Numerical methods

Main problem:

Look for roots of functions : $f(x) = 0$ or for approximations of these roots.

Approximation of the derivative:

Recall $$f'(x) = \frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

or $$= \lim_{\Delta x \to 0} \frac{\overbrace{y(x+\Delta x) - y(x)}^{\Delta y}}{\Delta x}$$

Then if Δx is small, we can expect

$$\frac{dy}{dx}(x) \simeq \frac{y(x+\Delta x) - y(x)}{\Delta x}$$

This can be used to calculate an approximate value of the derivative of y at x, i.e. $\frac{dy}{dx}(x)$

If Δx is small, then

$\dfrac{\Delta y(x)}{\Delta x}$ is an approximation of $f'(x)$, i.e.

$$f'(x) \simeq \frac{f(x+\Delta x) - f(x)}{\Delta x}.$$

Then $\Delta x \; f'(x) \simeq f(x+\Delta x) - f(x)$

and $f(x+\Delta x) \simeq \underline{f(x)} + \Delta x \cdot \underline{f'(x)}$

Suppose we know $f(x)$ and $f'(x)$, then we can have an estimate of $f(x+\Delta x)$

E.G. $f(x) = e^x$ then $f'(x) = e^x$

$f(0) = e^0 = 1$ $\qquad$ $f'(0) = e^0 = 1$

Take $\Delta x = 0{,}1$

$f(0+0{,}1) \simeq f(0) + 0{,}1 \; f'(0)$

$e^0 \simeq 1 + 0{,}1 \cdot 1 = 1{,}1$

We can repeat the process:

$$f(0,2) = f(\overbrace{0,1}^{x} + \overbrace{0,1}^{\Delta x}) \simeq f(0,1) + \overbrace{0,1}^{\Delta x}\, \underbrace{f'(\overbrace{0,1}^{x})}_{= f(0,1)}$$

$$\downarrow$$

$$e^{0,2}$$

$$\simeq 1,1 + 0,1 \cdot 1,1$$

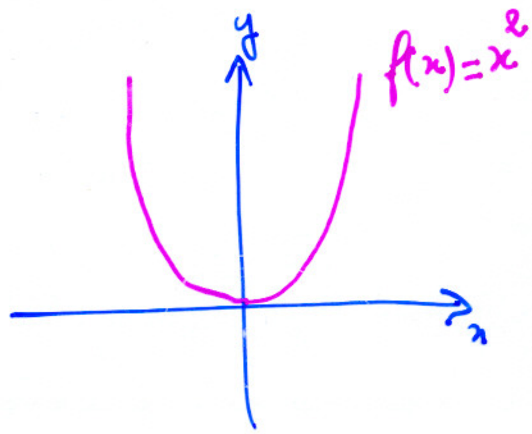
$$\simeq 1,21$$

Definition:

Let f be a given function and c a point in the domain of f.
The point c is called a critical point of f if

$$f'(c) = 0 .$$

Classification of critical points:



(1) $f(x) = x^2$

$f'(x) = 2x$

For critical points, solve $f'(x) = 0$

$2x = 0 \Rightarrow \underline{\underline{x = 0}}$

$c = 0$ is the only critical point of f.

In this particular example, $c=0$ is called a local minimum point of f., i.e. $c=0$ gives the smallest value of $f(x)$ for x near 0.

Remark: If we compute the second derivative f'':

$$\frac{d^2f}{dx^2}(x)=f''(x)=2 \quad , \text{ then } \quad f''(0)=2>0$$

For a critical point, if the second derivative is strictly positive, then this point is a local minimum.

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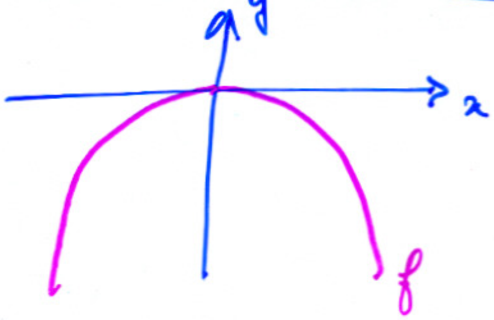
② $f(x)=-x^2$



$f'(x)=-2x$

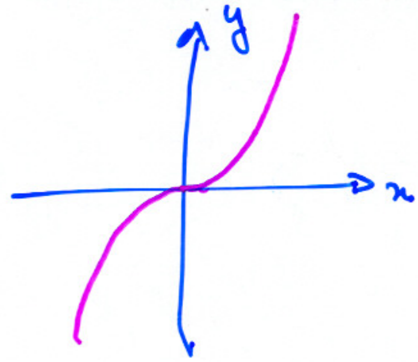
$f'(x)=0 \implies -2x=0$
$\implies x=0$

So $x=0$ is the only critical point of f.

$$\frac{d^2f}{dx^2}=f''(x)=-2 \quad , \text{ then } \quad f''(0)=-2<0$$

Here $c=0$ is a local maximum of f.

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



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

$f'(x) = 0 \implies 3x^2 = 0$

$\implies x = 0$

$f''(x) = \frac{d}{dx}(3x^2) = 6x$

$f''(0) = 6.0 = 0$

$c = 0$ is the only critical point of f.

$c = 0$ is called an inflection point of f.

$(f''(0) = 0)$

Critical point	$f'(c)$	$f''(c)$
Local Min	0	> 0
Local Max	0	< 0
Inflection point	0	$= 0$

c = critical point of f.

<u>Application:</u> The critical points can be useful to draw graphs of functions without evaluating the functions at many points.

E.G. $$f(x) = x^3 - 4x^2 + x + 6$$

<u>Note:</u> $$f(x) = \cancel{2}(x+1)(x-2)(x-3)$$

$$f(-1) = 0 \cdot (-3) \cdot (-4) = 0$$
$$f(2) = ? \cdot 0 \cdot ? = 0$$
$$f(3) = ? \cdot ? \cdot 0 = 0$$

We say that $\{-1, 2, 3\}$ are the <u>roots</u> of $f(x) = 0$.

<u>1st step</u> Determine critical points of f.

$$f'(x) = 3x^2 - 8x + 1 + 0$$

Critical points are solutions of:

$$3x^2 - 8x + 1 = 0$$

$$c = \frac{-(-8) \pm \sqrt{(-8)^2 - 4(3)(1)}}{2(3)}$$

$\Rightarrow$ 2 critical points $c \simeq \underbrace{2,53}_{c_1}$; $\underbrace{0,13}_{c_2}$

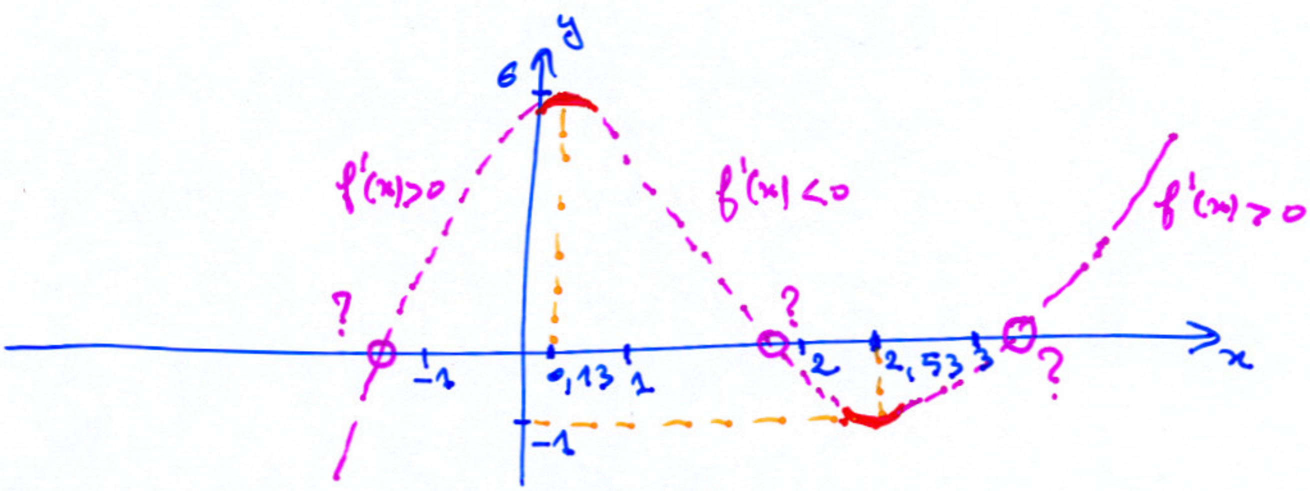
2nd step What kind of critical points are they?

$$f''(x) = \frac{d}{dx}\left(f'(x)\right) = 6x - 8$$

$$\Rightarrow \begin{cases} f''(c_2) \simeq 0{,}78 - 8 < 0 \\ f''(c_1) \simeq 15 - 8 > 0 \end{cases}$$

$$\Rightarrow \begin{cases} c_1 \text{ is local min} \\ c_2 \text{ is local max} \end{cases}$$

3rd step:
$$\begin{cases} f(0{,}13) \simeq 6 \\ f(2{,}53) \simeq -1 \end{cases}$$



The dashed lines are inferred from the sign of $f'(x)$.

We still need to know what the root are. (?)

We now study a numerical method to find the roots of an equation.

The Newton-Raphson method

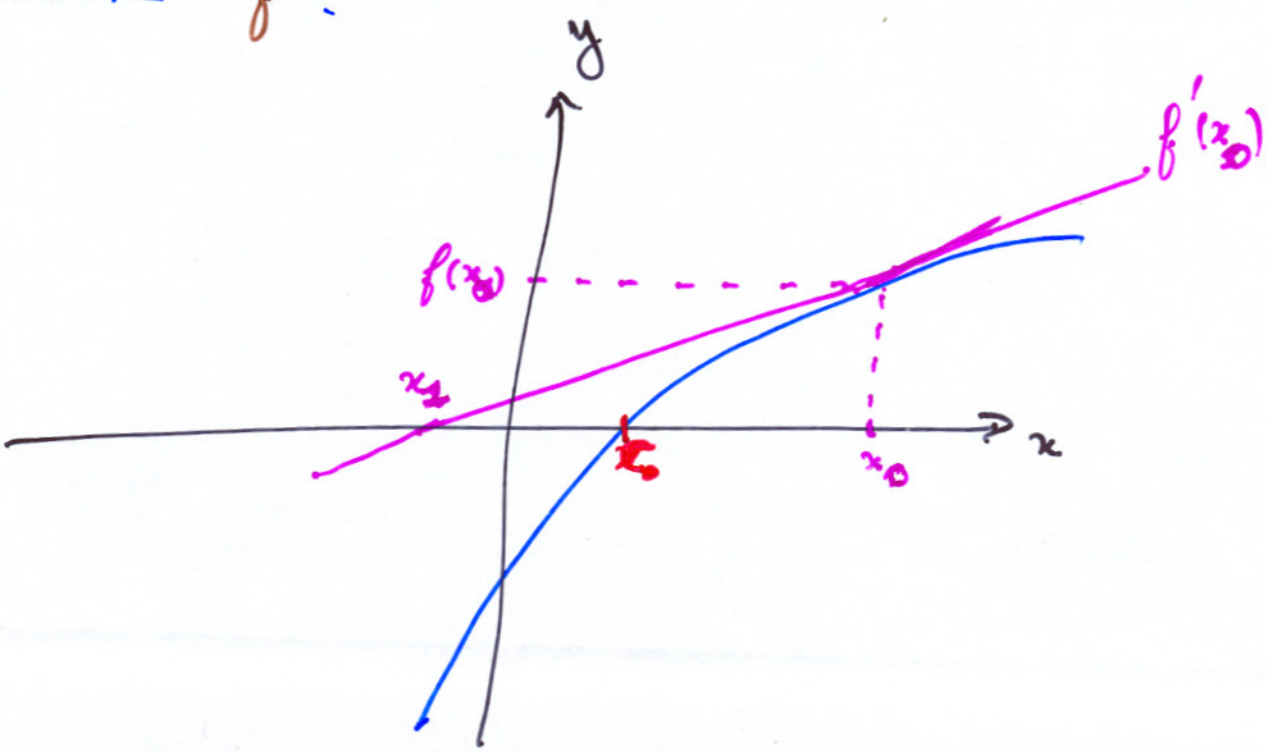
We look for roots ξ of an equation $f(x)=0$.

If f is of the form $f(x) = ax + b$ $(a \neq 0)$ then f represents a straight line and:

$$\xi = -\frac{b}{a}.$$

Remark: $\boxed{a = f'(x)}$

* Now suppose f is a general function having a derivative f'.



x_0 : a given number.

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}, \quad x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}, \quad x_3 = x_2 - \frac{f(x_2)}{f'(x_2)}, \ldots$$

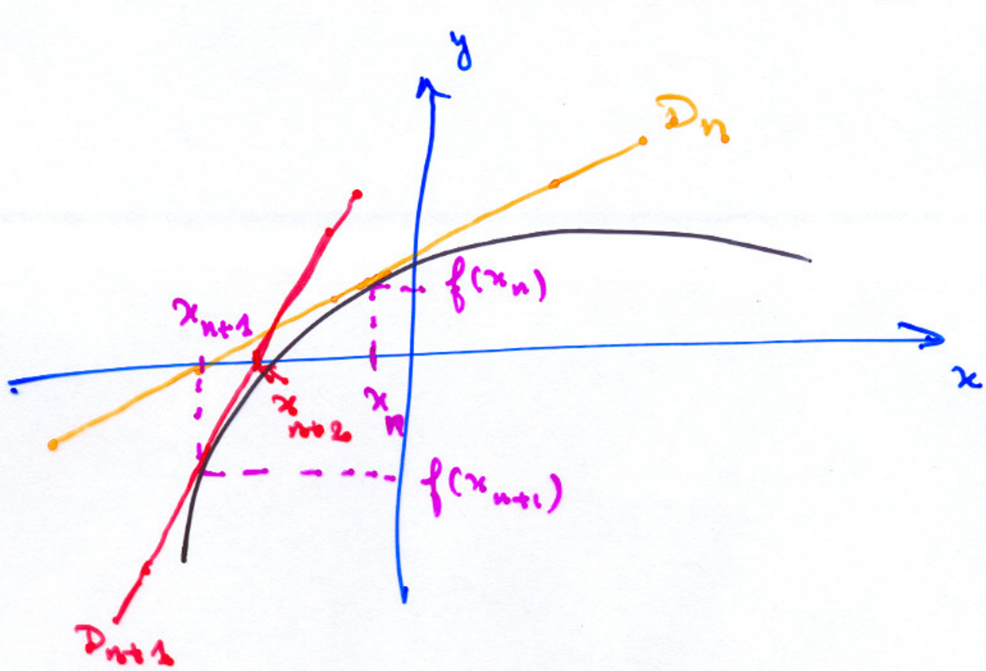
* x_0 = initial guess, has to be chosen reasonably close to the actual root.

* to find x_{n+1} starting from x_n we assimilate the curve of f to the straight line D_n passing at $(x_n, f(x_n))$ and having a slope $f'(x_n)$.

- D_n is the tangent to the curve at $(x_n, f(x_n))$
- The equation of D_n is: $y = (x - x_n) f'(x_n) + f(x_n)$
- x_{n+1} is given by the intersection of D_n with the x axis:

$$0 = (x_{n+1} - x_n) f'(x_n) + f(x_n)$$

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



For a large class of functions, the sequence $(x_n)_{n\geq 0}$ will converge to a limit ℓ that is a root of f, i.e. $f(\ell)=0$.

<u>Example:</u>

$$f(x) = x^3 - 4x^2 + x + 6$$

$$f'(x) = 3x^2 - 8x + 1$$

* set $x_0 = 0$ (arbitrary choice)
* $x_1 = 0 - \frac{f(0)}{f'(0)} = 0 - \frac{6}{1} = -6$
* $x_2 = -6 - \frac{f(-6)}{f'(-6)} \simeq -3,707$
* $x_3 \simeq -2,655$ $\quad x_4 = -1,4422 \quad x_5 = -1,0821$

$x_6 = -1,0037$

We clearly see that the N-R method is converging to the root -1. The roots of f are $-1, 2, 3$

. Setting $x_0 = 4$, will probably converge to the root 3.

```
x0 = 0
for i = 1:10
  x1 = x0 - f(x0)/f'(x0)
  x0 = x1
end
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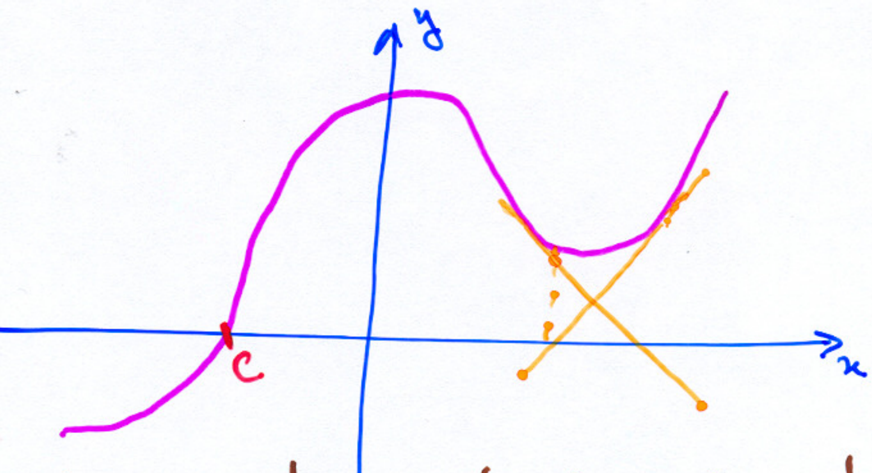
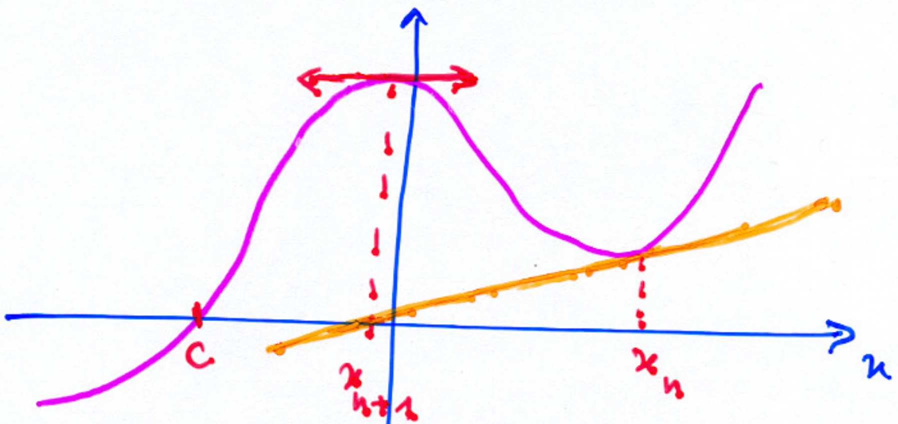
```
x0 = 0
while |f(x0)| < error
  x1 = x0 - f(x0)/f'(x0)
  x0 = x1
end
```

Shortcomings of the Newton-Raphson method



The sequence (x_n) is trapped; bouncing back and forth and will never converge to the root C

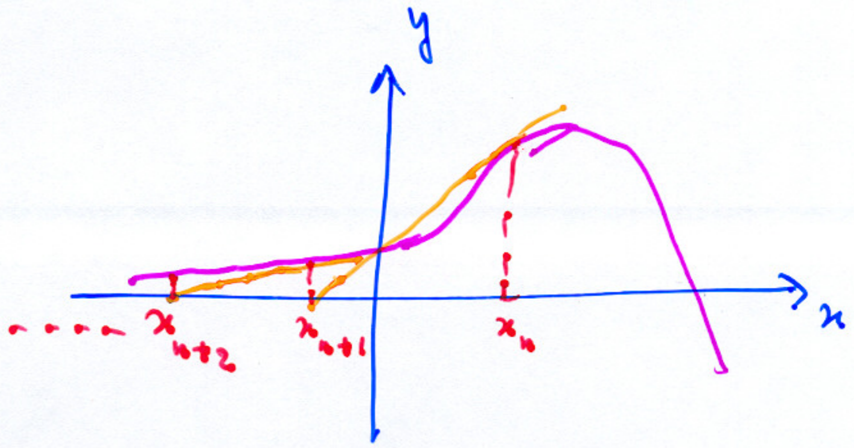
⟶ change starting point.



Here we can not apply the method after x_{n+1}:

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

← move x_{n+1} a little bit.



Here (x_n) will go to $-\infty$

⟶ change starting point.

Exercise :

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1) Sketch the graph of $f(x) = x^3 + 4x^2 + 7$ after having studied the sign of $f'(x)$.

2) Find the root of the ~~fun~~ f in the vicinity of $x = -4$ correct to 5 decimal places.