta)$$
  
= 
$$\prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y^{(i)} - \theta^{T} x^{(i)})^{2}}{2\sigma^{2}}\right).$$

log likelihood:

$$\begin{split} \ell(\theta) &= \log L(\theta) \\ &= \log \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^{T} x^{(i)})^{2}}{2\sigma^{2}}\right) \\ &= \sum_{i=1}^{m} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^{T} x^{(i)})^{2}}{2\sigma^{2}}\right) \\ &= m \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^{2}} \cdot \frac{1}{2} \sum_{i=1}^{m} (y^{(i)} - \theta^{T} x^{(i)})^{2}. \end{split}$$



Hence, maximizing  $\ell(\theta)$  gives the same answer as minimizing

$$\frac{1}{2}\sum_{i=1}^{m} (y^{(i)} - \theta^T x^{(i)})^2,$$

which we recognize to be  $J(\theta)$ , our original least-squares cost function.

To summarize: When errors follow a Gaussian distribution, least-squares regression can be justified as a very natural method that's just doing maximum likelihood estimation.

Note that, our final choice of  $\theta$  did not depend on what was  $\sigma^2$ .



## Part II. Classification and logistic regression





We need a  $h_{\theta}(x)$  for logistic regression.



#### Classification and logistic regression





<Machine learning> ex2 by Andrew Ng

Classification and logistic regression



Let us assume that

$$P(y = 1 | x; \theta) = h_{\theta}(x)$$
  

$$P(y = 0 | x; \theta) = 1 - h_{\theta}(x)$$

Note that this can be written more compactly as

$$p(y \mid x; \theta) = (h_{\theta}(x))^{y} (1 - h_{\theta}(x))^{1-y}$$

Write down the likelihood of the parameters as

$$L(\theta) = p(\vec{y} \mid X; \theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta) = \prod_{i=1}^{m} (h_{\theta}(x^{(i)}))^{y^{(i)}} (1 - h_{\theta}(x^{(i)}))^{1-y^{(i)}}$$

Classification and logistic regression



It will be easier to maximize the log likelihood:

$$\begin{split} \ell(\theta) &= \log L(\theta) \\ &= \sum^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)})) \\ \frac{\partial}{\partial \theta_{j}} \ell(\theta) &= \left( y \frac{1}{g(\theta^{T}x)} - (1 - y) \frac{1}{1 - g(\theta^{T}x)} \right) \frac{\partial}{\partial \theta_{j}} g(\theta^{T}x) \\ &= \left( y \frac{1}{g(\theta^{T}x)} - (1 - y) \frac{1}{1 - g(\theta^{T}x)} \right) g(\theta^{T}x) (1 - g(\theta^{T}x) \frac{\partial}{\partial \theta_{j}} \theta^{T}x \\ &= \left( y (1 - g(\theta^{T}x)) - (1 - y) g(\theta^{T}x) \right) x_{j} \\ &= \left( y - h_{\theta}(x) \right) x_{j} \end{split}$$

Stochastic Gradient ascent rule:

$$\theta_j := \theta_j + \alpha \left( y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}$$



## Part III. Generalized linear model



In statistics, the **generalized linear model** (**GLM**) is a flexible generalization of ordinary linear regression that allows for response variables that have error distribution models other than a normal distribution. The GLM generalizes linear regression by allowing the linear model to be related to the response variable via a *link function* and by allowing the magnitude of the variance of each measurement to be a function of its predicted value.

-By Wikipedia



The GLM consists of three elements:

- 1. A probability distribution from the exponential family.
- 2. A linear predictor  $\eta = \theta^T x$ .
- 3. A link function g such that  $E(Y) = \mu = g^{-1}(\eta)$



## $p(y;\eta) = b(y) \exp(\eta^T T(y) - a(\eta))$

Here,  $\eta$  is called the **natural parameter** (also called the **canonical parameter**) of the distribution; T(y) is the **sufficient statistic** (for the distributions we consider, it will often be the case that T(y) = y); and  $a(\eta)$  is the **log partition function**. The quantity  $e^{-a(\eta)}$  essentially plays the role of a normalization constant, that makes sure the distribution  $p(y; \eta)$  sums/integrates over y to 1.

The exponential family



$$p(y;\eta) = b(y) \exp(\eta^T T(y) - a(\eta))$$

$$P(y; \varphi) = \varphi^{y}(1 - \varphi)^{1-y} = \exp(\log\varphi^{y}(1 - \varphi)^{1-y})$$
$$= \exp(y\log\varphi + (1 - y)\log(1 - \varphi))$$
$$= \exp(y\log\frac{\varphi}{1 - \varphi} + \log(1 - \varphi))$$

For Bernoulli distribution

b(y) = 1  
T(y) = y  

$$\eta = \log \frac{\varphi}{1-\varphi} \Rightarrow \varphi = \frac{1}{1+e^{-\eta}}$$
a(\eta) = -log(1-\varphi) = 1 + e^{-\eta}
The logistic model is the pre-probability

estimation for Bernoulli distribution.

# The exponential family $p(y;\eta) = b(y) \exp(\eta^T T(y) - a(\eta))$ $\text{set } \sigma^2 = 1$ $N(\mu, 1) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(y-\mu)^2\right) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}y^2 - \frac{1}{2}\mu^2 + \mu y\right)$ $= \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}y^2) \exp(\mu y - \frac{1}{2}\mu^2)$

For Gaussian distribution

$$egin{aligned} b(y) &= rac{1}{\sqrt{2\pi}} \, exp(-rac{1}{2} \, y^2) \ && T(y) = y \ && \eta = \mu \ && a(\eta) = rac{1}{2} \, \mu^2 \end{aligned}$$



1.  $y \mid x; \theta \sim Exponential Family(\eta)$ . I.e., given x and  $\theta$ , the distribution of y follows some exponential family distribution, with parameter  $\eta$ .

2. Given x, our goal is to predict the expected value of T(y) given x. In most of our examples, we will have T(y) = y, so this means we would like the prediction h(x) output by our learned hypothesis h to satisfy h(x) = E[y|x].

3. The natural parameter  $\eta$  and the inputs x are related linearly:  $\eta = \theta^T x$ .

(1)  $y|x; \theta$  *ExponentialFamily* ( $\eta$ ); 给定样本x与参数 $\theta$ , 样本分类y 服从指数分布族中的某个分布; (2) 给定一个 x, 我们需要的目标函数为 $h_{\theta}(x) = E[T(y)|x];$ (3) $\eta = \theta^{T}x$ 。



From Bernoulli distribution to logistic regression model :

$$egin{aligned} h_{ heta}(x) &= E[T(y)|x] = E[y|x] = p(y=1|x; heta)\ &= arphi\ &= rac{1}{1+e^{-\eta}}\ &= rac{1}{1+e^{- heta Tx}} \end{aligned}$$

The first equality follows from Assumption 2, above; the second equality follows from the fact that y|x;  $\theta \sim Bernoulli(\varphi)$ ; the third equality follows from Bernoulli distribution is an exponential family distribution; the fourth equality follows from Assumption 3, above.



From Gaussian distribution to linear model:

$$egin{aligned} h_{ heta}(x) &= E(T(y)|x) = E[y|x] \ &= \mu \ &= \eta \ &= heta^T x \end{aligned}$$

The first equality follows from Assumption 2, above; the second equality follows from the fact that  $y|x; \theta \sim N(\mu, \sigma^2)$ , and so its expected value is given by  $\mu$ ; the third equality follows from Assumption 1; and the last equality follows from Assumption 3.





- η以不同的映射函数与其它概率分布函数中的参数发生联系,从 而得到不同的模型。
- GLM将指数分布族中的所有成员都作为linear model的扩展,
   通过各种非线性的映射函数g<sup>-1</sup>(η) = E[T(y); η]将线性函数映
   射到其他空间,从而大大扩大了线性模型可解决的问题。
- 广义线性模型通过假设一个概率分布,得到不同的模型,而梯度
   下降是为了求取模型中的线性部分(θ<sup>T</sup>x)的参数θ的。



