One Dimensional Non-Linear Problems

Lectures for PHD course on
Unconstrained Numerical Optimization

Enrico Bertolazzi

DIMS – Università di Trento

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Outline

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.

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

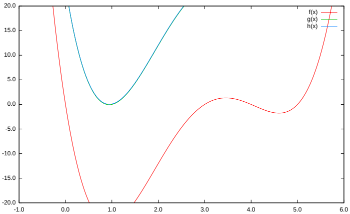
1. $f(x) = x^4 - 12x^3 + 47x^2 - 60x$;
2. $g(x) = x^4 - 12x^3 + 47x^2 - 60x + 24$;
3. $h(x) = x^4 - 12x^3 + 47x^2 - 60x + 24.1$;

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.

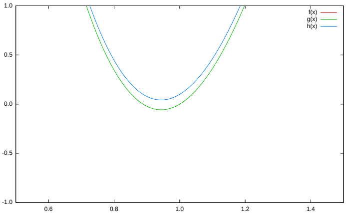
So in general a non linear problem may have

- One or more solutions;
- No solution.

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



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



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 $-0.1629 + 1.8371p = 0$ yileds $p = 0.08866$.
- 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 known 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, . . .

Algorithm (Newton iterative scheme)

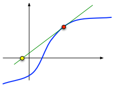
Let x_0 be assigned, then for $k = 0, 1, 2, \ldots$

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

The Newton procedure: a geometric point of view

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

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

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, if not we have

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

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

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.

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

Lemma (Taylor expansion)

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

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

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

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

□

Local Convergence

Newton scheme converges locally near simple roots:

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

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

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

$f' \in \mathtt{C}^1(a,b)$ so that there exist 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

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

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.

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 $x_k \in \mathbb{R}$, $k = 0, 1, 2, \ldots$ Then, the sequence $\{x_k\}$ is said to converge to α if

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

Definition (Q-order of a convergent sequence)

Let $\alpha \in \mathbb{R}$ and $x_k \in \mathbb{R}$, $k = 0, 1, 2, \ldots$ 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 $x_k \in \mathbb{R}$, $k = 0, 1, 2, \ldots$ 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 $x_k \in \mathbb{R}$, $k = 0, 1, 2, \ldots$ 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 exists 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 $\lim_{k\mapsto\infty} x_k = 1$ 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

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

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 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 $k = 0, 1, 2, \ldots$.

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.

Secant method

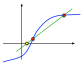
Newton method is a fast (q-order 2) numerical scheme to approximate the root of a function $f(x)$ but needs the knowledge of the first derivative of $f(x)$. Sometimes first derivative is not available or not computable, in this case a numerical procedure to approximate the root which does not use derivative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

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

The secant method: a geometric point of view

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

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



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

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

Algorithm (Secant scheme)

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

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

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

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

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* $k = 0, 1, 2, 3, \ldots$
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

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

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

$$\frac{\dfrac{f(x_k)}{x_k - \alpha} - \dfrac{f(x_{k-1})}{x_{k-1} - \alpha}}{f(x_k) - f(x_{k-1})} = \frac{\dfrac{f(x_k) - f(\alpha)}{x_k - \alpha} - \dfrac{f(x_{k-1}) - f(\alpha)}{x_{k-1} - \alpha}}{f(x_k) - f(x_{k-1})},$$

$$= \frac{\dfrac{f(x_k) - f(\alpha)}{x_k - \alpha} - \dfrac{f(x_{k-1}) - f(\alpha)}{x_{k-1} - \alpha}}{x_k - x_{k-1}} \left(\frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}\right)^{-1}$$

Proof of Local Convergence (2/5)

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

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

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

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

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

[1] Joseph-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 $k = 1, 2, 3, \ldots$

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

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

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

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

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 $E_{k+1} \leq C E_k^p$.

Divided difference bound

Lemma

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

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

The proof use the trick function

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

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 theorem[2] 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 $f'(x)$.

[2] Michel Rolle 1652–1719

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 $a_k = \dfrac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$ we obtain the secant method.
5. If $a_k = \dfrac{f(x_k) - f(x_k - h_k)}{h_k}$ 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.

Lemma

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

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

let α be a simple root and h_k satisfying

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

then the following inequality is true

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

Proof.

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

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

By using thed Taylor expansion Lemma we have

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

(cont.)

Proof.

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

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

and that the finite difference secant scheme satisfies:

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

Moreover, form

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

it follows that

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

□

Local convergence of quasi-Newton method

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

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

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

1. *If $\lim_{k\mapsto\infty} h_k = 0$ then $\{x_k\}$ q-super-linearlyconverges 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 with order $p = (1+\sqrt{5})/2 = 1.618\ldots$*

Fixed–Point procedure

Definition (Fixed point)

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

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

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

$$x_{k+1} = g(x_k), \qquad k = 1, 2, \ldots$$

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:

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

Contraction mapping Theorem

Theorem (Contraction mapping)

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

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

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

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

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

Proof of Contraction mapping (1/2)

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

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

and

$$\|\boldsymbol{x}_m - \boldsymbol{x}_0\| \leq \sum_{l=0}^{m-1} \|\boldsymbol{x}_{l+1} - \boldsymbol{x}_l\| \leq \sum_{l=0}^{m-1} L^l \|\boldsymbol{x}_1 - \boldsymbol{x}_0\|$$

$$\leq \frac{1 - L^m}{1 - L} \|\boldsymbol{x}_1 - \boldsymbol{x}_0\| \leq \frac{\|\boldsymbol{x}_1 - \boldsymbol{x}_0\|}{1 - L}$$

so that

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

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

Proof of Contraction mapping (2/2)

Prove existence, uniqueness and rate

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

$$\|\boldsymbol{x}_\star - \mathbf{G}(\boldsymbol{x}_\star)\| \leq \|\boldsymbol{x}_\star - \boldsymbol{x}_k\| + \|\boldsymbol{x}_k - \mathbf{G}(\boldsymbol{x}_k)\| + \|\mathbf{G}(\boldsymbol{x}_k) - \mathbf{G}(\boldsymbol{x}_\star)\|$$

$$\leq (1 + L) \|\boldsymbol{x}_\star - \boldsymbol{x}_k\| + L^k \|\boldsymbol{x}_1 - \boldsymbol{x}_0\| \quad \underset{k \mapsto \infty}{\longrightarrow} \quad 0$$

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

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

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

$$\|\boldsymbol{x}_k - \boldsymbol{x}_\star\| \leq \|\boldsymbol{x}_k - \boldsymbol{x}_{k+m}\| + \|\boldsymbol{x}_{k+m} - \boldsymbol{x}_\star\|$$

$$\leq \frac{L^k}{1 - L} \|\boldsymbol{x}_1 - \boldsymbol{x}_0\| + \|\boldsymbol{x}_{k+m} - \boldsymbol{x}_\star\|$$

Example

Newton-Raphson in fixed point form

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

If α is a simple root of $f(x)$ then

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

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

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

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 $g \in \mathbb{C}^p$ with

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

by Taylor Theorem

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

so that

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

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

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

If α is a multiple root, i.e.

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

it follows that

$$f'(x) = n(x-\alpha)^{n-1}h(x) + (x-\alpha)^n h'(x)$$
$$f''(x) = (x-\alpha)^{n-2}\left[(n^2-n)h(x) + 2n(x-\alpha)h'(x) + (x-\alpha)^2 h''(x)\right]$$

Slow convergence (2/2)

Consequently,

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

so that

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

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

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

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

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

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

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
$$
\begin{aligned}
|x_{k+1}-x_k| &\leq \tau && \text{Absolute tolerance} \\
|x_{k+1}-x_k| &\leq \tau \max\{|x_k|, |x_{k+1}|\} && \text{Relative tolerance}
\end{aligned}
$$

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

Estimation of the q-order (2/3)

1. The ratio
$$\log\frac{|x_{k+2}-\alpha|}{|x_{k+1}-\alpha|}\Big/\log\frac{|x_{k+1}-\alpha|}{|x_k-\alpha|} \approx p$$
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
$$\log\frac{|x_{k+2}-x_{k+3}|}{|x_{k+1}-x_{k+2}|}\Big/\log\frac{|x_{k+1}-x_{k+2}|}{|x_k-x_{k+1}|} \approx p$$
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:
$$\log\frac{|f(x_{k+2})|}{|f(x_{k+1})|}\Big/\log\frac{|f(x_{k+1})|}{|f(x_k)|} \approx p$$
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.

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