

One Dimensional Non-Linear Problems

Lectures for PHD course on
Numerical optimization

Enrico Bertolazzi

DIMS – Università di Trento

November 21 – December 14, 2011

- 1 The Newton–Raphson method
 - Standard Assumptions
 - Local Convergence of the Newton–Raphson method
 - Stopping criteria
- 2 Convergence order
 - Q -order of convergence
 - R -order of convergence
- 3 The Secant method
 - Local convergence of the the Secant Method
- 4 The quasi-Newton method
 - Local convergence of quasi-Newton method
- 5 Fixed–Point procedure
 - Contraction mapping Theorem
- 6 Stopping criteria and q -order estimation



In this lecture some classical numerical scheme for the approximation of the zeros of nonlinear one-dimensional equations are presented.

The methods are exposed in some details, moreover many of the ideas presented in this lecture can be extended to the multidimensional case.



The problem we want to solve

Formulation

Given $f : [a, b] \mapsto \mathbb{R}$

Find $\alpha \in [a, b]$ for which $f(\alpha) = 0$.

Example

Let

$$f(x) = \log(x) - 1$$

which has $f(\alpha) = 0$ for $\alpha = \exp(1)$.

Some example

Consider the following three one-dimensional problems

- 1 $f(x) = x^4 - 12x^3 + 47x^2 - 60x$;
- 2 $g(x) = x^4 - 12x^3 + 47x^2 - 60x + 24$;
- 3 $h(x) = x^4 - 12x^3 + 47x^2 - 60x + 24.1$;

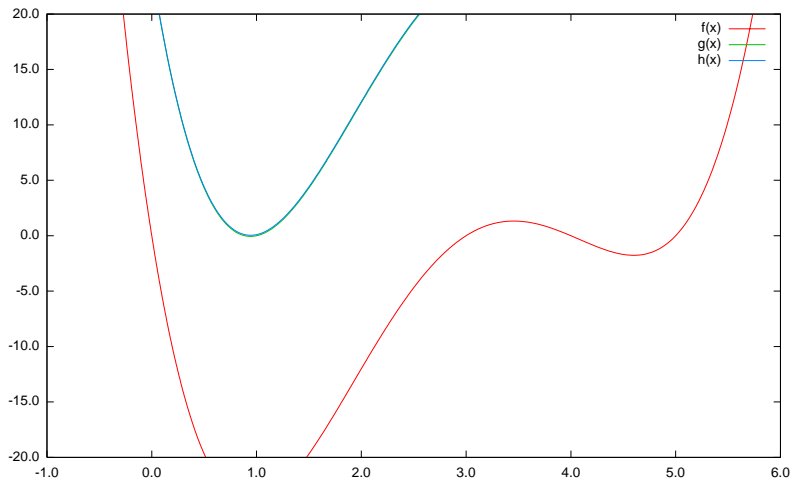
The roots of $f(x)$ are $x = 0$, $x = 3$, $x = 4$ and $x = 5$ the real roots of $g(x)$ are $x = 1$ and $x \approx 0.8888$; $h(x)$ has no real roots.

So in general a non linear problem may have

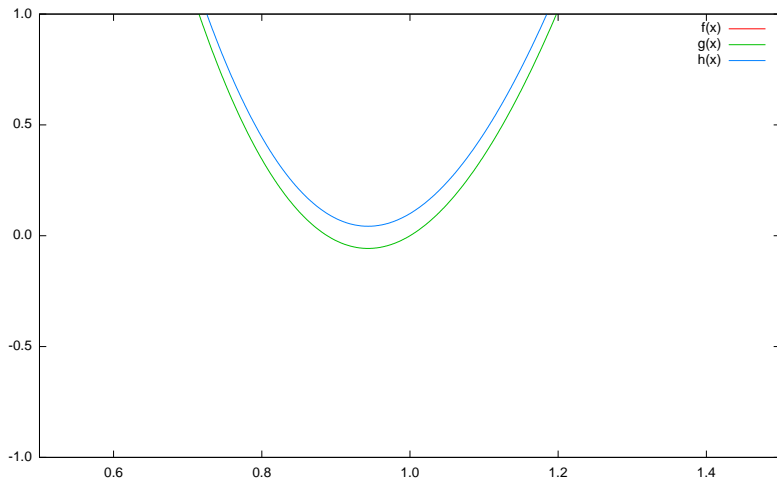
- One or more then one solutions;
- No solution.



Plotting of $f(x)$, $g(x)$ and $h(x)$



Plotting of $f(x)$, $g(x)$ and $h(x)$ (zoomed)



Outline

- 1 The Newton–Raphson method
 - Standard Assumptions
 - Local Convergence of the Newton–Raphson method
 - Stopping criteria
- 2 Convergence order
 - Q -order of convergence
 - R -order of convergence
- 3 The Secant method
 - Local convergence of the the Secant Method
- 4 The quasi-Newton method
 - Local convergence of quasi-Newton method
- 5 Fixed–Point procedure
 - Contraction mapping Theorem
- 6 Stopping criteria and q -order estimation



The original Newton procedure

Isaac Newton (1643-1727) used the following arguments

- Consider the polynomial $f(x) = x^3 - 2x - 5$ and take $x \approx 2$ as approximation of one of its root.
- Setting $x = 2 + p$ we obtain $f(2 + p) = p^3 + 6p^2 + 10p - 1$, if 2 is a good approximation of a root of $f(x)$ then p is a small number ($p \ll 1$) and p^2 and p^3 are very small numbers.
- Neglecting p^2 and p^3 and solving $10p - 1 = 0$ yields $p = 0.1$.
- Considering
 $f(2 + p + q) = f(2.1 + q) = q^3 + 6.3q^2 + 11.23q + 0.061$,
 neglecting q^3 and q^2 and solving $11.23q + 0.061 = 0$, yields
 $q = -0.0054$.
- Analogously considering $f(2 + p + q + r)$ yields
 $r = 0.00004863$.

The original Newton procedure

Further considerations

- The Newton procedure construct the approximation of the real root 2.094551482... of $f(x) = x^3 - 2x - 5$ by **successive correction**.
- The corrections are smaller and smaller as the procedure advances.
- The corrections are computed by using a **linear approximation** of the polynomial equation.



The Newton procedure: a modern point of view

(1/2)

- Consider the following function $f(x) = x^{3/2} - 2$ and let $x \approx 1.5$ an approximation of one of its root.
- Setting $x = 1.5 + p$ yields
 $f(1.5 + p) = -0.1629 + 1.8371p + \mathcal{O}(p^2)$, if 1.5 is a good approximation of a root of $f(x)$ then $\mathcal{O}(p^2)$ is a small number.
- Neglecting $\mathcal{O}(p^2)$ and solving $-0.1629 + 1.8371p = 0$ yields $p = 0.08866$.
- Considering
 $f(1.5 + p + q) = f(1.5886 + q) = 0.002266 + 1.89059q + \mathcal{O}(q^2)$, neglecting $\mathcal{O}(q^2)$ and solving $0.002266 + 1.89059q = 0$ yields $q = -0.001198$.



The Newton procedure: a modern point of view

(2/2)

The previous procedure can be resumed as follows:

- 1 Consider the following function $f(x)$. We know an approximation of a root x_0 .
- 2 Expand by Taylor series
$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \mathcal{O}((x - x_0)^2).$$
- 3 Drop the term $\mathcal{O}((x - x_0)^2)$ and solve
$$0 = f(x_0) + f'(x_0)(x - x_0).$$
 Call x_1 this solution.
- 4 Repeat 1 – 3 with x_1, x_2, x_3, \dots

Algorithm (Newton iterative scheme)

Let x_0 be assigned, then for $k = 0, 1, 2, \dots$

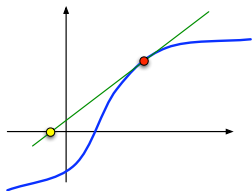
$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}.$$



The Newton procedure: a geometric point of view

Let $f \in C^1(a, b)$ and x_0 be an approximation of a root of $f(x)$. We approximate $f(x)$ by the tangent line at $(x_0, f(x_0))^T$.

$$y = f(x_0) + (x - x_0)f'(x_0). \quad (\star)$$



The intersection of the line (\star) with the x axis, that is $x = x_1$, is the new approximation of the root of $f(x)$,

$$0 = f(x_0) + (x_1 - x_0)f'(x_0), \quad \Rightarrow \quad x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}.$$



Standard Assumptions

Definition (Lipschitz function)

a function $g : [a, b] \mapsto \mathbb{R}$ is **Lipschitz** if there exists a constant γ such that

$$|g(x) - g(y)| \leq \gamma |x - y|$$

for all $x, y \in (a, b)$ satisfy

Example (Continuous non Lipschitz function)

Any Lipschitz function is continuous, but the converse is not true. Consider $g : [0, 1] \mapsto \mathbb{R}$, $g(x) = \sqrt{x}$. This function is not Lipschitz, because

$$\left| \sqrt{x} - \sqrt{0} \right| \leq \gamma |x - 0|$$

but $\lim_{x \rightarrow 0^+} \sqrt{x}/x = \infty$.



Standard Assumptions

In the study of convergence of numerical schemes, some standard regularity assumptions are assumed for the function $f(x)$.

Assumption (Standard Assumptions)

The function $f : [a, b] \mapsto \mathbb{R}$ is continuous, derivable with Lipschitz derivative $f'(x)$. i.e.

$$|f'(x) - f'(y)| \leq \gamma |x - y|. \quad \forall x, y \in [a, b]$$

Lemma (Taylor like expansion)

Let $f(x)$ satisfy the standard assumptions, then

$$|f(y) - f(x) - f'(x)(y - x)| \leq \frac{\gamma}{2} |x - y|^2. \quad \forall x, y \in [a, b]$$

Proof of Lemma

From basic Calculus:

$$f(y) - f(x) - f'(x)(y - x) = \int_x^y [f'(z) - f'(x)] dz$$

making the change of variable $z = x + t(y - x)$ we have

$$f(y) - f(x) - f'(x)(y - x) = \int_0^1 [f'(x + t(y - x)) - f'(x)](y - x) dt$$

and

$$|f(y) - f(x) - f'(x)(y - x)| \leq \int_0^1 \gamma t |y - x| |y - x| dt = \frac{\gamma}{2} |y - x|^2$$



Theorem (Local Convergence of Newton method)

Let $f(x)$ satisfy standard assumptions, and α be a simple root (i.e. $f'(\alpha) \neq 0$). If $|x_0 - \alpha| \leq \delta$ with $C\delta \leq 1$ where

$$C = \frac{\gamma}{|f'(\alpha)|}$$

then, the sequence generated by the Newton method satisfies:

- 1 $|x_k - \alpha| \leq \delta$ for $k = 0, 1, 2, 3, \dots$
- 2 $|x_{k+1} - \alpha| \leq C |x_k - \alpha|^2$ for $k = 0, 1, 2, 3, \dots$
- 3 $\lim_{k \rightarrow \infty} x_k = \alpha$.



proof of local convergence

Consider a Newton step with $|x_k - \alpha| \leq \delta$ and

$$x_{k+1} - \alpha = x_k - \alpha - \frac{f(x_k) - f(\alpha)}{f'(x_k)} = \frac{f(\alpha) - f(x_k) - f'(x_k)(\alpha - x_k)}{f'(x_k)}$$

taking absolute value and using the Taylor expansion like lemma

$$|x_{k+1} - \alpha| \leq \gamma |x_k - \alpha|^2 / (2 |f'(x_k)|)$$

$f' \in C^1(a, b)$ so that there exists a δ such that $2 |f'(x)| > |f'(\alpha)|$ for all $|x_k - \alpha| \leq \delta$. Choosing δ such that $\gamma\delta \leq |f'(\alpha)|$ we have

$$|x_{k+1} - \alpha| \leq C |x_k - \alpha|^2 \leq |x_k - \alpha|, \quad C = \gamma / |f'(\alpha)|$$

By induction we prove point 1. Point 2 and 3 follow trivially.



Stopping criteria

An iterative scheme generally does not find the solution in a **finite** number of steps. Thus, **stopping criteria** are needed to interrupt the computation. The major ones are:

- 1 $|f(x_{k+1})| \leq \tau$
- 2 $|x_{k+1} - x_k| \leq \tau |x_{k+1}|$
- 3 $|x_{k+1} - x_k| \leq \tau \max\{|x_k|, |x_{k+1}|\}$
- 4 $|x_{k+1} - x_k| \leq \tau \max\{\text{typ } \mathbf{x}, |x_{k+1}|\}$

Typ \mathbf{x} is the **typical size of \mathbf{x}** and $\tau \approx \sqrt{\varepsilon}$ where ε is the machine precision.



Outline

- 1 The Newton–Raphson method
 - Standard Assumptions
 - Local Convergence of the Newton–Raphson method
 - Stopping criteria
- 2 Convergence order
 - Q -order of convergence
 - R -order of convergence
- 3 The Secant method
 - Local convergence of the the Secant Method
- 4 The quasi-Newton method
 - Local convergence of quasi-Newton method
- 5 Fixed–Point procedure
 - Contraction mapping Theorem
- 6 Stopping criteria and q -order estimation



Convergence of a sequence of real number

The inequality $|x_{k+1} - \alpha| \leq C |x_k - \alpha|^2$ permits to say that Newton scheme is locally a **second order** scheme. We need a precise definition of convergence order; first we define a convergent sequence

Definition (Convergent sequence)

Let $\alpha \in \mathbb{R}$ and $x_k \in \mathbb{R}$, $k = 0, 1, 2, \dots$. Then, the sequence $\{x_k\}$ is said to **converge** to α if

$$\lim_{k \rightarrow \infty} |x_k - \alpha| = 0.$$



Definition (Q-order of a convergent sequence)

Let $\alpha \in \mathbb{R}$ and $x_k \in \mathbb{R}$, $k = 0, 1, 2, \dots$. Then $\{x_k\}$ is said:

- 1 **q-linearly convergent** if there exists a constant $C \in (0, 1)$ and an integer $m > 0$ such that for all $k \geq m$

$$|x_{k+1} - \alpha| \leq C |x_k - \alpha|$$

- 2 **q-super-linearly convergent** if there exists a sequence $\{C_k\}$ convergent to 0 such that

$$|x_{k+1} - \alpha| \leq C_k |x_k - \alpha|$$

- 3 **convergent sequence of q-order p** ($p > 1$) if there exists a constant C and an integer $m > 0$ such that for all $k \geq m$

$$|x_{k+1} - \alpha| \leq C |x_k - \alpha|^p$$

Quotient order of convergence

The prefix q in the q -order of convergence is a shortcut for **quotient**, and results from the quotient criteria of convergence of a sequence.

Remark

Let $\alpha \in \mathbb{R}$ and $x_k \in \mathbb{R}$, $k = 0, 1, 2, \dots$. Then $\{x_k\}$ is said:

- 1 **q -quadratic** if is q -convergent of order p with $p = 2$
- 2 **q -cubic** if is q -convergent of order p with $p = 3$

another useful generalization of q -order of convergence:

Definition (j -step q -order convergent sequence)

Let $\alpha \in \mathbb{R}$ and $x_k \in \mathbb{R}$, $k = 0, 1, 2, \dots$. Then $\{x_k\}$ is said **j -step q -convergent of order p** if there exists a constant C and an integer $m > 0$ such that for all $k \geq m$

$$|x_{k+j} - \alpha| \leq C |x_k - \alpha|^p$$



Root order of convergence

There may exist convergent sequences that do not have a q -order of convergence.

Example (convergent sequence without a q -order)

Consider the following sequence

$$x_k = \begin{cases} 1 + 2^{-k} & \text{if } k \text{ is not prime} \\ 1 & \text{otherwise} \end{cases}$$

it is easy to show that $\lim_{k \rightarrow \infty} x_k = 1$ but $\{x_k\}$ cannot be q -order convergent.



Root order convergence

A weaker definition of order of convergence is the following

Definition (R -order convergent sequence)

Let $\alpha \in \mathbb{R}$ and $\{x_k\}_{k=0}^{\infty} \subset \mathbb{R}$. Let $\{y_k\}_{k=0}^{\infty} \subset \mathbb{R}$ be a dominating sequence, i.e. there exists m and C such that

$$|x_k - \alpha| \leq C |y_k - \alpha|, \quad k \geq m.$$

Then $\{x_k\}$ is said *at least*:

- ① *r -linearly convergent* if $\{y_k\}$ is q -linearly convergent.
- ② *r -super-linearly convergent* if $\{y_k\}$ is q -super-linearly convergent.
- ③ *convergent sequence of r -order p* ($p > 1$) if $\{y_k\}$ is a convergent sequence of q -order p .

Convergent sequences without a q -order of convergence but with an r -order of convergence.

Example

Consider again the sequence

$$x_k = \begin{cases} 1 + 2^{-k} & \text{if } k \text{ is not prime} \\ 1 & \text{otherwise} \end{cases}$$

it is easy to show that the sequence

$$\{y_k\} = \{1 + 2^{-k}\}$$

is q -linearly convergent and that

$$|x_k - 1| \leq |y_k - 1|$$

for $k = 0, 1, 2, \dots$



The q -order and r -order measure the speed of convergence of a sequence. A sequence may be convergent but cannot be measured by q -order or r -order.

Example

The sequence $\{x_k\} = \{1 + 1/k\}$ may not be q -linearly convergent, unless $C < 1$ becomes

$$|x_{k+1} - 1| \leq C |x_k - 1| \quad \Rightarrow \quad \frac{1}{k+1} \leq \frac{C}{k}$$

also implies

$$\frac{k(1-C) - C}{k(k+1)} \leq 0$$

have that for $k > C/(1-C)$ the inequality is not satisfied.

Outline

- 1 The Newton–Raphson method
 - Standard Assumptions
 - Local Convergence of the Newton–Raphson method
 - Stopping criteria
- 2 Convergence order
 - Q -order of convergence
 - R -order of convergence
- 3 The Secant method
 - Local convergence of the the Secant Method
- 4 The quasi-Newton method
 - Local convergence of quasi-Newton method
- 5 Fixed–Point procedure
 - Contraction mapping Theorem
- 6 Stopping criteria and q -order estimation

Secant method

Newton method is a **fast** (q -order 2) numerical scheme to approximate the root of a function $f(x)$ but needs the knowledge of the first derivative of $f(x)$. Sometimes first derivative is not available or not computable, in this case a numerical procedure to approximate the root which does not use derivative is required. A simple modification of the Newton–Raphson scheme where the first derivative is approximated by a finite difference produces the **secant** method:

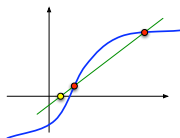
$$x_{k+1} = x_k - \frac{f(x_k)}{a_k}, \quad a_k = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$



The secant method: a geometric point of view

Let us take $f \in C(a, b)$ and x_0 and x_1 be different approximations of a root of $f(x)$. We can approximate $f(x)$ by the secant line for $(x_0, f(x_0))^T$ and $(x_1, f(x_1))^T$.

$$y = \frac{f(x_0)(x_1 - x) + f(x_1)(x - x_0)}{x_1 - x_0}. \quad (\star)$$



The intersection of the line (\star) with the x axes at $x = x_2$ is the new approximation of the root of $f(x)$,

$$0 = \frac{f(x_0)(x_1 - x_2) + f(x_1)(x_2 - x_0)}{x_1 - x_0}, \quad \Rightarrow \quad x_2 = x_1 - \frac{f(x_1)}{\frac{f(x_1) - f(x_0)}{x_1 - x_0}}.$$



Algorithm (Secant scheme)

Let $x_0 \neq x_1$ assigned, for $k = 1, 2, \dots$

$$x_{k+1} = x_k - \frac{f(x_k)}{\frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}} = \frac{x_{k-1}f(x_k) - x_k f(x_{k-1})}{f(x_k) - f(x_{k-1})}$$

Remark

*In the secant method near convergence we have $f(x_k) \approx f(x_{k-1})$, so that **numerical cancellation** problem may arise. In this case we must stop the iteration before such a problem is encountered, or we must modify the secant method near convergence.*

Local convergence of the Secant Method

Theorem

Let $f(x)$ satisfy standard assumptions, and α be a simple root (i.e. $f'(\alpha) \neq 0$); then, there exists $\delta > 0$ such that $C\delta \leq \exp(-p) < 1$ where

$$C = \frac{\gamma}{|f'(\alpha)|} \quad \text{and} \quad p = \frac{1 + \sqrt{5}}{2} = 1.618034 \dots$$

For all $x_0, x_1 \in [\alpha - \delta, \alpha + \delta]$ with $x_0 \neq x_1$ we have:

- 1 $|x_k - \alpha| \leq \delta$ for $k = 0, 1, 2, 3, \dots$
- 2 the sequence $\{x_k\}$ is convergent to α with r -order at least p .

Proof of Local Convergence

(1/5)

Subtracting α on both side of secant scheme

$$x_{k+1} - \alpha = (x_k - \alpha)(x_{k-1} - \alpha) \frac{\frac{f(x_k)}{x_k - \alpha} - \frac{f(x_{k-1})}{x_{k-1} - \alpha}}{f(x_k) - f(x_{k-1})}.$$

Moreover, because $f(\alpha) = 0$

$$\begin{aligned} \frac{\frac{f(x_k)}{x_k - \alpha} - \frac{f(x_{k-1})}{x_{k-1} - \alpha}}{f(x_k) - f(x_{k-1})} &= \frac{\frac{f(x_k) - f(\alpha)}{x_k - \alpha} - \frac{f(x_{k-1}) - f(\alpha)}{x_{k-1} - \alpha}}{f(x_k) - f(x_{k-1})}, \\ &= \frac{\frac{f(x_k) - f(\alpha)}{x_k - \alpha} - \frac{f(x_{k-1}) - f(\alpha)}{x_{k-1} - \alpha}}{x_k - x_{k-1}} \left(\frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \right)^{-1} \end{aligned}$$



Proof of Local Convergence

(2/5)

From Lagrange ¹ theorem and divided difference properties (see next lemma):

$$\frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} = f'(\eta_k), \quad \eta_k \in I[x_{k-1}, x_k],$$

$$\left| \frac{(f(x_k) - f(\alpha))/(x_k - \alpha) - (f(x_{k-1}) - f(\alpha))/(x_{k-1} - \alpha)}{x_k - x_{k-1}} \right| \leq \frac{\gamma}{2}$$

where $I[a, b]$ is the smallest interval containing a, b By using these equations, we can write

$$|x_{k+1} - \alpha| \leq |x_k - \alpha| |x_{k-1} - \alpha| \frac{\gamma}{2 |f'(\eta_k)|}, \quad \eta_k \in I[x_{k-1}, x_k]$$

¹Joseph-Louis Lagrange 1736—1813



Proof of Local Convergence

(3/5)

As α is a simple root, there exists $\delta > 0$ such that for all $x \in [\alpha - \delta, \alpha + \delta]$ we have $2|f'(x)| \geq |f'(\alpha)|$; if x_k and x_{k-1} are in $x \in [\alpha - \delta, \alpha + \delta]$ we have

$$|x_{k+1} - \alpha| \leq C |x_k - \alpha| |x_{k-1} - \alpha|$$

by reducing δ , we obtain $C\delta \leq \exp(-p) < 1$, and by induction, we can show that $x_k \in [\alpha - \delta, \alpha + \delta]$ for $k = 1, 2, 3, \dots$

To prove r -order, we set $e_i = C |x_i - \alpha|$ so that

$$|x_{k+1} - \alpha| \leq C |x_k - \alpha| |x_{k-1} - \alpha| \quad \Rightarrow \quad e_{i+1} \leq e_i e_{i-1}$$



Proof of Local Convergence

(4/5)

Now we build a majoring sequence $\{E_k\}$ defined as $E_1 = \max\{e_0, e_1\}$, $E_0 \geq E_1$ and $E_{k+1} = E_k E_{k-1}$. It is easy to show that $e_k \leq E_k$, in fact

$$e_{k+1} \leq e_k e_{k-1} \leq E_k E_{k-1} = E_{k+1}.$$

By searching a solution of the form $E_k = E_0 \exp(-z^k)$ we have

$$\exp(-z^{k+1}) = \exp(-z^k) \exp(-z^{k-1}) = \exp(-z^k - z^{k-1}),$$

so that z must satisfy:

$$z^2 = z + 1, \quad \Rightarrow \quad z_{1,2} = \frac{1 \pm \sqrt{5}}{2} = \begin{cases} 1.618034\dots \\ -0.618034\dots \end{cases}$$



Proof of Local Convergence

(5/5)

In order to have convergence we must choose the positive root so that $E_k = E_0 \exp(-p^k)$ where $p = (1 + \sqrt{5})/2$. Finally $E_0 \geq E_1 = E_0 \exp(-p)$. In this way we have produced a majoring sequence E_k such that

$$|x_k - \alpha| \leq ME_k = ME_0 \exp(-p^k)$$

let us now compute the q -order of $\{E_k\}$.

$$\frac{E_{k+1}}{E_k^r} = \frac{ME_0 \exp(-p^{k+1})}{M^r E_0^r \exp(-rp^k)} = C \exp(-p^{k+1} + rp^k), \quad C = (ME_0)^{1-1/r}$$

and, by choosing $r = p$, we obtain $E_{k+1} \leq CE_k^r$.



Lemma

Let $f(x)$ satisfying standard assumptions, then

$$\left| \frac{\frac{f(\alpha + h) - f(\alpha)}{h} - \frac{f(\alpha - k) - f(\alpha)}{k}}{h + k} \right| \leq \frac{\gamma}{2}$$

The proof use the **trick function**

$$G(t) := \frac{\frac{f(\alpha + th) - f(\alpha)}{h} - \frac{f(\alpha - tk) - f(\alpha)}{k}}{h + k},$$

Note that $G(1)$ is the finite difference of the lemma.



Proof of lemma

The function $H(t) := G(t) - G(1)t^2$ is 0 in $t = 0$ and $t = 1$. In view of Rolle's theorem² there exists an $\eta \in (0, 1)$ such that $H'(\eta) = 0$. But

$$H'(t) = G'(t) - 2G(1)t, \quad G'(t) = \frac{f'(\alpha + th) - f'(\alpha - tk)}{h + k},$$

by evaluating $H'(\eta)$ we have $G'(\eta) = 2G(1)\eta$. Then

$$G(1) = \frac{1}{2\eta}G'(\eta) = \frac{f'(\alpha + \eta h) - f'(\alpha - \eta k)}{2\eta(h + k)}$$

The thesis follows by taking $|G(1)|$ and using the Lipschitz property of $f'(x)$.

²Michel Rolle 1652–1719



Outline

- 1 The Newton–Raphson method
 - Standard Assumptions
 - Local Convergence of the Newton–Raphson method
 - Stopping criteria
- 2 Convergence order
 - Q -order of convergence
 - R -order of convergence
- 3 The Secant method
 - Local convergence of the the Secant Method
- 4 The quasi-Newton method
 - Local convergence of quasi-Newton method
- 5 Fixed–Point procedure
 - Contraction mapping Theorem
- 6 Stopping criteria and q -order estimation

Quasi-Newton method

A simple modification on Newton scheme produces a whole classes of numerical schemes. if we take

$$x_{k+1} = x_k - \frac{f(x_k)}{a_k},$$

different choice of a_k produce different numerical scheme:

- ① If $a_k = f'(x_k)$ we obtain the **Newton Raphson** method.
- ② If $a_k = f'(x_0)$ we obtain the **chord** method.
- ③ If $a_k = f'(x_m)$ where $m = [k/p]p$ we obtain the **Shamanskii** method.
- ④ If $a_k = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$ we obtain the **secant** method.
- ⑤ If $a_k = \frac{f(x_k) - f(x_k - h_k)}{h_k}$ we obtain the **secant finite difference** method.

Remark

By choosing $h_k = x_{k-1} - x_k$ in the secant finite difference method, we obtain the secant method, so that this method is a generalization of the secant method.

Remark

If $h_k \neq x_{k-1} - x_k$ the secant finite difference method needs **two** evaluation of $f(x)$ per step, while the secant method needs only **one** evaluation of $f(x)$ per step.

Remark

In the secant method near convergence we have $f(x_k) \approx f(x_{k-1})$, so that **numerical cancellation** problem can arise. The Secant Finite Difference scheme does not have this problem provided that h_k is not too small.

Local convergence of quasi-Newton method

(1/3)

Let α be a simple root of $f(x)$ (i.e. $f(\alpha) \neq 0$) and $f(x)$ satisfy standard assumptions, then we can write

$$\begin{aligned}x_{k+1} - \alpha &= x_k - \alpha - a_k^{-1} f(x_k) \\&= a_k^{-1} [f(\alpha) - f(x_k) - a_k(\alpha - x_k)] \\&= a_k^{-1} [f(\alpha) - f(x_k) - f'(x_k)(\alpha - x_k) \\&\quad + (f'(x_k) - a_k)(\alpha - x_k)]\end{aligned}$$

By using the **Taylor Like expansion Lemma** we have

$$|x_{k+1} - \alpha| \leq |a_k|^{-1} \left(\frac{\gamma}{2} |x_k - \alpha| + |f'(x_k) - a_k| \right) |x_k - \alpha|$$



Local convergence of quasi-Newton method

(2/3)

Lemma

If $f(x)$ satisfies standard assumptions, then

$$\left| f'(x) - \frac{f(x) - f(x-h)}{h} \right| \leq \frac{\gamma}{2}h$$

from the Lemma we have that the **finite difference secant** scheme satisfies:

$$|x_{k+1} - \alpha| \leq \frac{\gamma}{2|a_k|} \left(|x_k - \alpha| + h_k \right) |x_k - \alpha|$$

Moreover, from

$$|f'(x_k)| \leq |f'(x_k) - a_k| + |a_k| \leq |a_k| + \frac{\gamma}{2}h_k$$

it follows that

$$|x_{k+1} - \alpha| \leq \frac{\gamma}{2|f'(x_k)| - \gamma h_k} \left(|x_k - \alpha| + h_k \right) |x_k - \alpha|$$



Local convergence of quasi-Newton method

(3/3)

Theorem

Let $f(x)$ satisfies standard assumptions, and α be a simple root; then, there exists $\delta > 0$ and $\eta > 0$ such that if $|x_0 - \alpha| < \delta$ and $0 < |h_k| \leq \eta$; the sequence $\{x_k\}$ given by

$$x_{k+1} = x_k - \frac{f(x_k)}{a_k}, \quad a_k = \frac{f(x_k) - f(x_k - h_k)}{h_k},$$

for $k = 1, 2, \dots$ is defined and q -linearly converges to α . Moreover,

- 1 If $\lim_{k \rightarrow \infty} h_k = 0$ then $\{x_k\}$ q -super-linearly converges to α .
- 2 If there exists a constant C such that $|h_k| \leq C|x_k - \alpha|$ or $|h_k| \leq C|f(x_k)|$ then the convergence is q -quadratic.
- 3 If there exists a constant C such that $|h_k| \leq C|x_k - x_{k-1}|$ then the convergence is:
 - **two-step** q -quadratic;
 - **one-step** r -order $p = (1 + \sqrt{5})/2$.



Outline

- 1 The Newton–Raphson method
 - Standard Assumptions
 - Local Convergence of the Newton–Raphson method
 - Stopping criteria
- 2 Convergence order
 - Q -order of convergence
 - R -order of convergence
- 3 The Secant method
 - Local convergence of the the Secant Method
- 4 The quasi-Newton method
 - Local convergence of quasi-Newton method
- 5 Fixed-Point procedure
 - Contraction mapping Theorem
- 6 Stopping criteria and q -order estimation



Fixed-Point procedure

Definition (Fixed point)

Given a map $\mathbf{G} : D \subset \mathbb{R}^m \mapsto \mathbb{R}^m$ we say that \mathbf{x}_\star is a fixed point of \mathbf{G} if:

$$\mathbf{x}_\star = \mathbf{G}(\mathbf{x}_\star).$$

Searching a zero of $f(x)$ is the same as searching a fixed point of:

$$g(x) = x - f(x).$$

A natural way to find a fixed point is by using iterations. For example by starting from x_0 we build the sequence

$$x_{k+1} = g(x_k), \quad k = 1, 2, \dots$$

We ask when the sequence $\{x_i\}_{i=0}^{\infty}$ is convergent to α .

Example (Fixed point Newton)

Newton-Raphson scheme can be written in the fixed point form by setting:

$$g(x) = x - \frac{f(x)}{f'(x)}$$

Example (Fixed point secant)

Secant scheme can be written in the fixed point form by setting:

$$\mathbf{G}(\mathbf{x}) = \begin{pmatrix} \frac{x_2 f(x_1) - x_1 f(x_2)}{f(x_1) - f(x_2)} \\ x_1 \end{pmatrix}$$



Contraction mapping Theorem

Theorem (Contraction mapping)

Let $\mathbf{G} : D \mapsto D \subset \mathbb{R}^n$ such that there exists $L < 1$

$$\|\mathbf{G}(\mathbf{x}) - \mathbf{G}(\mathbf{y})\| \leq L \|\mathbf{x} - \mathbf{y}\|, \quad \forall \mathbf{x}, \mathbf{y} \in D$$

Let \mathbf{x}_0 such that $B_\rho(\mathbf{x}_0) = \{\mathbf{x} \mid \|\mathbf{x} - \mathbf{x}_0\| \leq \rho\} \subset D$ where $\rho = \|\mathbf{G}(\mathbf{x}_0) - \mathbf{x}_0\| / (1 - L)$, then

- 1 There exists a unique fixed point \mathbf{x}_* in $B_\rho(\mathbf{x}_0)$.
- 2 The sequence $\{\mathbf{x}_k\}$ generated by $\mathbf{x}_{k+1} = \mathbf{G}(\mathbf{x}_k)$ remains in $B_\rho(\mathbf{x}_0)$ and q -linearly converges to \mathbf{x}_* with constant L .
- 3 The following error estimate is valid

$$\|\mathbf{x}_k - \mathbf{x}_*\| \leq \|\mathbf{x}_1 - \mathbf{x}_0\| \frac{L^k}{1 - L}$$

Proof of Contraction mapping

(1/2)

Prove that $\{\mathbf{x}_k\}_0^\infty$ is a Cauchy sequence

$$\|\mathbf{x}_{k+m} - \mathbf{x}_k\| \leq L \|\mathbf{x}_{k+m-1} - \mathbf{x}_{k-1}\| \leq \dots \leq L^k \|\mathbf{x}_m - \mathbf{x}_0\|$$

and

$$\begin{aligned} \|\mathbf{x}_m - \mathbf{x}_0\| &\leq \sum_{l=0}^{m-1} \|\mathbf{x}_{l+1} - \mathbf{x}_l\| \leq \sum_{l=0}^{m-1} L^l \|\mathbf{x}_1 - \mathbf{x}_0\| \\ &\leq \frac{1 - L^m}{1 - L} \|\mathbf{x}_1 - \mathbf{x}_0\| \leq \frac{\|\mathbf{x}_1 - \mathbf{x}_0\|}{1 - L} \end{aligned}$$

so that

$$\|\mathbf{x}_{k+m} - \mathbf{x}_k\| \leq \frac{L^k}{1 - L} \|\mathbf{x}_1 - \mathbf{x}_0\| \leq \rho$$

This prove that $\{\mathbf{x}_k\}_0^\infty \subset B_\rho(\mathbf{x}_0)$ and that is a Cauchy sequence.



Proof of Contraction mapping

(2/2)

Prove existence, uniqueness and rate

The sequence $\{\mathbf{x}_k\}_0^\infty$ is a Cauchy sequence so that there is the limit $\mathbf{x}_\star = \lim_{k \rightarrow \infty} \mathbf{x}_k$. To prove that \mathbf{x}_\star is a fixed point:

$$\begin{aligned} \|\mathbf{x}_\star - \mathbf{G}(\mathbf{x}_\star)\| &\leq \|\mathbf{x}_\star - \mathbf{x}_k\| + \|\mathbf{x}_k - \mathbf{G}(\mathbf{x}_k)\| + \|\mathbf{G}(\mathbf{x}_k) - \mathbf{G}(\mathbf{x}_\star)\| \\ &\leq (1 + L) \|\mathbf{x}_\star - \mathbf{x}_k\| + L^k \|\mathbf{x}_1 - \mathbf{x}_0\| \xrightarrow[k \rightarrow \infty]{} 0 \end{aligned}$$

Uniqueness is proved by contradiction, let be \mathbf{x} and \mathbf{y} two fixed points:

$$\|\mathbf{x} - \mathbf{y}\| = \|\mathbf{G}(\mathbf{x}) - \mathbf{G}(\mathbf{y})\| \leq L \|\mathbf{x} - \mathbf{y}\| < \|\mathbf{x} - \mathbf{y}\|$$

To prove convergence rate notice that $\mathbf{x}_{k+m} \mapsto \mathbf{x}_\star$ for $m \mapsto \infty$:

$$\begin{aligned} \|\mathbf{x}_k - \mathbf{x}_\star\| &\leq \|\mathbf{x}_k - \mathbf{x}_{k+m}\| + \|\mathbf{x}_{k+m} - \mathbf{x}_\star\| \\ &\leq \frac{L^k}{1 - L} \|\mathbf{x}_1 - \mathbf{x}_0\| + \|\mathbf{x}_{k+m} - \mathbf{x}_\star\| \end{aligned}$$



Example

Newton-Raphson in fixed point form

$$g(x) = x - \frac{f(x)}{f'(x)}, \quad g'(x) = \frac{f(x)f''(x)}{(f'(x))^2},$$

If α is a simple root of $f(x)$ then

$$g'(\alpha) = \frac{f(\alpha)f''(\alpha)}{(f'(\alpha))^2} = 0,$$

If $f(x) \in \mathcal{C}^2$ then $g'(x)$ is continuous in a neighborhood of α and by choosing ρ small enough we have

$$|g'(x)| \leq L < 1, \quad x \in [\alpha - \rho, \alpha + \rho]$$

From the contraction mapping theorem, it follows from that the Newton-Raphson method is locally convergent when α is a simple root.



Fast convergence

Suppose that α is a fixed point of $g(x)$ and $g \in \mathcal{C}^p$ with

$$g'(\alpha) = g''(\alpha) = \dots = g^{(p-1)}(\alpha) = 0,$$

by Taylor Theorem

$$g(x) = g(\alpha) + \frac{(x - \alpha)^p}{p!} g^{(p)}(\eta),$$

so that

$$|x_{k+1} - \alpha| = |g(x_k) - g(\alpha)| \leq \frac{|g^{(p)}(\eta_k)|}{p!} |x_k - \alpha|^p.$$

If $g^{(p)}(x)$ is bounded in a neighborhood of α it follows that the procedure has locally q -order of p .



Slow convergence

(1/2)

Newton-Raphson in fixed point form

$$g(x) = x - \frac{f(x)}{f'(x)}, \quad g'(x) = \frac{f(x)f''(x)}{(f'(x))^2},$$

If α is a multiple root, i.e.

$$f(x) = (x - \alpha)^n h(x), \quad h(\alpha) \neq 0 \quad n > 1$$

it follows that

$$f'(x) = n(x - \alpha)^{n-1}h(x) + (x - \alpha)^n h'(x)$$

$$f''(x) = (x - \alpha)^{n-2} [(n^2 - n)h(x) + 2n(x - \alpha)h'(x) + (x - \alpha)^2 h''(x)]$$



Slow convergence

(2/2)

Consequently,

$$g'(\alpha) = \frac{n(n-1)h(\alpha)^2}{n^2h(\alpha)^2} = 1 - \frac{1}{n},$$

so that

$$|g'(\alpha)| = 1 - \frac{1}{n} < 1$$

and the Newton-Raphson scheme is locally q -linearly convergent with coefficient $1 - 1/n$.



Outline

- 1 The Newton–Raphson method
 - Standard Assumptions
 - Local Convergence of the Newton–Raphson method
 - Stopping criteria
- 2 Convergence order
 - Q -order of convergence
 - R -order of convergence
- 3 The Secant method
 - Local convergence of the the Secant Method
- 4 The quasi-Newton method
 - Local convergence of quasi-Newton method
- 5 Fixed–Point procedure
 - Contraction mapping Theorem
- 6 Stopping criteria and q -order estimation



Stopping criteria for q -convergent sequences

(1/2)

- 1 Consider an iterative scheme that produces a sequence $\{x_k\}$ that converges to α with q -order p .
- 2 This means that there exists a constant C such that

$$|x_{k+1} - \alpha| \leq C |x_k - \alpha|^p \quad \text{for } k \geq m$$

- 3 If $\lim_{k \rightarrow \infty} \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|^p}$ exists and converge say to C then we have

$$|x_{k+1} - \alpha| \approx C |x_k - \alpha|^p \quad \text{for large } k$$

- 4 We can use this last expression to obtain an estimate of the error even if the values of p is unknown by using the only known values.

Stopping criteria q -convergent sequences

(2/2)

- ① If $|x_{k+1} - \alpha| \leq C |x_k - \alpha|^p$ we can write:

$$\begin{aligned} |x_k - \alpha| &\leq |x_k - x_{k+1}| + |x_{k+1} - \alpha| \\ &\leq |x_k - x_{k+1}| + C |x_k - \alpha|^p \\ &\Downarrow \\ |x_k - \alpha| &\leq \frac{|x_k - x_{k+1}|}{1 - C |x_k - \alpha|^{p-1}} \end{aligned}$$

- ② If x_k is so near to the solution that $C |x_k - \alpha|^{p-1} \leq \frac{1}{2}$, then

$$|x_k - \alpha| \leq 2 |x_k - x_{k+1}|$$

- ③ This fact justifies the two stopping criteria

$$|x_{k+1} - x_k| \leq \tau \quad \text{Absolute tolerance}$$

$$|x_{k+1} - x_k| \leq \tau \max\{|x_k|, |x_{k+1}|\} \quad \text{Relative tolerance}$$



Estimation of the q -order

(1/3)

- 1 Consider an iterative scheme that produce a sequence $\{x_k\}$ converging to α with q -order p .
- 2 If $|x_{k+1} - \alpha| \approx C |x_k - \alpha|^p$ then the ratio:

$$\log \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|} \approx \log \frac{C |x_k - \alpha|^p}{|x_k - \alpha|} = (p - 1) \log C^{\frac{1}{p-1}} |x_k - \alpha|$$

and analogously

$$\log \frac{|x_{k+2} - \alpha|}{|x_{k+1} - \alpha|} \approx \log \frac{C^{1+p} |x_k - \alpha|^{p^2}}{C |x_k - \alpha|^p} = p(p - 1) \log C^{\frac{1}{p-1}} |x_k - \alpha|$$

- 3 From this two ratios we can deduce p as follows

$$\log \frac{|x_{k+2} - \alpha|}{|x_{k+1} - \alpha|} \bigg/ \log \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|} \approx p$$



Estimation of the q -order

(2/3)

1 The ratio

$$\log \frac{|x_{k+2} - \alpha|}{|x_{k+1} - \alpha|} \bigg/ \log \frac{|x_{k+1} - \alpha|}{|x_k - \alpha|} \approx p$$

is expressed in term of unknown errors uses the error which is not known.

2 If we are near to the solution, we can use the estimation

$|x_k - \alpha| \approx |x_{k+1} - x_k|$ so that

$$\log \frac{|x_{k+2} - x_{k+3}|}{|x_{k+1} - x_{k+2}|} \bigg/ \log \frac{|x_{k+1} - x_{k+2}|}{|x_k - x_{k+1}|} \approx p$$

nd three iterations are enough to estimate the q -order of the sequence.



Estimation of the q -order

(3/3)

- 1 if the the step length is proportional to the value of $f(x)$ as in the Newton-Raphson scheme, i.e. $|x_k - \alpha| \approx M |f(x_k)|$ we can simplify the previous formula as:

$$\log \frac{|f(x_{k+2})|}{|f(x_{k+1})|} \bigg/ \log \frac{|f(x_{k+1})|}{|f(x_k)|} \approx p$$

- 2 Such estimation are useful to check the code implementation. In fact, if we expect the order p and we see the order $r \neq p$, something is wrong in the implementation or in the theory!



Conclusions

The methods presented in this lesson can be generalized for higher dimension. In particular

- 1 Newton-Raphson
 - multidimensional Newton scheme
 - inexact Newton scheme
- 2 Secant
 - Broyden scheme
- 3 quasi-Newton
 - finite difference approximation of the Jacobian

moreover those method can be **globalized**.



References



J. Stoer and R. Bulirsch

Introduction to numerical analysis

Springer-Verlag, Texts in Applied Mathematics, **12**, 2002.



J. E. Dennis, Jr. and Robert B. Schnabel

Numerical Methods for Unconstrained Optimization and
Nonlinear Equations

SIAM, Classics in Applied Mathematics, **16**, 1996.