The upper-crossing/solution (US) algorithm for root-finding with strongly stable convergence

Xunjian LI† and Guo-Liang TIAN†,*

Department of Statistics and Data Science, Southern University of Science and Technology, Shenzhen 518055, Guangdong Province, P. R. China Email: 11930699@mail.sustech.edu.cn

†Equally contributed
*Corresponding author’s Email: tiangl@sustech.edu.cn

Abstract. In this paper, we propose a new and broadly applicable root–finding method, called as the upper-crossing/solution (US) algorithm, which belongs to the category of non-bracketing (or open domain) methods. The US algorithm is a general principle for iteratively seeking the unique root $\theta^*$ of a non-linear equation $g(\theta) = 0$ and its each iteration consists of two steps: an upper-crossing step (U-step) and a solution step (S-step), where the U-step finds an upper-crossing function or a $U$-function $U(\theta|\theta^{(t)})$ [whose form depends on $\theta^{(t)}$ being the $t$-th iteration of $\theta^*$] based on a new notion of so-called changing direction inequality, and the S-step solves the simple $U$-equation $U(\theta|\theta^{(t)}) = 0$ to obtain its explicit solution $\theta^{(t+1)}$. The US algorithm holds two major advantages: (i) It strongly stably converges to the root $\theta^*$; and (ii) it does not depend on any initial values, in contrast to Newton’s method. The key step for applying the US algorithm is to construct one simple $U$-function $U(\theta|\theta^{(t)})$ such that an explicit solution to the $U$-equation $U(\theta|\theta^{(t)}) = 0$ is available. Based on the first–, second– and third–derivative of $g(\theta)$, three methods are given for constructing such $U$-functions. We show various applications of the US algorithm in such as calculating quantile in continuous distributions, calculating exact $p$-values for skew null distributions, and finding maximum likelihood estimates of parameters in a class of continuous/discrete distributions. The analysis of the convergence rate of the US algorithm and some numerical experiments are also provided. Especially, because of the property of strongly stable convergence, the US algorithm could be one of the powerful tools for solving an equation with multiple roots.

Keywords: Changing direction inequality; Multiple roots; Non-bracketing methods; Strongly stable convergence; US algorithm.
1. Introduction

Solving roots of an equation or zeros of a function is the most fundamental problem in computational mathematics. Many problems in science and engineering can be formulated as: Given a continuous function \( g(x) \) of a single variable defined in the real line \( \mathbb{R} \), find the value \( x^* \in \mathbb{R} \) such that \( g(x^*) = 0 \). These problems are usually called root finding problems. Calculating the *maximum likelihood estimate* (MLE) of a parameter in classical statistics and computing the posterior mode in Bayesian statistics can be viewed as finding a solution to a non-linear equation. Let \( g(\theta) \) be a non-linear function of a single variable and there exist a unique root \( \theta^* \) to the following equation:

\[
g(\theta) = 0, \quad \theta \in \Theta \subseteq \mathbb{R},
\]

where \( \Theta \) is the parameter space or an interval in the real line \( \mathbb{R} \).

There exist many methods for seeking the root of (1.1) in numerical analysis and they are roughly categorized into two classes:

(i) Closed domain (bracketing) methods, for example, the bisection method and the false position method (Wood 1992, Chabert 1999 p.83–112).

(ii) Open domain (non-bracketing) methods such as Newton’s method, the secant method, and Muller’s method (Wolfe 1959, Boyd & Vandenberghe 2004 p.484–496, Costabile et al. 2006).

The bisection method (Wood 1992) can guarantee to obtain a solution since the root is trapped in the closed interval, while it converges slowly since the information about actual functions behavior is not utilized. By using information about the function \( g(\theta) \), the false position method (Chabert 1999) generally converges more rapidly than the bisection method, however it does not give a bound on the error of the root. Non-bracketing methods are not as robust as bracketing methods and may actually diverge. However, they use information about the function itself to refine the approximations of the root. Thus, they are considerably more efficient than bracketing ones.
It is well known that Newton’s method or the Newton–Raphson (NR) algorithm is a golden standard for seeking the root of (1.1) with the following NR iteration:

\[ \theta^{(t+1)} = \theta^{(t)} - \frac{g(\theta^{(t)})}{g'(\theta^{(t)})}, \]

where \( \theta^{(t)} \) denotes the \( t \)-th iteration/approximation of the root \( \theta^* \) and \( g'(\theta) \) is the first-order derivative of \( g(\theta) \). Although the NR algorithm converges quadratically, it is sensitive to initial values (Lindstrom & Bates 1988). This property hinders its applications in repeated use of the NR algorithm such as in bootstrapping calculation of the standard deviation of an MLE. One advantage of Newton’s method is that it is an optimization technique as well as a root–finding technique. In computational statistics, we know that the expectation–maximization (EM) algorithm (Dempster et al. 1977) and minorization–maximization (MM) algorithm (Lange et al. 2000, Hunter & Lange 2004) are two popular optimization tools for calculating MLEs of parameters with monotonic convergence, rather than two root–finding tools.

To overcome the drawback of sensitiveness to initial values associated with the NR algorithm and to retain a similar property to the monotonic convergence associated with the EM/MM algorithms, we in this paper propose a new root–finding method, called as the upper-crossing/solution (US) algorithm, which belongs to the category of open domain methods. The US algorithm is a general principle for iteratively seeking the root \( \theta^* \) of equation (1.1) with strongly stable convergence (its definition will be given in the beginning of Section 2), and its each iteration consists of an upper-crossing step (U-step) and a solution step (S-step), where

**U-step**: Find a \( U \)-function \( U(\theta|\theta^{(t)}) \) satisfying (2.5);

**S-step**: Solve the \( U \)-equation to obtain its root \( \theta^{(t+1)} \) as showed by (2.6).

The two-step process is repeated until convergence occurs.

The rest of the paper is organized as follows. In Section 2, first we define two new relation symbols on the changing direction inequality, and the concept of weakly/strongly stable convergence. Next we introduce new notions such as upper-crossing function or \( U \)-function
and \(U\)-equation. Finally each US iteration with two steps (i.e., **U-step** and **S-step**) is formulated and the strongly stable convergence of the US algorithm is proved. Three methods for constructing \(U\)-functions are given in Section 3. Section 4 presents various applications such as calculating quantile in continuous distributions, calculating exact \(p\)-values for skew null distributions, and finding MLEs of parameters in a class of continuous/discrete distributions. Section 5 provides the analysis of the convergence rate of the US algorithm. Numerical experiments and some discussions are given in Sections 6–7. More technical details are put in three Appendices. Here we first present one simple example to give the flavour of the US algorithm.

**Example 1 (Root of an equation involving a trigonometric function).** Suppose that we want to find the root of the equation \(g(x) \triangleq \cos(0.5\pi x) - x = 0\) for all \(x \in \mathbb{R}\). From (3.1), note that

\[
g'(x) = -0.5\pi \sin(\pi x/2) - 1 \geq -0.5\pi - 1 \triangleq b_1,
\]

then the **U-step** of the US iteration is to find an upper-crossing function or a \(U\)-function \(U(x|\alpha(t))\), in this example, it is given by (3.5); i.e.,

\[
U(x|\alpha(t)) = g(\alpha(t)) + b_1(\alpha - \alpha(t)) = g(\alpha(t)) - (0.5\pi + 1)x + (0.5\pi + 1)\alpha(t).
\]

And the **S-step** is to solve the \(U\)-equation: \(U(x|\alpha(t)) = 0\), and to obtain its root \(\alpha(t+1)\) as

\[
\alpha(t+1) = \alpha(t) - \frac{g(\alpha(t))}{b_1} = \frac{(0.5\pi + 1)\alpha(t) + g(\alpha(t))}{0.5\pi + 1}.
\]  

(1.3)

Figure 1 plots both \(g(x)\) and \(U(x|\alpha(t))\) with the root \(x^* = 0.594612\). Using the initial value \(x(0) = -1\), Figure 1(a) shows that the sequence \(\{x(t)\}_{t=0}^{\infty}\) generated by (1.3) strongly stably converges to \(x^*\) satisfying \(x(0) < x(1) < \cdots < x(t) < \cdots \leq x^*\); while Figure 1(b) shows that with \(x(0) = 2\), the sequence \(\{x(t)\}_{t=0}^{\infty}\) generated by (1.3) strongly stably converges to \(x^*\) satisfying \(x^* \leq \cdots < x(t) < \cdots < x(1) < x(0)\).

Table 1 displayed these numerical results of the US iterations for two different initial values \(x(0) = -1, 2\). With the rate of convergence being 0.1069, the US algorithm moved for 10 and 8 steps, respectively.
Figure 1. Plots of $g(x) = \cos(0.5\pi x) - x$ and $U(x|x^{(t)}) = -(0.5\pi + 1)x + (0.5\pi + 1)x^{(t)} + g(x^{(t)})$. The true root of the equation $g(x) = 0$ is $x^* = 0.594612$. (a) With the initial value $x^{(0)} = -1$, the sequence $\{x^{(t)}\}_{t=0}^{\infty}$ generated by (1.3) strongly stably converges to $x^*$ satisfying $x^{(0)} < x^{(1)} < \cdots < x^{(t)} < \cdots \leq x^*$; (b) With the initial value $x^{(0)} = 2$, the sequence $\{x^{(t)}\}_{t=0}^{\infty}$ generated by (1.3) strongly stably converges to $x^*$ satisfying $x^* \leq \cdots < x^{(t)} < \cdots < x^{(1)} < x^{(0)}$. 
Table 1. The US algorithm for solving the equation: \( \cos(0.5\pi x) - x = 0 \) with two different initial values \( x^{(0)} = -1, 2 \)

| \( t \) | \( x^{(t)} \) | \( g(x^{(t)}) \) | \( \varepsilon^{(t)} \) | Rate | \( x^{(t)} \) | \( g(x^{(t)}) \) | \( \varepsilon^{(t)} \) | Rate |
|---|---|---|---|---|---|---|---|---|
| 0 | -1 | 1 | -1.59461 | .7561 | 2 | -3 | 1.40539 | .1697 |
| 1 | -0.611015 | 1.18471 | -1.20563 | .6178 | .833046 | -0.573792 | .238435 | .0639 |
| 2 | -0.150180 | 1.12248 | -0.744791 | .4138 | .609850 | -0.034652 | .015239 | .1154 |
| 3 | 0.286449 | 0.614018 | -0.308163 | .2249 | .596371 | -0.003983 | .001759 | .1192 |
| 4 | 0.525293 | 0.153170 | -0.069319 | .1405 | .594821 | -0.000475 | .000025 | .1197 |
| 5 | 0.584874 | 0.021967 | -0.009738 | .1225 | .594607 | -0.000225 | .000005 | .1197 |
| 6 | 0.593418 | 0.002700 | -0.001193 | .1201 | .594615 | -0.000005 | .000000 | .1196 |
| 7 | 0.594468 | 0.000324 | -0.000143 | .1198 | .594612 | -0.000001 | .000000 | .1182 |
| 8 | 0.594594 | 0.000039 | -0.000017 | .1196 | .594612 | -0.000001 | .000000 | .1069 |
| 9 | 0.594610 | 0.000005 | -0.000002 | .1182 | – – – – | – – – – | – – – – | – – – – |
| 10 | 0.594611 | 0.000001 | 0.000000 | .1069 | – – – – | – – – – | – – – – | – – – – |

Note: \( \varepsilon^{(t)} \triangleq x^{(t)} - x^* \) is the difference between the current iteration and the root; \( \text{Rate} \triangleq |\varepsilon^{(t+1)}/\varepsilon^{(t)}| \) is the rate of convergence.

2. The US algorithm with strongly stable convergence

First, we define two new relation symbols on the changing direction (CD) inequalities, \( \text{sgn}(a) \geq \) and \( \text{sgn}(a) \leq \), as follows: For two functions \( h_1(x) \) and \( h_2(x) \) with the same domain \( X \),

\[
\begin{align*}
\text{sgn}(a) \geq & h_1(x) \geq h_2(x) \quad \text{means} \quad \\
& \begin{cases} 
  h_1(x) \geq h_2(x), & \text{if } a > 0, \\
  h_1(x) = h_2(x), & \text{if } a = 0, \\
  h_1(x) \leq h_2(x), & \text{if } a < 0,
\end{cases}
\end{align*}
\]

and

\[
\begin{align*}
\text{sgn}(a) \leq & h_1(x) \leq h_2(x) \quad \text{means} \quad \\
& \begin{cases} 
  h_1(x) \leq h_2(x), & \text{if } a > 0, \\
  h_1(x) = h_2(x), & \text{if } a = 0, \\
  h_1(x) \geq h_2(x), & \text{if } a < 0.
\end{cases}
\end{align*}
\]

For example, \( x^{2n-1} \geq 0 \) for any positive integer \( n \); \( \sin(x) \geq 0 \) for any \( x \in (0, 2\pi) \); and \( \cos(x) \leq 0 \) for any \( x \in (0, \pi) \) are three illustrative examples.

Next, a sequence \( \{\theta^{(t)}\}_{t=0}^{\infty} \) is called to weakly stably converge to a fixed point \( \theta^* \), if

\[
|\theta^{(t+1)} - \theta^*| < |\theta^{(t)} - \theta^*|, \quad \forall \ t = 0, 1, \ldots, \infty.
\]
A sequence \( \{ \theta^{(t)} \}_{t=0}^{\infty} \) is called to strongly stably converge to a fixed point \( \theta^* \), if
\[
\theta^{(0)} < \theta^{(1)} < \cdots < \theta^{(t)} < \cdots \leq \theta^* \quad \text{or} \quad \theta^* \leq \cdots < \theta^{(t)} < \cdots < \theta^{(1)} < \theta^{(0)}. 
\]

An algorithm is said to possess \textit{weakly (or strongly) stable convergence} if the sequence \( \{ \theta^{(t)} \}_{t=0}^{\infty} \) generated by this algorithm weakly (or strongly) stably converges to a fixed point \( \theta^* \). It is clear that a strongly stable convergence implies a weakly stable convergence.

### 2.1 Definition of a \( U \)-function

Suppose that directly solving the unique root \( \theta^* \) of the non-linear equation (1.1) is very difficult. Without loss of generality, we assume that
\[
g(\theta) > 0, \quad \forall \theta < \theta^* \quad \text{and} \quad g(\theta) < 0, \quad \forall \theta > \theta^*. \tag{2.1}
\]

If \( g(\theta) < 0 \) when \( \theta < \theta^* \), then we can multiplies \(-1\) on both sides of (1.1) and obtain a new equation \(-g(\theta) = 0\), which satisfies the assumption (2.1) and has the same root \( \theta^* \).

The idea of the US algorithm is as follows. Let \( \theta^{(t)} \) be the \( t \)-th iteration of \( \theta^* \) and \( U(\theta|\theta^{(t)}) \) be a real-valued function of \( \theta \) whose form depends on \( \theta^{(t)} \). The function \( U(\theta|\theta^{(t)}) \) is called a \( U \)-function for \( g(\theta) \) at \( \theta = \theta^{(t)} \) if the following three conditions are satisfied:

\[
\begin{align*}
g(\theta) &\leq U(\theta|\theta^{(t)}), \quad \text{if} \quad \theta < \theta^{(t)}, \tag{2.2} \\
g(\theta^{(t)}) &= U(\theta^{(t)}|\theta^{(t)}) \quad \text{if} \quad \theta = \theta^{(t)}, \tag{2.3} \\
g(\theta) &\geq U(\theta|\theta^{(t)}), \quad \text{if} \quad \theta > \theta^{(t)}. \tag{2.4}
\end{align*}
\]

The three conditions can be equivalently rewritten as
\[
g(\theta) \sgn(\theta - \theta^{(t)}) \geq U(\theta|\theta^{(t)}), \quad \forall \theta, \theta^{(t)} \in \Theta. \tag{2.5}
\]

The conditions (2.2)–(2.3) indicate that the \( U(\theta|\theta^{(t)}) \) function majorizes the objective function \( g(\theta) \) at \( \theta = \theta^{(t)} \) for all \( \theta \leq \theta^{(t)} \), and the conditions (2.4)–(2.3) show that the \( U(\theta|\theta^{(t)}) \) function minorizes \( g(\theta) \) at \( \theta = \theta^{(t)} \) for all \( \theta \geq \theta^{(t)} \). The geometric interpretations of the objective function \( g(\theta) \) (solid curve) and the \( U \)-function \( U(\theta|\theta^{(t)}) \) (dotted curve) are showed in Figure 1.
The assumption (2.1) implies \( \text{sgn}(\theta - \theta^*) \geq g(\theta) \) for all \( \theta, \theta^* \in \Theta \). By comparing this CD inequality with (2.5), we conclude that \( g(\theta) \) is a U-function for 0 at \( \theta = \theta^* \). Other properties on U-functions are listed in Property 1 below.

**Property 1 (Basic properties on U-functions).**

(a) Let \( g(\theta) \) be defined in \( \Theta \), then \( g(\theta) \) is a U-function for itself at any inner point in \( \Theta \);

(b) If \( U_1(\theta|\theta^{(t)}) \) and \( U_2(\theta|\theta^{(t)}) \) are two U-functions for \( g(\theta) \) at \( \theta = \theta^{(t)} \), then \( [U_1(\theta|\theta^{(t)}) + U_2(\theta|\theta^{(t)})]/2 \) is a U-function for \( g(\theta) \) at \( \theta = \theta^{(t)} \);

(c) For two functions \( g_1(\theta) \) and \( g_2(\theta) \) defined in \( \Theta \), if \( U_1(\theta|\theta^{(t)}) \) is a U-function for \( g_1(\theta) \) at \( \theta = \theta^{(t)} \), then \( U_1(\theta|\theta^{(t)}) + g_2(\theta) \) is a U-function for \( g_1(\theta) + g_2(\theta) \) at \( \theta = \theta^{(t)} \).

2.2 The U-equation and the US algorithm

If a \( U(\theta|\theta^{(t)}) \) function satisfying (2.5) could be found, then one need only solve the simple U-equation: \( U(\theta|\theta^{(t)}) = 0 \) to obtain its solution \( \theta^{(t+1)} \), denoted by

\[
\theta^{(t+1)} = \text{sol} \{ U(\theta|\theta^{(t)}) = 0, \ \forall \ \theta, \theta^{(t)} \in \Theta \},
\]

which defines a US algorithm. Therefore, the US algorithm is a general principle for iteratively seeking the root \( \theta^* \) with strongly stable convergence, and its each iteration consists of an upper-crossing step (U-step) and a solution step (S-step), where

**U-step:** Find a U-function \( U(\theta|\theta^{(t)}) \) satisfying (2.5);

**S-step:** Solve the U-equation to obtain its root \( \theta^{(t+1)} \) as showed by (2.6).

The two-step process is repeated until convergence occurs.

In general, the solution \( \theta^{(t+1)} \) in (2.6) has an explicit expression. Usually, the U-equation \( U(\theta|\theta^{(t)}) = 0 \) could be any equation with analytic solution, e.g., a quadratic equation, even a linear equation. Therefore, the US principle is iteratively solving a sequence of tractable surrogate equations \( U(\theta|\theta^{(t)}) = 0 \) instead of solving the intractable original non-linear equation \( g(\theta) = 0 \).
Theorem 1 below states that the US algorithm holds two characteristics: (i) It strongly stably converges to the root $\theta^*$; (ii) It does not depend on any initial values in $\Theta$, in contrast to Newton’s method. Its proof is put in Appendix A.

**Theorem 1 (Strongly stable convergence).** Let $\theta^*$ be the unique root of the equation (1.1), and $U(\theta|\theta^{(t)})$ be one $U$-function for $g(\theta)$ at $\theta = \theta^{(t)}$ in $\Theta$. Then, for any initial value $\theta^{(0)}$ in $\Theta$, the sequence $\{\theta^{(t+1)}\}_{t=0}^{\infty}$ specified by (2.6) strongly stably converges to $\theta^*$.

3. Three methods for constructing $U$-functions

For the same objective function $g(\theta)$, it is possible that there exist several $U$-functions. In other words, for the equation (1.1), it may exist more than one US algorithm. We know that the key for a US algorithm is how to find a $U$-function. In this section, we propose three general methods to construct $U$-functions based on the objective function $g(\theta)$.

3.1 The FLB function method

Suppose the first–order derivative $g'(\cdot)$ exists and it is bounded by some function $b(\cdot)$; i.e.,

$$g'(\theta) \geq b(\theta), \quad \forall \theta \in \Theta,$$

where $b(\theta)$ is called the **first-derivative lower bound** (FLB) function. It is easy to verify that

$$U(\theta|\theta^{(t)}) \triangleq g(\theta^{(t)}) + \int_{\theta^{(t)}}^{\theta} b(z) \, dz, \quad \forall \theta, \theta^{(t)} \in \Theta,$$

is a $U$-function for $g(\theta)$ at $\theta = \theta^{(t)}$. In fact, we have

$$g(\theta) - U(\theta|\theta^{(t)}) \overset{(3.2)}{=} [g(\theta) - g(\theta^{(t)})] - \int_{\theta^{(t)}}^{\theta} b(z) \, dz = \int_{\theta^{(t)}}^{\theta} g'(z) \, dz - \int_{\theta^{(t)}}^{\theta} b(z) \, dz$$

$$= \int_{\theta^{(t)}}^{\theta} [g'(z) - b(z)] \, dz \begin{cases} \leq 0, & \text{if } \theta < \theta^{(t)}, \text{ indicating (2.2)}, \\ = 0, & \text{if } \theta = \theta^{(t)}, \text{ indicating (2.3)}, \\ \geq 0, & \text{if } \theta > \theta^{(t)}, \text{ indicating (2.4)} \end{cases}$$

$$\geq 0, \quad \forall \theta, \theta^{(t)} \in \Theta,$$

where we have used the result $g'(z) - b(z) \overset{(3.1)}{\geq} 0$ for all $z \in \Theta$ in the above CD inequality.
3.1.1 Two special cases of the FLB function $b(\theta)$

Let $b(\theta) = b_1 + b_2 \theta$ be a linear function. Then the $U$-function defined by (3.2) becomes a quadratic function

$$U(\theta|\theta^{(t)}) = \frac{1}{2} b_2 \theta^2 + b_1 \theta + c_1^{(t)} \quad \text{with} \quad c_1^{(t)} \triangleq g(\theta^{(t)}) - \frac{1}{2} b_2 \theta^{(t)} - b_1 \theta^{(t)},$$

(3.3)

if $b_2 \neq 0$. From (2.6), the $U$-equation $U(\theta|\theta^{(t)}) = 0$ has two solutions

$$\theta^{(t+1)} = \frac{-b_1 \pm \sqrt{b_1^2 - 2b_2c_1^{(t)}}}{b_2},$$

(3.4)

but only one is the desired US iteration.

In particular, if $b_2 = 0$ (i.e., $g'(\theta) \geq b_1$ for all $\theta \in \Theta$, where $b_1$ is called the FLB constant), then (3.3) becomes to a linear function

$$U(\theta|\theta^{(t)}) = g(\theta^{(t)}) + b_1(\theta - \theta^{(t)})$$

(3.5)

and the corresponding US iteration is given by

$$\theta^{(t+1)} = \theta^{(t)} - \frac{g(\theta^{(t)})}{b_1}, \quad b_1 \neq 0,$$

(3.6)

which can be viewed as the NR iteration (1.2) by replacing $g'(\theta^{(t)})$ with $b_1$.

3.1.2 Motivation for constructing the $U$-function (3.2)

Under the assumption (3.1), the key for constructing the US algorithm is how to obtain $U(\theta|\theta^{(t)})$ function specified by (3.2). Our motivation is from the mean value theorem (i.e., the first–order Taylor expansion). It states that there exists a point $z^*$ between $\theta$ and $\theta^{(t)}$ such that

$$g(\theta) - g(\theta^{(t)}) = (\theta - \theta^{(t)}) g'(z^*) = \int_{\theta^{(t)}}^{\theta} g'(z) \, dz.$$  

(3.7)

Rewriting (3.7), we obtain

$$g(\theta) = g(\theta^{(t)}) + \int_{\theta^{(t)}}^{\theta} g'(z) \, dz$$

$$\begin{align*}
\text{sgn}(\theta - \theta^{(t)}) & \geq\prod g(\theta^{(t)}) + \int_{\theta^{(t)}}^{\theta} b(z) \, dz \triangleq U(\theta|\theta^{(t)}),
\end{align*}$$

where the result $g'(z) - b(z) \geq 0$ is used in the above CD inequality.
3.2 The SLUB constants method

Suppose that \( g''(\cdot) \) exists and there are two constants \( \{ b_{21}, b_{22} \} \) (which are called the second-derivative lower-upper bound (SLUB) constants) such that

\[
 b_{21} \leq g''(\theta) \leq b_{22}, \quad \forall \theta \in \Theta. \tag{3.8}
\]

Let \( I(\cdot) \) denote the indicator function and define a step constant

\[
 b_2(\theta|\theta^{(t)}) \triangleq b_{22} \cdot I(\theta \leq \theta^{(t)}) + b_{21} \cdot I(\theta > \theta^{(t)}). \tag{3.9}
\]

It is easy to verify that the quadratic function

\[
 U(\theta|\theta^{(t)}) \triangleq g(\theta^{(t)}) + g'(\theta^{(t)})(\theta - \theta^{(t)}) + \frac{1}{2} b_2(\theta|\theta^{(t)})(\theta - \theta^{(t)})^2, \quad \forall \theta, \theta^{(t)} \in \Theta, \tag{3.10}
\]

is a \( U \)-function for \( g(\theta) \) at \( \theta = \theta^{(t)} \).

Note that the second-order Taylor’s expansion

\[
 g(\theta) = g(\theta^{(t)}) + g'(\theta^{(t)})(\theta - \theta^{(t)}) + \frac{1}{2} g''(\tilde{\theta})(\theta - \theta^{(t)})^2, \quad \forall \theta, \theta^{(t)} \in \Theta,
\]

where \( \tilde{\theta} \) lies between \( \theta \) and \( \theta^{(t)} \), we only need to prove that \( b_2(\theta|\theta^{(t)})(\theta - \theta^{(t)})^2 \) is a \( U \)-function for \( g''(\tilde{\theta})(\theta - \theta^{(t)})^2 \) at \( \theta = \theta^{(t)} \). In fact, by using (3.8) and (3.9), we have

\[
 g''(\tilde{\theta})(\theta - \theta^{(t)})^2 \begin{cases} 
 \leq b_{22}(\theta - \theta^{(t)})^2, & \text{if } \theta < \theta^{(t)}, \text{ indicating (2.2)}, \\
 = 0, & \text{if } \theta = \theta^{(t)}, \text{ indicating (2.3)}, \\
 \geq b_{21}(\theta - \theta^{(t)})^2, & \text{if } \theta > \theta^{(t)}, \text{ indicating (2.4)}.
\end{cases}
\]

\[
 sgn(\theta - \theta^{(t)}) \geq b_2(\theta|\theta^{(t)})(\theta - \theta^{(t)})^2, \quad \forall \theta, \theta^{(t)} \in \Theta.
\]

3.3 The TLB constant method

Suppose that \( g'''(\theta) \) exists and is bounded by some constant \( b_3 \); i.e.,

\[
 g'''(\theta) \geq b_3, \quad \forall \theta \in \Theta, \tag{3.11}
\]

where \( b_3 \) is called the third-derivative lower bound (TLB) constant. It is easy to verify that the cubic function (if \( b_3 \neq 0 \))

\[
 U(\theta|\theta^{(t)}) \triangleq g(\theta^{(t)}) + g'(\theta^{(t)})(\theta - \theta^{(t)}) + \frac{1}{2} g''(\theta^{(t)})(\theta - \theta^{(t)})^2
\]

\[
 + \frac{1}{6} b_3(\theta - \theta^{(t)})^3, \quad \forall \theta, \theta^{(t)} \in \Theta, \tag{3.12}
\]
is a $U$-function for $g(\theta)$ at $\theta = \theta^{(t)}$. If $b_3 = 0$, then \[3.12\] becomes a quadratic function.

In fact, by applying the third-order Taylor expansion

$$g(\theta) = g(\theta^{(t)}) + g'(\theta^{(t)})(\theta - \theta^{(t)}) + \frac{1}{2} g''(\theta^{(t)})(\theta - \theta^{(t)})^2 + \frac{1}{6} g'''(\tilde{\theta})(\theta - \theta^{(t)})^3,$$ \[3.13\]

where $\tilde{\theta}$ lies between $\theta$ and $\theta^{(t)}$, we obtain

$$g(\theta) - U(\theta|\theta^{(t)}) \begin{cases} \leq 0, & \text{if } \theta < \theta^{(t)}, \text{ indicating } (2.2), \\ = 0, & \text{if } \theta = \theta^{(t)}, \text{ indicating } (2.3), \\ \geq 0, & \text{if } \theta > \theta^{(t)}, \text{ indicating } (2.4) \end{cases}$$

where we have used the result $g'''(\theta) - b_3 \geq 0$ for all $\theta \in \Theta$ in the above CD inequality.

4. Applications

4.1 Calculation of quantile in continuous distributions

Let $f(x|\theta)$ and $F(x|\theta)$ respectively denote the pdf and cdf of a population distribution. Given $\theta$ and a real number $p \in (0, 1)$, the $p$-th quantile $\xi_p$ of the distribution can be calculated as

$$\xi_p = \text{sol} \left\{ g(x|\theta) \triangleq p - F(x|\theta) = 0, \forall x \in \mathbb{X} \right\},$$

where we need to solve an integral equation. In this subsection, we will demonstrate that the US algorithm can be employed to iteratively find the $p$-th quantile $\xi_p$.

Assume that $g'(x|\theta) \triangleq \frac{dg(x|\theta)}{dx}$ is bounded by some function $b(x|\theta)$; i.e.,

$$g'(x|\theta) = -f(x|\theta) \geq b(x|\theta), \forall x \in \mathbb{X}. \quad (4.1)$$

Then, from \[2.6\], the US iteration is to solve

$$x^{(t+1)} = \text{sol} \left\{ U(x|x^{(t)}, \theta) \begin{cases} \geq g(x^{(t)}|\theta), & \text{if } x^{(t)} = x, \forall x, x^{(t)} \in \mathbb{X} \end{cases} \right\}.$$ \[3.14\]

In this subsection, we will consider two cases: (i) The mode $x_{\text{mod}}$ of the density $f(x|\theta)$ exists; (ii) The mode $x_{\text{mod}}$ of $f(x|\theta)$ does not exist.
4.1.1 The mode of the density exists

Let \( x_{\text{mod}} \) denote the mode of the density \( f(x|\theta) \), then we have \( -f(x|\theta) \geq -f(x_{\text{mod}}|\theta) \) for all \( x \in \mathbb{X} \). From (4.2), the US iteration is to solve

\[
x^{(t+1)} = \text{sol}\left\{ g(x^{(t)}|\theta) - f(x_{\text{mod}}|\theta)(x - x^{(t)}) = 0, \ \forall \ x, x^{(t)} \in \mathbb{X} \right\}
\]

\[
= x^{(t)} - \frac{F(x^{(t)}|\theta) - p}{f(x_{\text{mod}}|\theta)},
\]

(4.3)

Example 2 (Quantile of the normal distribution). To find the \( p \)-th quantile of the normal distribution with mean \( \mu \) and variance \( \sigma^2 \), we denote its cdf and pdf by \( \Phi(x|\mu,\sigma^2) \) and \( \phi(x|\mu,\sigma^2) = [1/(\sqrt{2\pi}\sigma)] \exp[-(x-\mu)^2/(2\sigma^2)] \), respectively. Note that the mode of \( \phi(x|\mu,\sigma^2) \) is given by \( x_{\text{mod}} = \mu \), then (4.3) becomes

\[
x^{(t+1)} = x^{(t)} - \sqrt{2\pi}\sigma \left[ \Phi(x^{(t)}|\mu,\sigma^2) - p \right].
\]

(4.4)

Example 3 (Quantile of the skew normal distribution). To find the \( p \)-th quantile of the skew normal distribution (Azzalini 1985) with pdf

\[
f(x|\mu,\sigma^2,\alpha) = \frac{2}{\sigma\sqrt{2\pi}} \exp \left[ -\frac{(x-\mu)^2}{2\sigma^2} \right] \Phi\left( \frac{\alpha(x-\mu)}{\sigma} \right),
\]

(4.5)

where \( x, \mu \in \mathbb{R}, \sigma^2 > 0, \alpha \geq 0 \) and \( \Phi(\cdot) \) is the cdf of \( N(0,1) \), in Appendix B, we proposed an MM algorithm to iteratively calculate the mode \( x_{\text{mod}} \) of the skew normal density as shown in (B.1). From (4.3), the US iteration for calculating the \( p \)-th quantile \( \xi_p \) is

\[
x^{(t+1)} = x^{(t)} - \frac{F(x^{(t)}|\mu,\sigma^2,\alpha) - p}{f(x_{\text{mod}}|\mu,\sigma^2,\alpha)},
\]

where \( F(x|\mu,\sigma^2,\alpha) \) is the cdf of the skew normal distribution.

4.1.2 The mode of the density does not exist

Let \( F(x|\alpha,\beta) \) denote the cdf of the beta distribution \( \text{Beta}(\alpha, \beta) \) and its pdf is

\[
f(x|\alpha,\beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1}(1-x)^{\beta-1}, \quad x \in (0,1), \ \alpha > 0, \ \beta > 0.
\]

(4.6)
Given $\alpha \in (0, 1), \beta \in (0, 1)$ and $p \in (0, 1)$, suppose that we want to calculate the $p$-th quantile of the distribution as $\xi_p = \text{sol} \{ g(x|\alpha, \beta) \triangleq p - F(x|\alpha, \beta) = 0, \forall x \in (0, 1) \}$. We know that if at least one of $\alpha$ and $\beta$ is less than 1, the mode of the beta density $f(x|\alpha, \beta)$ does not exist. Thus, the US iteration specified by (4.3) can not be used for such cases.

We employ (4.1)–(4.2) to calculate $\xi_p$. First, it is easy to verify the following inequality:

$$\frac{1}{x(1-x)} \leq \frac{1}{2x^2} + \frac{1}{2(1-x)^2}, \; \forall x \in (0, 1), \tag{4.7}$$

where the equality holds iff $x = 1/2$. Next,

$$g'(x|\alpha, \beta) \triangleq -f(x|\alpha, \beta) = -f(x|\alpha + 1, \beta + 1) \frac{B(\alpha + 1, \beta + 1)}{B(\alpha, \beta)} \cdot \frac{1}{x(1-x)} \tag{4.8} \geq -f(x|\alpha + 1, \beta + 1) \frac{B(\alpha + 1, \beta + 1)}{B(\alpha, \beta)} \left[ \frac{1}{2x^2} + \frac{1}{2(1-x)^2} \right] \geq -f(x_{\text{mod,1}}|\alpha + 1, \beta + 1) \frac{B(\alpha + 1, \beta + 1)}{2B(\alpha, \beta)} \left[ \frac{1}{x^2} + \frac{1}{(1-x)^2} \right] \geq \frac{a}{x^2} - \frac{a}{(1-x)^2} \triangleq b(x|\alpha, \beta), \; \forall x \in (0, 1),$$

where $x_{\text{mod,1}} \triangleq \alpha/\alpha + \beta$ denotes the mode of the beta density $f(x|\alpha + 1, \beta + 1)$ and

$$a \triangleq f(x_{\text{mod,1}}|\alpha + 1, \beta + 1) \frac{B(\alpha + 1, \beta + 1)}{2B(\alpha, \beta)}. \tag{4.8}$$

Finally, from (4.2), the US iteration for calculating the $p$-th quantile $\xi_p$ is

$$x^{(t+1)} = \text{sol} \left\{ g(x^{(t)}|\alpha, \beta) + \int_{x^{(t)}}^x b(z|\alpha, \beta) \, dz = 0, \; \forall x, x^{(t)} \in (0, 1) \right\}$$

$$= \text{sol} \left\{ g(x^{(t)}|\alpha, \beta) + \frac{a}{x} - \frac{a}{1-x} - \frac{a}{x^{(t)}} + \frac{a}{1-x^{(t)}} = 0, \; \forall x, x^{(t)} \in (0, 1) \right\}$$

$$= \text{sol} \left\{ a_1^{(t)} x^2 + a_2^{(t)} x + a = 0, \; \forall x, x^{(t)} \in (0, 1) \right\},$$

where $a_1^{(t)} \triangleq F(x^{(t)}|\alpha, \beta) - p + a/x^{(t)} - a/(1-x^{(t)})$ and $a_2^{(t)} \triangleq -a_1^{(t)} - 2a$.

### 4.2 Calculation of exact $p$-values for skew null distributions

#### 4.2.1 The chi-squared null distribution

Let $\{X_i\}_{i=1}^n \overset{iid}{\sim} N(\mu, \sigma^2)$ with unknown $\{\mu, \sigma^2\}$ and we want to test $H_0$: $\sigma^2 = \sigma_0^2$ against $H_1$: $\sigma^2 \neq \sigma_0^2$. The test statistic is $\chi = \nu S^2/\sigma_0^2$ with corresponding observed value $\chi_{\text{obs}} \triangleq \nu s^2/\sigma_0^2$. 


where $S^2 = (1/\nu) \sum_{i=1}^{n} (X_i - \bar{X})^2$ is the sample variance, $s^2$ is its observed value and $\nu \equiv n-1$. Under $H_0$, we have $\chi \sim \chi^2(\nu)$, which is called chi-squared null distribution. We denote the pdf of $\chi^2(\nu)$ by $h_\nu(x) = [2^{\nu/2}\Gamma(\nu/2)]^{-1}x^{\nu/2-1}e^{-x/2}$ for $x > 0$, whose mode is $\nu - 2 \triangleq m_0$.

(a) Case I: $\chi_{\text{obs}} < m_0$

The exact $p$-value can be calculated as $p\text{-value} = \Pr\{\chi^2(\nu) \leq \chi_{\text{obs}}\} + \Pr\{\chi^2(\nu) \geq m_0\}$, where $x_u (> m_0)$ satisfies $h_\nu(x_u) = h_\nu(\chi_{\text{obs}})$; i.e., $m_0 \log(x_u) - x_u = m_0 \log(\chi_{\text{obs}}) - \chi_{\text{obs}} \triangleq c_0$. Thus, finding $x_u$ is equivalent to finding the root to the equation $g(x_u) = c_0 - m_0 \log(x_u) + x_u = 0$. Since $g'(x_u) = -m_0/x_u + 1 > -m_0/x_u \triangleq b(x_u)$, the US iteration for calculating $x_u$ is

$$x_u^{(t+1)} = \text{sol}\left\{g(x_u^{(t)}) + \int_{x_u^{(t)}}^{x_u} b(z) \, dz = 0, \forall x_u, x_u > m_0\right\}$$

$$= \text{sol}\left\{g(x_u^{(t)}) - m_0 \log(x_u) + m_0 \log(x_u^{(t)}) = 0, \forall x_u, x_u^{(t)} > m_0\right\}$$

$$= x_u^{(t)} \exp\left[g(x_u^{(t)})/m_0\right].$$

(b) Case II: $\chi_{\text{obs}} > m_0$

The exact $p$-value can be calculated as $p\text{-value} = \Pr\{\chi^2(\nu) \leq x_l\} + \Pr\{\chi^2(\nu) \geq \chi_{\text{obs}}\}$, where $x_l \in (0, m_0)$ satisfies $h_\nu(x_l) = h_\nu(\chi_{\text{obs}})$; i.e., $m_0 \log(x_l) - x_l = m_0 \log(\chi_{\text{obs}}) - \chi_{\text{obs}} \triangleq c_0$. Thus, finding $x_l$ is equivalent to finding the root to the equation $g(x_l) = m_0 \log(x_l) - x_l - c_0 = 0$. Since $g'(x_l) = m_0/x_l - 1 > -1 \triangleq b(x_l)$, the US iteration for calculating $x_l$ is

$$x_l^{(t+1)} = \text{sol}\left\{g(x_l^{(t)}) + \int_{x_l^{(t)}}^{x_l} b(z) \, dz = 0, \forall x_l, x_l^{(t)} \in (0, m_0)\right\}$$

$$= \text{sol}\left\{g(x_l^{(t)}) - x_l + x_l^{(t)} = 0, \forall x_l, x_l^{(t)} \in (0, m_0)\right\}$$

$$= g(x_l^{(t)}) + x_l^{(t)} = m_0 \log(x_l^{(t)}/\chi_{\text{obs}}) + \chi_{\text{obs}}.$$

4.2.2 The $F$ null distribution

Let $\{X_{ij}\}_{j=1}^{n_i} \overset{\text{iid}}{\sim} N(\mu_i, \sigma_i^2)$ for $i = 1, 2$, and the two random samples be independent, where $\{\mu_i, \sigma_i^2\}$ are unknown. We want to test $H_0$: $\sigma_1^2 = \sigma_2^2$ against $H_1$: $\sigma_1^2 \neq \sigma_2^2$, and the test statistic is $F = S_1^2/S_2^2$ with corresponding observed value $F_{\text{obs}} \triangleq s_1^2/s_2^2$, where $S_i^2$ is the $i$-th
sample variance, \( s_i^2 \) is its observed value and \( \nu_i \triangleq n_i - 1 \). Under \( H_0 \), we have \( F \sim F(\nu_1, \nu_2) \), which is called \( F \) null distribution. We denote the pdf of \( F(\nu_1, \nu_2) \) by

\[
h_{\nu_1, \nu_2}(x) = \frac{\Gamma(\nu_1/2)\nu^{\nu_1/2}}{\Gamma(\nu_2/2)} x^{\nu_1/2-1}(1+\nu x)^{-\nu_1/2}, \quad x > 0, \quad \nu \triangleq \frac{\nu_1}{\nu_2}, \quad \nu_{12} \triangleq \nu_1 + \nu_2.
\]

The mode of \( h_{\nu_1, \nu_2}(x) \) is \( m_1\nu_2/[\nu_1(\nu_2 + 2)] \triangleq m_0 \), where \( m_1 \triangleq \nu_1 - 2 \).

(a) Case I: \( F_{\text{obs}} < m_0 \)

The exact \( p \)-value can be calculated as \( p \)-value = \( \Pr\{F(\nu_1, \nu_2) \leq F_{\text{obs}}\} + \Pr\{F(\nu_1, \nu_2) > x_u\} \), where \( x_u (> m_0) \) satisfies \( h_{\nu_1, \nu_2}(x_u) = h_{\nu_1, \nu_2}(F_{\text{obs}}) \); i.e., \( m_1 \log(x_u) - \nu_{12} \log(1 + \nu x_u) = m_1 \log(F_{\text{obs}}) - \nu_{12} \log(1 + \nu F_{\text{obs}}) \triangleq c_0 \). Thus, finding \( x_u \) is equivalent to finding the root to the equation \( g(x_u) = c_0 - m_1 \log(x_u) + \nu_{12} \log(1 + \nu x_u) = 0 \). Since \( g'(x_u) = -m_1/x_u + \nu_{12} \nu/(1 + \nu x_u) > -m_1/x_u \triangleq b(x_u) \), the US iteration for calculating \( x_u \) is

\[
x_u^{(t+1)} = \text{sol} \left\{ g\left(x_u^{(t)}\right) + \int_{x_u^{(t)}}^{x_u} b(z) \, dz = 0, \ \forall \ x_u, x_u^{(t)} > m_0 \right\}
\]

\[
= \text{sol} \left\{ g\left(x_u^{(t)}\right) - m_1 \log(x_u) + m_1 \log\left(x_u^{(t)}\right) = 0, \ \forall \ x_u, x_u^{(t)} > m_0 \right\}
\]

\[
= x_u^{(t)} \exp\left[g\left(x_u^{(t)}\right)/m_1\right].
\]

(b) Case II: \( F_{\text{obs}} > m_0 \)

The exact \( p \)-value can be calculated as \( p \)-value = \( \Pr\{F(\nu_1, \nu_2) \leq x_l\} + \Pr\{F(\nu_1, \nu_2) > F_{\text{obs}}\} \), where \( x_l \in (0, m_0) \) satisfies \( h_{\nu_1, \nu_2}(x_l) = h_{\nu_1, \nu_2}(F_{\text{obs}}) \); i.e., \( m_1 \log(x_l) - \nu_{12} \log(1 + \nu x_l) = m_1 \log(F_{\text{obs}}) - \nu_{12} \log(1 + \nu F_{\text{obs}}) \triangleq c_0 \). Thus, finding \( x_l \) is equivalent to finding the root to the equation \( g(x_l) = m_1 \log(x_l) - \nu_{12} \log(1 + \nu x_l) - c_0 = 0 \). Since \( g'(x_l) = m_1/x_l - \nu_{12} \nu/(1 + \nu x_l) > m_1/x_l - \nu_{12}/x_l = -(2 + \nu_2)/x_l \triangleq b(x_l) \), the US iteration for calculating \( x_l \) is

\[
x_l^{(t+1)} = \text{sol} \left\{ g\left(x_l^{(t)}\right) + \int_{x_l^{(t)}}^{x_l} b(z) \, dz = 0, \ \forall \ x_l, x_l^{(t)} \in (0, m_0) \right\}
\]

\[
= \text{sol} \left\{ g\left(x_l^{(t)}\right) - (2 + \nu_2) \log(x_l/x_l^{(t)}) = 0, \ \forall \ x_l, x_l^{(t)} \in (0, m_0) \right\}
\]

\[
= x_l^{(t)} \exp\left[g\left(x_l^{(t)}\right)/(2 + \nu_2)\right].
\]
4.3 MLEs of parameters in a class of continuous distributions

4.3.1 MLE of $\alpha$ in gamma distribution

Let $\{X_i\}_{i=1}^n \sim \text{Gamma}(\alpha, \beta)$ with pdf 
\[ f(x) = \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)}, \quad x > 0, \]
where $\{\alpha, \beta\}$ are two positive parameters. The log-likelihood function
\[ \ell(\alpha, \beta) = nG(x) + n\log(\beta) - n\psi(\alpha), \]
where $G(x) = \frac{1}{n} \sum_{i=1}^n \log(x_i)$ and $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$. Let
\[ 0 = \frac{\partial \ell(\alpha, \beta)}{\partial \alpha} = nG(x) - n\psi(\alpha), \quad (4.9) \]
\[ 0 = \frac{\partial \ell(\alpha, \beta)}{\partial \beta} = -n\bar{x} + \frac{n\alpha}{\beta}. \quad (4.10) \]

Given $\alpha$, from (4.10), we have $\beta = \frac{\alpha}{\bar{x}}$. Given $\beta$, from (4.9), the MLE of $\alpha$ is the root of the equation:
\[ g(\alpha) = c_0 - \psi(\alpha) = 0 \quad \text{for} \quad \alpha > 0, \]
where $c_0 \triangleq G(x) + \log(\beta)$ is a known constant, $\psi(\cdot)$ is the digamma function defined as
\[ \psi(\alpha) \triangleq \frac{\Gamma'(\alpha)}{\Gamma(\alpha)} = -\gamma + \sum_{m=0}^{\infty} \left( \frac{1}{m+1} - \frac{1}{m+\alpha} \right) \quad (4.11) \]
here $\gamma = \lim_{n \to \infty} (\sum_{m=1}^n m^{-1} - \log n) \approx 0.5772$ is the Euler–Mascheroni constant. Since
\[ g'(\alpha) = -\psi'(\alpha) = -\sum_{m=0}^{\infty} \frac{1}{(m+\alpha)^2} = -\frac{1}{\alpha^2} - \sum_{m=1}^{\infty} \frac{1}{(m+\alpha)^2} > -\frac{1}{\alpha^2} - \sum_{m=1}^{\infty} \frac{1}{m^2} = -\frac{1}{\alpha^2} - \frac{\pi^2}{6} \triangleq b(\alpha), \]
the US iteration for calculating the MLE $\hat{\alpha}$ is
\[ \alpha^{(t+1)} = \text{sol} \left\{ g(\alpha^{(t)}) + \int_{\alpha^{(t)}}^\alpha b(z) \, dz = 0, \quad \forall \alpha, \alpha^{(t)} > 0 \right\} \]
\[ = \text{sol} \left\{ g(\alpha^{(t)}) + \frac{1}{\alpha} - \frac{\pi^2}{6} \alpha - \frac{1}{\alpha^{(t)}} + \frac{\pi^2}{6} \alpha^{(t)} = 0, \quad \forall \alpha, \alpha^{(t)} > 0 \right\} \]
\[ = \text{sol} \left\{ \left( \frac{\pi^2}{6} \right) \alpha^2 - a_3^{(t)} \alpha - 1 = 0, \quad \forall \alpha, \alpha^{(t)} > 0 \right\}, \]
where $a_3^{(t)} = c_0 - \psi(\alpha^{(t)}) + \left( \frac{\pi^2}{6} \right) \alpha^{(t)} - 1/\alpha^{(t)}$.

4.3.2 MLE of $\theta$ in Weibull distribution

Let $\{X_i\}_{i=1}^n \sim \text{Weibull}(\theta, \lambda)$ with pdf 
\[ f(x) = \frac{\theta}{\lambda} \left( \frac{x}{\lambda} \right)^{\theta-1} \exp\left[ -\left( \frac{x}{\lambda} \right)^\theta \right], \quad x > 0, \]
where $\{\theta, \lambda\}$ are two positive parameters (Hallinan 1993, Rinne 2008). The log-likelihood function is
\[ \ell(\theta, \lambda) = n \log(\theta) - n \theta \log(\lambda) + n G(\mathbf{x})(\theta - 1) - \sum_{i=1}^{n} (x_i / \lambda)^{\theta}, \]

where \( G(\mathbf{x}) \triangleq (1/n) \sum_{i=1}^{n} \log(x_i). \)

Let \( 0 = \partial \ell(\theta, \lambda) / \partial \lambda = -n \theta \lambda^{-1} + \theta \lambda^{-\theta - 1} \sum_{i=1}^{n} x_i^{\theta}. \) Given \( \theta, \)

Replacing \( \lambda \) in \( \ell(\theta, \lambda) \) by \( [(1/n) \sum_{i=1}^{n} x_i^{\theta}]^{1/\theta}, \) we know that \( \ell(\theta, \lambda) \) will reduce to \( \ell(\theta) = \theta n G(\mathbf{x}) + n \log(\theta) - n \log(\sum_{i=1}^{n} x_i^{\theta}) + \text{constant}. \) Thus, the MLE of \( \theta \) is the root of \( \ell'(\theta) = 0 \)

or the root of the equation

\[ g(\theta) = G(\mathbf{x}) + \frac{1}{\theta} - \frac{\sum_{i=1}^{n} x_i^{\theta} \log(x_i)}{\sum_{i=1}^{n} x_i^{\theta}} = 0, \quad \theta > 0. \]

Since

\[
\begin{align*}
  g'(\theta) &= -\frac{1}{\theta^2} - \frac{[\sum_{i=1}^{n} x_i^{\theta}(\log x_i)]^2 [\sum_{i=1}^{n} x_i^{\theta}] - (\sum_{i=1}^{n} x_i^{\theta} \log x_i)^2}{(\sum_{i=1}^{n} x_i^{\theta})^2} \\
  &\geq -\frac{1}{\theta^2} - \frac{[\sum_{i=1}^{n} x_i^{\theta}(\log x_i)]^2}{\sum_{i=1}^{n} x_i^{\theta}} \\
  &\geq -\frac{1}{\theta^2} - \max_{1 \leq i \leq n} (\log x_i)^2 \triangleq -\frac{1}{\theta^2} - T_{\max} \triangleq b(\theta),
\end{align*}
\]

the US iteration for calculating the MLE \( \hat{\theta} \) is

\[ \theta^{(t+1)} \overset{3.2}{=} \operatorname{sol} \left\{ g(\theta^{(t)}) + \int_{\theta^{(t)}}^{\theta} b(z) \, dz = 0, \forall \theta, \theta^{(t)} > 0 \right\} \]

\[ = \operatorname{sol} \left\{ g(\theta^{(t)}) + \frac{1}{\theta} - T_{\max} \theta - \frac{1}{\theta^{(t)}} + T_{\max} \theta^{(t)} = 0, \forall \theta, \theta^{(t)} > 0 \right\} \]

\[ = \operatorname{sol} \left\{ T_{\max} \theta^{2} - a_{4}^{(t)} \theta - 1 = 0, \forall \theta, \theta^{(t)} > 0 \right\}, \]

where \( a_{4}^{(t)} \triangleq g(\theta^{(t)}) + T_{\max} \theta^{(t)} - 1/\theta^{(t)}. \)

### 4.4 MLEs of parameters in a class of discrete distributions

#### 4.4.1 MLE of \( \theta \) in zeta distribution

The zeta (or Zipf) distribution can be used to model the frequency of occurrence of a word randomly chosen from a text, or the population rank of a city randomly chosen from a country. Let \( \{X_i\}_{i=1}^{n} \overset{\text{iid}}{\sim} \text{Zeta}(\theta) \) with pmf \( Z^{-1}(\theta) x^{-\theta}, x = 1, 2, \ldots, \infty, \) where \( \theta (> 1) \) is a parameter and \( Z(\theta) = \sum_{x=1}^{\infty} x^{-\theta} \) is called Riemann’s zeta function (Nair et al. 2018, p.131–134). The log-likelihood is \( \ell(\theta) = -nG(\mathbf{x})\theta - n \log Z(\theta), \) where \( G(\mathbf{x}) \triangleq (1/n) \sum_{i=1}^{n} \log(x_i). \)
Let \( 0 = \ell'(\theta) = -nG(x) - nZ'(\theta)/Z(\theta) \), then the MLE of \( \theta \) is the root of the equation:
\[
g(\theta) = -G(x) - Z'(\theta)/Z(\theta) = 0 \quad \text{for} \quad \theta > 1.
\]
Note that
\[
g'(\theta) = -\frac{Z''(\theta)Z(\theta) - [Z'(\theta)]^2}{Z^2(\theta)} \geq -\frac{Z''(\theta)}{Z(\theta)} \Leftrightarrow a_5 - \frac{a_6}{(\theta - 1)^2} \triangleq b(\theta),
\]
where \( a_5 \triangleq -\log 2 \cdot (\log 2 + 2) \) and \( a_6 \triangleq 2 \log 2 + 2 \), then the US iteration for calculating the MLE \( \hat{\theta} \) is given by
\[
\theta^{(t+1)} \triangleq \text{sol } \left\{ g(\theta^{(t)}) + \int_{\theta^{(t)}}^\theta b(z) \, dz = 0, \ \forall \ \theta, \theta^{(t)} > 1 \right\}
\]
\[
\begin{align*}
&= \text{sol } \left\{ g(\theta^{(t)}) + a_5(\theta - \theta^{(t)}) + \frac{a_6}{\theta - 1} - \frac{a_6}{\theta^{(t)} - 1} = 0, \ \forall \ \theta, \theta^{(t)} > 1 \right\} \\
&= \text{sol } \left\{ a_5\theta^2 + a_7^t \theta + a_8^t = 0, \ \forall \ \theta, \theta^{(t)} > 1 \right\},
\end{align*}
\]
where \( a_7^t \triangleq g(\theta^{(t)}) - a_5(\theta^{(t)} + 1) - a_6/(\theta^{(t)} - 1) \) and \( a_8^t \triangleq -g(\theta^{(t)}) + a_5\theta^{(t)} + a_6\theta^{(t)}/(\theta^{(t)} - 1) \).

### 4.4.2 MLE of \( \theta \) in Yule–Simon distribution

The Yule–Simon distribution (Yule 1925, Garcia 2011) can be employed to model species among genera, words frequencies in texts, numbers of papers published by researchers, cities by population, income by size (Leisen, Rossini & Villa 2017). Let \( \{X_i\}_{i=1}^n \overset{iid}{\sim} \text{YS}(\theta) \) with pmf \( \theta \text{ Beta}(x, \theta + 1), \ x = 1, 2, \ldots, \infty \), where \( \theta > 0 \) is the shape parameter. The log-likelihood function is \( \ell(\theta) = n \log(\theta) + n \log \Gamma(\theta + 1) - \sum_{i=1}^n \log \Gamma(x_i + \theta + 1) + \text{constant} \). Thus, the MLE of \( \theta \) is the root of the following equation:
\[
0 = \ell'(\theta) = \frac{n}{\theta} + \sum_{i=1}^n \left[ \psi(\theta + 1) - \psi(x_i + \theta + 1) \right]
\]
\[
\begin{align*}
&= \frac{n}{\theta} + \sum_{i=1}^n \left( -\sum_{m=0}^{\infty} \frac{1}{m + \theta + 1} + \sum_{m=0}^{\infty} \frac{1}{m + x_i + \theta + 1} \right) \quad \text{[Let } m + x_i = k] \\
&= \frac{n}{\theta} + \sum_{i=1}^n \left( -\sum_{m=0}^{\infty} \frac{1}{m + \theta + 1} + \sum_{k=x_i}^{\infty} \frac{1}{k + \theta + 1} \right) \\
&= \frac{n}{\theta} + \sum_{i=1}^n \left( -\sum_{m=0}^{x_i-1} \frac{1}{m + \theta + 1} \right) \triangleq g(\theta).
\end{align*}
\]
Since

\[ g'(\theta) = -\frac{n}{\theta^2} + \sum_{i=1}^{n} \left[ \sum_{m=0}^{x_i-1} \frac{1}{(m + \theta + 1)^2} \right] \]

\[ = -\frac{n}{\theta^2} + \sum_{i=1}^{n} \left[ \frac{1}{(\theta + 1)^2} + I(x_i \geq 2) \sum_{m=0}^{x_i-1} \frac{1}{(m + \theta + 1)^2} \right] \geq -\frac{n}{\theta^2} + \frac{n}{(\theta + 1)^2} \triangleq b(\theta), \]

the US iteration for calculating the MLE \( \hat{\theta} \) is

\[ \theta^{(t+1)} = \text{sol} \left\{ g(\theta^{(t)}) + \int_{\theta^{(t)}}^{\theta} b(z) \, dz = 0, \forall \theta, \theta^{(t)} > 0 \right\} \]

\[ = \text{sol} \left\{ g(\theta^{(t)}) + \frac{n}{\theta} - \frac{n}{\theta + 1} - \frac{n}{\theta^{(t)}} + \frac{n}{\theta^{(t)} + 1} = 0, \forall \theta, \theta^{(t)} > 0 \right\} \]

\[ = \text{sol} \left\{ a_9^{(t)} \theta^2 + a_9^{(t)} \theta + n = 0, \forall \theta, \theta^{(t)} > 0 \right\}, \]

where \( a_9^{(t)} \triangleq g(\theta^{(t)}) - n/\theta^{(t)} + n/(\theta^{(t)} + 1) \).

### 4.4.3 MLE of \( \alpha \) in Gamma–Poisson distribution

Let \( \{X_i\}_{i=1}^{n} \overset{iid}{\sim} \text{GPoission}(\alpha, \beta) \) with pmf \( \Gamma(x + \alpha)\Gamma^{-1}(\alpha)\beta^{-x-\alpha}/x! \), \( x = 0, 1, 2, \ldots, \infty \), where \( \alpha \) and \( \beta \) are two positive parameters (Arbous & Kerrich 1951, Bates & Neyman 1952).

Define \( \bar{x} = (1/n) \sum_{i=1}^{n} x_i \), the log-likelihood function is

\[ \ell(\alpha, \beta) = \sum_{i=1}^{n} \log \Gamma(x_i + \alpha) - n \log \Gamma(\alpha) + n \alpha \log(\beta) - n(\alpha + \bar{x}) \log(\beta + 1) + \text{constant}. \]

Let \( 0 = \partial \ell(\alpha, \beta)/\partial \beta = n\alpha/\beta - n(\alpha + \bar{x})/(\beta + 1) \), we obtain \( \beta = \alpha/\bar{x} \). Replacing \( \beta \) in \( \ell(\alpha, \beta) \) by \( \alpha/\bar{x} \), we know that \( \ell(\alpha, \beta) \) becomes

\[ \ell(\alpha) = \sum_{i=1}^{n} \log \Gamma(x_i + \alpha) - n \log \Gamma(\alpha) + n \alpha \log \alpha - n(\alpha + \bar{x}) \log(\alpha + \bar{x}) + \text{constant}. \]

Thus, the MLE of \( \alpha \) is the root of the following equation:

\[ 0 = \ell'(\alpha) = \sum_{i=1}^{n} [\psi(x_i + \alpha) - \psi(\alpha)] + n \log \alpha - n \log(\alpha + \bar{x}) \]
\[ \sum_{i=1}^{n} \left[ -\sum_{m=0}^{\infty} \frac{1}{m + x_i + \alpha} + \sum_{m=0}^{\infty} \frac{1}{m + \alpha} \right] + n \log \alpha - n \log(\alpha + \bar{x}) \]

\[ = \sum_{i=1}^{n} \left[ -\sum_{m=0}^{\infty} \frac{1}{m + \alpha} + \sum_{m=0}^{\infty} \frac{1}{m + \alpha} \right] + n \log \alpha - n \log(\alpha + \bar{x}) \]

\[ = \sum_{i=1}^{n} \left[ I(x_i \geq 1) \sum_{m=0}^{x_i-1} \frac{1}{m + \alpha} \right] + n \log \alpha - n \log(\alpha + \bar{x}) \triangleq g(\alpha). \]

Since

\[ g'(\alpha) = \sum_{i=1}^{n} \left[ -I(x_i \geq 1) \sum_{m=0}^{x_i-1} \frac{1}{(m + \alpha)^2} \right] + \frac{n}{\alpha} - \frac{n}{\alpha + \bar{x}} \]

\[ \geq -\sum_{i=1}^{n} \left[ I(x_i \geq 2) \sum_{m=1}^{x_i-1} \frac{1}{m^2} \right] - \frac{1}{\alpha^2} \sum_{i=1}^{n} I(x_i \geq 1) + \frac{n\bar{x}}{\alpha(\alpha + \bar{x})} \]

\[ \geq a_{10} + a_{11}/\alpha^2 \triangleq b(\alpha), \]

where \( a_{10} \triangleq -\sum_{i=1}^{n} \left[ I(x_i \geq 2) \sum_{m=1}^{x_i-1} m^{-2} \right] \) and \( a_{11} \triangleq -\sum_{i=1}^{n} I(x_i \geq 1) \), the US iteration for calculating the MLE \( \hat{\theta} \) is

\[ \alpha^{(t+1)} \triangleq \text{sol} \left\{ g(\alpha^{(t)}) + \int_{\alpha^{(t)}}^{\alpha} b(z) \, dz = 0, \, \forall \, \alpha, \alpha^{(t)} > 0 \right\} \]

\[ = \text{sol} \left\{ g(\alpha^{(t)}) + a_{10}(\alpha - \alpha^{(t)}) - a_{11}/\alpha + a_{11}/\alpha^{(t)} = 0, \, \forall \, \alpha, \alpha^{(t)} > 0 \right\} \]

\[ = \text{sol} \left\{ a_{10}\alpha^2 + a_{12}\alpha - a_{11} = 0, \, \forall \, \alpha, \alpha^{(t)} > 0 \right\}, \]

where \( a_{12} \triangleq g(\alpha^{(t)}) - a_{10}\alpha^{(t)} + a_{11}/\alpha^{(t)}. \)

### 4.4.4 MLE of \( \theta \) in Generalized Poisson distribution

Let \( \{X_i\}_{i=1}^{n} \overset{\text{iid}}{\sim} \text{GP}(\lambda, \theta) \) with pmf \( \lambda(\lambda + \theta x)^{x-1}e^{-\lambda-\theta x}/x! \), \( x = 0, 1, 2, \ldots, \infty \), where \( \lambda > 0 \) and \( \max(-1, -\lambda/r) < \theta \leq 1 \) are two parameters and \( r (\geq 4) \) is the largest positive integer for which \( \lambda + \theta r > 0 \) when \( \theta < 0 \) (Consul & Jain 1973, Consul & Famoye 1989). The log-likelihood is \( \ell(\lambda, \theta) = \sum_{i=1}^{n} \log \lambda + (x_i - 1) \log(\lambda + \theta x_i) - \lambda - \theta x_i \) + constant. There is an MM algorithm for calculating the MLE of \( \theta \) for the case of \( \theta \in [0, 1] \), while, to the best of our knowledge, there is no efficient algorithm to calculate \( \hat{\theta} \) for the case of \( \theta < 0 \). In this
subsection, we only consider the case of $\theta < 0$. Let

$$0 = \frac{\partial \ell(\lambda, \theta)}{\partial \lambda} = \frac{n}{\lambda} + \sum_{i=1}^{n} \frac{x_i - 1}{\lambda + \theta x_i} - n \quad \text{and}$$

$$0 = \frac{\partial \ell(\lambda, \theta)}{\partial \theta} = \sum_{i=1}^{n} \frac{(x_i - 1)x_i}{\lambda + \theta x_i} - n \bar{x}. \quad (4.13)$$

By multiplying $\lambda$ and $\theta$ to the two partial differential equations \((4.12)\) and \((4.13)\), respectively, and then adding them together, we obtain $\lambda = (1 - \theta)\bar{x}$. Replacing $\lambda$ in $\ell(\lambda, \theta)$ by $(1 - \theta)\bar{x}$, we know that $\ell(\lambda, \theta)$ will reduce to $\ell(\theta) = n \log(1 - \theta) + \sum_{i=1}^{n} \{(x_i - 1) \log[\bar{x} + (x_i - \bar{x})\theta]\}$ + constant. Thus, the MLE of $\theta$ is the root of the following equation:

$$0 = \ell'(\theta) = -\frac{n}{1-\theta} + \sum_{i=1}^{n} \frac{(x_i - 1)(x_i - \bar{x})}{\bar{x} + (x_i - \bar{x})\theta} \triangleq g(\theta).$$

Since

$$g'(\theta) = -\frac{n}{(1-\theta)^2} - \sum_{i=1}^{n} \frac{(x_i - 1)(x_i - \bar{x})^2}{[\bar{x} + (x_i - \bar{x})\theta]^2} \geq -\frac{n}{(1-\theta)^2} - \sum_{i=1}^{n} \frac{x_i(x_i - \bar{x})^2}{[\bar{x}(1-\theta) + x_i\theta]^2}$$

$$= -\frac{n}{(1-\theta)^2} - \frac{\sum_{i=1}^{n} [x_i(x_i - \bar{x})^2/(x_{(n)} - \bar{x})^2]}{[\bar{x}/(x_{(n)} - \bar{x}) + \theta]^2} \triangleq -\frac{n}{(1-\theta)^2} - \frac{a_{13}}{(a_{14} + \theta)^2} \triangleq b(\theta),$$

where $x_{(n)} \triangleq \max(x_1, \ldots, x_n)$, $a_{13} \triangleq \sum_{i=1}^{n} [x_i(x_i - \bar{x})^2/(x_{(n)} - \bar{x})^2]$, and $a_{14} \triangleq \bar{x}/(x_{(n)} - \bar{x})$, the US iteration for calculating the MLE $\hat{\theta}$ is

$$\theta^{(t+1)} \overset{\text{sol}}{=} \begin{cases} \theta^{(t)} + \int_{\theta^{(t)}}^{\theta} b(z) \, dz = 0, \forall \theta, \theta^{(t)} < 0 \end{cases}$$

$$= \begin{cases} \theta^{(t)} - \frac{n}{1-\theta} + \frac{a_{13}}{a_{14} + \theta} + \frac{n}{(1-\theta^{(t)})} - \frac{a_{13}}{a_{14} + \theta^{(t)}} = 0, \forall \theta, \theta^{(t)} < 0 \end{cases}$$

$$= \begin{cases} a_{15}^{(t)} \theta^2 - a_{16}^{(t)} \theta + (n - a_{15}^{(t)})a_{14} - a_{13} = 0, \forall \theta, \theta^{(t)} < 0 \end{cases},$$

where $a_{15}^{(t)} \triangleq g(\theta^{(t)}) + n/(1 - \theta^{(t)}) - a_{13}/(a_{14} + \theta^{(t)})$ and $a_{16}^{(t)} \triangleq a_{15}^{(t)}(1 - a_{14}) - n - a_{13}.$
5. Analysis of the convergence rate

Let $\theta^*$ be the unique root of the equation $g(\theta) = 0$ for all $\theta \in \Theta$. To get the rate of convergence for the US iteration $\theta^{(t+1)} \triangleq h(\theta^{(t)})$, we consider the first-order Taylor expansion of $h(\theta^{(t)})$ around $\theta^*$: $h(\theta^{(t)}) = h(\theta^*) + (\theta^{(t)} - \theta^*)h'(\theta^*) + 0.5(\theta^{(t)} - \theta^*)^2 h''(\tilde{\theta})$, where $\tilde{\theta}$ is a point between $\theta^{(t)}$ and $\theta^*$. The convergence rate of the US algorithm is defined by

$$\lim_{t \to \infty} \frac{|\theta^{(t+1)} - \theta^*|}{|\theta^{(t)} - \theta^*|} = \lim_{t \to \infty} \frac{|h(\theta^{(t)}) - h(\theta^*)|}{|\theta^{(t)} - \theta^*|}$$

$$= \lim_{t \to \infty} |h'(\theta^*) + 0.5(\theta^{(t)} - \theta^*)h''(\tilde{\theta})| = |h'(\theta^*)|.$$

If $|h'(\theta^*)| \in (0, 1)$, then the US algorithm has a linear convergence rate.

In this section, we investigate the convergence rate of the US algorithm for the three methods of constructing $U$-functions presented in Section 3. Theorem 2 below states that the US algorithm holds a linear convergence rate, just like the EM and MM algorithms with monotonic convergence and linear convergence rate in maximization of an objective function. Theorems 3–4 below show that the US algorithm holds a quadratic and even a cubic convergence rates, corresponding to the SLUB constants method and the TLB constant method.

**Theorem 2** (Linear convergence rate for the FLB function method). Let the FLB function $b(\theta)$ be defined by (3.1), and the $U$-function $U(\theta|\theta^{(t)})$ be given by (3.2). Then the US iteration

$$\theta^{(t+1)} = \text{sol} \left\{ U(\theta|\theta^{(t)}) = g(\theta^{(t)}) + \int_{\theta^{(t)}}^{\theta} b(z) \, dz = 0, \forall \theta, \theta^{(t)} \in \Theta \right\} \triangleq h(\theta^{(t)})$$

holds a linear convergence rate given by

$$\lim_{t \to \infty} \frac{|\theta^{(t+1)} - \theta^*|}{|\theta^{(t)} - \theta^*|} = |h'(\theta^*)| = \left| 1 - \frac{g'(\theta^*)}{b(\theta^*)} \right| \in (0, 1).$$

**Theorem 3** (Quadratic convergence rate for the SLUB constants method). Let two SLUB constants $\{b_{21}, b_{22}\}$ be defined by (3.8), and the $U$-function $U(\theta|\theta^{(t)})$ be given by (3.10).
Then the US iteration
\[ \theta^{(t+1)} = \text{sol} \left\{ g(\theta^{(t)}) + g'(\theta^{(t)}) (\theta - \theta^{(t)}) + \frac{b_2(\theta^{(t)})}{2} (\theta - \theta^{(t)})^2 = 0, \quad \forall \theta, \theta^{(t)} \in \Theta \right\} \]
\[ \triangleq h(\theta^{(t)}) \] (5.3)
has a quadratic convergence rate given by
\[ \lim_{t \to \infty} \frac{|\theta^{(t+1)} - \theta^*|}{|\theta^{(t)} - \theta^*|^2} = \frac{|h''(\theta^*)|}{2} = \frac{|b_{22} - g''(\theta^*)|}{2g'(\theta^*)} \in (0, \infty). \] (5.4)

**Theorem 4 (Cubic convergence rate for the TLB constant method).** Let the TLB constant \( b_3 \) be defined by (3.11), and the \( U \)-function \( U(\theta|\theta^{(t)}) \) be given by (3.12). Then the US iteration
\[ \theta^{(t+1)} = \text{sol} \left\{ g(\theta^{(t)}) + g'(\theta^{(t)}) (\theta - \theta^{(t)}) + g''(\theta^{(t)}) (\theta - \theta^{(t)})^2 + \frac{b_3}{6} (\theta - \theta^{(t)})^3 = 0, \right\}
\[ \forall \theta, \theta^{(t)} \in \Theta \] \[ \triangleq h(\theta^{(t)}) \] (5.5)
has a cubic convergence rate given by
\[ \lim_{t \to \infty} \frac{|\theta^{(t+1)} - \theta^*|}{|\theta^{(t)} - \theta^*|^3} = \frac{|h'''(\theta^*)|}{6} = \frac{|b_3 - g'''(\theta^*)|}{6g'(\theta^*)} \in (0, \infty). \] (5.6)

6. Numerical experiments

To compare the proposed US algorithm with Newton’s method and bisection method by using numerical experiments, we consider two root-finding problems: Roots of a high-order polynomial equation and the \( p \)-th quantile of a normal distribution.

6.1 Root of a high-order polynomial equation

Assume that there exists a unique real root for the following polynomial equation in \((0, a)\):
\[ 0 = g(\theta) \triangleq a_3 \theta^m + a_2 \theta^2 + a_1 \theta + a_0 \triangleq g_1(\theta) + a_2 \theta^2 + a_1 \theta + a_0, \quad \theta \in (0, a), \] (6.1)
where $m \geq 3$ is a real number (unnecessary positive integer) and $a_0 > 0$. Based on

\[
g''_1(\theta) = a_3m(m-1)\theta^{m-2} \in (a_3m(m-1)a^{m-2}, 0), \quad \text{if } a_3 < 0,
\]

\[
g''_2(\theta) = a_3m(m-1)(m-2)\theta^{m-3} > 0, \quad \text{if } a_3 > 0,
\]

and Property 1(c), we can construct the following two quadratic $U$-functions:

\[
U_2(\theta|\theta^{(t)}) = a_3[\theta^{(t)}]^m + a_3m[\theta^{(t)}]^{m-1}(\theta - \theta^{(t)}) + 0.5b_2(\theta|\theta^{(t)})(\theta - \theta^{(t)})^2
\]

\[
+ a_2\theta^2 + a_1\theta + a_0
\]

\[
= \left[ 0.5b_2(\theta|\theta^{(t)}) + a_2 \right] \theta^2 + \left\{ a_3m[\theta^{(t)}]^{m-1} - b_2(\theta|\theta^{(t)})\theta^{(t)} + a_1 \right\} \theta
\]

\[
+ a_3(1-m)[\theta^{(t)}]^m + 0.5b_2(\theta|\theta^{(t)})[\theta^{(t)}]^2 + a_0 \quad \text{and}
\]

\[
U_3(\theta|\theta^{(t)}) = a_3[\theta^{(t)}]^m + a_3m[\theta^{(t)}]^{m-1}(\theta - \theta^{(t)}) + 0.5a_3m(m-1)[\theta^{(t)}]^{m-2}(\theta - \theta^{(t)})^2
\]

\[
+ a_2\theta^2 + a_1\theta + a_0
\]

\[
= \left\{ 0.5a_3m(m-1)[\theta^{(t)}]^{m-2} + a_2 \right\} \theta^2 + \left\{ a_3m(2-m)[\theta^{(t)}]^{m-1} + a_1 \right\} \theta
\]

\[
+ a_3(m-1)(0.5m-1)[\theta^{(t)}]^m + a_0.
\]

where $b_2(\theta|\theta^{(t)}) = 0 \cdot I(\theta \leq \theta^{(t)}) + a_3m(m-1)a^{m-2} \cdot I(\theta > \theta^{(t)})$.

For the purpose of numerical experiments, we set \{0, 1, 2\} = \{1, -1, 1, -1, 3\} in (6.2), \{0, 1, 2\} = \{1, -1, 3, 1, 3\} in (6.3), and $a = 2$. We know that the unique root of (6.1) in the interval $(0, 2)$ is $\theta^* = 0.4608111$ and $\theta^* = 1$ for the two cases. We use three algorithms (i.e., the US algorithm, Newton's method and bisection method) to seek the root of (6.1) by running each algorithm for 100,000 repetitions with initial values randomly chosen from the uniform distribution on the interval $(0, 2)$. The percentage of converged algorithms among 100,000 repetitions (denoted by Percentage), the average number of iterations for converged algorithms among 100,000 repetitions (denoted by N), and the total computation time in second of calculating $\theta^*$ for 100,000 repetitions [denoted by Time(s)] are recorded and reported in Table 2.

From Table 2, we can see that all three algorithms have 100% convergence performance according to Percentage. The US algorithm and Newton's methods have similar performance
in terms of $N$ and $\text{Time(s)}$. The bisection method performs worst among the three for the two cases.

Table 2. Comparisons of three algorithms in terms of the percentage of converged algorithms, the average number of iterations, and the total computation time in second

| Coefficients | Algorithms | US$_2$ | Newton | Bisection | US$_3$ | Newton | Bisection |
|--------------|-----------|-------|--------|-----------|-------|--------|-----------|
| $\{a_0, a_1, a_2, a_3, m\} = \{1, -1, 1, -1, 3\}$ | Percentage | 100.0% | 100.0% | 100.0% | \{1, -1, -3, 1, 3\} | 100.0% | 100.0% | 100.0% |
| | N | 7.0000 | 6.3672 | 41.000 | 7.0000 | 6.3630 | 40.000 |
| | Time(s) | 1.6931 | 1.5313 | 10.255 | 1.6931 | 1.6206 | 10.184 |

Note: US$_2$ denotes the US algorithm based on $U_2(\theta|\theta(t))$ in (6.2); US$_3$ denotes the US algorithm based on $U_3(\theta|\theta(t))$ in (6.3); Percentage is the percentage of converged algorithms among 100,000 repetitions for different initial values randomly chosen from $U(0, 2)$; $N$ is the average number of iterations for converged algorithms among 100,000 repetitions; Time(s) is the total computation time in second of calculating $\theta^*$ for 100,000 repetitions.

### 6.2 Calculation of the $p$-th quantile of normal distribution

In Example 2 of subsection 4.1.1, we have applied the US algorithm to find the $p$-th quantile of the normal distribution $N(\mu, \sigma^2)$; i.e., to iteratively calculate the solution to the integral equation $0 = g(x) \triangleq p - \Phi(x|\mu, \sigma^2)$ with US iteration given by (4.4). Theorem 2 shows that the US iteration (4.4) only has a linear rate of convergence. To speed the convergence, we first derive the second–derivative to the fourth–derivative of $g(x)$ as follows:

\[
g''(x) = \frac{x - \mu}{\sigma^2} \phi(x|\mu, \sigma^2),
\]

\[
g'''(x) = \frac{1}{\sigma^2} \left[ 1 - \frac{(x - \mu)^2}{\sigma^2} \right] \phi(x|\mu, \sigma^2) \quad \text{and}
\]

\[
g^{(4)}(x) = -\frac{x - \mu}{\sigma^4} \left[ 3 - \frac{(x - \mu)^2}{\sigma^2} \right] \phi(x|\mu, \sigma^2).
\]

Note that there are three roots $\{\mu, \mu \pm \sqrt{3}\sigma\}$ for the equation $0 = g^{(4)}(x)$, then $g'''(x)$ achieves its minimum $-2(\sqrt{2\pi}\sigma^3 e^{3/2})^{-1}$ when $x = \mu \pm \sqrt{3}\sigma$. Similarly, since $\mu \pm \sigma$ are two roots of the equation $0 = g''(x)$, we know that $g''(x)$ achieves its minimum $-(\sqrt{2\pi}\sigma^2 e^{1/2})^{-1}$ and
maximum \((\sqrt{2\pi\sigma^2e^{1/2}})^{-1}\) when \(x = \mu - \sigma\) and \(\mu + \sigma\), respectively. Thus, we obtain

\[
g''(x) \in \left[-(\sqrt{2\pi\sigma^2e^{1/2}})^{-1}, \ (\sqrt{2\pi\sigma^2e^{1/2}})^{-1}\right] \quad \text{and} \quad g'''(x) \geq -2(\sqrt{2\pi\sigma^3e^{3/2}})^{-1}, \ \forall x \in \mathbb{R},
\]

so that we can construct the following two \(U\)-functions:

\[
U_2(x|x^{(t)}) = \frac{3}{10} g(x^{(t)}) + g'(x^{(t)})(x - x^{(t)}) + 0.5b_2(x|x^{(t)})(x - x^{(t)})^2 \quad \text{and} \quad (6.4)
\]

\[
U_3(x|x^{(t)}) = \frac{3}{12} g(x^{(t)}) + g'(x^{(t)})(x - x^{(t)}) + 0.5g''(x^{(t)})(x - x^{(t)})^2 - (3\sqrt{2\pi\sigma^3e^{3/2}})^{-1}(x - x^{(t)})^3, \quad (6.5)
\]

where \(b_2(x|x^{(t)}) = (\sqrt{2\pi\sigma^2e^{1/2}})^{-1} \times [I(x \leq x^{(t)}) - I(x > x^{(t)})]\).

In numerical experiments, we set \(p = 0.01, 0.9, \mu = -2, 2\) and \(\sigma = 1\). For each combination of the four cases of \(\{p, \mu\}\), we use four algorithms (i.e., two US algorithms based on (6.4) and (6.5), Newton’s method and bisection method) to seek the root of (6.1) by running each algorithm for 100,000 repetitions with initial values randomly chosen from \(U(-4, 4)\). The percentage of converged algorithms among 100,000 repetitions (denoted by Percentage), the average number of iterations for converged algorithms among 100,000 repetitions (denoted by \(N\)), and the total computation time in second of calculating \(x^*\) for 100,000 repetitions [denoted by \(\text{Time(s)}\)] are recorded and displayed in Table 3.

In Table 3, we can see that Newton’s method has the worst convergence performance according to Percentage. In terms of \(N\), the US_3 performs the best. In terms of \(\text{Time(s)}\), although Newton’s method only takes about 2 seconds for 100,000 repetitions for Case 1, we can see that there are only about 40% valid computations, hence we prefer US_2.

### 6.3 Solving an equation with multiple roots

Thanks for the strongly stable convergence, the US algorithm could be one of the powerful tools for solving an equation with multiple roots. For the purpose of illustration, we consider the following toy equation:

\[
0 = g(x) \triangleq -0.5x - 2\sin(x) + 1, \quad x \in \mathbb{R}. \quad (6.6)
\]
Table 3. Comparisons of four algorithms in terms of the percentage of converged algorithms, the average number of iterations, and the total computation time in second

| Parameters \( \{p, \mu\} = \{0.01, -2\} \) | Algorithms | US₂ | US₃ | Newton | Bisection | US₂ | US₃ | Newton | Bisection |
|---------------------------------------------|------------|-----|-----|--------|-----------|-----|-----|--------|-----------|
| Percentage                                 | 100.0%     | 100.0% | 39.98% | 100.0% | 39.98% | 100.0% | 100.0% | 55.40% | 100.0% |
| N                                          | 10.544     | 5.3599 | 6.6532 | 33.000 | 33.000 | 10.2855 | 5.0179 | 6.3664 | 36.000 |
| Time(s)                                    | 7.7039     | 14.560 | 2.2438 | 12.678 | 12.678 | 7.62123 | 14.026 | 2.4824 | 13.852 |

| Parameters \( \{p, \mu\} = \{0.9, -2\} \) | Algorithms | US₂ | US₃ | Newton | Bisection | US₂ | US₃ | Newton | Bisection |
|---------------------------------------------|------------|-----|-----|--------|-----------|-----|-----|--------|-----------|
| Percentage                                 | 100.0%     | 100.0% | 42.74% | 100.0% | 42.74% | 100.0% | 100.0% | 38.65% | 100.0% |
| N                                          | 5.9959     | 4.1400 | 5.0428 | 39.000 | 39.000 | 6.7453 | 4.5215 | 4.9311 | 40.000 |
| Time(s)                                    | 4.7217     | 10.066 | 2.0309 | 14.832 | 14.832 | 5.2619 | 10.515 | 1.9345 | 15.421 |

Note: US₂ denotes the US algorithm based on \( U_2(\theta|\theta(t)) \) in (6.4); US₃ denotes the US algorithm based on \( U_3(\theta|\theta(t)) \) in (6.5); Percentage is the percentage of converged algorithms among 100,000 repetitions for different initial values randomly chosen from \( U(-4, 4) \); N is the average number of iterations for converged algorithms among 100,000 repetitions; Time(s) is the total computation time in second of calculating \( x^* \) for 100,000 repetitions.

Figure 2(a) shows the equation (6.6) with three roots, denoted by \( x^*_1 < x^*_2 < x^*_3 \), respectively. First, based on the first–order derivative \( g'(x) = -0.5 - 2 \cos(x) \geq -2.5 \), we can construct the first \( U \)-function for \( g(x) \) at \( x = x^{(t)} \) and obtain the corresponding US iterations as follows:

\[
U_{1,1}(x|x^{(t)}) \overset{3.5}{=} g(x^{(t)}) - 2.5(x - x^{(t)}) \quad \text{and} \quad x^{(t+1)} = x^{(t)} + \frac{g(x^{(t)})}{2.5} = x^{(t)} + \frac{-0.5x^{(t)} - 2 \sin(x^{(t)}) + 1}{2.5}. \tag{6.7}
\]

Given an initial value \( x^{(0)} \) (< \( x^*_1 \)), say \( x^{(0)} = 0 \), the US iterations \( \{x^{(t+1)}\}_{t=0}^\infty \) defined by (6.7) converged to the first root \( x^*_1 = 0.4090497 \) as shown in Figure 2(b1).

Second, once we obtained \( x^*_1 \), we define a new function

\[
g_2(x) \overset{\Delta}{=} -g(x) = 0.5x + 2 \sin(x) - 1, \quad x \in \mathbb{R}.
\]

Based on the first–order derivative \( g_2'(x) = 0.5 + 2 \cos(x) \geq -1.5 \), we can construct the second
$U$-function for $g_2(x)$ at $x = x^{(t)}$ and obtain the corresponding US iterations as follows:

$$U_{1,2}(x|x^{(t)}) \overset{\mathbf{3.5}}{=} g_2(x^{(t)}) - 1.5(x - x^{(t)}) \quad \text{and}$$

$$x^{(t+1)} = x^{(t)} + \frac{g_2(x^{(t)})}{1.5} = x^{(t)} + \frac{0.5x^{(t)} + 2\sin(x^{(t)}) + 1}{2.5}.$$

(6.8)

Set $x^{(0)} \overset{\Delta}{=} x^*_1 + \varepsilon$ as the initial value such that $g_2(x^{(0)}) > 0$, where $\varepsilon$ is a small positive real number, say $10^{-6}$. Then the US iterations $\{x^{(t+1)}\}_{t=0}^\infty$ defined by (6.8) converged to the second root $x^*_2 = 3.535612$ as shown in Figure 2(b2).

Third, once we obtained $x^*_2$, we set $x^{(0)} \overset{\Delta}{=} x^*_3 + \varepsilon$ as the initial value such that $g(x^{(0)}) > 0$, then the US iterations $\{x^{(t+1)}\}_{t=0}^\infty$ defined by (6.7) converged to the second root $x^*_3 = 5.308993$ as shown in Figure 2(b3).

### 7. Discussions

To solve the root of a non-linear equation $g(\theta) = 0$, in this paper, we have established a general framework of a new root–finding method, called as the US algorithm. Its each iteration consists of a **U-step** and an **S-step**, where the **U-step** is to construct one $U$-function $U(\theta|\theta^{(t)})$ based on a new notion of changing direction inequality for the original function $g(\theta)$, while the **S-step** solves the $U$-equation $U(\theta|\theta^{(t)}) = 0$ with respect to the left argument to obtain the next iterate $\theta^{(t+1)}$. Unlike the NR algorithm, which is sensitive to initial values and may diverge if a poor initial value is chosen, from Theorem 1, we know that the US algorithm has the property of strongly stable convergence; that is, it does not depend on any initial values in $\Theta$ and strongly stably converges to the root $\theta^*$. Especially, because of the property of strongly stable convergence, the US algorithm could be one of the powerful tools for solving an equation with multiple roots as shown in Section 6.3.

The critical requirement for applying the US algorithm is to construct one $U$-function $U(\theta|\theta^{(t)})$ for $g(\theta)$ at $\theta = \theta^{(t)}$ (i.e., to satisfy the CD inequality $g(\theta) - U(\theta|\theta^{(t)}) \overset{sgn(\theta-\theta^{(t)})}{\geq} 0$) such that an explicit solution to the surrogate equation $U(\theta|\theta^{(t)}) = 0$ is available. By using Taylor expansion, we have developed three methods for constructing $U$-functions based on the FLB function, SLUB constants and TLB constant. The resulting US algorithms
Figure 2. (a) Plots of $0 = g(x) = -0.5x - 2\sin(x) + 1$ with three roots $x_1^* = 0.4090497$, $x_2^* = 3.535612$ and $x_3^* = 5.308993$. (b) With the initial values $x^{(0)} = 0$, $x^{(0)} = x_1^* + 10^{-6}$ and $x^{(0)} = x_2^* + 10^{-6}$, the sequence $\{x^{(t+1)}\}_{t=0}^\infty$ generated respectively by (6.7), (6.8), (6.7) strongly stably converges to $\{x_k^*\}_{k=1}^3$, satisfying $x^{(0)} < x^{(1)} < \cdots < x^{(t)} < \cdots \leq x_k^*$ for $k = 1, 2, 3$. 
have linear/quadratic/cubic convergence rates as shown in Theorems 2–4, respectively. In
the future studies, we will develop other methods for constructing $U$-functions. Although
the US algorithm enjoys strongly stable convergence, we would like to accelerate the US
algorithm with slow convergence rate if the bound functions/constants are not tight enough,
particularly for the FLB function-based US algorithms. Some accelerating techniques for
the proposed US algorithms may significantly spark the method’s potential.

In Section 4, we successfully applied the US algorithms to deal with a wide range of sta-
tistical issues that are not perfectly solved by the traditional numerical algorithms. Beyond
those problems, we are trying to use the US algorithms to handle other attractive statistical
models that are still remained to be conquered.

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**References**

Arbous AG and Kerrich JE (1951). Accident statistics and the concept of accident-
proneness. *Biometrics* 7(4): 340–432.

Azzalini A (1985). A class of distributions which includes the normal ones. *Scandinavian
Journal of Statistics* 12(2): 171–178.

Bates GE and Neyman J (1952). Contributions to the theory of accident proneness. 1. an
optimistic model of the correlation between light and severe accidents. *University of
California Publications in Statistics* 1(9): 215–254.

Boyd S and Vandenberghe L (2004). *Convex Optimization*. Cambridge: Cambridge Uni-
versity Press.

Chabert JL (1999). *A History of Algorithms: From the Pebble to the Microchip*, Chapter 3:
Methods of false position. Berlin: Springer.

Consul PC and Famoye F (1989). The truncated generalized Poisson distribution and its
estimation. *Communications in Statistics — Theory and Methods* **18**(10): 3635–3648.
Consul PC and Jain GC (1973). A generalization of the Poisson distribution. *Technometrics* **15**(4): 791–799.
Costabile F, Gualtieri MI and Luceri R (2006). A modification of Muller’s method. *Calcolo*, **43**(1): 39–50.
Dempster AP, Laird NM and Rubin DB (1977). Maximum likelihood from incomplete data via the EM algorithm (with discussions). *Journal of the Royal Statistical Society: Series B (Methodological)* **39**: 1–38.
Garcia JMG (2011). A fixed–point algorithm to estimate the Yule–Simon distribution parameter. *Applied Mathematics and Computation* **217**(21): 8560–8566.
Hallinan JAJ (1993). A review of the Weibull distribution. *Journal of Quality Technology* **25**(2): 85–93.
Hunter DR and Lange K (2004). A tutorial on MM algorithms. *The American Statistician* **58**(1): 30–37.
Lange K, Hunter DR and Yang I (2000). Optimization transfer using surrogate objective functions (with discussions). *Journal of Computational and Graphical Statistics* **9**, 1–20.
Leisen F, Rossini L and Villa C (2017). A note on the posterior inference for the Yule–Simon distribution. *Journal of Statistical Computation and Simulation* **87**(6), 1179–1188.
Nair U, Sankaran PG and Balakrishnan N (2018). *Reliability Modelling and Analysis in Discrete Time* Chapter 3: Discrete Lifetime Models. London: Academic Press.
Rinne H (2008). *The Weibull Distribution: A Handbook*. Florida: CRC Press.
Wolfe P (1959). The secant method for simultaneous nonlinear equations. *Communications of the ACM* **2**(12): 12–13.
Wood GR (1992). The bisection method in higher dimensions. *Mathematical Programming* **55**: 319–337.
Yule GU (1925). A mathematical theory of evolution, based on the conclusions of Dr. JC Willis, FR S. *Philosophical Transactions of the Royal Society of London. Series B, Containing Papers of A Biological Character* **213**(402–410): 21–87.
Appendix A: Proofs of Theorem 1–4

Proof of Theorem 1. (i) We first prove that the US algorithm strongly stably converges to the unique root $\theta^*$. Let $\theta^{(t)}$ be the $t$-th iteration of $\theta^*$, then we only need to prove that

$$ \theta^{(t)} < \theta^{(t+1)} \leq \theta^*, \quad \text{if } \theta^{(t)} < \theta^*, \tag{A.1} $$

$$ \theta^* \leq \theta^{(t+1)} < \theta^{(t)}, \quad \text{if } \theta^{(t)} > \theta^*. \tag{A.2} $$

For the case of $\theta^{(t)} < \theta^*$, note that $U(\theta^{(t)}|\theta^{(t)})$ is a $U$-function for $g(\theta)$ at $\theta = \theta^{(t)}$, then we have

$$ U(\theta^{(t)}|\theta^{(t)}) \geq g(\theta) \quad \text{if } \theta \leq \theta^{(t)} (< \theta^*), \tag{A.3} $$

$$ U(\theta^{(t)}|\theta^{(t)}) \leq g(\theta), \quad \text{if } \theta > \theta^{(t)}. \tag{A.4} $$

Let $\theta^{(t+1)}$ be the $(t+1)$-th US iteration; i.e., $U(\theta^{(t+1)}|\theta^{(t)}) = 0$. Then we can show

$$ \theta^{(t+1)} > \theta^{(t)}. \tag{A.5} $$

In fact, if (A.5) is not true (i.e., $\theta^{(t+1)} \leq \theta^{(t)}$ is true), by replacing $\theta$ in (A.3) with $\theta^{(t+1)}$, we have $0 = U(\theta^{(t+1)}|\theta^{(t)}) \geq g(\theta^{(t+1)}) > 0$, which is contradictory. So (A.5) is true.

Next, we can show that

$$ \theta^{(t+1)} \leq \theta^*. \tag{A.6} $$

In fact, if (A.6) is not true (i.e., $\theta^{(t+1)} > \theta^*$ is true), by replacing $\theta$ in (A.4) with $\theta^{(t+1)}$, we have $g(\theta^{(t+1)}) \geq U(\theta^{(t+1)}|\theta^{(t)}) = 0$, which is contradictory to the fact that $g(\theta) < 0$ for any $\theta > \theta^*$ as shown by (2.1). So (A.6) is true. By combining (A.5) with (A.6), we obtain (A.1).

For the case of $\theta^{(t)} > \theta^*$, similarly, we can prove (A.2).

(ii) From (A.1) and (A.2), we can see that the US algorithm does not depend on any initial values in $\Theta$. □

Proof of Theorem 2. From (5.1), we have

$$ 0 = U(h(\theta^{(t)})|\theta^{(t)}) = g(\theta^{(t)}) + \int_{\theta^{(t)}}^{h(\theta^{(t)})} b(z) \, dz. $$

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By taking derivative with respect to \( \theta(t) \) on the both sides of the above equation, we obtain

\[
0 = g'(\theta(t)) + b(h(\theta(t)))h'(\theta(t)) - b(\theta(t)),
\]

so that

\[
h'(\theta(t)) = \frac{b(\theta(t)) - g'(\theta(t))}{b(h(\theta(t)))}.
\]

Note that the rate of convergence for the US algorithm is

\[
|g'(\theta^*)| = \lim_{t \to \infty} |h'(\theta(t))| = \lim_{t \to \infty} \left| \frac{b(\theta(t)) - g'(\theta(t))}{b(h(\theta(t)))} \right| = \left| \frac{b(h(\theta^*))}{b(\theta^*)} \right|.
\]

we only need to show that

\[
|1 - g'(\theta^*)/b(\theta^*)| < 1. \tag{A.7}
\]

If the condition, \( b(\theta^*) \leq g'(\theta^*) < 0 \), holds, then it is easy to check the correctness of (A.7).

From (3.1), we of course have \( b(\theta^*) \leq g'(\theta^*)\).

Now, we only need to prove \( g'(\theta^*) < 0 \). For any \( \varepsilon > 0 \), from the assumption (2.1), we have \( g(\theta^* + \varepsilon) < 0 \) and \( g(\theta^* - \varepsilon) > 0 \) so that we obtain

\[
\begin{align*}
g'_+(\theta^*) & \triangleq \lim_{\varepsilon \to 0^+} \frac{g(\theta^* + \varepsilon) - g(\theta^*)}{\varepsilon} = \lim_{\varepsilon \to 0^+} \frac{g(\theta^* + \varepsilon)}{\varepsilon} < 0 \quad \text{and} \\
g'_-(\theta^*) & \triangleq \lim_{\varepsilon \to 0^+} \frac{g(\theta^* - \varepsilon) - g(\theta^*)}{-\varepsilon} = \lim_{\varepsilon \to 0^+} \frac{g(\theta^* - \varepsilon)}{-\varepsilon} < 0.
\end{align*}
\]

Since the first-order derivative \( g'(\cdot) \) exists, we have \( g'(\theta^*) = g'_+(\theta^*) = g'_-(\theta^*) < 0 \).

\[
\square
\]

**Proof of Theorem 3.** From (5.3), we have

\[
g(\theta(t)) + g'(\theta(t))[h(\theta(t)) - \theta(t)] + \frac{b_2(h(\theta(t)), \theta(t))}{2}[h(\theta(t)) - \theta(t)]^2 = 0. \tag{A.8}
\]

By taking the first-derivative about \( \theta(t) \) on the both sides of (A.8), we obtain

\[
g'(\theta(t))h'(\theta(t)) + \left( g''(\theta(t)) + b_2(h(\theta(t)), \theta(t))[h'(\theta(t))] - 1 \right)[h(\theta(t)) - \theta(t)] = 0.
\]

By letting \( t \to \infty \), we have \( g'(\theta^*)h'(\theta^*) = 0 \) because

\[
\lim_{t \to \infty} [h(\theta(t)) - \theta(t)] = h(\theta^*) - \theta^* = 0. \tag{A.9}
\]
Usually, we know that $g'(\theta^*) \neq 0$ so that

$$h'(\theta^*) = 0. \quad (A.10)$$

By taking the second-derivative with respect to $\theta^{(t)}$ on the both sides of (A.8), we have

$$0 = g''(\theta^{(t)}) h'(\theta^{(t)}) + g'(\theta^{(t)}) h''(\theta^{(t)}) + \left\{ g'''(\theta^{(t)}) + b_2(h(\theta^{(t)}), \theta^{(t)}) h''(\theta^{(t)}) \right\} [h(\theta^{(t)}) - \theta^{(t)}]$$

$$+ \left\{ g''(\theta^{(t)}) + b_2(h(\theta^{(t)}), \theta^{(t)}) [h'(\theta^{(t)}) - 1] \right\} [h'(\theta^{(t)}) - 1].$$

By letting $t \to \infty$ and using (A.9) & (A.10), we obtain

$$|h''(\theta^*)| = \lim_{t \to \infty} |h''(\theta^{(t)})| = \left| \frac{b_2(\theta^*, \theta^*) - g''(\theta^*)}{g'(\theta^*)} \right| = \left| \frac{b_{22} - g''(\theta^*)}{g'(\theta^*)} \right|,$$

indicating that the US iteration (5.3) has a quadratic convergence rate given by (5.4). $\square$

**Proof of Theorem 4.** From (5.5), we have

$$0 = g(\theta^{(t)}) + g'(\theta^{(t)})[h(\theta^{(t)}) - \theta^{(t)}] + \frac{g''(\theta^{(t)})}{2} [h(\theta^{(t)}) - \theta^{(t)}]^2 + \frac{b_2}{6} [h(\theta^{(t)}) - \theta^{(t)}]^3. \quad (A.11)$$

By taking the first-derivative about $\theta^{(t)}$ on the both sides of (A.11), we obtain

$$0 = g'(\theta^{(t)}) h'(\theta^{(t)}) + g''(\theta^{(t)}) [h(\theta^{(t)}) - \theta^{(t)}] + \frac{g'''(\theta^{(t)})}{2} [h(\theta^{(t)}) - \theta^{(t)}]^2$$

$$+ g''(\theta^{(t)}) [h(\theta^{(t)}) - \theta^{(t)}] [h'(\theta^{(t)}) - 1] + \frac{b_2}{2} [h(\theta^{(t)}) - \theta^{(t)}]^2 [h'(\theta^{(t)}) - 1].$$

By letting $t \to \infty$, we have $h'(\theta^*) = 0$ when $g'(\theta^*) \neq 0$, because

$$\lim_{t \to \infty} [h(\theta^{(t)}) - \theta^{(t)}] = h(\theta^*) - \theta^* = 0. \quad (A.12)$$

By taking the second-derivative about $\theta^{(t)}$ on the both sides of (A.11), we obtain

$$0 = g''(\theta^{(t)}) h'(\theta^{(t)}) + g'(\theta^{(t)}) h''(\theta^{(t)}) + g''(\theta^{(t)}) [h(\theta^{(t)}) - \theta^{(t)}] + g''(\theta^{(t)}) [h'(\theta^{(t)}) - 1]$$

$$+ \frac{g'''(\theta^{(t)})}{2} [h(\theta^{(t)}) - \theta^{(t)}]^2 + g''(\theta^{(t)}) [h(\theta^{(t)}) - \theta^{(t)}] [h'(\theta^{(t)}) - 1]$$

$$+ \left\{ g''(\theta^{(t)}) + \frac{b_3}{2} [h'(\theta^{(t)}) - 1] \right\} \cdot [h(\theta^{(t)}) - \theta^{(t)}] [h'(\theta^{(t)}) - 1]$$

$$+ \left\{ g''(\theta^{(t)}) + \frac{b_3}{2} [h(\theta^{(t)}) - \theta^{(t)}] \right\} \cdot \left\{ [h'(\theta^{(t)}) - 1]^2 + [h(\theta^{(t)}) - \theta^{(t)}] h''(\theta^{(t)}) \right\}.$$
By letting \( t \to \infty \), we have \( h''(\theta^*) = 0 \), because \( h'(\theta^*) = 0 \) and (A.12). By taking the third-derivative about \( \theta^{(t)} \) on the both sides of equation (A.11), we obtain

\[
0 = g'''(\theta^{(t)})h'(\theta^{(t)}) + g''(\theta^{(t)})h''(\theta^{(t)}) + g''(\theta^{(t)})h''(\theta^{(t)}) + g'(\theta^{(t)})h'''(\theta^{(t)})
+ g^{(4)}(\theta^{(t)})[h(\theta^{(t)}) - \theta^{(t)}] + g'''(\theta^{(t)})[h'(\theta^{(t)}) - \theta^{(t)}] + g''(\theta^{(t)})[h'(\theta^{(t)}) - \theta^{(t)}] - 1
+ g''(\theta^{(t)})h''(\theta^{(t)}) + \frac{1}{2} g^{(5)}(\theta^{(t)})[h(\theta^{(t)}) - \theta^{(t)}]^2 + g^{(4)}(\theta^{(t)})[h(\theta^{(t)}) - \theta^{(t)}][h'(\theta^{(t)}) - \theta^{(t)}]
+ \left\{ 2g^{(4)}(\theta^{(t)}) + \frac{b_3}{2} h''(\theta^{(t)}) \right\} \cdot [h(\theta^{(t)}) - \theta^{(t)}][h'(\theta^{(t)}) - \theta^{(t)}] - 1
+ \left\{ 2g'''(\theta^{(t)}) + \frac{b_3}{2} [h'(\theta^{(t)}) - \theta^{(t)}] \right\} \cdot \left\{ [h'(\theta^{(t)}) - 1]^2 + [h(\theta^{(t)}) - \theta^{(t)}]h''(\theta^{(t)}) \right\}
+ \left\{ g''(\theta^{(t)}) + \frac{b_3}{2} [h'(\theta^{(t)}) - \theta^{(t)}] \right\} \cdot \left\{ 3[h'(\theta^{(t)}) - 1]h''(\theta^{(t)}) + [h(\theta^{(t)}) - \theta^{(t)}]h'''(\theta^{(t)}) \right\}.
\]

By letting \( t \to \infty \) and using \( h'(\theta^*) = 0 \), (A.12) and \( h''(\theta^*) = 0 \), we obtain

\[
|h'''(\theta^*)| = \left| \frac{b_3 - g'''(\theta^*)}{g'(\theta^*)} \right|,
\]

indicating that the US iteration (5.5) has a cubic convergence rate given by (5.6). \( \square \)

### Appendix B: Mode of the skew normal distribution

Let \( x_{\text{mod}} \) denote the mode of the skew normal distribution with pdf given by (4.5), in this appendix, we will propose an MM algorithm to iteratively calculate

\[
x_{\text{mod}} = \arg \max_{x \in \mathbb{R}} \log[f(x|\mu, \sigma^2, \alpha)] = \arg \max_{x \in \mathbb{R}} \left\{ -\frac{(x - \mu)^2}{2\sigma^2} + \log \left[ \Phi \left( \frac{x - \mu}{\sigma_*} \right) \right] \right\},
\]

where \( \sigma_* \equiv \sigma / \alpha \). Let \( \theta = (\mu, \sigma_*^2)^\top \) and define the left-truncated normal density as

\[
h(x|x^{(s)}, \theta) \equiv \phi \left( x + x^{(s)} - \mu | \theta \right) \cdot \Phi^{-1} \left( \frac{x^{(s)} - \mu}{\sigma_*} \right) \cdot I(x < \mu),
\]
where \( \phi(\cdot | \theta) \) denotes the pdf of \( N(\mu, \sigma^2) \). By applying the integral version of Jensen’s inequality, we have
\[
\log \left[ \Phi \left( \frac{x - \mu}{\sigma^2} \right) \right] = \log \left[ \int_{-\infty}^{x} \phi(y | \theta) \, dy \right] = \log \left[ \int_{-\infty}^{\mu} \phi(z + x - \mu | \theta) \, dz \right]
\]
\[
= \log \left[ \int_{-\infty}^{\mu} \frac{\phi(z + x - \mu | \theta)}{h(z | x(s), \theta)} \cdot h(z | x(s), \theta) \, dz \right] \geq \int_{-\infty}^{\mu} \log \left[ \frac{\phi(z + x - \mu | \theta)}{h(z | x(s), \theta)} \right] \cdot h(z | x(s), \theta) \, dz,
\]
where the equality holds iff \( x = x(s) \). Thus, the minorizing function can be constructed as
\[
Q(x | x(s)) \triangleq -\frac{(x - \mu)^2}{2\sigma^2} + \int_{-\infty}^{\mu} \log \left[ \frac{\phi(z + x - \mu | \theta)}{h(z | x(s), \theta)} \right] \cdot h(z | x(s), \theta) \, dz
\]
\[
= -\frac{(x - \mu)^2}{2\sigma^2} - \int_{-\infty}^{\mu} \frac{(z + x - 2\mu)^2}{2\sigma^2} \cdot h(z | x(s), \theta) \, dz + \text{constant}
\]
\[
= -\left( \frac{1}{2\sigma^2} + \frac{1}{2\sigma^2_*} \right) x^2 + \left[ \frac{\mu}{\sigma^2} + \frac{2\mu}{\sigma_*^2} - \frac{1}{\sigma_*^2} \int_{-\infty}^{\mu} z \cdot h(z | x(s), \theta) \, dz \right] \cdot x + \text{constant}.
\]
Let \( dQ(x | x(s)) / dx = 0 \), we obtain the \((s + 1)\)-th MM iteration:
\[
x^{(s+1)} = \frac{1}{1 + \alpha^2} \left[ \mu(1 + 2\alpha^2) - \alpha^2 \int_{-\infty}^{\mu} z \cdot h(z | x(s), \theta) \, dz \right]. \tag{B.1}
\]

**Appendix C: Inequalities on Riemann’s zeta function**

First, for any \( \theta > 1 \), we have
\[
\left( \theta - \frac{3}{2} \right)^2 + 3 \quad \Rightarrow \quad \theta^2 - 3\theta + 3 > 0 \quad \Rightarrow \quad \frac{1}{\theta - 1} < \frac{1}{(\theta - 1)^2} + 1. \tag{C.1}
\]

Next, we prove the following key inequality:
\[
\int_{1}^{\infty} \frac{\log(z + 1)}{z^\theta} \, dz = \frac{1}{1 - \theta} \int_{1}^{\infty} \log(z + 1) \, dz^{1-\theta}
\]
\[
= \log(2) \frac{\theta}{\theta - 1} + \frac{1}{\theta - 1} \int_{1}^{\infty} \frac{z^{1-\theta}}{z + 1} \, dz
\]
\[
< \log(2) \frac{\theta}{\theta - 1} + \frac{1}{\theta - 1} \int_{1}^{\infty} \frac{z^{1-\theta}}{z} \, dz \tag{C.1}
\]
\[
= \log(2) \frac{\theta}{\theta - 1} + \frac{1}{(\theta - 1)^2} < \log(2) + \frac{1}{(\theta - 1)^2} + \log(2). \tag{C.2}
\]
Finally, we obtain

\[
Z(\theta) = \sum_{x=1}^{\infty} \frac{1}{x^\theta} \geq \int_{1}^{\infty} \frac{1}{x^\theta} \, dx = \frac{1}{\theta - 1}, \tag{C.3}
\]

\[
Z'(\theta) = -\sum_{x=2}^{\infty} \frac{\log(x)}{x^\theta} \geq -\int_{1}^{\infty} \frac{\log(z+1)}{z^\theta} \, dz \tag{C.2} > -\frac{\log(2) + 1}{(\theta - 1)^2} - \log(2),
\]

\[
Z''(\theta) = \sum_{x=2}^{\infty} \frac{\log^2(x)}{x^\theta} \leq \int_{1}^{\infty} \frac{\log^2(z+1)}{z^\theta} \, dz = \int_{1}^{\infty} \frac{\log^2(z+1)}{1-\theta} \, dz^{1-\theta}
\]

\[
\leq \frac{\log^2(2)}{\theta - 1} + \frac{2}{\theta - 1} \int_{1}^{\infty} \frac{z}{z+1} \cdot z^{-\theta} \log(z+1) \, dz
\]

\[
\leq \frac{\log^2(2)}{\theta - 1} + \frac{2}{\theta - 1} \int_{1}^{\infty} \frac{\log(z+1)}{z^\theta} \, dz \tag{C.2}
\]

\[
\leq \frac{\log^2(2)}{\theta - 1} + \frac{2}{\theta - 1} \left[ \frac{\log(2) + 1}{(\theta - 1)^2} + \log(2) \right]. \tag{C.4}
\]

**Appendix D: R program for solving the root of high–order polynomial equation**

```r
root.HPE = function(a3, a2, a1, a0, a.max = 10, m, x0 = 0)
{
# Function name: root.HPE(a3, a2, a1, a0, a.max = 10, m, x0 = 0)
# ---------------------------Aim------------------------------------------
# Solve the equation: 0 = a3*x^m + a2*x^2 + a1*x + a0, 0 < x < a.max
# ---------------------------Input----------------------------------------
# a3: The coefficient of x^m
# a2: The coefficient of x^2
# a1: The coefficient of x
# a0: The constant, that is a positive real number
# a.max: The maximum of x
# m: The highest order of the equation
# x0: An initial value and the default value is 0
# ---------------------------Output---------------------------------------
# The unique root of the polynomial equation in (0, a.max)
# xt.save = c(); yt.save = c();
```

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xt = x0; y1t = a3*xt^m + a2*xt^2 + a1*xt + a0
xt.save[1] = xt; yt.save[1] = y1t
k = 1; esp = 1
while(esp>1e-8){
    if(a3<0){
        ### When a3<0, we apply the SLUF method
        if(y1t>0){ b2 = a3*m*(m-1)*a.max^(m-2) }else{b2 = 0}
        A2 = b2/2+a2
        A1 = a3*m*xt^(m-1)-b2*xt + a1
        A0 = a3*(1-m)*xt^m+b2/2*xt^2 + a0
    }
    else{
        ### When a3>0, we apply the TLF method
        A2 = a3*m*(m-1)/2*xt^(m-2)+a2
        A1 = a3*m*(2-m)*xt^(m-1)+a1
        A0 = a3*(m-1)*(m/2-1)*xt^m+a0
    }
    Delta.det = A1^2-4*A2*A0
    if(Delta.det >= 0){
        xt.save[k+1] = -(A1+sqrt(Delta.det))/(2*A2)
        yt.save[k+1] = a3*xt.save[k+1]^m + a2*xt.save[k+1]^2 +
                        a1*xt.save[k+1]+a0
        esp = abs(yt.save[k+1])
        xt = xt.save[k+1]
        y1t = yt.save[k+1]
        k = k+1
    }
    else{
        stop(paste('There exists no root in (0,',a.max,')'))
    }
}
return(xt)

# --------------------------------------------------------------------------
# --------Example: x^3-3x^2+x+1 = 0---------------------------------------------------------------------
> a3 = 1; a2 = -3; a1 = 1; a0 = 1
> root.HPE(a3, a2, a1, a0, a.max=2, m=3, x0=0)
[,1]      [,2]      [,3]      [,4]      [,5]
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xt.save 0 0.7675919 0.99418291 9.999999e-01 1
yt.save 1 0.4522631 0.01163398 1.968315e-07 0