# Unconstrained Problem and Algorithm II 

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## CONTENTS

- Secant method
- MM algorithm
- Applications


## SECANT METHOD

## Newton method vs. Secant Method

The common goal is to find the solution of $f^{\prime}(x)=0$

- (Newton method) For an existing approximator $x^{(t)}$, the next solution is updated by a linear equation, $f^{\prime}\left(x^{(t)}\right)+f^{\prime \prime}\left(x^{(t)}\right)\left(x-x^{(t)}\right)=0$.

$$
x^{(t+1)}=x^{(t)}-f^{\prime \prime}\left(x^{(t)}\right) f\left(x^{(t)}\right)
$$

- (Secant method) For two existing approximators $x^{(t)}$ and $x^{(t+1)}$, the next solution is updated by a linear equation, $f^{\prime}\left(x^{(t)}\right)+\left(\frac{f^{\prime}\left(x^{(t+1)}\right)-f^{\prime}\left(x^{(t)}\right)}{x^{(t+1)}-x^{(t)}}\right)\left(x-x^{(t)}\right)=0$.

$$
x^{(t+2)}=x^{(t)}-\left(\frac{f^{\prime}\left(x^{(t+1)}\right)-f^{\prime}\left(x^{(t)}\right)}{x^{(t+1)}-x^{(t)}}\right)^{-1} f^{\prime}\left(x^{(t)}\right)
$$



Figure 1: Left: Newton method. Right: Secant method

## Secant condition

The next solution is equally given by the two different equations:

$$
\begin{align*}
f^{\prime}\left(x^{(t)}\right)+B\left(x-x^{(t)}\right) & =0  \tag{1}\\
f^{\prime}\left(x^{(t+1)}\right)+B\left(x-x^{(t+1)}\right) & =0 \tag{2}
\end{align*}
$$

where $B=\left(\frac{f^{\prime}\left(x^{(t+1)}\right)-f^{\prime}\left(x^{(t)}\right)}{x^{(t+1)}-x^{(t)}}\right)$.
That is, $x^{(t+2)}=x^{(t)}-B^{-1} f^{\prime}\left(x^{(t)}\right)=x^{(t+1)}-B^{-1} f^{\prime}\left(x^{(t+1)}\right)$ and $x^{(t+1)}-x^{(t)}=B^{-1}\left(f^{\prime}\left(x^{(t+1)}\right)-\right.$ $f^{\prime}\left(x^{(t)}\right)$ ). Thus,

$$
B\left(x^{(t+1)}-x^{(t)}\right)=\left(f^{\prime}\left(x^{(t+1)}\right)-f^{\prime}\left(x^{(t)}\right)\right) .
$$

## Definition 1 (Secant condition)

An approximation of the hessian matrix $B$ satisfies that

$$
B\left(x^{(t+1)}-x^{(t)}\right)=\nabla f\left(x^{(t+1)}\right)-\nabla f\left(x^{(t)}\right)
$$

## Approximation of Hessian matrix

Let $f: \mathbb{R}^{n} \mapsto \mathbb{R}$ be convex and twice differentiable. The Hessian matrix satisfies

$$
\nabla f(x)-\nabla f(x+s) \simeq-\nabla^{2} f(x+s) s
$$

Let $x^{(k+1)}=x^{(k)}+s^{(k)}$. When the computation of $\nabla^{2} f\left(x^{(k+1)}\right)$ is practically difficult, an approximation of $\nabla^{2} f\left(x^{(k+1)}\right), B_{k+1}$, is desired to satisfy

$$
\nabla f\left(x^{(k+1)}\right) \simeq \nabla f\left(x^{(k)}\right)+B_{k+1}\left(x^{(k+1)}-x^{(k)}\right) .
$$

The secant condition for $B_{k+1}$ is written by

$$
\nabla f\left(x^{(k+1)}\right)-\nabla f\left(x^{(k)}\right)=B_{k+1}\left(x^{(k+1)}-x^{(k)}\right)
$$

## Outline of Quasi-Newton Method

1. For $k=0, x^{(k)}$ and $B_{k}$ are initialized.
2. $\nabla f\left(x^{(k)}\right)$ is computed and $x^{(k+1)}$ follows by

$$
x^{(k+1)}=x^{(k)}-\left(B_{k}\right)^{-1} \nabla f\left(x^{(k)}\right)
$$

3. $\nabla f\left(x^{(k+1)}\right)$ is computed.
4. $B_{k+1}$ is updated.

Before the step 4, new information is $s_{k}=x^{(k+1)}-x^{(k)}$ and $y_{k}=\nabla f\left(x^{(k+1)}\right)-\nabla f\left(x^{(k)}\right)$. Note that we let $B_{k+1} s_{k}=y_{k}$ by the secant condition.

Update of $B_{k+1}$

- Rank 1 update

$$
B_{k+1}=B_{k}+a v_{k} v_{k}^{\top}
$$

- Rank 2 update

$$
B_{k+1}=B_{k}+\alpha u_{k} u_{k}^{\top}+\beta v_{k} v_{k}^{\top}
$$

(Symmetric Rank-1 update)
Since $B_{k+1} s_{k}=B_{k} s_{k}+a v_{k} v_{k}^{\top} s_{k}$ or $y_{k}-B_{k} s_{k}=a\left(v_{k}^{\top} s_{k}\right) v_{k}, v_{k} \propto y_{k}-B_{k} s_{k}$. Let $v_{k}=$ $d\left(y_{k}-B_{k} s_{k}\right)$ then

$$
y_{k}-B_{k} s_{k}=a d^{2}\left(\left(y_{k}-B_{k} s_{k}\right)^{\top} s_{k}\right)\left(y_{k}-B_{k} s_{k}\right)
$$

Let $d^{2}=1 /\left(\left(y_{k}-B_{k} s_{k}\right)^{\top} s_{k}\right)$ and $a=\operatorname{sign}\left(\left(y_{k}-B_{k} s_{k}\right)^{\top} s_{k}\right)$. Thus,

$$
v_{k}=\frac{1}{\sqrt{\left(y_{k}-B_{k} s_{k}\right)^{\top} s_{k}}}\left(y_{k}-B_{k} s_{k}\right)
$$

and the update rule is given by

$$
B_{k+1}=B_{k}+\frac{\left(y_{k}-B_{k} s_{k}\right)\left(y_{k}-B_{k} s_{k}\right)^{\top}}{\left(y_{k}-B_{k} s_{k}\right)^{\top} s_{k}}
$$

(Rank-2 update: BFGS)
Since $B_{k+1} s_{k}=B_{k} s_{k}+\alpha\left(u_{k}^{\top} s_{k}\right) u_{k}+\beta\left(v_{k}^{\top} s_{k}\right) v_{k}$,

$$
y_{k}-B_{k} s_{k}=\alpha\left(u_{k}^{\top} s_{k}\right) u_{k}+\beta\left(v_{k}^{\top} s_{k}\right) v_{k}
$$

Let $u_{k}=y_{k}$ and $v_{k}=B_{k} s_{k}$ then $\alpha\left(u_{k}^{\top} s_{k}\right)=1$ and $\beta\left(v_{k}^{\top} s_{k}\right)=-1$. Since $\alpha=1 /\left(y_{k}^{\top} s_{k}\right)$ and $\beta=-1 /\left(s_{k}^{\top} B_{k} s_{k}\right)$,

$$
B_{k+1}=B_{k}+\frac{y_{k} y_{k}^{\top}}{y_{k}^{\top} s_{k}}-\frac{B_{k} s_{k} s_{k}^{\top} B_{k}^{\top}}{s_{k}^{\top} B_{k} s_{k}} .
$$

## Broyden-Fletcher-Goldfarb-Shanno algorithm

(1) Set $k=0$, let an initial $x^{(k)}$ and an initial Hessian matrix $B_{k}$.
(2) Find the direction $s_{k}=-B_{k}^{-1} \nabla f\left(x^{(k)}\right)$.
(4) Update $x^{(k+1)}=x^{(k)}+s_{k}$.
(5) Update $B_{k+1}=B_{k}+\frac{y_{k} y_{k}^{\top}}{y_{k}^{\top} s_{k}}-\frac{B_{k} s_{s} s_{k}^{\top} B_{k}^{\top}}{s_{k}^{\top} B_{k} s_{k}}$, where $y_{k}=\nabla f\left(x^{(k+1)}\right)-\nabla f\left(x^{(k)}\right)$.
(6) Repeat (2)-(5) until the solution converges.

Broyden-Fletcher-Goldfarb-Shanno update rule
(1) Set $k=0$, let an initial $x^{(k)}$ and an initial Hessian matrix $B_{k}$.
(2) Find the direction $p_{k}=-B_{k}^{-1} \nabla l\left(x^{(k)}\right)$.
(3) (Line search) Find a step size $\alpha_{k}=\operatorname{argmin}_{\alpha} l\left(x^{(k)}+\alpha p_{k}\right)$.
(4) Update $x^{(k+1)}=x^{(k)}+\alpha_{k} p_{k}$.
(5) Update $B_{k+1}=B_{k}+\frac{y_{k} \varphi_{k}^{\top}}{y_{k}^{\top} s_{k}}-\frac{B_{k} s_{k} s_{k}^{\top} B_{k}^{\top}}{s_{k}^{\top} B_{k} s_{k}}$,
where $s_{k}=\alpha_{k} p_{k}$ and $y_{k}=\nabla l\left(x^{(k+1)}\right)-\nabla l\left(x^{(k)}\right)$.
(6) Repeat (2)-(5) until the solution converges.

## Symmetric Rank-1 algorithm

Let $H_{k}=B_{k}^{-1}$ For step (5), by Sherman-Morrison formula,

$$
\begin{equation*}
H_{k+1}=H_{k}+\frac{\left(s_{k}-H_{k} y_{k}\right)\left(s_{k}-H_{k} y_{k}\right)^{\top}}{\left(s_{k}-H_{k} y_{k}\right)^{\top} y_{k}} \tag{3}
\end{equation*}
$$

- When $\left(s_{k}-H_{k} y_{k}\right)^{\top} y_{k}<0$, the nonnegative definiteness of $H_{k+1}$ can be violated.
- When $\left(s_{k}-H_{k} y_{k}\right)^{\top} y_{k}$ is close to zero, the updating process becomes unstable.


## BFGS algorithm

For step 5, by Sherman-Morrison formula,

$$
\begin{equation*}
H_{k+1}=\left(I-\frac{s_{k} y_{k}^{\top}}{y_{k}^{\top} s_{k}}\right) H_{k}\left(I-\frac{y_{k} s_{k}^{\top}}{y_{k}^{\top} s_{k}}\right)+\frac{s_{k} s_{k}^{\top}}{y_{k}^{\top} s_{k}} . \tag{4}
\end{equation*}
$$

When $H_{k}$ is positive definite and $y_{k}^{\top} s_{k}>0$, then $H_{k+1}$ is also positive definite. The line search is required for $y_{k}^{\top} s_{k}>0$ (see the strong Wolfe Condition).

## Total derivatives of $f$

Let $f: \mathbb{R}^{n} \mapsto \mathbb{R}^{k}$ If there exists a linear map $g: \mathbb{R}^{n} \mapsto \mathbb{R}^{k}$ such that

$$
\left\|f\left(x_{0}+h\right)-f\left(x_{0}\right)-g h\right\| \rightarrow 0
$$

as $\|h\| \rightarrow 0$
we call $g$ the total derivative of $f$ at $x_{0}$. Note that $g$ is a linear map depending on $x_{0}$ (in fact $n \times k$ matrix). Let $d\left(h ; x_{0}\right)=f\left(x_{0}+h\right)-f\left(x_{0}\right)$ then $g$ is an approximation of the map $d$. Now replace $f$ by $\nabla f$. What is $g$ ?

## L-BFGS algorithm

## Limited-memory BFGS

(1) Set $k=0$, and let an initial $x^{(k)}$.
(2) Let an $q=\nabla l\left(x^{(k)}\right)$.
(3) For $i=k-1, \ldots, k-m$ :

- $\alpha_{i}=\frac{s_{i}^{\top} q}{y_{i}^{\top} s_{i}}$.
- $q=q-\alpha_{i} y_{i}$.
(4) $\gamma_{k}=\frac{s_{k-1}^{\top} y_{k-1}}{y_{k-1}^{\top} y_{k-1}}, H_{k}^{0}=\gamma_{k} I$ and $z=-H_{k}^{0} q$.
(5) For $i=k-m, \ldots, k-1$ :
- $\beta_{i}=\frac{y_{i}^{\top} z}{y_{i}^{\top} s_{i}}$.
- $z=z-s_{i}\left(\alpha_{i}-\beta_{i}\right)$
(6) Repeat (2)-(5) until the solution converges.


## MM ALGORITHM

## Definition 2 (Majorized function)

Let $f, g: \mathbb{R}^{p} \rightarrow \mathbb{R}$. If $g\left(x \mid x^{(t)}\right) \geq f(x)$ for all $x$ and $g\left(x^{(t)} \mid x^{(t)}\right)=f\left(x^{(t)}\right)$ then we call $g\left(x \mid x^{(t)}\right)$ is a majorized function of $f$ at $x^{(t)}$.

## Example 3 (Quantile loss function)

The loss function $l(\cdot ; q): \mathbb{R} \rightarrow \mathbb{R}$ is given by

$$
l(x ; q)=\left\{\begin{array}{cl}
q x & , x \geq 0 \\
-(1-q) x & , x<0
\end{array}\right.
$$

for $0<q<1$. Then a majorized function of $f$ at $x^{*} \neq 0$ is given by

$$
g\left(x \mid x^{*}\right)=\frac{1}{4\left|x^{*}\right|} x^{2}+\left(q-\frac{1}{2}\right) x+\frac{\left|x^{*}\right|}{4}
$$



Figure 2: A majorized function of quantile loss
proof) Let $g\left(x \mid x^{*}\right)=a x^{2}+b x+c$. There are four sufficient conditions for $g\left(x \mid x^{*}\right)$ to be a majorized function of $f$ at $x^{*} \neq 0$ :

- $(b-q)^{2}-4 a c=0$ and $(b-q+1)^{2}-4 a c=0: b=q-1 / 2$
- $2 a x^{*}+b=q: a=1 / 4 x^{*}$
- $a\left(x^{*}\right)^{2}+b x^{*}+c=q x^{*}: c=x^{*} / 4$


## Example 4 (Quantile regression)

Let the risk function

$$
L(\boldsymbol{\beta})=\sum_{i=1}^{n} l\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta} ; q\right)
$$

for $0<q<1$. Then a majorized function of $L(\boldsymbol{\beta} ; q)$ at $\boldsymbol{\beta}^{*}$ is given by

$$
g\left(\boldsymbol{\beta} \mid \boldsymbol{\beta}^{*}\right)=\sum_{i=1}^{n} \frac{1}{4\left|r_{i}^{*}\right|}\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta}\right)^{2}+\left(q-\frac{1}{2}\right)\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta}\right)+\frac{\left|r_{i}^{*}\right|}{4}
$$

where $r_{i}^{*}=y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta}^{*}$. Note that $g\left(\boldsymbol{\beta} \mid \boldsymbol{\beta}^{*}\right)$ is quadratic function.

MM algorithm (Majorize-Minimization or Minorize-Maximization)

$$
\operatorname{minimize}_{x} f(x)
$$

- Give a initial solution $x^{(0)}$ and let $t=0$.
- Obtain the majorized function at $x^{(t)}: q\left(x \mid x^{(t)}\right)$
- Minimize the majorized function and let the minimizer $x^{(t+1)}$.
- $t \leftarrow t+1$ and repeat steps 2-4 until the solution converges.


## Proposition 1 (Descent property of MM algorithm)

If a sequence of $x^{(t)}$ for $t=1,2, \cdots$ is obtained by $M M$ algorithm, then

$$
f\left(x^{(t+1)}\right) \leq f\left(x^{(t)}\right)
$$

for all $t$. It means that the value of the object function evaluated at the solution always non-decreasing. Moreover, if $f$ is strictly convex and $x^{(t+1)} \neq x^{(t)}$, then the values are always decreasing.
proof)

$$
\begin{aligned}
f\left(x^{(t)}\right) & =q\left(x^{(t)} \mid x^{(t)}\right) \\
& \geq q\left(x^{(t+1)} \mid x^{(t)}\right) \\
& \geq f\left(x^{(t+1)}\right)
\end{aligned}
$$

- By definition of the majorized function the first equality holds.
- Since $x^{(t+1)}$ is the minimizer of $q\left(x \mid x^{(t)}\right)$, the first inequality holds.
- By definition of the majorized function the third inequality holds.


Figure 3: illustration of MM algorithm
(Q) What is the key to the success of MM algorithm?

## APPLICATIONS

- Huberized regression
- Logistic regression (for stable computation)
- Bradley-Terry model


## Huberized regression

Let a loss function $l(z ; d)=\frac{1}{2} z^{2} \mathbb{I}(|z| \leq d)+\left(d|z|-d^{2} / 2\right) \mathbb{I}(|z|>d)$ where $\mathbb{I}(\cdot)$ is the indicator function. When $d=\infty$, the loss function is $L_{2}$ loss function.

The regression estimator of regression model with huberized loss function is defined by

$$
\hat{\boldsymbol{\beta}}=\underset{\beta}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} l\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta} ; d\right)
$$

$\hat{\boldsymbol{\beta}}$ is robust to the error distribution of the assumed linear model. When the error variance is infinite, the estimator enjoys good asymptotic properties.

Here we will show the algorithm to obtain the Huberized regression estimator. We can decompose the function as

$$
l(z ; d)=l^{(1)}(z ; d)+l^{(2)}(z ; d)
$$

where

$$
l^{(1)}(z ; d)=z^{2} / 2
$$

and

$$
l^{(2)}(z ; d)=\left(|z|+d^{2} / 2-z^{2} / 2-d\right) I(|z|>d) .
$$



Figure 4: decomposition of Huber loss

Then, $l^{(2)}(z ; d)$ is a differentiable concave function and

$$
l^{(1)}(z ; d)+\nabla l^{(2)}\left(z^{*} ; d\right)\left(z-z^{*}\right)+l^{(2)}\left(z^{*} ; d\right)
$$

is a majorized function of $l(z ; d)$ at $z^{*}$ (by concavity of $l^{(2)}$ ). That is,

$$
l(z ; d) \leq l^{(1)}(z ; d)+\nabla l^{(2)}\left(z^{*} ; d\right)\left(z-z^{*}\right)+l^{(2)}\left(z^{*} ; d\right)
$$

Using this inequality, we construct MM algorithm for regression model with huber loss.
cf) CCCP algorithm

## MM algorithm for the huberized regression

1. Let $k=0$ and set an initial estimator $\boldsymbol{\beta}^{(k)}$
2. Repeat:

- Obtain the majorized function of $\frac{1}{n} \sum_{i=1}^{n} l\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta} ; d\right)$ at $\boldsymbol{\beta}^{(k)}$ :

$$
\begin{aligned}
Q\left(\boldsymbol{\beta} \mid \boldsymbol{\beta}^{(k)}\right)= & \sum_{i=1}^{n} l^{(1)}\left(\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta} ; d\right)\right. \\
& +\nabla l^{(2)}\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta}^{(k)} ; d\right)\left(\mathbf{x}_{i}^{\top} \boldsymbol{\beta}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta}^{(k)}\right) \\
& \left.+l^{(2)}\left(y_{i}-\mathbf{x}_{i}^{\top} \boldsymbol{\beta}^{(k)} ; d\right)\right)
\end{aligned}
$$

which is a quadratic function.

- Minimize $Q\left(\boldsymbol{\beta} \mid \boldsymbol{\beta}^{(k)}\right)$ and update $\boldsymbol{\beta}^{(k)}$
- $k \rightarrow k+1$


## Logistic regression

- $y \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^{p}$ and $y \mid \mathbf{x} \sim \operatorname{Bernoulli}(\theta(\mathbf{x} ; \boldsymbol{\beta}))$, where

$$
\theta(\mathbf{x} ; \boldsymbol{\beta})=\frac{\exp \left(\mathbf{x}^{\top} \boldsymbol{\beta}\right)}{1+\exp \left(\mathbf{x}^{\top} \boldsymbol{\beta}\right)} .
$$

- Let $\left(y_{i}, \mathbf{x}_{i}\right)$ for $i=1, \cdots, n$ be independent random samples, then the negative loglikelihood function is given by

$$
l(\boldsymbol{\beta})=\frac{1}{n} \sum_{i=1}^{n}\left[-y_{i} \mathbf{x}_{i}^{\top} \boldsymbol{\beta}+\log \left(1+\exp \left(\mathbf{x}_{i}^{\top} \boldsymbol{\beta}\right)\right)\right]
$$

Assume that $\sum_{i=1}^{n} \mathbf{x}_{i} \mathbf{x}_{i}^{\top} / n \in \mathbb{R}^{p \times p}$ is positive definite. For a fixed $\boldsymbol{\beta}$ there exists $\tilde{\boldsymbol{\beta}} \in B=\{b \in$ $\left.\mathbb{R}^{p}: b=h \boldsymbol{\beta}+(1-h) \hat{\boldsymbol{\beta}}^{(k)}, 0 \leq h \leq 1\right\}$ such that

$$
l(\boldsymbol{\beta})=l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)+\nabla l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)^{\top}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)+\frac{1}{2}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\top} \nabla^{2} l(\tilde{\boldsymbol{\beta}})\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) .
$$

Let $A=\frac{1}{4} \sum_{i=1}^{n} \mathbf{x}_{i} \mathbf{x}_{i}^{\top}$ then it can be shown that $A-\nabla^{2} l(\tilde{\boldsymbol{\beta}})$ is nonnegative definite, that is

$$
\begin{equation*}
\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\top} A\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) \geq\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\top} \nabla^{2} l(\tilde{\boldsymbol{\beta}})\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) . \tag{5}
\end{equation*}
$$

Moreover, we know that $\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\top} A\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) \geq \sup _{\tilde{\beta}}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\top} \nabla^{2} l(\tilde{\boldsymbol{\beta}})\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)$.
Hence, from (5),

$$
l(\boldsymbol{\beta}) \leq l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)+\nabla l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)^{\top}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)+\frac{1}{2}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\top} A\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right),
$$

which is a majorizing function of $l(\boldsymbol{\beta})$ at $\boldsymbol{\beta}^{(k)}$.

Consider a trick to solve logistic regression by $L_{2}$ regression package for stable computation. Let $X=\left[\mathbf{x}_{1}: \mathbf{x}_{2}: \cdots: \mathbf{x}_{n}\right]^{\prime}$, and $Y=\left(y_{1}, \cdots, y_{n}\right)^{\prime}$, and $\theta\left(\mathbf{x}_{i} ; \boldsymbol{\beta}\right)=\frac{\exp \left(\mathbf{x}_{i}^{\prime} \boldsymbol{\beta}\right)}{\left(1+\exp \left(\mathbf{x}_{i}^{\prime} \boldsymbol{\beta}\right)\right)}$. For convenience denote $\theta\left(\mathbf{x}_{i} ; \hat{\boldsymbol{\beta}}^{(k)}\right)$ by $\hat{\theta}_{i}$ and let $\hat{\boldsymbol{\theta}}=\left(\hat{\theta}_{1}, \cdots, \hat{\theta}_{n}\right)^{\prime}$. Note that

- $X^{\prime} X=\sum_{i=1}^{n} \mathbf{x}_{i} \mathbf{x}_{i}^{\prime}$
- $X^{\prime}(\hat{\boldsymbol{\theta}}-Y)=\nabla l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)$.

Write the majorized function of $l(\boldsymbol{\beta})$ at $\boldsymbol{\beta}^{(k)}$ by

$$
\begin{aligned}
Q\left(\boldsymbol{\beta} \mid \boldsymbol{\beta}^{(k)}\right)= & l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)+\nabla l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)^{\prime}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) \\
& +\frac{1}{2}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\prime} A\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) \\
= & l\left(\hat{\boldsymbol{\beta}}^{(k)}\right)-(Y-\hat{\boldsymbol{\theta}})^{\prime} X\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) \\
& +\frac{1}{8}\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right)^{\prime} X^{\prime} X\left(\boldsymbol{\beta}-\boldsymbol{\beta}^{(k)}\right) \\
= & \frac{1}{2}\left\|2(Y-\hat{\boldsymbol{\theta}})+X \boldsymbol{\beta}^{(k)} / 2-X \boldsymbol{\beta} / 2\right\|^{2}+\text { const }
\end{aligned}
$$

Let $\tilde{Y}=2(Y-\hat{\boldsymbol{\theta}})+X \boldsymbol{\beta}^{(k)} / 2$ and $\tilde{X}=X / 2$, then the $Q\left(\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}^{(k)}\right)$ can be regarded as the empirical risk function of the regression models

$$
\tilde{Y}=\tilde{X} \boldsymbol{\beta}+\epsilon .
$$

Thus, we can use the $l_{2}$ regression package to minimize $Q\left(\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}^{(k)}\right)$. The algorithm for logistic regression models by $l_{2}$ regression package follows (you can see the original idea in Section 3 of [Friedman et al., 2010]).

## Logistic regression with $l_{2}$ regression package

1. Set $k=0$ and an initial $\hat{\boldsymbol{\beta}}^{(k)}$ and let $\tilde{X}=X / 2$
2. Compute $\tilde{Y}=2(Y-\hat{\boldsymbol{\theta}})+X \boldsymbol{\beta}^{(k)} / 2$
3. Solve $\tilde{Y} \sim \tilde{X}$ by $l_{2}$ regression package, and obtain the solution $\hat{\boldsymbol{\beta}}$
4. Update $\hat{\boldsymbol{\beta}}^{(k+1)}$ by $\hat{\boldsymbol{\beta}}$
5. $k \rightarrow k+1$ and repeat (2-4) until the solution converges.

## Bradley-Terry model

Ranking data commonly arise from situations where it is desired to rank a set of individuals or objects in accordance with some criterion.

Two types of ranking data

- Ranking comes from a set of assigned scores.
ex) University ranking
- Ranking directly observed.
ex) Horse racing game

There are three components consisting in ranking data.

- Comparison(game): a unit acting to assign orders for some criterion.
- Item(player): object to be assigned orders in a game.
- Ranking: resulting orders from a game.


## Notation

- Let $S$ be a set of items in a comparison.
- Let $R$ be rank-vector obtained from the comparison.
- Denote the events that an item $j_{1}$ is ranked higher than $j_{2}$ by $\left(j_{1} \rightarrow j_{2}\right)$.

The Bradley-Terry Model [Bradley and Terry, 1952] is one of the most popular parametric probability models for ranking (see [Hunter, 2004]).

- When $p$ items are to be ranked, the model assumes positive valued $p$ parameters ( $u_{1}, \cdots, u_{p}$ ) representing utilities of items.
- Higher $u_{i}$, higher the probability of the item $i$ being top ranked.

For identifiability, let $u_{p}=1$.

Consider an event

$$
\left(j_{1} \rightarrow j_{2}\right)
$$

and let $r$ be the rank-vector corresponding to the event.
Then,

$$
\operatorname{Pr}(R=r)=\frac{u_{j_{1}}}{u_{j_{1}}+u_{j_{2}}}
$$

## Likelihood

Let $D_{i}=\left\{(j, k): j, k \in S_{i}, j \neq k\right\}$ and $y_{i j k}=I\left(R_{i j}<R_{i k}\right)$.

$$
L(u)=\prod_{i=1}^{n} \prod_{(j, k) \in D_{i}}\left(\frac{u_{j}}{u_{j}+u_{k}}\right)^{y_{i j k}}\left(\frac{u_{k}}{u_{j}+u_{k}}\right)^{1-y_{i j k}}
$$

subject to $u_{p}=1$ and $u_{j}>0$.

Let $w_{j k}$ be the number of winnings of item $j$ against $k$. Then the loglikelihood is simply written by

$$
l(\mathbf{u})=\log L(\mathbf{u})=\sum_{j=1}^{p} \sum_{k=1}^{p}\left[w_{j k} \log \left(u_{j}\right)-w_{j k} \log \left(u_{j}+u_{k}\right)\right]
$$

MLE is given by

$$
\hat{\mathbf{u}}=\operatorname{argmin}_{\mathbf{u}>0, u_{p}=1}-l(\mathbf{u})
$$

$$
\begin{aligned}
-l(\mathbf{u}) & =-\sum_{j=1}^{p} \sum_{k=1}^{p} w_{j k}\left[\log \left(u_{j}\right)-\log \left(u_{j}+u_{k}\right)\right] \\
& \leq-\sum_{j=1}^{p} \sum_{k=1}^{p} w_{j k}\left[\log \left(u_{j}\right)-\frac{u_{j}+u_{k}}{\tilde{u}_{j}+\tilde{u}_{k}}-\log \left(\tilde{u}_{j}+\tilde{u}_{k}\right)+1\right]
\end{aligned}
$$

by $\log x \leq \log (\tilde{x})+\frac{1}{\tilde{x}}(x-\tilde{x})=\log \tilde{x}+x / \tilde{x}-1$.

Thus,

$$
Q(\mathbf{u} \mid \tilde{\mathbf{u}})=-\sum_{j=1}^{p} \sum_{k=1}^{p} w_{j k}\left[\log \left(u_{j}\right)-\frac{u_{j}+u_{k}}{\tilde{u}_{j}+\tilde{u}_{k}}-\log \left(\tilde{u}_{j}+\tilde{u}_{k}\right)+1\right]
$$

is the majorized function of $-l(\mathbf{u})$ at $\tilde{\mathbf{u}}$, where $\tilde{\mathbf{u}}=\left(\tilde{u}_{1}, \cdots, \tilde{u}_{p}\right)$.

- Note that $Q(\mathbf{u} \mid \tilde{\mathbf{u}}) \geq-l(\mathbf{u})$, and the equality holds only when $\mathbf{u}=\tilde{\mathbf{u}}$
- Next, define the $m$-th coordinate function of $Q(\mathbf{u} \mid \tilde{\mathbf{u}})$ by

$$
Q_{m}(\mathbf{u} \mid \tilde{\mathbf{u}})=Q\left(\left(\tilde{u}_{1}, \cdots, \tilde{u}_{m-1}, u, \tilde{u}_{m+1}, \cdots, \tilde{u}_{p}\right) \mid \tilde{\mathbf{u}}\right)
$$

$Q_{m}(\mathbf{u} \mid \tilde{\mathbf{u}}) \geq-l(\mathbf{u})$ for all $u>0$ and the equality holds when $u=\tilde{u}_{m}$.
We use the majorized function of $-l(\mathbf{u})$ at $\tilde{u}$ by $Q_{m}(\mathbf{u} \mid \tilde{u})$.

In finding maximizer $Q(\mathbf{u} \mid \tilde{\mathbf{u}})$, we just consider a function of $u_{m}$ that

$$
g\left(u_{m}\right)=\sum_{k=1}^{p} w_{m k}\left[\log \left(u_{m}\right)-\frac{u_{m}}{\tilde{u}_{m}+\tilde{u}_{k}}\right]+\sum_{k=1}^{p} w_{k m}\left[-\frac{u_{m}}{\tilde{u}_{m}+\tilde{u}_{k}}\right]
$$

- Note that the differential function of $g\left(u_{m}\right)$ is given by

$$
g^{\prime}\left(u_{m}\right)=\sum_{k=1}^{p} w_{m k}\left[\frac{1}{u_{m}}-\frac{1}{\tilde{u}_{m}+\tilde{u}_{k}}\right]+\sum_{k=1}^{p} w_{k m}\left[-\frac{1}{\tilde{u}_{m}+\tilde{u}_{k}}\right]
$$

- Hence the minimizer of $g\left(u_{m}\right)$ is obtained by the solution of $g^{\prime}\left(u_{m}\right)=0$, which is given by

$$
\hat{u}_{m}=\left[\sum_{k=1}^{p} w_{m k}\right] \sum_{k=1}^{p}\left[\frac{N_{m k}}{\tilde{u}_{m}+\tilde{u}_{k}}\right]^{-1}
$$

where $N_{m k}=w_{m k}+w_{k m}$ ( the number of games between $j$ and $\left.k\right)$.

| $(j, k)$ | 1 | 2 | 3 | $\cdots$ | k | $\cdots$ | p | $\sum_{k=1}^{p} w_{j k}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 1 | 2 | $\cdots$ | $w_{1 k}$ | $\cdots$ | 2 | 17 |
| 2 | 3 | 0 | 1 | $\cdots$ | $w_{2 k}$ | $\cdots$ | 0 | 12 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| p | 1 | 1 | 0 | $\cdots$ | $w_{p k}$ | $\cdots$ | 0 | 21 |
| $\sum_{j=1}^{p} w_{j k}$ | 10 | 5 | 2 | $\cdots$ | $w_{p k}$ | $\cdots$ | 0 | $N$ |

Table 1: summary of pairwise comparisons
$\left(w_{j k}: \#\right.$ of $i$ 's wins against $j, N_{j k}=w_{j k}+w_{k j}: \#$ of matches between $i$ and $\left.j\right)$

## One cycle of MM algorithm

(1) Let $\tilde{\mathbf{u}}$ and set $m=1$
(2) Obtain $\hat{u}_{m}$.
(3) Update the $m$-th coordinate of $\tilde{\mathbf{u}}$ by $\hat{u}_{m}$ and $m \leftarrow m+1$.
(4) Repeat (2)-(3) until $m=p$.

Repeat the one cycle MM algorithm, we obtain the MLE of the Bradley-Terry model.

## Discussion

- Newton Raphson algorithm is applicable to obtaining MLE of the Bradley-Terry model?
- What's the advantage of the MM algorithm for obtaining the MLE of the Bradley-Terry model?
- Read [Hunter and Lange, 2004]
- Prove (3).
- Prove (4).
- Prove (5).
- Write three manual codes of the logistic regression model with the gradient descent method, the Newton-Raphson method, and the BFGS algorithm.
- Write a manual code of the Huberized regression with MM-algorithm and check the descent property.
- Write a manual code of the Bradley-Terry model with MM algorithm and check the descent property.

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