

# One Dimensional Non-Linear Problems

Lectures for PHD course on  
Numerical Optimization

Enrico Bertolazzi

DII – Università di Trento



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- 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



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# Introduction

In this lecture some classical numerical scheme for the approximation of the zeroes 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.



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# 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  $\alpha = \exp(1)$ .



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# 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 solutions;
- No solution.



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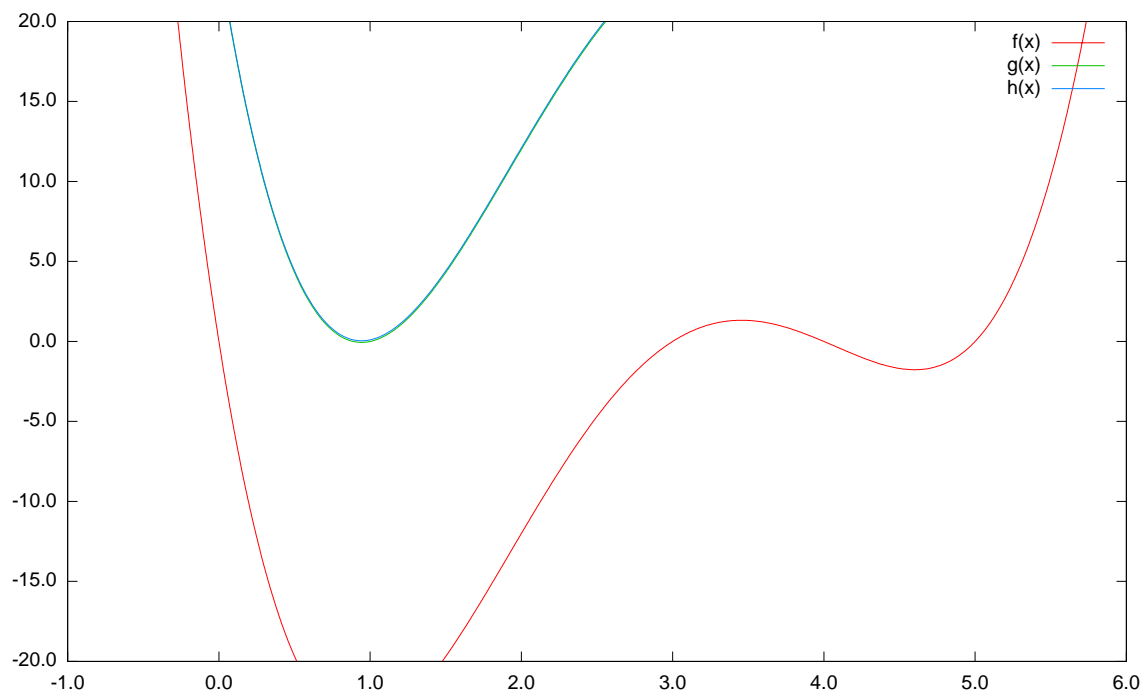
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# Plotting of $f(x)$ , $g(x)$ and $h(x)$



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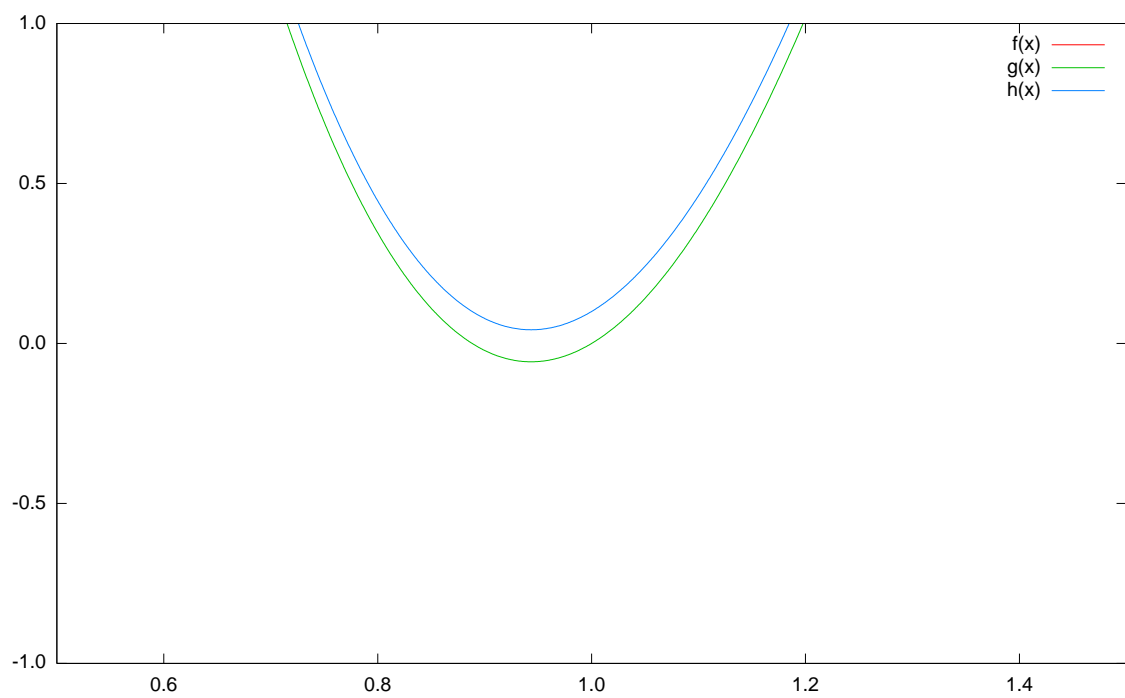
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# Plotting of $f(x)$ , $g(x)$ and $h(x)$ (zoomed)



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# Outline

## 1 The Newton–Raphson method

- Standard Assumptions
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- 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

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# 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  $r = 0.00004863$ .



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# The original Newton procedure

## Further considerations

- The Newton procedure constructs the approximation of the real root  $2.094551482\dots$  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.



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- 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  $q = -0.001198$ .



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

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



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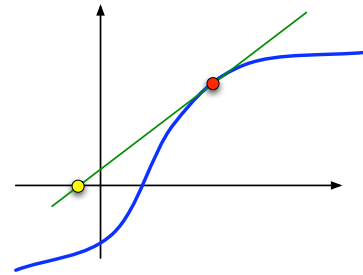
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# Newton scheme: Geometric point of view

Let  $f \in \mathcal{C}^1(a, b)$  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  $f(x)$ ,

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



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# Standard Assumptions

## Definition (Lipschitz function)

a function  $g : [a, b] \mapsto \mathbb{R}$  is **Lipschitz** if there exists a constant  $\gamma > 0$  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, if not we have

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

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



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# Standard Assumptions

In the study of convergence of numerical scheme, 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 expansion)

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

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



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**Proof:** 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

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

and

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



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# Local Convergence

Newton scheme converges locally near simple roots:

## Theorem (Local Convergence of Newton method)

Let  $f(x)$  satisfy standard assumptions, and  $\alpha$  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  $\lim_{k \rightarrow \infty} x_k = \alpha$ .



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**Proof:** 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 lemma

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

$f' \in \mathcal{C}^1(a, b)$  so that there exist a  $\delta$  such that  $2 |f'(x)| > |f'(\alpha)|$  for all  $|x_k - \alpha| \leq \delta$ . Choosing  $\delta$  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. □



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# Error estimation

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# 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  $\varepsilon$  is the machine precision.



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# Convergence of a sequence

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  $\alpha$  if

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



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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  $k \geq m$

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



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# 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  $k \geq m$

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



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# Root order of convergence

There may exist convergent sequence 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.



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# 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  $p$ .



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Convergent sequences without a  $q$ -order of converge 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  $k = 0, 1, 2, \dots$



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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.



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# 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:

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



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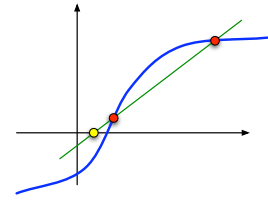
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# Geometric point of view of secant method

Let us take  $f \in \mathcal{C}(a, b)$  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  $(x_1, f(x_1))^T$ .



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

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

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



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## 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.



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# Local convergence of the Secant Method

## Theorem

Let  $f(x)$  satisfy standard assumptions, and  $\alpha$  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  $\alpha$  with  $r$ -order at least  $p$ .



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Subtracting  $\alpha$  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  $f(\alpha) = 0$

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



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From Lagrange <sup>1</sup> 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

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

<sup>1</sup>Joseph-Louis Lagrange 1736—1813



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As  $\alpha$  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  $\delta$ , 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

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



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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  $\exp(-z^{k-1}(z^2 - z - 1)) = 1$  or:

$$z^2 - z - 1 = 0, \quad \Rightarrow \quad z_{1,2} = \frac{1 \pm \sqrt{5}}{2} = \begin{cases} 1.618034 \dots \\ -0.618034 \dots \end{cases}$$



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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

$$|x_k - \alpha| \leq M E_k = M E_0 \exp(-p^k)$$

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

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

with  $C = (M E_0)^{1-1/r}$  and, by choosing  $r = p$ , we obtain  $\exp(-p^{k+1} + r p^k) = 1$  and  $E_{k+1} \leq C E_k^p$ .



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# Divided difference bound

## 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.



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# 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 theorem<sup>2</sup> 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  $f'(x)$ .

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<sup>2</sup>Michel Rolle 1652–1719



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# 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
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# 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.



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## 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.



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## Lemma

Let  $f(x)$  satisfies standard assumptions and consider the sequence generated by

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

let  $\alpha$  be a simple root and  $h_k$  satisfying

$$\gamma |h_k| < |f'(x_k)|$$

then the following inequality is true

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



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**Proof:** Let  $\alpha$  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 expansion Lemma** we have

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

□



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**Proof:** If  $f(x)$  satisfies standard assumptions, then

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

and 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

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



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## quasi-Newton method local convergence

## Theorem

Let  $f(x)$  satisfies standard assumptions, and  $\alpha$  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  $\alpha$ . Moreover,

- 1 If  $\lim_{k \rightarrow \infty} h_k = 0$  then  $\{x_k\}$   $q$ -super-linearly converges to  $\alpha$ .
- 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 with order  $p = (1 + \sqrt{5})/2 = 1.618\dots$



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# Fixed-Point procedure

## Definition (Fixed point)

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

$$x_* = \mathbf{G}(x_*).$$

Searching for a zero of  $f(x)$  is the same as searching for 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  $\alpha$ .



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### 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:

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



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# 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  $\mathbf{x}_\star$  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  $\mathbf{x}_\star$  with constant  $L$ .
- 3 The following error estimate is valid

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



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# Proof of Contraction mapping

(1/2)

Prove that  $\{x_k\}_0^\infty$  is a Cauchy sequence

$$\|x_{k+m} - x_k\| \leq L \|x_{k+m-1} - x_{k-1}\| \leq \dots \leq L^k \|x_m - x_0\|$$

and

$$\begin{aligned} \|x_m - x_0\| &\leq \sum_{l=0}^{m-1} \|x_{l+1} - x_l\| \leq \sum_{l=0}^{m-1} L^l \|x_1 - x_0\| \\ &\leq \frac{1 - L^m}{1 - L} \|x_1 - x_0\| \leq \frac{\|x_1 - x_0\|}{1 - L} \end{aligned}$$

so that

$$\|x_{k+m} - x_k\| \leq \frac{L^k}{1 - L} \|x_1 - x_0\| \leq \rho$$

This prove that  $\{x_k\}_0^\infty \subset B_\rho(x_0)$  and that is a Cauchy sequence.



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# Proof of Contraction mapping

(2/2)

Prove existence, uniqueness and rate

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

$$\begin{aligned} \|x_\star - G(x_\star)\| &\leq \|x_\star - x_k\| + \|x_k - G(x_k)\| + \|G(x_k) - G(x_\star)\| \\ &\leq (1 + L) \|x_\star - x_k\| + L^k \|x_1 - x_0\| \xrightarrow{k \rightarrow \infty} 0 \end{aligned}$$

Uniqueness is proved by contradiction, let be  $x$  and  $y$  two fixed points:

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

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

$$\begin{aligned} \|x_k - x_\star\| &\leq \|x_k - x_{k+m}\| + \|x_{k+m} - x_\star\| \\ &\leq \frac{L^k}{1 - L} \|x_1 - x_0\| + \|x_{k+m} - x_\star\| \end{aligned}$$



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## 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  $\alpha$  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  $\alpha$  and by choosing  $\rho$  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  $\alpha$  is a simple root.



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# Fast convergence

Suppose that  $\alpha$  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  $\alpha$  it follows that the procedure has locally  $q$ -order of  $p$ .



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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  $\alpha$  is a multiple root, i.e.

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

it follows that

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

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



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Consequently,

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

so that

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

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



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# Outline

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  - Local convergence of quasi-Newton method
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- 1 Consider an iterative scheme that produces a sequence  $\{x_k\}$  that converges to  $\alpha$  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.



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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

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

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



## Notes

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- 1 Consider an iterative scheme that produce a sequence  $\{x_k\}$  converging to  $\alpha$  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

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



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### 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

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

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



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- 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!



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# 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**.



## Notes

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