## Nonlinear Equations

## Introduction

In this Section we briefly discuss nonlinear equations (what they are and what their solutions might be) before noting that many such equations which crop up in applications cannot be solved exactly. The remainder (and majority) of the Section then goes on to discuss methods for approximating solutions of nonlinear equations.

| Prerequisites | - understand derivatives of simple functions <br> - understand the quadratic formula |
| :--- | :--- |
| Lefore starting this Section you should $\ldots$ | - understand exponentials and logarithms |

## 1. Nonlinear Equations

A linear equation is one related to a straight line, for example $f(x)=m x+c$ describes a straight line with slope $m$ and the linear equation $f(x)=0$, involving such an $f$, is easily solved to give $x=-c / m$ (as long as $m \neq 0$ ). If a function $f$ is not represented by a straight line in this way we say it is nonlinear.

The nonlinear equation $f(x)=0$ may have just one solution, like in the linear case, or it may have no solutions at all, or it may have many solutions. For example if $f(x)=x^{2}-9$ then it is easy to see that there are two solutions $x=-3$ and $x=3$. The nonlinear equation $f(x)=x^{2}+1$ has no solutions at all (unless the application under consideration makes it appropriate to consider complex numbers).
Our aim in this Section is to approximate (real-valued) solutions of nonlinear equations of the form $f(x)=0$. The definitions of a root of an equation and a zero of a function have been gathered together in Key Point 13.

## Key Point 13

If the value $x$ is such that $f(x)=0$ we say that

1. $x$ is a root of the equation $f(x)=0$
2. $x$ is a zero of the function $f$.

## Example 22

Find any (real valued) zeros of the following functions. (Give 3 decimal places if you are unable to give an exact numerical value.)
(a) $f(x)=x^{2}+x-20$
(b) $f(x)=x^{2}-7 x+5$
(c) $f(x)=2^{x}-3$
(d) $f(x)=e^{x}+1$
(e) $f(x)=\sin (x)$

## Solution

(a) This quadratic factorises easily into $f(x)=(x-4)(x+5)$ and so the two zeros of this $f$ are $x=4, x=-5$.
(b) The nonlinear equation $x^{2}-7 x+5=0$ requires the quadratic formula and we find that the two zeros of this $f$ are $x=\frac{7 \pm \sqrt{7^{2}-4 \times 1 \times 5}}{2}=\frac{7 \pm \sqrt{29}}{2}$ which are equal to $x=0.807$ and $x=6.193$, to 3 decimal places.

## Solution (contd.)

(c) Using the natural logarithm function we see that

$$
x \ln (2)=\ln (3)
$$

from which it follows that $x=\ln (3) / \ln (2)=1.585$, to 3 decimal places.
(d) This $f$ has no zeros because $e^{x}+1$ is always positive.
(e) $\sin (x)$ has an infinite number of zeros at $x=0, \pm \pi, \pm 2 \pi, \pm 3 \pi, \ldots$ To 3 decimal places these are $x=0.000, \pm 3.142, \pm 6.283, \pm 9.425, \ldots$.

Find any (real valued) zeros of the following functions.
(a) $f(x)=x^{2}+2 x-15$,
(b) $f(x)=x^{2}-3 x+3$,
(c) $f(x)=\ln (x)-2$,
(d) $f(x)=\cos (x)$.

For parts (a) to (c) give your answers to 3 decimal places if you cannot give an exact answer; your answers to part (d) may be left in terms of $\pi$.

## Your solution

## Answer

(a) This quadratic factorises easily into $f(x)=(x-3)(x+5)$ and so the two zeros of this $f$ are $x=3, x=-5$.
(b) The equation $x^{2}-3 x+3=0$ requires the quadratic formula and the two zeros of this $f$ are

$$
x=\frac{3 \pm \sqrt{3^{2}-4 \times 1 \times 3}}{2}=\frac{3 \pm \sqrt{-3}}{2}
$$

which are complex values. This $f$ has no real zeros.
(c) Solving $\ln (x)=2$ gives $x=e^{2}=7.389$, to 3 decimal places.
(d) $\cos (x)$ has an infinite number of zeros at $x=\frac{\pi}{2}, \frac{\pi}{2} \pm \pi, \frac{\pi}{2} \pm 2 \pi, \ldots$.

Many functions that crop up in engineering applications do not lend themselves to finding zeros directly as was achieved in the examples above. Instead we approximate zeros of functions, and this Section now goes on to describe some ways of doing this. Some of what follows will involve revision of material you have seen in HELM 12 concerning Applications of Differentiation.

## 2. The bisection method

Suppose that, by trial and error for example, we know that a single zero of some function $f$ lies between $x=a$ and $x=b$. The root is said to be bracketed by $a$ and $b$. This must mean that $f(a)$ and $f(b)$ are of opposite signs, that is that $f(a) f(b)<0$.

## Example 23

The single positive zero of the function $f(x)=x \tanh \left(\frac{1}{2} x\right)-1$ models the wave number of water waves at a certain frequency in water of depth 0.5 (measured in some units we need not worry about here). Find two points which bracket the zero of $f$.

## Solution

We simply evaluate $f$ at a selection of $x$-values.

| $x$ | $f(x)=x \tanh \left(\frac{1}{2} x\right)-1$ |  |
| ---: | :--- | :--- |
| 0 | $0 \times \tanh (0)-1$ | $=-1$ |
| 0.5 | $0.5 \times \tanh (0.25)-1=0.5 \times 0.2449-1$ | $=-0.8775$ |
| 1 | $1 \times \tanh (0.5)-1=1 \times 0.4621-1$ | $=-0.5379$ |
| 1.5 | $1.5 \times \tanh (0.75)-1=1.5 \times 0.6351-1$ | $=-0.0473$ |
| 2 | $2 \times \tanh (1)-1=2 \times 0.7616-1$ | $=0.5232$ |

From this we can see that $f$ changes sign between 1.5 and 2 . Thus we can take $a=1.5$ and $b=2$ as the bracketing points. That is, the zero of $f$ is in the bracketing interval $1.5<x<2$.

The function $f(x)=\cos (x)-x$ has a single positive zero. Find bracketing points $a$ and $b$ for the zero of $f$. Arrange for the difference between $a$ and $b$ to be equal to $\frac{1}{2}$.
(NB - be careful to use radians on your calculator!)

## Your solution

## Answer

We evaluate $f$ for a range of values:

| $x$ | $f(x)$ |
| :---: | :---: |
| 0 | 1 |
| 0.5 | 0.37758 |
| 1 | -0.459698 |

Clearly $f$ changes sign between the bracketing values $a=0.5$ and $b=1$.
(Other answers are valid of course, it depends which values of $f$ you tried.)

The aim with the bisection method is to repeatedly reduce the width of the bracketing interval $a<x<b$ so that it "pinches" the required zero of $f$ to some desired accuracy. We begin by describing one iteration of the bisection method in detail.

Let $m=\frac{1}{2}(a+b)$, the mid-point of the interval $a<x<b$. All we need to do now is to see in which half (the left or the right) of the interval $a<x<b$ the zero is in. We evaluate $f(m)$. There is a (very slight) chance that $f(m)=0$, in which case our job is done and we have found the zero of $f$. Much more likely is that we will be in one of the two situations shown in Figure 13 below. If $f(m) f(b)<0$ then we are in the situation shown in (a) and we replace $a<x<b$ with the smaller bracketing interval $m<x<b$. If, on the other hand, $f(a) f(m)<0$ then we are in the situation shown in (b) and we replace $a<x<b$ with the smaller bracketing interval $a<x<m$.


(b)

Figure 13

Either way, we now have a bracketing interval that is half the size of the one we started with. We have carried out one iteration of the bisection method. By successively reapplying this approach we can make the bracketing interval as small as we wish.

## Example 24

Carry out one iteration of the bisection method so as to halve the width of the bracketing interval $1.5<x<2$ for

$$
f(x)=x \tanh \left(\frac{1}{2} x\right)-1 .
$$

## Solution

The mid-point of the bracketing interval is $m=\frac{1}{2}(a+b)=\frac{1}{2}(1.5+2)=1.75$. We evaluate

$$
f(m)=1.75 \times \tanh \left(\frac{1}{2} \times 1.75\right)-1=0.2318
$$

to 4 decimal places. We found earlier (Example 20, page 63) that $f(a)<0$ and $f(b)>0$, the fact that $f(m)$ is of the opposite sign to $f(a)$ means that the zero of $f$ lies in the bracketing interval $1.5<x<1.75$.


Carry out one iteration of the bisection method so as to halve the width of the bracketing interval $0.5<x<1$ for

$$
f(x)=\cos (x)-x .
$$

## Your solution

## Answer

Here $a=0.5, b=1$. The mid-point of the bracketing interval is $m=\frac{1}{2}(a+b)=\frac{1}{2}(0.5+1)=0.75$. We evaluate

$$
f(m)=\cos (0.75)-0.75=-0.0183
$$

We found earlier (Task, pages 58-59) that $f(a)>0$ and $f(b)<0$, the fact that $f(m)$ is of the opposite sign to $f(a)$ means that the zero of $f$ lies in the bracketing interval $0.5<x<0.75$.

So we have a way of halving the size of the bracketing interval. By repeatedly applying this approach we can make the interval smaller and smaller.

The general procedure, involving (possibly) many iterations, is best described as an algorithm:

1. Choose an error tolerance.
2. Let $m=\frac{1}{2}(a+b)$, the mid-point of the bracketing interval.
3. There are three possibilities:
(a) $f(m)=0$, this is very unlikely in general, but if it does happen then we have found the zero of $f$ and we can go to step 7,
(b) the zero is between $m$ and $b$,
(c) the zero is between $a$ and $m$.
4. If the zero is between $m$ and $b$, that is if $f(m) f(b)<0$ (as in Figure 13(a)) then let $a=m$.
5. Otherwise the zero must be between $a$ and $m$ (as in Figure 13(b)) so let $b=m$.
6. If $b-a$ is greater than the required tolerance then go to step 2 .
7. End.

One feature of this method is that we can predict in advance how much effort is required to achieve a certain level of accuracy.

## Example 25

A given problem using the bisection method starts with the bracketing points $a=1.5$ and $b=2$. How many iterations will be required so that the error in the approximation is less that $\frac{1}{2} \times 10^{-6}$ ?

## Solution

Before we carry out any iterations we can write that the zero to be approximated is $1.75 \pm 0.25$ so that the maximum magnitude of the error in 1.75 may be taken to be equal to 0.25 .
Each successive iteration will halve the size of the error, so that after $n$ iterations the error is equal to

$$
\frac{1}{2^{n}} \times 0.25
$$

We require that this quantity be less than $\frac{1}{2} \times 10^{-6}$. Now,

$$
\frac{1}{2^{n}} \times 0.25<\frac{1}{2} \times 10^{-6} \quad \text { implies that } \quad 2^{n}>\frac{1}{2} \times 10^{6} .
$$

The smallest value of $n$ which satisfies this inequality can be found by trial and error, or by using logarithms to see that $n>\left(\ln \left(\frac{1}{2}\right)+6 \ln (10)\right) / \ln (2)$. Either way, the smallest integer which will do the trick is

$$
n=19 .
$$

It takes 19 iterations of the bisection method to ensure the required accuracy.

A function $f$ is known to have a single zero between the points $a=3.2$ and $b=4$. If these values were used as the initial bracketing points in an implementation of the bisection method, how many iterations would be required to ensure an error less than $\frac{1}{2} \times 10^{-3}$ ?

## Your solution

## Answer

We require that

$$
\frac{1}{2^{n}} \times\left(\frac{4-3.2}{2}\right)<\frac{1}{2} \times 10^{-3}
$$

or, after a little rearranging,

$$
2^{n}>\frac{4}{5} \times 10^{3} .
$$

The smallest value of $n$ which satisfies this is $n=10$. (This can be found by trial-and-error or by using logarithms.)

## Pros and cons of the bisection method

## Pros

- the method is easy to understand and remember
- the method always works (once you find values $a$ and $b$ which bracket a single zero)
- the method allows us to work out how many iterations it will take to achieve a given error tolerance because we know that the interval will exactly halve at each step


## Cons

- the method is very slow
- the method cannot find roots where the curve just touches the $x$-axis but does not cross it (e.g. double roots)

The slowness of the bisection method will not be a surprise now that you have worked through an example or two! Significant effort is involved in evaluating $f$ and then all we do is look at this $f$-value and see whether it is positive or negative! We are throwing away hard won information.

Let us be realistic here, the slowness of the bisection method hardly matters if all we are saying is that it takes a few more fractions of a second of computing time to finish, when compared with a competing approach. But there are applications in which $f$ may be very expensive (that is, slow) to calculate and there are applications where engineers need to find zeros of a function many thousands of times. (Coastal engineers, for example, may employ mathematical wave models that involve finding the wave number we saw in Example 20 at many different water depths.) It is quite possible that you will encounter applications where the bisection method is just not good enough.

## 3. The Newton-Raphson method

You may recall (e.g. HELM 13.3) that the Newton-Raphson method (often simply called Newton's method) for approximating a zero of the function $f$ is given by

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

where $f^{\prime}$ denotes the first derivative of $f$ and where $x_{0}$ is an initial guess to the zero of $f$. A graphical way of interpreting how this method works is shown in Figure 14.


Figure 14
At each approximation to the zero of $f$ we extrapolate so that the tangent to the curve meets the $x$-axis. This point on the $x$-axis is the new approximation to the zero of $f$. As is clear from both the figure and the mathematical statement of the method above, we require that $f^{\prime}\left(x_{n}\right) \neq 0$ for $n=0,1,2, \ldots$.

## Example 26

Let us consider the example we met earlier in Example 24. We know that the single positive zero of

$$
f(x)=x \tanh \left(\frac{1}{2} x\right)-1
$$

lies between 1.5 and 2. Use the Newton-Raphson method to approximate the zero of $f$.

## Solution

We must work out the derivative of $f$ to use Newton-Raphson. Now

$$
f^{\prime}(x)=\tanh \left(\frac{1}{2} x\right)+x\left(\frac{1}{2} \operatorname{sech}^{2}\left(\frac{1}{2} x\right)\right)
$$

on differentiating a product and recalling that $\frac{d}{d x} \tanh (x)=\operatorname{sech}^{2}(x)$. (To evaluate sech on a calculator recall that $\operatorname{sech}(x)=\frac{1}{\cosh (x)}$.)
We must choose a starting value $x_{0}$ for the iteration and, given that we know the zero to be between 1.5 and 2, we take $x_{0}=1.75$. The first iteration of Newton-Raphson gives

$$
x_{1}=x_{0}-\frac{f\left(x_{0}\right)}{f^{\prime}\left(x_{0}\right)}=1.75-\frac{f(1.75)}{f^{\prime}(1.75)}=1.75-\frac{0.231835}{1.145358}=1.547587,
$$

where 6 decimal places are shown. The second iteration gives

$$
x_{2}=x_{1}-\frac{f\left(x_{1}\right)}{f^{\prime}\left(x_{1}\right)}=1.547587-\frac{f(1.547587)}{f^{\prime}(1.547587)}=1.547587-\frac{0.004585}{1.09687}=1.543407 .
$$

Clearly this method lends itself to implementation on a computer and, for example, using a spreadsheet package, it is not hard to compute a few more iterations. Here is output from Microsoft Excel where we have included the two lines of hand-calculation above:

| $n$ | $x_{n}$ | $f\left(x_{n}\right)$ | $f^{\prime}\left(x_{n}\right)$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 1.75 | 0.231835 | 1.145358 | 1.547587 |
| 1 | 1.547587 | 0.004585 | 1.09687 | 1.543407 |
| 2 | 1.543407 | $2.52 E-06$ | 1.095662 | 1.543405 |
| 3 | 1.543405 | $7.69 E-13$ | 1.095661 | 1.543405 |
| 4 | 1.543405 | 0 | 1.095661 | 1.543405 |

and all subsequent lines are equal to the last line here. The method has converged (very quickly!) to 1.543405 , to six decimal places.

Earlier, in Example 25, we found that the bisection method would require 19 iterations to achieve 6 decimal place accuracy. The Newton-Raphson method gave an answer good to this number of places in just two or three iterations.

Use the starting value $x_{0}=0$ in an implementation of the Newton-Raphson method for approximating the zero of

$$
f(x)=\cos (x)-x .
$$

(If you are doing these calculations by hand then just perform two or three iterations. Don't forget to use radians.)

## Your solution

## Answer

The derivative of $f$ is $f^{\prime}(x)=-\sin (x)-1$. The first iteration is

$$
x_{1}=x_{0}-\frac{f\left(x_{0}\right)}{f^{\prime}\left(x_{0}\right)}=0-\frac{1-0}{-0-1}=1
$$

and the second iteration is

$$
x_{2}=x_{1}-\frac{f\left(x_{1}\right)}{f^{\prime}\left(x_{1}\right)}=1-\frac{\cos (1)-1}{-\sin (1)-1}=1-\frac{-0.459698}{-1.841471}=0.750364,
$$

and so on. There is little to be gained in our understanding by doing more iterations by hand, but using a spreadsheet we find that the method converges rapidly:

| $n$ | $x_{n}$ | $f\left(x_{n}\right)$ | $f^{\prime}\left(x_{n}\right)$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 1 | -1 | 1 |
| 1 | 1 | -0.4597 | -1.84147 | 0.750364 |
| 2 | 0.750364 | -0.01892 | -1.6819 | 0.739113 |
| 3 | 0.739113 | $-4.6 E-05$ | -1.67363 | 0.739085 |
| 4 | 0.739085 | $-2.8 E-10$ | -1.67361 | 0.739085 |
| 5 | 0.739085 | 0 | -1.67361 | 0.739085 |

It is often necessary to find zeros of polynomials when studying transfer functions. Here is a Task involving a polynomial.

The function $f(x)=x^{3}+2 x+4$ has a single zero near $x_{0}=-1$. Use this value of $x_{0}$ to perform two iterations of the Newton-Raphson method.

## Your solution

## Answer

Using the starting value $x_{0}=-1$ you should find that $f\left(x_{0}\right)=1$ and $f^{\prime}\left(x_{0}\right)=5$. This leads to

$$
x_{1}=x_{0}-\frac{f\left(x_{0}\right)}{f^{\prime}\left(x_{0}\right)}=-1-\frac{1}{5}=-1.2
$$

The second iteration should give you $\quad x_{2}=x_{1}-\frac{f\left(x_{1}\right)}{f^{\prime}\left(x_{1}\right)}=-1.2-\frac{-0.128}{6.32}=-1.17975$.
Subsequent iterations will home in on the zero of $f$. Using a computer spreadsheet gives:

| $n$ | $x_{n}$ | $f(x)$ | $f^{\prime}(x)$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | -1 | 1 | 5 | -1.2 |
| 1 | -1.2 | -0.128 | 6.32 | -1.17975 |
| 2 | -1.17975 | -0.00147 | 6.175408 | -1.17951 |
| 3 | -1.17951 | $-2 E-07$ | 6.173725 | -1.17951 |
| 4 | -1.17951 | 0 | 6.173725 | -1.17951 |

where we have recomputed the hand calculations for the first two iterations.
We see that the method converges to the value -1.17951 .

## Engineering Example 2

## Pressure in an ideal multi-component mixture

## Introduction

An ideal multi-component mixture consists of

1. n-pentane (5\%)
2. $n$-hextane ( $15 \%$ )
3. $n$-heptane ( $50 \%$ )
4. $n$-octane $(30 \%)$

In general, the total pressure, $P(\mathrm{~Pa})$ of an ideal four-component mixture is related to the boiling point, $T(\mathrm{~K})$ through the formula:

$$
P=x_{1} p_{1}^{*}+x_{2} p_{2}^{*}+x_{3} p_{3}^{*}+x_{4} p_{4}^{*}
$$

where, for component $i$, the mole fraction is $x_{i}$ and the vapour pressure is $p_{i}^{*}$, given by the formula:

$$
p_{i}^{*}=\exp \left\{A_{i}-\frac{B_{i}}{\left(T+C_{i}\right)}\right\} \quad i=1,2,3,4
$$

Here $p_{i}^{*}$ is in $\mathrm{mm} \mathrm{Hg}(1 \mathrm{~mm} \mathrm{Hg}=133.32 \mathrm{~Pa}), T$ is the absolute temperature $(\mathrm{K})$ and the constants $A_{i}, B_{i}$ and $C_{i}$ are given in the table below.

| $i$ | component | $x_{i}$ | $A_{i}$ | $B_{i}$ | $C_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | $n$-pentane | 0.05 | 15.8333 | 2477.07 | -39.94 |
| 2 | $n$-hexane | 0.15 | 15.8366 | 2697.55 | -48.78 |
| 3 | $n$-heptane | 0.50 | 15.8737 | 2911.32 | -56.51 |
| 4 | $n$-octane | 0.30 | 15.9426 | 3120.29 | -63.63 |

## Problem 1

For the liquid compositions, $x_{i}$ given in the table above, plot a graph of the total pressure, $P(\mathrm{~Pa})$ against temperature ( K ) over the range 250 to 500 K .

## Solution

$p_{i}^{*}=\exp \left(A_{i}-\frac{B_{i}}{T+C_{i}}\right)$, expressed in millimetres of mercury, and so it is 133.32 times that in pascals. Therefore, expressed in pascals, we have

$$
P=133.32 \sum_{i=1}^{4} x_{i} \exp \left(A_{i}-\frac{B_{i}}{T+C_{i}}\right)
$$

Plotting this from $T=250$ to 500 gives the following graph


Figure 15

## Problem 2

Using the Newton-Raphson method, solve the equations to find the boiling points at total pressures of $1,2,5$ and 10 bars. Show the sequence of iterations and perform sufficient calculations for convergence to three significant figures. Display these solutions on the graph of the total pressure, $P(\mathrm{~Pa})$ against temperature $T(\mathrm{~K})$.

## Solution

We wish to find $T$ when $P=1,2,5$ and 10 bars, that is, $10^{5}, 2 \times 10^{5}, 5 \times 10^{5}$ and $10 \times 10^{5} \mathrm{~Pa}$.
Reading crude approximations to $T$ from the graph gives a starting point for the Newton-Raphson process. We see that for $10^{5}, 2 \times 10^{5}, 5 \times 10^{5}$ and $10 \times 10^{5} \mathrm{~Pa}$, temperature $T$ is roughly $365,375,460$ and 485 degrees K , respectively, so we shall use these values as the start of the iteration.

In this case it is easy to calculate the derivative of $P$ with respect to $T$ exactly, rather than numerically, giving

$$
P^{\prime}(T)=133.32 \sum_{i=1}^{4} x_{i} \exp \left(A_{i}-\frac{B_{i}}{T+C_{i}}\right) \times\left(\frac{B_{i}}{\left(T+C_{i}\right)^{2}}\right)
$$

Therefore to solve the equation $P(T)=y$, we set $T_{0}$ to be the starting value above and use the iteration

$$
T_{n+1}=T_{n}-\frac{P\left(T_{n}\right)-y}{P^{\prime}\left(T_{n}\right)}
$$

For $y=100000$ this gives the iterations

| $T_{0}$ | $T_{1}$ | $T_{2}$ | $T_{3}$ | $T_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| 365 | 362.7915 | 362.7349 | 362.7349 | 362.7349 |

We conclude that, to three significant figures $T=363^{\circ} \mathrm{K}$ when $P=100000 \mathrm{~Pa}$.
For $y=200000$ this gives the iterations

| $T_{0}$ | $T_{1}$ | $T_{2}$ | $T_{3}$ | $T_{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| 375 | 390.8987 | 388.8270 | 388.7854 | 388.7854 |

We conclude that, to three significant figures $T=389^{\circ} \mathrm{K}$ when $P=200000 \mathrm{~Pa}$.
For $y=500000$ this gives the iterations

| $T_{0}$ | $T_{1}$ | $T_{2}$ | $T_{3}$ | $T_{4}$ | $T_{5}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 460 | 430.3698 | 430.4640 | 430.2824 | 430.2821 | 430.2821 |

We conclude that, to three significant figures $T=430^{\circ} \mathrm{K}$ when $P=500000 \mathrm{~Pa}$.
For $y=1000000$ this gives the iterations

| $T_{0}$ | $T_{1}$ | $T_{2}$ | $T_{3}$ | $T_{4}$ | $T_{5}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 475 | 469.0037 | 468.7875 | 468.7873 | 468.7873 | 468.7873 |

We conclude that, to three significant figures $T=469^{\circ} \mathrm{K}$ when $P=1000000 \mathrm{~Pa}$.

## An approximate Newton-Raphson method

The Newton-Raphson method is an excellent way of approximating zeros of a function, but it requires you to know the derivative of $f$. Sometimes it is undesirable, or simply impossible, to work out the derivative of a function and here we show a way of getting around this.

We approximate the derivative of $f$. From Section 31.3 we know that

$$
f^{\prime}(x) \approx \frac{f(x+h)-f(x)}{h}
$$

is a one-sided (or forward) approximation to $f^{\prime}$ and another one, using a central difference, is

$$
f^{\prime}(x) \approx \frac{f(x+h)-f(x-h)}{2 h}
$$

The advantage of the forward difference is that only one extra $f$-value has to be computed. If $f$ is especially complicated then this can be a considerable saving when compared with the central difference which requires two extra evaluations of $f$. The central difference does have the advantage, as we saw when we looked at truncation errors, of being a more accurate approximation to $f^{\prime}$.

The spreadsheet program Microsoft Excel has a built in "solver" command which can use Newton's method. (It may be necessary to use the "Add in" feature of Excel to access the solver.) In reality Excel has no way of working out the derivative of the function and must approximate it. Excel gives you the option of using a forward or central difference to estimate $f^{\prime}$.

We now reconsider the problem we met in Examples 24 to 26.

## Example 27

We know that the single positive zero of $f(x)=x \tanh \left(\frac{1}{2} x\right)-1$ lies between 1.5 and 2. Use the Newton-Raphson method, with an approximation to $f^{\prime}$, to approximate the zero of $f$.

## Solution

There is no requirement for $f^{\prime}$ this time, but the nature of this method is such that we will resort to a computer straight away. Let us choose $h=0.1$ in our approximations to the derivative.
Using the one-sided difference to approximate $f^{\prime}(x)$ we obtain this sequence of results from the spreadsheet program:

| $n$ | $x_{n}$ | $f\left(x_{n}\right)$ | $\frac{f(x+h)-f(x)}{h}$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 1.75 | 0.231835 | 1.154355 | 1.549165 |
| 1 | 1.549165 | 0.006316 | 1.110860 | 1.543479 |
| 2 | 1.543479 | $8.16 E-05$ | 1.109359 | 1.543406 |
| 3 | 1.543406 | $1.01 E-06$ | 1.109339 | 1.543405 |
| 4 | 1.543405 | $1.24 E-08$ | 1.109339 | 1.543405 |
| 5 | 1.543405 | $1.53 E-10$ | 1.109339 | 1.543405 |
| 6 | 1.543405 | $1.89 E-12$ | 1.109339 | 1.543405 |
| 7 | 1.543405 | $2.31 E-14$ | 1.109339 | 1.543405 |
| 8 | 1.543405 | 0 | 1.109339 | 1.543405 |

And using the (more accurate) central difference gives

| $n$ | $x_{n}$ | $f\left(x_{n}\right)$ | $\frac{f(x+h)-f(x-h)}{2 h}$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 1.75 | 0.231835 | 1.144649 | 1.547462 |
| 1 | 1.547462 | 0.004448 | 1.095994 | 1.543404 |
| 2 | 1.543404 | $-1 E-06$ | 1.094818 | 1.543405 |
| 3 | 1.543405 | $7.95 E-10$ | 1.094819 | 1.543405 |
| 4 | 1.543405 | $-6.1 E-13$ | 1.094819 | 1.543405 |
| 5 | 1.543405 | 0 | 1.094819 | 1.543405 |

We see that each of these approaches leads to the same value (1.543405) that we found with the Newton-Raphson method.

Use a spreadsheet to recompute the approximations shown in Example 24, for the following values of $h$ :

$$
h=0.001, \quad 0.00001, \quad 0.000001 .
$$

## Your solution

## Answer

You should find that as $h$ decreases, the numbers get closer and closer to those shown earlier for the Newton-Raphson method. For example, when $h=0.0000001$ we find that for a one-sided difference the results are

| $n$ | $x_{n}$ | $f\left(x_{n}\right)$ | $\frac{f(x+h)-f(x)}{h}$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 1.75 | 0.231835 | 1.145358 | 1.547587 |
| 1 | 1.547587 | 0.004585 | 1.096870 | 1.543407 |
| 2 | 1.543407 | $2.52 E-06$ | 1.095662 | 1.543405 |
| 3 | 1.543405 | $8.08 E-13$ | 1.095661 | 1.543405 |
| 4 | 1.543405 | 0 | 1.095661 | 1.543405 |

and those for a central difference with $h=0.0000001$ are

| $n$ | $x_{n}$ | $f\left(x_{n}\right)$ | $\frac{f(x+h)-f(x-h)}{2 h}$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 1.75 | 0.231835 | 1.145358 | 1.547587 |
| 1 | 1.547587 | 0.004585 | 1.096870 | 1.543407 |
| 2 | 1.543407 | $2.52 E-06$ | 1.095662 | 1.543405 |
| 3 | 1.543405 | $7.7 E-13$ | 1.095661 | 1.543405 |
| 4 | 1.543405 | 0 | 1.095661 | 1.543405 |

It is clear that these two tables very closely resemble the Newton-Raphson results seen earlier.

## Exercises

1. It is given that the function

$$
f(x)=x^{3}+2 x+8
$$

has a single negative zero.
(a) Find two integers $a$ and $b$ which bracket the zero of $f$.
(b) Perform one iteration of the bisection method so as to halve the size of the bracketing interval.
2. Consider a simple electronic circuit with an input voltage of 2.0 V , a resistor of resistance 1000 $\Omega$ and a diode. It can be shown that the voltage across the diode can be found as the single positive zero of

$$
f(x)=1 \times 10^{-14} \exp \left(\frac{x}{0.026}\right)-\frac{2-x}{1000}
$$

Use one iteration of the Newton-Raphson method, and an initial value of $x_{0}=0.75$ to show that

$$
x_{1}=0.724983
$$

and then work out a second iteration.
3. It is often necessary to find the zeros of polynomials as part of an analysis of transfer functions. The function

$$
f(x)=x^{3}+5 x-4
$$

has a single zero near $x_{0}=1$. Use this value of $x_{0}$ in an implementation of the Newton-Raphson method performing two iterations. (Work to at least 6 decimal place accuracy.)
4. The smallest positive zero of

$$
f(x)=x \tan (x)+1
$$

is a measure of how quickly certain evanescent water waves decay, and its value, $x_{0}$, is near 3 . Use the forward difference

$$
\frac{f(3.01)-f(3)}{0.01}
$$

to estimate $f^{\prime}(3)$ and use this value in an approximate version of the Newton-Raphson method to derive one improvement on $x_{0}$.

## Answers

1. (a) By trial and error we find that $f(-2)=-4$ and $f(-1)=5$, from which we see that the required bracketing interval is $a<x<b$ where $a=-2$ and $b=-1$.
(b) For an iteration of the bisection method we find the mid-point $m=-1.5$. Now $f(m)=$ 1.625 which is of the opposite sign to $f(a)$ and hence the new smaller bracketing interval is $a<x<m$.
2. The derivative of $f$ is $f^{\prime}(x)=\frac{1 \times 10^{-14}}{0.026} \exp \left(\frac{x}{0.026}\right)+\frac{1}{1000}$, and therefore the first iteration of Newton-Raphson gives $\quad x_{1}=0.75-\frac{0.032457}{1.297439}=0.724983$.

The second iteration gives $\quad x_{2}=0.724983-\frac{0.011603}{0.496319}=0.701605$.
Using a spreadsheet we can work out some more iterations. The result of this process is tabulated below

| $n$ | $x_{n}$ | $f\left(x_{n}\right)$ | $f^{\prime}\left(x_{n}\right)$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 2 | 0.701605 | 0.003942 | 0.202547 | 0.682144 |
| 3 | 0.682144 | 0.001161 | 0.096346 | 0.670092 |
| 4 | 0.670092 | 0.000230 | 0.060978 | 0.666328 |
| 5 | 0.666328 | $1.56 E-05$ | 0.052894 | 0.666033 |
| 6 | 0.666033 | $8.63 E-08$ | 0.052310 | 0.666031 |
| 7 | 0.666031 | $2.68 E-12$ | 0.052306 | 0.666031 |
| 8 | 0.666031 | 0 | 0.052306 | 0.666031 |

and we conclude that the required zero of $f$ is equal to 0.666031 , to 6 decimal places.
3. Using the starting value $x_{0}=1$ you should find that $f\left(x_{0}\right)=2$ and $f^{\prime}\left(x_{0}\right)=8$. This leads to

$$
x_{1}=x_{0}-\frac{f\left(x_{0}\right)}{f^{\prime}\left(x_{0}\right)}=1-\frac{2}{8}=0.75 .
$$

The second iteration should give you $\quad x_{2}=x_{1}-\frac{f\left(x_{1}\right)}{f^{\prime}\left(x_{1}\right)}=0.75-\frac{0.171875}{6.6875}=0.724299$.
Subsequent iterations can be used to 'home in' on the zero of $f$ and, using a computer spreadsheet program, we find that

| $n$ | $x_{n}$ | $f(x)$ | $f^{\prime}(x)$ | $x_{n+1}$ |
| :---: | :---: | :---: | :---: | :---: |
| 2 | 0.724299 | 0.001469 | 6.573827 | 0.724076 |
| 3 | 0.724076 | $1.09 E-07$ | 6.572856 | 0.724076 |
| 4 | 0.724076 | 0 | 6.572856 | 0.724076 |

We see that the method converges to the value 0.724076 .

## Answers

4. We begin with

$$
f^{\prime}(3) \approx \frac{f(3.01)-f(3)}{0.01}=\frac{0.02924345684}{0.01}=2.924345684
$$

to the displayed number of decimal places, and hence an improvement on $x_{0}=0.75$ is

$$
x_{1}=3-\frac{f(3)}{2.924345684}=2.804277,
$$

to 6 decimal places. (It can be shown that the root of $f$ is 2.798386 , to 6 decimal places.)

