

STA6171: Statistical Computing for DS 1

Solving Nonlinear Equations

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Optimization. \Rightarrow Finding maximum or minimum

\Rightarrow Calculate the derivative

$$\frac{f'(x) = 0}{\hookrightarrow \text{analytic form}}$$

\Rightarrow When $f'(x) = 0$ does not have an analytic form,
how we can find a solution

1 Motivating Example

2 Univariate Optimization

3 Multivariate Optimization

Motivating Example

- A simple univariate numerical optimization problem is to maximize

$$g(x) = \frac{\log x}{1+x} \quad (1)$$

with respect to x .

- The derivative of $g(x)$ is

$$g'(x) = \frac{1 + \frac{1}{x} - \log x}{(1+x)^2} = 0 \quad (2)$$

and no analytic solution can be found in maximization.

optimal function
ex) MLE → find maximum numerical optimization → no analytic solution. ← denominator includes x

Motivaing Example

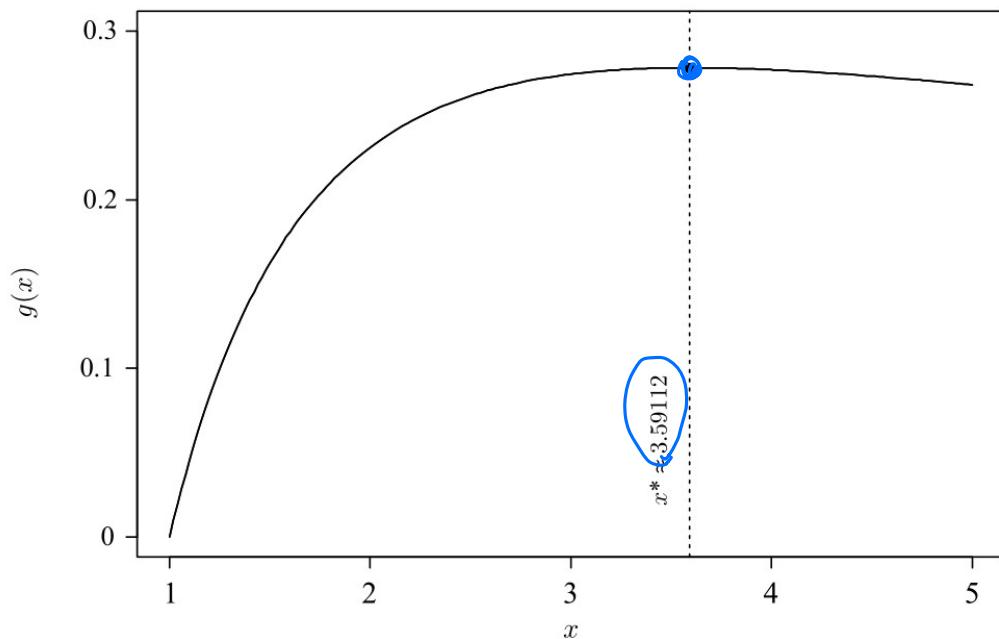


FIGURE 2.1 The maximum of $g(x) = (\log x) / (1 + x)$ occurs at $x^* \approx 3.59112$, indicated by the vertical line.

Convergence Criterion

↳ optimization \Rightarrow solution

↳ convergence criterion.

numerical optimization
we use computer
 \Rightarrow We cannot run algorithm forever.

- We cannot allow the algorithm to run indefinitely, so we require a stopping rule based on convergence criteria, to trigger an end to the successive approximation.
stop running algorithm $\xrightarrow{\text{check}}$
 - At each iteration, the stopping rule should be checked and the new $x^{(t+1)}$ is taken as the solution when the convergence criteria are met.
when newly updated $x^{(t+1)}$ satisfies the stopping rule, we stop running optimization algorithm.
 - Two reasons to stop if the algorithm appears
 - to have achieved satisfactory convergence.
 - unlikely to converge soon.
- ↳ Diverge.

Convergence Criterion

$$g'(x^{(t+1)}) \approx 0$$

Object : $g'(x) = 0$ If $g'(x^{(t)}) \approx 0$, can we declare it converge?

~~By other types of algorithm, there exists a large change.~~

- Monitor convergence by tracking the proximity of $g'(x^{(t+1)})$ to zero is not reliable because large changes from $x^{(t)}$ to $x^{(t+1)}$ can occur even when $g'(x^{(t+1)})$ is very small.
from $x^{(t)} \rightarrow x^{(t+1)}$
- On the other hand, a small change from $x^{(t)}$ to $x^{(t+1)}$ is most frequently associated with $g'(x^{(t+1)})$ near zero.
the change of $x^{(t)} \rightarrow x^{(t+1)}$ \hookrightarrow small $\Rightarrow g'(x^{(t+1)}) \approx 0$
- Assess convergence by monitoring $|x^{(t+1)} - x^{(t)}|$ and use $g'(x^{(t+1)})$ as a backup check.

Convergence criterion :

$$|x^{(t+1)} - x^{(t)}| < \epsilon$$

Then we declare it converges.

stopping rule

Types of Convergence Criterion

- Absolute convergence criterion mandates stopping when

$$\left| x^{(t+1)} - x^{(t)} \right| < \epsilon,$$

↑ stopping rule
tolerable imprecision.

where ϵ is a constant chosen to indicate tolerable imprecision.

- Relative convergence criterion mandates stopping when iterations have reached a point for which

$$\frac{\left| x^{(t+1)} - x^{(t)} \right|}{\left| x^{(t)} \right|} < \epsilon.$$

↑ scaling.

↑ Why we need relative convergence criterion?

This criterion enables the specification of a target specification of a target precision (e.g., within 1%) without worrying about the units of x .

Preference of Convergence Criterion

$$\frac{|x^{(t+1)} - x^{(t)}|}{|x^{(t)}|} \quad \epsilon = 0.001 \quad \text{if } |x^{(t)}| \approx 0 \text{ then } |x^{(t+1)} - x^{(t)}| \text{ will be large} \Rightarrow \text{algorithm will be unstable.}$$

- Preference between the absolute and relative convergence criteria depends on the problem at hand.
- If the scale of x is huge (or tiny) relative to ϵ , an absolute convergence criterion may stop iterations too reluctantly (or too soon). *relative*
- The relative convergence criterion corrects for the scale of x , but can become unstable if $x^{(t)}$ values (or true solution) lie too close to zero.
- For the latter case, monitor relative convergence by stopping when

$$\frac{|x^{(t+1)} - x^{(t)}|}{|x^{(t)}| + \epsilon} < \epsilon.$$

reduce the instability of relative convergence criterion

Stopping Rule for Failure

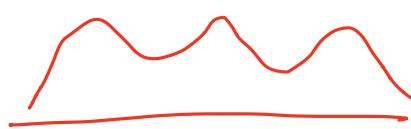
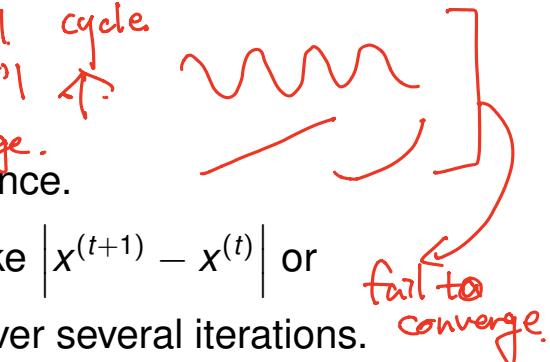
Monitor Convergence Criterion.

→ We have to set N suff. large.

- Stop after N iterations regardless of convergence.
- Stop if one or more convergence measures like $|x^{(t+1)} - x^{(t)}|$ or $|x^{(t+1)} - x^{(t)}| / |x^{(t)}|$ fail to decrease or cycle over several iterations.
- Stop if the procedure appears to be converging to a point at which $g(x)$ is inferior to another value you have already found. (Finding a false peak or local maximum.)
 $\text{We already found some other point } f(\text{Convergence point}) \leftarrow f(\text{Other point})$
- Any indication of poor convergence behavior means that $x^{(t+1)}$ must be discarded that the algorithm somehow restarted.

local maximum optimum

Multi-modality



Starting Points

- A bad starting value can lead to divergence, cycling, discovery of a misleading local maximum or a local minimum or other problems.
- The outcome depends on g , the starting value, and the optimization algorithm tried.
$$\text{Outcome} \leftarrow \begin{pmatrix} \text{function} \\ \text{the starting point} \\ \text{algorithm} \end{pmatrix}$$
- Methods for generating a reasonable starting values include graphing, preliminary estimates, educated guesses, and trial and error.
- Using a collection of runs from multiple starting values can be an effective way to gain confidence in your result.

[Convergence criterion
Starting points]

Bisection Method

Single parameter.

Bisection Method

- Iterative root-finding algorithm
- If g' is continuous on $[a_0, b_0]$ and $g'(a_0)g'(b_0) \leq 0$, then there exists at least one $x^* \in [a_0, b_0]$ for which $g'(x^*) = 0$ and hence x^* is a local optimum of g .
- The bisection method systematically shrinks the interval from $[a_0, b_0]$ to $[a_1, b_1]$ to $[a_2, b_2]$ and so on, where $[a_0, b_0] \supset [a_1, b_1] \supset [a_2, b_2] \supset \dots$ and so forth.

Bisection Method

- Let $x^{(0)} = \frac{a_0+b_0}{2}$ be the starting value. The updating equations are

$$[a_{t+1}, b_{t+1}] = \begin{cases} [a_t, x^{(t)}] & \text{if } g'(a_t)g'(x^{(t)}) \leq 0, \\ [x^{(t)}, b_t] & \text{if } g'(a_t)g'(x^{(t)}) > 0 \end{cases}$$

and

$$x^{(t+1)} = \frac{1}{2} (a_{t+1} + b_{t+1}).$$

Graphical Illustration: Bisection Method

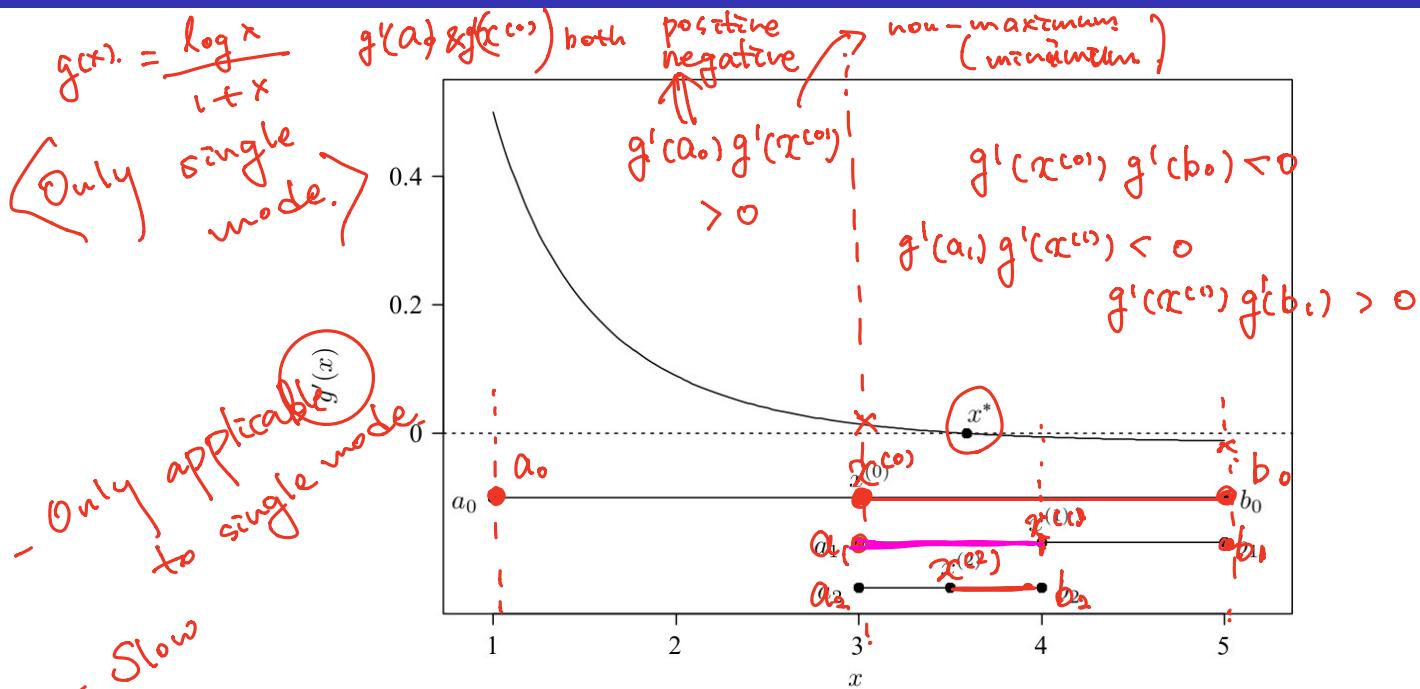


FIGURE 2.2 Illustration of the bisection method from Example 2.1. The top portion of this graph shows $g'(x)$ and its root at x^* . The bottom portion shows the first three intervals obtained using the bisection method with $(a_0, b_0) = (1, 5)$. The t th estimate of the root is at the center of the t th interval.

Newton's Method

$$\underbrace{g'(x^*) = 0}_{\text{Root}}$$
$$g'(x^*) \approx g'(x^{(t)}) + (x^* - x^{(t)}) g''(x^{(t)})$$

$\xrightarrow{\text{Taylor Series Expansion.}} + \frac{1}{2} (x^* - x^{(t)})^2 g'''(x^{(t)}) + \text{Remainder}$

Suppose that g' is continuously differentiable and that $g''(x^*) \neq 0$. At iteration t , the approach approximates $g'(x^*)$ by the Taylor series expansion:

$$0 = g'(x^*) \approx g'(x^{(t)}) + (x^* - x^{(t)}) g''(x^{(t)}).$$

Since g' is approximately by its tangent line at $x^{(t)}$, it seems sensible to approximate the root of g' by the root of the tangent line. Thus,

$$x^{(t+1)} = x^{(t)} - \frac{g'(x^{(t)})}{g''(x^{(t)})}.$$

$$g(x^*) \approx g'(x^{(t)}) + (x^* - x^{(t)}) g''(x^{(t)}) = 0$$

$$x^* - x^{(t)} \underset{\curvearrowright}{=} -\frac{g'(x^{(t)})}{g''(x^{(t)})}$$

$$x^{(t+1)} = x^{(t)} - \frac{g'(x^{(t)})}{g''(x^{(t)})}$$

Updating Equation of

Newton-Raphson Algorithm

Graphical Illustration: Newton's Method

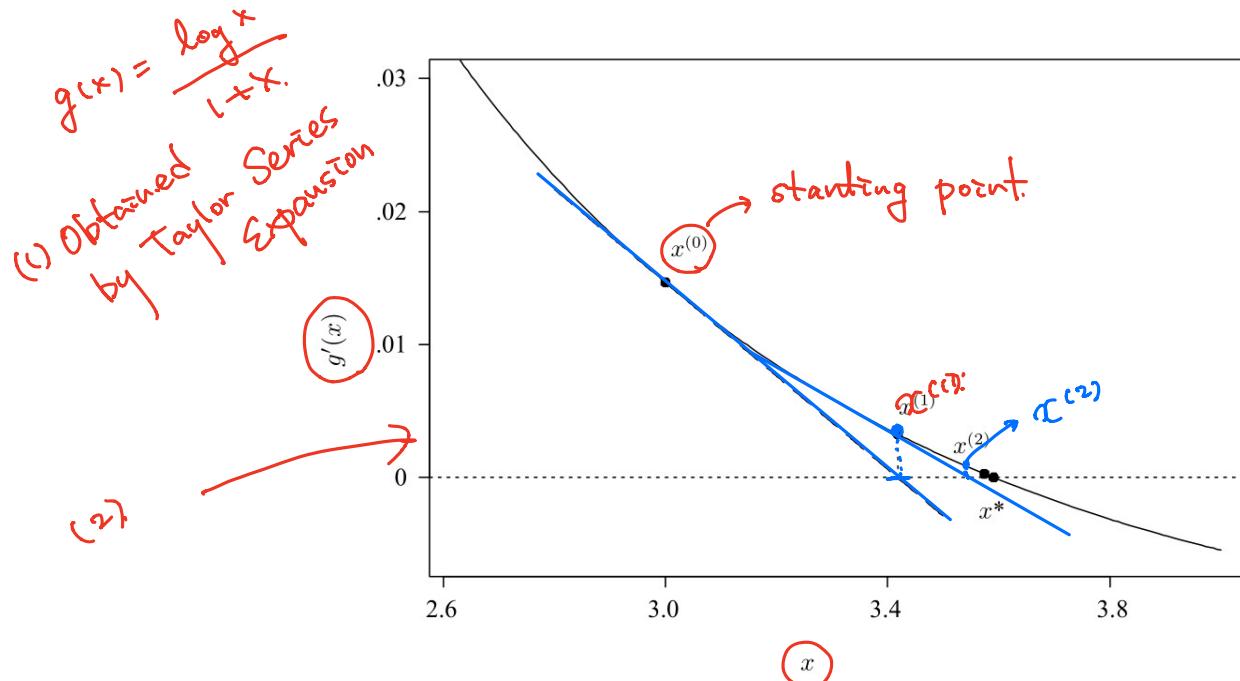


FIGURE 2.3 Illustration of Newton's method applied in Example 2.2. At the first step, Newton's method approximates g' by its tangent line at $x^{(0)}$, whose root $x^{(1)}$ serves as the next approximation of the true root x^* . The next step similarly yields $x^{(2)}$, which is already quite close to x^* .

Example: Newton's Method

Recall our motivating example. The Newton-Raphson increment for this problem is given by

$$\frac{g'(x^{(t)})}{g''(x^{(t)})} = \frac{\left(x^{(t)} + 1\right) \left(1 + 1/x^{(t)} - \log x^{(t)}\right)}{3 + 4/x^{(t)} + 1/(x^{(t)})^2 - 2 \log x^{(t)}}.$$

Starting from $x^{(0)} = 3.0$.

Example: Newton's Method

(Question) Find the root of the equation $f'(x) = e^{-x} - 5x = 0$.

(Answer)

$$f'(x) = e^{-x} - 5x, \quad \text{and} \quad f''(x) = -e^{-x} - 5.$$

The solution of the Newton-Raphson algorithm can be updated as

$$x^{(t+1)} = x^{(t)} - \frac{e^{-x} - 5x}{-e^{-x} - 5} = x^{(t)} + \frac{e^{-x} - 5x}{e^{-x} + 5}.$$

Implement the Newton-Raphson algorithm by yourselves. (Homework!!!)

Divergence of the Newton's Method

Whether Newton's method convergence depends on the shape of g and the starting value.

Convergence of Newton's Method

shape of g
starting value.

Disadvantage
- need to calculate
the second derivative.

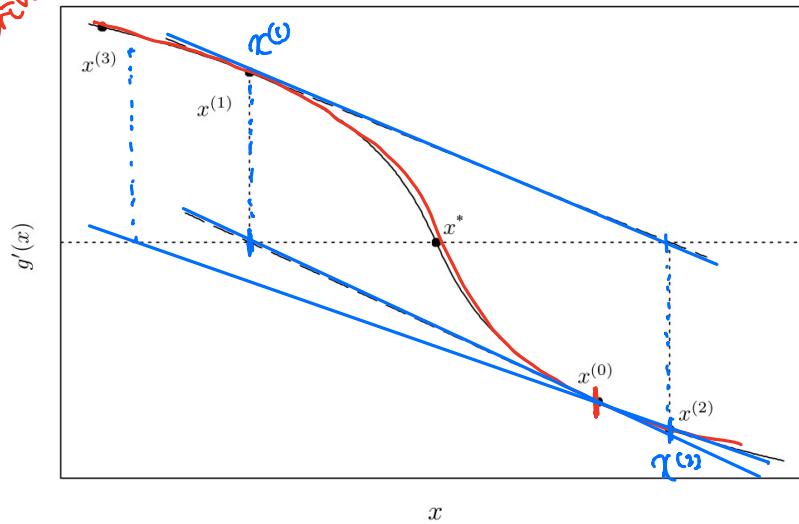


FIGURE 2.4 Starting from $x^{(0)}$, Newton's method diverges by taking steps that are increasingly distant from the true root, x^* .

Need to run with multiple starting points.

Fisher Scoring

We use for finding the MLE. $\Rightarrow l'(\theta) = 0 \Rightarrow$ When we use Newton-Raphson method,
 Variant of Newton-Raphson method. related to Fisher information $I''(\theta)$

- Recall $I(\theta)$ can be approximated by $-I''(\theta)$. Therefore, when the optimization of g corresponds to an MLE problem, it is reasonable to replace $-I''(\theta)$ in the Newton update with $I(\theta)$. $I(\theta) = -I''(\theta)$
- The updating equation of the Fisher scoring method is

$$\theta^{(t+1)} = \theta^{(t)} + I'(\theta^{(t)})I(\theta^{(t)})^{-1},$$

where $I(\theta^{(t)})$ is the expected Fisher information evaluated at $\theta^{(t)}$.

- Generally, Fisher scoring works better in the beginning to make rapid improvements, while Newton's method works better for refinement near the end.

$$\theta^{(t+1)} = \theta^{(t)} - \frac{l'(x^{(t)})}{l''(x^{(t)})} = \theta^{(t)} - \frac{l'(x^{(t)})}{I(\theta^{(t)})}$$

$\Rightarrow \theta^{(t+1)} = \theta^{(t)} + l'(\theta^{(t)})[I(\theta^{(t)})]^{-1}$

Secant Method

- ↳ Variant of
 Newton-Raphson method
 \Rightarrow We need to calculate the second derivative
- The updating increment for Newton-Raphson's method relies on the second derivative, $g''(x^{(t)})$. Instead of calculating the second derivative, use the definition of derivative.
 - If calculating the derivative is difficult, it might be replaced by the discrete-difference approximation. The result is the secant method,

↳ Updating equation of Secant method.

$$x^{(t+1)} = x^{(t)} - g'(x^{(t)}) \frac{x^{(t)} - x^{(t-1)}}{g'(x^{(t)}) - g'(x^{(t-1)})}$$

for $t \geq 1$.

$$g''(x) = \lim_{x^{(t)} - x^{(t-1)} \rightarrow 0} \frac{g(x^{(t)}) - g(x^{(t-1)})}{x^{(t)} - x^{(t-1)}}$$

- This approach requires two starting points, $x^{(0)}$ and $x^{(1)}$.

Secant Method

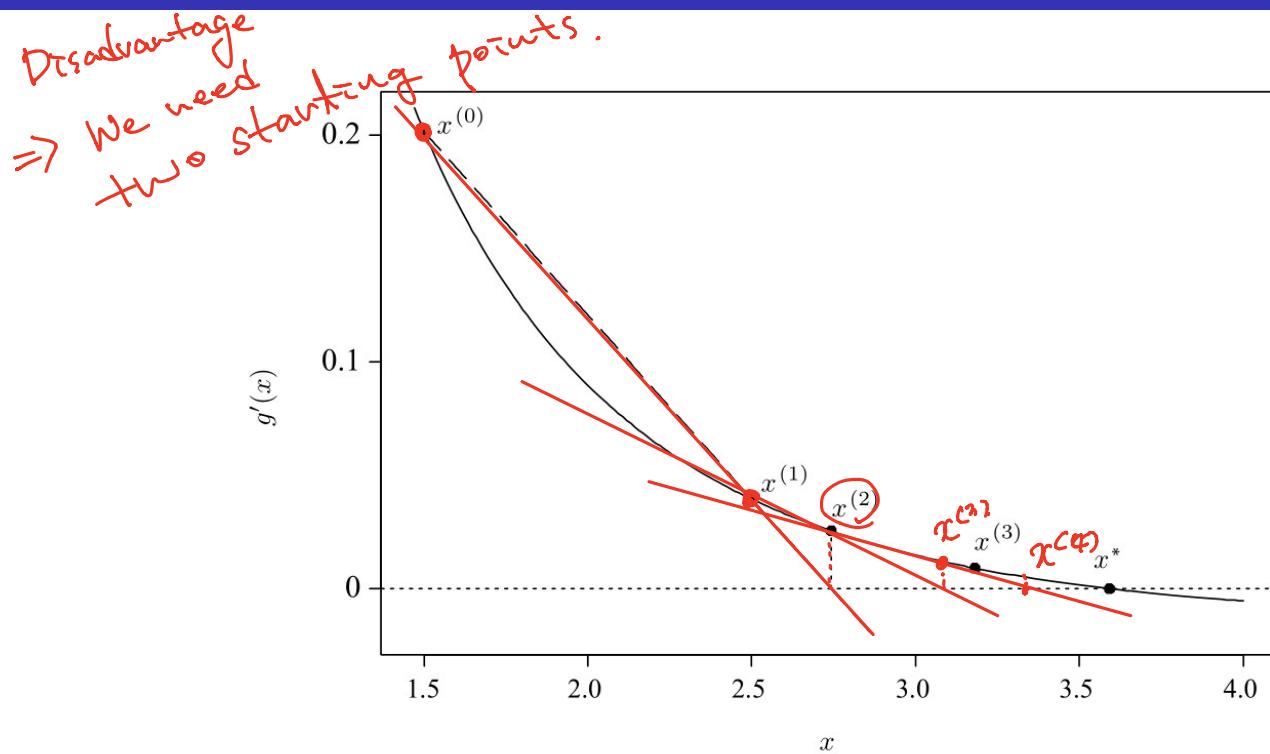


FIGURE 2.5 The secant method locally approximates g' using the secant line between $x^{(0)}$ and $x^{(1)}$. The corresponding estimated root, $x^{(2)}$, is used with $x^{(1)}$ to generate the next approximation.

Fixed Point: Fixed points of a function is an element of the function's domain that is mapped to itself by the function.

$$f(c) = c$$

c is a fixed point

$$(\text{Ex}) \quad f(x) = x^2 - 3x + 4 = x. \quad \text{fixed point } x=2$$

$$x^2 - 4x + 4 = 0$$

$$(x-2)^2 = 0 \quad x=2.$$

Do all functions have fixed points? No.

$$f(x) = \underline{x+1} \neq x$$

$0 \neq 1 \Rightarrow$ No fixed point.

Fixed Point Iteration

$$g'(x) = 0 \quad (G(x) = x) \xrightarrow{\text{has fixed point}}$$

- The fixed-point strategy for finding roots is to determine a function G for which $g'(x) = 0$ if and only if $G(x) = x$.

$$\alpha g'(x) = 0$$

$$g'(x) = 0 \Rightarrow g'(x) + x = x \Rightarrow G(x) = x.$$

$$\xrightarrow{\quad} g'(x) + x = x \Rightarrow G(x) = x$$

This transforms the problem of finding a root of g' into a problem of finding a fixed point of G . $\xrightarrow{\quad} g'(x) + x$. will be used as a updating equation,

- The simplest way to hunt for a fixed point is to use the updating

equation $x^{(t+1)} = G(x^{(t)})$. This yields the updating equation

$$x^{(t+1)} = x^{(t)} + g'(x^{(t)})$$

$$x^{(t+1)} = x^{(t)} + g'(x^{(t)})$$

$$\text{or } = x^{(t)} + \alpha g'(x^{(t)})$$

- Scaling: When g'' is bounded and does not change sign on $[a, b]$, we can rescaling nonconvergent problems by choosing $G(x) = \alpha g'(x) + x$ for $\alpha \neq 0$. \Rightarrow Newton-Raphson method \Rightarrow Variant of fixed-point iteration

Fixed Point Iteration

$$\exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right) \quad \text{normal density}$$

- Suppose an MLE is sought for the parameter of a quadratic log-likelihood, ℓ . Then, the score function is locally linear and ℓ'' is roughly a constant.

- For quadratic log likelihoods, Newton's method would use the updating equation

$$\theta^{(t+1)} = \theta^{(t)} - \frac{\ell'(\theta)}{\gamma} = \theta^{(t)} + \alpha \ell'(\theta)$$

- If we use scaled fixed-point iteration with $\alpha = -1/\gamma$, we get the same updating equation.

$$\alpha = -1/\gamma$$

fixed point iteration method

- Since many log-likelihoods are approximately locally quadratic, scaled fixed-point iteration can be very effective.

Fixed Point Iteration

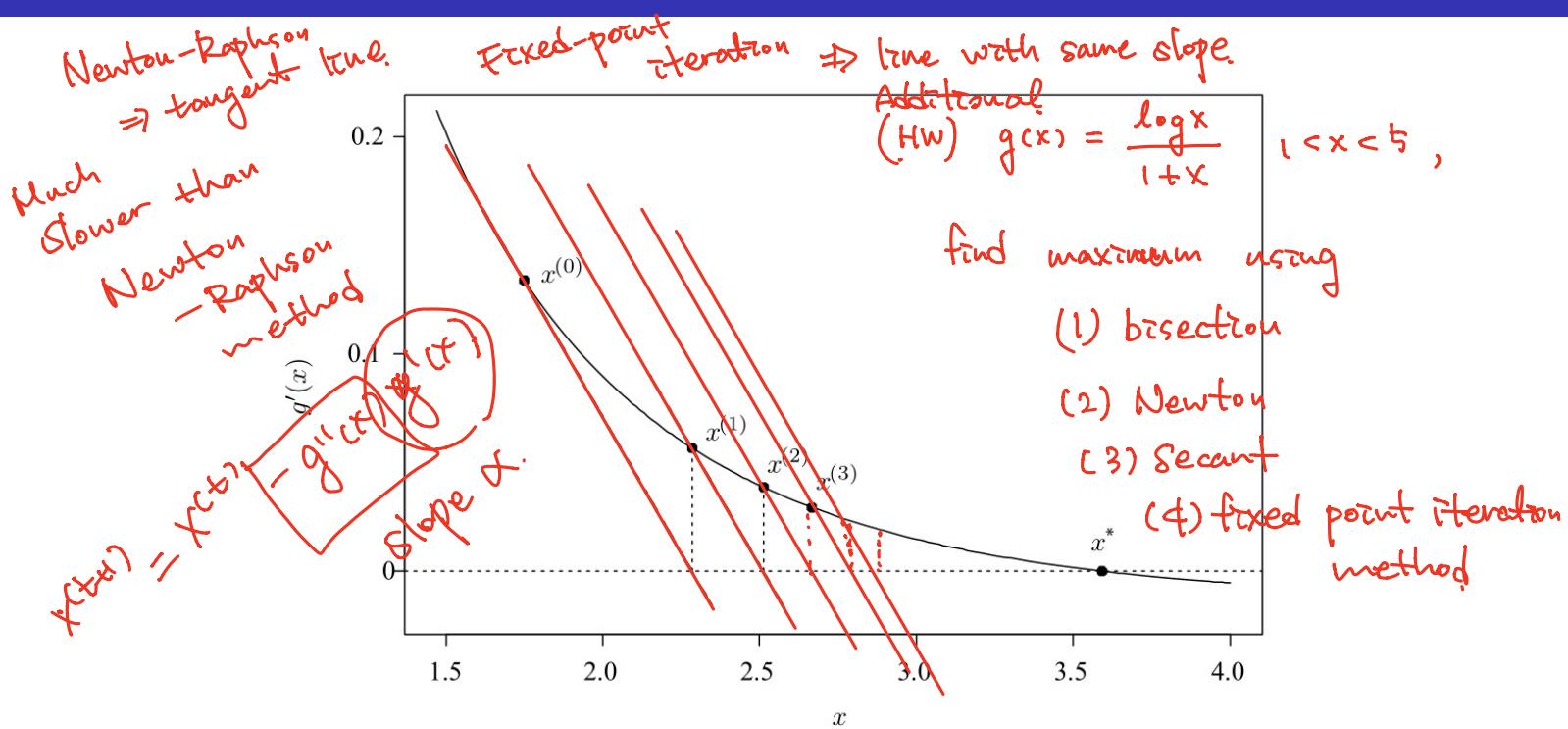


FIGURE 2.6 First three steps of scaled fixed-point iteration to maximize $g(x) = (\log x)/(1 + x)$ using $G(x) = g'(x) + x$ and scaling with $\alpha = 4$, as in Example 2.3.

Convergence Criteria

distance between

$x^{(t+1)}$ & $x^{(t)}$

$x_{\tilde{t}}$

- Let $D(\mathbf{u}, \mathbf{v})$ be a distance measure for p -dimensional vectors where

→ absolute difference

$$D(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^p |u_i - v_i|, \quad \text{and} \quad D(\mathbf{u}, \mathbf{v}) = \sqrt{\sum_{i=1}^p (u_i - v_i)^2}.$$

$\therefore (x_{\tilde{t}} - 0)$

↳ Euclidean distance,

- Absolute and relative convergence criteria can be formed from the inequalities

Absolute Convergence

$$D(\mathbf{x}^{(t+1)}, \mathbf{x}^{(t)}) < \epsilon, \quad \frac{D(\mathbf{x}^{(t+1)}, \mathbf{x}^{(t)})}{D(\mathbf{x}^{(t)}, \mathbf{0})} < \epsilon.$$

Relative

$\mathbf{x}^{(t)}$ & $\mathbf{0}$ distance.

$g'(\mathbf{x}) = 0$

Newton's Method and Fisher Scoring

small boldic letter : vector
 Capital : Matrix

- Approximate $g(\mathbf{x}^*)$ by the Taylor series expansion

$$g(\mathbf{x}^*) = g(\mathbf{x}^{(t)}) + (\mathbf{x}^* - \mathbf{x}^{(t)})' g'(\mathbf{x}^{(t)}) + \frac{1}{2} (\mathbf{x}^* - \mathbf{x}^{(t)})' g''(\mathbf{x}^{(t)}) (\mathbf{x}^* - \mathbf{x}^{(t)})$$

and maximize this quadratic function with respect to \mathbf{x}^* .

- The gradient of the right-hand side of previous equation equal to zero yields

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - g''(\mathbf{x}^{(t)})^{-1} g'(\mathbf{x}^{(t)})$$

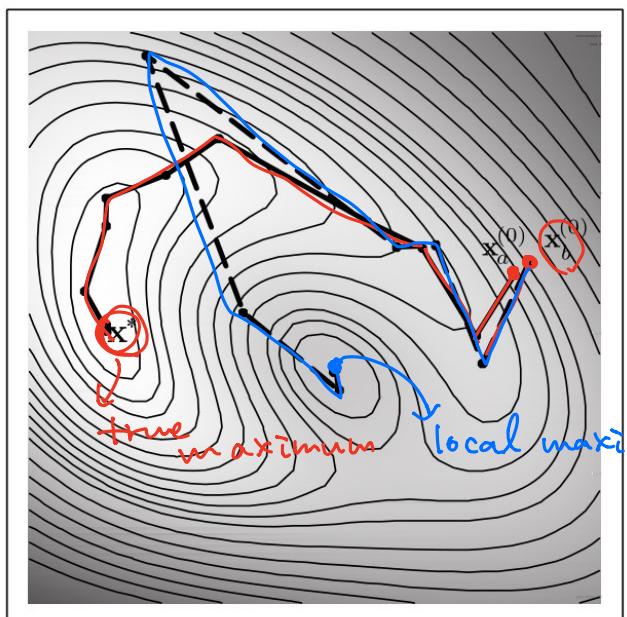
$$g'(\mathbf{x}^{(t)}) + g''(\mathbf{x}^{(t)}) (\mathbf{x}^* - \mathbf{x}^{(t)}) = 0 \quad \text{and} \quad \mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - g''(\mathbf{x}^{(t)})^{-1} g'(\mathbf{x}^{(t)}).$$

vector

- Multivariate Fisher scoring approach is given by

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} + \mathbf{I}(\boldsymbol{\theta}^{(t)})^{-1} l'(\boldsymbol{\theta}^{(t)}).$$

Example: Multivariate Newton's Methods



Multivariate case
=> Multimodality
more severe
than univariate
case.

FIGURE 2.7 Application of Newton's method for maximizing a complicated bivariate function, as discussed in Example 2.4. The surface of the function is indicated by shading and contours, with light shading corresponding to high values. Two runs starting from $\mathbf{x}_a^{(0)}$ and $\mathbf{x}_b^{(0)}$ are shown. These converge to the true maximum and to a local minimum, respectively.

Iteratively Reweighted Least Squares

→ Generalize Linear Model \Rightarrow Parameter Estimation.

- Suppose the observed data consist of p covariate values

$\mathbf{x}_i = (1, x_{i1}, \dots, x_{ip})'$ and a binary response value y_i , for $i = 1, \dots, n$.

Let $\beta = (\beta_0, \beta_1, \dots, \beta_p)'$ denote a vector of parameter. x_i

- GLM used for logistic regression is based on the Bernoulli distribution.

Model the response variables as $y_i | x_i \sim \text{Bernoulli}(\pi_i)$. $y_i | x_i \sim \text{Bernoulli}(\pi_i)$

- Let π_i be the probability of a binary response. $\pi_i \in [0, 1]$ \Rightarrow map π_i into $[-\infty, \infty]$ link function.

$$\log \frac{\pi_i}{1 - \pi_i} = \beta' \mathbf{x}_i \Rightarrow \pi_i = \frac{\exp(\beta' \mathbf{x}_i)}{1 + \exp(\beta' \mathbf{x}_i)}$$

Then, the likelihood function is

$$L(\beta) = \prod_{i=1}^n \pi_i^{y_i} (1 - \pi_i)^{1-y_i} = \left[\prod_{i=1}^n \left(\frac{\exp(\beta' \mathbf{x}_i)}{1 + \exp(\beta' \mathbf{x}_i)} \right)^{y_i} \left(\frac{1}{1 + \exp(\beta' \mathbf{x}_i)} \right)^{1-y_i} \right]$$

$$\log \frac{\pi_i}{1 - \pi_i} = \beta' \mathbf{x}_i \Rightarrow \pi_i = \frac{\exp(\beta' \mathbf{x}_i)}{1 + \exp(\beta' \mathbf{x}_i)}$$

Find β that maximize the likelihood

plug-in
Bernoulli dist

Binary
 \Rightarrow logit link
(probit)

Iteratively Reweighted Least Squares

- The log-likelihood is

$$l(\beta) = \mathbf{y}' \mathbf{X} \beta - \mathbf{b}' \mathbf{1},$$

where $\mathbf{1}$ is a column vector of 1, $\mathbf{y} = (y_1, \dots, y_n)'$,

$\mathbf{b} = (\log\{1 + \exp(\mathbf{x}_1' \beta)\}, \dots, \log\{1 + \exp(\mathbf{x}_n' \beta)\})$, and \mathbf{X} is the $n \times (p+1)$ matrix whose i -th row is \mathbf{x}_i' .

- The score function is

$$l'(\beta) = \mathbf{X}' (\mathbf{y} - \boldsymbol{\pi})$$

$$l'(\beta) = \mathbf{X}' (\mathbf{y} - \boldsymbol{\pi}),$$

where $\boldsymbol{\pi} = (\pi_1, \dots, \pi_n)'$ and the Hessian matrix is given by

$$l''(\beta) = \frac{d}{d\beta} \mathbf{X}' (\mathbf{y} - \boldsymbol{\pi}) = -\mathbf{X}' W \mathbf{X},$$

where W is a diagonal matrix with i -th diagonal entry equal to $\pi_i(1 - \pi_i)$.

$$\begin{aligned} \mathbf{b}' &= \begin{bmatrix} \log(1 + \exp(\mathbf{x}_1' \beta)) \\ \log(1 + \exp(\mathbf{x}_2' \beta)) \\ \vdots \\ \log(1 + \exp(\mathbf{x}_n' \beta)) \end{bmatrix} \\ \boldsymbol{\pi} &= \begin{bmatrix} \frac{\exp(\mathbf{x}_1' \beta)}{1 + \exp(\mathbf{x}_1' \beta)} \\ \frac{\exp(\mathbf{x}_2' \beta)}{1 + \exp(\mathbf{x}_2' \beta)} \\ \vdots \\ \frac{\exp(\mathbf{x}_n' \beta)}{1 + \exp(\mathbf{x}_n' \beta)} \end{bmatrix} \end{aligned}$$

$$W = \begin{bmatrix} \frac{\exp(x_i^T \beta)}{1 + \exp(x_i^T \beta)} & \dots & 1 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix}$$

$$= \begin{bmatrix} \pi_1(1 - \pi_1) & & & & \\ & \ddots & & & \\ & & \pi_2(1 - \pi_2) & & \\ & & & \ddots & \\ & & & & \pi_n(1 - \pi_n) \end{bmatrix}$$

\rightarrow Determined by β

$$\begin{pmatrix} \pi \\ W \end{pmatrix} \quad l''(\beta) = -X^T W X \quad -[l''(\beta)]^{-1}$$

$$l'(\beta) = X^T(y - \pi)$$

\rightarrow Updating equation from Newton-Raphson method

$$\beta^{(t+1)} = \beta^{(t)} + [X^T W^{(t)} X]^{-1} X^T (y - \pi^{(t)})$$

$$(X^T X)^{-1} X^T y$$

\Rightarrow Iteratively reweighted least square

Iteratively Reweighted Least Squares

Starting points-

Delay hw 1 due
 $a/b \rightarrow a/c$

- Therefore, Newton's update is

$$\begin{aligned}\boldsymbol{\beta}^{(t+1)} &= \boldsymbol{\beta}^{(t)} - I \left(\boldsymbol{\beta}^{(t)} \right)^{-1} I' \left(\boldsymbol{\beta}^{(t)} \right) \\ &= \boldsymbol{\beta}^{(t)} + \left(X' W^{(t)} X \right)^{-1} \left(X' \left(\mathbf{y} - \pi^{(t)} \right) \right),\end{aligned}$$

where $\pi^{(t)}$ is the value of π corresponding to $\boldsymbol{\beta}^{(t)}$, and $W^{(t)}$ is the diagonal weight matrix evaluated at $\pi^{(t)}$.

Similarly, you can derive IRLS for Poisson regression (HW). a/q

