Numerical Methods in Physics

Numerische Methoden in der Physik, 515.421.

Instructor: Ass. Prof. Dr. Lilia Boeri
Room: PH 03 090
Tel: +43-316-873 8191
Email Address: l.boeri@tugraz.at

Room: TDK Seminarraum

Time: 8:30-10 a.m.

Exercises: Computer Room, PH EG 004 F

http://itp.tugraz.at/LV/boeri/NUM_METH/index.html

(Lecture slides, Script, Exercises, etc).

TOPICS (this year):

- **Chapter 1: Introduction.** ✖
- **Chapter 2: Numerical methods for the solution of linear inhomogeneous systems.** ✖
- Chapter 3: Interpolation of point sets.
- **Chapter 4: Least-Squares Approximation.** ✖
- **Chapter 5: Numerical solution of transcendental equations.**
- Chapter 6: Numerical Integration.
- Chapter 7: Eigenvalues and Eigenvectors of real matrices.
- **Chapter 8: Numerical Methods for the solution of ordinary differential equations: initial value problems.**
- Chapter 9: Numerical Methods for the solution of ordinary differential equations: marginal value problems.

This week(19/11/2013)

- **Zeroes of a Trascendental Equation: Definition.**
- Iterative method: general concepts and convergence criteria.
- The Newton-Raphson method: definition, convergence.
- The Newton-Raphson method: a program.

Zeroes of a Trascendental Equation: Definition.

$$F(x) = 0$$

The values of *x* which satisfy this equation are called **zeroes**, **solutions** or **roots** of the function.

Finding the **zeroes** of a function is one of the most important problems of numerical analysis.

We will treat the following:

- Newton-Raphson and Regula Falsi (False position): Iterative Methods.
- Method of the nested intervals.

$$F(x) \equiv P_m(x) = \sum_{j=1}^{m} \alpha_j x^{j-1} = 0$$

We will not treat the **special** methods for **algebraic** equations.

Iterative methods: definition.

$$F(x) = 0 \quad \Rightarrow \quad f(x) = x$$

reduces to:

This permits to define an ***iterative method*** to find the solution:

$$\begin{aligned}
&x_0 \ \text{starting value} \\
&x_1 = f(x_0) \\
&x_2 = f(x_1) \\
&\ldots \\
&x_{t+1} = f(x_t)
\end{aligned}$$

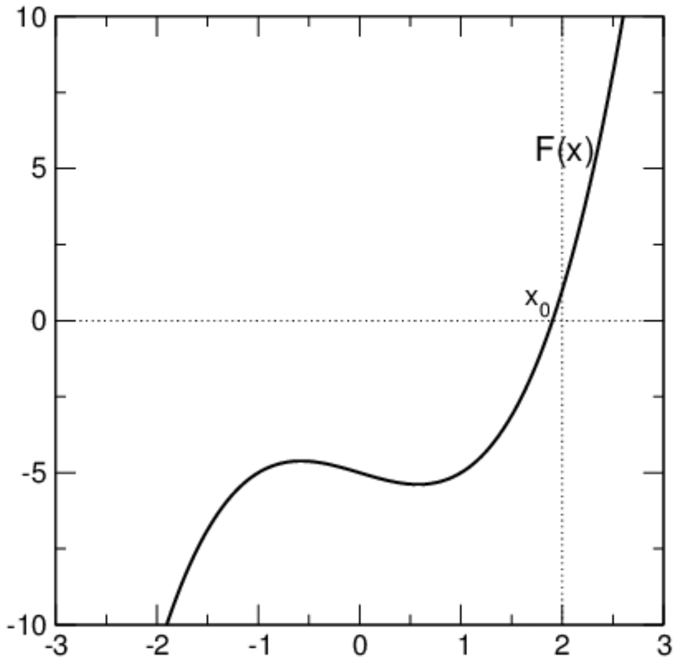
If the method converges, x_t can get arbitrarily close to the exact solution (x_{ex}).

$$\lim_{t \to \infty} x_t = x_{ex}$$

$$x_{t+1} = f(x_t)$$

The convergence of the iteration depends on the way in which the reformulation **F(x) = 0 -> f(x) =x** is performed.

Example:



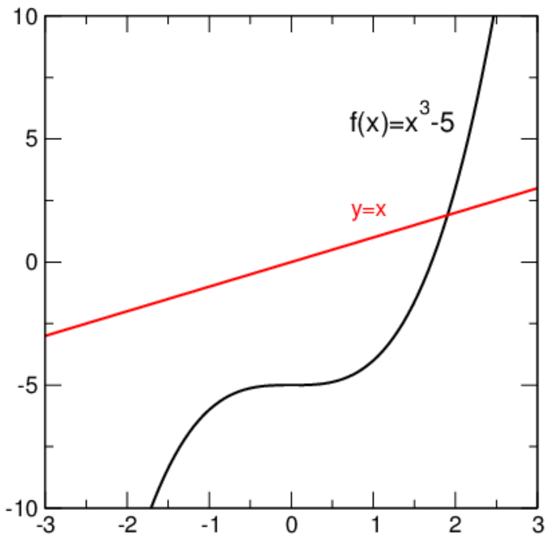
$$F(x) = x^3 - x - 5$$

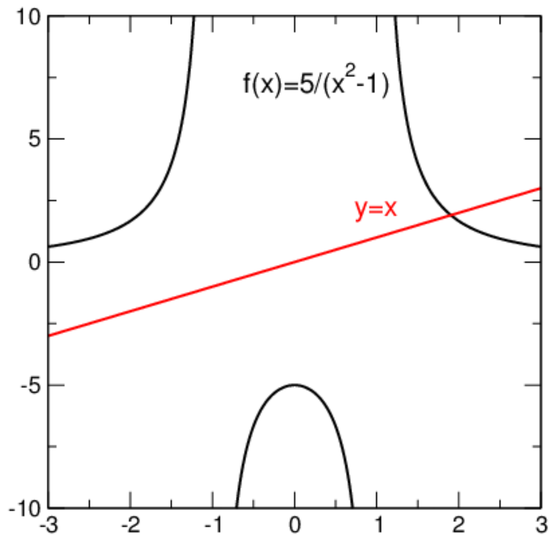
This function has **one** zero in *x≈1.9…*

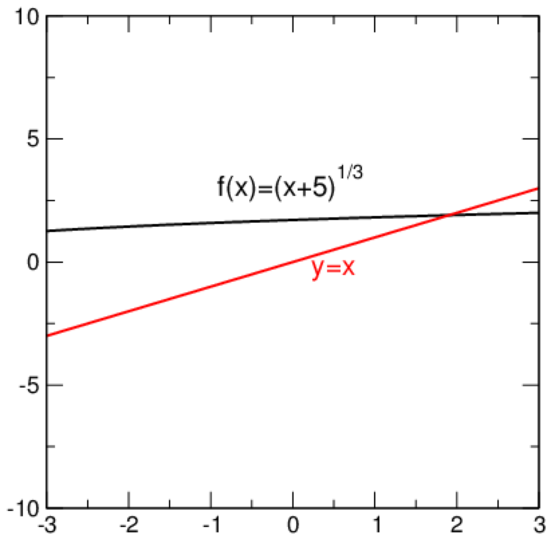
$$F(x) = x^3 - x - 5 = 0$$

There are three possible ways to reformulate this equation: **F(x) = 0 -> f(x) =x**.

$$x = x^3 - 5 \qquad x = \frac{5}{x^2 - 1} \qquad x = \sqrt[3]{x+5}$$







x0 = 2.0

t	(a)	(b)	(c)
0	2	2	2
1	3	1.6667	1.9129
2	22	2.8125	1.9050
3	10643	0.7236	1.9042
4	.	-10.4944	1.9042
.	.	.	.
.	.	.	.
	DIV	DIV	CONV

Error estimate:

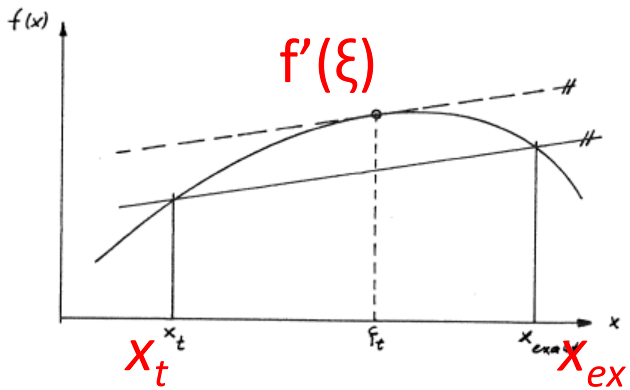
$$x_{ex} = f(x_{ex})$$

Exact Solution

$$x_{t+1} = f(x_t) - \delta_t$$

$$x_{ex} - x_{t+1} = f(x_{ex}) - f(x_t) + \delta_t$$

Roundoff error



The **mean value theorem** gives:

$$\frac{f(x_{ex}) - f(x_t)}{x_{ex} - x_t} = f'(\xi), \ \xi \in [x_t, x_{ex}]$$

We thus obtain:

$$x_{ex} - x_{t+1} = f'(\xi_t)\cdot(x_{ex} - x_t) + \delta_t$$

And iterating down to x_0:

$$\begin{aligned} x_{ex} - x_{t+1} = {} & f'(\xi_t)\cdot f'(\xi_{t-1})\cdot\ldots\cdot f'(\xi_0)(x_{ex} - x_0) + \delta_t + \\ & + f'(\xi_t)\delta_{t-1} + f'(\xi_t)f'(\xi_{t-1})\delta_{t-2} + \\ & + f'(\xi_t)\cdot f'(\xi_{t-1})\cdot\ldots\cdot f'(\xi_1)\delta_0 \end{aligned}$$

We further assume that:

- *m* is the maximum value of the abs. value of the first derivative of f in the interval I
- δ is independent of t.

Proof of

$$x_{ex} - x_{t+1} = f'(\xi_t)\,(x_{ex} - x_t) + \delta_t$$

$$x_{ex} - x_t = f'(\xi_{t-1})\,(x_{ex} - x_{t-1}) + \delta_{t-1}$$

$$x_{ex} - x_{t+1} = f'(\xi_t)\cdot f'(\xi_{t-1})\,(x_{ex} - x_{t-1}) + f'(\xi_t)\cdot \delta_{t-1} + \delta_0$$

...

$$x_1 - x_0 = f'(\xi_0)\cdot(x_{ex} - x_0) + \delta_0$$

$\Rightarrow$

$$(x_{ex} - x_{t+1}) = f'(\xi_t)\cdot f'(\xi_{t-1})\cdots f'(\xi_0)\,(x_{ex} - x_0) + \delta_t + f'(\xi_t)\,\delta_{t-1} + f'(\xi_t)\,f'(\xi_{t-1})\,\delta_{t-2} + \dots + f'(\xi_t)\cdots f'(\xi_1)\,\delta_0$$

c.v.d.

With these assumptions we derive an upper boundary for the error in the iteration:

$$\left|x_{ex} - x_{t+1}\right| \le m^{t+1}\left|x_{ex} - x_0\right| + \left|\delta\right|(1 + m + m^2 + \ldots + m^t)$$

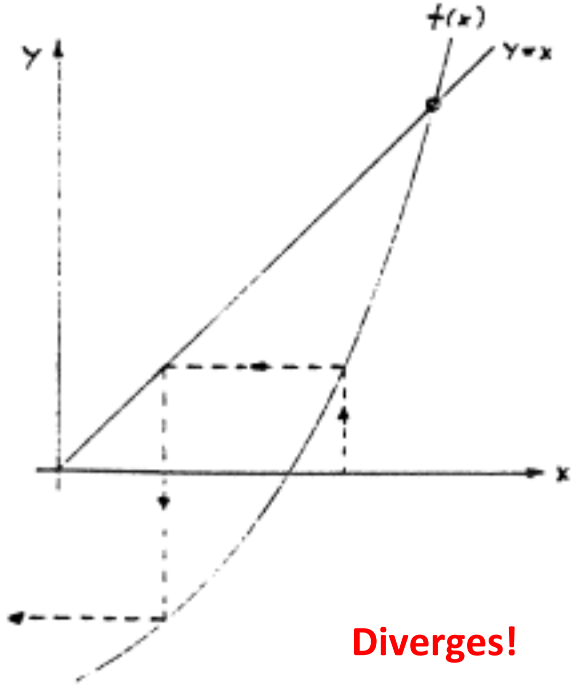
$$\lim_{t\to\infty}\left|x_{ex} - x_{t+1}\right| \le \underbrace{\left|x_{ex} - x_0\right| \cdot \lim_{t\to\infty} m^{t+1}}_{\text{Methodological Error}} + \underbrace{\frac{\left|\delta\right|}{1-m}}_{\text{Roundoff Error}}$$

Both terms diverge for $m \ge 1$; the **methodological error** converges for $0 \le m \le 1$.

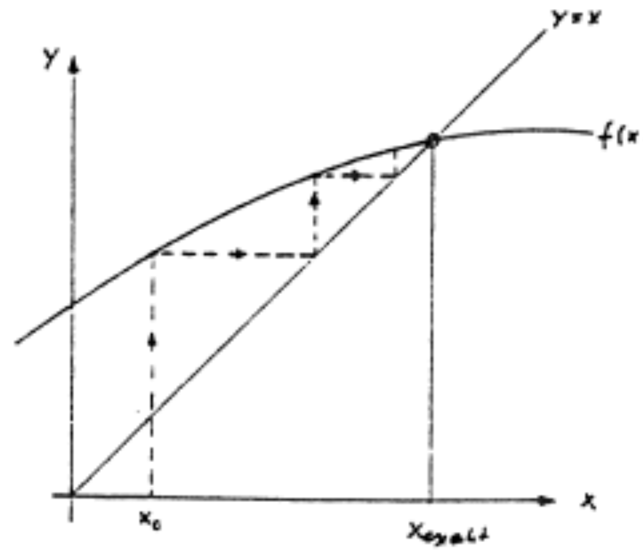
$$\lim_{t\to\infty}\left|x_{ex} - x_{t+1}\right| \le \frac{\left|\delta\right|}{1-m}$$

The convergence criterion for the iteration is:

$$0 \leq m \leq 1 \qquad m = \max_I f'(x)$$



Diverges!



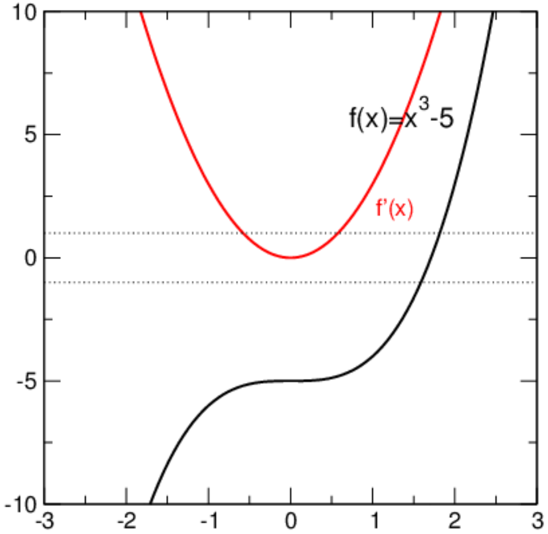
Converges!

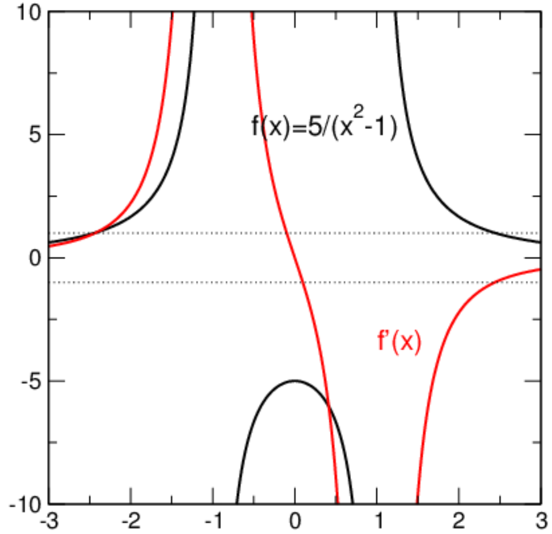
Going back to our original example:

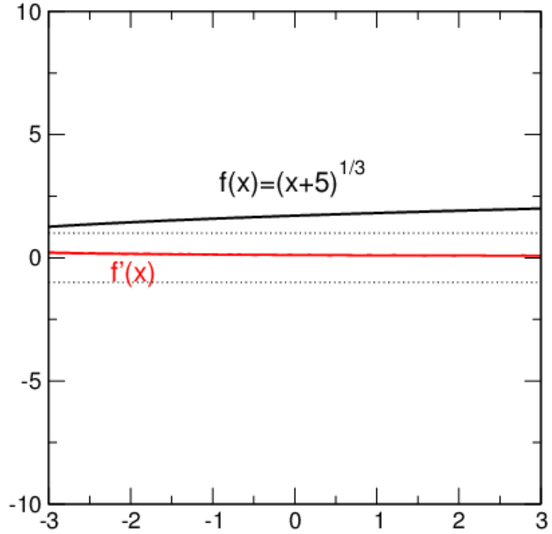
$$x = x^3 - 5$$

$$x = \frac{5}{x^2 - 1}$$

$$x = \sqrt[3]{x + 5}$$







$$f'(x) = 3x^2$$

$$f'(x) = -\frac{10x}{(x^2 - 1)}$$

$$f'(x) = \frac{1}{3}(x+5)^{-2/3}$$

Upper boundary for the convergence of the iteration:

From the iteration rule for the error one can derive an upper boundary for the error in the iteration:

$$\left|x_{ex} - x_{t+1}\right| \leq \frac{m}{1-m}\left|x_{t+1} - x_t\right| + \frac{|\delta|}{1-m}$$

A simpler expression can be used if m and δ are not known:

$$\left|x_{ex} - x_{t+1}\right| \leq \left|x_{t+1} - x_t\right|$$

However, **this expression works only if m≤1/2 or until the methodological error is larger than the roundoff error!**

Proof of

$$x_{ex} - x_{t+1} = f'(\xi_t)(x_{ex} - x_t) + \delta_t$$

$$x_{ex} - x_{t+1} = f'(\xi_t)(x_{ex} - x_t + x_{t+1} - x_{t+1}) + \delta_t$$

$$(x_{ex} - x_{t+1})(1 - f'(\xi_t)) = f'(\xi_t)(x_{t+1} - x_t) + \delta_t$$

$$|f'(\xi_t)| \leq m \leq 1; \quad |\delta_t| \leq \delta$$

$\Rightarrow$

$$|x_{ex} - x_{t+1}| \leq \frac{|f'(\xi_t)|}{|1 - |f'(\xi_t)||} |x_{t+1} - x_t| + \frac{\delta_t}{|1 - f'(\xi_t)|}$$

$\Rightarrow$

$$|x_{ex} - x_{t+1}| \leq \frac{m}{1 - m} |x_{t+1} - x_t| + \frac{\delta}{|1 - m|}$$

Example:

$$F(x) = a + (1-a)x^2 - x$$

The two zeroes are:

$$x_1 = 1 \qquad x_2 = \frac{a}{1-a}$$

We want to find a good approximation for x_1=1 using the **iterative** method:

$$x_{t+1} = f(x_t)$$

$$x_{t+1} = a + (1-a)x_t^2$$

The first derivative is:

$$f'(x) = 2x(1-a)$$

The upper limit for the first derivative is:

$$m = \max_I \left|2x(1-a)\right|$$

If we approach x=1 from below, $m \leq 2(1-a)$; the iteration converges for $|(1-a)| \leq 1/2$.

$$\left|1-a\right| \leq \frac{1}{2}$$

$$1-a \leq \frac{1}{2} \Rightarrow a \geq \frac{1}{2}$$

$$a-1 \leq \frac{1}{2} \Rightarrow a \leq \frac{3}{2}$$

The iteration converges for: $\frac{1}{2} \leq a \leq \frac{3}{2}$

Parameter a = 2.500 > 1.5 i.e. Divergence expected:

t	x_{t}	x_{ex}-x_{t+1}	x_{t+1}-x_{t}
0	.1200000E+01		
1	.3400000E+00	.6600000E+00	-.8600000E+00
2	.2326600E+01	-.1326600E+01	.1986600E+01
3	-.5619601E+01	.6619601E+01	-.7946201E+01
4	-.4486988E+02	.4586988E+02	-.3925028E+02
5	-.3017459E+04	.3018459E+04	-.2972589E+04
6	-.1365759E+08	.1365759E+08	-.1365457E+08
7	-.2797945E+15	.2797945E+15	-.2797945E+15
8	-.1174274E+30	.1174274E+30	-.1174274E+30
9	-.2068380E+59	.2068380E+59	-.2068380E+59
10	-.6417295+117	.6417295+117	-.6417295+117

Parameter a = 0.600 ===> m=0.8 i.e.: convergence, but breakdown of (5.11):

t	x_{t}	x_{ex}-x_{t+1}	x_{t+1}-x_{t}
0	.6000000E+00		
1	.7440000E+00	.2560000E+00	.1440000E+00
2	.8214144E+00	.1785856E+00	.7741440E-01
3	.8698886E+00	.1301114E+00	.4847425E-01
4	.9026825E+00	.9731750E-01	.3279386E-01
5	.9259343E+00	.7406572E-01	.2325178E-01
6	.9429417E+00	.5705828E-01	.1700744E-01
7	.9556556E+00	.4434437E-01	.1271392E-01
8	.9653111E+00	.3468892E-01	.9655443E-02
9	.9727302E+00	.2726981E-01	.7419114E-02
10	.9784816E+00	.2151839E-01	.5751419E-02

Parameter a = 1.200 ===> m=0.4 d.h.: convergence and validity of (5.11):

0	.6000000E+00		
1	.1128000E+01	-.1280000E+00	.5280000E+00
2	.9455232E+00	.5447680E-01	-.1824768E+00
3	.1021197E+01	-.2119718E-01	.7567398E-01
4	.9914313E+00	.8568734E-02	-.2976591E-01
5	.1003413E+01	-.3412809E-02	.1198154E-01
6	.9986325E+00	.1367453E-02	-.4780262E-02
7	.1000547E+01	-.5466072E-03	.1914060E-02
8	.9997813E+00	.2187027E-03	-.7653099E-03
9	.1000087E+01	-.8747150E-04	.3061742E-03
10	.9999650E+00	.3499013E-04	-.1224616E-03

The Newton-Raphson Method

Iterative method

Definition:

In the **Newton-Raphson** method the reduction:

$$F(x) = 0 \quad \Rightarrow \quad f(x) = x$$

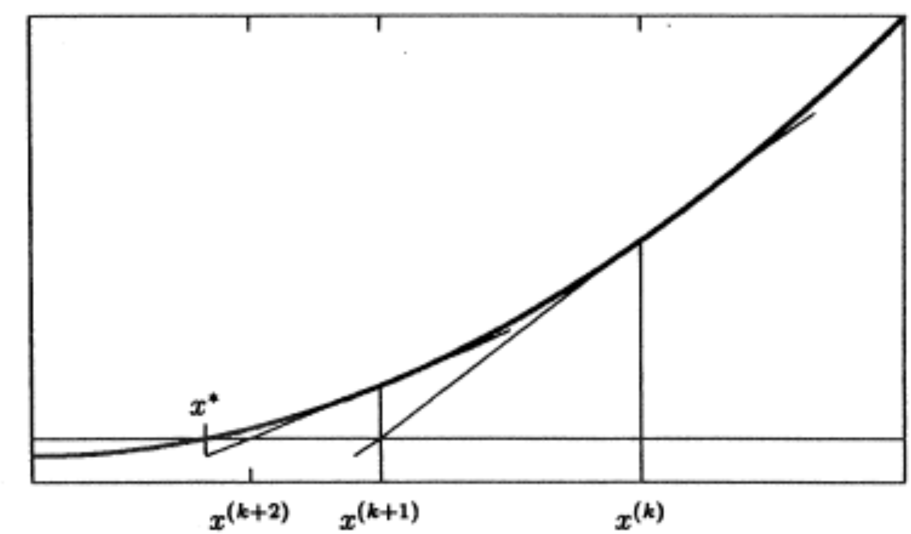
is obtained by setting:

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

This gives the iteration rule:

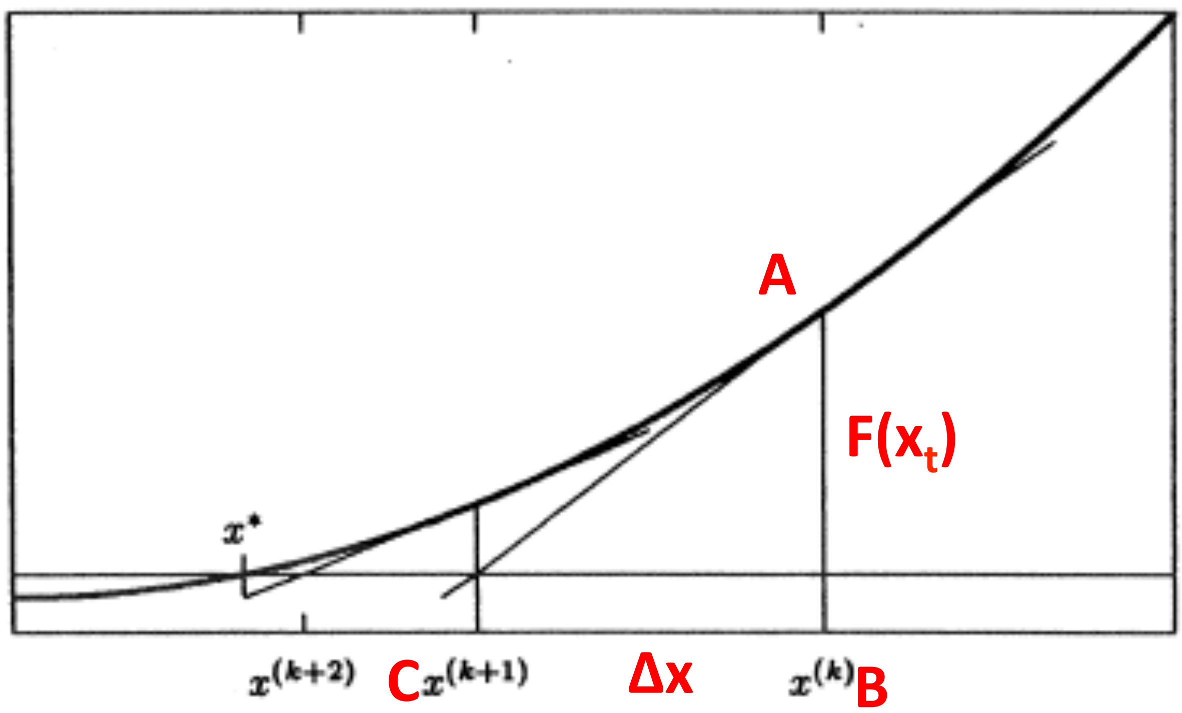
$$x_{t+1} = x_t - \frac{F(x_t)}{F'(x_t)}$$

Newton-Raphson iteration



Newton-Raphson (tangent) method:

$$x_{t+1} = x_t - \frac{F(x_t)}{F'(x_t)}$$



$$\frac{AB}{BC} = F'(x_t)$$

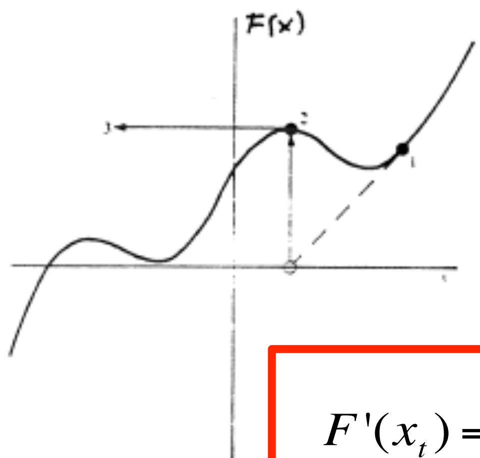
$$\frac{f(x_t)}{\Delta x_t} = F'(x_t) \Rightarrow \Delta x_t = \frac{F(x_t)}{F'(x_t)}$$

The error estimate gives:

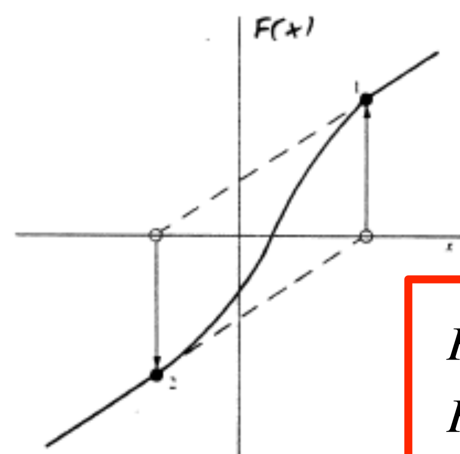
$$m = \max_I \frac{d}{dx}\left(x - \frac{F(x)}{F'(x)}\right) = \max_{x_0, x_{ex}}\left(\frac{xF''(x)}{(F'(x))^2}\right)$$

The Newton-Raphson method converges badly if the slope (F'(x)) is small. This happens, for example, if two zeroes lie close to each other.

Problematic cases:



$$F'(x_t) = 0$$



$$F(x_{t+1}) = -F(x_t)$$
$$F'(x_{t+1}) = F'(x_t)$$

Convergence of the Newton-Raphson Method:

In case of convergence, the Newton-Raphson method converges **quadratically**.

$$\Delta x_{t+1} = -\frac{1}{2}\frac{F''(x_t)}{F'(x_t)}(\Delta x_t)^2$$

PROOF:

$$F(x) = F(x_t) + F'(x_t)\cdot(x - x_t) + \frac{1}{2}F''(x_t)(x - x_t)^2$$

In $x = x_{ex}$ we have: $(F(x_{ex} = 0))$

$$\underset{=\emptyset}{F(x_{ex})} = F(x_t) + F'(x_t)(x_{ex} - x_t) + \frac{1}{2}F''(x_t)(x_{ex} - x_t)^2 + \dots$$

Dividing by $F'(x_t)$

$$0 = -\frac{F(x_t)}{F'(x_t)} + (x_{ex} - x_t) + \frac{1}{2}\frac{F''(x_t)}{F'(x_t)}(x_{ex} - x_t)^2 + \dots$$

$$\left\{\emptyset = -(x_{t+1} - x_t) + (x_{ex} - x_t) + \frac{1}{2}\frac{F''(x_t)}{F'(x_t)}(x_{ex} - x_t)^2\right\} \Leftrightarrow$$

$$\emptyset = (x_{ex} - x_{t+1}) + \frac{1}{2}\frac{F''(x_t)}{F'(x_t)}(x_{ex} - x_t)^2 \Rightarrow \Delta x_{t+1} = -\frac{1}{2}\frac{F''(x_t)}{F'(x_t)}\Delta x_t$$

q.e.d

RTNEWT(X1,X2,JMAX,XACC,ERROR)

INPUT parameters:

X1,X2: Beginning and end of the interval where the zero lies.

JMAX: Maximum number of iterations.

XACC: Relative precision limit according to Eq.(4.11).

OUTPUT parameters:

RTNEWT: Approximate value of the solution.

ERROR: Error diagnostics:

ERROR = 0:	Newton iteration ok.
ERROR = 1:	No sign change in [X1,X2]
ERROR = 2:	No convergence within JMAX iterations
ERROR = 3:	'Jumped out of brackets' during Newton.

Internal Variables:

FUNC,DF: $F(x)$ and $F'(x)$. The function that calculates these quantities must be called **FUNC**.

DX: Iteration correction.

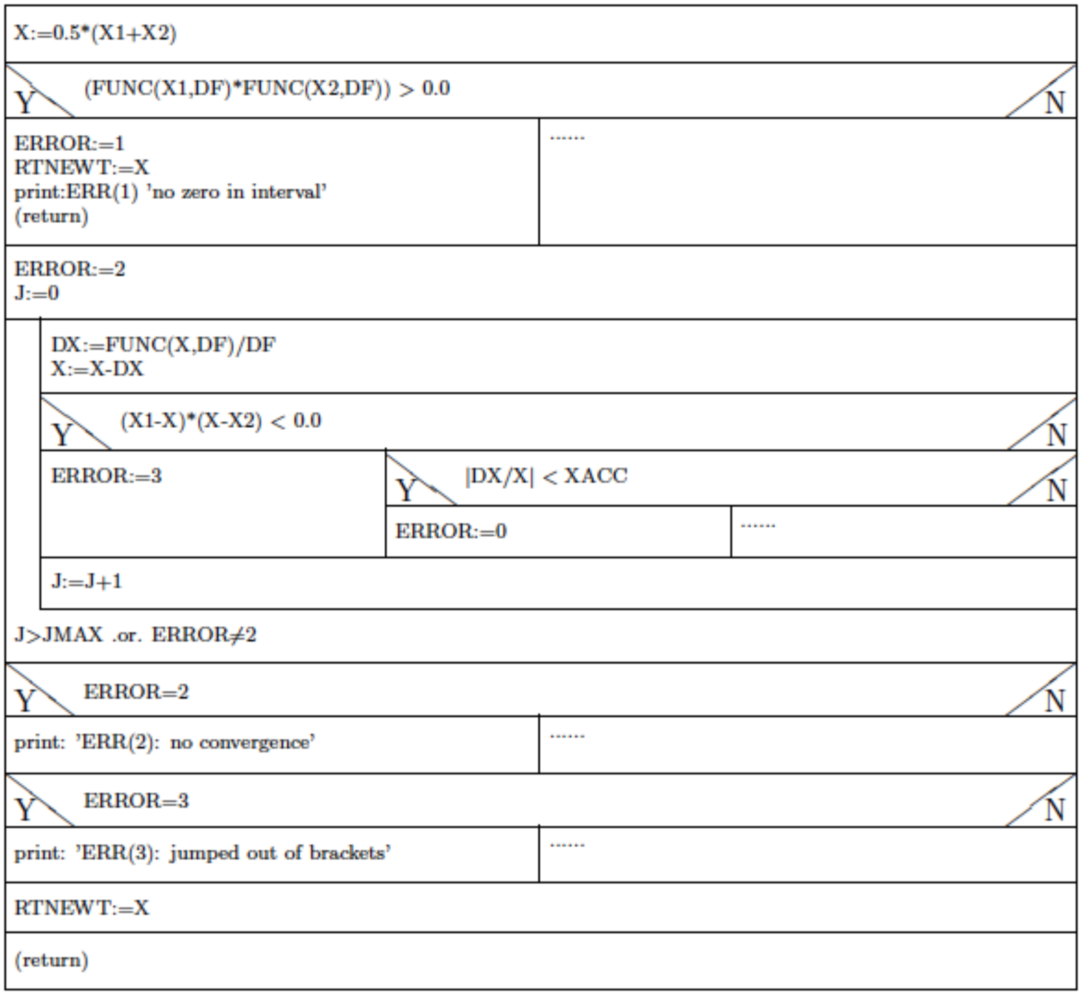
Remarks:

- At the beginning, the program tries to understand whether (at least) one of the two zeroes lies in the interval specified [X1,X2]. This is done checking whether the function $F(x)$ changes sign at least once.

- The formula for the *relative* error used in the program leads to convergence problems if the zero of the function is found exactly in $x = 0.0$.

- The first 'emergency exit' of the program RTNEWT ('jumped out of brackets') occurs if during the iterations the program jumps out of the interval specified by the external program that calls the routine (see Fig.4.6, left).

- The second 'emergency exit' ('exceeding maximum iterations') happens in case of a divergence or also of a too slow convergence, but also in those special cases, in which the iteration gets caught in a loop (see Fig.4.6, right).


X:=0.5*(X1+X2)
(FUNC(X1,DF)*FUNC(X2,DF)) > 0.0
Y
N
ERROR:=1
RTNEWT:=X
print:ERR(1) 'no zero in interval'
(return)
......
ERROR:=2
J:=0
DX:=FUNC(X,DF)/DF
X:=X-DX
(X1-X)*(X-X2) < 0.0
Y
N
ERROR:=3
|DX/X| < XACC
Y
N
ERROR:=0
......
J:=J+1
J>JMAX .or. ERROR≠2
ERROR=2
Y
N
print: 'ERR(2): no convergence'
......
ERROR=3
Y
N
print: 'ERR(3): jumped out of brackets'
......
RTNEWT:=X
(return)

This week(19/11/2013)

- **Zeroes of a Trascendental Equation: Definition.**
- Iterative method: general concepts and convergence criteria.
- The Newton-Raphson method: definition, convergence.
- The Newton-Raphson method: a program.