Learning From Data
Lecture 2: Linear Regression & Logistic Regression

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Outline

Introduction

Today's Lecture

Supervised Learning (Part I)

- Linear Regression
- Binary Classification
- Multi-Class Classification

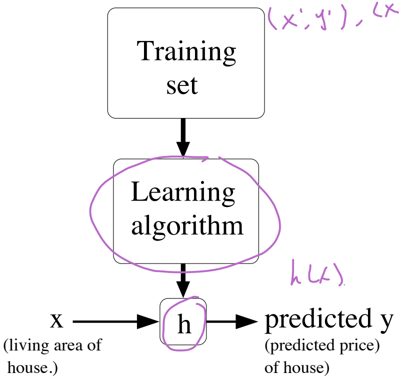
Review: Supervised Learning

- Input space: $\mathcal{X}$, Target space: $\mathcal{Y}$

Review: Supervised Learning

- Input space: $\mathcal{X}$, Target space: $\mathcal{Y}$
- Given training examples, we want to learn a **hypothesis** function $h : \mathcal{X} \to \mathcal{Y}$ so that $h(x)$ is a "good" predictor for the corresponding y.

$(x^1, y^1), (x^2, y^2), \ldots, (x^m, y^m)$



Review: Supervised Learning

- y is discrete (categorical): **classification problem**
- y is continuous (real value): **regression problem**

Outline

$h(x)$ is a linear function

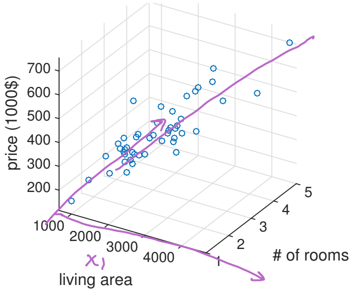
Linear Regression

Linear Regression Model
Ordinary Least Square
Maximum Likelihood Estimation

Linear Regression

Example: predict Portland housing price

Living area (ft^2)	# bedrooms	Price (\$1000)
x_1	x_2	y
2104	3	400
1600	3	330
2400	3	369
⋮	⋮	⋮



Linear Approximation

bias.

A linear model

$$h(x) = \underline{\theta_0} + \underline{\theta_1} x_1 + \underline{\theta_2} x_2$$

θ_i's are called **parameters**.

Linear Approximation

A linear model

bias

weights

$$h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

θ

θ_i's are called **parameters**.

Using vector notation,

$$h(x) = \theta^T x, \quad \text{where } \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}, \quad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}$$

← pad 1

$$= \theta_0 \cdot 1 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2$$

Alternative Notation

$$h(x) = w_1 x_1 + w_2 x_2 + b$$

w_1, w_2 are called **weights**, b is called the **bias**

$h(x) = \theta^T x$

$$h(x) = w^T x + b, \quad \text{where } w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$ $\quad b \in \mathbb{R}$

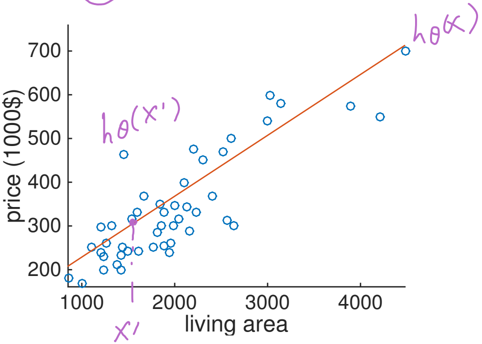
Apply model to new data

Suppose we have the optimal parameters θ , e.g.

```
> h = LinearRegression().fit(X, y)
> theta = h.coef
array([89.60, 0.1392, -8.738])
```

make a prediction of new feature x:

$$\hat{y} = h_\theta(x) = \theta^T x$$



Model Estimation

How to estimate model parameters θ (or w and b) from data?

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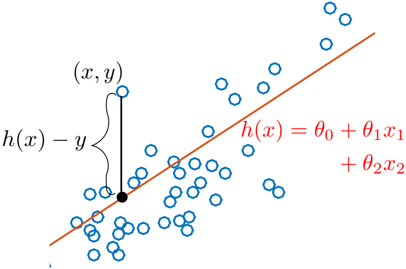
Least Square Estimation

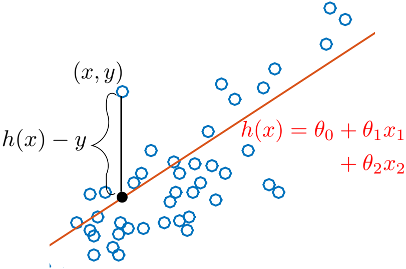


geometric approach

Model Estimation

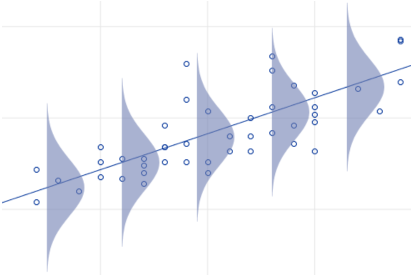
How to estimate model parameters θ (or w and b) from data?

Least Square Estimation



geometric approach

Maximum Likelihood Estimation



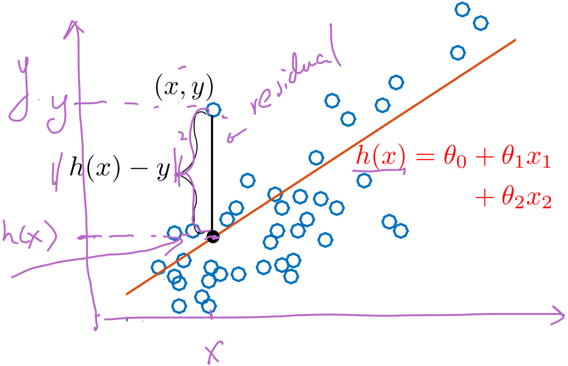
Probabilistic approach

Ordinary Least Square

$\frac{1}{m}$

Cost function:

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



Ordinary Least Square

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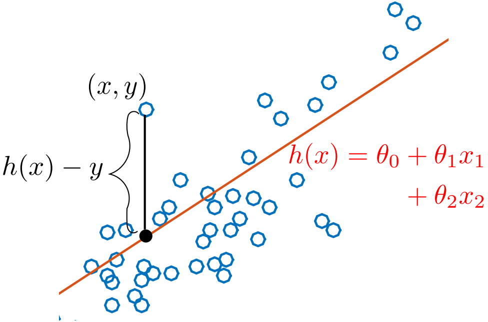

Ordinary Least Square

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Ordinary Least Square

Cost function:

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

The **ordinary Least square problem** is:

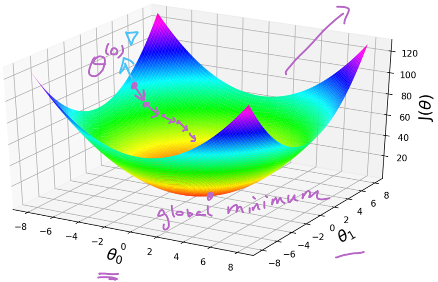
$$\begin{aligned} &\min_{\theta} J(\theta) \\ &= \min_{\theta} \frac{1}{2}\sum_{i=1}^{m}(h(x^{(i)}) - y^{(i)})^2 \end{aligned}$$

How to minimize $J(\theta)$?

- Numerical solution: gradient descent, Newton's method
- Analytical solution: normal equation

Gradient descent

A first-order iterative optimization algorithm for finding the minimum of a function $J(\theta)$.



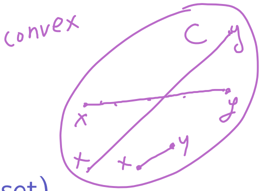
Key idea

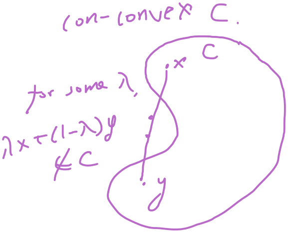
Start at an initial guess, $\theta^{(0)}$ repeatedly change θ to decrease $J(\theta)$:

$$\theta := \theta - \alpha \cdot \nabla J(\theta)$$

α is the **learning rate**

Review: Convex function





Definition (Convex set)

Let S be a vector space, any subset $C \subseteq S$ is **convex** if for any $x, y \in C$, $0 \leq \lambda \leq 1$, affine combination[1] $\lambda x + (1 - \lambda)y \in C$

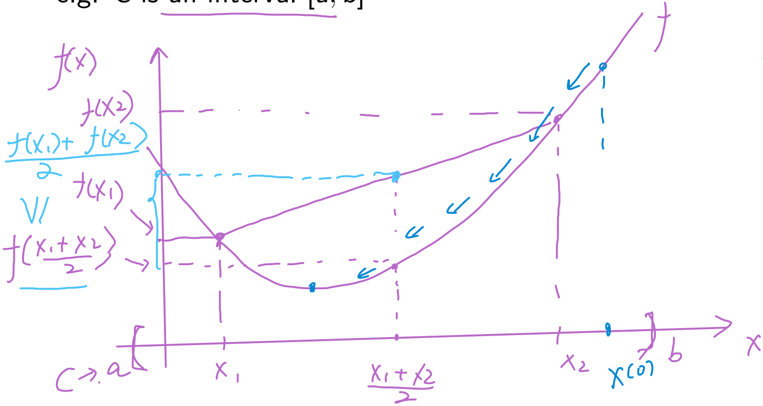
[1] An affine combination is a linear combination where coefficients sum to 1.

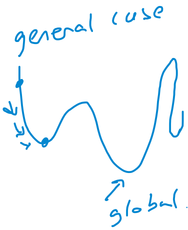
Definition (Convex function)

A function $f(x)$ is **convex** on a convex set C if for any $x_1, x_2 \in C$ and $0 \leq \lambda \leq 1$,

$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda) f(x_2)$$

e.g. C is an interval $[a, b]$





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Theorem

If $J(\theta)$ is convex, gradient descent finds the global minimum.

$\underline{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$

For the ordinary least square problem,

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

m samples

$\theta \in \mathbb{R}^n$.

$$\underline{\nabla J(\theta)} = \begin{bmatrix} \boxed{\frac{\partial J(\theta)}{\partial \theta_1}} \\ \boxed{\vdots} \\ \frac{\partial J(\theta)}{\partial \theta_n} \end{bmatrix}, \text{ where } \frac{\partial J(\theta)}{\partial \theta_j} = \frac{\partial}{\partial \theta_j}\frac{1}{2}\sum_{i=1}^{m}(\theta^T x^{(i)} - y^{(i)})^2$$

jth

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

$$= \cancel{\frac{1}{2}}\sum_{i=1}^{m}\cancel{2}\cdot(\theta^T x^{(i)} - y^{(i)})\underbrace{\frac{\partial}{\partial \theta_j}(\theta^T x^{(i)})}_{x_j^{(i)}}.$$

$\theta^T x^{(i)} = \theta_1 \cdot x_1^{(i)} + \underline{\theta_2 x_2^{(i)}} + \cdots \theta_n x_n^{(i)}$

if $j=2$, then only $\theta_j x_j^{(i)}$ depends on θ_j.

For the ordinary least square problem,
$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h(x^{(i)}) - y^{(i)})^2 = \frac{1}{2}\sum_{i=1}^{m}(\theta^T x^{(i)} - y^{(i)})^2$,

$$\nabla J(\theta) = \begin{bmatrix} \frac{\partial J(\theta)}{\partial \theta_1} \\ \vdots \\ \frac{\partial J(\theta)}{\partial \theta_n} \end{bmatrix}, \text{ where } \frac{\partial J(\theta)}{\partial \theta_j} = \frac{\partial}{\partial \theta_j}\left[\frac{1}{2}\sum_{i=1}^{m}\left(\theta^T x^{(i)} - y^{(i)}\right)^2\right]$$

$$= \sum_{i=1}^{m}\left(\theta^T x^{(i)} - y^{(i)}\right)\boxed{x_j^{(i)}}$$

Gradient descent for ordinary least square

Gradient of cost function: $\nabla J(\theta)_j = \sum_{i=1}^{m} \left(\theta^T x^{(i)} - y^{(i)}\right) x_j^{(i)}$
Gradient descent update: $\theta := \theta - \alpha \nabla J(\theta)$

Batch Gradient Descent

Repeat until convergence{
  $\boxed{\theta_j} = \theta_j + \alpha \sum_{i=1}^{m} (y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)}$ for every j
}

for $j = 1 \cdots n$:
  $\Delta = 0$
  for $i = 1 \cdots m$:
    $\Delta = \Delta + (y^i - h_\theta(x^i))x_j$
  $\theta_j = \theta_j + \alpha \cdot \Delta$

Gradient descent for ordinary least square

Gradient of cost function: $\nabla J(\theta)_j = \sum_{i=1}^{m} \left(\theta^T x^{(i)} - y^{(i)}\right) x_j^{(i)}$
Gradient descent update: $\theta := \theta - \alpha \nabla J(\theta)$

Batch Gradient Descent

```
Repeat until convergence{
    θ_j = θ_j + α Σ_{i=1}^m (y^(i) − h_θ(x^(i))) x_j^(i)  for every j
}
```

θ is only updated after we have seen all m training samples.

Batch gradient descent

```
Repeat until convergence{
```
$$\theta_j = \theta_j + \alpha \boxed{\sum_{i=1}^{m}} (y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)} \quad \texttt{for every j}$$
```
}
```

outer loop.

Stochastic gradient descent

```
Repeat until convergence{
```
$\texttt{for } i = 1 \ldots m$ {

$$\theta_j = \theta_j + \alpha(y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)} \quad \texttt{for every j}$$
```
  }
}
```

θ is updated each time a training example is read

Batch gradient descent

Repeat until convergence{

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

}

Stochastic gradient descent

Repeat until convergence{

for $i = 1 \ldots m$ {

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

}

}

θ is updated each time a training example is read

- Stochastic gradient descent gets θ close to minimum much faster (Video)
- Good for regression on large data

Minimize $J(\theta)$ Analytically

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

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

The matrix notation

$$\overbrace{x_1^{(1)} \; x_2^{(1)} \; \cdots \; x_n^{(1)}}^{n} \qquad \theta.$$

$$X = \underbrace{\begin{bmatrix} - \left(x^{(1)}\right)^T - \\ - \left(x^{(2)}\right)^T - \\ \vdots \\ - \left(x^{(m)}\right)^T - \end{bmatrix}}_{m} \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}, \quad \vec{y} = \underbrace{\begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}}_{m \times 1}$$

X is called the **design matrix**.

Minimize $J(\theta)$ Analytically

The matrix notation

$$X = \begin{bmatrix} — (x^{(1)})^T — \\ — (x^{(2)})^T — \\ \vdots \\ — (x^{(m)})^T — \end{bmatrix}, \quad \vec{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

X is called the **design matrix**. The least square function can be written as

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

Compute the gradient of $J(\theta)$:

$$\nabla_\theta J(\theta) = \nabla_\theta \left[\underbrace{\frac{1}{2}(X\theta - y)^T (X\theta - y)} \right]$$

① $\frac{\partial x^T A x}{\partial x} = Ax + A^T x = (A + A^T)x.$

if A is symmetric $A = A^T$; $\frac{\partial x^T A x}{\partial x} = 2Ax.$

② $\frac{\partial x^T a}{\partial x} = a$

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

$$= \frac{1}{2}(\theta^T X^T X \theta - \underbrace{\theta^T X^T y}_{\in \mathbb{R}} - \underbrace{y^T X \theta}_{\in \mathbb{R}} + y^T y)$$

$$= \underline{\frac{1}{2}\theta^T X^T X \theta} - \cancel{\frac{1}{2}} \cancel{2}\, \theta^T X^T y + \frac{1}{2} y^T y.$$

$$\nabla_\theta J(\theta) = \frac{\partial}{\partial \theta} J(\theta) = \frac{1}{2} \cdot \frac{\partial(\theta^T X^T X \theta)}{\partial \theta} - \frac{\partial}{\partial \theta} \theta^T \underline{X^T y}_{a} + \cancel{\frac{\partial y^T y}{\partial \theta}} \quad 0.$$

$$X^T X \theta - X^T y = 0.$$

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

Compute the gradient of $J(\theta)$:

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Compute the gradient of $J(\theta)$:

$$\nabla_\theta J(\theta) = \nabla_\theta \left[\frac{1}{2}(X\theta - y)^T(X\theta - y) \right]$$

$$=$$

Compute the gradient of $J(\theta)$:

$$
\begin{aligned}
\nabla_\theta J(\theta) =& \nabla_\theta \left[\frac{1}{2} (X\theta - y)^T (X\theta - y) \right] \\
=& X^T X\theta - X^T y
\end{aligned}
$$

Since $J(\theta)$ is **convex**, x is a global minimum of $J(\theta)$ when $\nabla J(\theta) = 0$.

Compute the gradient of $J(\theta)$:

$$\begin{aligned}\nabla_\theta J(\theta) =& \nabla_\theta \left[\frac{1}{2}(X\theta - y)^T(X\theta - y)\right] \\ =& X^T X\theta - X^T y\end{aligned}$$

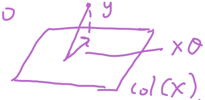
Since $J(\theta)$ is **convex**, x is a global minimum of $J(\theta)$ when $\nabla J(\theta) = 0$.

The Normal equation

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

$X^TX\theta - X^Ty = 0$

$\underbrace{X^T(X\theta - y)}_{\text{residual}} = 0.$



if X^TX is not full rank, solution θ^* is not unique.

Compute the gradient of $J(\theta)$:

$$\nabla_\theta J(\theta) = \nabla_\theta \left[\frac{1}{2}(X\theta - y)^T(X\theta - y)\right]$$
$$= X^TX\theta - X^Ty$$

Since $J(\theta)$ is **convex**, x is a global minimum of $J(\theta)$ when $\nabla J(\theta) = 0$.

When is X^TX not invertible?

① features are not independent.

② # of linearly independent samples are fewer than # of features.

The Normal equation

$$\theta = \boxed{(X^TX)^{-1}X^T}y$$

$(X^TX)^{-1}X^T$ is called the **Moore-Penrose pseudoinverse of** X

rank deficiency.

$X = \begin{bmatrix}1&0&0\\0&1&0\end{bmatrix}$ (2×3)

$X^TX = \begin{bmatrix}1&0&0\\0&1&0\\0&0&0\end{bmatrix}$ rank(X^TX) = 2

$Ax = y$

$(X^TX)\theta = X^Ty.$

Which method to use?

numerical analytical

gradient descent	**normal equation**
iterative solution	exact solution

Which method to use?

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need to choose proper learning parameter α for cost function to converge	

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gradient descent	**normal equation**
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works well for large number of samples m	

Which method to use?

gradient descent	**normal equation**
iterative solution	exact solution
need to choose proper learning parameter α for cost function to converge	numerically unstable when X is ill-conditioned. e.g. features are highly correlated
works well for large number of samples m	solving equation is slow when m is large

Minimize $J(\theta)$ using Newton's Method

Numerically solve for θ in $\nabla_\theta J(\theta) = 0$

Newton's method

Solves real functions $f(x) = 0$ by iterative approximation:

- Start an initial guess $x^{(0)}$
- Update x until convergence

$$x := x - \frac{f(x)}{f'(x)}$$

Minimize $J(\theta)$ using Newton's Method

Geometric intuition of Newton's method

At step $n+1$:

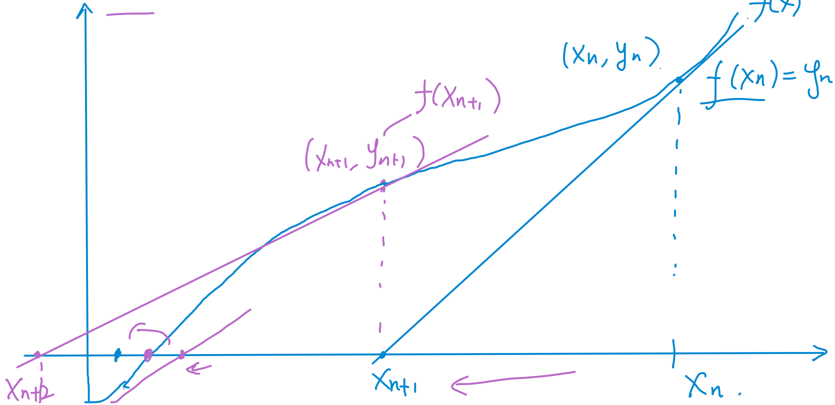
- Find tangent line of f at (x_n, y_n)
- $x_{n+1} \leftarrow$ x-intercept of the tangent line
- $y_{n+1} \leftarrow f(x_{n+1})$

$y - f(x_n) = f'(x)(x - x_n)$

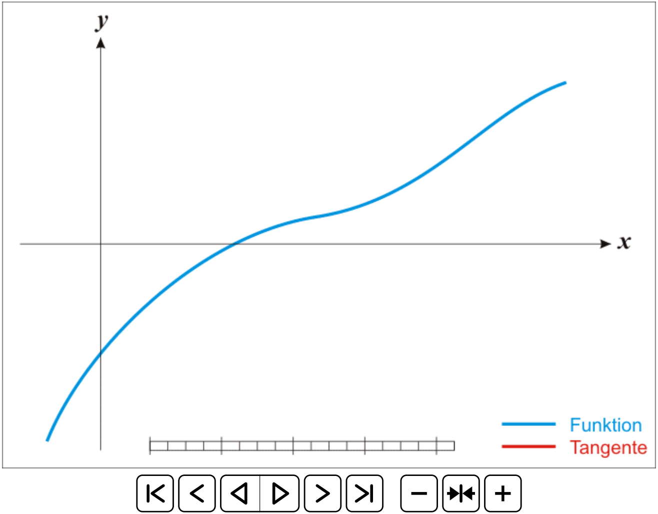
$y = f'(x)(x - x_n) + f(x_n) = 0$

$x_{n+1} = -\frac{f(x_n)}{f'(x_n)} + x_n$

$f(x) = 0$



Newton's Method Demo



https://en.wikipedia.org/wiki/File:NewtonIteration_Ani.gif

Minimize $J(\theta)$ using Newton's Method

$x = x - \frac{f(x)}{f'(x)}$

Newton's method for optimization $\min_\theta J(\theta)$

Use newton's method to solve $\nabla_\theta J(\theta) = 0$:

- θ is one-dimensional:

$f = J'(\theta) = \nabla_\theta J(\theta)$.

$$\theta := \theta - \frac{J'(\theta)}{J''(\theta)}$$

$f' = J''(\theta) = H_\theta(J(\theta))$

Minimize $J(\theta)$ using Newton's Method

Newton's method for optimization $\min_\theta J(\theta)$

Use newton's method to solve $\nabla_\theta J(\theta) = 0$:

- θ is one-dimensional:

$$\theta := \theta - \frac{J'(\theta)}{J''(\theta)}$$

$$\underset{(n\times n)}{H(\theta)} = \begin{bmatrix} \frac{\partial^2}{\partial\theta_1^2}J(\theta) & \frac{\partial^2}{\partial\theta_1\partial\theta_2}J(\theta) & \cdots & \frac{\partial^2}{\partial\theta_1\partial\theta_n}J(\theta) \\ \vdots & \vdots & & \\ \frac{\partial^2}{\partial\theta_n\partial\theta_1}J(\theta) & \cdots & \cdots & \frac{\partial^2}{\partial\theta_n^2}J(\theta) \end{bmatrix}$$

- θ is multidimensional: $\theta \in \mathbb{R}^n$.

$$\boxed{\theta = \theta - H^{-1}(\theta)\nabla J(\theta)}$$

where H is the Hessian matrix of $J(\theta)$.

a.k.a Newton-Raphson method

Newton's Method for Optimization

```
Initialize θ
While θ has not coverged {
  θ := θ − H^{-1}(θ)∇J(θ)
}
```

$$\theta := \theta - H^{-1}(\theta)\nabla J(\theta)$$

Newton's Method for Optimization

Initialize θ
While θ has not coverged {
  $\theta := \theta - H^{-1}(\theta)\nabla J(\theta)$
}

Performance of Newton's method:

- Needs fewer interations than batch gradient descent

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Performance of Newton's method:

- Needs fewer interations than batch gradient descent :)
- Computing H^{-1} is time consuming :(

Newton's Method for Optimization

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Initialize θ
While θ has not coverged {
  θ := θ − H^{-1}(θ)∇J(θ)
}
```

Performance of Newton's method:

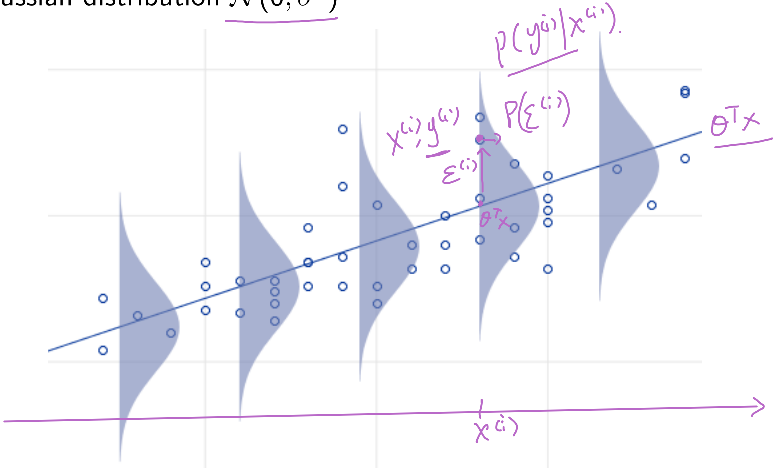
- Needs fewer interations than batch gradient descent
- Computing H^{-1} is time consuming
- Faster in practice when n is small

Maximum Likelihood Estimation

Consider target y is modeled as

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

and $\epsilon^{(i)}$ are *independently and identically distributed (IID)* to Gaussian distribution $\mathcal{N}(0, \sigma^2)$



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and $\epsilon^{(i)}$ are *independently and identically distributed (IID)* to Gaussian distribution $\mathcal{N}(0, \sigma^2)$, then

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

Maximum Likelihood Estimation

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Maximum Likelihood Estimation

Consider target y is modeled as

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

and $\epsilon^{(i)}$ are *independently and identically distributed (IID)* to Gaussian distribution $\mathcal{N}(0, \sigma^2)$, then

$\varepsilon^{(i)} = \underline{y^{(i)} - \theta^T x^{(i)}}$

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

likelihood of one sample

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

Maximum Likelihood Estimation

$\varepsilon^{(i)}$ / $y^{(i)}|x^{(i)} \sim$ i.i.d. $\mathcal{N}(0, \sigma^2)$

The **likelihood** of this model with respect to θ is

(m) (m×n)

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

Maximum Likelihood Estimation

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

Maximum likelihood estimation of θ:

$$\theta_{MLE} = \underset{\theta}{\operatorname{argmax}}\, L(\theta)$$

Maximum Likelihood Estimation

We compute log likelihood,

$L(\theta)$.

$$\log L(\theta) = \log \prod_{i=1}^{m} p(y^{(i)}|x^{(i)};\theta) = \sum_{i=1}^{m} \log p(y^{(i)}|x^{(i)};\theta)$$

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

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$$= m \log \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{m} (y^{(i)} - \theta^T x^{(i)})^2$$

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J(θ) in ordinary least square

$$= \underbrace{m \log \frac{1}{\sqrt{2\pi\sigma^2}}}_{\text{doesn't depend on } \theta} - \frac{1}{\sigma^2} \cdot \boxed{\frac{1}{2} \sum_{i=1}^{m} (y^{(i)} - \theta^T x^{(i)})^2}$$

Then $\text{argmax}_\theta \log L(\theta) \equiv \text{argmin}_\theta \frac{1}{2} \sum_{i=1}^{m} (y^{(i)} - \theta^T x^{(i)})^2$.

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Under the assumptions on $\epsilon^{(i)}$, least-squares regression corresponds to the maximum likelihood estimate of θ.

Linear Regression Summary

How to estimate model parameters θ (or w and b) from data?

- Least square regression (geometry approach)
- Maximum likelihood estimation (probabilistic modeling approach)

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Other estimation methods exist, e.g. Bayesian estimation MAP.

How to solve for solutions ?

- normal equation (close-form solution) analytical
- gradient descent
- newton's method

numerical

Outline

Logistic Regression

A binary classification problem

Classify binary digits

normalize

$[0, 255] \rightarrow [0,1]$

- Training data: 12600 grayscale images of handwritten digits

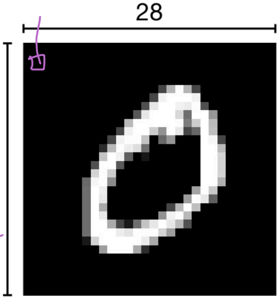
- Each image is represent by a vector $x^{(i)}$ of dimension $28 \times 28 = 784$
- Vectors $x^{(i)}$ are normalized to [0,1]

28

28

784

$x^{(i)}$



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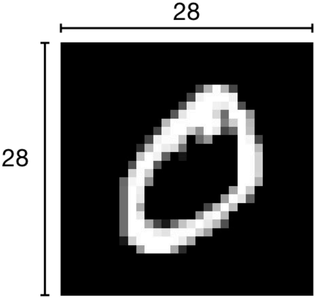


Binary classification: $\mathcal{Y} = \{0, 1\}$

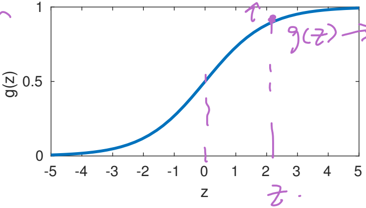
- negative class: $y^{(i)} = 0$
- positive class: $y^{(i)} = 1$

Logistic Regression Hypothesis Function

Sigmoid function

$$g(z) = \frac{1}{1 + e^{-z}}$$ → parameter

round



$g(z) \to 1$

z.

- $g : \mathbb{R} \to (0, 1)$
- $g'(z) =$

$$\frac{\partial}{\partial z}\left(\frac{1}{1+e^{-z}}\right)$$

Logistic Regression Hypothesis Function

Sigmoid function

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- $g : \mathbb{R} \to (0, 1)$
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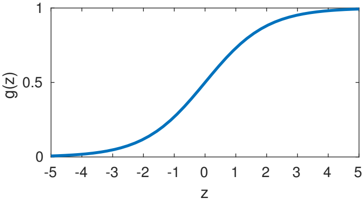

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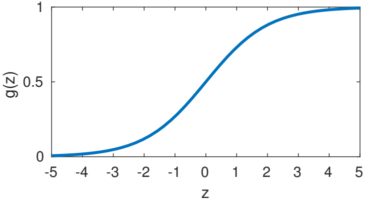

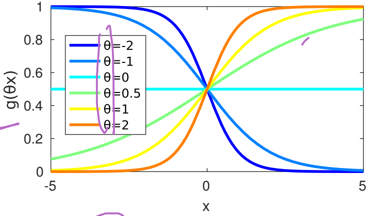

Hypothesis function for logistic regression:

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

$$\theta^T x = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_{n-1} \end{bmatrix} \cdot \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_{n-1} \end{bmatrix}$$

Review: Bernoulli Distribution

A discrete probability distribution of a binary random variable $x \in \{0, 1\}$:

landing on (H, H)

$0.7 \cdot 0.7 = 0.49$

(H, T) : $0.7 \cdot (1 - 0.7) = 0.21$

$$p(x) = \begin{cases} \lambda & \text{if } x = 1 \\ 1 - \lambda & \text{if } x = 0 \end{cases}$$

$$= \boxed{\lambda^x (1-\lambda)^{1-x}}$$

$x = 1$, $p(x) = \lambda \cancel{(1-\lambda)^0} = \lambda$

$x = 0$, $p(x) = \lambda^0 (1-\lambda)^1$
$= 1 - \lambda$

$\lambda = 0.7$

$p(\text{head})$
$= P(x=1) = \lambda = 0.7$

$P(\text{tail})$
$= P(x=0) = 1 - \lambda = 0.3$

Maximum likelihood estimation for logistic regression

model for λ $\quad \varepsilon^{(i)}$ $\quad \mathbb{E}[y|x] = \lambda$

$= h_\theta(x)$

Logistic regression assumes $y|x$ is **Bernoulli distributed**.

- $p(y = 1 \mid x; \theta) = h_\theta(x)$
- $p(y = 0 \mid x; \theta) = \underbrace{1 - h_\theta(x)}_{\text{model for } 1-\lambda}$

Maximum likelihood estimation for logistic regression

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

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Given m **independently generated** training examples, the likelihood function is:

i.i.d.

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

$$l(\theta) = \log(L(\theta)) = \sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

Maximum likelihood estimation for logistic regression

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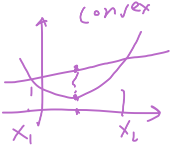

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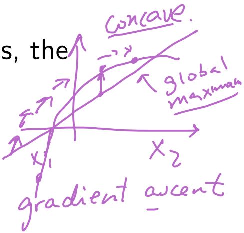

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$l(\theta)$ is concave!

Maximum likelihood estimation for logistic regression

$$l(\theta) = \sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

Solve $\text{argmax}_\theta \, l(\theta)$ using gradient ascent:

$$\frac{\partial l(\theta)}{\partial \theta_j} =$$

Maximum likelihood estimation for logistic regression

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Solve $\text{argmax}_\theta \, l(\theta)$ using gradient ascent:

similar to $\nabla J(\theta)$ in linear regression

$h_\theta(x) = \theta^T x$

$$\underline{\frac{\partial l(\theta)}{\partial \theta_j} = \sum_{i=1}^{m} \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}}$$

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

Stocastic Gradient Ascent

```
Repeat until convergence{
  for i = 1...m {
    θj = θj + α(y^(i) − hθ(x^(i)))xj^(i)   for every j
  }
}
```

- Update rule has the same form as least square regression, but with different hypothesis function $\underline{h_\theta}$

Binary Digit Classification

$0 < g(\theta^T x) < 1$

Using the learned classifier

Given an image x, the predicted label is

$$\hat{y} = \begin{cases} 1 & g(\theta^T x) > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

rounding

Binary digit classification results

	sample size	accuracy
Training	16200	100%
Testing	1225	100%

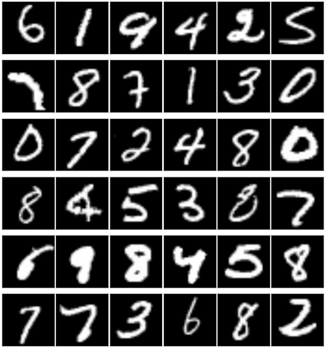
- Testing accuracy is 100% since this problem is relatively easy.

Multi-class classification

Each data sample belong to one of $k > 2$ different classes.

$$\mathcal{Y} = \{1, \ldots, k\}$$

$k = 10.$



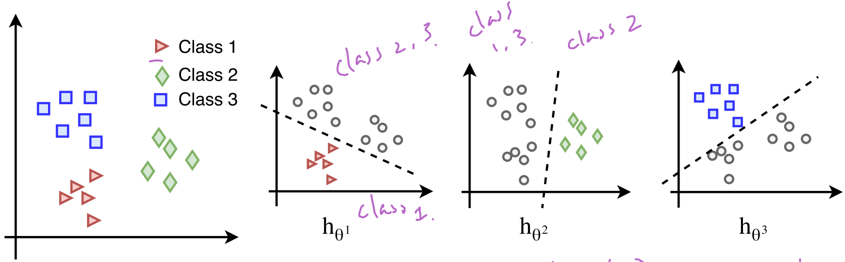
Given new sample $x \in \mathbb{R}^k$, predict which class it belongs.

Naive Approach: Convert to binary classification

One-Vs-Rest

Learn k classifiers $h_1, \ldots, h_k$. Each h_i classify one class against the rest of the classes.
Given a new data sample x, its predicted label $\hat{y}$:

$$\hat{y} = \operatorname*{argmax}_i h_i(x)$$



max (P(y=1|x) , P(y=2|x) , P(y=3|x))

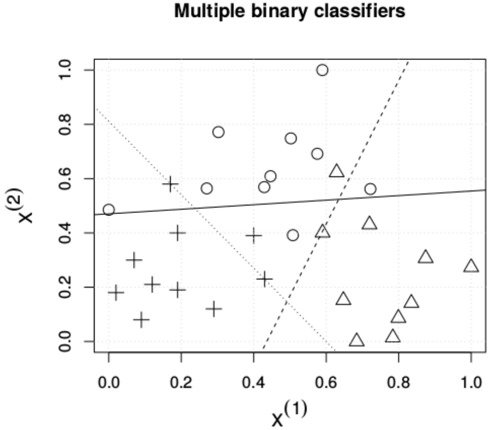
Multiple binary classifiers

50-class classification

$(\frac{1}{50}, \frac{49}{50})$

Drawbacks of One-Vs-Rest:

- Class unbalance: more negative samples than positive samples
- Different classifiers may have different confidence scales



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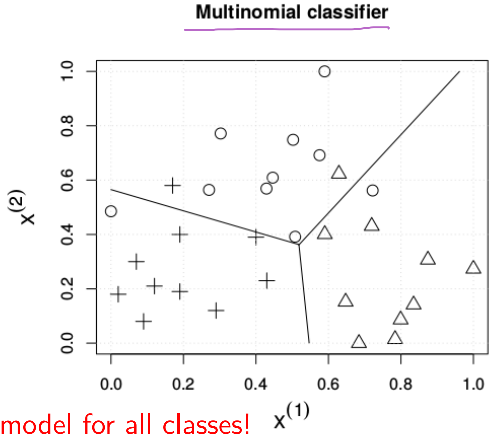


Learn one model for all classes!

Review: Multinomial Distribution

fair die

$\phi = [\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}]$

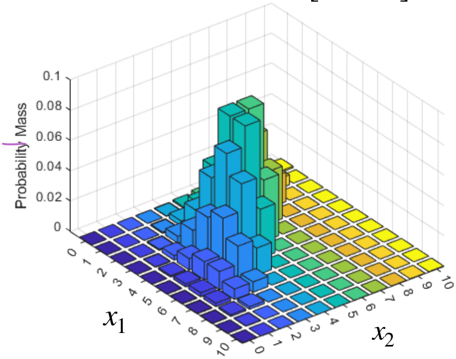
Models the probability of counts for each side of a k-sided die rolled m times, each side with independent probability ϕ_i

ϕ:

$$\sum_{i=1}^{k} \phi_i = 1$$

$$\phi_1 + \cdots + \phi_k = 1$$

$$k = 3, \; n = 10 \qquad \phi = \left[\frac{1}{2}, \frac{1}{3}, \frac{1}{6}\right]$$



Extend logistic regression: Softmax Regression

i.i.d.

Assume $p(y|x)$ is **multinomial distributed**, $k = |\mathcal{Y}|$

Extend logistic regression: Softmax Regression

$h_\theta(x) = \begin{bmatrix} \lambda \\ 1-\lambda \end{bmatrix}$

Assume $p(y|x)$ is **multinomial distributed**, $k = |\mathcal{Y}|$

Hypothesis function for sample x:

$p(y=\ell|x;\theta) = \dfrac{e^{\theta_\ell^T x}}{\sum_{\nu=1}^{k} e^{\theta_j^T x_j}}$

$$h_\theta(x) = k.\left\{ \begin{bmatrix} p(y=1|x;\theta) \\ \vdots \\ p(y=k|x;\theta) \end{bmatrix} \right. = \frac{1}{\sum_{j=1}^{k} e^{\theta_j^T x_j}} \begin{bmatrix} e^{\theta_1^T x} \\ \vdots \\ e^{\theta_k^T x} \end{bmatrix} = \text{softmax}(\underbrace{\theta^T x}_{z.})$$

$$\text{softmax}(z_i) = \frac{e^{z_i}}{\sum_{j=1}^{k} e^{(z_j)}}$$

Extend logistic regression: Softmax Regression

Assume $p(y|x)$ is **multinomial distributed**, $k = |\mathcal{Y}|$

Hypothesis function for sample x:

$$h_\theta(x) = \begin{bmatrix} p(y=1|x;\theta) \\ \vdots \\ p(y=k|x;\theta) \end{bmatrix} = \frac{1}{\sum_{j=1}^{k} e^{\theta_j^T x_j}} \begin{bmatrix} e^{\theta_1^T x} \\ \vdots \\ e^{\theta_k^T x} \end{bmatrix} = \text{softmax}(\theta^T x)$$

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$$\begin{array}{c} \theta_{1,1} \cdots\cdots \theta_{1,n} \\ \end{array}$$

$$\text{Parameters: } \theta = \underbrace{\begin{bmatrix} - & \theta_1^T & - \\ & \vdots & \\ - & \theta_k^T & - \end{bmatrix}}_{(k \times n)}$$

Θ

Softmax Regression

Bernoulli $p(y|x) = \underline{\lambda}^{y}(1-\lambda)^{\underline{y}}.$

$\lambda = h_\theta(x)$

Given $(x^{(i)}, y^{(i)}), i = 1, \dots, m$, the log-likelihood of the Softmax model is

$1\{y^i = l\} = \begin{cases} 1 & y^i = l \\ 0 & y^i \neq l. \end{cases}$

$$\ell(\theta) = \sum_{i=1}^{m} \log \underbrace{p(y^{(i)}|x^{(i)};\theta)}$$

$$= \sum_{i=1}^{m} \log \prod_{l=1}^{k} p(y^{(i)} = l|x^{(i)})^{\boxed{\mathbf{1}\{y^{(i)}=l\}}}$$

Softmax Regression

Given $(x^{(i)}, y^{(i)}), i = 1, \ldots, m$, the log-likelihood of the Softmax model is

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^{m} \log p(y^{(i)} | x^{(i)}; \theta) \\ &= \sum_{i=1}^{m} \log \prod_{l=1}^{k} p(y^{(i)} = l | x^{(i)})^{\mathbf{1}\{y^{(i)} = l\}} \\ &= \sum_{i=1}^{m} \sum_{l=1}^{k} \mathbf{1}\{y^{(i)} = l\} \log p(y^{(i)} = l | x^{(i)})\end{aligned}$$

Softmax Regression

Given $(x^{(i)}, y^{(i)}), i = 1, \ldots, m$, the log-likelihood of the Softmax model is

$$\begin{aligned}
\ell(\theta) &= \sum_{i=1}^{m} \log p(y^{(i)}|x^{(i)};\theta) \\
&= \sum_{i=1}^{m} \log \prod_{l=1}^{k} p(y^{(i)} = l|x^{(i)})^{\mathbf{1}\{y^{(i)}=l\}} \\
&= \sum_{i=1}^{m} \sum_{l=1}^{k} \mathbf{1}\{y^{(i)} = l\} \log p(y^{(i)} = l|x^{(i)}) \\
&= \sum_{i=1}^{m} \sum_{l=1}^{k} \mathbf{1}\{y^{(i)} = l\} \log \frac{e^{\theta_l^T x^{(i)}}}{\sum_{j=1}^{k} e^{\theta_j^T x^{(i)}}}
\end{aligned}$$

Softmax Regression

Derive the stochastic gradient descent update:

- Find $\nabla_{\theta_l} \ell(\theta)$

$$\nabla_{\theta_l} \ell(\theta) = \sum_{i=1}^{m} \left[\left(\mathbf{1}\{y^{(i)} = l\} - P\left(y^{(i)} = l | x^{(i)}; \theta\right) \right) x^{(i)} \right]$$

Property of Softmax Regression

- Parameters $\theta_1, \dots \theta_k$ are not independent: $\sum_j p(y = j|x) = \sum_j \phi_j = 1$
- Knowning $k - 1$ parameters completely determines model.

Invariant to scalar addition

$$p(y|x; \theta) = p(y|x; \theta - \psi)$$

Proof.

Relationship with Logistic Regression

When K = 2,

$$h_\theta(x) = \frac{1}{e^{\theta_1^T x} + e^{\theta_2^T x}} \begin{bmatrix} e^{\theta_1^T x} \\ e^{\theta_2^T x} \end{bmatrix}$$

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Replace $\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$ with $\theta* = \theta - \begin{bmatrix} \theta_2 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} \theta_1 - \theta_2 \\ 0 \end{bmatrix}$,

$$\begin{aligned} h_\theta(x) &= \frac{1}{e^{\theta_1^T x - \theta_2^T x} + e^{0x}} \begin{bmatrix} e^{(\theta_1 - \theta_2)^T x} \\ e^{0^T x} \end{bmatrix} \\ &= \begin{bmatrix} \frac{e^{(\theta_1-\theta_2)^T x}}{1+e^{(\theta_1-\theta_2)^T x}} \\ \frac{1}{1+e^{(\theta_1-\theta_2)^T x}} \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{1+e^{-(\theta_1-\theta_2)^T x}} \\ 1 - \frac{1}{1+e^{-(\theta_1-\theta_2)^T x}} \end{bmatrix} = \begin{bmatrix} g(\theta *^T x) \\ 1 - g(\theta *^T x) \end{bmatrix} \end{aligned}$$

When to use Softmax?

- When classes are mutually exclusive: use Softmax
- Not mutually exclusive: multiple binary classifiers may be better