IB CATAM Project 0.1 (Preliminary Project)

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based on work by S.J.Cowley & M.Spivack

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Root finding in 1D

Given $F(x)$, find x_* so that $F(x_*) = 0$

1. $F = 2x - 3\sin x + 5 \quad (x_* = -2.88323687)$
2. $F = \left(x - \frac{1}{2}\right)(x-4)^2$

Methods

1. Bisection: if $F(a) < 0 < F(b)$, consider mid-point $\frac{1}{2}(a+b)$
2. Picard iteration: rearrange to $x = f(x)$, then iterate $x_{n+1} = f(x_n)$
3. Newton-Raphson: $x_{n+1} = x_n - F(x_n)/F'(x_n)$

Writing program + obtain numerical results $\rightarrow$ only half marks.

Need to demonstrate reported results are reliable

1. Does process behave as expected? – converge/diverge, when?
2. Error reduce as expected? – order of convergence?

Combine a little theory with numerical evidence

Question 1

Find the root of

$$F(x) \equiv 2x - 3\sin x + 5 = 0$$

Show graphically has exactly one root.

Think about $3\sin x$ and $2x+5$. Need only plot $[-4,-1]$ because

- $-|3\sin x| \geq -3 > 2x+5 \quad$ for $x < -4$
- $|3\sin x| \leq \ \ 3 < 2x+5 \quad$ for $x > -1$

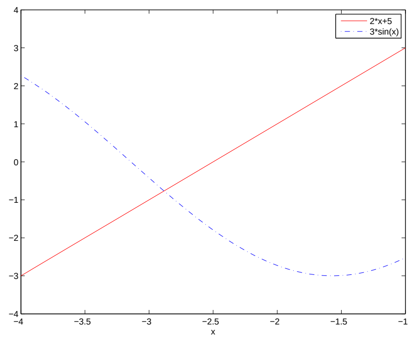


Figure: Plot of $2x+5$ and $3\sin x$.

But $2x+5$ and $3\sin x$ have same signs only in $-\pi \leq x \leq -\frac{5}{2}$, where have opposite slopes, so single root.

Programming Task 1 – bisection

Write a program for bisection method.

Terminate when $|x_{n+1} - x_n| < 0.5\,10^{-5}$.

Printout x_n and number of iterations n.

Run for a number of suitable starting values to check working.

Bisection program

Various comments and inputting code, then

```
n=0;
while( (xu-xl) > 2.0*tol )
  n=n+1;
  xm=0.5*(xl+xu);
  fprintf('%2d %11.7f %13.6e %13.6e %13.6e\n',n,xm,(xu-xl)/2,yl,yu)
  ym=f(xm);
  if yl*ym < 0
    xu=xm;
    yu=ym;
  else
    xl=xm;
    yl=ym;
  end
end
```

and then outputting code.

Programming Task 1 – bisection

Write a program for bisection method.
Terminate within $0.5\,10^{-5}$.
Printout x and number of iterations n.
Run for a number of suitable starting values to check working.

Initial Interval	Final Iterate	Truncation Error
$[-3.0, -2.0]$	$x_{18} = -2.8832359\ldots$	$\pm 0.0000038\ldots$
$[-\pi, -5/2]$	$x_{17} = -2.8832414\ldots$	$\pm 0.0000049\ldots$
$[-5\pi/4, -3\pi/4]$	$x_{19} = -2.8832397\ldots$	$\pm 0.0000030\ldots$

NB: all runs give same answer to $0.5\,10^{-5}$.
NB: more iterations for wider initial interval.

Question 2

Question: Suppose numerical error δ in evaluating function,
i.e. $F_{\text{exact}} = F_{num}(x) \pm \delta$.
What is effect on root?
Hint: $|F'| \geq 4$ in range of interest.

Answer: correct x_* is within $\pm\delta/F'(x_*)$ of program answer.
Thus error bound is $0.5\,10^{-5} + \frac{1}{4}\delta$

Programming Task 2 – iteration

Write a program for Pichard iteration method.
Terminate when $|x_{n+1} - x_n| < \epsilon$ or $n > n_{\max}$.
Printout x_n and n so can monitor progress.

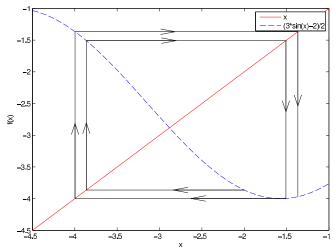
Question 3
Rearrange $F = 2x - 3\sin x + 5$ to iteration

$$x_{n+1} = f(x_n) = \frac{3\sin x_n + kx_n - 5}{2 + k}$$

(i) $k = 0$, $\epsilon = 10^{-5}$, $x_0 = -2$, $n_{max} = 10$.
Plot $y = f(x)$ and $y = x$. Why no convergence?

Question 3 (i)

Iteration diverges:



Question Explain the divergence by identifying a theoretical criterion that has been violated.

Contraction mapping theory:

$$\epsilon_{n+1} = x_{n+1} - x_* = f'(x)\epsilon_n$$

So converges if $|f'| < 1$, not true $k = 0$.

Question 3 (ii)

Question: Determine values of k for which convergence is guaranteed if x_n remains in the range $(-\pi, -\frac{1}{2}\pi)$.

Answer:

$$|f'| = \left|\frac{(3\cos x + k)}{(2 + k)}\right| < 1 \quad \text{for all } x \in [-\pi, -\tfrac{1}{2}\pi] \text{ if } k > \tfrac{1}{2}.$$

Question 3 (iii)

Question: Choose, *giving reasons*, a values of k which give (a) monotonic and (b) oscillatory convergence.
Verify expected behaviour, with $n_{max} = 20$.

Answer: $f'(x_*)$ changes from negative at $k \approx 2.9$.

Oscillating case with $k = 2.5$ and $x_0 = -2$.

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$f'(x_n)$
0	-2.0000000	8.832369e-01		
1	-2.8284205	5.481637e-02	0.0620630	-0.0786852
2	-2.8878412	-4.604324e-03	-0.0839954	-0.0897628
3	-2.8828254	4.115123e-04	-0.0893752	-0.0889152
4	-2.8832735	-3.660414e-05	-0.0889503	-0.0889916
5	-2.8832336	3.257347e-06	-0.0889885	-0.0889848
6	-2.8832372	-2.898553e-07	-0.0889851	-0.0889854

. . . question 3 (iii)

Monotone case with $k = 3.5$ and $x_0 = -2$.

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$f'(x_n)$
0	-2.0000000	8.832369e-01		
1	-2.6777986	2.054383e-01	0.2325970	0.1485300
2	-2.8571507	2.608618e-02	0.1269782	0.1128263
3	-2.8803442	2.892679e-03	0.1108894	0.1094173
4	-2.8829210	3.159219e-04	0.1092143	0.1090560
5	-2.8832024	3.444623e-05	0.1090340	0.1090168
6	-2.8832331	3.755134e-06	0.1090144	0.1090125
7	-2.8832365	4.093556e-07	0.1090122	0.1090120

Question 3 (iv)

Question: Run $k = 16$. This should converge slowly, so set $n_{max} = 50$.
Discuss if expect truncation error to be less than 10^{-5}.
Answer:

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$f'(x_n)$
0	-2.0000000	8.832369e-01		
1	-2.2071051	6.761317e-01	0.7655158	0.7898504
2	-2.3736981	5.095388e-01	0.7536087	0.7689931
⋮	⋮	⋮	⋮	⋮
32	-2.8831971	3.981016e-05	0.7277548	0.7277554
33	-2.8832079	2.897202e-05	0.7277545	0.7277549
34	-2.8832158	2.108451e-05	0.7277543	0.7277546

$$x_{n+1} - x_* \approx \frac{(x_{n+1} - x_n) f'(x_*)}{f'(x_n) - 1}$$

i.e. error is $2.673\times$ difference in iterates for $k = 16$

Question 3 (v)

Question: Discuss whether your results are consistent with first-order convergence.

Answer:
Theory is first-order convergence if $|f'(x_*)| < 1$ and $f'(x_*) \neq 0$.

Also the smaller $|f'(x_*)|$, the quicker the convergence
– faster than bisection if $|f'(x_*)| < \frac{1}{2}$.

Tables give evidence that error going down by factor f'.

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$f'(x_n)$
32	-2.8831971	3.981016e-05	0.7277548	0.7277554
33	-2.8832079	2.897202e-05	0.7277545	0.7277549
34	-2.8832158	2.108451e-05	0.7277543	0.7277546

Question 4 – double root

Rearrange $F = \left(x - \frac{1}{2}\right)(x-4)^2$ to iteration

$$x_{n+1} = f(x_n) = \frac{1}{20}\left(-x^3 + 8.5x^2 + 8\right)$$

Question: Set $n_{\max} = 1000$, and just print out final n & x_n, terminate when $|x_{n+1} - x_n| < 10^{-5}$.
Answer:

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$7n\epsilon_n/40$
0	4.5000000	5.000000e-01		
1	4.4500000	4.500000e-01	0.9000000	0.0787500
2	4.4100063	4.100063e-01	0.9111250	0.1435022
3	4.3771416	3.771416e-01	0.9198436	0.1979994
⋮	⋮	⋮	⋮	⋮
734	4.0075549	7.554867e-03	0.9986733	0.9704226
735	4.0075449	7.544857e-03	0.9986750	0.9704572
736	4.0075349	7.534874e-03	0.9986768	0.9704917

NB: error very much bigger than difference between iterates.

. . . question 4

Taylor series at double root

$$x_{n+1} = x_n + \tfrac{1}{2} f''(x_*)(x_n - x_*)^2 + \dots$$

so

$$\epsilon_{n+1} = \epsilon_n + \tfrac{1}{2} f''(x_*)\epsilon_n^2$$

i.e. $\epsilon_{n+1}/\epsilon_n \to 1$, so slower than first-order convergence.

See this in table

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$7n\epsilon_n/40$
734	4.0075549	7.554867e-03	0.9986733	0.9704226
735	4.0075449	7.544857e-03	0.9986750	0.9704572
736	4.0075349	7.534874e-03	0.9986768	0.9704917

Can show

$$\epsilon_n \sim -\frac{2}{f''(x_*)\, n} = \frac{40}{7n}$$

See this in table

Programming Task 3 – Newton-Raphson

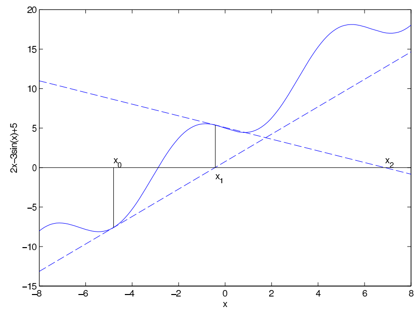
Write a program for Newton-Raphson for the two given functions.

Question 5 – single root

For $F = 2x - 3\sin x + 5$, find an x_0 that converges, and one that does not converged in 10 iterations.

In the unconverged case, show graphically what happened in the first few iterations.

$x_0 = -4.8$ divergences (initially).



. . . question 5 – single root

$x_0 = -4$ converges

n	x_n	ϵ_n	$\frac{\epsilon_n}{(\epsilon_{n-1})^2}$	$\frac{\log\|\epsilon_n\|}{\log\|\epsilon_{n-1}\|}$	$\frac{F''(x_n)}{2F'(x_n)}$
0	-4.000000000000000	-1.116763e+00			
1	-2.669401797516753	2.138351e-01	0.1714576	-13.9680184	-0.1460399
2	-2.888959367133085	-5.722495e-03	-0.1251490	3.3472819	-0.0764422
3	-2.883239394297850	-2.521740e-06	-0.0770069	2.4965498	-0.0782039
4	-2.883236872558781	-4.969358e-13	-0.0781448	2.1977565	-0.0782047
5	-2.883236872558284	4.440892e-16	1.798e+09	1.2477978	-0.0782047

. . . question 5 – single root

Question: do your results bear out the theoretical orders of convergence? Comment on the effects of rounding error.

Answer: Taylor series

$$\epsilon_{n+1} \sim K\epsilon_n^2 \quad \text{where} \quad K = \frac{F''(x_*)}{2F'(x_*)} \approx -0.0782\,.$$

i.e. 2nd order convergence. OR $\frac{\log|\epsilon_{n+1}|}{\log|\epsilon_n|} \to 2$

See table

n	x_n	ϵ_n	$\frac{\epsilon_n}{(\epsilon_{n-1})^2}$	$\frac{\log\|\epsilon_n\|}{\log\|\epsilon_{n-1}\|}$	$\frac{F''(x_n)}{2F'(x_n)}$
0	-4.000000000000000	-1.116763e+00			
1	-2.669401797516753	2.138351e-01	0.1714576	-13.9680184	-0.1460399
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4	-2.883236872558781	-4.969358e-13	-0.0781448	2.1977565	-0.0782047
5	-2.883236872558284	4.440892e-16	1.798e+09	1.2477978	-0.0782047

NB: Different behaviour of 5th iteration, because of rounding error.

Question 5 – double root

Starting at $x_0 = 5$ until $|x_{n+1} - x_n| < 10^{-5}$

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$\log|\epsilon_n|/\log|\epsilon_{n-1}|$
0	5.000000000	1.000000e+00		
1	4.550000000	5.500000e-01	0.5500000	
2	4.292485549	2.924855e-01	0.5317919	2.0563130
3	4.151672687	1.516727e-01	0.5185647	1.5341813
4	4.077379237	7.737924e-02	0.5101725	1.3568375
5	4.039103573	3.910357e-02	0.5053497	1.2667037
⋮	⋮	⋮	⋮	⋮
13	4.000154442	1.544418e-04	0.5000221	1.0857526
14	4.000077223	7.722263e-05	0.5000111	1.0789824
15	4.000038612	3.861176e-05	0.5000057	1.0732019
16	4.000019306	1.930602e-05	0.5000038	1.0682093
17	4.000009653	9.652994e-06	0.4999991	1.0638547

i.e. 1st order convergence. Taylor series gives $\epsilon_{n+1} = \frac{1}{2}\epsilon_n$.

... question 5 – double root

Question: Comment on the effect of rounding error.

Answer: If make error δ in numerically evaluating F and F', say

$$F(x_n) \sim \frac{1}{2}F''\epsilon_n^2 + \delta, \quad \text{and} \quad F'(x_n) \sim F''\epsilon_n + \delta$$

then Newton-Raphson gives

$$\epsilon_{n+1} \sim \epsilon_n - \frac{\frac{1}{2}F''\epsilon_n^2 + \delta}{F''\epsilon_n + \delta} \sim \tfrac{1}{2}\epsilon_n - \frac{\delta}{F''\epsilon_n}$$

So rounding error becomes comparable with update when $\epsilon_n = O(\delta^{1/2})$

... question 5 – double root

Rounding error in MATLAB's double precision is 10^{-16}
i.e. problem when $\epsilon = 10^{-8}$

Starting at $x_0 = 5$ until $|x_{n+1} - x_n| < 10^{-10}$

n	x_n	ϵ_n	$\epsilon_n/\epsilon_{n-1}$	$\log|\epsilon_n|/\log|\epsilon_{n-1}|$
18	4.000004826	4.826398e-06	0.4999897	1.0600237
19	4.000002413	2.413255e-06	0.5000116	1.0566212
20	4.000001206	1.206080e-06	0.4997730	1.0536240
21	4.000000602	6.017966e-07	0.4989692	1.0510129
22	4.000000302	3.015609e-07	0.5011010	1.0482393
23	4.000000147	1.467238e-07	0.4865479	1.0479823
24	4.000000064	6.370571e-08	0.4341880	1.0530215
25	4.000000032	3.183852e-08	0.4997750	1.0418612
26	3.999999968	-3.192455e-08	-1.0027018	0.9998437
27	3.999999968	-3.192455e-08	1.0000000	1.0000000

i.e. problem when $\epsilon = 10^{-8}$

Conclusion

Writing program + obtain numerical results → only half marks.

Need to demonstrate reported results are reliable

1. Does process behave as expected? – converge/diverge, when?
2. Error reduce as expected? – order of convergence?

Combine a little theory with numerical evidence