# ACCELERATED ITERATIVE METHOD FOR FINDING ZEROS OF NONLINEAR FUNCTIONS

**M.Sc Thesis**

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**DISCIPLINE OF MATHEMATICS**
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# ACCELERATED ITERATIVE METHOD FOR FINDING ZEROS OF NONLINEAR FUNCTIONS

*A THESIS*

*Submitted in partial fulfillment of the*
*requirements for the award of the degree*

***of***
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*by*
**Akshita Aggarwal**

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CANDIDATE'S DECLARATION

I hereby certify that the work which is being presented in the thesis entitled **ACCELERATED ITERATIVE METHOD FOR FINDING ZEROS OF NONLINEAR FUNCTIONS** in the partial fulfillment of the requirements for the award of the degree of **MASTER OF SCIENCE** and submitted in the **DISCIPLINE OF MATHEMATICS, Indian Institute of Technology Indore**, is an authentic record of my own work carried out during the time period from July 2017 to June 2019 under the supervision of **Dr. V. Antony Vijesh**, Associate Professor, Discipline of Mathematics, IIT Indore.

The matter presented in this thesis by me has not been submitted for the award of any other degree of this or any other institute.

Signature of the student with date

(**AKSHITA AGGARWAL**)

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This is to certify that the above statement made by the candidate is correct to the best of my knowledge.

Signature of Thesis Supervisor with date

(**Dr. V. ANTONY VIJESH**)

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**AKSHITA AGGARWAL** has successfully given her M.Sc. Oral Examination held on $3^{rd}$ July,2019

Signature of supervisor of M.Sc Thesis

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Signature of Convener, DPGC

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Signature of PSPC Member #1

Date:

Signature of PSPC Member #2

Date:

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# ABSTRACT

**Keywords:** Halley's method, Gamma distribution, Newton's method, Schwarzian Newton method.

The dissertation in three chapters presents interesting results on convergence of Newton's method, Halley's method and Schwarzian Newton's method and their applications to find the inversion of gamma distribution. This dissertation also presents an interesting numerical simulation result by comparing the iterative methods Newton's method, Schwarzian Newton's method and Average Newton's method.

**Chapter 1** provides basic results towards the convergence of Newton's method and the development of various modification of Newton's method.

**Chapter 2** presents the Schwarzian Newton's method and its nonlocal convergence property and its application to find the inversion of gamma distribution. This chapter is based on the recent work of J. Segura.

**Chapter 3** presents the numerical simulation results by comparing various Newton's methods. In this section, the Schwarzian Newton's method is applied to the normal distribution and generalize gamma distribution.

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## CHAPTER 1

# INTRODUCTION

Finding the zeros of a nonlinear function is one of the oldest and important problems in mathematics. One of the famous results of Abel [**5**] ensures that polynomial of degree greater than or equal to five can not be solved by radicals. Similarly finding the zeros of transcendental function is a much more difficult job. Recently, finding zeros and inversion of special functions that are the solutions of second order differential equation have attained a lot of attention due to their frequent appearance in various science and engineering problems. For example, Airy's function is used in transmittance of Fabry-Perotinter-ferometer, Marcum-Q-function and its generalization are used in the detection theories for radar systems and wireless communications. Additionally, Marcum-Q-function is also used in the error performance analysis of digital communication problems and the error function is used in determining the bit error rate of digital communication etc. Similarly, elliptic integrals of first and second kind and Fresnal integral are some of the special functions which are very frequently appear in numerous practical problems. For example, Fresnal integral has been used in the calculation of electromagnetic field intensity in an environment where light bends around opaque objects. Furthermore, special functions also play an important role in probability and statistics. For example, the gamma function, beta function and their variations, appear very frequently in probability and statistics. Even some of the special functions have been found advantageous to express the solution of some important differential equations. Though these special functions have numerous applications, there is still a critical need to evaluate these special functions numerically. There is also a challenge to find their inversion numerically. Developing mathematical techniques to find the zero of nonlinear function is a vital step to solve real life problems. Iterative methods such as bisection method, successive iteration method, secant method, Newton's method and their variation are widely used to find the zeros of nonlinear functions. The aim of this section is to summarize some basic results for Newton's method to find the zeros of a real valued function.

## 1.1. Newton's Method

Newton's method is one of the iterative scheme to find the zeros of nonlinear function which converges faster than the bisection method, successive iteration method and secant method. Though this method studied by Newton in 1669 for finding the zeros of polynomial, this idea was used by Heron [**2**] to find the square root of a positive number. More specifically, he used the iterative scheme $x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$ to find the square root of a positive number $a$. Mesopotamia [**1**] also used these iterative procedure to find the square root of a positive number $a$ before 1500 B.C.

In 1669, Newton demonstrated this procedure to find the zeros of the cubic polynomial $f(x) = x^3 - 2x - 5 = 0$. Newton's demonstration is as follows:

Step 1 Start with an initial guess $x_0 = 2$.

Step 2 Improve the initial guess by adding $\alpha$ to $x_0$. The value of $\alpha$ is obtained by solving the linear equation $10\alpha - 1 = 0$ i.e. $\alpha = 0.1$. This linear equation is obtained by neglecting the higher order terms of degree greater than or equal to two from the relation $g(\alpha) = f(2 + \alpha) = 0$.

Step 3 This value is further improved by adding $\beta$ with $x_0 + \alpha$. The value of $\beta$ is obtained by solving the linear equation $11.23\beta + 0.061 = 0$ i.e. $\beta = -0.0054$. This linear equation is obtained by neglecting the higher order terms of degree greater than or equal to two from the relation $h(\beta) = g(\beta + 0.1) = 0$.

Step 4 Improve this value by adding $\gamma$ with $x_0 + \alpha + \beta$. The above procedure is repeated and we obtain $\gamma = 0.00004853$.

Thus $x_0 + \alpha + \beta + \gamma = 2.09464853$ is the new approximation for the zero of $f(x)$ which is close to zero of $f(x)$. It is interesting to note that

$$\alpha = x_1 - x_0 = -\frac{f(x_0)}{f'(x_0)} \tag{1.1}$$

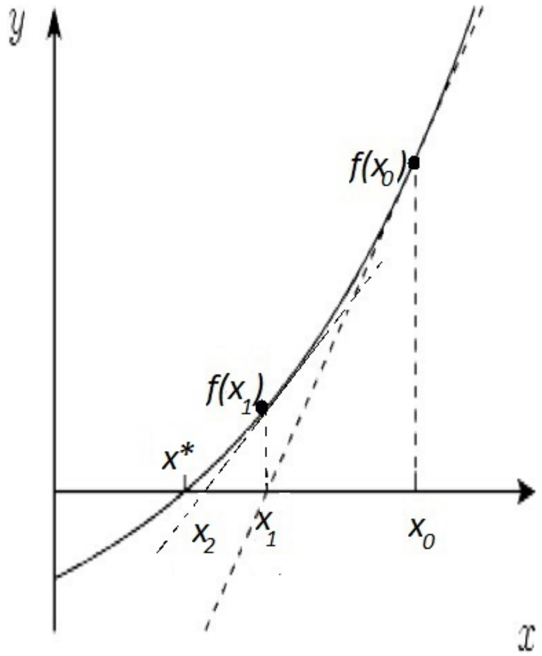
$$\beta = x_2 - x_1 = -\frac{f(x_1)}{f'(x_1)}. \tag{1.2}$$

Thus the Newton's method can be summarized as follows: If $x_k$ is an approximation for the zero $x*$ one can get the improved approximation $x_{k+1}$ by adding $x_k + h$, where $h$ is the solution of the linear equation $f(x_k) + f'(x_k)h = 0$. Raphson independently provided the iterative scheme $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$ in 1690 for finding the zero of polynomial of the form $f(x) = x^3 - ax - b$.

### 1.1.1. Geometrical interpretation of Newton's method

From Figure 1.1, one can conclude that $\tan q = \frac{f(x_0)}{x_0 - x_1}$. The geometrical interpretation of derivative leads to $f'(x_0) = \tan q$. Using these relations one can get $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$. Thus to find $x_2$ draw the tangent line at $(x_1, f(x_1))$. The point of intersection of tangent line and the x-axis will be taken as $x_2$. Moreover, $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$. Repeat the above procedure to obtain the better approximation for the zero of $f(x)$.

FIGURE 1.1. Geometrical interpretation of Newton's method




It is interesting to note that one can obtain the Newton's method from Taylor's series representation for the given function $f(x)$. Let $x$ be an approximation to the zero $x^*$ of $f(x)$. From Taylor's series one can have

$$0 = f(x^*) = f(x+h) = f(x) + hf'(x) + \mathcal{O}(h^2) \tag{1.3}$$

where $h = x^* - x$. Note that if $x$ is very close to $x^*$ then $h$ will be very small. Consequently, one can neglect the higher order terms $\mathcal{O}(h^2)$ to obtain the value $h = -\frac{f(x)}{f'(x)}$. Thus $x + h$ will be better approximation than $x$ to $x^*$. Consequently, this leads to the iterative procedure $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, n = 0, 1, 2, \cdots$ .
The following definition helps us to quantify how much faster an iterative scheme converge to the zero of a nonlinear function $f(x)$.

**Definition 1.1.1.** [**2**] *Let* $(x_n)$ *be a sequence of real numbers that converges to* $x^*$. *If* $\exists$ *positive constants* $c$ *and* $\alpha$ *and an integer* $n_0 \in \mathbb{N}$ *such that*

$$|x_{n+1} - x^*| \leq c|x_n - x^*|^{\alpha} \quad \forall \quad n \geq n_0$$

*then we say that the order of convergence is* $\alpha$ *at least.*

Interesting example is provided in [**2**] to show that Newton's method may not converge to the zero of the nonlinear function. In other words, the convergence of Newton's method depends on the initial approximation. Hence the study of convergence analysis of Newton's method is very important. In literature two types of convergence analysis results are available for Newton's method namely local convergence theorem and semilocal convergence theorem. If one assumes the existence of zeros of the nonlinear function $f(x)$ and proves the convergence of the Newton's iterative scheme, then this type of convergence theorem is known as local convergence theorem. If one assumes sufficient condition on the initial guess and proves the convergence of Newton's iterative scheme as well as the existence of zero of $f(x)$, then this type of convergence theorem is known as semilocal convergence theorem.

The first semilocal convergence theorem for Newton's method was proved by Cauchy in 1829. The Cauchy's version semilocal convergence theorem is given below.

**Theorem 1.1.1.** [**12**]

$$\text{Let } X = \mathbb{R},\ f \in C^2,\ x_0 \in X,\ f'(x_0) \neq 0,\ \sigma_0 = -\tfrac{f(x_0)}{f'(x_0)},\ \eta = |\sigma_0|,$$

$$I = \big\langle x_0, x_0 + 2\sigma_0 \big\rangle \equiv \begin{cases} [x_0, x_0 + 2\sigma_0] & \text{if } \sigma_0 \geq 0, \\ [x_0 + 2\sigma_0, x_0] & \text{if } \sigma_0 < 0 \end{cases}$$

*and* $|f''(x)| \leq K$ *in* $I$. *Then the following results hold: If* $2K\eta < |f'(x_0)|$, *then* $f(x) = 0$ *has a unique solution* $x^*$ *in* $I$. *Also if* $|f'(x)| \geq m$ *in* $I$ *and* $2K\eta < m$, *then the Newton's sequence* $x_k$ *starting from* $x_0$ *satisfies the following:*

$$|x_{k+1} - x_k| \leq \frac{K}{2m}|x_k - x_{k-1}|^2, \quad k \geq 1$$

*and*

$$x^* \in \big\langle x_k, x_k + 2\sigma_k \big\rangle,$$

*where,* $\sigma_k = -f(x_k)/f'(x_k) = x_{k+1} - x_k$, *so that*

$$|x^* - x_k| \leq 2\eta\Big(\frac{K\eta}{2m}\Big)^{2^k - 1} \quad (k \geq 0).$$

One of the local convergence theorem for Newton's iterative scheme is given below.

**Theorem 1.1.2.** [**2**]
*Let* $f''$ *be a continuous function and* $r$ *be a simple zero of* $f$. *Then there is a neighborhood of* $r$ *and a constant* $C$ *such that if Newton's method is started in that neighborhood, then the Newton's iterative method converges and satisfies*

$$|x_{n+1} - r| \leq C|x_n - r|^2.$$

Though the convergence of the Newton's iterative scheme is very sensitive to the initial guess, but if the nonlinear function $f(x)$ is convex or concave then it provides a greater flexibility in selecting the initial guess. To find the zeros of convex function one can use the following theorem.

**Theorem 1.1.3.** [**2**]
*Let* $f \in C^2(\mathbb{R})$. *If* $f$ *is strictly increasing, strictly convex and has a zero then the Newton's iteration converges from any starting point to the unique zero of* $f(x)$.

In the above theorem convex property of the nonlinear function $f(x)$ is assumed throughout the real line. By assuming the convex property of the nonlinear function on a closed and bounded interval the convergence of the Newton's iterative scheme studied in the following theorem.

**Theorem 1.1.4.** [**6**]*(Theorem 2.1)*
*Let $f''$ be a continuous function and $f' \neq 0$ in a neighborhood of an simple zero $r$, namely, in $[\alpha_0, \beta_0]$ say. If $f'(x) > 0$, $f(\alpha_0) < 0$, $f(\beta_0) > 0$, $\alpha_0 < \beta_0$ and $f''(x) > 0$, then there exist monotone sequences $\{\alpha_n\}, \{\beta_n\}$ satisfying*

$$\alpha_0 < \alpha_1 < \alpha_2 < ... < \alpha_n < r < \beta_n < ... < \beta_1 < \beta_0, \tag{1.4}$$

*which are generated by the iterative schemes*

$$f(\beta_n) + f'(\beta_n)(\beta_{n+1} - \beta_n) = 0 \tag{1.5}$$

$$f(\alpha_n) + f'(\beta_n)(\alpha_{n+1} - \alpha_n) = 0. \tag{1.6}$$

*Moreover, the sequences $\{\alpha_n\}, \{\beta_n\}$ converge to the unique zero $r$ quadratically.*

*Proof.* From (1.5) for $n = 0$ and $f(\beta_0) > 0$, we have
$0 < f(\beta_0) - [f(\beta_0) + f'(\beta_0)(\beta_1 - \beta_0)] = -f'(\beta_0)(\beta_1 - \beta_0)$,
hence $\beta_0 > \beta_1$ as $f'(\beta_0) > 0$. Similarly one can get $\alpha_1 > \alpha_0$. In the next step we prove that $\alpha_1 < r < \beta_1$. Using relation (1.5) we have

$$\begin{aligned} 0 &= f(r) - f(\beta_0) - f'(\beta_0)(\beta_1 - \beta_0) \\ &= f'(\sigma)(r - \beta_0) - f'(\beta_0)(\beta_1 - \beta_0) > f'(\beta_0)[r - \beta_0 - \beta_1 + \beta_0] \\ 0 &> f'(\beta_0)(r - \beta_1), \end{aligned}$$

Thus $\beta_1 > r$. Using similar argument one can show that $r > \alpha_1$. Consequently,

$$\alpha_0 < \alpha_1 < r < \beta_1 < \beta_0.$$

Using induction, we can show (1.4) holds. Hence $\{\alpha_n\}$ is an increasing sequence and bounded above by $\alpha$. Similarly $\{\beta_n\}$ is a decreasing sequence bounded below by $r$. Thus $\exists$ $\alpha$ and $\beta$ such that $\{\alpha_n\}$ converges to $\alpha$ and $\{\beta_n\}$ converges to $\beta$.

Using the continuity of $f'$ and the relations (1.5) and (1.6) ensure that $f(\alpha) = 0 = f(\beta)$. The monotone property of the function in the interval $[\alpha_0, \beta_0]$ guarantees that $\alpha = \beta = r$.

Now we show that the sequences $\{\alpha_n\}, \{\beta_n\}$ converge quadratically to $r$. Since $[f'(x)]^{-1}$ and $f''(x)$ are continuous function, $\exists$ a contant $K$ such that

$$\sup_{x,y\in[\alpha_0,\beta_0]} |f'(x)^{-1}f''(y)| \leq K$$

Note that

$$\begin{aligned}
|r-\alpha_{n+1}| &= |r-\alpha_n + [f'(\beta_n)]^{-1}f(\alpha_n)| \\
&= |[f'(\beta_n)]^{-1}[f'(\beta_n)(r-\alpha_n) + f(\alpha_n) - f(r)]| \\
&= |[f'(\beta_n)]^{-1}[f'(\beta_n)(r-\alpha_n) + f'(\zeta)(\alpha_n - r)],\ \zeta \in (\alpha_n, r)| \\
&= |[f'(\beta_n)]^{-1}[(r-\alpha_n)(f'(\beta_n) - f'(\zeta)]| \\
&< |[f'(\beta_n)]^{-1}[(r-\alpha_n)(f'(\beta_n) - f'(\alpha_n)]| \\
&< |[f'(\beta_n)]^{-1}[(r-\alpha_n)f''(\zeta_1)(\beta_n - \alpha_n)]| \\
&\leq K|r-\alpha_n|[\beta_n - r + r - \alpha_n] \\
&= K|r-\alpha_n|^2 + K(\beta_n - r)(r-\alpha_n) \\
&\leq K|r-\alpha_n|^2 + \frac{K}{2}(\beta_n - r)^2 + \frac{K}{2}(r-\alpha_n)^2 \\
&= \frac{3K}{2}|r-\alpha_n|^2 + \frac{K}{2}|\beta_n - r|^2 \\
|r-\alpha_{n+1}| &< \frac{3K}{2}[|r-\alpha_n|^2 + |\beta_n - r|^2].
\end{aligned}$$

Similar estimate can be obtained for $\{\beta_n\}$. Hence the proof. $\square$

**Remark 1.1.1.** *Let $f''$ be a continuous function and $f' \neq 0$ in a neighborhood of a simple zero $r$, namely, in $[\alpha_0, \beta_0]$ say. If $f'(x) < 0, f(\alpha_0) > 0, f(\beta_0) < 0, \alpha_0 < \beta_0$ and $f''(x) < 0$, then there exist monotone sequences $\{\alpha_n\}, \{\beta_n\}$ satisfying*

$$\alpha_0 < \alpha_1 < \alpha_2 < ... < \alpha_n < r < \beta_n < ... < \beta_1 < \beta_0, \tag{1.7}$$

*which are generated by the iterative schemes*

$$f(\alpha_n) + f'(\beta_n)(\alpha_{n+1} - \alpha_n) = 0, \tag{1.8}$$

$$f(\beta_n) + f'(\beta_n)(\beta_{n+1} - \beta_n) = 0. \tag{1.9}$$

*Moreover, the sequences $\{\alpha_n\}, \{\beta_n\}$ converge to the unique zero $r$ quadratically.*

## 1.2. Higher Order Convergence Method

Though Newton's method converges quadratically, consistent efforts were made to improve the order of convergence. This subsection provides some of the modification in Newton's method which leads to third order convergence.

### 1.2.1. Halley's method

One of the well known third order convergence method is given by Halley. Halley's iterative method with initial guess $x_0$ can be written as

$$x_{n+1} = x_n - \frac{2f(x_n)f'(x_n)}{2[f'(x_n)]^2 - f(x_n)f''(x_n)}, \quad n = 1, 2, \cdots .$$

The above iterative method can be rewritten as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}\left[1 - \frac{f(x_n)}{f'(x_n)}\frac{f''(x_n)}{2f'(x_n)}\right]^{-1}. \tag{1.10}$$

It is clear from (1.10) that as $f''(x) \to 0$ Halley's method approaches Newton's method. If $f(r) = 0$, under suitable assumption one can show that Halley's iterative scheme satisfies the following inequality

$$|x_{n+1} - r| \leq K|x_n - r|^3$$

for some $K > 0$.
Consequently, Halley's method has third order convergence.

### 1.2.2. Newton's method based on quadrature rules

Though the Halley's method provides third order convergence, it requires the evaluation of the second derivative of the function. In this direction, a third order method will require the evaluation of only the first order derivative was proposed by S. Weerakoon and T. G. I. Fernando [**10**]. They obtained the method as follows: Let $f$ be a smooth function from $\mathbb{R}$ to $\mathbb{R}$. By Fundamental theorem of calculus one can write

$$f(x) = f(x_n) + \int_{x_n}^{x} f'(\lambda) d\lambda. \tag{1.11}$$

Evaluate the integral using trapezoidal rule. Thus (1.11) becomes

$$f(x) \approx f(x_n) + \frac{1}{2}(x - x_n)(f'(x_n) + f'(x)). \tag{1.12}$$

Let $x = x_{n+1} = r$ be the zero of $f(x)$ then (1.12) becomes

$$x_{n+1} = x_n - \frac{2f(x_n)}{[f'(x_n) + f'(x_{n+1})]}. \tag{1.13}$$

To make this iterative scheme explicit one can replace $f'(x_{n+1})$ by $f(x_n{}^*)$ where $x_n^* = x_n - \frac{f(x_n)}{f'(x_n)}$.
Thus (1.13) becomes the following iterative procedure

$$x_{n+1} = x_n - \frac{2f(x_n)}{[f'(x_n) + f'(x_n^*)]}. \tag{1.14}$$

This method can be considered as **Average Newton's method.**

In 2000, S. Weerakoon and T. G. I. Fernando [**10**] provided the third order convergence of this method.

One can get a different variants of Newton's method if one approximate the integral term in (1.11) by different quadrature formula. M. Frontini and E. Sormani proved the more general local convergence theorem for Newton's method based on quadrature formula.

**Theorem 1.2.1.** [**3**] *Let $f$ be a sufficiently smooth function and $\zeta$ is a simple zero of $f$. The order of convergence of the modified Newton's method $x_{n+1} = x_n - \frac{f(x_n)}{\sum_{i=1}^{m} A_i f'(\eta_i{}^*)}$, obtained by approximating the integral in (1.11) by an interpolatory quadrature formula is three. Here $\tau_i$ are knots in $[0,1]$, $A_i$ are the weights of the interpolatory quadrature formula used and $\eta_i{}^* = x_n - \tau_i \frac{f(x_n)}{f'(x_n)}$.*

The following theorem is a semilocal convergence theorem for Newton's method obtained from the quadrature formula.

**Theorem 1.2.2.** [**4**]*(Theorem 2.2.1)*
*Let $f : \mathbb{R} \to \mathbb{R}$ be a differentiable function. Let $\lambda_i \in [0,1]$, $1 \leq i \leq m$ be such that $\sum_{i=1}^{m} \lambda_i = 1$. Assume further that*

1. $f'(x_0) \neq 0$;
2. *for some* $\eta > 0, |f'(x_0)^{-1} f(x_0)| \leq \eta$;
3. $|(f'(x_0)^{-1}(f'(x_0) - f'(x)))| < \epsilon$ *whenever* $x \in [x_0 - 2r, x_0 + 2r]$. *Set* $c_0 = \frac{(\lambda_1 + \sum_{i=2}^{m} 2\lambda_i)\epsilon}{1-\epsilon}$, $c = \frac{2\epsilon}{1-\epsilon}$ *such that* $(1 + \frac{c_0}{1-c})\eta < r$ *and* $0 < 3\epsilon < 1$;
4. *for some* $x_0^{(i)} \in [x_0 - r, x_0 + r], |\sum_{i=1}^{m} (\lambda_i f'(x_0^{(i)}))^{-1} f(x_0)| \leq \eta$.

*Then, the sequence of iterates $(x_n)$ generated by*

$$x_{n+1} = x_n - (\sum_{i=1}^{m} \lambda_i f'(x_n^{(i)}))^{-1} f(x_n), \quad x_n^{(i)} = x_n - \frac{i}{m} \frac{f(x_n)}{f'(x_n)} \tag{1.15}$$

*is well-defined, remains in* $[x_0 - r, x_0 + r] \quad \forall n \geq 0$ *and converges to a unique solution* $x^* \in [x_0 - r, x_0 + r]$ *of the equation* $f(x) = 0$*. Moreover, for* $n \geq 2$*, the following error-estimates hold*

$$|x_{n+1} - x_n| \leq c^{n-1} c_0 \eta,$$
$$|x_n - x^*| \leq \frac{c^{n-1} c_0 \eta}{1 - c}.$$

## 1.3. Normal Form of Second Order Ordinary Differential Equation.

Consider a second order ordinary differential equation:

$$y'' + p(x)y' + q(x)y = 0. \tag{1.16}$$

By putting

$$y = u.e^{-\frac{1}{2}\int p(x)dx},$$

we get normal form of (1.16) i.e.

$$u'' + u\left( -\frac{1}{2}p' - \frac{1}{4}p^2 + q \right) = 0$$

where $u = ye^{\frac{1}{2}\int p(x)dx}$.

**For Example:** Bessel's equation is

$$y'' + \frac{1}{x}y' + \left(1 - \frac{n^2}{x^2}\right)y = 0.$$

Normal form of Bessel's equation is

$$u'' + u\left(1 + \frac{1 - 4n^2}{4x^2}\right) = 0.$$

CHAPTER 2

# SCHWARZIAN NEWTON'S METHOD AND ITS APPLICATIONS

In the direction of improving the order of convergence of Newton's method Schwarzian derivative plays a crucial role. In 1993, Julian Palmore [**7**] studied the relation between the Schwarzian derivative and Newton's method. Recently, J. Segura [**9, 8**] derived a Newton's method based on Schwarzian derivative and applied this technique to find the zero as well as inversion of special function which is a solution of second order differential equation. This chapter is based on the work of J. Palmore [**7**] and J. Segura [**9, 8**].

## 2.1. Schwarzian Derivative and Newton's Method

The following definitions are useful to understand the theorems in later of this chapter. The Schwarzian derivative of a smooth function $f : \mathbb{R} \to \mathbb{R}$ is given below.

**Definition 2.1.1.** *The* ***Schwarzian derivative*** *of $f$ is denoted by $S[f]$ or $\{f, x\}$. It is defined by $S[f](x) = f'''(x)/f'(x) - \frac{3}{2}[f''(x)/f'(x)]^2 \;\; \forall \;\; x \in \mathbb{R} \setminus f'^{-1}(0)$.*

Define

$$\tan(\lambda, x) = \frac{1}{\sqrt{\lambda}} \tan(\sqrt{\lambda} x) = \begin{cases} \frac{1}{\sqrt{\lambda}} \tan(\sqrt{\lambda} x) & \lambda > 0 \\ x & \lambda = 0 \\ \frac{1}{\sqrt{-\lambda}} \tanh(\sqrt{-\lambda} x) & \lambda < 0 \end{cases} \tag{2.1}$$

and similarly for the inverse function,

$$\arctan(\lambda, x) = \arctan(\sqrt{\lambda}x)/\sqrt{\lambda}.$$

**Remark 2.1.1.** *General functions for which the schwarzian derivative is constant are*

$$S_\lambda(x) = \frac{\tan(\lambda, x) + P}{Q\tan(\lambda, x) + R}. \tag{2.2}$$

*Proof.* Given that schwarzian derivative is a constant $\lambda$ (say).

$$\frac{1}{2}\left(\frac{f'''}{f'} - \frac{3}{2}\left(\frac{f''}{f'}\right)^2\right) = \lambda \tag{2.3}$$

Now Let

$$\begin{aligned}
y &= \frac{f''}{f'} \\
y' &= \frac{f'f''' - f''^2}{f'^2} \\
&= \frac{f'''}{f'} - \left(\frac{f''}{f'}\right)^2 \\
&= \frac{f'''}{f'} - \frac{3}{2}\left(\frac{f''}{f'}\right)^2 + \frac{1}{2}\left(\frac{f''}{f'}\right)^2 \\
y' &= 2\lambda + \frac{1}{2}y^2 \\
2y' &= 4\lambda + y^2
\end{aligned}$$

Integerating both sides we get

$$\frac{1}{\sqrt{\lambda}}\arctan(\frac{y}{2\sqrt{\lambda}}) = x + C_1.$$

Solving for $y$, we get

$$y = 2\sqrt{\lambda}\tan(\sqrt{\lambda}(x + C_1)).$$

Now Putting the value of $y$, we have

$$\frac{f''}{f'} = 2\sqrt{\lambda}\tan(\sqrt{\lambda}(x + C_1))$$

Integerating both sides we get

$$\begin{aligned}
\log(f') &= 2\log(\sec(\sqrt{\lambda}(x + C_1))) + \log(C_2) \\
f' &= \sec^2(\sqrt{\lambda}(x + C_1))C_2.
\end{aligned}$$

Integerating both sides we get

$$\begin{aligned}
f(x) &= \frac{C_2}{\sqrt{\lambda}}\tan(\sqrt{\lambda}(x + C_1)) + C_3 \\
&= \frac{C_2}{\sqrt{\lambda}}\left[\frac{\tan(\sqrt{\lambda}x) + \tan(\sqrt{\lambda}C_1)}{1 - tan(\sqrt{\lambda}x)\tan(\sqrt{\lambda}C_1)}\right] + C_3 \\
&= \frac{\frac{C_2}{\sqrt{\lambda}} + \frac{C_2}{\sqrt{\lambda}}\tan(\sqrt{\lambda}C_1) + C_3 - \frac{C_3}{\sqrt{\lambda}}\tan(\sqrt{\lambda}x)\tan(\sqrt{\lambda}C_1)\sqrt{\lambda}}{1 - tan(\sqrt{\lambda}x)\tan(\sqrt{\lambda}C_1)} \\
&= \frac{\tan(\lambda, x) + P}{Q\tan(\lambda, x) + R}
\end{aligned}$$

where

$$\begin{aligned}
P &= \frac{\frac{C_2}{\sqrt{\lambda}}\tan(\sqrt{\lambda}C_1) + C_3}{C_2 - \sqrt{\lambda}C_3\tan(\sqrt{\lambda}C_1)} \\
Q &= \frac{-\sqrt{\lambda}\tan(\sqrt{\lambda}C_1)}{C_2 - \sqrt{\lambda}C_3\tan(\sqrt{\lambda}C_1)} \\
R &= \frac{1}{C_2 - \sqrt{\lambda}C_3\tan(\sqrt{\lambda}C_1)}.
\end{aligned}$$

Hence the remark. $\square$

**Remark 2.1.2.** *General functions for which the schwarzian derivative is zero are*

$$S_0(x) = \frac{x + P}{Qx + R}. \tag{2.4}$$

*Proof.* Given that schwarzian derivative is zero.

$$\frac{1}{2}\left(\frac{f'''}{f'} - \frac{3}{2}\left(\frac{f''}{f'}\right)^2\right) = 0 \tag{2.5}$$

Now Let

$$\begin{aligned}
y &= \frac{f''}{f'} \\
y' &= \frac{f'f''' - f''^2}{f'^2} \\
&= \frac{f'''}{f'} - \left(\frac{f''}{f'}\right)^2 \\
&= \frac{f'''}{f'} - \frac{3}{2}\left(\frac{f''}{f'}\right)^2 + \frac{1}{2}\left(\frac{f''}{f'}\right)^2 \\
y' &= \frac{1}{2}y^2
\end{aligned}$$

Integerating both sides, we get

$$\begin{aligned}
y &= \frac{-2}{x+C} \\
\frac{f''}{f'} &= \frac{-2}{x+C}
\end{aligned}$$

Solving for $f$ we get

$$\begin{aligned}
f(x) &= \frac{1}{C'}\frac{-1}{x+C} + C'' \\
&= \frac{-1 + C'C''(x+C)}{C'(x+C)} \\
&= \frac{x+P}{Qx+R}
\end{aligned}$$

where

$$P = \frac{CC'C'' - 1}{C'C''}$$
$$Q = \frac{1}{C''}$$
$$R = \frac{C}{C''}.$$

Hence the remark. $\square$

**Definition 2.1.2.** *Let $f$ be a smooth function from $\mathbb{R}$ to $\mathbb{R}$. Function $g$ is said to be Newton's map of $f$ if $g(x) = x - \frac{f(x)}{f'(x)}$ for $x \in \mathbb{R} \setminus f'^{-1}(0)$.*

The following theorem due to J. Palmore [**7**] provides the relation between Newton's method and Schwarzian derivative.

**Theorem 2.1.1.** [**7**]*(Theorem 1)*
*Let $g$ be Newton's map of a 4 times continuously differentiable function $f$. Let $\zeta \in \mathbb{R} \setminus f'^{-1}(0)$ be such that $f(\zeta) = 0$. Then we have $g'''(\zeta) = S[f](\zeta)$.*

The following theorem due to J. Palmore [**7**] provides the relation between the order of convergence of Newton's method and Schwarzian derivative.

**Theorem 2.1.2.** [**7**]*(Theorem 2)*
*Let $g$ be a rational function and let $\zeta \in \mathbb{C}$ be a fixed point. Let $f$ be an entire function such that $g$ is Newton's map of $f$, $f(\zeta) = 0$ and $f'(\zeta) \neq 0$. If $f''(\zeta) = 0$, then Newton's map has convergence to $\zeta$ of order 3 or greater. If $S[f](\zeta) = 0$, then convergence of $g$ to $\zeta$ has order 4 or greater.*

## 2.2. The Schwarzian Newton's Method

It is well known that Newton's method is exact (gives exact root in one iteration) for linear functions. In other words, Newton's method is exact for functions whose derivative is constant. Recently, J. Segura [**9, 8**] derived Schwarzian Newton's method based on Schwarzian derivative which is exact for functions whose Schwarzian derivative is constant. Moreover, J. Segura also studied the nonlocal convergence properties of Schwarzian Newton's method. His study also ensures that the Schwarzian Newton's method has fourth order convergence. The derivation of Schwarzian Newton's method goes as follows.

Let $f$ be a smooth function which satisfies the second order ordinary differential equation

$$f''(x) + B(x)f'(x) = 0 \tag{2.6}$$

Let

$$\Phi'' + \Omega\Phi = 0, \;\; \Phi = \frac{f}{\sqrt{f'}} \tag{2.7}$$

be the corresponding normal form of the second order ODE.
Hence

$$\Omega = -\frac{1}{4}B^2 - \frac{1}{2}B' = \frac{1}{2}\left(\frac{f'''}{f'} - \frac{3}{2}\left(\frac{f''}{f'}\right)^2\right) = \frac{1}{2}\{f, x\},$$

where $\{f, x\}$ is the Schwarzian derivative of $f$ with respect to $x$. Note that the zeros of $f$ and the zeros of $\Phi$ are same. One can rewrite (2.7) as

$$y'(x) = 1 + \Omega(x)y^2(x), \;\; y(x) = \frac{\Phi}{\Phi'} \tag{2.8}$$

Let $\Omega(x) > 0$. Let $\alpha$ be the simple zero of $f$. Hence it is a simple zero of $\Phi$. Consequently $\alpha$ is a zero of $y(x)$.
Using (2.8) we get,

$$x - \alpha = \int_{\alpha}^{x} \frac{y'(t)}{1 + \Omega(t)y^2(t)} dt \approx \frac{1}{\sqrt{\Omega(x)}} \arctan(\sqrt{\Omega(x)}y(x)). \tag{2.9}$$

Thus one can endup with the iterative scheme

$$x_{n+1} = x_n - \frac{1}{\sqrt{\Omega(x_n)}} \arctan(\sqrt{\Omega(x_n)}y(x_n)). \tag{2.10}$$

This iterative scheme is known as **Schwarzian Newton's method.**

**Remark 2.2.1.** *If $\Omega < 0$, then the Schwarzian Newton's method becomes*

$$x_{n+1} = x_n - \frac{1}{\sqrt{|\Omega(x_n)|}} \operatorname{artanh}(\sqrt{|\Omega(x_n)|}\, y(x_n)). \tag{2.11}$$

**Remark 2.2.2.** *It is interesting to note that Halley's method for finding zero of $f$ is nothing but the Newton's method to find the zero of $\Phi$. One can get this conclusion from the following relation.*

$$x_{n+1} = x_n - \frac{\Phi(x_n)}{\Phi'(x_n)} \approx x_n - \frac{2f(x_n)f'(x_n)}{2[f'(x_n)]^2 - f(x_n)f''(x_n)}. \tag{2.12}$$

**Remark 2.2.3.** *From equation* (2.10) *and equation* (2.11) *one can easily conclude that as the Schwarzian derivative approaches zero, Schwarzian Newton's method approaches Halley's method.*

**Remark 2.2.4.** *From equation* (2.9) *it is easy to conclude that Schwarzian Newton's method is exact for function whose Schwarzian derivative is constant.*

**Theorem 2.2.1.** *The order of convergence of SNM is 4.*

*Proof.* Let $\Omega > 0$ and $g(x) = x - \frac{1}{\sqrt{\Omega(x)}} \arctan(\sqrt{\Omega(x)}\, y(x))$.

To prove the theorem it is enough to show that $g'(\alpha) = g''(\alpha) = g'''(\alpha) = 0$, where $\alpha$ is a zero of $f(x)$.

SNM is $\quad x_{n+1} = g(x_n)$,

where $\quad g(x) = x - \frac{1}{\sqrt{\Omega}} \arctan\left(\sqrt{\Omega}\frac{\Phi}{\Phi'}\right)$.

Now Let $\quad \omega(x) = \sqrt{\Omega(x)}, \quad h(x) = \frac{\Phi(x)}{\Phi'(x)}$, which satisfies the Riccati equation i.e.

$$h'(x) = 1 + (\omega(x)h(x))^2. \tag{2.13}$$

So $g(x)$ becomes

$$g(x) = x - \frac{1}{\omega(x)} \arctan(\omega(x)h(x)).$$

Now

$$
\begin{aligned}
g'(x) &= 1 - \left[ \frac{\frac{\omega(x)}{1+(\omega(x)h(x))^2}(\omega(x)h'(x) + h(x)\omega'(x)) - \arctan(\omega(x)h(x))\omega'(x)}{\omega(x)^2} \right] \\
&= 1 - \left[ \frac{\frac{\omega(x)^2}{1+(\omega(x)h(x))^2} + \frac{\omega(x)h(x)\omega'(x)}{1+(\omega(x)h(x))^2} - \arctan(\omega(x)h(x))\omega'(x)}{\omega(x)^2} \right] \\
&= \frac{\omega'(x)}{\omega^2(x)} \left[ \arctan(\omega(x)h(x)) - \frac{\omega(x)h(x)}{1+(\omega(x)h(x))^2} \right] \\
&= q(x)[K(p(x)],
\end{aligned}
$$

where $q(x) = \frac{\omega'(x)}{\omega^2(x)}$, $p(x) = \omega(x)h(x)$ and $K(z) = \arctan(z) - \frac{z}{1+z^2}$.

Now

$$K(0) = K'(0) = K''(0) = 0, K'''(0) = 4, \tag{2.14}$$

$$p(\alpha) = 0, \;\; p'(\alpha) = \omega(\alpha) \tag{2.15}$$

$$g''(x) = q(x)K'(p(x))p'(x) + K(p(x))q'(x)$$

$g'''(x) = q(x)K'(p(x))p''(x) + q(x)K''(p(x))p'(x)^2 + K'(p(x))q'(x)p'(x) + K(p(x))q''(x) + q'(x)K'(p(x))p'(x)$

$g^{(4)}(x) = q(x)K'(p(x))p'''(x) + p''(x)[q(x)K''(p(x))p'(x) + K'(p(x))q'(x)] + 2q(x)K''(p(x))p'(x)p''(x$ $p''(x)^2[q(x)K'''(p(x))p'(x) + K''(p(x))q'(x)] + K'(p(x))[q'(x)p''(x) + p'(x)q''(x)] + q'(x)p'(x)^2K''(p(x)) + K(p(x))q'''(x) + q''(x)K'(p(x))p'(x) + K'(p(x))[q'(x)p''(x) + p'(x)q''(x)] + q'(x)p'(x)[K''(p(x))p'(x)]$

Now from equation (2.14) and equation (2.15) we get

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

and

$$
\begin{aligned}
g^{(4)}(\alpha) &= 4\omega(\alpha)\omega'(\alpha) \\
&= 2\Omega'(\alpha)
\end{aligned}
$$

which proves the theorem. $\square$

The following theorem ensures the covergence of Halley's method for finding zeros of the function $f$.

**Theorem 2.2.2.** *Let $\Phi$ be a sufficiently differentiable function in some interval $J$ satisfying $\Phi'' + \Omega\Phi = 0$, $\Phi' \neq 0$, and $\Phi(\alpha) = 0$ for some $\alpha \in J$. If $\Omega < 0$ in $J$, then Halley's method converges monotonically to $\alpha$ for any starting value $x_0 \in J$.*

### 2.2.1. Geometrical interpretation of the Halley's method and Schwarzian Newton's method.

The Halley's method and Schwarzian Newton's method can be obtained from osculating curves for function $f$. The following definition provides the formal definition for osculating curves for the function $f$.

**Definition 2.2.1.** [**11**] *An **osculating curve** is a plane curve from a given family that has the highest possible order of contact with another curve. That is, if F is a family of smooth curves, C is a smooth curve (not in general belonging to F), and p is a point on C, then an osculating curve from F at p is a curve from F that passes through p and has as many of its derivatives at p equal to the derivatives of C as possible.*

**Theorem 2.2.3.** [**9**]*(Theorem 2.2)*

*Let $S_0(x)$ be as in (2.4) and define $y(x) = S_0(x - x_n)$. The HM* (1) *is obtained by setting $y(x_n) = f(x_n)$, $y'(x_n) = f'(x_n)$, $y''(x_n) = f''(x_n)$ and $y'''(x_n) = f'''(x_n)$(thus determining the three constants) and obtaining $x_{n+1}$ from $y(x_{n+1}) = 0$. The three constants are given by*

$$P = \frac{2f(x_n)f'(x_n)}{D(x_n)},\ Q = \frac{-f''(x_n)}{D(x_n)},\ R = \frac{2f'(x_n)}{D(x_n)}, \tag{2.16}$$

*where*

$$D(x_n) = 2f'(x_n)^2 - f(x_n)f''(x_n). \tag{2.17}$$

*Proof.* Given that

$$y(x) = \frac{x - x_n + P}{Q(x - x_n) + R}$$

and

$$f(x_n) = y(x_n) = \frac{P}{R}. \tag{2.18}$$

$$S_0'(x) = \frac{R - PQ}{(Qx + R)^2}$$

$$y'(x) = \frac{R - PQ}{(Q(x - x_n) + R)^2}$$

$$f'(x_n) = y'(x_n) = \frac{R - PQ}{R^2} \tag{2.19}$$

$$S_0''(x) = \frac{(-2Q)R - PQ}{(Qx + R)^3}$$

$$y''(x) = \frac{(-2Q)R - PQ}{(Q(x - x_n) + R)^3}$$

$$f''(x_n) = y''(x_n) = \frac{(-2Q)R - PQ}{R^3} \tag{2.20}$$

Solving equations (2.18), (2.19) and (2.20), we get the desired value of $P$, $Q$ and $R$.

Now putting

$$y(x_{n+1}) = 0$$

$$\frac{x_{n+1} - x_n + P}{Q(x_{n+1} - x_n) + R} = 0$$

$$x_{n+1} - x_n + P = 0.$$

Putting the value of $P$ we get

$$x_{n+1} - x_n + \frac{2f(x_n)f'(x_n)}{2f'(x_n)^2 - f(x_n)f''(x_n)} = 0$$
$$x_{n+1} = x_n - \frac{2f(x_n)f'(x_n)}{2f'(x_n)^2 - f(x_n)f''(x_n)}$$

which is Halley's method. □

The following theorem due to J. Segura [**9**] provides the geometrical interpretation of Schwarzian Newton's method i.e. it can be obtained from osculating curves for the function $f$.

**Theorem 2.2.4.** [**9**]*(Theorem 2.3)*
*Let $S_\lambda(x)$ be as in (2.2) and define $y(x) = S_\lambda(x - x_n)$. The SNM* (2) *is obtained by setting $y(x_n) = f(x_n)$, $y'(x_n) = f'(x_n)$, $y''(x_n) = f''(x_n)$ and $y'''(x_n) = f'''(x_n)$ (thus determining the three constants) and obtaining $x_{n+1}$ from $y(x_{n+1}) = 0$. The constant $\lambda$ is given by*

$$\lambda = \Omega(x_n) \tag{2.21}$$

*and the other three constants $P$,$Q$ and $R$ are as in Theorem 2.2.3.*

### 2.2.2. Non-local convergence properties of the Schwarzian Newton's method.

Schwarzian Newton's method posses some good non local convergence properties. In this subsection, nonlocal convergence theorem and a comparison between Halley's method and Schwarzian Newton's method due to J. Segura [**9**] is presented.

**Theorem 2.2.5.** [**9**]*(Theorem 2.7)*
*Consider $f' \neq 0$ , $f'''$ continuous in an interval $J$ and $\alpha \in J$ be such that $f(\alpha) = 0$, the following hold.*

- *Let $\{f,x\}$ be decreasing in $I=[a,\alpha]\subset J$, then the SNM converges monotonically to $\alpha$ for any starting value $x_0\in[a,\alpha]$. If $\{f,x\}>0$ in part of the interval, the same is true if, in addition, the SNM iteration satisfies $g(a)>a$.*
- *Let $\{f,x\}$ be increasing in $I=[\alpha,b]\subset J$, then the SNM converges monotonically to $\alpha$ for any starting value $x_0\in[\alpha,b]$. If $\{f,x\}>0$ in part of the interval, the same is true if, in addition, the SNM iteration satisfies $g(b)<b$.*

**Corollary 2.2.1.** [**9**]*(Theorem2.8)*
*Consider $f'\neq 0$ , $f'''$ continuous in an interval $J$ and $\alpha\in J$ be such that $f(\alpha)=0$, if $\{f,x\}$ has one and only one extremum at $x_e\in J$ and it is a maximum, then*

- *If $\{f,x\}$ is negative the SNM converges monotonically to $\alpha$ starting from $x_0=x_e$.*
- *If $(x_e-\alpha)(x_e-g(x_e))>0$ the SNM converges monotonically to $\alpha$ starting from $x_0=x_e$.*

**Theorem 2.2.6.** [**9**]*(Theorem 2.9)*
*The steps of the SNM $(x_{n+1}-x_n)$ are of the same sign and greater (smaller) in absolute value than those for HM when $\{f,x\}$ is negative(positive).*

### 2.2.3. Application of Schwarzian Newton's method

In this section the SNM is successfully applied for finding the inversion of central gamma distribution function. This function appears very frequently in probability. Consider the central gamma distribution function

$$F(a,x)=\frac{1}{\Gamma(a)}\int_0^x t^{a-1}e^{-t}dt, a>0, x>0.$$

Let $a \geq 1$. Consider the problem of numerical inversion of central gamma distribution as $f(x) = F(a,x) - p$.

It is easy to verify that $f$ satisfies the second order ODE

$$f''(x) + B(x)f'(x) = 0 \tag{2.22}$$

with

$$B(x) = 1 + \frac{1-a}{x}.$$

The normal form of our differential equation is

$$\Phi'' + \Omega\Phi = 0 \tag{2.23}$$

where $\Omega(x) = -\frac{1}{4}\left(1 + 2\frac{1-a}{x} + \frac{a^2-1}{x^2}\right)$ and $\Phi(x) = \exp(\frac{x}{2})x^{\frac{1-a}{2}}f(x)$.

When $a = 1$, $\Omega$ is a constant. Hence when $a = 1$ the SNM is exact.

We claim $\Omega < 0 \ \forall x > 0$.

As

$$a > 1$$

$$1 - a < 0$$

$$2 - 2a < 0$$

$$1 - 2a < -1$$

$$a^2 + 1 - 2a < a^2 - 1$$

$$\frac{a^2 + 1 - 2a}{x^2} < \frac{a^2 - 1}{x^2}$$

$$(\frac{1-a}{x})^2 < \frac{a^2 - 1}{x^2}$$

$$1 + (\frac{1-a}{x})^2 + 2\frac{1-a}{x} < 1 + \frac{a^2 - 1}{x^2} + 2\frac{1-a}{x}$$

$$\left(1 + \frac{1-a}{x}\right)^2 < 1 + \frac{a^2 - 1}{x^2} + 2\frac{1-a}{x}$$

Hence $\Omega < 0 \ \forall x > 0$.

Note that $\Omega'(x) = \frac{1}{2x^3}(x(1-a) + a^2 - 1)$. Consequently, $x = a+1$ is the only relative extremum. The second derivative of $\Omega$ at $a+1$ is $\frac{(1-a)}{2(a+1)^3}$ which is negative. Hence $\Omega$ attains its maximum at $x = a+1$ which is $\Omega(a+1) = \frac{-1}{2(a+1)} < 0$. Hence corollary 2.2.1 ensures that the SNM will converge to zero of $f(x)$ if $x_0 = a+1$. For $0 < a < 1$ use the change of variable $z(x) = log(x)$ in (2.23). Hence (2.23) becomes

$$\frac{d^2\Phi}{dz^2} - \frac{d\Phi}{dz} + R(z)\Phi = 0 \tag{2.24}$$

where $R(z) = \frac{-1}{4}(e^{2z} + 2e^z(1-a) + a^2 - 1)$.

The normal form of (2.24) is $\tilde{\Phi}''(z) + \tilde{\Omega}(z)\tilde{\Phi}(z) = 0$ where $\tilde{\Phi}(z) = \frac{1}{e^{\frac{z}{2}}}\Phi(e^z)$ and $\tilde{\Omega}(z) = \frac{-1}{4}[e^{2z} + a^2 + 2e^z(1-a)]$.

Consequently , $\tilde{\Omega}(z(x)) = \frac{-1}{4}[x^2 + a^2 + 2x(1-a)] < 0 \ \forall x > 0$. It is easy to verify that $x = a - 1$ *i.e.* $z = \log(x)$ is the only extremum point for $\tilde{\Omega}$. Hence it does not have any real extremum value. Consequently, $\tilde{\Omega}'$ does not change sign for $x > 0$. Thus $\tilde{\Omega}' < 0 \ \forall x > 0$. Let $\alpha$ be the zero of $f(x)$. By Theorem 2.2.5, for any $x_0 > 0$ such that $\log(x_0) < \log(\alpha)$ the SNM converges to $\alpha$.

CHAPTER 3

# Numerical Simulation

Finding inversion of special functions is one of the central problems in numerical analysis with many applications. Finding inverse of a function can be seen as finding zeros of a suitable function. In other words, if one wants to find $f^{-1}(\alpha)$, it is equivalent to find the zero of a function $g(x)$ where $g(x) = f(x) - \alpha$. Recently, J. Segura [**9**] proposed Schwarzian Newton's method for finding the zero of a function which is a solution to a second order differential equation. A detailed discussion is provided in [**9**] for finding the inverse of central gamma function, central beta distribution and the incomplete elliptical integral of second kind. In this section, using the idea of [**9**], the inversion of Normal distribution is discussed. This section also extends the Schwarzian Newton's method [**9**] to find the inversion of generalized gamma distribution. This section also provides an interesting numerical simulation results by comparing Newton's method, average Newton's method and Schwarzian Newton's method.

## 3.1. Inversion of Normal Distribution.

In this section, the inversion of cumulative distribution function of Normal distribution is discussed. The cumulative distribution function $\Phi$ of Normal distribution is given by

$$\Phi(x) = \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{x} e^{-\left(\frac{t-\mu}{\sigma\sqrt{2}}\right)^2} dt$$

where $\mu$ is mean of distribution and $\sigma$ is standard deviation.

Let $f(x) = \Phi(x) - \alpha$ , where $\alpha \in (0,1)$. Consequently, $f$ satisfies the following differential equation.

$$f''(x) + B(x)f'(x) = 0, \quad B(x) = \frac{x-\mu}{\sigma}.$$

Note that

$$\begin{aligned}
\Omega &= -\frac{1}{4}B^2 - \frac{1}{2}B' \\
&= -\frac{1}{4}\Big(\frac{x-\mu}{\sigma}\Big)^2 - \frac{1}{2\sigma^2} \\
\Omega &< 0.
\end{aligned}$$

Consequently, $\Omega'(x) = -\frac{1}{2\sigma^3}(x-\mu)$ and $\Omega''(x) = -\frac{1}{2\sigma^3} < 0$.
Thus $\Omega$ has only one extremum at $x = \mu$, which is maximum. Hence by corollary 2.2.1 for the initial guess $x_0 = \mu$, the Schwarzian Newton's method converges to the zero of $f(x)$. The zero of $f(x)$ is nothing but $\Phi^{-1}(\alpha)$.

| S No. | $\mu$ | $\sigma$ | $x$ | SM | NM | AM | $T_1$ | $T_2$ | $T_3$ |
|---|---|---|---|---|---|---|---|---|---|
| 1. | 5 | 3 | 6.2922 | 4 | 4 | 3 | 0.059825 | 0.018026 | 0.057159 |
| 2. | 5 | 7 | 8.0151 | 5 | 5 | 3 | 0.023748 | 0.017570 | 0.017260 |
| 3. | 25 | 22 | 34.4760 | 5 | 5 | 3 | 0.020559 | 0.008716 | 0.015228 |
| 4. | 25 | 30 | 37.9218 | 5 | 5 | 3 | 0.023723 | 0.008436 | 0.014324 |
| 5. | 100 | 70 | 130.1509 | 5 | 5 | 3 | 0.024717 | 0.008457 | 0.015759 |
| 6. | 100 | 150 | 164.6091 | 6 | 6 | 3 | 0.027541 | 0.030277 | 0.015288 |
| 7. | 1000 | 600 | 1.2584e+3 | 6 | 6 | 3 | 0.029290 | 0.021522 | 0.035796 |
| 8. | 1000 | 1100 | 1.4738e+3 | 6 | 6 | 3 | 0.023727 | 0.007852 | 0.018042 |

TABLE 3.1. Comparison table for CDF of Normal distribution when $\alpha = \frac{2}{3}$.

| S No. | $\mu$ | $\sigma$ | $x$ | SM | NM | AM | $T_1$ | $T_2$ | $T_3$ |
|---|---|---|---|---|---|---|---|---|---|
| 1. | 20 | 50 | -22.0810 | 9 | 9 | 3 | 0.059120 | 0.025797 | 0.097967 |
| 2. | 70 | 50 | 27.9189 | 9 | 9 | 3 | 0.013711 | 0.0380 | 0.023046 |
| 3. | 70 | 100 | -14.1621 | 9 | 9 | 3 | 0.018320 | 0.024547 | 0.024856 |
| 4. | 150 | 100 | 65.8379 | 9 | 9 | 3 | 0.032012 | 0.029797 | 0.033761 |
| 5. | 250 | 500 | -170.8106 | 10 | 10 | 4 | 0.026628 | 0.036347 | 0.044347 |
| 6. | 700 | 500 | 279.1894 | 10 | 10 | 4 | 0.019391 | 0.104458 | 0.029608 |
| 7. | 500 | 1000 | -341.6212 | 10 | 10 | 4 | 0.013928 | 0.023380 | 0.056030 |
| 8. | 700 | 1000 | -141.6212 | 10 | 10 | 4 | 0.021235 | 0.029702 | 0.043973 |

TABLE 3.2. Comparison table for CDF of Normal distribution when $\alpha = \frac{1}{5}$.

| S No. | $\mu$ | $\sigma$ | $x$ | SM | NM | AM | $T_1$ | $T_2$ | $T_3$ |
|---|---|---|---|---|---|---|---|---|---|
| 1. | 6 | 3 | 5.46 | 3 | 3 | 3 | 0.011371 | 0.035329 | 0.057669 |
| 2. | 6 | 5 | 5.0999 | 3 | 3 | 3 | 0.011608 | 0.010414 | 0.022659 |
| 3. | 6 | 9 | 4.3799 | 3 | 3 | 3 | 0.019088 | 0.008030 | 0.010461 |
| 4. | 6 | 15 | 3.2998 | 4 | 4 | 3 | 0.025483 | 0.010257 | 0.011161 |
| 5. | 6 | 40 | -1.2005 | 4 | 4 | 3 | 0.028250 | 0.009705 | 0.012167 |
| 6. | 6 | 55 | -3.9007 | 4 | 4 | 3 | 0.020419 | 0.017162 | 0.009093 |
| 7. | 6 | 73 | -7.1409 | 4 | 4 | 3 | 0.022754 | 0.010264 | 0.011807 |
| 8. | 6 | 80 | -8.4010 | 4 | 4 | 3 | 0.023331 | 0.011013 | 0.012584 |

TABLE 3.3. Comparison table for CDF of Normal distribution when $\alpha = \frac{3}{7}$.

| S No. | $\mu$ | $\sigma$ | $x$ | SM | NM | AM | $T_1$ | $T_2$ | $T_3$ |
|---|---|---|---|---|---|---|---|---|---|
| 1. | 2 | 10 | 11.6742 | 9 | 9 | 3 | 0.128476 | 0.039262 | 0.0736519 |
| 2. | 8 | 10 | 17.6742 | 9 | 9 | 3 | 0.026881 | 0.020104 | 0.038409 |
| 3. | 20 | 10 | 29.6742 | 9 | 9 | 3 | 0.016834 | 0.053632 | 0.026987 |
| 4. | 50 | 10 | 59.6742 | 9 | 9 | 3 | 0.016123 | 0.014745 | 0.018822 |
| 5. | 200 | 10 | 209.6742 | 9 | 9 | 3 | 0.014272 | 0.013809 | 0.021979 |
| 6. | 520 | 10 | 529.6742 | 9 | 9 | 3 | 0.040001 | 0.011254 | 0.020548 |
| 7. | 1110 | 10 | 1.1197e+03 | 9 | 9 | 3 | 0.060823 | 0.016459 | 0.028956 |
| 8. | 1506 | 10 | 1.5157e+03 | 9 | 9 | 3 | 0.018749 | 0.013352 | 0.031925 |

TABLE 3.4. Comparison table for CDF of Normal distribution when $\alpha = \frac{5}{6}$.

Table 3.1 to table 3.4 provide the numerical simulation results for various algorithms applied on CDF of Normal distribution. Throughout the tables SM, NM and AM denote the number of iterations taken by Schwarzian Newton's method [**9**], Newton's method and Average Newton's method [**10**] respectively. $T_1, T_2$ and $T_3$ denote the time (in seconds) taken by the algorithms Schwarzian Newton's method, Newton's method and Average Newton's method respectively.

## 3.2. Generalized Gamma Distribution

In [**9**], the inverse of the cumulative distribution function of central gamma distribution is discussed using Schwarzian Newton's method. In this section, we extend this result to cumulative distribution function of generalized gamma distribution. The cumulative distribution function of generalized gamma distribution is given by

$$P(a,p,x) = \frac{\gamma(\frac{a}{p}, x^p)}{\Gamma(\frac{a}{p})}$$

where $\gamma(\frac{a}{p}, x^p) = \int_0^x t^{\frac{a}{p}-1} e^{-t^p} dt$ and $\Gamma(\frac{a}{p}) = \int_0^\infty t^{\frac{a}{p}-1} e^{-t} dt$

Let $f(x) = P(a,p,x) - \alpha$. It is easy to verify that $f$ satisfies the following second order differential equation.

$$f''(x) + B(x)f'(x) = 0, \quad B(x) = px^{p-1} - \frac{a}{px} + \frac{1}{x}.$$

Note that

$$\Omega = -\frac{1}{4}B^2 - \frac{1}{2}B'$$

$$\Omega = -\frac{p^2x^{2p-2}}{4} + \frac{1}{4x^2}\left(1 - \frac{a^2}{p^2}\right) + \frac{x^{p-2}}{2}(a - p^2). \tag{3.1}$$

**Lemma 3.2.1.** *If $p < \sqrt{2a-1}$ and $1 \leq p < a$, then $\Omega < 0$ for $x > 0$.*

*Proof.* From (3.1)

$$\Omega = -\frac{p^2x^{2p-2}}{4} + \frac{1}{4x^2}\left(1 - \frac{a^2}{p^2}\right) + \frac{x^{p-2}}{2}(a - p^2)$$

$$\Omega = \frac{1}{x^2}\Bigg( - \frac{p^2x^{2p}}{4} + \frac{1}{4}\left(1 - \frac{a^2}{p^2}\right) + \frac{x^p}{2}(a - p^2)\Bigg). \tag{3.2}$$

Let $x^p = t$, then equation (3.2) becomes

$$\Omega(t^{\frac{1}{p}}) = \tfrac{1}{t^{\frac{2}{p}}}\Bigg( - \tfrac{p^2t^2}{4} + \tfrac{t}{2}(a - p^2) + \tfrac{1}{4}\Big(1 - \tfrac{a^2}{p^2}\Big)\Bigg).$$

Note that using the hypothesis $p < \sqrt{2a-1}$ and $1 \leq p < a$, the discriminant of $\Bigg( - \tfrac{p^2t^2}{4} + \tfrac{t}{2}(a-p^2) + \tfrac{1}{4}\Big(1 - \tfrac{a^2}{p^2}\Big)\Bigg)$ is negative. Consequently, $\Omega$ does not have any real zeros. Thus $\Omega(x)$ has same sign for $x > 0$. Using the following limit

$$\lim_{x\to 0}\Omega(x) = \lim_{x\to 0} -\frac{p^2x^{2p-2}}{4} + \frac{1}{4x^2}\Big(1-\frac{a^2}{p^2}\Big) + \frac{x^{p-2}}{2}(a-p^2) = -\infty, \tag{3.3}$$

one can conclude that $\Omega(x) < 0$ for all $x > 0$. Hence the result.

□

**Lemma 3.2.2.** *If $p < \sqrt{2a-1}$ and $1 \le p < a$, then $\Omega(x)$ has only one extremum i.e. maximum.*

*Proof.*

$$\Omega'(x) = \frac{-p^2(p-1)}{2}x^{2p-3} + \frac{1}{2x^3}\left(\frac{a^2}{p^2}-1\right) + \frac{1}{2}(a-p^2)(p-2)x^{p-3}$$

$$\Omega'(x) = \frac{1}{x^3}\left(\frac{-p^2(p-1)}{2}x^{2p} + \frac{1}{2}\left(\frac{a^2}{p^2}-1\right) + \frac{1}{2}(a-p^2)(p-2)x^p\right). \tag{3.4}$$

Use the change of variable $x^p = t$, in equation (3.4) which leads to $\Omega'(t^{\frac{1}{p}}) = \frac{1}{t^{\frac{3}{p}}}\left(\frac{-p^2(p-1)}{2}t^2 + \frac{1}{2}(a-p^2)(p-2)t + \frac{1}{2}\left(\frac{a^2}{p^2}-1\right)\right)$. Note that the discriminant of the quadratic polynomial is $(p^2-a)^2(p-2)^2 + 4(p-1)(a^2-p)$ which is always positive. Hence $\Omega'$ has two real roots.

Consider the first real root

$$t_1 = \frac{(p^2-a)(p-2) + \sqrt{(p^2-a)^2(p-2)^2 + 4(p-1)(a^2-p)}}{-2p^2(p-1)} < 0.$$

This root can be neglected as our focus is only on positive real axis. The other root is

$$t_2 = \frac{(p^2-a)(p-2) - \sqrt{(p^2-a)^2(p-2)^2 + 4(p-1)(a^2-p)}}{-2p^2(p-1)} > 0$$

Consequently, $x^p = t$ has only one real root. Thus $x_0 = \left(\frac{(p^2-a)(p-2) - \sqrt{(p^2-a)^2(p-2)^2+4(p-1)(a^2-p)}}{-2p^2(p-1)}\right)^{\frac{1}{p}}$ is the only extremum of $\Omega(x)$ which is maximum. □

Hence for the choice $x_0$ as the initial guess Schwarzian Newton's method will converge to the zero of $f(x)$ by corollary 2.2.1. The zero of $f(x)$ is nothing but $P^{-1}(\alpha)$.

| S No. | $a$ | $x$ | SM | NM | ANM | $T_1$ | $T_2$ | $T_3$ |
|---|---|---|---|---|---|---|---|---|
| 1. | 2 | 1.3051 | 3 | 4 | 4 | 0.007161 | 0.006621 | 0.014429 |
| 2. | 3 | 2.1915 | 5 | 5 | 4 | 0.009937 | 0.008383 | 0.016406 |
| 3. | 5 | 4.0196 | 10 | 10 | 9 | 0.022883 | 0.030964 | 0.033505 |
| 4. | 6 | 4.9485 | 26 | 26 | 24 | 0.052943 | 0.034876 | 0.067967 |
| 5. | 8 | 6.8235 | 673 | 702 | 613 | 0.585162 | 0.513897 | 1.355498 |

TABLE 3.5. Comparison table for CDF of Central gamma distribution when $\alpha = \frac{3}{8}$.

Table 3.5 provides the numerical simulation results for various algorithms applied on CDF of central gamma distribution. Here SM, NM and AM denote the number of iterations taken by Schwarzian Newton's method [**9**], Newton's method and Average Newton's method [**10**] respectively. $T_1, T_2$ and $T_3$ denote the time (in seconds) taken by the algorithms Schwarzian Newton's method, Newton's method and Average Newton's method respectively.

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