**EE226 Big Data Mining Lecture 4** 

# Supervised Learning

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#### **Reference and Acknowledgement**

• Most of the course materials are credited to Andrew Ng's CS229 lecture notes.

### Outline

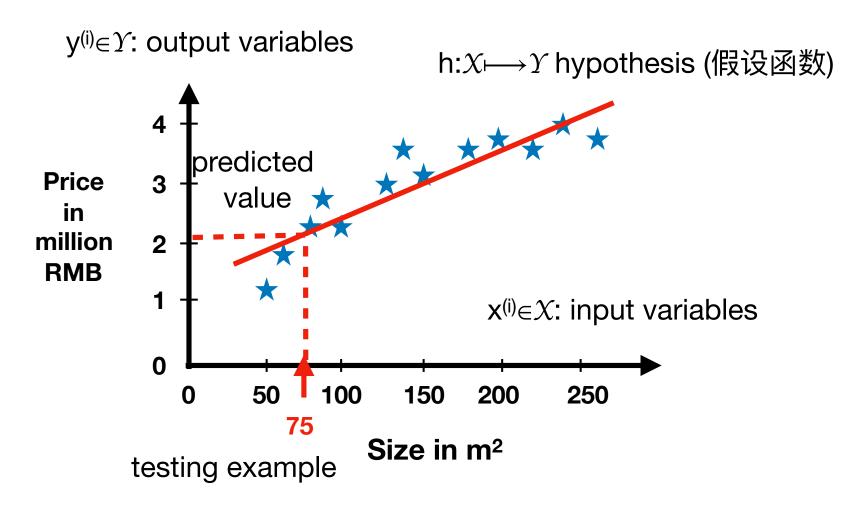
- Linear Regression (线性回归)
- Classification and Logistic Regression (逻辑回归)
- Generalized Linear Models

### Outline

- Linear Regression (线性回归)
- Classification and Logistic Regression (逻辑回归)
- Generalized Linear Models

#### Supervised Learning Example Revisited

 $(x^{(i)}, y^{(i)})$ : a training example { $(x^{(i)}, y^{(i)})$ ; i = 1,..., m}: training set



#### Supervised Learning Example Revisited

Let's consider a richer dataset in which we also know the number of bedrooms in each apartment

Size	#bedrooms	Price (million ¥ )
40	0	1.2
65	1	1.9
80	2	2.2
89	2	3.3
120	3	5.3

Why a linear function?

- x: two-dimensional vectors in  $\mathcal{R}^2$
- x<sub>1</sub><sup>(i)</sup>: the size of the i-th apartment in the training set
- x2<sup>(i)</sup>: the number of bedrooms of the i-th apartment in the training set
- We decide hypothesis h as a linear function:  $h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$
- θ<sub>i</sub>: parameters/weights of h
- By letting  $\mathbf{x}_0 = \mathbf{1}$ , we rewrite h as  $h(x) = \sum_{i=0}^n \theta_i x_i = \theta^T x$

#### Supervised Learning Example Revisited

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40	0	1.2	
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120	3	5.3	
Why a least-squares cost?			

• By letting 
$$x_0 = 1$$
, we rewrite h as

$$h(x) = \sum_{i=0}^{\infty} \theta_i x_i = \theta^T x$$

- How can we learn θ? Making h(x) close to y for the training examples!
- cost function (损失函数):

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

# Least-Mean Square Alg

 How to choose θ to minimize J(θ)? Let's start with some "initial guess" for θ, and use gradient descent (梯度下降) alg. repeatedly to make J(θ) smaller:

$$\theta_j := \theta_j - \alpha \underbrace{\partial J(\theta)}_{\theta_j}$$
 direction of steepest decrease of J  $\alpha$ : learning rate

• What is the partial derivative (偏导数) term?

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_{\theta}(x) - y)^2$$

$$= 2 \cdot \frac{1}{2} (h_{\theta}(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_{\theta}(x) - y)$$

$$= (h_{\theta}(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left( \sum_{i=0}^n \theta_i x_i - y \right)$$

$$= (h_{\theta}(x) - y) x_j$$

# Least-Mean Square Alg

- Two ways to modify the method:
  - batch gradient descent: scan through the entire training set before taking a single step

Repeat until convergence {

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

• stochastic gradient descent: update parameters according to the gradient of the error w.r.t. a single training example

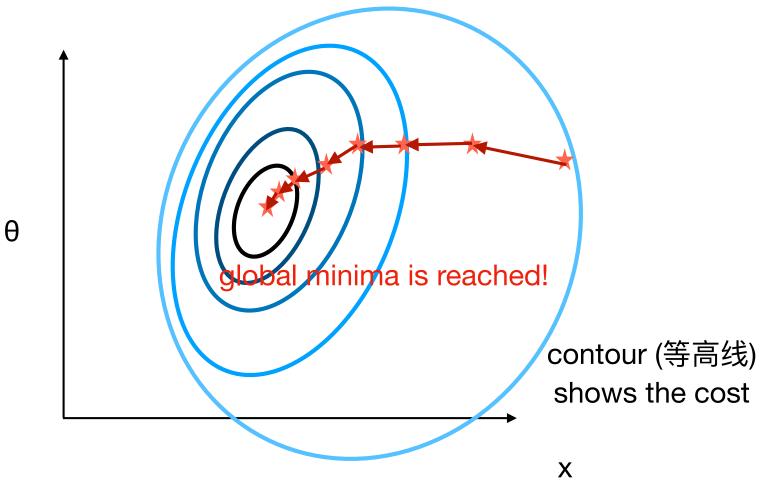
Loop {

for i=1 to m, {  

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

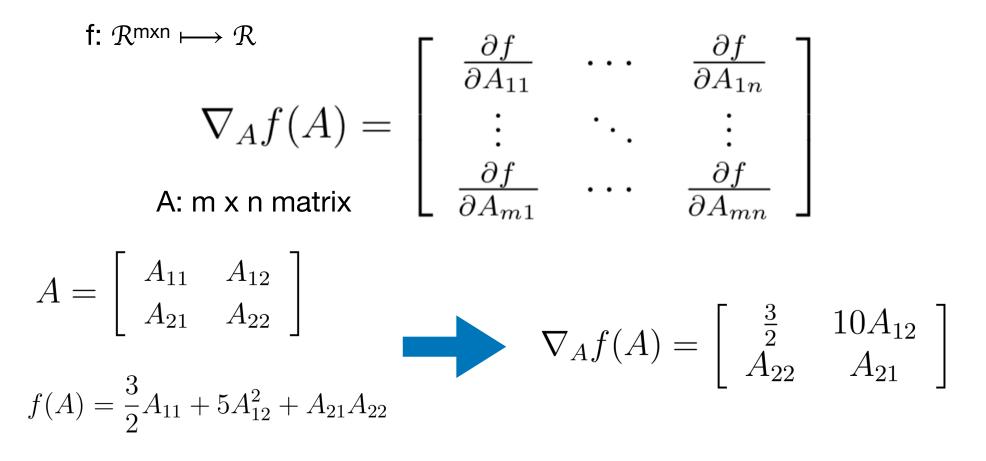
# Convergence

• In most cases, gradient descent converges to local minima. Linear regression only has one global minima, which the gradient descent always converges to. This is because the cost function J is a convex quadratic function (二次凸函数).



# Normal Equations (标准方程)

- Gradient descent gives one way of minimizing J. How about others?
- We minimize J by explicitly taking derivatives w.r.t. θ and setting them to 0s. And solve the equations!



### Normal Equations (标准方程)

1. trace (迹):  $trA = \sum_{i=1}^{n} A_{ii}$ , the trace of a real number is itself

- 2. trace of a matrix = trace of its transpose (转置矩阵)  $trA = trA^T$
- 3. tr(A+B) = trA + trB, trAB = trBA
- 4.  $\nabla_A \operatorname{tr} AB = B^T$
- 5.  $\nabla_{A^T} \operatorname{tr} ABA^T C = B^T A^T C^T + BA^T C$

 $X = \begin{bmatrix} -(x^{(1)})^T - \\ -(x^{(2)})^T - \\ \vdots \\ -(x^{(m)})^T - \end{bmatrix} \quad \vec{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad X\theta - \vec{y} = \begin{bmatrix} (x^{(1)})^T \theta \\ \vdots \\ (x^{(m)})^T \theta \end{bmatrix} - \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}$  $= \begin{bmatrix} h_{\theta}(x^{(1)}) - y^{(1)} \\ \vdots \\ h_{\theta}(x^{(m)}) - y^{(m)} \end{bmatrix}.$ 

# Normal Equations (标准方程)

$$\nabla_{\theta} J(\theta) = \nabla_{\theta} \frac{1}{2} (X\theta - \vec{y})^{T} (X\theta - \vec{y})$$

$$= \frac{1}{2} \nabla_{\theta} (\theta^{T} X^{T} X \theta - \theta^{T} X^{T} \vec{y} - \vec{y}^{T} X \theta + \vec{y}^{T} \vec{y})$$
Property 1
$$= \frac{1}{2} \nabla_{\theta} \operatorname{tr} (\theta^{T} X^{T} X \theta - \theta^{T} X^{T} \vec{y} - \vec{y}^{T} X \theta + \vec{y}^{T} \vec{y})$$
Property 2, 3
$$= \frac{1}{2} \nabla_{\theta} (\operatorname{tr} \theta^{T} X^{T} X \theta - 2 \operatorname{tr} \vec{y}^{T} X \theta)$$
Property 4, 5
$$= \frac{1}{2} (X^{T} X \theta + X^{T} X \theta - 2 X^{T} \vec{y})$$

$$= X^{T} X \theta - X^{T} \vec{y} = 0$$

$$\theta = (X^{T} X)^{-1} X^{T} \vec{y}.$$

### **Probabilistic View**

• The target variables and the inputs are related by

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

- Assume  $\epsilon^{(i)}$  are distributed IID (independently and identically distributed 独立同分布) and  $\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$
- Implies

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

• Given X and  $\theta$ , what is the distribution of  $y^{(i)}$ 's? Likelihood function:

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

### **Probabilistic View**

- Maximum likelihood: we should choose θ to make the data as high probability as possible
- Equivalently, we maximize the log likelihood:

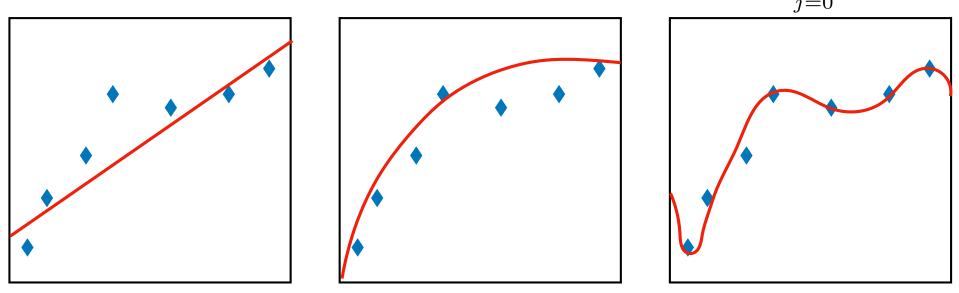
$$\ell(\theta) = \log L(\theta) = \log \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y^{(i)} - \theta^{T} x^{(i)})^{2}}{2\sigma^{2}}\right) = \sum_{i=1}^{m} \log \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y^{(i)} - \theta^{T} x^{(i)})^{2}}{2\sigma^{2}}\right) = m \log \frac{1}{\sqrt{2\pi\sigma}}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

minimizing this term instead! original least-squares cost

# **Underfitting & Overfitting**

• Fitting to different hypotheses:

$$y = \theta_0 + \theta_1 x \qquad \qquad y = \theta_0 + \theta_1 x + \theta_2 x^2$$



#### underfitting

overfitting

 $\sum \theta_j x^j$ 

y =

The more features we add, the better. However, there is also a risk in adding too many features.

#### Locally Weighted Linear Regression

- The choice of features is important to learning performance!
- Locally weighted linear regression
  - 1. Fit  $\theta$  to minimize  $\sum_{i} w^{(i)} (y^{(i)} \theta^T x^{(i)})^2$
  - 2. Output  $\theta^T x$
- larger w<sup>(i)</sup> -> try harder to make (y<sup>(i)</sup> θ<sup>T</sup>x<sup>(i)</sup>)<sup>2</sup> small; otherwise, ignore the corresponding error term
- Standard choice for the weight:

$$w^{(i)} = \exp\left(-\frac{(x^{(i)} - x)^2}{2\tau^2}\right)$$

Non-parametric Alg: keep the entire training dataset when making predictions

 $\theta$  is giving a higher weight to the training examples close to the testing data x

# Summary

- Linear regression

  - Linear hypothesis class  $h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x$  Cost function  $J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) y^{(i)})^2$  Least mean square algorithm:  $\theta_j := \theta_j + \alpha \left( y^{(i)} h_{\theta}(x^{(i)}) \right) x_j^{(i)}$
  - - Batch/stochastic gradient descent
  - Probabilistic view:  $\bullet$ 
    - Errors ~ I.I.D. Gaussian distribution
    - Maximum likelihood
  - **Overfitting & Underfitting**
  - Locally weighted linear regression

### Outline

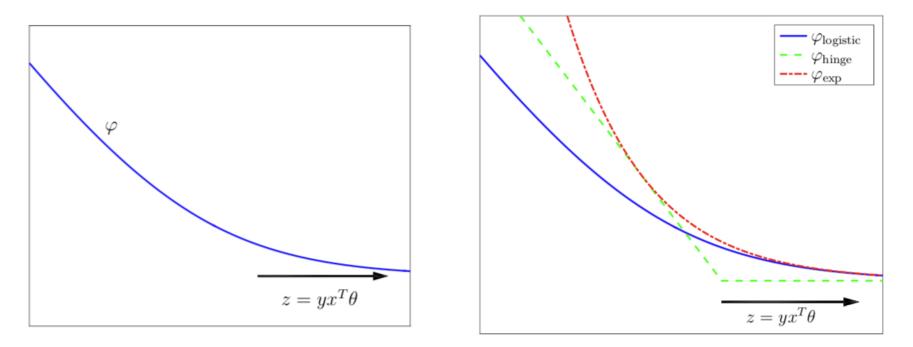
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# **Binary Classification**

- The target y can only take two values: y ∈ {-1, +1}. y = 1 if the example belongs to the positive class, otherwise, it is a member of the negative class
- Hypothesis:  $h(x) = \theta^T x$ . Given x, we classify it as positive or negative depending on the sign of  $\theta^T x$ , i.e.,  $sign(\theta^T x) = y \iff y\theta^T x > 0$
- Margin for the example (x, y): yθ<sup>T</sup>x the more θ<sup>T</sup>x is negative (or positive), the stronger the belief that y is negative (or positive)
- loss function: should penalize the  $\theta$  for which  $y(i)\theta^T x(i) < 0$  frequently in the training data. Loss value should be small if  $y(i)\theta^T x(i) > 0$  and large if  $y(i)\theta^T x(i) < 0$
- We expect the loss function to be continuous and convex (easy to converge to the global minima!)

# **Binary Classification**

 Expect the loss to satisfy: Loss\_func (y(i)θ<sup>T</sup>x(i)) → 0 as y(i)θ<sup>T</sup>x(i) →∞ and Loss\_func (y(i)θ<sup>T</sup>x(i)) → ∞ as y(i)θ<sup>T</sup>x(i) →-∞



 $Loss_{logistic}(z) = \log(1 + e^{-z})$  logistic regression  $Loss_{hinge} = \max\{1 - z, 0\}$  support vector machines  $Loss_{exp} = e^{-z}$  boosting

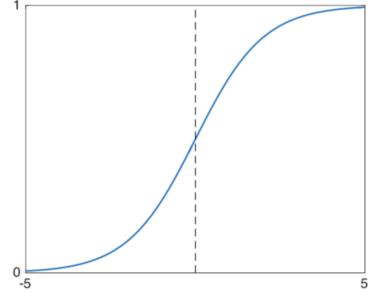
# Logistic Regression

• Choose θ to minimize

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} Loss_{logistic}(y^{(i)}\theta^{T} x^{(i)}) = \frac{1}{m} \sum_{i=1}^{m} \log(1 + \exp(-y^{(i)}\theta^{T} x^{(i)}))$$

which hopefully yields  $\theta$  that  $y(i)\theta^T x(i) > 0$  for most training examples

- Alternative view: Logistic (Sigmoid) function  $g(z) = \frac{1}{1 + e^{-z}}$  $\rightarrow 1 \text{ as } z \rightarrow \infty \text{ and } g(z) \rightarrow 0 \text{ as } z \rightarrow -\infty$
- g(z) + g(-z) = 1 we could use it to define the probability model for binary classification.



### **Probabilistic View**

• For  $y \in \{-1, +1\}$ , we define the logistic model as

$$p(Y=y|x;\theta)=g(yx^T\theta)=\frac{1}{1+e^{-yx^T\theta}}~$$
, & refine hypothesis class as 
$$h_\theta(x)=\frac{1}{1+e^{-x^T\theta}}$$

• The likelihood of the training data is

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

• The log-likelihood is

$$\ell(\theta) = \sum_{i=1}^{m} \log h_{\theta}(y^{(i)}x^{(i)}) = -\sum_{i=1}^{m} \log \left(1 + e^{-y^{(i)}\theta^{T}x^{(i)}}\right) = -mJ(\theta)$$

maximizing likelihood in the logistic model = minimizing the average logistic loss

#### **Gradient Descent**

• For the  $Loss_{logistic}(z) = \log(1 + e^{-z})$ , the derivative is

Sigmoid function

$$\frac{\mathrm{d}}{\mathrm{d}z} Loss_{logistic}(z) = \frac{1}{1+e^{-z}} \cdot \frac{\mathrm{d}}{\mathrm{d}z} e^{-z} = -\frac{e^{-z}}{1+e^{-z}} = -g(-z)$$

• For a single training example (x, y):

$$\frac{\partial}{\partial \theta_k} Loss_{logistic}(yx^T\theta) = -g(-yx^T\theta)\frac{\partial}{\partial \theta_k}(yx^T\theta) = -g(-yx^T\theta)yx_k$$

• Update rule for stochastic gradient descent:

$$\theta^{t+1} = \theta^t - \alpha_t \cdot \nabla_\theta Loss_{logistic}(-y^{(i)}x^{(i)T}\theta^t) \quad \text{incorrect label}$$
$$= \theta^{(t)} + \alpha_t g(-y^{(i)}x^{(i)T}\theta^{(t)})y^{(i)}x^{(i)} = \theta^{(t)} + \alpha_t h_{\theta^{(t)}} \underbrace{-y^{(i)}x^{(i)}}_{-y} \underbrace{$$

# Update Rule when $y \in \{0, 1\}$

$$P(y = 1 | x; \theta) = h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$
$$P(y = 0 | x; \theta) = 1 - h_{\theta}(x)$$

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

$$L(\theta) = p(\vec{y} \mid X; \theta) \qquad \ell(\theta) = \log L(\theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta) \qquad = \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)})) = \prod_{i=1}^{m} (h_{\theta}(x^{(i)}))^{y^{(i)}} (1 - h_{\theta}(x^{(i)}))^{1 - y^{(i)}}$$

gradient ascent:

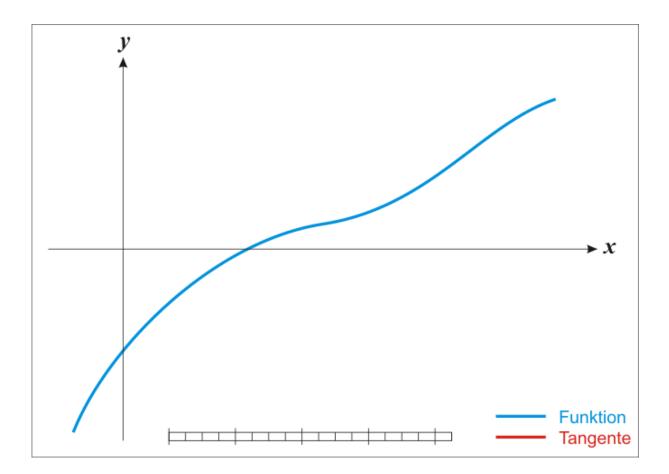
 $\theta := \theta + \alpha \nabla_{\theta} \ell(\theta)$ 

similar to least mean square update rule, but h is non-linear!

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

#### Another Update Rule to Maximize $l(\theta)$

- Newton's method for finding a zero of a function:  $f(\theta) = 0$
- Update rule:  $\theta := \theta f(\theta)/f'(\theta)$



#### Another Update Rule to Maximize $l(\theta)$

- Newton's method for finding a zero of a function:  $f(\theta) = 0$
- What if we want to maximize some loss function? The maxima of the loss corresponds to points where its first derivative is 0
- Update rule:  $\theta := \theta \frac{l'(\theta)}{l''(\theta)}$
- Multidimensional setting:  $\theta := \theta H^{-1} \nabla_{\theta} l(\theta)$  Hessian matrix
- Advantage: Newton's method typically enjoys faster convergence than gradient descent, and requires many fewer iterations to get very close to the minimum.
- Disadvantage: more expensive in one iteration

# Summary

- Logistic regression
  - Hypothesis  $h(x) = \theta^T x$
  - Cost function  $Loss_{logistic}(z) = \log(1 + e^{-z})$
  - Update rule:  $\theta^{t+1} = \theta^t \alpha_t \cdot \nabla_{\theta} Loss_{logistic}(-y^{(i)}x^{(i)T}\theta^t)$ 
    - Newton's method  $\theta := \theta \frac{l'(\theta)}{l''(\theta)}$
  - Probabilistic view:
    - maximizing likelihood in the logistic model = minimizing the average logistic loss

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- Generalized Linear Models

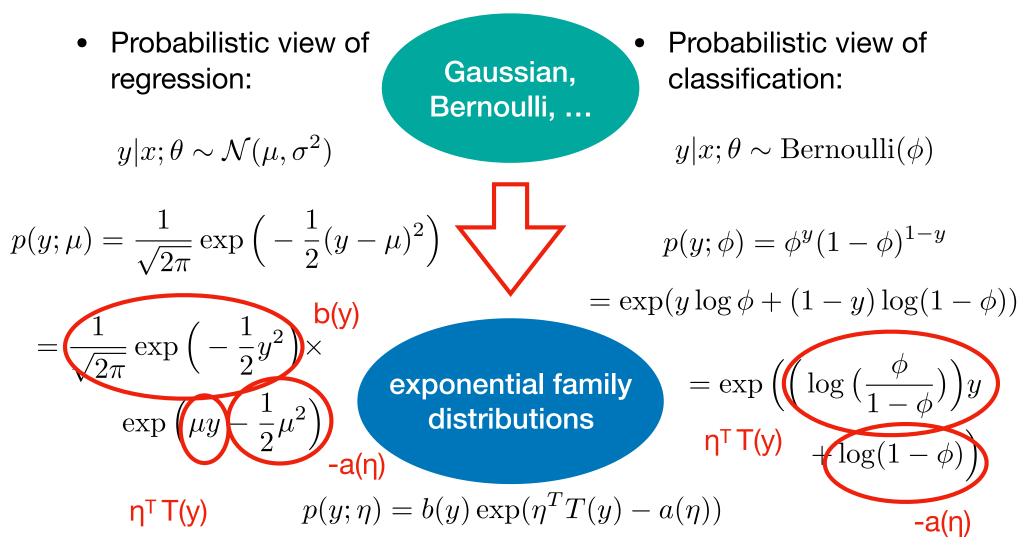
# **Generalized Linear Models**

- Given the distributions of y | x, how do we come up with the hypothesis?
  - linear regression:  $y|x; \theta \sim \mathcal{N}(\mu, \sigma^2)$ , hypothesis:  $h_{\theta}(x) = \theta^T x$
  - logistic regression:  $y|x; \theta \sim \text{Bernoulli}(\phi)$ , hypothesis:

$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$

• We show both of the methods are special cases of generalized linear models

### **Generalized Linear Models**



A fixed choice of T, a, and b defines a family of distributions parameterized by  $\eta$ 

# Construct GLMs

- Knowing the distribution, how to construct GLMs?
- Assumptions about P(y | x) and hypothesis:
  - 1.  $y|x; \theta$  follows a distribution that belongs to exponential family
  - 2.  $h(x) = \mathbb{E}[T(y)|x]$ . E.g., in logistic regression,

$$h_{\theta}(x) = p(y = 1 | x; \theta) = 0 \cdot p(y = 0 | x; \theta) + 1 \cdot p(y = 1 | x; \theta) = \mathbb{E}[y | x]$$

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

#### **Construct Linear Regression Model**

• Target variable follows Gaussian distribution:  $y|x; \theta \sim \mathcal{N}(\mu, \sigma^2)$ 

 $h_{\theta}(x) = \mathbb{E}[y|x; \theta]$  Assumption 2

$$= \mu \qquad y|x; \theta \sim \mathcal{N}(\mu, \sigma^2)$$

 $=\eta$ 

Assumption 1: Write the Gaussian distribution in the form of exponential family distribution  $p(y;\mu) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}y^2\right) \times \exp\left(\mu y - \frac{1}{2}\mu^2\right)$ 

 $= \theta^T x$  Assumption 3

#### **Construct Logistic Regression Model**

• Target variable is binary-valued. Thus we choose the Bernoulli family distributions to model the conditional distribution:

 $y|x; \theta \sim \text{Bernoulli}(\phi)$ 

 $h_{\theta}(x) = \mathbb{E}[y|x;\theta] \quad \text{Assumption 2}$   $= \phi \quad \text{Bernoulli distribution} = \eta$   $= 1/(1+e^{-\eta}) \quad \text{Assumption 1}$   $p(y;\phi) = \exp\left(\left(\log\left(\frac{\phi}{1-\phi}\right)\right)y + \log(1-\phi)\right)$   $= 1/(1+e^{-\theta^{T}x}) \quad \text{Assumption 3}$ 

# k-Classification

- Target variable takes on any of k values:  $y \in \{1, 2, \dots, k\}$
- We choose multinomial distribution to model: k parameters  $\phi_1, \ldots, \phi_k$  denoting the probability of each outcome

• 
$$\sum_{i=1}^{n} \phi_{i} = 1, \text{ k - 1 parameters}$$
  
• 
$$T(1) = \begin{bmatrix} 1\\0\\0\\\vdots\\0 \end{bmatrix}, T(2) = \begin{bmatrix} 0\\1\\0\\\vdots\\0 \end{bmatrix}, T(3) = \begin{bmatrix} 0\\0\\1\\\vdots\\0 \end{bmatrix}, \dots, T(k-1) = \begin{bmatrix} 0\\0\\0\\\vdots\\1 \end{bmatrix}, T(k) = \begin{bmatrix} 0\\0\\0\\\vdots\\1 \end{bmatrix}$$

$$(T(y))_i = 1\{y = i\}$$
  $\mathbb{E}[(T(y))_i] = P(y = i) = \phi_i$ 

# k-Classification

• Multinomial is a member of the exponential family.

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

probability of class i! known as softmax function

# Softmax Regression Model

 $h_{\theta}(x) = \mathrm{E}[T(y)|x;\theta]$  Assumption 2

$$= E \begin{bmatrix} 1\{y=1\} \\ 1\{y=2\} \\ \vdots \\ 1\{y=k-1\} \end{bmatrix} x; \theta$$

Our hypothesis outputs the estimated probability that  $p(y=i \mid x; \theta)$  for every  $i \in \{1, ..., k\}$ .

 $= \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{k-1} \end{bmatrix} = \begin{bmatrix} \overline{\Sigma}_j^k \\ \overline{\Sigma}_j^k \\ e_1 \\ e_2 \\ \overline{\Sigma}_j^k \end{bmatrix}$ 

$$\frac{\exp(\theta_1^T x)}{\sum_{j=1}^k \exp(\theta_j^T x)} \\ \frac{\exp(\theta_2^T x)}{\sum_{j=1}^k \exp(\theta_j^T x)} \\ \vdots \\ \frac{\exp(\theta_{k-1}^T x)}{\sum_{j=1}^k \exp(\theta_j^T x)} \\ \end{array}$$

 $\langle AT \rangle$ 

Express the multinomial distribution in the form of Exponential family & Assumption 3

Multinomial distribution

# Softmax Regression

 Training by maximizing the log-likelihood by gradient ascent or Newton's method

$$\ell(\theta) = \sum_{i=1}^{m} \log p(y^{(i)} | x^{(i)}; \theta)$$
  
= 
$$\sum_{i=1}^{m} \log \prod_{l=1}^{k} \left( \frac{e^{\theta_{l}^{T} x^{(i)}}}{\sum_{j=1}^{k} e^{\theta_{j}^{T} x^{(i)}}} \right)^{1\{y^{(i)} = l\}}$$

# Summary

- Generalized Linear Models
  - distribution of the target variable —> hypothesis
    - 1. rewrite the distribution in the form of exponential family distributions
    - 2. find the relation between the expected value of the target variable and the natural parameter  $\eta$
    - 3. express the natural parameter η in terms of inputs x (linear in most cases)