Numerical Analysis : [MA214]
Lecture 9

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Recall

Last time we did numerical differentiation.

The first formula is

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

This is an $\theta(h)$ formula.

The central difference formula is

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

This is an $\theta(h^2)$ approximation.

Another $\theta(h^2)$ formula is

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

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 formula enables us to solve linear boundary value problem.

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

$$y(a) = \alpha,\ y(b) = \beta,\ x \in [a, b].$$

One of the most frequently occurring problem 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", *i.e.* a point x^* for which $|f(x^*)|$ is small.

Some iterative methods of root finding:-

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 $a_0 = a$ and $b_0 = b$, $m = \frac{a_0+b_0}{2}$.

$f(a_0)f(m) < 0$ then set $a_1 = a_0$ and $b_1 = m$
Otherwise set $a_1 = m$ and $b_1 = b$

So root lies in $[a_1, b_1]$

Example of Bisection method

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

$$a_0 = 1 \qquad f(a_0) = -1$$
$$b_0 = 2 \qquad f(b_0) = 2$$
$$m = \frac{1+2}{2} = 1.5$$
$$f(m) = 2.25 - 2 = 0.25$$
$$a_0 = 1 \qquad b_1 = 1.5$$

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 $n = 0, 1, 2, \cdots$ until satisfied do

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

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

Otherwise set $a_{n+1} = m$ and $b_{n+1} = b_n$

Then $f(x)$ has a root in the interval $[a_{n+1}, b_{n+1}]$

Example:-

$$f(x) = x^2 - 2 \ \ (\text{ in 4 sig digits })$$

n	a_n	b_n	$f(a_n)$	$f(b_n)$
0	1	2	-1	2
1	1	1.5	-1	$2.5E-1$
2	1.25	1.5	$-4.375E-1$	$2.5E-1$
3	1.375	1.5	$-1.094E-1$	$2.5E-1$
4	1.375	1.438	$-1.094E-1$	$6.641E-1$
5	1.407	1.438	$-2.035E-2$	$6.641E-1$
6	1.407	1.423	$-2.035E-2$	$2.493E-2$
7	1.407	1.415	$-2.035E-2$	$2.225E-3$
8	1.411	1.415	$-9.079E-3$	$2.225E-3$
9	1.413	1.415	$-3.431E-3$	$2.225E-3$
10	1.414	1.415	$-6.040E-4$	$2.225E-3$

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

So algorithm ends, roots 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 midpoint 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 $f(1)$ and $f(2)$ 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 algorithm is known as **Regula-falsi** or **false-position method**

Algorithm (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 $n = 0, 1, 2, \cdots$ until satisfied do

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

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

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

Then $f(x)$ has a root in the interval $[a_{n+1}, b_{n+1}]$

Example

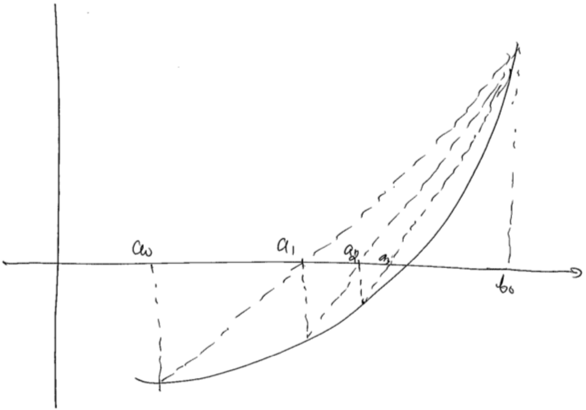
$$f(x) = x^2 - 2 \quad (\text{ in 4 sig digits })$$

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	$-4.086E-2$	2	1.412
3	1.412	2	$-6.256E-2$	2	1.414
4	1.414	2	$-6.040E-4$	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 $f(x)$.

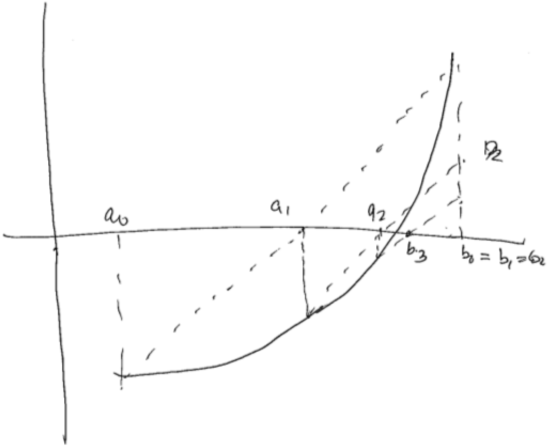
Consequently w always lies to the left of the zero (in our example).

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 method

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



Algorithm (Modified Regula-Falsi)

Given a function $f(x)$ continuous on the interval $[a_0, b_0]$ and such that $f(a_0)f(b_0) < 0$. Set $F = f(a_0)$, $G = f(b_0)$ and $w_0 = a_0$.

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

Calculate $w_{n+1} = \frac{Ga_n - Fb_n}{G - F}$

If $f(a_n)f(w_{n+1}) \leq 0$, then set $a_{n+1} = a_n$, $b_{n+1} = w_{n+1}$ and $G = f(w_{n+1})$

If also $f(w_n)f(w_{n+1}) > 0$, Set $F = \frac{F}{2}$

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

If also $f(w_n)f(w_{n+1}) > 0$, Set $G = \frac{G}{2}$

Then $f(x)$ has a zero in the interval $[a_{n+1}, b_{n+1}]$

Example

$$f(x) = x^2 - 2 \quad (\text{ in 4 sig digits })$$

$$a_0 = 0, \;\; b_0 = 2, \;\; w_0 = 1$$

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 $[1.414, 1.415]$.

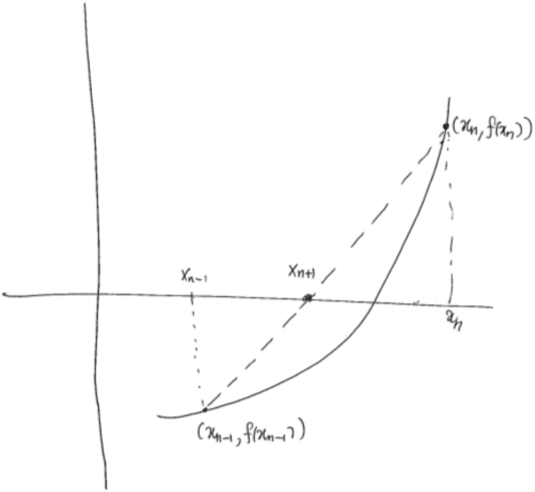
It retains the use of secants throughout but gives up the bracketing of the root.

Algorithm (Secant method)

Given a function $f(x)$ and two points x_1 and x_0.

For $n = 0, 1, 2, \cdots$ until satisfied calculate

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



Example

$$f(x) = x^2 - 2 \quad (\text{ in 4 sig digits })$$

$$x_{-1} = 1, \; x_0 = 2$$

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

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

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

Remarks

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

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

If x_n close to x_{n-1} then we get $[f(x_n), f(x_{n-1})] \approx f'(x_n)$.

This gives the famous **Newton's method**.

Newton's method

Given $f(x)$ continuously differentiable and a point x_0.

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

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

Example:-

$$f(x) = x^2 - 2 \quad \text{and } x_0 = 1$$

$$\begin{aligned}
x_1 &= 1.5 \\
x_2 &= 1.416666667 \\
x_3 &= 1.414215686 \\
x_4 &= 1.414213562 \\
x_n &= x_4 \quad \text{for} \quad n \geq 4
\end{aligned}$$

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".

$$\begin{aligned} g(x) &= x - \frac{f(x)}{f'(x)} \\ x_{n+1} &= g(x_n) \end{aligned}$$

$g : I \to I$, I is closed interval containing root. If the sequence $x_1, x_2, \cdots$ converges to some point ξ and $g(x)$ is continuous.

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

So ξ is a "fixed point" of g

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

Fixed point Iteration

Our goal is to find root of

$$f(x) = 0 \tag{4}$$

One derives from (4) an equation of the form

$$x = g(x) \tag{5}$$

So any solution of (5) (*i.e.*, a fixed point of $g(x)$) is a solution for (4)

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 $n = 0, 1, 2 \cdots$ until satisfied calculate $x_{n+1} = g(x_n)$.

Question: When does the sequence converge?

Remark: Not all sequences converge

Example: $g(x) = x^3 - 1$, $x_0 = 1$

$$\begin{aligned} x_1 &= 0 \\ x_2 &= -1 \\ x_3 &= -2 \\ x_4 &= -9 \\ x_5 &= -730 \\ x_6 &= -3.89 \times 10^8 \end{aligned}$$

This sequence diverges.

One the other hand $g(x) = (1+x)^{\frac{1}{3}}$, $x_0 = 0$

$$
\begin{aligned}
x_1 &= 1 \\
x_2 &= 1.25992 \\
x_3 &= 1.31229 \\
x_4 &= 1.32235 \\
x_5 &= 1.32427 \\
x_6 &= 1.32463 \\
x_7 &= 1.32470 \\
x_8 &= 1.32471 \\
x_9 &= 1.32472 \\
x_{10} &= 1.32472 \\
x_j &= x_{10} \quad \text{for } j \geq 10 \\
f(x) = x^3 - x - 1 & \\
f(x_{10}) = -9.001E - 8 &
\end{aligned}
$$

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 $g : I \longrightarrow I$ be continuous in $I = [a, b]$. Then g has a fixed point.

Proof.

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

Otherwise $g(a) \neq a$ and $g(b) \neq b$ and $g(a),\ g(b) \in I$.

So $g(a) > a$ and $g(b) < b$. Let $h(x) = g(x) - x$. Then $h(a) > 0$ and $h(b) < 0$.

So by intermediate value theorem (as h is continuous)

$$h(x_0) = 0 \quad \text{for some} \quad x_0$$

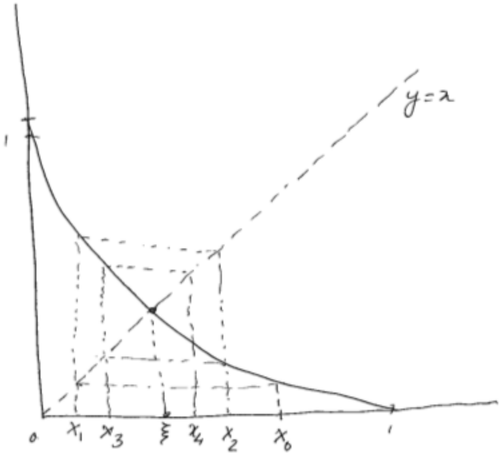
$$g(x_0) = x_0$$

$\square$

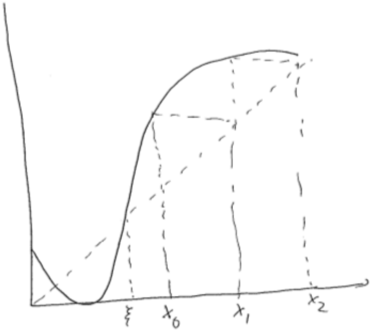
Still we have not found condition guaranteeing convergence.

It is better to look at iteration graphically.

Iteration graphically



Here $x_i \longrightarrow \xi$ (fixed point)



$$x_n \not\to \xi$$

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

$$|g'(x)| \leq K \quad \text{for all } x \in I$$

Theorem

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

Proof of theorem

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

Let $x_0 \in I$ be any point. For $n \geq 1$ set $x_n = g(x_{n-1})$.

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

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

$$\begin{aligned} e_n &= g(\xi) - g(x_{n-1}) \\ &= g'(\eta_n)(\xi - x_{n-1}) \quad \text{by MVT } \eta_n \text{ between } \xi \text{ and } x_{n-1} \\ \text{So} \quad & e_n = g'(\eta_n)e_{n-1} \\ & |e_n| = |g'(\eta_n)||e_{n-1}| \leq K|e_{n-1}| \end{aligned}$$

By induction on n we get

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

Since $0 \leq K < 1$ we have $\lim_{n\to\infty} K^n = 0$. So

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

$$i.e. \;\; x_n \longrightarrow \xi$$

Uniqueness of fixed point:-

Say α is another fixed point $\alpha \neq \xi$.

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

$$\begin{aligned} \alpha - \xi &= g(\alpha) - g(\xi) \\ &= g'(u)(\alpha - \xi) \;\; u \text{ between } \alpha \text{ and } \xi \\ |\alpha - \xi| &\leq K|\alpha - \xi| \;\; \text{where } K < 1 \end{aligned}$$

which is a contradiction.

Example

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

$$\begin{aligned} e^x - 4x^2 &= 0 \\ \iff \quad & e^x = 4x^2 \\ \iff \quad & x = \frac{1}{2}e^{\frac{x}{2}} \end{aligned}$$

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

$$g(0) = \frac{1}{2}$$

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

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

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

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

Calculations in 6 sig digits

$$
\begin{aligned}
x_0 &= 0 \\
x_1 &= 0.5 \\
x_2 &= 0.642013 \\
x_3 &= 0.689257 \\
&\vdots \\
x_{13} &= 0.714805 \\
x_{14} &= 0.714806 \\
x_n &= x_{14} \quad \text{for } n \geq 14 \\
f(0.714806) &= -3.2E - 7
\end{aligned}
$$

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