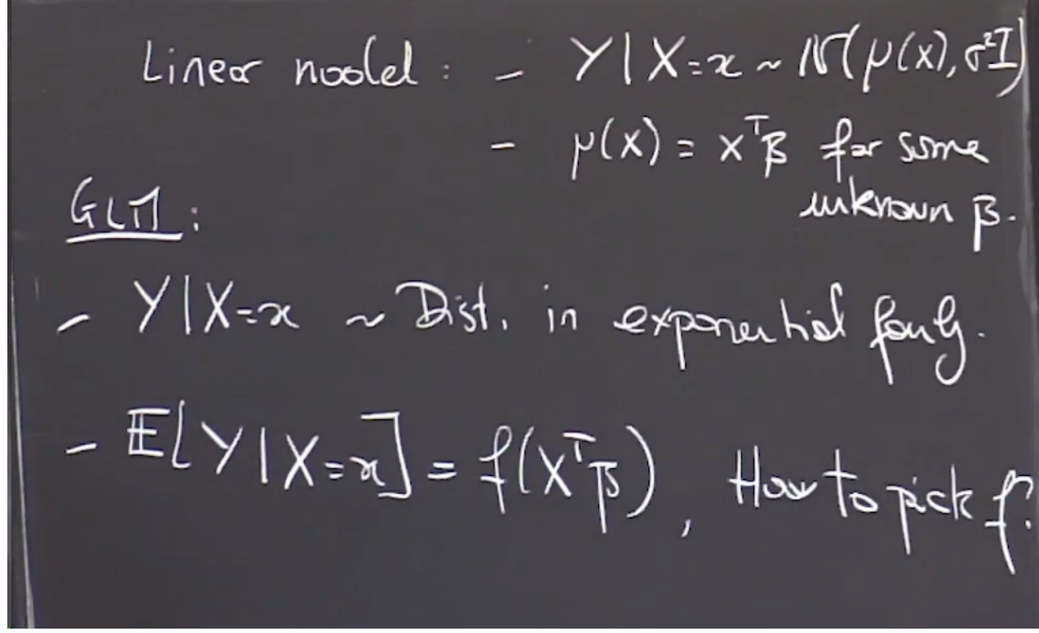
18.650 – Fundamentals of Statistics

7. Generalized linear models

Linear model



A Gaussian linear model assumes

$$\underbrace{Y|X=x}\sim\underbrace{\mathcal{N}}(\underbrace{\mu(x)},\underbrace{\sigma^2 I}),$$

1，假设一个特定族的分布

And[1]

$$\mathbb{E}(Y|X=x)=\mu(x)=x^\top\beta,$$

2，把Y|X和x联系起来。（有无限种联系的方式，这里我们只讨论线性的。）

regression function

[1] Throughout we drop the boldface notation for vectors

Components of a linear model

The two model components (that we are going to relax) are

1. Random component: the response variable Y is continuous and $Y|X = x$ is Gaussian with mean $\mu(x)$.

2. Regression function: $\mu(x) = x^\top \beta$. linear

Kyphosis

The Kyphosis data consist of measurements on 81 children following corrective spinal surgery. The binary response variable, Y, indicates the presence or absence of a postoperative deforming.

The three covariates are:

- $X^{(1)}$: Age of the child in month,
- $X^{(2)}$: Number of the vertebrae involved in the operation, and
- $X^{(3)}$: Start of the range of the vertebrae involved.

Write $X = (1, X^{(1)}, X^{(2)}, X^{(3)})^\top \in \mathbb{R}^4$

mean response；
此时X1,X2,X3都是0
也就是当没有任何信息的时候，
你的预测值。

Kyphosis

- The response variable is binary so there is no choice:
  $Y|X = x$ is Bernoulli with expected value
  $\mu(x) = \mathbb{E}[Y|X = x] \in (0, 1)$
- We cannot write

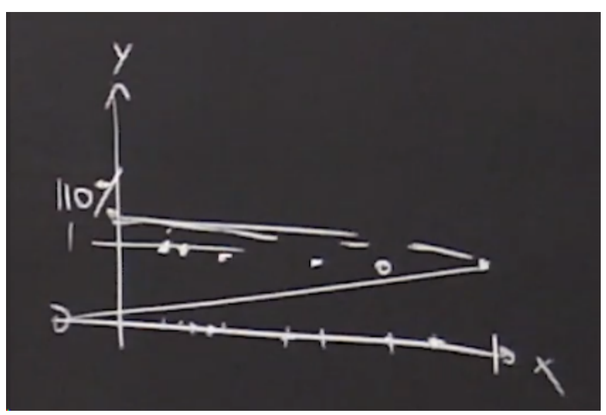
$$\mu(x) = x^\top \beta$$

because the right-hand side ranges through $\mathbb{R}$

- We need an invertible function f such that $f(x^\top \beta) \in (0, 1)$

我们需要的预测值应该符合我们的理解，
在这个例子中预测值应该在0和1中间。

所以我们需要一个逆函数将我们的Ymap到(0,1)



Generalization

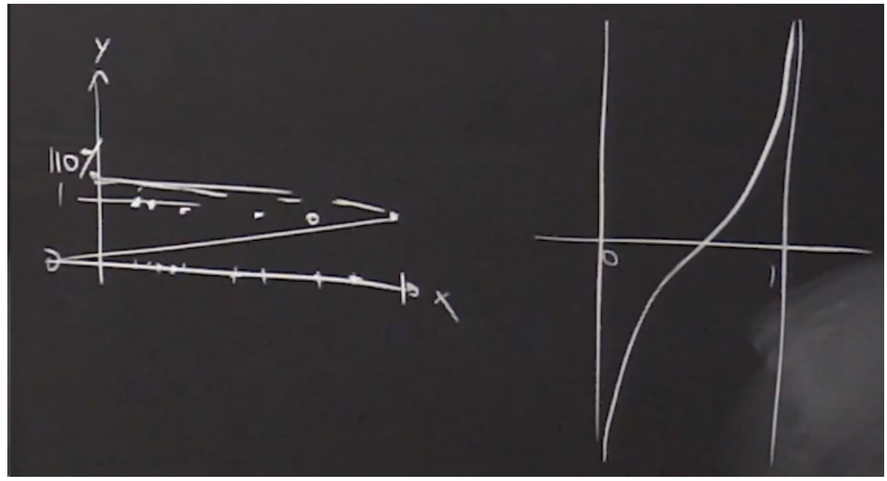
A generalized linear model (GLM) generalizes normal linear regression models in the following directions.

1. Random component:

$$Y|X = x \sim \text{some distribution}$$

(e.g. Bernoulli, exponential, Poisson)

左图是一个不符合事实的情况，
右图将(0,1)map to R



2. Regression function:

值域是(0,1)

$$g(\mu(x)) = x^\top \beta$$

其实也就是mu(x) = f(x'β)
这里g是f（上一页）的反函数

where g called **link function** and $\mu(x) = \mathbb{E}(Y|X = x)$ is the regression function.

Predator/Prey

Consider the following model for the number of preys Y that a predator (Hawk) catches per day ~~a predator~~ given a number X of preys (mice) in its hunting territory.

Random component: $Y > 0$ and the variance of capture rate is known to be approximately equal to its expectation so we propose the following model:

$$Y|X = x \sim \text{Poiss}(\mu(x))$$

very large n, small p

Where $\mu(x) = \mathbb{E}[Y|X = x]$.

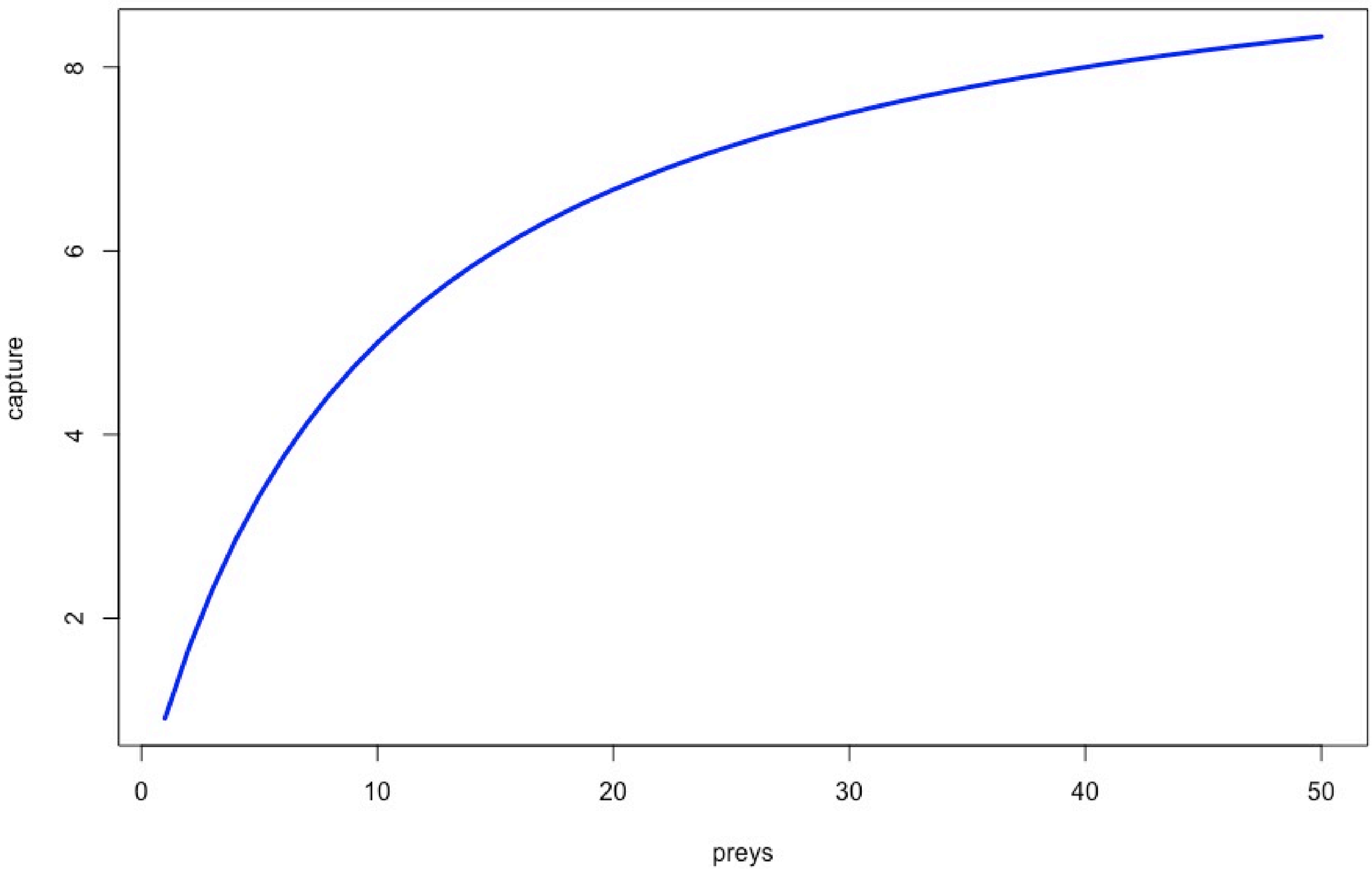
Regression function: We assume

$$\mu(x) = \frac{mx}{h + x}, \qquad \text{for some unknown } m, h > 0.$$

where:

- m is the max expected daily preys the predator can cope with
- h is the number of preys such that $\mu(h) = m/2$

The regression function $m(x)$ for $m = h = 10$



Example 2: Prey Capture Rate

$\mu(x) = \frac{mx}{h+x}$ [0,inf)

$\frac{1}{\mu(x)} = \frac{h+x}{mx}$

mu(x)已经确定，此时需要找出一个g(x)，
使得我们最后能得到一个linear model

不需要将[0,inf) maps to R, 因为在这个问题中我们知道x>0。

Obviously $\mu(x)$ is not linear but using **reciprocal link**: $g(x) = \frac{1}{x}$, the right-hand side can be made linear in the parameters:

$$g(\mu(x)) = \frac{1}{\mu(x)} = \frac{1}{m} + \frac{h}{m}\cdot\frac{1}{x} = \beta_0 + \beta_1 \frac{1}{x}.$$

这种形式的回归方程不行是因为和问题不兼容

$\mu(x) = \beta_0 + \beta_1 x$

Exponential Family

A family of distribution $\{\mathbb{P}_\theta : \theta \in \Theta\}$, $\Theta \subset \mathbb{R}^k$ is said to be a k-**parameter exponential family** on $\mathbb{R}^q$, if there exist real valued functions:

Y的维度

- $\eta_1, \eta_2, \cdots, \eta_k$ and B of θ, 我们通过regression function和X的data来构造这个B(θ)
- T_1, $T_2, \cdots, T_k$, and h of $y \in \mathbb{R}^q$ such that the density function (pmf or pdf) of $\mathbb{P}_\theta$ can be written as

k：theta的维度

$$f_\theta(y) = \exp\left[\sum_{i=1}^{k} \eta_i(\theta) T_i(y) - B(\theta)\right] h(y)$$

normalized term

$f_\theta(y) = \exp\left(e^{\frac{\theta}{y}} - B(\theta)\right) h(y)$

$(\eta_1(\theta) \cdots \eta_k(\theta)) \begin{pmatrix} T_1(y) \\ \vdots \\ T_k(y) \end{pmatrix}$

$f_\theta(y) = \exp\left(\eta(\theta)^T T(y) - B(\theta) + \log h(y)\right)$

$f_\theta(y) = \exp\left(\eta(\theta)^T T(y)\right) e^{-B(\theta)} h(y)$

化简的形式有多种写法

Normal distribution example

- Consider $Y \sim \mathcal{N}(\mu, \sigma^2)$, $\theta = (\mu, \sigma^2)$. The density is

$$f_\theta(y) = \exp\left(\frac{\mu}{\sigma^2}y - \frac{1}{2\sigma^2}y^2 - \frac{\mu^2}{2\sigma^2}\right)\frac{1}{\sigma\sqrt{2\pi}},$$

which forms a two-parameter exponential family with

可以任意分解，但是不要这样做

$$\eta_1 = \frac{\mu}{\sigma^2},\ \eta_2 = -\frac{1}{2\sigma^2},\ T_1(y) = y,\ T_2(y) = y^2,$$

$$B(\theta) = \frac{\mu^2}{2\sigma^2} + \log(\sigma\sqrt{2\pi}),\ h(y) = 1.$$

- When σ^2 is known, it becomes a one-parameter exponential family on $\mathbb{R}$:

$$\eta = \frac{\mu}{\sigma^2},\ T(y) = y,\ B(\theta) = \frac{\mu^2}{2\sigma^2},\ h(y) = \frac{e^{-\frac{y^2}{2\sigma^2}}}{\sigma\sqrt{2\pi}}.$$

Examples of discrete distributions

The following distributions form **discrete** exponential families of distributions with **pmf**

- Bernoulli(p): $p^y(1-p)^{1-y}$, $y \in \{0,1\}$

$$\exp\left(y \log p + (1-y)\log(1-p)\right)$$
$$= \exp\left(\underbrace{y}_{T(y)}\ \underbrace{\log\left(\frac{p}{1-p}\right)}_{\eta(p)} - \underbrace{\left(-\log(1-p)\right)}_{B(p)}\right)\cdot \underbrace{1}_{h(y)}$$

- Poisson(λ): $\dfrac{\lambda^y}{y!}e^{-\lambda}$, $y = 0, 1, \ldots$.

$$\text{Poisson}\quad \frac{\lambda^y}{y!}e^{-\lambda} = \exp\left(\underbrace{-\lambda}_{B(\lambda)} + \underbrace{y}_{T(y)}\underbrace{\log\lambda}_{\eta(\lambda)}\right)\frac{1}{y!}$$

Examples of Continuous distributions

The following distributions form **continuous** exponential families of distributions with **pdf**:

- Gamma(a, b): $\frac{1}{\Gamma(a)b^a} y^{a-1} e^{-\frac{y}{b}}$;
  - above: a: shape parameter, b: scale parameter
  - reparametrize: $\mu = ab$: mean parameter

$$\frac{1}{\Gamma(a)} \left(\frac{a}{\mu}\right)^a y^{a-1} e^{-\frac{ay}{\mu}}.$$

- Inverse Gamma(α, β): $\frac{\beta^\alpha}{\Gamma(\alpha)} y^{-\alpha-1} e^{-\beta/y}$.
- Inverse Gaussian(μ, σ^2): $\sqrt{\frac{\sigma^2}{2\pi y^3}} e^{\frac{-\sigma^2(y-\mu)^2}{2\mu^2 y}}$.

Others: Chi-square, Beta, Binomial, Negative binomial distributions.

One-parameter canonical exponential family

- **Canonical exponential family** for $k = 1$, $y \in \mathbb{R}$

这一项前面是减号

$$f_\theta(y) = \exp\left(\frac{y\theta - b(\theta)}{\phi} + c(y, \phi)\right)$$

h(y)

for some *known* functions $b(\cdot)$ and $c(\cdot, \cdot)$.

- If ϕ is known, this is a one-parameter exponential family with θ being the canonical parameter .
- If ϕ is unknown, this may/may not be a two-parameter exponential family.
- ϕ is called **dispersion parameter**.
- In this class, we always assume that ϕ is *known*.

$f_\theta(y) = \exp\left(\frac{y\theta - b(\theta)}{\phi}\right) \cdot h(y)$ where $h(y) = e^{c(y,\phi)}$

Normal distribution example

- Consider the following Normal density function with known variance σ^2,

$$\begin{aligned} f_\theta(y) &= \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(y-\mu)^2}{2\sigma^2}} \\ &= \exp\left\{ \frac{y\mu - \frac{1}{2}\mu^2}{\sigma^2} - \frac{1}{2}\left(\frac{y^2}{\sigma^2} + \log(2\pi\sigma^2) \right) \right\}, \end{aligned}$$

- Therefore $\theta = \mu,\ \phi = \sigma^2,\ b(\theta) = \frac{\theta^2}{2}$, and

$$c(y, \phi) = -\frac{1}{2}\left(\frac{y^2}{\phi} + \log(2\pi\phi)\right).$$

Other distributions

Table 1: Exponential Family

	Normal	Poisson	Bernoulli
Notation	$\mathcal{N}(\mu, \sigma^2)$	$\mathcal{P}(\mu)$	$\mathcal{B}(p)$
Range of y	$(-\infty, \infty)$	$[0, -\infty)$	$\{0, 1\}$
ϕ	σ^2	1	1
$b(\theta)$	$\frac{\theta^2}{2}$	e^θ	$\log(1 + e^\theta)$
$c(y, \phi)$	$-\frac{1}{2}(\frac{y^2}{\phi} + \log(2\pi\phi))$	$-\log y!$	0

Likelihood

Let $\ell(\theta) = \log f_\theta(Y)$ denote the log-likelihood function.
The mean $\mathbb{E}(Y)$ and the variance $\mathrm{var}(Y)$ can be derived from the following identities

- First identity

$$\mathbb{E}(\frac{\partial \ell}{\partial \theta}) = 0$$

$$\begin{aligned}
\mathbb{E}\left[\frac{d\ell}{d\theta}\right] &= \int_Y \frac{d\ell}{d\theta} f_\theta(y)\, dy \\
&= \int_Y \frac{d \ln f_\theta(y)}{d\theta} f_\theta(y)\, dy \\
&= \int_Y \frac{1}{f_\theta(y)} \frac{d f_\theta(y)}{d\theta} f_\theta(y)\, dy \\
&= \frac{d}{d\theta} \int_Y f_\theta(y)\, dy = \frac{d}{d\theta} 1 = 0.
\end{aligned}$$

微分和导数互换（在这里可以）

- Second identity

$$\mathbb{E}\left[\ell'(\theta)\right] = \mathbb{E}\left[\frac{\frac{\partial}{\partial\theta} f_\theta(X)}{f_\theta(X)}\right] = \int_{-\infty}^{\infty} \left(\frac{\frac{\partial}{\partial\theta} f_\theta(x)}{f_\theta(x)}\right) f_\theta(x)\, dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial\theta} f_\theta(x)\, dx = 0$$

$$\mathbb{E}(\frac{\partial^2 \ell}{\partial \theta^2}) + \mathbb{E}(\frac{\partial \ell}{\partial \theta})^2 = 0.$$

$$\begin{aligned}
\mathrm{Var}\left(\ell'(\theta)\right) &= \mathbb{E}\left[\ell'(\theta)^2\right] - \mathbb{E}[\ell'(\theta)]^2 \\
&= \mathbb{E}\left[\left(\ell'(\theta)\right)^2\right] \\
&= \mathbb{E}\left[\left(\frac{\frac{\partial}{\partial\theta} f_\theta(X)}{f_\theta(X)}\right)^2\right] \\
&= \int_{-\infty}^{\infty} \frac{\left(\frac{\partial}{\partial\theta} f_\theta(x)\right)^2}{f_\theta(x)}\, dx
\end{aligned}$$

$\left(\Leftrightarrow \underbrace{\mathbb{E}\left[\left(\frac{\partial \ell}{\partial \theta}\right)^2\right]}_{\text{F.I}} = \underbrace{-\mathbb{E}\left[\frac{\partial^2 \ell}{\partial \theta^2}\right]}_{\text{F.I}}\right.$ (reminder)

两种fisher information的表达方式

Expected value

Note that

$$\ell(\theta) = \frac{Y\theta - b(\theta)}{\phi} + c(Y;\phi),$$

Therefore

$$\frac{\partial \ell}{\partial \theta} = Y - b'(\theta)$$

It yields

$$0 = \mathbb{E}(\frac{\partial \ell}{\partial \theta}) = \frac{\mathbb{E}(Y) - b'(\theta)}{\phi},$$

which leads to

$$\mathbb{E}(Y) = b'(\theta)$$

Variance

On the other hand we have we have

$$\frac{\partial^2 \ell}{\partial \theta^2} + (\frac{\partial \ell}{\partial \theta})^2 = -\frac{b''(\theta)}{\phi} + \left(\frac{Y - b'(\theta)}{\phi}\right)^2$$

and from the previous result,

$$\frac{Y - b'(\theta)}{\phi} = \frac{Y - \mathbb{E}(Y)}{\phi}$$

Together, with the second identity, this yields

$$0 = -\frac{b''(\theta)}{\phi} + \frac{\mathsf{var}(Y)}{\phi^2},$$

which leads to

$$\mathsf{var}(Y) = b''(\theta) \cdot \phi$$

Example: Poisson distribution

$b(\theta) = \mu = e^{\theta}$

$\log \mu = \theta \Rightarrow \mu = e^{\theta}$

Example: Consider a Poisson likelihood,

这里的mu是Y的参数

$$f(y) = \frac{\mu^y}{y!} e^{-\mu} = \exp\left(y \log \mu - \mu - \log(y!)\right)$$

$b(\theta)$

θ

$c(y, \phi)$, $\phi = 1$

mu不是回归方程的参数，log(mu)才是
这样做转化成一个GLM

Thus,

$$\theta = \log \mu \quad b(\theta) = e^{\theta} \quad \phi = 1 \quad c(y, \phi) = -\log(y!),$$

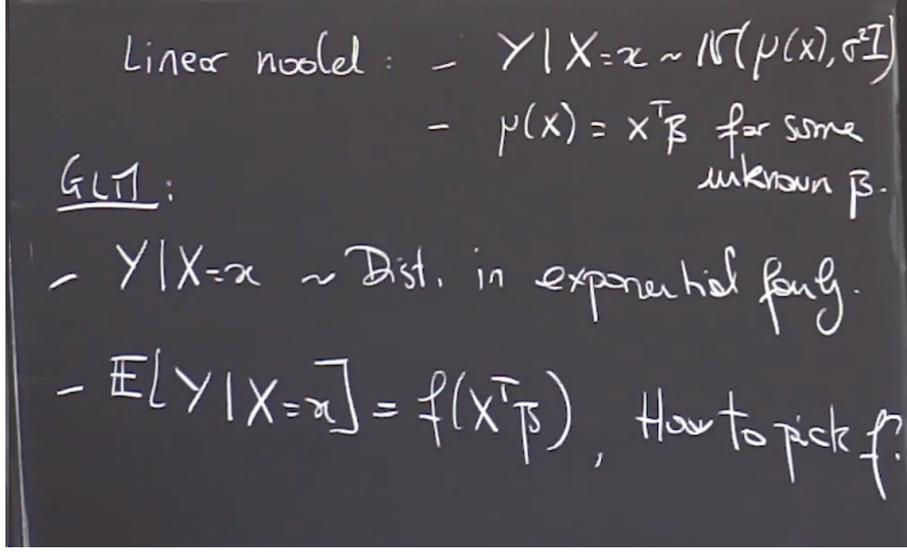
So

$$\mu = e^{\theta}, \quad b(\theta) = \mu \quad b''(\theta) = \mu$$

$\mathbb{E}[Y] = \mu$, $\mathrm{Var}[Y] = \mu \cdot 1 = \mu$

Link function

前面用概率论构建了一个有parameter的模型
这里我们要把我们的data和parameter联系起来



- β is the parameter of interest, and needs to appear somehow in the likelihood function to use maximum likelihood.
- A link function g relates the linear predictor $X^\top\beta$ to the mean parameter μ,

mu在上一页中，是Y的参数，我们要用X'β来表达mu
用predictor表达parameter

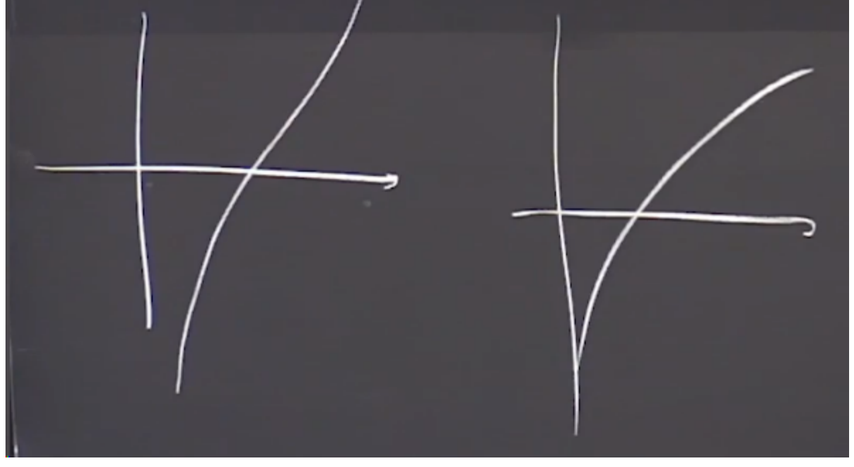
$$X^\top\beta = g(\mu). = g(\mu(X))$$

- g is required to be monotone increasing and differentiable

invertible

$$\mu = g^{-1}(X^\top\beta).$$

Examples of link functions



linear model中的function g就相当于啥都不用做

- For LM, $g(\cdot) = \text{identity}$.
- Poisson data. Suppose $Y|X \sim \text{Poisson}(\mu(X))$.
  - $\mu(X) > 0$;
  - $\log(\mu(X)) = X^\top \beta$;
  - In general, a link function for the count data should map $(0, +\infty)$ to $\mathbb{R}$.
    - The log link is a natural one.

把(0,inf)的数据map到R

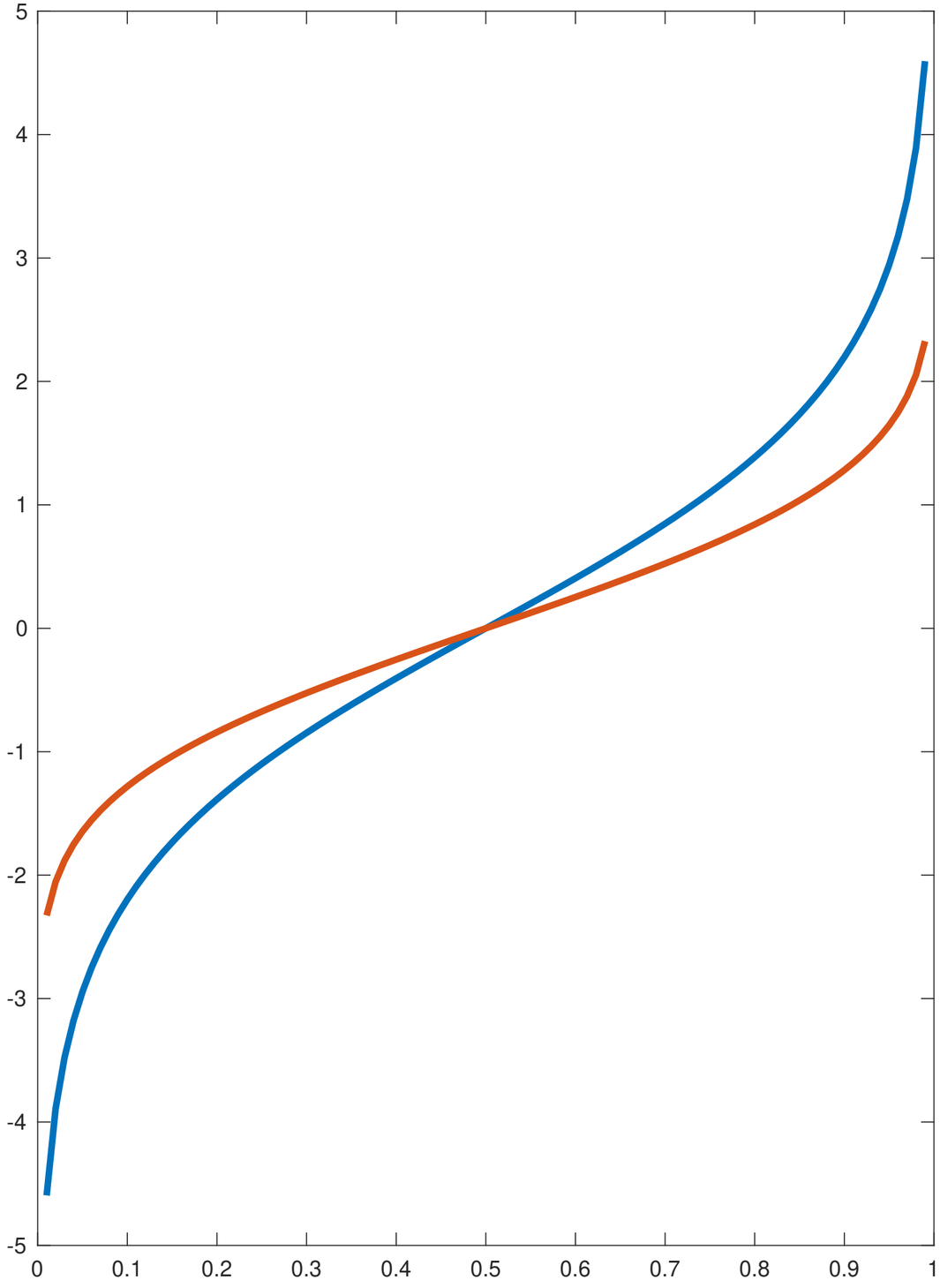
log-link

- Bernoulli/Binomial data.
  - $0 < \mu < 1$;
  - g should map $(0, 1)$ to $\mathbb{R}$:
  - 3 choices:
    1. logit: $\log\left(\frac{\mu(X)}{1-\mu(X)}\right) = X^\top \beta$;
    2. probit: $\Phi^{-1}(\mu(X)) = X^\top \beta$ where $\Phi(\cdot)$ is the normal cdf;

先把(0,1)map到R+，再用log map到R

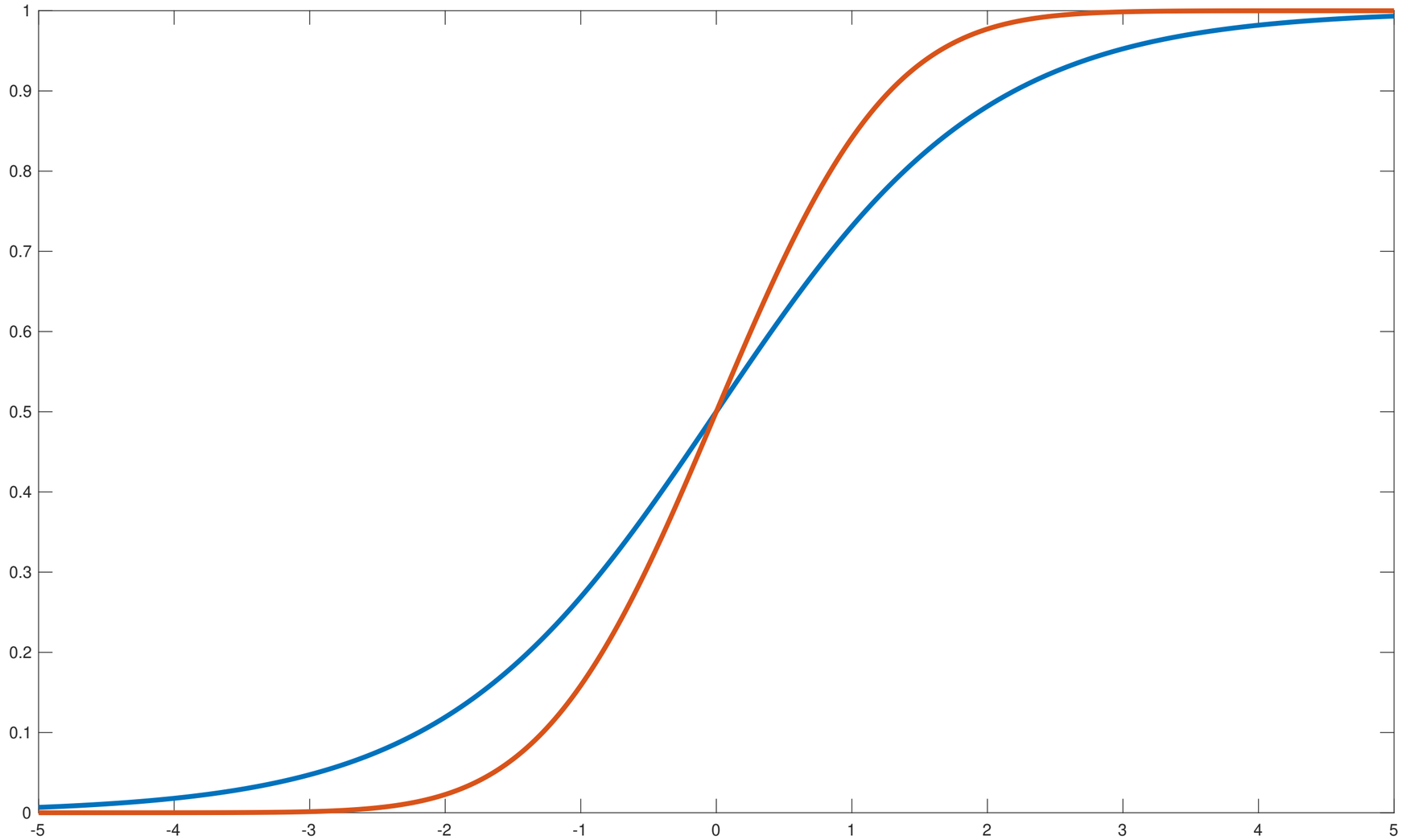
  - The logit link is the natural choice.

Examples of link functions for Bernoulli response



- in blue:
  $g_1(x) = f_1^{-1}(x) = \log\left(\frac{x}{1-x}\right)$ (logit link)
- in red:
  $g_2(x) = f_2^{-1}(x) = \Phi^{-1}(x)$
  (probit link)

Examples of link functions for Bernoulli response



- in blue: $f_1(x) = \dfrac{e^x}{1+e^x}$
- in red: $f_2(x) = \Phi(x)$ (Gaussian CDF)

Canonical Link

- The function g that links the mean μ to the canonical parameter θ is called **Canonical Link**:

$$g(\mu) = \theta$$

- Since $\mu = b'(\theta)$, the canonical link is given by

b是构造出来的函数
g是link函数

$b'(g(\mu)) = \mu$

$$g(\mu) = (b')^{-1}(\mu)\,.$$

- If $\phi > 0$, the canonical link function is **strictly increasing**.

Why?

$g \nearrow$ str. $\Leftrightarrow$ $g^{-1} \nearrow$ str. $\Leftrightarrow$ $(g^{-1})' > 0$ $\Leftrightarrow$ $b'' > 0$ $(\Leftarrow)$ $\mathrm{Var} > 0$
$\phi > 0$

Example: the Bernoulli distribution

- We can check that

$$b(\theta) = \log(1 + e^{\theta})$$

- Hence we solve

$$b'(\theta) = \frac{\exp(\theta)}{1 + \exp(\theta)} = \mu \qquad \Leftrightarrow \qquad \theta = \log\left(\frac{\mu}{1-\mu}\right)$$

- The canonical link for the Bernoulli distribution is the logit link

Other examples

$$\mu = b'(\theta)$$

link functions

前三个mean都正好等于参数

	$b(\theta)$	$g(\mu)$
Normal	$\theta^2/2$	μ
Poisson	$\exp(\theta)$	$\log \mu$
Bernoulli	$\log(1+e^\theta)$	$\log \frac{\mu}{1-\mu}$
Gamma	$-\log(-\theta)$	$-\frac{1}{\mu}$

exercise

Model and notation

Xi是一个p维的观测变量,Yi是一个预测变量
通过Xi预测Yi一共有n对Xi和Yi

- Let $(X_i, Y_i) \in \mathbb{R}^p \times \mathbb{R}$, $i = 1, \ldots, n$ be independent random pairs such that the conditional distribution of Y_i given $X_i = x_i$ has density in the canonical exponential family:

给了Y的分布，b，phi
我们就知道了任何Y|X的信息

每个Yi有不同的模型，θ将所有的Yi和Xi联系起来。
θi = Xi'β

$$f_{\theta_i}(y_i) = \exp\left\{\frac{y_i\theta_i - b(\theta_i)}{\phi} + c(y_i, \phi)\right\}.$$

β是唯一的未知参数，当我们有Y和X的数据的后，用这些数据来估计β

- $\mathbf{Y} = (Y_1, \ldots, Y_n)^\top$, $\mathbb{X} = (X_1, \ldots, X_n)^\top =$  $\in \mathbb{R}^{n\times p}$
- Here the mean $\mu_i = \mathbb{E}[Y_i|X_i]$ is related to the canonical parameter θ_i via

$$\mu_i = b'(\theta_i)$$

这里的θ是canonical模型的θ，我们通过构建canonical模型，将mu转换成θ
那么，我们用反函数，也能把mu找回来。
这么做的原因也是指数分布族的优点

- and μ_i depends linearly on the covariates through a link function g:

$$g(\mu_i) = X_i^\top \beta \ .$$

我们要将Y的期望和βX通过link function联系起来。

$b'(g(\mu)) = \mu$

Back to β

likelihood function里面只有θ
我们想要的是β，所以我们把θ替换成β

- Given a link function g, note the following relationship between β and θ:

$$g(\mu) = \theta$$
$$\mu = b'(\theta)$$

$$\begin{aligned} \theta_i &= (b')^{-1}(\mu_i) \\ &= (b')^{-1}(g^{-1}(X_i^\top \beta)) \equiv h(X_i^\top \beta), \end{aligned}$$

where h is defined as

$$h = (b')^{-1} \circ g^{-1} = (g \circ b')^{-1}.$$

- Remark: if g is the **canonical** link function, h is the identity

$g = (b')^{-1}$

Log-likelihood

- The log-likelihood is given by

$$\ell_n(\mathbf{Y}, \mathbb{X}, \beta) = \sum_i \frac{Y_i\theta_i - b(\theta_i)}{\phi} + \text{cst}$$

$\theta_i = \theta_i(X_i) = h(X_i^\top \beta)$

$$= \sum_i \frac{Y_i h(X_i^\top \beta) - b(h(X_i^\top \beta))}{\phi} + \text{cst}$$

up to a constant term.

- Note that when we use the **canonical** link function, we obtain the simpler expression

$$\ell_n(\mathbf{Y}, \mathbb{X}, \beta) = \sum_i \frac{Y_i X_i^\top \beta - b(X_i^\top \beta)}{\phi} + \text{cst}$$

$$-\nabla_\beta \ell_n = -\sum_i \nabla_\beta \frac{b(X_i^\top \beta)}{\phi} = -\frac{1}{\phi}\sum_{i=1}^n b''(X_i^\top \beta)\, X_i X_i^\top$$

$$-\nabla^2_\beta \ell_n = \frac{1}{\phi}\sum_{i=1}^n b''(X_i^\top \beta)(X^\top X_i)^2$$

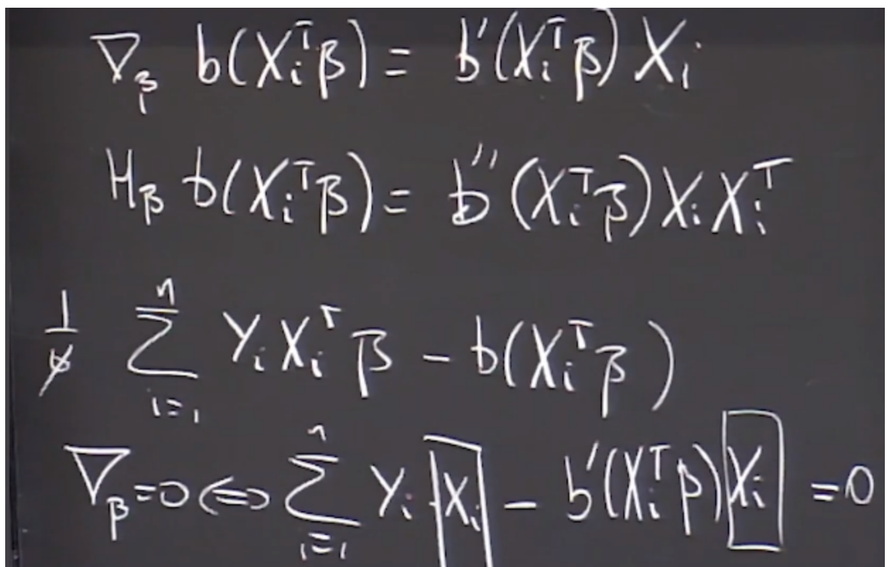
Strict concavity

- The log-likelihood $\ell(\theta)$ is **strictly concave** using the canonical function when $\phi > 0$. Why? if Rank($\mathbf{X}$) = p

  full rank

- As a consequence the maximum likelihood estimator is unique

- On the other hand, if another parameterization is used, the likelihood function may not be strictly concave leading to **several local maxima**.



solve the p equations
if b' is Gaussian canonical, it's LSE.
if b' is non-linear, it's nasty
so we use optimization algorithms.

Concluding remarks

- Maximum likelihood for Bernoulli Y and the logit link is called canonical logistic regression.
- In general, there is no closed form for the MLE and we have to use optimization algorithms (gradient ascent)
- The asymptotic normality of the MLE also applies to GLMs.

don't have Gaussian error, so rely on CLT

测试β是不是显著不等于0