## Statistics for Applications

## Chapter 10: Generalized Linear Models (GLMs)

## Linear model

A linear model assumes

$$
Y \mid X \sim \mathcal{N}\left(\mu(X), \sigma^{2} I\right)
$$

And

$$
\mathbb{E}(Y \mid X)=\mu(X)=X^{\top} \beta
$$

## Components of a linear model

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

1. Random component: the response variable $Y \mid X$ is continuous and normally distributed with mean $\mu=\mu(X)=\mathbb{E}(Y \mid X)$.
2. Link: between the random and covariates

$$
X=\left(X^{(1)}, X^{(2)}, \cdots, X^{(p)}\right)^{\top}: \mu(X)=X^{\top} \beta
$$

## Generalization

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

1. Random component:

$$
Y \sim \text { some exponential family distribution }
$$

2. Link: between the random and covariates:

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

where $g$ called link function and $\mu=\mathbb{E}(Y \mid X)$.

## Example 1: Disease Occuring Rate

In the early stages of a disease epidemic, the rate at which new cases occur can often increase exponentially through time. Hence, if $\mu_{i}$ is the expected number of new cases on day $t_{i}$, a model of the form

$$
\mu_{i}=\gamma \exp \left(\delta t_{i}\right)
$$

seems appropriate.

- Such a model can be turned into GLM form, by using a log link so that

$$
\log \left(\mu_{i}\right)=\log (\gamma)+\delta t_{i}=\beta_{0}+\beta_{1} t_{i}
$$

- Since this is a count, the Poisson distribution (with expected value $\mu_{i}$ ) is probably a reasonable distribution to try.


## Example 2: Prey Capture Rate(1)

The rate of capture of preys, $y_{i}$, by a hunting animal, tends to increase with increasing density of prey, $x_{i}$, but to eventually level off, when the predator is catching as much as it can cope with. A suitable model for this situation might be

$$
\mu_{i}=\frac{\alpha x_{i}}{h+x_{i}},
$$

where $\alpha$ represents the maximum capture rate, and $h$ represents the prey density at which the capture rate is half the maximum rate.

## Example 2: Prey Capture Rate (2)



## Example 2: Prey Capture Rate (3)

- Obviously this model is non-linear in its parameters, but, by using a reciprocal link, the right-hand side can be made linear in the parameters,

$$
g\left(\mu_{i}\right)=\frac{1}{\mu_{i}}=\frac{1}{\alpha}+\frac{h}{\alpha} \frac{1}{x_{i}}=\beta_{0}+\beta_{1} \frac{1}{x_{i}} .
$$

- The standard deviation of capture rate might be approximately proportional to the mean rate, suggesting the use of a Gamma distribution for the response.


## Example 3: Kyphosis Data

The Kyphosis data consist of measurements on 81 children following corrective spinal surgery. The binary response variable, Kyphosis, indicates the presence or absence of a postoperative deforming. The three covariates are, Age of the child in month, Number of the vertebrae involved in the operation, and the Start of the range of the vertebrae involved.

- The response variable is binary so there is no choice: $Y \mid X$ is Bernoulli with expected value $\mu(X) \in(0,1)$.
- 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 $f\left(X^{\top} \beta\right) \in(0,1)$


## GLM: motivation

- clearly, normal LM is not appropriate for these examples;
- need a more general regression framework to account for various types of response data
- Exponential family distributions
- develop methods for model fitting and inferences in this framework
- Maximum Likelihood estimation.


## Exponential Family

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

- $\eta_{1}, \eta_{2}, \cdots, \eta_{k}$ and $B$ of $\theta$,
- $T_{1}, T_{2}, \cdots, T_{k}$, and $h$ of $x \in \mathbb{R}^{q}$ such that the density function (pmf or pdf) of $P_{\theta}$ can be written as

$$
p_{\theta}(x)=\exp \left[\sum_{i=1}^{k} \eta_{i}(\theta) T_{i}(x)-B(\theta)\right] h(x)
$$

## Normal distribution example

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

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

which forms a two-parameter exponential family with

$$
\begin{gathered}
\eta_{1}=\frac{\mu}{\sigma^{2}}, \eta_{2}=-\frac{1}{2 \sigma^{2}}, T_{1}(x)=x, T_{2}(x)=x^{2} \\
B(\theta)=\frac{\mu^{2}}{2 \sigma^{2}}+\log (\sigma \sqrt{2 \pi}), h(x)=1
\end{gathered}
$$

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

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

## Examples of discrete distributions

The following distributions form discrete exponential families of distributions with pmf

- Bernoulli $(p): \quad p^{x}(1-p)^{1-x}, x \in\{0,1\}$
- Poisson $(\lambda): \frac{\lambda^{x}}{x!} e^{-\lambda}, x=0,1, \ldots$.


## Examples of Continuous distributions

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

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

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

- Inverse Gamma $(\alpha, \beta): \frac{\beta^{\alpha}}{\Gamma(\alpha)} x^{-\alpha-1} e^{-\beta / x}$.
- Inverse Gaussian $\left(\mu, \sigma^{2}\right): \sqrt{\frac{\sigma^{2}}{2 \pi x^{3}}} e^{\frac{-\sigma^{2}(x-\mu)^{2}}{2 \mu^{2} x}}$.

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

## Components of GLM

1. Random component:
$Y \sim$ some exponential family distribution
2. Link: between the random and covariates:

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

where $g$ called link function and $\mu(X)=\mathbb{E}(Y \mid X)$.

## One-parameter canonical exponential family

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

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

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

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


## Normal distribution example

- Consider the following Normal density function with known variance $\sigma^{2}$,

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

- 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 | $\mathcal{N}\left(\mu, \sigma^{2}\right)$ | $\mathcal{P}(\mu)$ | $\mathcal{B}(p)$ |
| Range of $y$ | $(-\infty, \infty)$ | $[0,-\infty)$ | $\{0,1\}$ |
| $\phi$ | $\sigma^{2}$ | 1 | 1 |
| $b(\theta)$ | $\frac{\theta^{2}}{2}$ | $e^{\theta}$ | $\log \left(1+e^{\theta}\right)$ |
| $c(y, \phi)$ | $-\frac{1}{2}\left(\frac{y^{2}}{\phi}+\log (2 \pi \phi)\right)$ | $-\log y!$ | 1 |

## Likelihood

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

- First identity

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

- Second identity

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

Obtained from $\int f_{\theta}(y) d y \equiv 1$.

## Expected value

Note that

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

Therefore

$$
\frac{\partial \ell}{\partial \theta}=\frac{Y-b^{\prime}(\theta)}{\phi}
$$

It yields

$$
0=\mathbb{E}\left(\frac{\partial \ell}{\partial \theta}\right)=\frac{\left.\mathbb{E}(Y)-b^{\prime}(\theta)\right)}{\phi}
$$

which leads to

$$
\mathbb{E}(Y)=\mu=b^{\prime}(\theta)
$$

## Variance

On the other hand we have we have

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

and from the previous result,

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

Together, with the second identity, this yields

$$
0=-\frac{b^{\prime \prime}(\theta)}{\phi}+\frac{\operatorname{var}(Y)}{\phi^{2}}
$$

which leads to

$$
\operatorname{var}(Y)=V(Y)=b^{\prime \prime}(\theta) \phi
$$

## Example: Poisson distribution

Example: Consider a Poisson likelihood,

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

Thus,

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

## Link function

- $\beta$ 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 $\mu$,

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

- $g$ is required to be monotone increasing and differentiable

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

## Examples of link functions

- For LM, $g(\cdot)=$ identity.
- Poisson data. Suppose $Y \mid X \sim \operatorname{Poisson}(\mu(X))$.
- $\mu(X)>0$;
- $\log (\mu(X))=X^{\top} \beta$;
- In general, a link function for the count data should map $(0,+\infty)$ to $\mathbb{R}$.
- The log link is a natural one.
- 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;
3. complementary log-log: $\log (-\log (1-\mu(X)))=X^{\top} \beta$

- The logit link is the natural choice.


## Examples of link functions for Bernoulli response (1)



- in blue: $f_{1}(x)=\frac{e^{x}}{1+e^{x}}$
- in red: $f_{2}(x)=\Phi(x)$ (Gaussian CDF)


## Examples of link functions for Bernoulli response (2)



- in blue:
$g_{1}(x)=f_{1}^{-1}(x)=$
$\log \frac{x}{1-x} \quad$ (logit link)
- in red:
$g_{2}(x)=f_{2}^{-1}(x)=\Phi^{-1}(x)$ (probit link)


## Canonical Link

- The function $g$ that links the mean $\mu$ to the canonical parameter $\theta$ is called Canonical Link:

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

- Since $\mu=b^{\prime}(\theta)$, the canonical link is given by

$$
g(\mu)=\left(b^{\prime}\right)^{-1}(\mu) .
$$

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


## Example: the Bernoulli distribution

- We can check that

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

- Hence we solve

$$
b^{\prime}(\theta)=\frac{\exp (\theta)}{1+\exp (\theta)}=\mu \quad \Leftrightarrow \quad \theta=\log \left(\frac{\mu}{1-\mu}\right)
$$

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


## Other examples

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

## Model and notation

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

$$
f_{\theta_{i}}\left(y_{i}\right)=\exp \left\{\frac{y_{i} \theta_{i}-b\left(\theta_{i}\right)}{\phi}+c\left(y_{i}, \phi\right)\right\} .
$$

- $\mathbf{Y}=\left(Y_{1}, \ldots, Y_{n}\right)^{\top}, \mathbb{X}=\left(X_{1}^{\top}, \ldots, X_{n}^{\top}\right)^{\top}$
- Here the mean $\mu_{i}$ is related to the canonical parameter $\theta_{i}$ via

$$
\mu_{i}=b^{\prime}\left(\theta_{i}\right)
$$

- and $\mu_{i}$ depends linearly on the covariates through a link function $g$ :

$$
g\left(\mu_{i}\right)=X_{i}^{\top} \beta
$$

## Back to $\beta$

- Given a link function $g$, note the following relationship between $\beta$ and $\theta$ :

$$
\begin{aligned}
\theta_{i} & =\left(b^{\prime}\right)^{-1}\left(\mu_{i}\right) \\
& =\left(b^{\prime}\right)^{-1}\left(g^{-1}\left(X_{i}^{\top} \beta\right)\right) \equiv h\left(X_{i}^{\top} \beta\right)
\end{aligned}
$$

where $h$ is defined as

$$
h=\left(b^{\prime}\right)^{-1} \circ g^{-1}=\left(g \circ b^{\prime}\right)^{-1} .
$$

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


## Log-likelihood

- The log-likelihood is given by

$$
\begin{aligned}
\ell_{n}(\beta ; \mathbf{Y}, \mathbb{X}) & =\sum_{i} \frac{Y_{i} \theta_{i}-b\left(\theta_{i}\right)}{\phi} \\
& =\sum_{i} \frac{Y_{i} h\left(X_{i}^{\top} \beta\right)-b\left(h\left(X_{i}^{\top} \beta\right)\right)}{\phi}
\end{aligned}
$$

up to a constant term.

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

$$
\ell_{n}(\beta, \phi ; \mathbf{Y}, \mathbb{X})=\sum_{i} \frac{Y_{i} X_{i}^{\top} \beta-b\left(X_{i}^{\top} \beta\right)}{\phi}
$$

## Strict concavity

- The $\log$-likelihood $\ell(\theta)$ is strictly concave using the canonical function when $\phi>0$. Why?
- 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.


## Optimization Methods

Given a function $f(x)$ defined on $\mathcal{X} \subset \mathbb{R}^{m}$, find $x^{*}$ such that $f\left(x^{*}\right) \geq f(x)$ for all $x \in \mathcal{X}$.

We will describe the following three methods,

- Newton-Raphson Method
- Fisher-scoring Method
- Iteratively Re-weighted Least Squares.


## Gradient and Hessian

- Suppose $f: \mathbb{R}^{m} \rightarrow \mathbb{R}$ has two continuous derivatives.
- Define the Gradient of $f$ at point $x_{0}, \nabla_{f}=\nabla_{f}\left(x_{0}\right)$, as

$$
\left(\nabla_{f}\right)=\left(\partial f / \partial x_{1}, \ldots, \partial f / \partial x_{m}\right)^{\top}
$$

- Define the Hessian (matrix) of $f$ at point $x_{0}, H_{f}=H_{f}\left(x_{0}\right)$, as

$$
\left(H_{f}\right)_{i j}=\frac{\partial^{2} f}{\partial x_{i} \partial x_{j}}
$$

- For smooth functions, the Hessian is symmetric. If $f$ is strictly concave, then $H_{f}(x)$ is negative definite.
- The continuous function:

$$
x \mapsto H_{f}(x)
$$

is called Hessian map.

## Quadratic approximation

- Suppose $f$ has a continuous Hessian map at $x_{0}$. Then we can approximate $f$ quadratically in a neighborhood of $x_{0}$ using

$$
f(x) \approx f\left(x_{0}\right)+\nabla_{f}^{\top}\left(x_{0}\right)\left(x-x_{0}\right)+\frac{1}{2}\left(x-x_{0}\right)^{\top} H_{f}\left(x_{0}\right)\left(x-x_{0}\right) .
$$

- This leads to the following approximation to the gradient:

$$
\nabla_{f}(x) \approx \nabla_{f}\left(x_{0}\right)+H_{f}\left(x_{0}\right)\left(x-x_{0}\right)
$$

- If $x^{*}$ is maximum, we have

$$
\nabla_{f}\left(x^{*}\right)=0
$$

- We can solve for it by plugging in $x^{*}$, which gives us

$$
x^{*}=x_{0}-H_{f}\left(x_{0}\right)^{-1} \nabla_{f}\left(x_{0}\right)
$$

## Newton-Raphson method

- The Newton-Raphson method for multidimensional optimization uses such approximations sequentially
- We can define a sequence of iterations starting at an arbitrary value $x_{0}$, and update using the rule,

$$
x^{(k+1)}=x^{(k)}-H_{f}\left(x^{(k)}\right)^{-1} \nabla_{f}\left(x^{(k)}\right) .
$$

- The Newton-Raphson algorithm is globally convergent at quadratic rate whenever $f$ is concave and has two continuous derivatives.


## Fisher-scoring method (1)

- Newton-Raphson works for a deterministic case, which does not have to involve random data.
- Sometimes, calculation of the Hessian matrix is quite complicated (we will see an example)
- Goal: use directly the fact that we are minimizing the KL divergence

$$
\mathrm{KL} "="-\mathbb{E}[\text { log-likelihood }]
$$

- Idea: replace the Hessian with its expected value. Recall that

$$
\mathbb{E}_{\theta}\left(H_{\ell_{n}}(\theta)\right)=-I(\theta)
$$

is the Fisher Information

## Fisher-scoring method (2)

- The Fisher Information matrix is positive definite, and can serve as a stand-in for the Hessian in the Newton-Raphson algorithm, giving the update:

$$
\theta^{(k+1)}=\theta^{(k)}+I\left(\theta^{(k)}\right)^{-1} \nabla_{\ell_{n}}\left(\theta^{(k)}\right) .
$$

This is the Fisher-scoring algorithm.

- It has essentially the same convergence properties as Newton-Raphson, but it is often easier to compute $I$ than $H_{\ell_{n}}$.


## Example: Logistic Regression (1)

- Suppose $Y_{i} \sim \operatorname{Bernoulli}\left(p_{i}\right), i=1, \ldots, n$, are independent $0 / 1$ indicator responses, and $X_{i}$ is a $p \times 1$ vector of predictors for individual $i$.
- The log-likelihood is as follows:

$$
\ell_{n}(\theta \mid \mathbf{Y}, \mathbb{X})=\sum_{i=1}^{n}\left(Y_{i} \theta_{i}-\log \left(1+e^{\theta_{i}}\right)\right)
$$

- Under the canonical link,

$$
\theta_{i}=\log \left(\frac{p_{i}}{1-p_{i}}\right)=X_{i}^{\top} \beta
$$

## Example: Logistic Regression (2)

- Thus, we have

$$
\ell_{n}(\beta \mid \mathbf{Y}, \mathbb{X})=\sum_{i=1}^{n}\left(Y_{i} X_{i}^{\top} \beta-\log \left(1+e^{X_{i}^{\top} \beta}\right)\right)
$$

- The gradient is

$$
\nabla_{\ell_{n}}(\beta)=\sum_{i=1}^{n}\left(Y_{i} X_{i}-\frac{e^{X_{i}^{\top} \beta}}{1+e^{X_{i}^{\top} \beta}} X_{i}\right) .
$$

- The Hessian is

$$
H_{\ell_{n}}(\beta)=-\sum_{i=1}^{n} \frac{e^{X_{i}^{\top} \beta}}{\left(1+e^{X_{i}^{\top} \beta}\right)^{2}} X_{i} X_{i}^{\top} .
$$

- As a result, the updating rule is

$$
\beta^{(k+1)}=\beta^{(k)}-H_{\ell_{n}}\left(\beta^{(k)}\right)^{-1} \nabla_{\ell_{n}}\left(\beta^{(k)}\right) .
$$

## Example: Logistic Regression (3)

- The score function is a linear combination of the $X_{i}$, and the Hessian or Information matrix is a linear combination of $X_{i} X_{i}^{\top}$. This is typical in exponential family regression models (i.e. GLM).
- The Hessian is negative definite, so there is a unique local maximizer, which is also the global maximizer.
- Finally, note that that the $Y_{i}$ does not appear in $H_{\ell_{n}}(\beta)$, which yields

$$
H_{\ell_{n}}(\beta)=\mathbb{E}\left[H_{\ell_{n}}(\beta)\right]=-I(\beta)
$$

## Iteratively Re-weighted Least Squares

- IRLS is an algorithm for fitting GLM obtained by Newton-Raphson/Fisher-scoring.
- Suppose $Y_{i} \mid X_{i}$ has a distribution from an exponential family with the following log-likelihood function,

$$
\ell=\sum_{i=1}^{n} \frac{Y_{i} \theta_{i}-b\left(\theta_{i}\right)}{\phi}+c\left(Y_{i}, \phi\right)
$$

- Observe that

$$
\begin{gathered}
\mu_{i}=b^{\prime}\left(\theta_{i}\right), X_{i}^{\top} \beta=g\left(\mu_{i}\right), \frac{d \mu_{i}}{d \theta_{i}}=b^{\prime \prime}\left(\theta_{i}\right) \equiv V_{i} \\
\theta_{i}=\left(b^{\prime}\right)^{-1} \circ g^{-1}\left(X_{i}^{\top} \beta\right):=h\left(X_{i}^{\top} \beta\right)
\end{gathered}
$$

## Chain rule

- According to the chain rule, we have

$$
\begin{aligned}
& \frac{\partial \ell_{n}}{\partial \beta_{j}}=\sum_{i=1}^{n} \frac{\partial \ell_{i}}{\partial \theta_{i}} \frac{\partial \theta_{i}}{\partial \beta_{j}} \\
= & \sum_{i} \frac{Y_{i}-\mu_{i}}{\phi} h^{\prime}\left(X_{i}^{\top} \beta\right) X_{i}^{j} \\
= & \sum_{i}\left(\tilde{\mathbf{Y}}_{i}-\tilde{\mu}_{i}\right) W_{i} X_{i}^{j} \quad\left(W_{i} \equiv\left(\frac{h^{\prime}\left(X_{i}^{\top} \beta\right)}{g^{\prime}\left(\mu_{i}\right) \phi}\right)\right) .
\end{aligned}
$$

- Where $\tilde{\mathbf{Y}}=\left(g^{\prime}\left(\mu_{1}\right) Y_{1}, \ldots g^{\prime}\left(\mu_{n}\right) Y_{n}\right)^{\top}$ and $\tilde{\mu}=\left(g^{\prime}\left(\mu_{1}\right) \mu_{1}, \ldots g^{\prime}\left(\mu_{n}\right) \mu_{n}\right)^{\top}$


## Gradient

- Define

$$
W=\operatorname{diag}\left\{W_{1}, \ldots, W_{n}\right\}
$$

- Then, the gradient is

$$
\nabla_{\ell_{n}}(\beta)=\mathbb{X}^{\top} W(\tilde{\mathbf{Y}}-\tilde{\mu})
$$

## Hessian

- For the Hessian, we have

$$
\begin{aligned}
\frac{\partial^{2} \ell}{\partial \beta_{j} \partial \beta_{k}}=\sum_{i} & \frac{Y_{i}-\mu_{i}}{\phi} h^{\prime \prime}\left(X_{i}^{\top} \beta\right) X_{i}^{j} X_{i}^{j} \\
& -\frac{1}{\phi} \sum_{i}\left(\frac{\partial \mu_{i}}{\partial \beta_{k}}\right) h^{\prime}\left(X_{i}^{\top} \beta\right) X_{i}^{j}
\end{aligned}
$$

- Note that

$$
\frac{\partial \mu_{i}}{\partial \beta_{k}}=\frac{\partial b^{\prime}\left(\theta_{i}\right)}{\partial \beta_{k}}=\frac{\partial b^{\prime}\left(h\left(X_{i}^{\top} \beta\right)\right)}{\partial \beta_{k}}=b^{\prime \prime}\left(\theta_{i}\right) h^{\prime}\left(X_{i}^{\top} \beta\right) X_{i}^{k}
$$

It yields

$$
\mathbb{E}\left(H_{\ell_{n}}(\beta)\right)=-\frac{1}{\phi} \sum_{i} b^{\prime \prime}\left(\theta_{i}\right)\left[h^{\prime}\left(X_{i}^{\top} \beta\right)\right]^{2} X_{i} X_{i}^{\top}
$$

## Fisher information

- Note that $g^{-1}(\cdot)=b^{\prime} \circ h(\cdot)$ yields

$$
b^{\prime \prime} \circ h(\cdot) \cdot h^{\prime}(\cdot)=\frac{1}{g^{\prime} \circ g^{-1}(\cdot)}
$$

Recall that $\theta_{i}=h\left(X_{i}^{\top} \beta\right)$ and $\mu_{i}=g^{-1}\left(X_{i}^{\top} \beta\right)$, we obtain

$$
b^{\prime \prime}\left(\theta_{i}\right) h^{\prime}\left(X_{i}^{\top} \beta\right)=\frac{1}{g^{\prime}\left(\mu_{i}\right)}
$$

- As a result

$$
\mathbb{E}\left(H_{\ell_{n}}(\beta)\right)=-\sum_{i} \frac{h^{\prime}\left(X_{i}^{\top} \beta\right)}{g^{\prime}\left(\mu_{i}\right) \phi} X_{i} X_{i}^{\top}
$$

- Therefore,

$$
I(\beta)=-\mathbb{E}\left(H_{\ell_{n}}(\beta)\right)=\mathbb{X}^{\top} W \mathbb{X} \quad \text { where } \quad W=\operatorname{diag}\left(\frac{h^{\prime}\left(X_{i}^{\top} \beta\right)}{g^{\prime}\left(\mu_{i}\right)}\right)
$$

## Fisher-scoring updates

- According to Fisher-scoring, we can update an initial estimate $\beta^{(k)}$ to $\beta^{(k+1)}$ using

$$
\beta^{(k+1)}=\beta^{(k)}+I\left(\beta^{(k)}\right)^{-1} \nabla_{\ell_{n}}\left(\beta^{(k)}\right),
$$

- which is equivalent to

$$
\begin{aligned}
\beta^{(k+1)} & =\beta^{(k)}+\left(\mathbb{X}^{\top} W \mathbb{X}\right)^{-1} \mathbb{X}^{\top} W(\tilde{\mathbf{Y}}-\tilde{\mu}) \\
& =\left(\mathbb{X}^{\top} W \mathbb{X}\right)^{-1} \mathbb{X}^{\top} W\left(\tilde{\mathbf{Y}}-\tilde{\mu}+\mathbb{X} \beta^{(k)}\right)
\end{aligned}
$$

## Weighted least squares (1)

Let us open a parenthesis to talk about Weighted Least Squares.

- Assume the linear model $\mathbf{Y}=\mathbb{X} \beta+\varepsilon$, where $\varepsilon \sim \mathcal{N}_{n}\left(0, W^{-1}\right)$, where $W^{-1}$ is a $n \times n$ diagonal matrix. When variances are different, the regression is said to be heteroskedastic.
- The maximum likelihood estimator is given by the solution to

$$
\min _{\beta}(\mathbf{Y}-\mathbb{X} \beta)^{\top} W(\mathbf{Y}-\mathbb{X} \beta)
$$

This is a Weighted Least Squares problem

- The solution is given by

$$
\left(\mathbb{X}^{\top} W \mathbb{X}\right)^{-1} \mathbb{X}^{\top} W\left(\mathbb{X}^{\top} W \mathbb{X}\right) \mathbf{Y}
$$

- Routinely implemented in statistical software.


## Weighted least squares (2)

Back to our problem.
Recall that

$$
\beta^{(k+1)}=\left(\mathbb{X}^{\top} W \mathbb{X}\right)^{-1} \mathbb{X}^{\top} W\left(\tilde{\mathbf{Y}}-\tilde{\mu}+\mathbb{X} \beta^{(k)}\right)
$$

- This reminds us of Weighted Least Squares with

1. $W=W\left(\beta^{(k)}\right)$ being the weight matrix,
2. $\tilde{\mathbf{Y}}-\tilde{\mu}+\mathbb{X} \beta^{(k)}$ being the response.

So we can obtain $\beta^{(k+1)}$ using any system for WLS.

## IRLS procedure (1)

Iteratively Reweighed Least Squares is an iterative procedure to compute the MLE in GLMs using weighted least squares.
We show how to go from $\beta^{(k)}$ to $\beta^{(k+1)}$

1. Fix $\beta^{(k)}$ and $\mu_{i}^{(k)}=g^{-1}\left(X_{i}^{\top} \beta^{(k)}\right)$;
2. Calculate the adjusted dependent responses

$$
Z_{i}^{(k)}=X_{i}^{\top} \beta^{(k)}+g^{\prime}\left(\mu_{i}^{(k)}\right)\left(Y_{i}-\mu_{i}^{(k)}\right)
$$

3. Compute the weights $W^{(k)}=W\left(\beta^{(k)}\right)$

$$
W^{(k)}=\operatorname{diag} \frac{h^{\prime}\left(X_{i}^{\top} \beta^{(k)}\right)}{g^{\prime}\left(\mu_{i}^{(k)}\right) \phi}
$$

4. Regress $\mathbf{Z}^{(k)}$ on the design matrix $\mathbb{X}$ with weight $W^{(k)}$ to derive a new estimate $\beta^{(k+1)}$;

We can repeat this procedure until convergence.

## IRLS procedure (2)

- For this procedure, we only need to know $\mathbb{X}, \mathbf{Y}$, the link function $g(\cdot)$ and the variance function $V(\mu)=b^{\prime \prime}(\theta)$.
- A possible starting value is to let $\mu^{(0)}=\mathbf{Y}$.
- If the canonical link is used, then Fisher scoring is the same as Newton-Raphson.

$$
\mathbb{E}\left(H_{\ell_{n}}\right)=H_{\ell_{n}} .
$$

There is no random component $(\mathbf{Y})$ in the Hessian matrix.

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