Lecture 9

Last time we did Numerical differentiation.

The first formula is

$$f'(a) \approx \frac{f(a+h) - f(a)}{h} \qquad (1)$$

This is an $O(h)$ formula.

The Central difference formula is

$$f'(a) \approx \frac{f(a+h) - f(a-h)}{2h} \qquad (2)$$

is an $O(h^2)$ approximation

Another $O(h^2)$ formula is

$$f'(a) \approx \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h} \qquad (3)$$

The central diff formula (2) is usually the best formula to find $f'(a)$ whenever it is applicable.

At the end-points only formula (1) and (3) are applicable. Here (3) gives better approximation.

Richardson Extrapolation can be used to get better approximation.

Numerical differentiation is an unstable process.

Numerical differentiation formulas enables us to solve linear boundary value problem

$$y'' + f(x)\,y' + g(x)\,y = q(x)$$

$$y(a) = \alpha \qquad y(b) = \beta$$

$$x \in [a, b].$$

Today we do

The solution of Non-linear equations

One of the most frequently occuring problems in scientific work is to find roots of equations of the form

$$f(x) = 0$$

In general we can only hope to find "approximate solution" ie a point x^* for which $|f(x^*)|$ is small

Some iterative methods of root finding

1. Bisection method

Recall intermediate value theorem.

If $f(x)$ is continuous and $f(a)f(b) < 0$ then f has a zero in (a, b)

Suppose $f(a)f(b) < 0$

Set $a_0 = a$ $\quad b_0 = b$

$$m = \frac{a_0 + b_0}{2}$$

If $f(a_0)f(m) < 0$ then set

$b_1 = m$ $\quad a_1 = a_0$

Otherwise set $a_1 = m$ $\quad b_1 = b$

So root lies in $[a_1, b_1]$

Example $f(x) = x^2 - 2$

$a_0 = 1 \qquad f(a_0) = -1$

$b_0 = 2 \qquad f(b_0) = 2$

$m = \frac{1+2}{2} = 1.5$

$f(1.5) = 2.25 - 2 = 0.25$

$a_0 = 1 \quad b_1 = 1.5$

root lies in $[1, 1.5]$

Algorithm for Bisection method

Given a function f continuous on $[a_0, b_0]$

and such that $f(a_0) f(b_0) < 0$

For $n = 0, 1, 2, \ldots$ until satisfied do

Set $m = \frac{a_n + b_n}{2}$

If $f(a_n) f(m) < 0$ then set $a_{n+1} = a_n$, $b_{n+1} = m$

Otherwise set $a_{n+1} = m$, $b_{n+1} = b$

Then $f(x)$ has a root in the interval

$[a_{n+1}, b_{n+1}]$

Example

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

(4 sig digits)

n	a_n	b_n	$f(a_n)$	$f(b_n)$
0	1	2	−1	2
1	1	1·5	−1	2·5 E−1
2	1·25	1·5	−4·375 E−1	2·5 E−1
3	1·375	1·5	−1·094 E−1	2·5 E−1
4	1·375	1·438	−1·094 E−1	6·641 E−1
5	1·407	1·438	−2·035 E−2	6·641 E−1
6	1·407	1·423	−2·035 E−2	2·493 E−2
7	1·407	1·415	−2·035 E−2	2·225 E−3
8	1·411	1·415	−9·079 E−3	2·225 E−3
9	1·413	1·415	−3·431 E−3	2·225 E−3
10	1·414	1·415	−6·040 E−4	2·225 E−3

$\frac{1.414 + 1.415}{2} = 1.415$ in 4 sig digits

So algorithm ends

root lies in $[1.414, 1.415]$

- Bisection method always converges to the root
- Convergence is slow

One can hope to get to root faster by using fully the information about $f(x)$ available at each step.

In our example

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

$f(1) = -1$ and $f(2) = 2$

Since $|f(1)|$ is closer to zero than $|f(2)|$ the root ξ is likely to be closer to 1 than 2.

Hence rather than check the mid point or average value of 1 and 2 we check f(x) at the weighted average

$$w = \frac{|f(2)|1 + |f(1)|2}{|f(2)| + |f(1)|}$$

Since f(1) & f(2) have opposite signs

$$w = \frac{f(2)1 - f(1)2}{f(2) - f(1)}$$

In our example

$$w = \frac{2+2}{3} = 1.333$$

$$f(w) < 0$$

So the root lies in [1.333, 2]

Repeating the process we get

$w = 1.400$ and so on

This algorithim is known as Regula-Falsi or false position method

Algorithim (Regula-Falsi)

Given a function $f(x)$ continuous on the interval $[a_0, b_0]$ and such that

$f(a_0) f(b_0) < 0$

For $n = 0, 1, 2, \ldots$ until satisfied do

Calculate $w = \dfrac{f(b_n) a_n - f(a_n) b_n}{f(b_n) - f(a_n)}$

If $f(a_n) f(w) \leq 0$ set $a_{n+1} = a_n$, $b_{n+1} = w$

Otherwise set $a_{n+1} = w$, $b_{n+1} = b_n$

Example

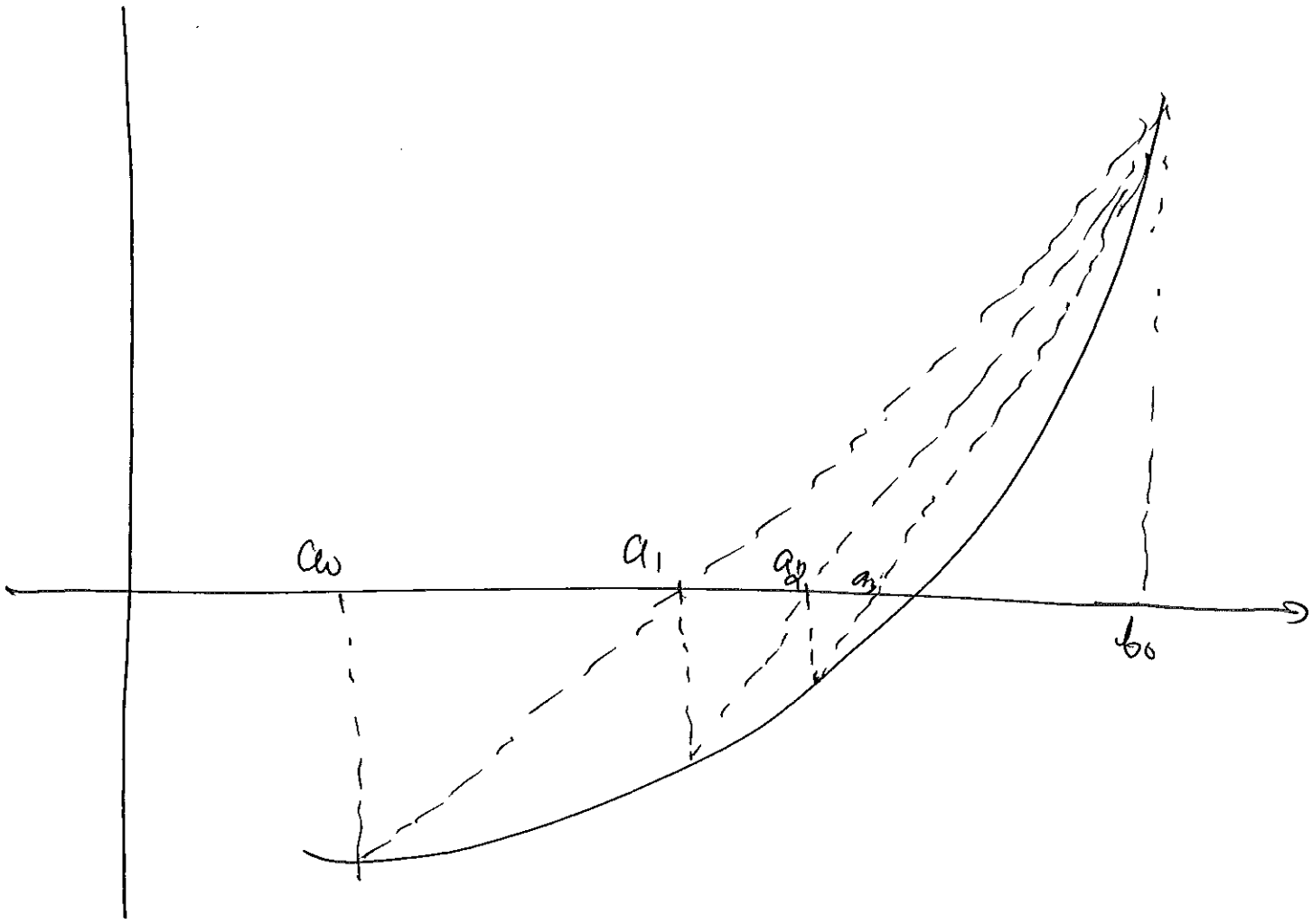
$$f(x) = x^2 - 2$$

4 sig digits

n	a_n	b_n	$f(a_n)$	$f(b_n)$	w_n
0	1	2	−1	2	1.333
1	1.333	2	−2.222E-1	2	1.400
2	1.400	2	−4.086 E-2	2	1.412
3	1.412	2	−6.256E-3	2	1.414
4	1.414	2	−6.060 E-4	2	-

Regula-falsi method produces a point at which $|f(x)|$ is "small" somewhat faster than the bisection-method, it fails completely to give a "small interval" where the root is known to lie.

Analysis of Regula-Falsi Method



$$w = \frac{f(b_n)a_n - f(a_n)b_n}{f(b_n) - f(a_n)}$$

is the point at which the straight line passing through $(a_n, f(a_n))$, $(b_n, f(b_n))$ intersects the x-axis.

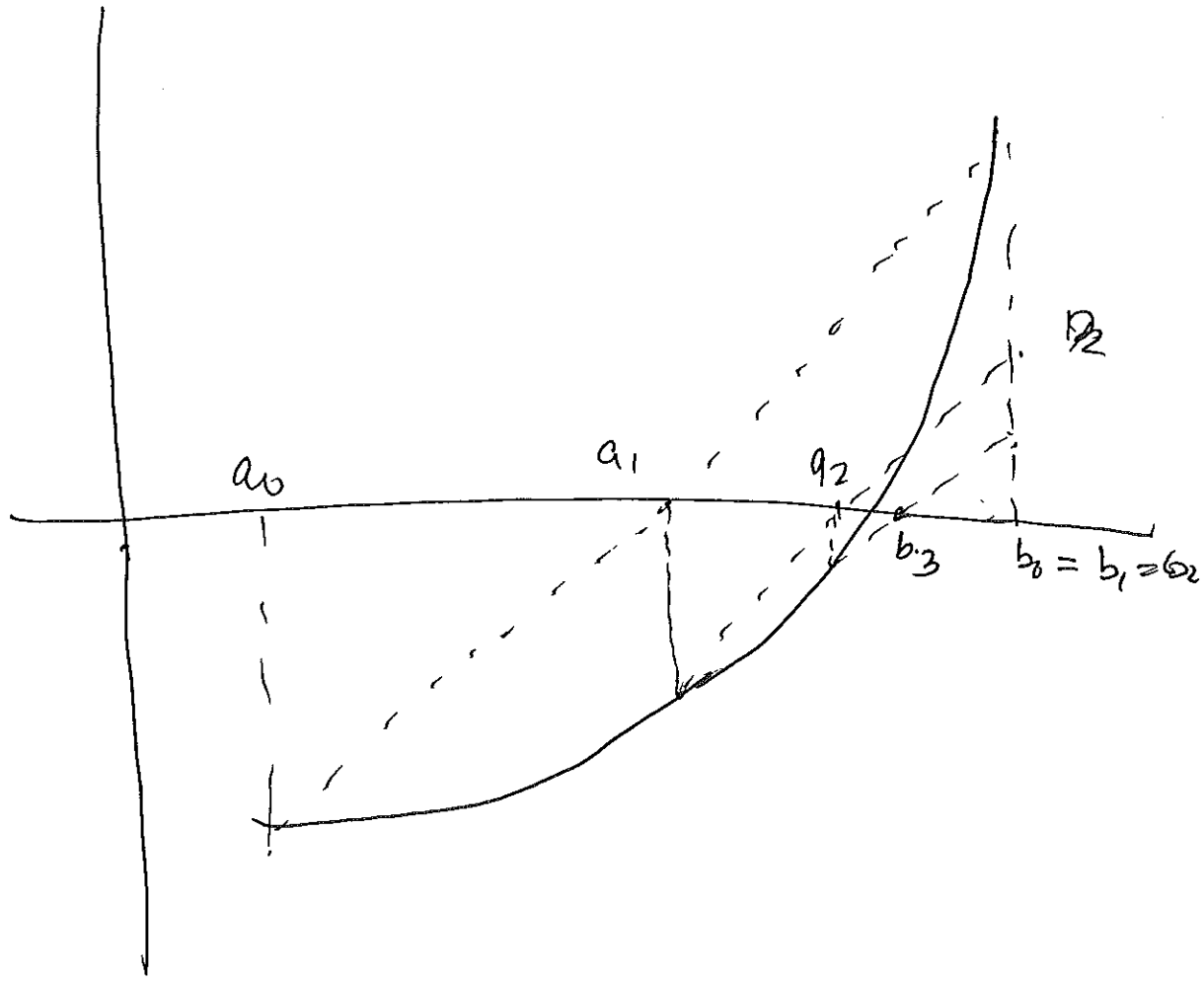
Such a straight-line is secant to $f(x)$. In our example $f(x)$ is concave upward and increasing (in the interval $[1, 2]$ of interest), hence the secant is always above the graph of $f(x)$. Consequently w always lies to the left of the zero (in our example).

If $f(x)$ were concave downward and increasing w would always lie to the right of the zero.

Two ways of improving regula-falsi method.

(1) "Modified Regula-Falsi"

It replaces secants by straight lines of ever smaller slope until w falls to the opposite side of the root



Algorithm (Modified Regula falsi)

Given $f(x)$ continuous on $[a_0, b_0]$ and such that $f(a_0) f(b_0) < 0$

Set $F = f(a_0)$ $\quad G = f(b_0)$

$w_0 = a_0$

For $n = 0, 1, 2, \ldots$ until satisfied do

Calculate $w_{n+1} = \dfrac{G a_n - F b_n}{G - F}$

If $f(a_n) f(w_{n+1}) \leq 0$ set $a_{n+1} = a_n$

$b_{n+1} = w_{n+1}$

$G = f(w_{n+1})$

If also $f(w_n) f(w_{n+1}) > 0$ set $F = F/2$

Otherwise set

$a_{n+1} = w_{n+1}$, $F = f(w_{n+1})$ $b_{n+1} = b_n$

If also $f(w_n) f(w_{n+1}) > 0$ set $G = G/2$

Then $f(x)$ has a zero in the interval

$[a_{n+1}, b_{n+1}]$.

Example

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

$$a_0 = 0 \qquad b_0 = 2 \qquad w_0 = 1$$

n	a_n	b_n	F	G	w_n
0	1	2	−1	2	1
1	1.333	2	−2.222E−1	1	1.333
2	1.333	1.454	−2.222E−1	1.141E−1	1.454
3	1.413	1.454	−3.431E−3	1.141E−1	1.413
4	1.414	1.454	−6.040E−4	5.705E−2	1.414
5	1.414	1.454	−6.040E−4	2.853E−2	1.414
6	1.414	1.415	−6.040E−4	1.742E−2	1.415

root lies in $[1.414, 1.415]$

② Secant Method

It retains the use of secants throughout but gives up the bracketing of the root.

Algorithim (secant method)

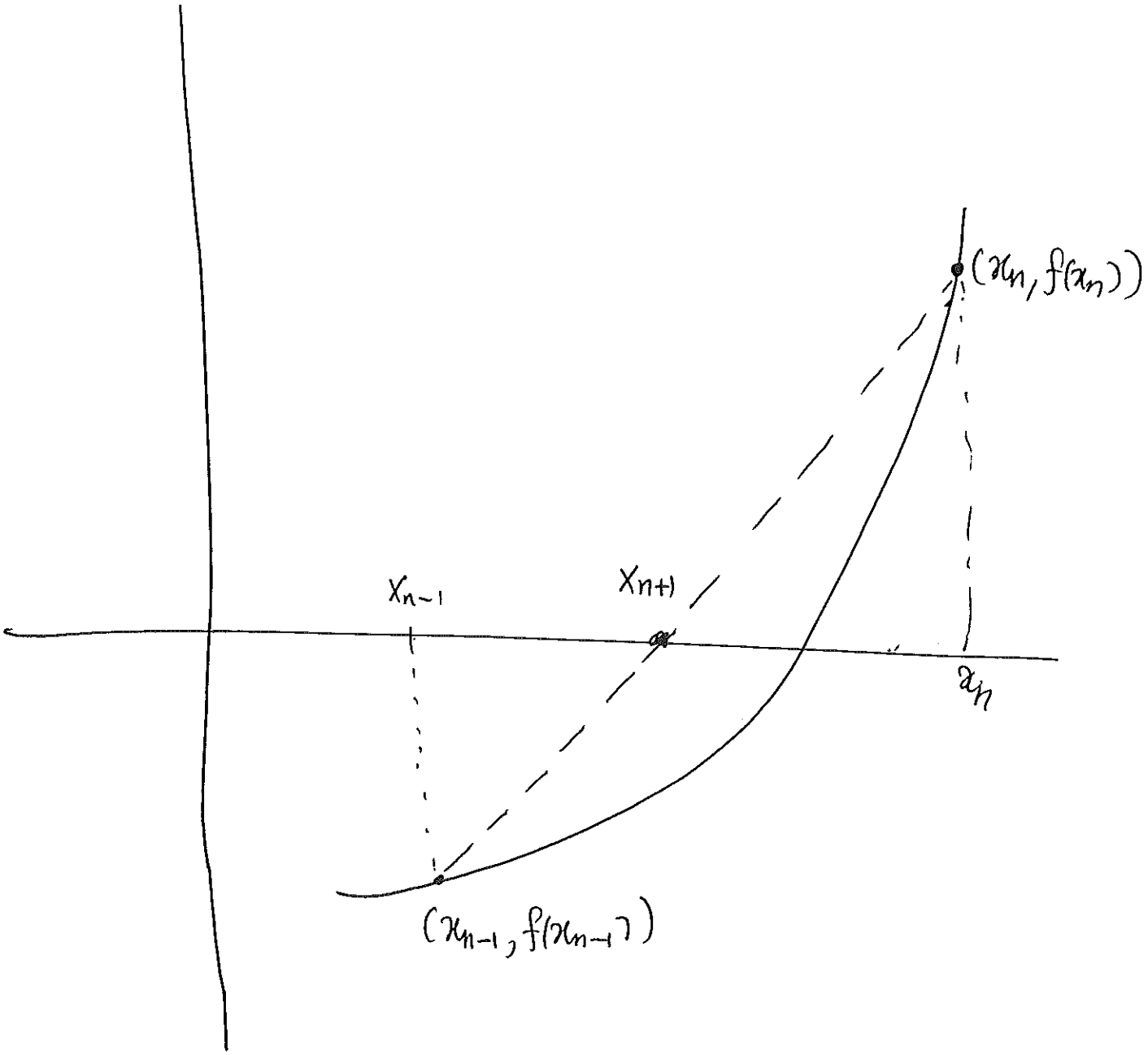
Given a function $f(x)$ and two points x_{-1} and x_0

FOR $n = 0, 1, 2, \ldots$ until satisfied

do Calculate

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

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


$(x_n, f(x_n))$
x_{n-1}
x_{n+1}
x_n
$(x_{n-1}, f(x_{n-1}))$

Example

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

$$x_{-1} = 1$$

$$x_0 = 2$$

(4 sig digits)

n	x_n	$f(x_n)$
-1	1	-1
0	2	2
1	1.333	-2.222 E-1
2	1.400	-4.000 E-2
3	1.415	2.225 E-3
4	1.414	-6.040 E-4
5	1.414	-6.040 E-4

Process ends

Note algorithm ends if $f(x_n) = f(x_{n-1})$

This makes the calculation of x_{n+1} impossible.

Remark

1. The expression

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

is prone to round-off errors since $f(x_n)$ and $f(x_{n-1})$ need not be of opposite signs

2. It is better to calculate x_{n+1} from the equivalent expression

$$x_{n+1} = x_n - f(x_n)\left\{\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}\right\}$$

in which x_{n+1} is obtained from x_n by adding the correction term

$$\frac{-f(x_n)}{\dfrac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}} = \frac{-f(x_n)}{[f(x_n), f(x_{n-1})]}$$

If x_n close to x_{n-1} then we get

$$[f(x_n), f(x_{n-1})] \simeq f'(x_n).$$

This gives the famous Newton's method

Given $f(x)$ continuously differentiable and a pt x_0

For $n = 0, 1, 2, \ldots$ until satisfied do

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

Example

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

$x_0 = 1$

$x_1 = 1.5$

$x_2 = 1.41666667$

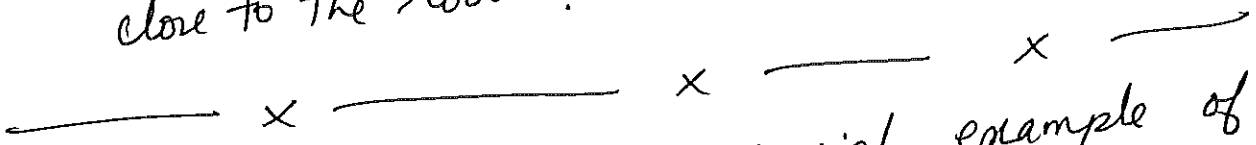
$x_3 = 1.41421568$

$x_4 = 1.41421356$

$X_n = x_4$ for $n \geq 4$.

Newton's method converges if x_0 is "close" to the root.

Question How to determine whether x_0 is close to the root?



Newton's method is a special example of "fixed-point iteration".

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

$$x_{n+1} = g(x_n)$$

$g : I \to I$
I closed interval containing root and $g(x)$ is cts

If the sequence $x_1, x_2, \cdots$ converges to some point ξ

$$\begin{aligned} \xi &= \lim_{n\to\infty} x_{n+1} \\ &= \lim_{n\to\infty} g(x_n) \\ &= g\left(\lim_{n\to\infty} x_n\right) \\ &= g(\xi) \end{aligned}$$

So ξ is a "fixed point" of g

$g(\xi) = \xi \iff f(\xi) = 0$ (assuming $f'(\xi) \neq 0$)

Fixed point iteration

Our goal is to find root of

$$f(x) = 0 \quad (1)$$

One derives from (1) an equation of the form

$$x = g(x) \quad (2)$$

So any solution of (2) (i.e., a fixed point of $g(x)$) is a solution for (1)

Usually there are many choices of $g(x)$

Example

$$f(x) = x^3 - x - 1$$

choices of $g(x)$ are

(1) $g(x) = x^3 - 1$

(2) $g(x) = \sqrt[3]{1+x}$

Algorithm for fixed point iteration

Given an iteration function $g(x)$ and a starting point x_0

For $n = 0, 1, 2, \ldots$ until satisfied

calculate $x_{n+1} = g(x_n)$.

Q When does the sequence converge?

Remark Not all sequences converge

Example $g(x) = x^3 - 1$

$x_0 = 1$

$x_1 = 0$

$x_2 = -1$

$x_3 = -2$

$x_4 = -9$

$x_5 = -730$

$x_6 = -3.89 \times 10^8$

This sequence diverges

On the other hand

$$g(x) = (1+x)^{1/3}$$

$x_0 = 0$

$x_1 = 1$

$x_2 = 1.25992$

$x_3 = \cancel{1.32235}$ 1.31229

$x_4 = \cancel{1.32427}$ 1.32235

$x_5 = 1.32427$

$x_6 = 1.32463$

$x_7 = 1.32470$

$x_8 = 1.32471$

$x_9 = 1.32472$

$x_{10} = 1.32472$

$x_j = x_{10}$ for $j \geq 10$

$$f(x) = x^3 - x - 1$$

$f(x_{10}) = -9.0001 \; E-8$

Condition for convergence of fixed point iteration

Condition 1 There is an interval $I = [a, b]$ such that for all $x \in I$, $g(x)$ is defined and $g(x) \in I$ i.e the function $g(x)$ maps I to itself.

Condition 2 The iteration function $g(x)$ is continuous on $I = [a, b]$.

Theorem Let $g : I \to I$ be continuous. $I = [a, b]$.

Then g has a fixed point.

Proof If $g(a) = a$ or $g(b) = b$ then obviously g has a fixed point

Otherwise $g(a) \neq a$ $\quad g(b) \neq b$

$g(a), g(b) \in I$. So

$g(a) > a$ $\quad g(b) < b$

$h(x) = g(x) - x$ $\quad h(a) > 0$ $\quad h(b) < 0$

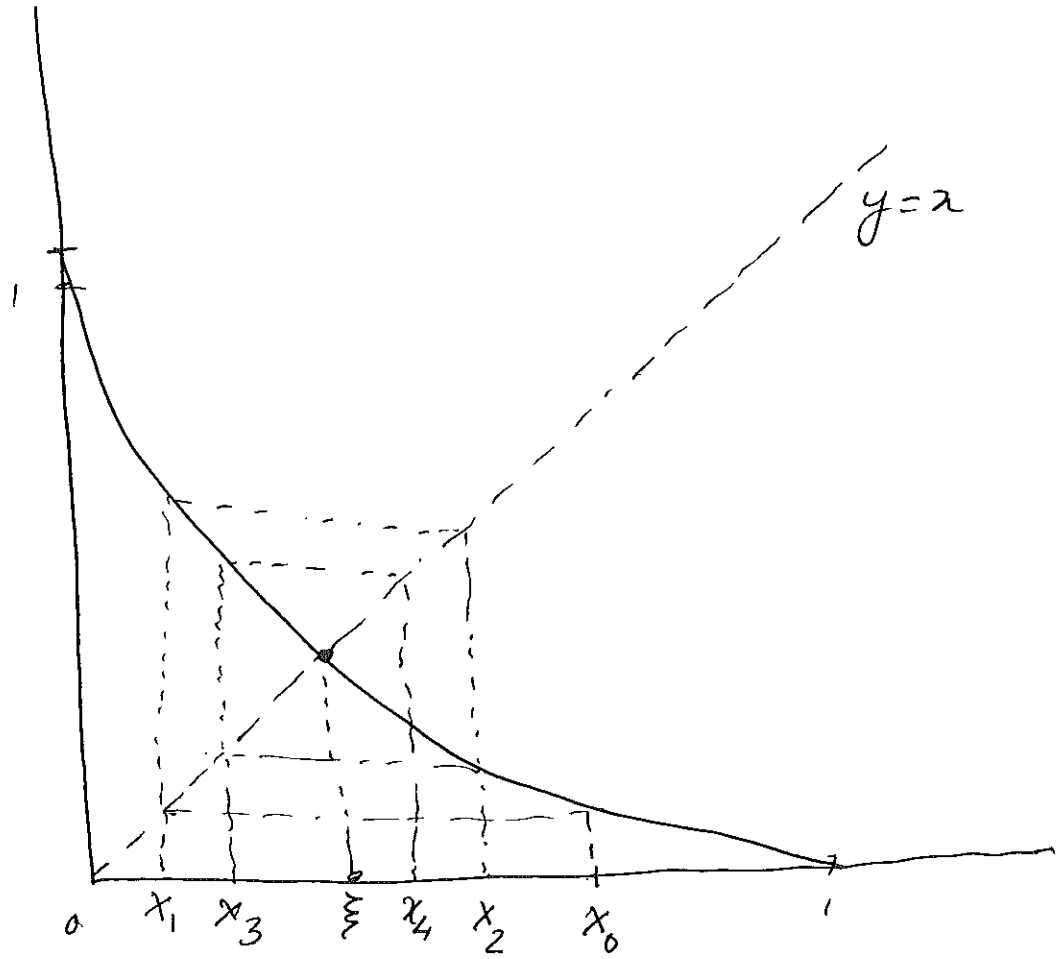
So by intermediate value theorem (as h is cts)

$h(x_0) = 0$ for some x_0

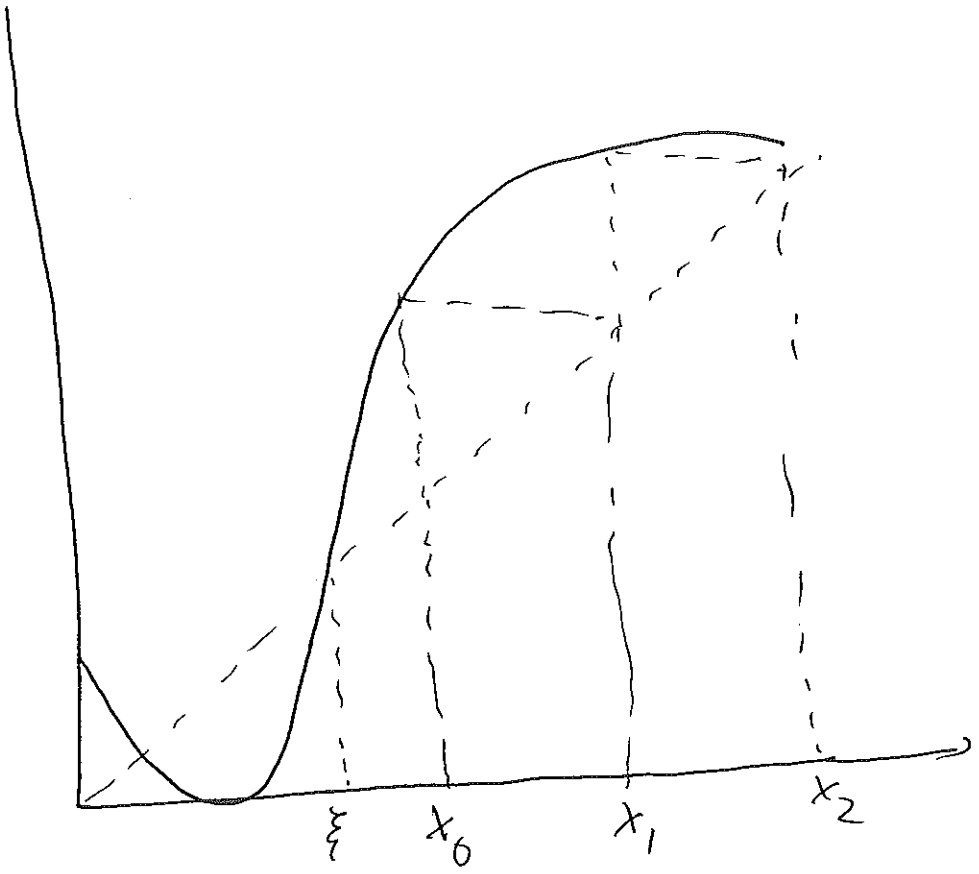
$\Rightarrow \quad g(x_0) = x_0$

Still we have not found conditions guaranteeing convergence.

It is better to look at iteration graphically



Here $x_i \to \xi \leftarrow$ fixed pt.



$x_1 \not\to \xi$

Reason :- slope of $g(x)$ is too large in absolute value, near ξ.

Condition 3 The iteration function $g(x)$ is differentiable on $I = [a, b]$. Furthermore there exists a non-negative constant $k < 1$ such that

$$|g'(x)| \leq k \qquad \forall\, x \in I$$

Theorem :- Let $g : I \to I$ be a function satisfying condition 1, 2, 3. Then g has a unique fixed point ξ in $I = [a, b]$. Furthermore with any point $x_0 \in I$, the sequence $x_0, x_1, \ldots, x_n = g(x_{n-1}), \ldots$ generated by fixed point iteration converges to ξ.

Proof :- By earlier result there exists a fixed point ξ of $g(x)$ in I

Let $x_0 \in I$ be any.

For $n \geq 1$ set $x_n = g(x_{n-1})$

Set $e_n = \xi - x_n$ the error in the n^{th} iterate

$\xi = g(\xi)$ and $x_n = g(x_{n-1})$

$e_n = g(\xi) - g(x_{n-1})$

$= g'(\eta_n)(\xi - x_{n-1})$ by MVT

η_n between ξ and x_{n-1}

So $e_n = g'(\eta_n) e_{n-1}$

$|e_n| = |g'(\eta_n)||e_{n-1}| \leq k|e_{n-1}|$

By induction on n we get

$|e_n| \leq k|e_{n-1}| \leq k^2|e_{n-2}| \leq \ldots \leq k^n|e_0|$

Since $0 \leq k < 1$ we have

$\lim_{n\to\infty} k^n = 0$

So $\lim_{n\to\infty} |e_n| = 0$

$\Rightarrow \lim_{n\to\infty} e_n = 0$

i.e $x_n \to \xi$.

Uniqueness of fixed pt.

Say α is another fixed pt $\quad \alpha \neq \xi$

$\alpha = g(\alpha) \qquad \xi = g(\xi)$

$\alpha - \xi = g(\alpha) - g(\xi)$

$= g'(u)(\alpha - \xi) \qquad u$ between α & ξ

$|\alpha - \xi| \leq K |\alpha - \xi|$ where $K < 1$

$\not\leq$ a contradiction

Example

Find root of $f(x) = e^x - 4x^2$ between 0 and 1

$e^x - 4x^2 = 0$

$4x^2 = e^x$

$x = \frac{1}{2} e^{\frac{x}{2}}$

$g(x) = \frac{1}{2} e^{\frac{x}{2}}$

$g(0) = \frac{1}{2} \qquad g(1) = \frac{1}{2} e^{1/2} = 0.82$

$$g'(x) = \frac{1}{4} e^{x/2}$$

$$|g'(x)| \leq |g(1)| = \frac{e}{2} = 0.41$$

Thus fixed point iteration of g will converge on interval $I = [0, 1]$

calculations in 6 sig digits

$x_0 = 0$

$x_1 = 0.5$

$x_2 = 0.642013$

$x_3 = 0.689257$

$\vdots$

$x_{13} = 0.714805$

$x_{14} = 0.714806$

$x_n = x_{14}$ for $n \geq 14$

$f(0.714806) = -3.2\ E{-7}$

Thus 0.714806 is approximately a root of $f(x)$.