Optimization

August 29, 2022

Optimization problem

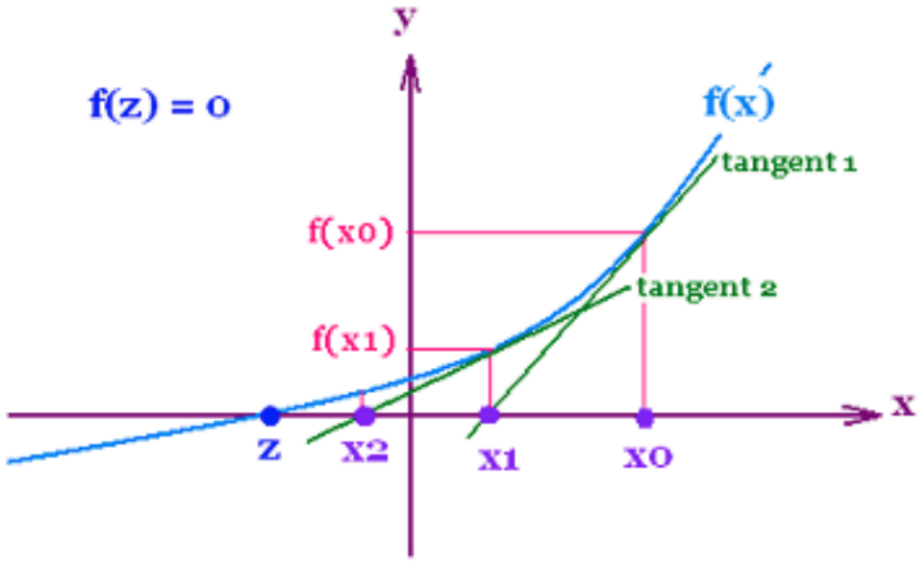
- An optimization problem is the problem of finding the best solution for an objective function.
- Optimization method plays an important role in statistics, for example, to find maximum likelihood estimate (MLE).
- Unconstrained vs. constrained optimization problem: whether there is constraint in the solution space.
- Most algorithms are based on iterative procedures.
- We'll spend next few lectures on several optimization methods, under the context of statistics:
  - New-Raphson, Fisher scoring, etc.
  - EM and MM.
  - Hidden Markov models.
  - Linear and quadratic programming.

Review: Newton-Raphson (NR) method

Goal: Find the root for equation $f(\theta) = 0$.

Approach:

1. Choose an initial value $\theta^{(0)}$ as the starting point.
2. By Taylor expansion at $\theta^{(0)}$, we have $\tilde{f}(\theta) = f(\theta^{(0)}) + f'(\theta^{(0)})(\theta - \theta^{(0)})$.
3. Setting $\tilde{f}(\theta) = 0$ gives an update of the parameter: $\theta^{(1)} = \theta^{(0)} - f(\theta^{(0)})/f'(\theta^{(0)})$.
4. Repeated update until convergence: $\theta^{(k+1)} = \theta^{(k)} - f(\theta^{(k)})/f'(\theta^{(k)})$.



Newton-Raphson Method

NR method convergence rate

Quadratic convergence: θ^* is the solution.

$$\lim_{k\to\infty} \frac{|\theta^{(k+1)} - \theta^*|}{|\theta^{(k)} - \theta^*|^2} = c \qquad (\text{rate} = c > 0, \text{order} = 2)$$

The # of significant digits nearly doubles at each step (in the neighborhood of θ^*).

Proof: By Taylor expansion (to the second order) at $\theta^{(k)}$,

$$0 = f(\theta^*) = f(\theta^{(k)}) + f'(\theta^{(k)})(\theta^* - \theta^{(k)}) + \frac{1}{2} f''(\xi^{(k)})(\theta^* - \theta^{(k)})^2, \quad \xi^{(k)} \in [\theta^*, \theta^{(k)}]$$

Dividing the equation by $f'(\theta^{(k)})$ gives

$$-f(\theta^{(k)})/f'(\theta^{(k)}) - (\theta^* - \theta^{(k)}) = \frac{f''(\xi^{(k)})}{2f'(\theta^{(k)})}(\theta^* - \theta^{(k)})^2.$$

The definition of $\theta^{(k+1)} = \theta^{(k)} - f(\theta^{(k)})/f'(\theta^{(k)})$ gives

$$\theta^{(k+1)} - \theta^* = \frac{f''(\xi^{(k)})}{2f'(\theta^{(k)})}(\theta^* - \theta^{(k)})^2.$$

What conditions are needed?

- $f'(\theta^{(k)}) \neq 0$ in the neighborhood of θ^*.
- $f''(\xi^{(k)})$ is bounded.
- Starting point is sufficiently close to the root θ^* (in order for the Taylor expansion to work).

Review: maximum likelihood

Here is a list of some definitions related to maximum likelihood estimate:

Parameter	θ, a p-vector
Data	X
Log likelihood	$l(\theta) = \log \Pr(X\|\theta)$
Score function (p-vector)	$\dot{l}(\theta) = (\partial l/\partial\theta_1, \ldots, \partial l/\partial\theta_p)'$
Hessian matrix ($p \times p$)	$\ddot{l}(\theta) = \{\partial^2 l/\partial\theta_i\partial\theta_j\}_{i,j=1,\ldots,p}$
Fisher information	$I(\theta) = -\mathrm{E}\ddot{l}(\theta) = \mathrm{E}\dot{l}(\theta)\{\dot{l}(\theta)\}'$
Observed information	$-\ddot{l}(\hat{\theta})$

When θ^* is a local maximum of l, $\dot{l}(\theta^*) = 0$, and $\ddot{l}(\theta^*)$ is negative definite.

Application of NR method in MLE: when θ is a scalar

Maximum Likelihood Estimation (MLE): $\hat{\theta} = \arg\max_\theta l(\theta)$.

Approach Find $\hat{\theta}$ such that $\dot{l}(\hat{\theta}) = 0$.

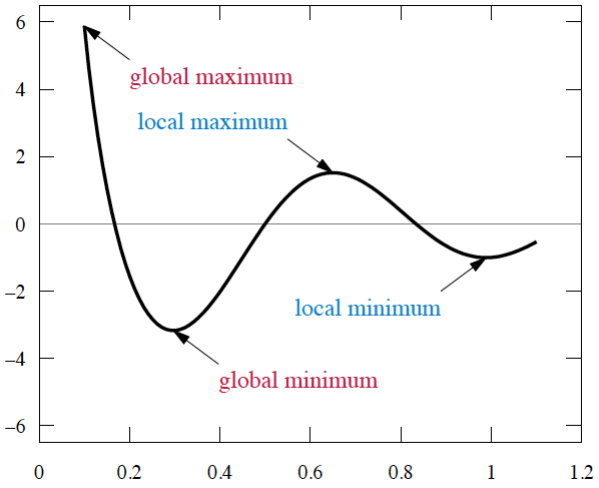
If the closed form solution for $\dot{l}(\hat{\theta}) = 0$ is difficult to obtain, one can use NR method (replace f by $\dot{l}$). The the NR update for solving MLE is:

$$\theta^{(k+1)} = \theta^{(k)} - \dot{l}(\theta^{(k)})/\ddot{l}(\theta^{(k)}).$$

What can go wrong?

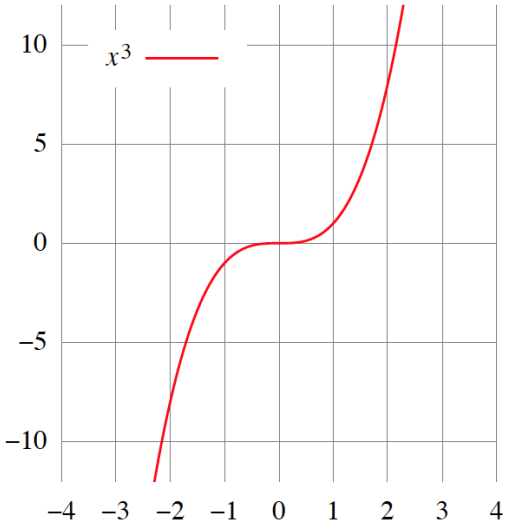
- Bad starting point
- May not converge to the global maximum
- Saddle point: $\dot{l}(\hat{\theta}) = 0$, but $\ddot{l}(\hat{\theta})$ is neither negative definite nor positive definite (stationary point but not a local extremum; can be used to check the likelihood)

starting point & local extremum



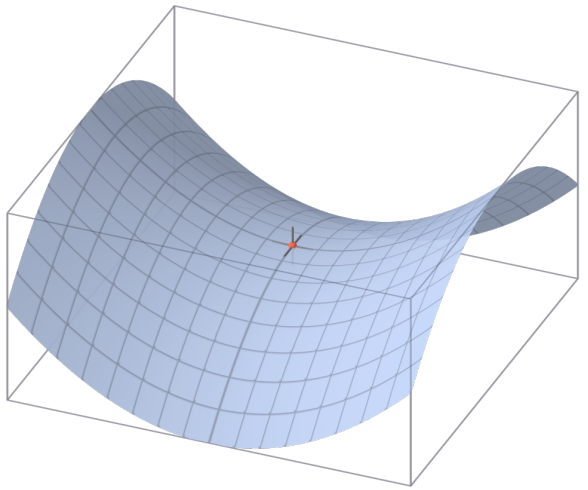
saddle point

$l(\theta) = \theta^3$



saddle point

$l(\theta_1, \theta_2) = \theta_1^2 - \theta_2^2$



Generalization to higher dimensions: when θ is a p-vector

General Algorithm

1. **(Starting point)** Pick a starting point $\theta^{(0)}$ and let $k = 0$
2. **(Iteration)** Determine the direction $d^{(k)}$ (a p-vector) and the step size $\alpha^{(k)}$ (a scalar) and calculate

$$\theta^{(k+1)} = \theta^{(k)} + \alpha^{(k)} d^{(k)},$$

such that the likelihood will increase, i.e.:

$$l(\theta^{(k+1)}) > l(\theta^{(k)})$$

3. **(Stop criteria)** Stop iteration if

$$|l(\theta^{(k+1)}) - l(\theta^{(k)})|/(|l(\theta^{(k)})| + \epsilon_1) < \epsilon_2$$

or

$$|\theta_{k+1,j} - \theta_{k,j}|/(|\theta_{k,j}| + \epsilon_1) < \epsilon_2, \quad j = 1, \ldots, p$$

for precisions such as $\epsilon_1 = 10^{-4}$ and $\epsilon_2 = 10^{-6}$. Otherwise go to 2.

Key: Determine the direction and the step size

Determining the direction (general framework, details later)

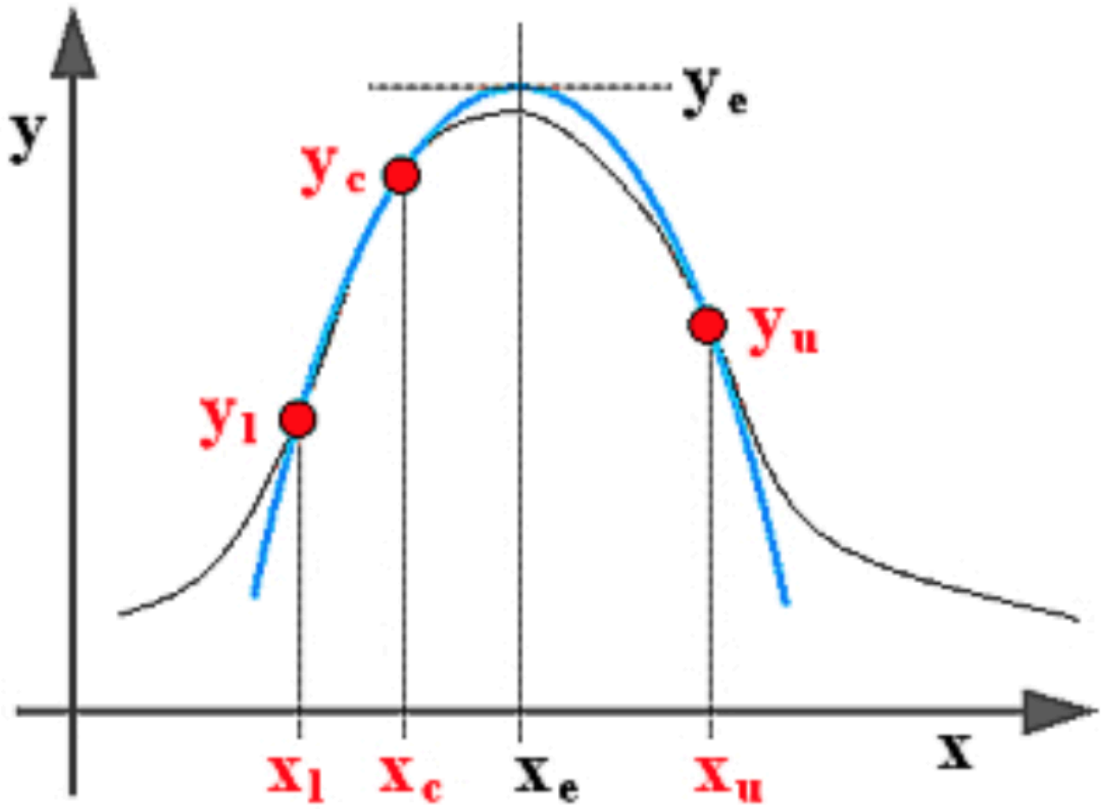
We generally pick $d^{(k)} = R^{-1}\dot{l}(\theta^{(k)})$, where R is a positive definite matrix.

Choosing a step size (given the direction). The goal is to find $\alpha^{(k)}$ so that $l(\theta^{(k+1)}) > l(\theta^{(k)})$

- Step halving
  - Start at a large value of $\alpha^{(k)}$. Halve $\alpha^{(k)}$ until $l(\theta^{(k+1)}) > l(\theta^{(k)})$
  - Simple, robust, but relatively slow
- Linear search
  - To find $\alpha^{(k)} = \arg\max_\alpha l(\theta^{(k)} + \alpha d^{(k)})$
  - Approximate $l(\theta^{(k)} + \alpha d^{(k)})$ by doing a **polynomial interpolation** and find $\alpha^{(k)}$ maximizing the polynomial
  - Fast

Polynomial interpolation

Given a set of $p+1$ data points from the function $f(\alpha) \equiv l(\theta^{(k)} + \alpha d^{(k)})$, we can find a unique polynomial with degree p that goes through the $p+1$ data points. (For a quadratic approximation, we only need 3 data points.)



1. Steepest ascent: $R = I$ = identity matrix

$$d^{(k)} = \dot{l}(\theta^{(k)})$$
$$\alpha^{(k)} = \arg\max_{\alpha} l(\theta^{(k)} + \alpha \dot{l}(\theta^{(k)})) \text{ or a small fixed number}$$
$$\theta^{(k+1)} = \theta^{(k)} + \alpha^{(k)} \dot{l}(\theta^{(k)})$$

$\dot{l}(\theta^{(k)})$ is the steepest ascent direction

Proof: By Taylor expansion at $\theta^{(k)}$,

$$l(\theta^{(k)} + \Delta) - l(\theta^{(k)}) = \Delta^T \dot{l}(\theta^{(k)}) + o(||\Delta||)$$

By Cauchy-Schwarz inequality,

$$\Delta^T \dot{l}(\theta^{(k)}) \leq ||\Delta|| \cdot ||\dot{l}(\theta^{(k)})||$$

The equality holds at $\Delta = \alpha \dot{l}(\theta^{(k)})$. So when $\Delta = \alpha \dot{l}(\theta^{(k)})$, $l(\theta^{(k)} + \Delta)$ increases the most. □

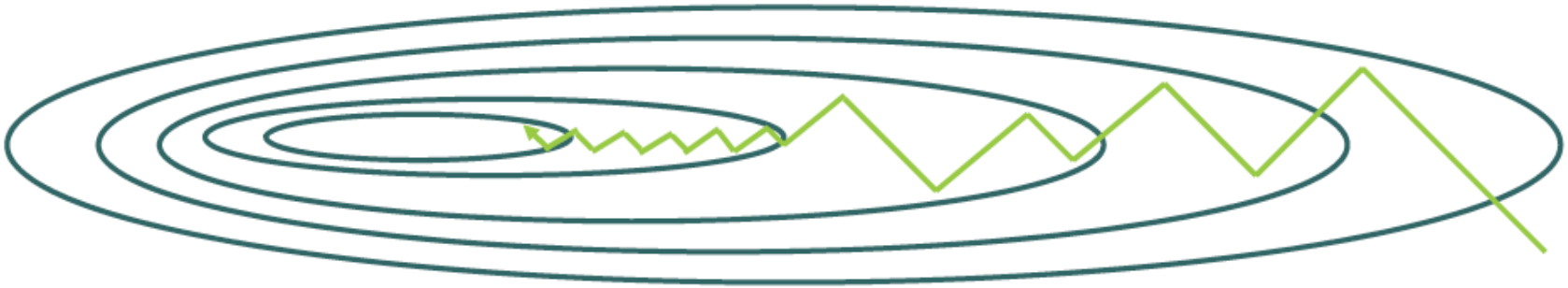
- Easy to implement; only require the first derivative/gradient/score
- Guarantee an increase at each step no matter where you start
- Converge slowly. The directions of two consecutive steps are orthogonal, so the algorithm “zigzags” to the maxima.

When $\alpha^{(k)}$ is chosen as $\arg\max_\alpha l(\theta^{(k)} + \alpha \dot{l}(\theta^{(k)}))$, the directions of two consecutive steps are orthogonal, i.e.,

$$[\dot{l}(\theta^{(k)})]^T \dot{l}(\theta^{(k+1)}) = 0.$$

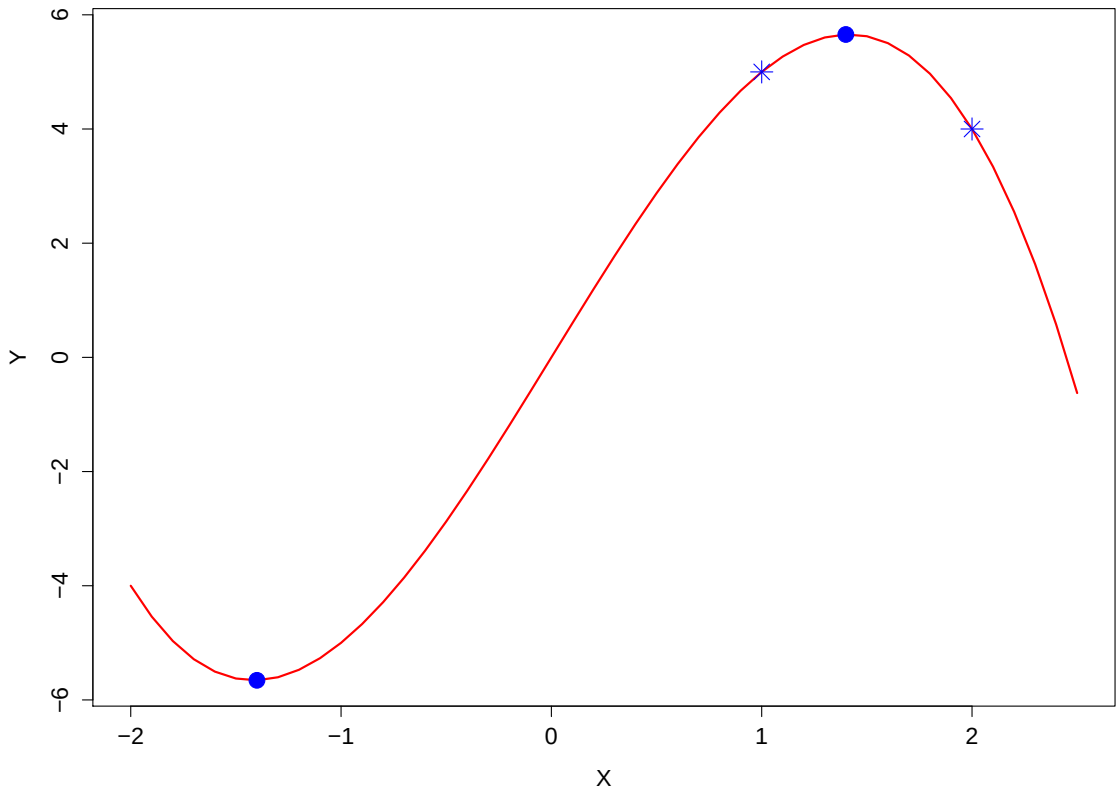
Proof: By the definition of $\alpha^{(k)}$ and $\theta^{(k+1)}$

$$0 = \frac{\partial l(\theta^{(k)} + \alpha \dot{l}(\theta^{(k)}))}{\partial \alpha}\Big|_{\alpha=\alpha^{(k)}} = \dot{l}(\theta^{(k)} + \alpha^{(k)} \dot{l}(\theta^{(k)}))^T \dot{l}(\theta^{(k)}) = \dot{l}(\theta^{(k+1)})^T \dot{l}(\theta^{(k)}).$$



Example: Steepest Ascent

Find the maximum of the function $f(x) = 6x - x^3$.



Example: Steepest Ascent (cont.)

```
fun0 <- function(x) return(- x^3 + 6*x)   # target function
grd0 <- function(x) return(- 3*x^2 + 6)   # gradient

# Steepest Ascent Algorithm
Steepest_Ascent <- function(x, fun=fun0, grd=grd0, step=0.01, kmax=1000, tol1=1e-6, tol2=1e-4)
{
        diff <- 2*x  # use a large value to get into the following "while" loop
        k <- 0       # count iteration

        while ( all(abs(diff) > tol1*(abs(x)+tol2) )  & k <= kmax) # stop criteria
        {
                g_x <- grd(x)          # calculate gradient using x
                diff <- step * g_x     # calculate the update
                x <- x + diff          # update x
                k <- k + 1             # update iteration
        }

        f_x = fun(x)

        return(list(iteration=k, x=x, f_x=f_x, g_x=g_x))
}
```

Example: Steepest Ascent (cont.)

```
> Steepest_Ascent(x=2, step=0.01)

$iteration
[1] 117
$x
[1] 1.414228
$f_x
[1] 5.656854
$g_x
[1] -0.0001380379
```

In large dataset

The data log-likelihood is usually summed over n observations: $l(\theta) = \sum_{i=1}^{n} l(x_i; \theta)$. When n is large, this poses heavy computational burden.

One can implement a "stochastic" version of the algorithm: **stochastic gradient descent** (SGD). Note: Gradient descent is just steepest descent.

Simple SGD algorithm: replace the gradient $\dot{l}(\theta)$ by the gradient computed from a single sample $\dot{l}(x_i; \theta)$, where x_i is randomly sampled.

"Mini-batch" SGD algorithm: compute the gradient based on a small number of observations.

- Advantage of SGD:
  - Evaluate gradient at one (or a few) observations, requires less memory.
  - Has better property to escape from local minimum (gradient is noisy).
- Disdvantage of SGD: even slower convergence.

2. Newton-Raphson: $R = -\ddot{l}(\theta^{(k)}) =$ observed information

$$d^{(k)} = [-\ddot{l}(\theta^{(k)})]^{-1}\dot{l}(\theta^{(k)})$$
$$\theta^{(k+1)} = \theta^{(k)} + [-\ddot{l}(\theta^{(k)})]^{-1}\dot{l}(\theta^{(k)})$$
$$\alpha^{(k)} = 1 \text{ for all } k$$

- Fast, quadratic convergence
- Need very good starting points

Theorem: If R is positive definite, the equation set $Rd^{(k)} = \dot{l}(\theta^{(k)})$ has a unique solution for the direction $d^{(k)}$, and the direction ensures ascent of $l(\theta)$.

Proof: When R is positive definite, it is invertible. So we have a unique solution $d^{(k)} = R^{-1}\dot{l}(\theta^{(k)})$.

Let $\theta^{(k+1)} = \theta^{(k)} + \alpha d^{(k)} = \theta^{(k)} + \alpha R^{-1}\dot{l}(\theta^{(k)})$. By Taylor expansion,

$$l(\theta^{(k+1)}) \approx l(\theta^{(k)}) + \alpha\dot{l}(\theta^{(k)})^T R^{-1}\dot{l}(\theta^{(k)}).$$

The positive definite matrix R ensures that $l(\theta^{(k+1)}) > l(\theta^{(k)})$ for positive α. □

Newton-Raphson vs. steepest ascent

- Newton-Raphson converges much faster than steepest ascent (gradient descent).
- NR requires the computation of second derivative, which can be difficult and computationally expensive. In contrast, gradient descent requires only the first derivative, which is easy to compute.
- For poorly behaved objective function (non-convex), gradient-based methods are often more stable.
- Gradient-based method (especially SGD) is widely used in modern machine learning.

Example: Newton Raphson


```
fun0 <- function(x) return(- x^3 + 6*x)   # target function
grd0 <- function(x) return(- 3*x^2 + 6)   # gradient
hes0 <- function(x) return(- 6*x)         # Hessian

# Newton-Raphson Algorithm
Newton_Raphson <- function(x, fun=fun0, grd=grd0, hes=hes0, kmax=1000, tol1=1e-6, tol2=1e-4)
{
        diff <- 2*x
        k <- 0

        while ( all(abs(diff) > tol1*(abs(x)+tol2) )  & k <= kmax)
        {
                g_x <- grd(x)
                h_x <- hes(x)         # calculate the second derivative (Hessian)
                diff <- -g_x/h_x      # calculate the update
                x <- x + diff
                k <- k + 1
        }

        f_x = fun(x)

        return(list(iteration=k, x=x, f_x=f_x, g_x=g_x, h_x=h_x))
}
```

Example: Newton Raphson


```
> Newton_Raphson(x=2)

$iteration
[1] 5
$x
[1] 1.414214
$f_x
[1] 5.656854
$g_x
[1] -1.353229e-11
$h_x
[1] -8.485281
```

3. Modification of Newton-Raphson

- **Fisher scoring**: replace $-\ddot{l}(\theta)$ with $-\mathrm{E}\ddot{l}(\theta)$
  - $-\mathrm{E}\ddot{l}(\theta) = \mathrm{E}\dot{l}(\theta)\dot{l}(\theta)'$ is always positive and stabilize the algorithm
  - $-\mathrm{E}\ddot{l}(\theta)$ can have a simpler form than $-\ddot{l}(\theta)$
  - Newton-Raphson and Fisher scoring are equivalent for parameter estimation in GLM with canonical link.

- **Quasi-Newton**: aka "variable metric methods" or "secant methods". Approximate $\ddot{l}(\theta)$ in a way that
  - avoids calculating Hessian and its inverse
  - has convergence properties similar to Newton

Fisher Scoring example: Poisson regression

In the Poisson regression model of n subjects,

- The responses $Y_i \sim \text{Poisson}(\lambda_i) = (Y_i!)^{-1}\lambda_i^{Y_i}e^{-\lambda_i}$. We know that $\lambda_i = \text{E}(Y_i|X_i)$.
- We relate the mean of Y_i to X_i by $g(\lambda_i) = X_i\beta$. Taking derivative on both sides,

$$g'(\lambda_i)\frac{\partial \lambda_i}{\partial \beta} = X_i \quad \Rightarrow \quad \frac{\partial \lambda_i}{\partial \beta} = \frac{X_i}{g'(\lambda_i)}$$

- Log likelihood: $l(\beta) = \sum_{i=1}^n (Y_i \log \lambda_i - \lambda_i)$, where λ_i's satisfy $g(\lambda_i) = X_i\beta$.
- Maximum likelihood estimation: $\hat{\beta} = \arg\max_\beta l(\beta)$

Newton-Raphson needs

$$\begin{aligned}
\dot{l}(\beta) &= \sum_i \left(\frac{Y_i}{\lambda_i} - 1\right)\frac{\partial \lambda_i}{\partial \beta} = \sum_i \left(\frac{Y_i}{\lambda_i} - 1\right)\frac{1}{g'(\lambda_i)}X_i \\
\ddot{l}(\beta) &= -\sum_i \frac{Y_i}{\lambda_i^2}\frac{\partial \lambda_i}{\partial \beta}\frac{1}{g'(\lambda_i)}X_i - \sum_i \left(\frac{Y_i}{\lambda_i} - 1\right)\frac{g''(\lambda_i)}{g'(\lambda_i)^2}\frac{\partial \lambda_i}{\partial \beta}X_i \\
&= -\sum_i \frac{1}{\lambda_i}\frac{1}{g'(\lambda_i)^2}X_i^2 - \sum_i \left(\frac{Y_i}{\lambda_i} - 1\right)\frac{1}{\lambda_i}\frac{1}{g'(\lambda_i)^2}X_i^2 - \sum_i \left(\frac{Y_i}{\lambda_i} - 1\right)\frac{g''(\lambda_i)}{g'(\lambda_i)^3}X_i^2
\end{aligned}$$

Fisher scoring needs $\dot{l}(\beta)$ and

$$\mathrm{E}\left[\ddot{l}(\beta)\right] = -\sum_i \frac{1}{\lambda_i} \frac{1}{g'(\lambda_i)^2} X_i^2$$

which is $\ddot{l}(\beta)$ without the extra terms involving Y.

With the canonical link for Poisson regression:

$$g(\lambda_i) = \log \lambda_i,$$

we have

$$g'(\lambda_i) = \lambda_i^{-1} \quad \text{and} \quad g''(\lambda_i) = -\lambda_i^{-2}.$$

So that the extra terms equal to zero (check this!) and we conclude that Newton-Raphson and Fisher scoring are equivalent.

Data: (x_i, y_i) for $i = 1, \ldots, n$

Notation and assumptions

- Model: $y_i = h(x_i, \beta) + \epsilon_i$, where $\epsilon_i \overset{i.i.d}{\sim} N(0, \sigma^2)$ and $h(.)$ is known and non-linear
- Residual: $e_i(\beta) = y_i - h(x_i, \beta)$
- Jacobian: $\{J(\beta)\}_{ij} = \frac{\partial h(x_i,\beta)}{\partial \beta_j} = -\frac{\partial e_i(\beta)}{\partial \beta_j}$, a $n \times p$ matrix

Goal: to obtain MLE $\hat{\beta} = \arg\min_\beta S(\beta)$, where $S(\beta) = \sum_i \{y_i - h(x_i, \beta)\}^2 = [e(\beta)]^T e(\beta)$ is the residual sum of squares.

We could use **Newton-Raphson algorithm**.

- Gradient: $g_j(\beta) = \frac{\partial S(\beta)}{\partial \beta_j} = 2 \sum_i e_i(\beta) \frac{\partial e_i(\beta)}{\partial \beta_j}$, i.e., $g(\beta) = -2J(\beta)^T e(\beta)$
- Hessian: $H_{jr}(\beta) = \frac{\partial^2 S(\beta)}{\partial \beta_j \partial \beta_r} = 2 \sum_i \{e_i(\beta) \frac{\partial^2 e_i(\beta)}{\partial \beta_j \partial \beta_r} + \frac{\partial e_i(\beta)}{\partial \beta_j} \frac{\partial e_i(\beta)}{\partial \beta_r}\}$

Problem: Hessian could be hard to obtain.

Gauss-Newton algorithm

Recall in linear regression models, we minimize

$$S(\beta) = \sum_i \left\{ y_i - x_i^T \beta \right\}^2$$

Because $S(\beta)$ is a quadratic function, it is easy to get MLE

$$\hat{\beta} = \left(\sum_i x_i x_i^T \right)^{-1} \left(\sum_i x_i y_i \right)$$

Now in the nonlinear regression models, we want to minimize

$$S(\beta) = \sum_i \{ y_i - h(x_i, \beta) \}^2$$

Idea: Approximate $h(x_i, \beta)$ by a linear function, iteratively at $\beta^{(k)}$

Given $\beta^{(k)}$ and by Taylor expansion of $h(x_i, \beta)$ at $\beta^{(k)}$, $S(\beta)$ becomes

$$S(\beta) \approx \sum_i \left\{ y_i - h(x_i, \beta^{(k)}) - (\beta - \beta^{(k)})^T \frac{\partial h(x_i, \beta^{(k)})}{\partial \beta} \right\}^2 = \sum_i \left\{ e(\beta^{(k)}) - (\beta - \beta^{(k)})^T J(\beta^{(k)}) \right\}^2$$

Gauss-Newton algorithm (cont.)

1. Find a good starting point $\beta^{(0)}$

2. At step $k+1$,

   (a) Form $e(\beta^{(k)})$ and $J(\beta^{(k)})$

   (b) Use a standard linear regression routine to obtain
   $\delta^{(k)} = [J(\beta^{(k)})^T J(\beta^{(k)})]^{-1} J(\beta^{(k)})^T e(\beta^{(k)})$

   (c) Obtain the new estimate $\beta^{(k+1)} = \beta^{(k)} + \delta^{(k)}$

- Does not need computing Hessian matrix.
- Needs good starting values.
- Requires $J(\beta^{(k)})^T J(\beta^{(k)})$ to be invertible.
- This is not a general optimization method. Only applicable to lease square problem.

Data: (y_i, x_i) for $i = 1, \ldots, n$

Notation and assumptions

- Mean: $\mathrm{E}(y|x) = \mu$
- Link g: $g(\mu) = x'\beta$
- Variance function V: $\mathrm{Var}(y|x) = \phi V(\mu)$: mean-variance dependency.
- Log likelihood (exponential dispersion model with canonical parameter θ and dispersion parameter ϕ): $l(\theta, \phi; y) = \{y\theta - b(\theta)\}/a(\phi) + c(y, \phi)$

We can obtain

- Score function: $\dot{l} = \{y - b'(\theta)\}/a(\phi)$
- Observed information: $-\ddot{l} = b''(\theta)/a(\phi)$
- Mean (in θ): $\mathrm{E}(y|x) = a(\phi)\mathrm{E}(\dot{l}) + b'(\theta) = b'(\theta)$ (expected score at true θ is 0).
- Variance (in θ, ϕ): $\mathrm{Var}(y|x) = \mathrm{E}(y - b'(\theta))^2 = a(\phi)^2\mathrm{E}(\dot{l}\dot{l}') = a(\phi)^2\mathrm{E}(-\ddot{l}) = b''(\theta)a(\phi)$

Canonical link: Function g satisfies $g(\mu) = \theta$. Thus $g = (b')^{-1}$

Model	Normal	Poisson	Binomial	Gamma
ϕ	σ^2	1	$1/m$	$1/\nu$
$b(\theta)$	$\theta^2/2$	$\exp(\theta)$	$\log(1+e^\theta)$	$-\log(-\theta)$
μ	θ	$\exp(\theta)$	$e^\theta/(1+e^\theta)$	$-1/\theta$
Canonical link g	identity	log	logit	reciprocal
Variance function V	1	μ	$\mu(1-\mu)$	μ^2

Iteratively reweighted least squares for GLM

In linear regression models, $\mathrm{E}(y_i|x_i) = x_i^T\beta$, so we minimize

$$S(\beta) = \sum_i \left\{y_i - x_i^T\beta\right\}^2$$

Because $S(\beta)$ is a quadratic function, it is easy to get MLE

$$\hat{\beta} = \left(\sum_i x_i x_i^T\right)^{-1}\left(\sum_i x_i y_i\right)$$

In GLM, consider to construct a similar quadratic function $S(\beta)$.

Question: Can we minimize $S(\beta) = \sum_i \left\{g(y_i) - x_i^T\beta\right\}^2$?

Answer: No, because $\mathrm{E}\{g(y_i)|x_i\} \neq g(\mathrm{E}\{y_i|x_i\}) = x_i^T\beta$, since g is nonlinear. This means we cannot transform y_i by g and then run linear regression.

Iteratively reweighted least squares

Idea: Approximate $g(y_i)$ by a linear function so that the LS formula can be used. iteratively update $\beta^{(k)}$.

Algorithm: at step k with current solution $\beta^{(k)}$, linearize $g(y_i)$ around $\hat{\mu}_i^{(k)} = g^{-1}(x_i^T \beta^{(k)})$ (remember our linear model is $g(\mu) = x'\beta$).

Denote the linearized value by $\tilde{y}_i^{(k)}$.

$$\tilde{y}_i^{(k)} = g(\hat{\mu}_i^{(k)}) + (y_i - \hat{\mu}_i^{(k)}) g'(\hat{\mu}_i^{(k)})$$

Now we can regress $\tilde{y}_i^{(k)}$ on x_i to estimate $\beta^{(k+1)}$. However, $\tilde{y}_i^{(k)}$ is heteroscedastic, i.e., the variances are not identical. Note: for most distributions the variances is related to the mean.

Derive the variances of $\tilde{y}_i^{(k)}$, and use the inverse of the variance as weights in a weighted least square (WLS):

$$W_i^{(k)} = \left\{ \text{Var}(\tilde{y}_i^{(k)}) \right\}^{-1} = \left[\{g'(\hat{\mu}_i^{(k)})\}^2 V(\hat{\mu}_i^{(k)}) \right]^{-1}$$

Given $\beta^{(k)}$, we consider to minimize

$$S(\beta) = \sum_i W_i^{(k)} \left\{ \tilde{y}_i^{(k)} - x_i^T \beta \right\}^2$$

IRLS algorithm:

1. Start with initial estimates, generally $\hat{\mu}_i^{(0)} = y_i$
2. Form $\tilde{y}_i^{(k)}$ and $W_i^{(k)}$, both depend on $\hat{\mu}_i^{(k)}$
3. Estimate $\beta^{(k+1)}$ by regressing $\tilde{y}_i^{(k)}$ on x_i with weights $W_i^{(k)}$
4. Form $\hat{\mu}_i^{(k+1)} = g^{-1}(x_i^T \beta^{(k+1)})$ and return to step 2.

Model	Poisson	Binomial	Gamma
$\mu = g^{-1}(\eta)$	e^{η}	$e^{\eta}/(1+e^{\eta})$	$1/\eta$
$g'(\mu)$	$1/\mu$	$1/[\mu(1-\mu)]$	$-1/\mu^2$
$V(\mu)$	μ	$\mu(1-\mu)$	μ^2

- McCullagh and Nelder (1983) showed that IRLS is equivalent to Fisher scoring.
- Using the canonical link, IRLS is also equivalent to Newton-Raphson.
- IRLS is attractive because no special optimization algorithm is required, just a subroutine that computes weighted least square estimates.

A quick review

- Optimization method is important in statistics, (i.e., to find MLE), or in general machine learning (minimize some loss function).
- Maximizing/minimizing an objective function is achieved by solving the equation that the first derivative is 0 (need to check second derivative).
- Steepest ascent method:
  - Only need gradient.
  - Slow convergence.
  - In large dataset with ill-behaved objective function, stochastic version (SGD) usually works better.

- Newton-Raphson (NR) method:
  - Quadratic convergence rate.
  - Could stuck in local maximum.
  - In higher dimension, the problems are to find directions and step sizes in each iteration.

- Fisher scoring: use expected information matrix.
  - NR use observed information matrix.
  - The expected information is more stable and simpler.
  - Fisher scoring and Newton-Raphson are equivalent under canonical link.

- Gauss-Newton algorithm for non-linear regression: Hessian matrix is not needed.