AMA252 Lecture 1: Infinite Series

6th September 2007

1 Taylor-MaClaurin Series

In this Chapter we examine how functions can be expressed in terms of power series. Power series are an extremely useful way of expressing functions since we can replace complicated functions with simple polynomials. The only requirement is that the complicated function should be smooth; this means that at a point of interest, it must be possible to differentiate the function as many times as is necessary. We begin with a reminder of ideas covered earlier

1.1 The Binomial Theorem

A very important infinite series which occurs often in various applications has the form:

$$1 + \alpha x + \frac{\alpha(\alpha-1)}{2!}x^2 + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}x^3 + ...$$

This series is valid (i.e. convergent) for $|x| < 1$ (that is, $-1 < x < +1$) and where α is any real number. The binomial theorem can be directly obtained from the binomial series if α is chosen to be a **positive integer.** In this case the binomial theorem is states that if n is positive integer then the expansion (a+b) raised to the power n is given by:

$$(a+b)^n = a^n + na^{n-1}b + \frac{n(n-1)}{2!}a^{n-2}b^2 + ... + b^n$$

If α is a *positive integer (*eg $\alpha = 2, 3$ etc) then the series terminates. For example,

$$\begin{aligned}(1+x)^3 &= 1 + \frac{3}{1!}x + \frac{3(2)}{2!}x^2 + \frac{3(2)(1)}{3!}x^3 \\ &= 1 + 3x + 3x^2 + x^3.\end{aligned}$$

This, and all similar series, is valid for all x. But, whenever α is *not* a positive integer, then there will always be an infinite number of terms.

Example

$$\begin{aligned}(1-x)^{-1} &= 1 + \frac{(-1)(-x)}{1!} + \frac{(-1)(-2)(-x)^2}{2!} + \frac{(-1)(-2)(-3)(-x)^3}{3!} + ... \\ &= 1 + x + x^2 + x^3 + x^4 + ...\end{aligned}$$

Example

$$\begin{aligned}(3+x)^{-2} &= \left[3\left(1+\frac{x}{3}\right)\right]^{-2} = \frac{1}{9}\left(1+\frac{x}{3}\right)^{-2} \\ &= \frac{1}{9}\left[1+(-2)\frac{x}{3}+\frac{(-2)(-3)}{2!}\left(\frac{x}{3}\right)^2+...\right] \\ &= \frac{1}{9}\left[1-\frac{2x}{3}+\frac{x^2}{3}+...\right]\end{aligned}$$

This series is valid for $|x/3|<1$ - that is, for $-3<x<+3$.
Series which are expressed in terms of *positive integral* powers of x are called *power series.* In principle, we should always examine our series to see if it converges/diverges for some range of x-values. Various tests are available - fortunately, we shall *not* need to investigate these for our applications where - mainly - only a few terms are used near the origin. For example, the expansion for $(1-x)^{-1}$ is valid for $-1\le x<1$ and not just for $-1<x<1$.
We shall soon see how to generate power series for many different kinds of functions, but first we look briefly at one way of generating useful results by differentiating and integrating power series:

1.2 Differentiation and Integration of Power Series

If

$$f(x)=c_0+c_1x+c_2x^2+c_3x^3+...+c_nx^n+...$$

is convergent for some range of x, then

$$f'(x)=c_1+2c_2x+3c_3x^2+...+nc_nx^{n-1}+...$$

and

$$\int_0^x f(t)\,dt=c_0x+c_1\frac{x^2}{2}+c_2\frac{x^3}{3}+...+c_n\frac{x^{n+1}}{n+1}+...$$

are also convergent for some range of x.

Example 1

Show that

$$x+\frac{x^2}{2}+\frac{x^3}{3}+...+\frac{x^n}{n}+...=-\ln(1-x)$$

Solution

Differentiating $-\ln(1-x)$ gives $1/(1-x)$ and we already know that

$$(1-x)^{-1}=1+x+x^2+x^3+...+x^n+...$$

for $-1\le x<1$. Integrating the series term by term gives

$$x+\frac{x^2}{2}+\frac{x^3}{3}+...+\frac{x^n}{n}+...=\int_0^x\frac{1}{1-t}\,dt=-\ln(1-x)$$

which is also convergent for $-1\le x<1$.

1.3 Taylor and MacLaurin Series

We have already seen that many simple functions have power series expansions.

Question: Does *any* function have a power series expansion?
To answer this, we suppose that some function, $f(x)$, can be represented as

$$f(x) = c_0 + c_1(x-a) + c_2(x-a)^2 + c_3(x-a)^3 + c_4(x-a)^4 + \dots$$

Then we have

$$\begin{aligned} f'(x) &= c_1 + 2c_2(x-a) + 3c_3(x-a)^2 + 4c_4(x-a)^3 + \dots \\ f''(x) &= 2c_2 + (3)(2)c_3(x-a) + (4)(3)c_4(x-a)^2 + \dots \\ f'''(x) &= 3!c_3 + 4!c_4(x-a) + \dots \\ f^{iv}(x) &= 4!c_4 + \dots \end{aligned}$$

Putting $x = a$ gives directly

$$c_0 = f(a),\ c_1 = f'(a),\ c_2 = \frac{1}{2!}f''(a),\ c_3 = \frac{1}{3!}f'''(a), \dots etc$$

so that

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \frac{(x-a)^3}{3!}f'''(a) + \dots + \frac{(x-a)^{n-1}}{(n-1)!}f^{(n-1)}(a) + \dots \quad (1)$$

This method works fine *as long as* $f(a)$, $f'(a)$, $f''(a)$,... etc exist (that is, have finite values). The equation (1) is called the *Taylor expansion* of $f(a)$ about $x = a$. The value of a is chosen according to circumstances (ie, what we need). In the particular case of $a = 0$, the series is called the *MacLaurin's expansion.*

Example 2

Find the MacLaurin expansion for $f(x) = \sin x$.

Solution

Since we want the MacLaurin expansion, we have $a = 0$.

$$\begin{aligned} f(x) = \sin x &\rightarrow f(0) = 0 \\ f'(x) = \cos x &\rightarrow f'(0) = 1 \\ f''(x) = -\sin x &\rightarrow f''(0) = 0 \\ f'''(x) = -\cos x &\rightarrow f'''(0) = -1 \\ f^{iv}(x) = \sin(x) &\rightarrow f^{iv}(0) = 0 \end{aligned}$$

The pattern should be clear, and we get

$$\begin{aligned}\sin x &= 0 + \frac{x}{1!}(1) + \frac{x^2}{2!}(0) + \frac{x^3}{3!}(-1) + \frac{x^4}{4!}(0) + \frac{x^5}{5!}(1) + ... \\ &= x - \frac{x^3}{3!} + \frac{x^5}{5!} - ...\end{aligned}$$

which converges for *all* x. The general term is given by

$$(-1)^m \frac{x^{2m+1}}{(2m+1)!}, \quad m = 0, 1, 2, ...$$

Example 3

Find the MacLaurin expansion of $\ln(1+x)$.

Solution

$$\begin{aligned} f(x) = \ln(1+x) &\quad\rightarrow\quad f(0) = \ln 1 = 0 \\ f'(x) = \frac{1}{1+x} &\quad\rightarrow\quad f'(0) = 1 \\ f''(x) = \frac{-1}{(1+x)^2} &\quad\rightarrow\quad f''(0) = -1 \\ f'''(x) = \frac{2}{(1+x)^3} &\quad\rightarrow\quad f'''(0) = 2! \\ f^{iv}(x) = \frac{-3!}{(1+x)^4} &\quad\rightarrow\quad f^{iv}(0) = -3! = -6 \end{aligned}$$

so that

$$\begin{aligned}\ln(1+x) &= 0 + \frac{x}{1!}(1) + \frac{x^2}{2!}(-1) + \frac{x^3}{3!}(2!) + \frac{x^4}{4!}(-3!) + ... \\ &= x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + ...\end{aligned}$$

The general term is

$$(-1)^{n-1}\frac{x^n}{n}, \; n = 1, 2, ...$$

We would expect this series to give reasonable answers for x close to 0 (that is, the point about which the expansion was made). Thus, if $x = 0.1$ the first three terms give

$$\ln 1.1 \approx 0.1 - \frac{0.1^2}{2} + \frac{0.1^3}{3} = 0.09533$$

The true value is $\ln 1.1 = 0.09531$ to 5dp.

Example 4

We can easily show that

$$\mathrm{e}^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots$$

which is true for *all* values of x.

Notes

- Remember that for a Taylor expansion to exist, then $f(a),\ f'(a),\ f''(a),\ f'''(a), \ldots$ must exist - that is, be *finite.*
- Thus, since a MacLaurin expansion is the special case of Taylor with $a = 0$, then $f(0),\ f'(0),\ f''(0), \ldots$ must exist.
- For this reason, there are no MacLaurin expansions for $\ln x$, or $\cot x$ or e^x/x or for any other function for which $f(0) = \infty$.
- However, for such functions, we will usually be able to expand about some other point.

Example 5

Thus, for $\ln x$ we can expand about $x = 1$ to get

$$\ln x = (x-1) - \frac{1}{2}(x-1)^2 + \frac{1}{3}(x-1)^3 + \ldots$$

1.4 Taylor's Theorem and Error Estimation

If we expand $f(x)$ about $x = a$, then the Taylor expansion of the function will be

$$f(x) = f(a) + (x-a)\, f^{(1)}(a) + \frac{(x-a)^2}{2!}\, f^{(2)}(a) + \ldots + \frac{(x-a)^{n-1}}{(n-1)!}\, f^{(n-1)}(a) + R_n(a,x)$$

where $R_n(x,a)$ is the - so-called - *remainder* term. This term represents the remaining part of the series that has not been included. It can be shown to be given by

$$R_n(a,x) = \frac{(x-a)^n}{n!}\, f^{(n)}(c), \quad \text{where} \;\; a < c < x$$

That is, there is a value of c in the range $a < c < x$ such that the given expression for $R_n(a,x)$ is equal to all the remaining series. Note that it is impossible to specify c more closely. Thus if, for any given x, we choose c such that $R_n(a,x)$ is *maximised* then this value of $R_n(a,x)$ can be considered as an estimate of the error involved in approximating $f(x)$ by the $n-1$ degree polynomial

$$f(x) \approx f(a) + (x-a)\, f^{(1)}(a) + \frac{(x-a)^2}{2!}\, f^{(2)}(a) + \ldots + \frac{(x-a)^{n-1}}{(n-1)!}\, f^{(n-1)}(a).$$

Example 6

Use the first two terms of the MacLaurin series for $\sin x$ to estimate $\sin 0.5$, and estimate the associated error.

Solution

We already have the MacLaurin series for $\sin x$:

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + ...$$

Hence, using the first two terms, we get

$$\sin 0.5 \approx 0.5 - \frac{0.5^3}{3!} = 0.47917$$

Since $a = 0$ here, the the error term is given by

$$R_5(0, x) = \frac{x^5}{5!} f^{(5)}(c), \quad 0 < c < x.$$

Since $x = 0.5$ then $0 < c < 0.5$ and since $f(x) = \sin x$ then $f^{(5)}(x) = \cos x$ so that $f^{(5)}(c) = \cos c$. We do not know c but, obviously, the maximum possible value for $f^{(5)}(c)$ in the range $0 < c < 0.5$ occurs when $c = 0$ and is given by $f^{(5)}(0) = 1$. So, we get

$$|R_5(0, 0.5)| \leq \frac{0.5^5}{5!} (1) = 2.604 \times 10^{-4} \approx 0.000260$$

In fact, we find true $\sin 0.5 = 0.479426$ to 6dp, whereas our estimate above gives $\sin 0.5 \approx 0.47917$ giving an actual error of 0.000256. Thus, the estimated error is very close to the true error.

Example 7

Repeat the above using the first four terms.

Solution

We get

$$R_9(0, x) = \frac{x^9}{9!} \cos c, \quad \text{where} \;\; 0 < c < 0.5$$

Hence

$$|R_9(0, 0.5)| \leq \frac{0.5^9}{9!} = 5.38 \times 10^{-9}$$

If we do the actual calculation and compare with the actual value, we find a true error of 5.39×10^{-9}

2 L'Hopital's Rule: Calculation of Limits

L'Hopital's rule is extremely useful in the evaluation of a limit which might otherwise be difficult to obtain, i.e. we are interested in the value of $0 \div 0$! For example,

$$\lim_{x \to 2} \frac{x^2 + x - 6}{x^2 - 4} = \frac{0}{0}$$

In fact, this example is easily solved

$$\lim_{x\to 2}\frac{x^2+x-6}{x^2-4}=\lim_{x\to 2}\frac{(x+3)(x-2)}{(x+2)(x-2)}=\lim_{x\to 2}\frac{x+3}{x+2}=\frac{5}{4}.$$

We now introduce a more general method known as *L'Hopital's Rule* for evaluating limits of the type

$$\lim_{x\to a}\frac{f(x)}{g(x)}$$

where $f(a)=g(a)=0$.
To obtain the general method, we begin by expanding $f(x)$ and $g(x)$ about $x=a$ using Taylor's Theorem:

$$\frac{f(x)}{g(x)}=\frac{f(a)+(x-a)f^{(1)}(a)+(x-a)^2f^{(2)}(a)/2!+...+(x-a)^nf^{(n)}(a)/n!+...}{g(a)+(x-a)g^{(1)}(a)+(x-a)^2g^{(2)}(a)/2!+...+(x-a)^ng^{(n)}(a)/n!+...}$$

Next, we note that, since we are assuming $f(a)=g(a)=0$, then

$$\begin{aligned}\frac{f(x)}{g(x)} &= \frac{(x-a)f^{(1)}(a)+(x-a)^2f^{(2)}(a)/2!+...+(x-a)^nf^{(n)}(a)/n!+...}{(x-a)g^{(1)}(a)+(x-a)^2g^{(2)}(a)/2!+...+(x-a)^ng^{(n)}(a)/n!+...}\\ &= \frac{f^{(1)}(a)+(x-a)f^{(2)}(a)/2!+...+(x-a)^{n-1}f^{(n)}(a)/n!+...}{g^{(1)}(a)+(x-a)g^{(2)}(a)/2!+...+(x-a)^{n-1}g^{(n)}(a)/n!+...}\end{aligned}$$

so that, finally,

$$\lim_{x\to a}\frac{f(x)}{g(x)}=\frac{f^{(1)}(a)}{g^{(1)}(a)}.$$

This is known as *L'Hopital's Rule.* However, in some cases, we might also find that $f^{(1)}(a)=g^{(1)}(a)=0$ in which case we simply apply the rule again so that

$$\lim_{x\to a}\frac{f^{(1)}(x)}{g^{(1)}(x)}=\frac{f^{(2)}(a)}{g^{(2)}(a)}$$

and so on.

Notes

The rule also applies directly for cases where $x\to\infty$ and to cases which involve the form ∞/∞.
For other indeterminate forms such as $0\times\infty$ or $\infty-\infty$, it is necessary to manipulate the algebra into either $0/0$ or ∞/∞ before the L'Hopital's Rule can be applied.

Example 8

Evaluate

$$\lim_{x\to\infty}\frac{\pi/2-\tan^{-1}x}{x^{-1}}.$$

Solution

$$
\begin{aligned}
\lim_{x\to\infty} \frac{\pi/2 - \tan^{-1} x}{x^{-1}} &= \lim_{x\to\infty} \frac{-1/(1+x^2)}{-1/x^2} = \lim_{x\to\infty} \frac{x^2}{1+x^2} \\
&= \lim_{X\to\infty} \frac{2x}{2x} = 1
\end{aligned}
$$

Example 9

Evaluate

$$\lim_{x\to 0+} x \, \ln x$$

Note that this has the form of $0 \times \infty$.

Solution

$$
\begin{aligned}
\lim_{x\to 0+} x \, \ln x &= \lim_{x\to 0+} \frac{\ln x}{1/x} \\
&= \lim_{x\to 0+} \frac{1/x}{-1/x^2} = \lim_{x\to 0+} (-x) = 0.
\end{aligned}
$$

Example 10

Evaluate

$$\lim_{x\to 1} \left(\frac{1}{\ln x} - \frac{x}{x-1} \right)$$

Note that this has the form $\infty - \infty$.

Solution

We begin by rearranging the form $\infty - \infty$ into the form $0/0$:

$$\lim_{x\to 1} \left(\frac{1}{\ln x} - \frac{x}{x-1} \right) = \lim_{x\to 1} \left[\frac{x - 1 - x \ln x}{(x-1)\ln x} \right]$$

Now apply L'Hopital's Rule:

$$
\begin{aligned}
= \lim_{x\to 1} \left[\frac{1 - (\ln x + x(1/x))}{\ln x + (x-1)(1/x)} \right] &= \lim_{x\to 1} \left[\frac{-\ln x}{\ln x + 1 - 1/x} \right] \\
= \lim_{x\to 1} \left[\frac{-1/x}{1/x + 1/x^2} \right] &= -\frac{1}{2}
\end{aligned}
$$

Example 11
When an alternating electromagnetic field (EMF) of the form $E \sin nt$ is applied to a quiescent LC circuit, the current *i* at time *t* is given by

$$i = \frac{nE}{L(n^2 - w^2)} [\cos wt - \cos nt]$$

where $w^2 = 1/LC$ and w is not equal to n. Show that when *n* is tuned to the natural frequency w of the circuit the current intensity will be

$$i = \frac{Et \sin wt}{2L}$$

Solution
In fact we need to calculate the limit

$$A = \lim_{n \to w} \frac{nE}{L(n^2 - w^2)} [\cos wt - \cos nt]$$

Clearly this is a *0/0* case, so we have to use the L'Hopital's rule, i.e. to differentiate the nominator and denominator with respect to *n*.

$$A = \lim_{n \to w} \frac{E\,[\cos wt - \cos nt] + nEt \sin nt}{2Ln} = \lim_{n \to w} \left[\frac{E\,(\cos wt - \cos nt)}{2Ln} + \frac{nEt \sin nt}{2Ln} \right]$$

It is obvious that the first limit will tend to zero, while the second term (after simplication) leads to the requested result.
AMA252 Lecture 2: Solving Non-Linear Equations

3 Approximate Estimation of Roots

Perhaps one of the most fundamental mathematical tasks is the problem of finding a root of a function $f(x)$, in other words, find the value(s) of x, say α, which solves the equation $f(x) = 0$. Specific values of α are called *roots* or zeros of the function or solutions of the equation, in either case $f(\alpha) = 0$. In the special case of a first order ($f(x) = ax + b$) or second order ($f(x) = ax^2 + bx + c$) equations the roots are very well known from algebra. On the other hand, for many simple functions, say, $f(x) = e^x - x$, it is not possible to determine an algebraic expression for the solution.
Geometrically, the fact that α is a solution of the equation $f(x) = 0$ means that the graph of the function crosses the horizontal axis at $x = \alpha$, or the graph just touches the horizontal axis at $x = \alpha$. In the case of differentiable functions, the graph may have a horizontal tangent at the point $(0, \alpha)$ on the horizontal axis; this indicates a multiple root. We are concerned with solving equations of the general form $f(x) = 0$: for example

$$x^3 - 2x - 5 = 0, \quad \text{or } \mathrm{e}^x = 3x$$

etc, for which it is generally impossible (or extremely difficult) to obtain analytical solutions. We begin by considering how to obtain rough estimates of the required solutions.

Graphical Methods

Here we simply sketch $y = f(x)$ and note the value of x which makes $y = 0$. It is often easier to split $f(x)$ into $f(x) = f_1(x) - f_2(x)$, where $f_1(x)$ and $f_2(x)$ are simpler functions, then plot these separately, noting where $f_1 = f_2$.

Example 2

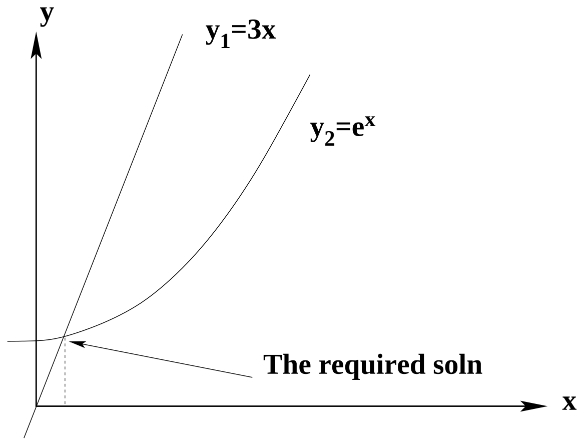


Figure 1: Graphical method used to evaluate the root of a function in the case of Example 2

Consider $f(x) = \mathrm{e}^x - 3x$ and let $f_1(x) = \mathrm{e}^x$ and $f_2(x) = 3x$.

Tabular Methods

We simply tabulate $f(x)$ over some suitable range and find where a sign change occurs:

Example 3

Consider the equation $f(x) \equiv x^3 - 3x^2 + 2x - 7 = 0$ and tabulate $f(x)$ as shown below:

x	0	1	2	3	4
$f(x)$	-7	-7	-7	-1	17

We see that a root lies between 3 and 4 - and probably nearer to 3. So, we could take 3.1 as a reasonable guess for x_0.

Polynomials: Descartes Rule Of Signs

This is a rule which applies to polynomial-type equations and gives us an upper limit to the *number* of *real* roots that the equation has:

> *The polynomial equation, $f(x) = 0$,cannot possess more $+ve$ real roots than there are changes of signs in the coefficients of $f(x)$ and cannot possess more $-ve$ real roots than there are changes of signs in the coefficients of $f(-x)$.*

Example 4

What are the possibilities for the roots of $f(x) = x^3 - 3x^2 + 2x - 7$? We remember that, if a polynomial has *real* coefficients, then any complex roots it has will always occur in complex-conjugate pairs.

Solution

There are *three* sign-changes in $f(x) = +x^3 - 3x^2 + 2x - 7$ so that there can be no more than *three* $+ve$ real roots. Conversely, there are *no* sign-changes in $f(-x) = -x^3 - 3x^2 - 2x - 7$ so that there are *no* $-ve$ real roots. Therefore, the possibilities are:

- Three $+ve$ real roots;
- One $+ve$ real root and two complex roots.

Series Expansion

Example 5

Consider $f(x) \equiv 2\cos x - x = 0$. This expands to give

$$f(x) \equiv 2\left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - ...\right) - x = 0$$

So, as a very crude approximation, we could use

$$2 - x \approx 0 \quad \rightarrow \quad x \approx 2$$

A better approximation would be

$$2 - x - x^2 \approx 0 \quad \rightarrow \quad x \approx 1, \, -2.$$

If we wanted a $+ve$ root, we could use $x_0 = 1$.

4 Iterative Methods for Refining Solutions

We are concerned with solving equations of the general form $f(x) = 0$, for example

$$x^3 - 2x - 5 = 0, \quad \text{or} \;\; \mathrm{e}^x = 3x$$

etc, for which it is generally impossible (or extremely difficult) to obtain analytical solutions. We shall consider *iterative* methods for the real solution of real equations having the form

$$f(x) = 0 \tag{2}$$

The general idea is to rearrange $f(x) = 0$ into some *equivalent* equation $x = g(x)$ and then to use this new equation to *define* the iteration (or *recurrence relation*)

$$x_{n+1} = g(x_n), \;\; n = 0, 1, 2, ... \tag{3}$$

Given some initial value, x_0 say, then (3) can be used to generate a sequence of values $x_1, x_2, x_3, ...$ Such a sequence will do one of three things:

- it will either *converge* - meaning that successive values in the sequence get closer and closer to some fixed value x^*say;

- or it will *diverge* - meaning that successive values get larger and larger;
- or it will *oscillate* - meaning that successive values meander around getting neither generally larger, not converging on some fixed value.

Only the first case is of interest for then, we must have, finally, $x^* = g(x^*)$. Since $x = g(x)$ is some rearrangement of (2), then x^* is a solution of the original equation.

Example 1

The equation $2x - 1 = 0$ can be rearranged as $x = x/2 + 1/4$. Use this latter equation to *define* the iteration

$$x_{n+1} = \frac{1}{2}x_n + \frac{1}{4}, \;\; n = 0, 1, 2, ...$$

Choose $x_0 = 0$ (*any* guess will do for this example), then the iteration generates the sequence (working to three decimal places)

$$0, \; 0.250, \; 0.375, \; 0.438, \; 0.469, \; 0.485, \; 0.493, \; ...$$

If we continued, and used more decimal places, this sequence would converge to the value $x^* = 0.5$ which is the actual solution of the original equation.

5 The Newton-Raphson Iterative Method For $f(x) = 0$

We wish to solve $f(x) = 0$ by some iteration method. We could simply rearrange the equation into the form $x = g(x)$ to get the iteration $x_{n+1} = g(x_n)$ and hope for the best. However, a much more effective way of getting $x_{n+1} = g(x_n)$ is given by the Newton-Raphson (N-R) method:
Suppose x_0 is our initial guess for the solution, x^*. Then we expand $f(x^*)$ about x_0 using Taylor's Theorem:

$$f(x^*) = f(x_0) + \frac{(x^* - x_0)}{1!}f'(x_0) + \frac{(x^* - x_0)^2}{2!}f''(x_0) + ...$$

Now, if x_0 is *sufficiently* close to x^*(and $f''(x^*)$ etc is not unduly large) then we can reasonably say

$$f(x^*) \approx f(x_0) + (x^* - x_0)f'(x_0).$$

Since we require x^* such that $f(x^*) = 0$, then the above gives

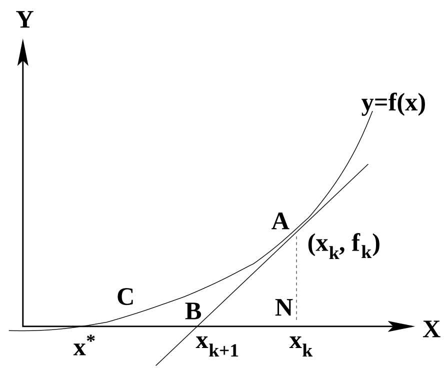
$$\begin{aligned} 0 &\approx f(x_0) + (x^* - x_0)f'(x_0) \\ & \;\;\downarrow \\ x^* &\approx x_0 - \frac{f(x_0)}{f'(x_0)} \end{aligned}$$

We now use this latter aproximation to *define* the Newton-Raphson iteration:

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

If our intial guess, x_0, is sufficiently close to the solution, x^*, then the method is *guaranteed* to work.

Y



(a) Geometrical interpretation of the Newton-Raphson method

Example 6

The equation $x^3 - 2x - 5 = 0$ has a real root near to $x = 2$. Use N-R to obtain this root correct to 4dp.

Solution

We have

$$f(x) = x^3 - 2x - 5, \quad f'(x) = 3x^2 - 2$$

so that N-R gives

$$x_{n+1} = x_n - \frac{x_n^3 - 2x_n - 5}{3x_n^2 - 2}$$

Since we know there is a root near 2 then we put $x_0 = 2$ to get:

$$\begin{aligned} x_1 &= 2 - \frac{(8 - 4 - 5)}{(12 - 2)} = 2.1 \\ x_2 &= 2.1 - \frac{(2.1^3 - 2(2.1) - 5)}{3(2.1)^2 - 2} = 2.0946 \\ x_3 &= ... = 2.094552 \end{aligned}$$

Hence, to 4dp, root is 2.0946

5.1 Geometric Interpretation of N-R

Let us suppose that the graph of f(x) intersects the x axis in the point x^*which is going to be the root we are looking for. In order to find this root we need an initial guess, denoted by x_k on the graph. Next we draw a tangent line to the curve of $f(x)$ through the point A, which is the point on the curve corresponding to x_k. The point where this tangent line meets the x axis will form the second guess, denoted here by x_{k+1}. From this point we can draw a vertical line to the curve and then a second tangent to the curve through this second point. Teh second

tangent will intersect the axis in a new point closer to the real root. This procedure is repetead as long as we obtain the root with the required precision.
From the figure, we have

$$f'(x_k) = \frac{AN}{BN} = \frac{f(x_k)}{BN}$$

Label the x-coordinate at B as x_{k+1}. Hence

$$\begin{aligned} f'(x_k) &= \frac{f(x_k)}{x_k - x_{k+1}} \\ & \downarrow \\ x_{k+1} &= x_k - \frac{f(x_k)}{f'(x_k)} \end{aligned}$$

The iteration process can be stopped when the algorithm meets the condition imposed by us. Typical termination (*truncation*) conditions are:

- Stop at x_n for some specified n
- Stop when x_n meets a specified error tolerance (ϵ),
- Stop if an unanticipated situation is encountered.

6 Convergence of Methods

- Consider the general iterative method

$$x_{n+1} = g(x_n) \tag{4}$$

and suppose that the error at the n-th step is ϵ_n so that $x_n = x^* + \epsilon_n$. Then (4) can be written as

$$x^* + \epsilon_{n+1} = g(x^* + \epsilon_n)$$

which can be expanded by Taylor's Theorem about $x = x^*$ to give

$$x^* + \epsilon_{n+1} = g(x^*) + \epsilon_n g'(x^*) + \frac{1}{2!}\epsilon_n^2 g''(x^*) + ...$$

Since, by definiton, $x^* = g(x^*)$, then this can be simplified to become

$$\epsilon_{n+1} = \epsilon_n g'(x^*) + \frac{1}{2!}\epsilon_n^2 g''(x^*) + ...$$

If the method converges then, at some point, ϵ_n must be very small so that ϵ_n^2 and higher order terms can be ignored. In this case, the above becomes

$$\epsilon_{n+1} \approx \epsilon_n g'(x^*) \tag{5}$$

But, since the method is converging by our assumption then we must have $|\epsilon_{n+1}| < |\epsilon_n|$ by definition. Inspection of (5) shows that the only way this can happen is if $|g'(x^*)| < 1$. Thus, we conclude that a *neccessary* condition for the convergence of an iterative method like (4) is $|g'(x^*)| < 1$.

6.1 Convergence of Newton-Raphson

In this case, the iteration (4) has the specific form

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

Therefore, to discuss the convergence of N-R, we firstly need to calculate $g'(x)$:

$$g'(x) = 1 - \frac{f'(x)f'(x) - f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2}$$

Next, we need to evaluate this latter expression at $x = x^*$. We get

$$g'(x^*) = \frac{f(x^*)f''(x^*)}{[f'(x^*)]^2}$$

Now, since $f(x^*) = 0$ by definition then, *except in the case* $f'(x^*) = 0$ then $g'(x^*) = 0$ *always* and the method is guaranteed to converge so long as our initial guess is close enough to x^*.

7 Bisection Method (Always works)

To find x^* such that $f(x^*) = 0$, the algorithm is given as:

1. Find an interval (x_0, X_0) which contains x^* - this implies that $f(x_0)f(X_0) < 0$;
2. Calculate the mid-point of this interval, say x_1, and determine if x^* lies in (x_0, x_1) or in (x_1, X_0)
3. Repeat the halving process in the interval which contains x^*;
4. Continue until some required accuracy is reached.

Example 7

The function $f(x) = x - e^{1/x}$ has a root in the interval $(1, 2)$. Perform three steps of the bisection method to determine an approximation to this root.

Solution

An initial interval is given by $x_0 = 1$ and $X_0 = 2$. Check: $f(1) = -1.7... < 0$ and $f(2) = 0.35... > 0$ so, OK.
From this point on, the process can be efficiently laid out in tabular form as follows:

x_0	x_1	X_0
$f(x_0) < 0$		$f(X_0) > 0$
1		2
	1.5000 ($f_1 < 0$)	
1.5		2
	1.7500 ($f_1 < 0$)	
1.75		2
	1.8750 ($f_1 > 0$)	
1.75		1.875
	1.8125 ($f_1 > 0$)	
1.75		1.8125
	1.7813 ($f_1 > 0$)	
1.75		1.7813
	1.7657 ($f_1 > 0$)	

The error in 1.7657 is about 0.0157. But we can continue to obtain whatever precision we require.

Comment

Bisection is very slow, and N-R (which is very fast) is to be preferred ... can use bisection to determine an interval within which a root lies, and then use N-R to carry out a very rapid and high-precision estimate of the root.

AMA252 Lecture 3: Numerical ODEs:

Differential equations are among the most important mathematical tools used in producing models for physics, biology and engineering. Here we consider numerical methods for solving ordinary differential equations (ODE), that is, those differential equations that have only one independent variable and they are of the form

$$\frac{dy}{dx} = f(x)$$

where $y(x)$ is the unknown function depending on the variable, x and $f(x)$ is a function which must be continuous. The solution of the above equation is given by the fundamental theorem of calculus

$$y(x) = C + \int_{x_0}^{x} f(x')dx'$$

This equation describes a family of solutions determined by the constant C. A particular solution is computed by requiring that the solution pass through the point (x_0, y_0). In other words, $y(x_0) = y_0$ The problem specified by the last two equations is called an *initial value problem* (IVP) and has the solution $y(x) = y_0 + \int_{x_0}^{x} f(x')dx'$ A general *first order* IVP consists of a differential equation and an initial value as follows

$$y'(x) = f(x, y), \quad y(x_0) = y_0$$

Unfortunately, many IVPs cannot be solved by analytical techniques. This leads to the need for numerical methods. This chapter will focus on some elementary methods for the numerical solution of IVPs. This means that we wish to compute a set of points $(x_i, \hat{y}_i)$, $i =$

$0, 1, 2, \ldots, n$ to approximate the true solution $y(x)$ where we have noted $\hat{y}_i = y(x_i)$. In many cases we assume that $x_i = x_0 + ih$ where h is a constant called *step size*. Obviously, the first point is (x_0, y_0).
Typical ode's you can meet in engineering are:

- The growth equation (also called the Malthus equation)

$$\frac{dy}{dt} = ky, \quad k = \text{constant}$$

- The pendulum equation

$$\frac{d^2y}{dt^2} + \frac{g}{l}\sin(y) = F(t)$$

- The LRC equation

$$L\frac{d^2y}{dt^2} + R\frac{dy}{dt} + \frac{y}{C} = E(t)$$

8 Approximate Methods for solving ODEs: Taylor Series:

This method uses the Taylor expansion of functions in a certain point, say, x_0. Recall

$$y(x) = y(x_0) + (x - x_0)y'(x_0) + \frac{(x - x_0)^2}{2!}y''(x_0) + \frac{(x - x_0)^3}{3!}y'''(x_0) + \ldots$$

provided all necessary derivatives exist.

Example: First order equation.

Solve

$$\frac{dy}{dx} = x^4 - xy$$

where $x_0 = 0$ and $y(x_0) = 1$

Solution

We have

$$\begin{array}{lll} y' = x^4 - xy & \rightarrow & y'(0) = 0 \\ y'' = 4x^3 - y - xy' & \rightarrow & y''(0) = -1 \\ y''' = 12x^2 - 2y' - xy'' & \rightarrow & y'''(0) = 0 \\ y^{iv} = 24x - 3y'' - xy''' & \rightarrow & y^{iv}(0) = 3 \end{array}$$

etc. Hence, we obtain

$$y = 1 - \frac{x^2}{2} + \frac{3x^4}{4!} + \frac{24}{5!}x^5 + \ldots$$

Example: Second order equation.

Solve

$$\frac{d^2y}{dx^2} + x\,\frac{dy}{dx} + y = 0,$$

where $y = 1$ and $y' = 0$ when $x = 0$.

Solution

When solving second order differential equations there will be two integration constants. In order to find their value we need two conditions. One condition could be when we specify the value of the function $y(x)$in two different points, or we specify the value of the function and its derivative in a certain point. For this particular exmple we have

$$\begin{array}{lll} y'' = -xy' - y & \rightarrow & y''(0) = -1 \\ y''' = -2y' - xy'' & \rightarrow & y'''(0) = 0 \\ y^{iv} = -3y'' - xy''' & \rightarrow & y^{iv}(0) = 3 \\ ... & ... & ... \end{array}$$

etc. Hence, we have

$$y = 1 - \frac{x^2}{2} + \frac{3x^4}{4!} - \frac{15}{6!}x^6 + ...$$

9 Runga-Kutta Methods

We begin by considering *first order* equations of the type

$$\frac{dy}{dx} = f(x, y), \text{ given } y = y_0 \text{ when } x = x_0$$

We seek to find y at intervals in x - usually x-values which are equally spaced so that $x_n = x_0 + nh,\ \ n = 0, 1, 2, ...$ and h is the *step-length.* The set of values $y_0,\ y_1,\ y_2, ...$ is the *numerical solution* $y(x_0),\ y(x_1),\ y(x_2), ...$ So, how are these values determined? One possibility is to use the series solution - but this is very likely to converge only for a limited range of x. (We exclude the possibility of *exact* solutions, since these arise only rarely in real life.)

9.1 Euler's First Method

We shall develop our methods from a geometrical approach (see Figure 2). Suppose the point (x_n, y_n) has been reached along the solution curve (since we know the initial point anyway, this is an OK asumption). In the figure, L_1 is the tangent at (x_n, y_n) and has slope $y'_n = f(x_n, y_n)$.

We can proceed to x_{n+1} by approximating $y(x_{n+1})$ by y_{n+1} - that is, we let y_{n+1} be the point where L_1 intersects the ordinate at x_{n+1}. The equation of L_1 is

$$y = y_n + y'_n(x - x_n)$$

Hence, at $x = x_{n+1}$ we get

$$y_{n+1} = y_n + y'_n(x_{n+1} - x_n)$$

which can be written as

$$y_{n+1} = y_n + h\,f(x_n, y_n). \tag{6}$$

This is often called the *First Euler method* or Euler-1. It is very simple, but performs very poorly unless extremely small values of h are used.

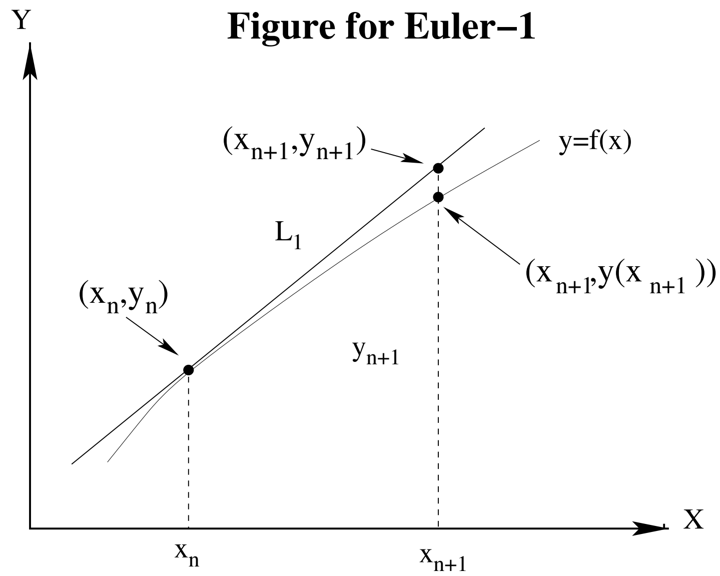


Figure 2:

An Alternative Derivation by Taylor ...

For an alternative derivation, we easily see that the Taylor expansion of y about x_n is given by

$$y(x) = y(x_n) + (x - x_n)y'_n + ...$$

so that, immediately,

$$y(x_{n+1}) = y(x_n) + h\,f(x_n, y_n) + O(h^2)$$

Thus, we see that Euler-1 agrees with the Taylor expansion with truncation error $O(h^2)$.

Example

Consider $y' = xy^{1/3}$ given that $y = 1$ when $x = 1$. Using $h = 0.01$ we obtain

$$\begin{aligned} y(1.01) \equiv\ & y_1 \approx y_0 + hf(x_0, y_0) = 1 + 0.01(1)(1)^{1/3} = 1.01 \\ y(1.02) \equiv\ & y_2 \approx y_1 + hf(x_1, y_1) = 1.01 + 0.01(1.01)(1.01)^{1/3} = 1.0201 \\ y(1.03) \equiv\ & y_3 \approx ... = 1.0304 \end{aligned}$$

In fact, the equation has an exact solution which gives $y_3 = 1.0306$ to 4dp.

9.2 Euler's Second Method

Euler-1 works by using the slope at (x_n, y_n), given by $y' = f(x_n, y_n)$, to *extrapolate* the solution to (x_{n+1}, y_{n+1}). Euler-2 is a refinement of this idea which goes as follows:

- One estimate of the average slope of $y(x)$ between $x_n$and x_{n+1} is given by $(y_{n+1} - y_n)/h$ where $h = (x_{n+1} - x_n)$;
- Using the differential equation $y' = f(x, y)$, another estimate is given by $(f(x_n, y_n) + f(x_{n+1}, y_{n+1}))/2$;
- These two estimates can be approximately equated so that

$$\frac{y_{n+1} - y_n}{h} \approx \frac{1}{2}\left(f(x_n, y_n) + f(x_{n+1}, y_{n+1})\right).$$

- Rearrangement then gives

$$y_{n+1} \approx y_n + \frac{h}{2}\left(f(x_n, y_n) + f(x_{n+1}, y_{n+1})\right).$$

Of course, we do not actually know the value of y_{n+1}, so this is useless as it stands - but we can use Euler-1, given at (6) to *estimate* this latter quantity. If we do this, we get *Euler-2:*

$$y_{n+1} = y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_n + h, y_n + hy_n')\right] \tag{7}$$

It can be shown that this relation agrees with the Taylor expansion up to terms $O(h^2)$.

9.3 Euler-2 written in Runga-Kutta Form:

Euler-2, given by (7), can be written in standard Runga-Kutta form as:

$$\begin{aligned} k_1 &= h\,f(x_n, y_n) \\ k_2 &= h\,f(x_n + h, y_n + k_1) \\ y_{n+1} &= y_n + (k_1 + k_2)/2 \end{aligned} \tag{8}$$

where we remember that $y_n' = f(x_n,\ y_n)$.

Example

We use Euler-2 to solve $y' = -10xy^2$ for $1 \le x \le 2$ given $y = 1$ when $x = 1$. To illustrate the need for *sufficiently small* h, we solve using $h = 0.05,\ 0.1$ and 0.2 respectively.

$h =$	0.05
x	y
1.00	1.00000
1.05	0.68437
1.10	0.50856
1.15	0.39885
1.20	0.32477
1.25	0.27176
1.30	0.23214
1.35	0.20151
1.40	0.17720
1.45	0.15748
1.50	0.14119
1.55	0.12754
1.60	0.11595
1.65	0.10601
1.70	0.09740
1.75	0.08987
1.80	0.08325
1.85	0.07739
1.90	0.07217
1.95	0.06749
2.00	0.06328

$h =$	0.1
x	y
1.0	1.00000
1.1	0.50000
1.2	0.33213
1.3	0.24000
1.4	0.18348
1.5	0.14597
1.6	0.11959
1.7	0.10020
1.8	0.08545
1.9	0.07390
2.0	0.06468

$h =$	0.2
x	y
1.0	1.00000
1.2	-1.2000
1.4	-33.278
1.6	-1.6×10^7
1.8	-1.1×10^{30}

We see that the solutions for $h = 0.1$ and $h = 0.05$ are reasonably similar, but that the solution for $h = 0.2$ is completely useless - the solution is seriously *unstable!!*

9.4 A Third-Order Runga-Kutta Method

The R-K method of (8) is a *second-order* method - which means that the errors are $O(h^2)$. A similar *third-order* method is given by

$$\begin{aligned} k_1 &= h\,f(x_n, y_n) \\ k_2 &= h\,f(x_n + h/2, y_n + k_1/2) \\ k_3 &= h\,f(x_n + h, y_n + 2k_2 - k_1) \\ y_{n+1} &= y_n + (k_1 + 4k_2 + k_3)/6 \end{aligned}$$

which is sometimes referred to as *Heun's Method*.

9.5 A Fourth-Order Runga-Kutta Method (Standard)

The following R-K method is probably the most widely used - being relatively simple and highly accurate. It is frequently referred to as simply *the* R-K method, and is given by

$$\begin{aligned}
k_1 &= h\,f(x_n,\,y_n) \\
k_2 &= h\,f(x_n+h/2,\,y_n+k_1/2) \\
k_3 &= h\,f(x_n+h/2,\,y_n+k_2/2) \\
k_4 &= h\,f(x_n+h,\,y_n+k_3) \\
y_{n+1} &= y_n+(k_1+2k_2+2k_3+k_4)/6.
\end{aligned}$$

A formal derivation of this method involves very lengthy algebra and so is omitted!! The R-K methods so far discussed are called *one-step* methods - that is information at the new point is determined entirely by information at the previous point only.

Example 1

Use $h=0.1$ to calculate $y(1.1)$ for the system

$$y'=xy^{1/3} \quad \text{given } y=1 \text{ when } x=1$$

We have $x_0=1,\ y_0=1$ so that, using $h=0.1$ we find:

$$\begin{aligned}
k_1 &= 0.1\,f(1,1)=0.1 \\
k_2 &= 0.1\,f(1.05,1.05)=0.1(1.05)(1.05)^{1/3}=0.10672 \\
k_3 &= 0.1\,f(1.05,1.05336)=0.1(1.05)(1.05336)^{1/3}=0.10684 \\
k_4 &= 0.1\,f(1.1,1.10684)=0.1(1.1)(1.10684)^{1/3}=0.11378 \\
y_1 &= 1+(0.1+2(0.10672)+2(0.10684)+0.11378)/6=1.10682
\end{aligned}$$

We can then proceed to calculate $y(1.2)$, $y(1.3)$ etc etc. After 40 similar steps we find $y(5)=26.99998$. In fact, the exact value is $y(5)=27$.
In practice, we do not usually have the exact solution available to determine accuracy - but this is generally done by repeating the calculation by repeatedly halving h until successive solutions agree to the accuracy required. That is, find a complete soln using h; then using $h/2$, $h/4$, etc etc.

Example 2

Use the 4th order R-K method to estimate $y(0.1)$ for the system

$$\frac{dy}{dx}=2y-x,\;\; y(0)=1$$

using a step $h=0.1$.

Solution

Note that $x_0 = 0$ and $y_0 = 1$ here so that:

$$
\begin{aligned}
k_1 &= hf(x_0, y_0) = 0.1(2y_0 - x_0) = 0.2 \\
k_2 &= hf(x_0 + h/2, y_0 + k_1/2) = 0.1\left[2(y_0 + k_1/2) - (x_0 + h/2)\right] = 0.1[2(1 + 0.1) - 0.05] = 0.2150 \\
k_3 &= hf(x_0 + h/2, y_0 + k_2/2) = 0.1\left[2\left(y_0 + k_2/2\right) - (x_0 + h/2)\right] = 0.1[2(1 + 0.1075) - 0.05] = 0.2165 \\
k_4 &= hf(x_0 + h, y_0 + k_3) = 0.1[2(y_0 + k_4) - (x_0 + h)] = 0.1[2(1 + 0.2165) - 0.1] = 0.2333 \\
y_1 &= y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 1 + \frac{1}{6}(0.2 + 0.4300 + 0.4330 + 0.2333) = 1.21605
\end{aligned}
$$

9.6 How is h to be chosen?

- We might expect that any approximate method used should tend to the original ode as $h \to 0$.

By Euler-2, we have

$$
y_{n+1} = y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_n + h, y_n + hy'_n\right]
$$

so that

$$
\frac{y_{n+1} - y_n}{h} = \frac{1}{2}\left[f(x_n, y_n) + f(x_n + h, y_n + hy'_n)\right].
$$

Letting $h \to 0$ this becomes

$$
\left.\frac{dy}{dx}\right|_{x_n} = f(x_n, y_n).
$$

A method which has this property is said to be *consistent* with the ode. The 4th-order R-K method above can be shown *consistent* in this sense.

- We know that for Euler-2 (for example) the error introduced *per step* is approximately proportional to h^3. The error per step is called the *local truncation error.* In practice, we are naturally more interested in the accumulated error after many steps (that is, the *global error*) at some point x_n.

- It can be shown that if a one-step method is *consistent* with the ode and if the local error is approx proportional to h^{p+1} for some $p > 0$, then the *global error* at x_n (for small h) is given by

  $$
  Y(x_n) - y(x_n) \approx C\,h^p
  $$

  where $Y(x_n)$ denotes the *exact* solution at $x = x_n$ and $y(x_n)$ is the numerical solution and C is some constant (for any given x_n).

- Thus, for Euler-2, which has local truncation error $O(h^3)$, we find

$$Y(x_n) - y(x_n) \approx C_1 h^2$$

whilst for the 4th-order R-K method, we find a local error of $O(h^5)$ and hence

$$Y(x_n) - y(x_n) \approx C_2 h^4.$$

Thus, for example, if we are using Euler-2, then replacing h by $h/2$ will reduce the global error by a factor of 4 whilst, if we are using the 4th-order R-K method, the replacement will reduce the global error by a factor of 16!!

- Clearly, as $h \to 0$ then (in general) global error will $\to 0$, and the method is said to be *convergent*.

Example

For $y' = xy^{1/3}$, given $y = 1$ when $x = 1$, the Euler-2 method gives the result in the table at $x = 2$:

	$h = 0.1$	$h = 0.05$
$y(2)$	2.827609	2.828218

Estimate the step-length required to achieve 6dp in $y(2)$.

Solution

- We have

$$\begin{aligned} Y - 2.827609 &\approx C(0.1)^2 \\ Y - 2.828218 &\approx C(0.05)^2 \end{aligned}$$

Subtracting gives $2.828218 - 2.827609 = C\,(0.01 - 0.0025)$ so that $C \approx 0.0812$.

- But we require $Ch^2 \leq 10^{-5} \to h^2 \leq 10^{-6}/0.0812 \to h \approx 0.0035$.

- In fact, if we use $h = 0.0025$, we find $y(2) = 2.828428$. The analytical solution gives $Y(2) = 2.828427$. Thus, to obtain 6dp accuracy using Euler-2 requires $h = 0.0025$.

- It transpires that the same accuracy can be obtained with the 4-th order R-K using $h = 0.1$ - thus forty fewer steps are required when R-K is used. However, each step requires about twice as much work so that the overall saving is twenty times less work $= 95\%$ saving.

9.7 Stability

In crude terms, a method is *stable* if it produces solutions which behave more-or-less like the exact solutions, and *unstable* otherwise.
We limit ourselves to a purely qualitative discussion by reference to a particular example. Consider the equation:

$$y' = -10xy, \quad \text{given } \; y = 1 \; \text{ when } \; \mathrm{x} = 1$$

solved by the Euler-2 method. We have already done this in §9.3 where it is clear that for $h = 0.05$ and $h = 0.1$ the solutions are reasonable - they could be used to perform an analysis similar to that of the previous section. However, for $h = 0.2$ the results are hopeless!!
The explanation for this can be given as follows: In any numerical calculation, there are *unavoidable* errors introduced at *every* step. In the above calculation, the errors for the cases $h = 0.05$ and $h = 0.1$ tended to balance out as the calculation progressed (positive errors tended to cancel out with negative errors). This is the situation of *stability.* But, for the $h = 0.2$ case, this self-cancellation process fails, and the errors start to cascade (think of *negative feedback* compared with *positive feedback*). This is the situation of *instability.*
The behaviour of errors generally varies from equation to equation and from method to method, and detailed analyses are usually very complicated. Thus, for the above example, whilst Euler-2 is *unstable* when $h = 0.2$, the 4th-order R-K is *stable* for all $h \leq 0.2$ and *unstable* otherwise.

10 Generalizations of the R-K Method

10.1 Simultaneous 1st Order Equations

Consider the pair of 1st-order eqns

$$\begin{aligned} y' &= F(x, y, z) \\ z' &= G(x, y, z) \end{aligned}$$

given $y = y_0$, $z = z_0$ when $x = x_0$. The 4th-order R-K for this more general type of system generalizes in a straightforward way:

$$\begin{aligned} k_1 &= h\, F(x_n, y_n z_n) \\ m_1 &= h\, G(x_n, y_n, z_n) \\ \\ k_2 &= h\, F(x_n + h/2, y_n + k_1/2, z_n + m_1/2) \\ m_2 &= h\, G(x_n + h/2, y_n + k_1/2, z_n + m_1/2) \\ \\ k_3 &= h\, F(x_n + h/2, y_n + k_2/2, z_n + m_2/2) \\ m_3 &= h\, G(x_n + h/2, y_n + k_2/2, z_n + m_2/2) \\ \\ k_4 &= h\, F(x_n + h, y_n + k_3, z_n + m_3) \\ m_4 &= h\, G(x_n + h, y_n + k_3, z_n + m_3) \end{aligned}$$

$$\begin{aligned} y_{n+1} &= y_n + (k_1 + 2k_2 + 2k_3 + k_4)/6 \\ z_{n+1} &= z_n + (m_1 + 2m_2 + 2m_3 + m_4)/6 \end{aligned}$$

Note the similarity with the basic R-K 4-th order method. This manner of generalization applies to any R-K method.

Example 1

Use the 4th order R-K method to estimate $y(0.2)$ for the system

$$\begin{aligned} \frac{dy}{dx} &= f(x,y,z) = x + y - z^2, \quad y(0) = 0 \\ \frac{dz}{dx} &= g(x,y,z) = x^2 - z + y^2, \quad z(0) = 1 \end{aligned}$$

using $h = 0.2$.

Solution

Note that $x_0 = 0,\ y_0 = 0,\ z_0 = 1$ here:

$$\begin{aligned} k_1 &= 0.2f(0,0,1) = 0.2(0+0-1) = -0.2 \\ m_1 &= 0.2g(0,0,1) = 0.2(0-1+0) = -0.2 \end{aligned}$$

$$\begin{aligned} k_2 &= 0.2f(0.1,\ -0.1,\ 0.9) = 0.2(0.1 - 0.1 - 0.9^2) = -0.162 \\ m_2 &= 0.2g(0.1,\ -0.1,\ 0.9) = 0.2(0.1^2 - 0.9 + (-0.1)^2) = -0.176 \end{aligned}$$

$$\begin{aligned} k_3 &= 0.2f(0.1,\ -0.081,\ 0.912) = 0.2(0.1 - 0.081 - 0.912^2) = -0.16255 \\ m_3 &= 0.2g(0.1,\ -0.081,\ 0.912) = 0.2(0.1^2 - 0.912 + (-0.081)^2) = -0.17909 \end{aligned}$$

$$\begin{aligned} k_4 &= 0.2f(0.2,\ -0.16255,\ 0.82091) = 0.2(0.2 - 0.16255 - 0.82091^2) = -0.12729 \\ m_4 &= 0.2g(0.2,\ -0.16255,\ 0.82091) = 0.2(0.2^2 - 0.82091 + (-0.16255)^2) = -0.15090 \end{aligned}$$

$$\begin{aligned} y(0.2) &= y(0) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = -0.1627 \\ z(0.2) &= z(0) + \frac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4) = 0.8232 \end{aligned}$$

Example 2

Consider

$$\begin{aligned} \frac{dy}{dx} &= x + y + z \\ \frac{dz}{dx} &= 1 + y + z \end{aligned}$$

with $y = 1$, $z = -1$ when $x = 0$. A direct application of the above using $h = 0.1$ gives $y(0.1) = 1.01053$ and $z(0.1) = -0.89448$ (Check this !!)

10.2 Second Order Equations

Consider the second order de

$$y'' = G(x, y, y') \text{ given } y = y_0 \text{ and } z = z_0 \text{ when } x = x_0.$$

This can be turned into a pair of 1st order equations as follows:

Put $y' = z$ so that $y'' = G(x, y, y')$ becomes $z' = G(x, y, z)$. That is, the 2nd-order eqn above can be written as

$$\begin{aligned} y' &= z \\ z' &= G(x, y, z) \\ y = y_0, \quad z = z_0 &\quad \text{when } x = x_0 \end{aligned}$$

This is a special case $F(x, y, z) \equiv z$, of the general first-order pair considered above. Hence

$$\begin{aligned}
k_1 &= h\, z_n \\
m_1 &= h\, G(x_n, y_n, z_n) \\
\\
k_2 &= h\,(z_n + m_1/2) \\
m_2 &= h\, G(x_n + h/2,\ y_n + k_1/2,\ z_n + m_1/2) \\
\\
k_3 &= h\,(z_n + m_2/2) \\
m_3 &= h\, G(x_n + h/2,\ y_n + k_2/2,\ z_n + m_2/2) \\
\\
k_4 &= h\,(z_n + m_3) \\
m_4 &= h\, G(x_n + h, y_n + k_3, z_n + m_3) \\
\\
y_{n+1} &= y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
z_{n+1} &= z_n + \frac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4)
\end{aligned}$$

Example

Use the 4-th order R-K method with $h = 0.5$ to determine $y(0.5)$ and $y'(0.5)$ for the eqn

$$y'' + xy' - y + x\,\mathrm{e}^{-x} = 0$$

given $y = 1$, $y' = 0$ when $x = 0$. Note: This is an *initial value* problem. We shall deal with *boundary value* problems later.

Solution

We have $y'' = -xy' + y - x\,\mathrm{e}^{-x} \equiv f(x, y, y')$ so put $y' = z \equiv f(x, y, z)$ so that ode becomes

$$\begin{aligned} y' &= z \equiv f(x, y, z), \\ z' &= -xz + y - x\,\mathrm{e}^{-x} \equiv g(x, y, z) \end{aligned}$$

$$y(0) = 1, \quad z(0) = 0$$

Note that $x_0 = 0,\ \ y_0 = 1,\ \ z_0 = 0$ and $h = 0.5$. Hence

$$\begin{aligned} k_1 &= hf(x_0, y_0, z_0) = hz_0 = 0 \\ m_1 &= hg(x_0, y_0, z_0) = hg(0, 1, 0) = 0.5(1) = 0.5 \\[1em] k_2 &= h(z_0 + m_1/2) = 0.5(0 + 0.25) = 0.125 \\ m_2 &= hg(x_0 + h/2,\ y_0 + k_1/2,\ z_0 + m_1/2) = 0.5g(0.25,\ 1.0,\ 0.25) = 0.3714 \\[1em] k_3 &= h(z_0 + m_2/2) = 0.5(0 + 0.1857) = 0.09285 \\ m_3 &= hg(x_0 + h/2,\ y_0 + k_2/2,\ z_0 + m_2/2) = 0.5g(0.25,\ 1.0625,\ 0.1857) = 0.41069 \\[1em] k_4 &= h(z_0 + m_3) = 0.5(0 + 0.41069) = 0.205345 \\ m_4 &= hg(x_0 + h,\ y_0 + k_3,\ z_0 + m_3) = 0.5g(0.5,\ 1.09285,\ 0.41069) = 0.29212 \end{aligned}$$

$$\begin{aligned} y(0.5) &= y(0) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 1.10684 \\ z(0.5) &= z(0) + \frac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4) = 0.39272 \end{aligned}$$

If we advance this solution further with $h = 0.5$ we eventually find, after ten steps, $y(5) = 5.005429$. With $h = 0.25$ we find, after 20 steps, $y(5) = 5.006649$.These together give $C = 0.0208$. For six-figure accuracy we then find that we must have $h \leq 0.08$.

11 Comments

- The general solution of a second-order linear eqn consists of a linear combination of solutions like $y(x) = Ay_1(x) + By_2(x)$. A particular choice of initial condition may make A or B zero. *But* the numerical soln will introduce the unwanted soln, $y_2(x)$ (with small B) due to the propagation of errors. The step-size suitable for calculating $y_1(x)$ may or may not be small enough to avoid instabilities in the computation of $y_2(x)$. Difficult cases require *very* small h. Such eqns are call *stiff* equations, and require special methods. Similar problems arise in non-linear eqns.

- Use of R-K requires continuity of appropriate number of derivatives - this condition is not always met. Eg: suppose $y(x) \sim x^{1/2}$. Here, $y'(x)$ does not exist at $x = 0$. In such a case, we would use *Frobenius series* to get away from $x = 0$, and then use R-K thereafter. Many physical problems (eg involving corners etc) are like this.

- There exist many other methods.

AMA252 Lecture 4: Partial Differentiation

12 Partial Differentiation

Let $z = f(x, y)$ be a real valued function of two *independent* variables, x and y. We *define* the *partial derivative* of f wrt x as:

$$\frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \left[\frac{f(x + \Delta x, y) - f(x, y)}{\Delta x} \right]$$

where in this limit y *is assumed to have a fixed value.* Similarly, we define the partial derivative of f wrt y as

$$\frac{\partial f}{\partial y} = \lim_{\Delta y \to 0} \left[\frac{f(x, y + \Delta y) - f(x, y)}{\Delta y} \right]$$

where, this time, x *is assumed to have a fixed value.*

Example 1

Find $\partial f / \partial x$ and $\partial f / \partial y$ for

1. $f(x, y) = x^3 + y^2$
2. $f(x, y) = x \tan^{-1} y + x^3 y + y^{3/2}$

Solution 1

$$\frac{\partial f}{\partial x} = 3x^2, \quad \frac{\partial f}{\partial y} = 2y$$

Solution 2

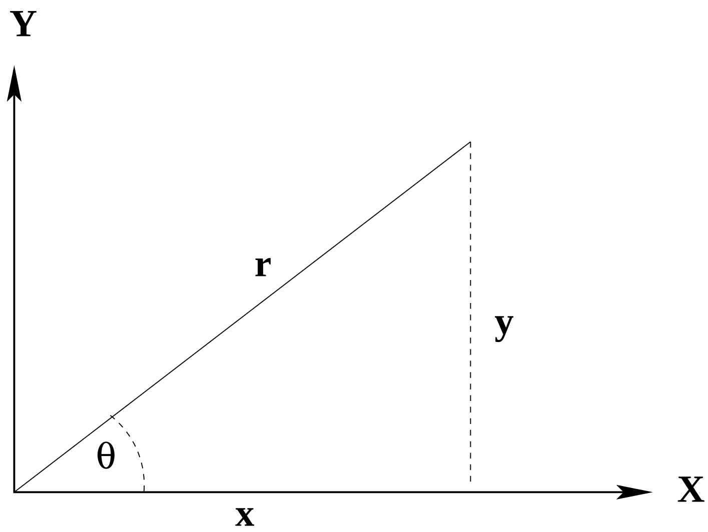


Figure 3: The transformation into polar coordinates

$$\frac{\partial f}{\partial x} = \tan^{-1} y + 3x^2 y$$
$$\frac{\partial f}{\partial y} = \frac{x}{1+y^2} + x^3 + \frac{3}{2} y^{1/2}$$

Note: All the standard rules of ordinary differentiation (eg product rule, quotient rule etc) apply unchanged.

Example 2

If $f(x, y) = \mathrm{e}^y \ln(x + y)$ then find $\partial f/\partial y$.

Solution

$$\frac{\partial f}{\partial y} = \mathrm{e}^y \ln(x+y) + \frac{\mathrm{e}^y}{x+y}$$

Example 3

Consider the transformation to plane-polar coordinates: From the figure, we have

$$x = r\cos\theta, \qquad y = r\sin\theta$$
$$\downarrow$$
$$r^2 = x^2 + y^2, \qquad \tan\theta = \frac{y}{x}$$

We could, for example, write x as a function of (r, θ), (r, y) or (θ, y):

$$x = r\cos\theta, \quad x = \sqrt{r^2 - y^2}, \quad x = y\cot\theta$$

From these we can compute the following partial derivatives in turn:

$$\frac{\partial x}{\partial r} = \cos\theta, \quad \frac{\partial x}{\partial r} = \frac{r}{\sqrt{r^2 - y^2}} = \frac{r}{x} = \sec\theta, \quad \frac{\partial x}{\partial y} = \cot\theta$$

Note: When computing any partial derivative, all the independent variables in the expression being differentiated - *except* the one in the differentiation - are assumed to be held *constant!!*
Question: Why do we get two *different* results for $\partial x/\partial r$ above?

12.1 Higher Order Derivatives

We mean, for example,

$$
\begin{aligned}
\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) &= \frac{\partial^2 f}{\partial x^2} \\
\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) &= \frac{\partial^2 f}{\partial y^2} \\
\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) &= \frac{\partial^2 f}{\partial x \partial y} \\
\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) &= \frac{\partial^2 f}{\partial y \partial x}
\end{aligned}
$$

Example 4

$$
\begin{aligned}
&f(x,y) = x^3 + y^2 \\
&\frac{\partial f}{\partial x} = 3x^2, \quad \frac{\partial^2 f}{\partial x^2} = 6x \\
&\frac{\partial f}{\partial y} = 2y, \quad \frac{\partial^2 f}{\partial y^2} = 2 \\
&\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}(2y) = 0 \\
&\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y}\left(3x^2\right) = 0
\end{aligned}
$$

Example 5

$$
\begin{aligned}
&f(x,y) = x\tan^{-1} y + x^3 y + y^{3/2} \\
&\frac{\partial f}{\partial x} = \tan^{-1} y + 3x^2 y, \quad \frac{\partial f}{\partial y} = \frac{x}{1+y^2} + x^3 + \frac{3}{2}y^{1/2} \\
&\frac{\partial^2 f}{\partial x^2} = 6xy, \qquad \frac{\partial^2 f}{\partial y^2} = -\frac{2xy}{(1+y^2)^2} + \frac{3}{4}y^{-1/2} \\
&\frac{\partial^2 f}{\partial y \partial x} = \frac{1}{1+y^2} + 3x^2, \quad \frac{\partial^2 f}{\partial x \partial y} = \frac{1}{1+y^2} + 3x^2
\end{aligned}
$$

Note: For all *well behaved* functions, then

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$$

can be assumed true - all functions considered on this course al well-behaved.

Example 6

Given $f(x,y) = x^2 \tan^{-1}(y/x)$ find f_{xy} at $(1,1)$.

Solution

Note that f_{xy} is short notation for $\partial^2 f/\partial x \partial y$.

$$\begin{aligned}\frac{\partial f}{\partial y} &= x^2\left(\frac{1}{1+(y/x)^2}\right)\frac{\partial}{\partial y}\left(\frac{y}{x}\right) \\ &= \frac{x^4}{x^2+y^2}\,\frac{1}{x} = \frac{x^3}{x^2+y^2}\end{aligned}$$

Hence

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = \frac{3x^2}{x^2+y^2} - \frac{2x^4}{(x^2+y^2)^2}$$

Thus, at $(1,1)$, we find

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{3}{2} - \frac{2}{4} = 1$$

12.2 Notes

A common notation is defined as follows:

$$f_x \equiv \frac{\partial f}{\partial x}, \quad f_y = \frac{\partial f}{\partial y}, \quad f_{xx} = \frac{\partial^2 f}{\partial x^2}, \quad \text{etc}$$

Partial differentiation can be extended to functions of more than two variables in a natural way.

Example 7

Suppose $f(x,y,z) = x^3 + x^2 z^4 + xy^5$, then

$$\frac{\partial f}{\partial x} = 3x^2 + 2xz^4 + y^5, \quad \frac{\partial f}{\partial y} = 5xy^4, \quad \frac{\partial f}{\partial z} = 4x^2 z^3$$

12.3 The Ordinary Chain Rule

The ordinary chain rule can be stated as follows: If $y = f(x)$ where $x = g(t)$ then

$$\frac{dy}{dt} = \frac{dy}{dx}\frac{dx}{dt}$$

12.4 The Generalized Chain Rule

The ordinary chain rule extends in an obvious way to functions of two or more variables. Thus, if $z = f(x,y)$ where $x = g(t)$ and $y = h(t)$ then

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt}$$

Example 8

Thus, if $z = \sin(xy^2)$ where $x = \mathrm{e}^{\mathrm{t}}$ and $y = t^3$ then

$$\begin{aligned}
\frac{dz}{dt} &= \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt} \\
&= y^2\cos(xy^2)\mathrm{e}^t + 2xy\cos(xy^2)3t^2 \\
&= t^6\cos(t^6\mathrm{e}^t)\mathrm{e}^t + 6\mathrm{e}^t t^5\cos(t^6\mathrm{e}^t) \\
&= (t+6)t^5\mathrm{e}^t\cos(t^6\mathrm{e}^t)
\end{aligned}$$

12.5 A Special Case of the Generalized Chain Rule

For the general case, the problem is: if $z = f(x, y)$ where $x \equiv g(t)$ and $y \equiv h(t)$ then find dz/dt, and the solution is:

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt}$$

Now suppose that $x = t$: then the problem becomes: if $z = f(x, y)$ where $y \equiv h(x)$, then find dz/dx, and the solution is:

$$\frac{dz}{dx} = \frac{\partial z}{\partial x} + \frac{\partial z}{\partial y}\frac{dy}{dx}$$

Example 9

If $z = x^2y + 1/y$ and $y = \ln x$ then find dz/dx.

Solution

$$\frac{dz}{dx} = 2xy + \left(x^2 - \frac{1}{y^2}\right)\frac{1}{x} = 2xy + x - \frac{1}{xy^2}$$

12.6 Implicit Differentiation

A further application of the above is to find dy/dx when y is defined as an *implicit* function of x: That is, find dy/dx when $f(x, y) = 0$. In this case, we write $z \equiv f(x, y)$ so that, firstly

$$\frac{dz}{dx} = \frac{\partial z}{\partial x} + \frac{\partial z}{\partial y}\frac{dy}{dx}$$

and then we note that, since $z = 0$ then we must have $dz/dx = 0$ also so that the above gives directly:

$$\frac{dy}{dx} = -\left(\frac{\partial f}{\partial x}\right) / \left(\frac{\partial f}{\partial y}\right)$$

Example 10

Given $f(x, y) \equiv x^2 + 3xy + 4y^2 = 0$ find dy/dx.

Solution

$$\frac{dy}{dx} = -(2x + 3y)/(3x + 8y).$$

13 Small Error Estimates

The total derivative formula can be used to estimate errors in calculations: Clearly, if $z \equiv z(x, y)$ then

$$\delta z \approx \frac{\partial z}{\partial x}\delta x + \frac{\partial z}{\partial y}\delta y \tag{9}$$

where δx and δy are small changes (which can be errors) in x and y, and δz is the corresponding change (or error) in z.

Example 11

The value of z is to be calculated from

$$z = \sqrt{xy}$$

for $x = 4$ and $y = 9$ and where the corresponding errors in x and y are ± 0.1 and ± 0.2 respectively. What is the corresponding maximum modulus for the error in z?

Solution

We have

$$\frac{\partial z}{\partial x} = \frac{1}{2}\sqrt{\frac{y}{x}} = \frac{3}{4}, \quad \frac{\partial z}{\partial y} = \frac{1}{2}\sqrt{\frac{x}{y}} = \frac{1}{3}$$

Consequently, (9) gives

$$\begin{aligned} \delta z &\approx \frac{3}{4}\delta x + \frac{1}{3}\delta y \\ |\delta z\,| &\approx |\frac{3}{4}\delta x + \frac{1}{3}\delta y| \\ |\delta z\,| &\leq \frac{3}{4}|\delta x\,| + \frac{1}{3}|\delta y\,| = \frac{3}{4}(0.1) + \frac{1}{3}(0.2) \approx 0.14 \end{aligned}$$

That is, $|\delta z\,| \leq 0.14$.

Notes:

- We have used $|a + b| \leq |a| + |b|$.
- The three-variable extension is

$$\delta f = \frac{\partial f}{\partial x}\delta x + \frac{\partial f}{\partial y}\delta y + \frac{\partial f}{\partial z}\delta z$$

- The chain-rule is mainly used when we change form one independent variable to another - as in coordinate transormation:

Example 12

If $f \equiv f(x,y)$ and $x = r\mathrm{e}^{\theta}$ and $y = r\mathrm{e}^{-\theta}$ then show that

$$\begin{aligned} 2x\frac{\partial f}{\partial x} &= r\frac{\partial f}{\partial r} + \frac{\partial f}{\partial \theta} \\ 2y\frac{\partial f}{\partial y} &= r\frac{\partial f}{\partial r} - \frac{\partial f}{\partial \theta} \end{aligned}$$

Solution

$$\begin{aligned} \frac{\partial f}{\partial r} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial r} = \mathrm{e}^{\theta}\frac{\partial f}{\partial x} + \mathrm{e}^{-\theta}\frac{\partial f}{\partial y} \\ &\downarrow \\ r\frac{\partial f}{\partial r} &= x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} \qquad (10) \end{aligned}$$

Similarly

$$\begin{aligned} \frac{\partial f}{\partial \theta} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial \theta} = r\mathrm{e}^{\theta}\frac{\partial f}{\partial x} - r\mathrm{e}^{-\theta}\frac{\partial f}{\partial y} \\ &\downarrow \\ \frac{\partial f}{\partial \theta} &= x\frac{\partial f}{\partial x} - y\frac{\partial f}{\partial y} \qquad (11) \end{aligned}$$

Adding and subtracting (10) and (11) gives, respectively:

$$\begin{aligned} 2x\frac{\partial f}{\partial x} &= r\frac{\partial f}{\partial r} + \frac{\partial f}{\partial \theta} \\ 2y\frac{\partial f}{\partial y} &= r\frac{\partial f}{\partial r} - \frac{\partial f}{\partial \theta} \end{aligned}$$

Alternative Solution

We could have rearranged $x = r\mathrm{e}^{\theta}$ and $y = r\mathrm{e}^{-\theta}$ as

$$\begin{aligned} \frac{x}{y} &= \mathrm{e}^{2\theta} \to \theta = \frac{1}{2}\ln\left(\frac{x}{y}\right) \\ xy = r^2 &\to r = (xy)^{1/2} \end{aligned}$$

and then used the relations

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x}$$

etc. *Students: Do this as exercise*

Example 13

This is Question 9 from the tutorial sheet: By putting $u = xy$ and $v = x^2/y$ show that the partial differential equation

$$x\frac{\partial z}{\partial x} + 2y\frac{\partial z}{\partial y} = 3x^3\cos(xy)$$

can be written in the form

$$\frac{\partial z}{\partial u} = v\cos u.$$

Hence, find the general solution of the equation.

Solution

We have

$$\begin{aligned}
\frac{\partial z}{\partial x} &= \frac{\partial z}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial z}{\partial v}\frac{\partial v}{\partial x} \\
&= y\frac{\partial z}{\partial u} + \frac{2x}{y}\frac{\partial z}{\partial v} \\
&\downarrow \\
x\frac{\partial z}{\partial x} &= xy\frac{\partial z}{\partial u} + \frac{2x^2}{y}\frac{\partial z}{\partial v} = u\frac{\partial z}{\partial u} + 2v\frac{\partial z}{\partial v}
\end{aligned}$$

Similarly,

$$\begin{aligned}
\frac{\partial z}{\partial y} &= \frac{\partial z}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial z}{\partial v}\frac{\partial v}{\partial y} \\
&= x\frac{\partial z}{\partial u} - \frac{x^2}{y^2}\frac{\partial z}{\partial v} \\
&\downarrow \\
2y\frac{\partial z}{\partial y} &= 2xy\frac{\partial z}{\partial u} - \frac{2x^2}{y}\frac{\partial z}{\partial v} = 2u\frac{\partial z}{\partial u} - 2v\frac{\partial z}{\partial v}
\end{aligned}$$

Adding these together gives, finally,

$$\begin{aligned}
x\frac{\partial z}{\partial x} + 2y\frac{\partial z}{\partial y} &= 3u\frac{\partial z}{\partial u} = 3x^3\cos(xy) \\
&\downarrow \\
3u\frac{\partial z}{\partial u} &= 3uv\cos u \\
&\downarrow \\
\frac{\partial z}{\partial u} &= v\cos u.
\end{aligned}$$

This pde can now be solved as follows: Integrate wrt to u:

$$\begin{aligned}
z &= v\sin u + f(v) \\
&\downarrow \\
z(x,y) &= \frac{x^2}{y}\sin(xy) + f\left(\frac{x^2}{y}\right)
\end{aligned}$$

Example 14
The potential function $V(x,t) = Ae^{-qt} sin\, k(x - ct)$ represents an attenuating wave travelling to the right along a cable with speed c. Here the quantities A, q, k, c are constants. Find (a) the rate of change of V with time t at any fixed point x; (b) the 'potential gradient' $\partial V/\partial x$ along the wire at any moment.
Solution:
For calculating (a) we note that V(x,t) is a product of two functions, i.e. we use the product rule

$$\frac{\partial V}{\partial t} = Ae^{-qt}\left[-kc\cos k(x-ct)\right]+(-qAe^{-qt}\sin k(x-ct) = Ae^{-qt}\left[kc\cos k(x-ct)+q\sin k(x-ct)\right]$$

(b) In order to calculate the gradient, we have

$$\frac{\partial V}{\partial x} = Ae^{-qt}\frac{\partial}{\partial x}\sin k(x-ct) = kAe^{-qt}\cos k(x-ct)$$

AMA252 Lecture 5: Fourier Series 1

14 Introduction

Consider the Taylor expansion of e^x:

$$\mathrm{e}^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + ...$$

This is an example of one function, e^x, be expressed in terms of simpler functions - powers of x. In general, we have

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \tag{12}$$

as the Taylor expansion of $f(x)$ about $x = 0$. There are many reasons why we might want to express a function, $f(x)$, in this way. In fact, (12) is a special case of the general expansion

$$f(x) = \sum_{n=0}^{\infty} a_n F_n(x) \tag{13}$$

where $F_n(x),\ n = 0, 1, 2, ...$ is some set of functions. In the particular case where $F_n(x) = \cos nx$ or $F_n(x) = \sin nx$ then (13) is said to be a *Fourier Series* which are a very useful class of function expansions - with many important applications in engineering and science in general.

15 Trigonometric Series: General Comments

A *trigonometric series* is a series of the type

$$\frac{1}{2}a_0 + \sum_{n=1}^{\infty}(a_n\cos nx + b_n\sin nx) \tag{14}$$

where the coefficients $a_0, a_1, ..., a_n, b_0, b_1, ..., b_n$ are independend of x. **Note:** The term $a_0/2$ (rather than simply a_0) is used for later convenience. It could be incorporated in the $\sum$ by starting at $n = 0$.

If the series (14) converges to a sum $f(x)$ then we see that, for any integer k, we must have

$$f(x + 2\pi k) = f(x)$$

since $\cos[n(x + 2\pi k)] = \cos nx$ etc. It follows that $f(x)$ as defined is *periodic* with period 2π. Thus, for such functions, we need only study the series expansion in an interval of 2π. We choose $-\pi \leq x \leq +\pi$.

15.1 Construction of Trigonometric Series

Suppose

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx) \tag{15}$$

and that this series is convergent. How do we construct such a series? We make use of the following useful results for which m, n are *integer* :

$$\int_{-\pi}^{+\pi} \sin nx \, dx = \int_{-\pi}^{+\pi} \cos nx \, dx = 0, \tag{16}$$

$$\int_{-\pi}^{+\pi} \cos mx \cos nx \, dx = \begin{cases} 0 & \text{if } m \neq n \\ \pi & \text{if } m = n \neq 0 \\ 2\pi & \text{if } m = n = 0 \end{cases} \tag{17}$$

$$\int_{-\pi}^{+\pi} \sin mx \sin nx \, dx = \begin{cases} 0 & \text{if } m \neq n \\ \pi & \text{if } m = n \neq 0 \\ 0 & \text{if } m = n = 0 \end{cases} \tag{18}$$

$$\int_{-\pi}^{+\pi} \sin mx \cos nx \, dx = 0 \;\; (\text{odd function}) \tag{19}$$

We prove (17) as an illustration of how the proofs go:

Proof of (17)

We remember

$$\begin{aligned} \cos(A+B) &= \cos A \cos B - \sin A \sin B \\ \cos(A-B) &= \cos A \cos B + \sin A \sin B \\ &\downarrow \\ \cos A \cos B &= \frac{1}{2}[\cos(A+B) + \cos(A-B)] \end{aligned}$$

Hence

$$\begin{aligned} \int_{-\pi}^{+\pi} \cos mx \cos nx \, dx &= \frac{1}{2}\int_{-\pi}^{+\pi} [\cos(m+n)x + \cos(m-n)x] \, dx \\ &= \frac{1}{2}\left[\frac{\sin(m+n)x}{m+n} + \frac{\sin(m-n)x}{m-n}\right]_{-\pi}^{+\pi} = 0 \quad \text{if } m \neq n \end{aligned}$$

The cases $m = n \neq 0$ and $m = n = 0$ must be treated separately: For $m = n \neq 0$ we have

$$\begin{aligned} \int_{-\pi}^{+\pi} \cos mx \cos mx \, dx &= \frac{1}{2}\int_{-\pi}^{+\pi} [1 + \cos 2mx] \, dx \\ &= \frac{1}{2}\left[x + \frac{\sin 2mx}{2m}\right]_{-\pi}^{+\pi} = \pi, \quad (m = n \neq 0) \end{aligned}$$

For the case $m = n = 0$ we have

$$\int_{-\pi}^{+\pi} \cos mx \cos nx \, dx = \int_{-\pi}^{+\pi} 1 = 2\pi, \quad (m = n = 0)$$

The other results follow in a similar fashion.

15.2 Determination of a_n and b_n

We have

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx) \tag{20}$$

and we wish to find the coefficients $a_0, a_1, ..., b_1, b_2, ...$

Case a_m: $m > 0$

Multiply the above through by $\cos mx$ and integrate over $[-\pi, +\pi]$:

$$\begin{aligned}\int_{-\pi}^{+\pi} f(x)\cos mx\,dx &= \frac{1}{2}a_0\int_{-\pi}^{+\pi}\cos mx\,dx + \sum_{n=1}^{\infty}\int_{-\pi}^{+\pi} a_n \cos nx \cos mx\,dx \\ &\quad + \sum_{n=1}^{\infty}\int_{-\pi}^{+\pi} b_n \sin nx \cos mx\,dx\end{aligned}$$

We now use results (16), (17) and (19) to get

$$\begin{aligned}\int_{-\pi}^{+\pi} f(x)\cos mx\,dx &= 0 + \int_{-\pi}^{+\pi} a_m \cos^2 mx\,dx + 0 \\ &= \pi a_m\end{aligned} \tag{21}$$

$$\downarrow$$

$$a_m = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos mx\,dx \tag{22}$$

Case a_m: $m = 0$

We integrate (20) directly wrt x:

$$\int_{-\pi}^{+\pi} f(x)\,dx = \pi a_0$$

$$\downarrow$$

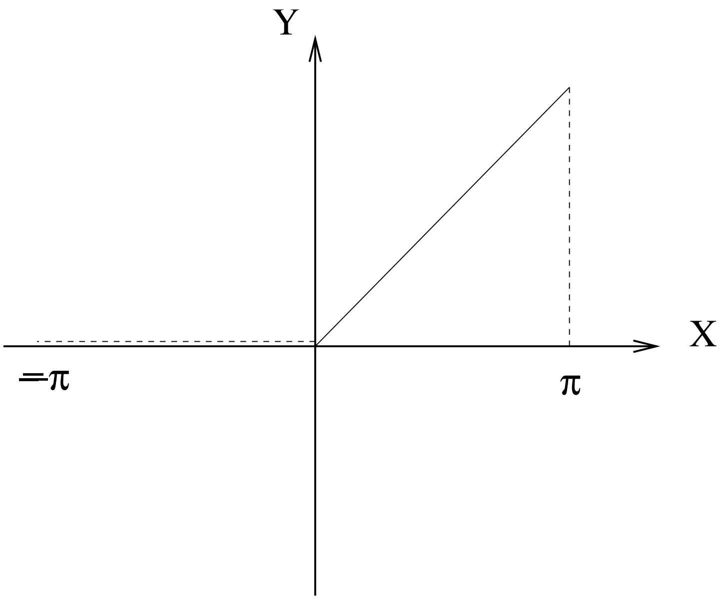
$$a_0 = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\,dx \tag{23}$$

If we compare (22) and (23), we see that the latter is just the special case of the former for $m = 0$. *This is the reason we used the notation $a_0/2$ in (20) - rather than simply a_0!!*

Case b_m

Now we multiply (20) through by $\sin mx$ and integrate: Following the same pattern as above we find

$$b_m = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\sin mx\,dx \tag{24}$$



15.3 Fourier (Trigonometric) Series: Summary and Notes

The series

$$
\begin{aligned}
f(x) &= \frac{1}{2}a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx) \\
\text{where} & \\
a_m &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos mx\, dx, \quad m = 0, 1, 2, ... \\
b_m &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\sin mx\, dx, \quad m = 1, 2, 3, ...
\end{aligned}
$$

is called the *Full-range Fourier Series* expansion of $f(x)$ in $(-\pi, +\pi)$. Note that b_0 does not appear.

General Comments

The Fourier series can represent either

- An arbitrary function $f(x)$ defined in the interval $(-\pi < x < +\pi)$, or:
- A periodic function, period 2π defined for *all* x.

Example 1

Find the Fourier representation of

$$
f(x) = \begin{cases} 0 & -\pi \le x \le 0 \\ x & 0 \le x \le \pi \end{cases}
$$

which is also shown in the figure.

Solution

For a_0 we have

$$\begin{aligned} a_0 &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\,dx \\ &= \frac{1}{\pi}\int_0^{\pi} x\,dx = \frac{\pi}{2} \end{aligned}$$

For a_m we have

$$\begin{aligned} a_m &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos mx\,dx = \frac{1}{\pi}\int_0^{\pi} x\cos mx\,dx \\ &= \frac{1}{\pi}\left[\frac{x\sin mx}{m}\right]_0^{\pi} - \frac{1}{m\pi}\int_0^{\pi}\sin mx\,dx \\ &= \frac{1}{m^2\pi}\left[\cos m\pi\right]_0^{\pi} = \frac{1}{m^2\pi}\left[\cos m\pi - 1\right] \\ &= \frac{1}{m^2\pi}\left[(-1)^m - 1\right] \end{aligned}$$

For b_m we have, by a similar calculation

$$b_m = \frac{1}{\pi}\int_0^{\pi} x\sin mx\,dx = \ldots = \frac{(-1)^{m+1}}{m}$$

Putting everything together we get, finally:

$$f(x) = \frac{\pi}{4} + \sum_{n=1}^{\infty}\left[\left(\frac{(-1)^n - 1}{n^2\pi}\right)\cos nx + \frac{(-1)^{n+1}}{n}\sin nx\right]$$

Example 2

Find the Fourier representation of

$$f(x) = \begin{cases} -1 & -\pi \le x \le 0 \\ +1 & 0 < x \le \pi \end{cases}$$

shown in the figure.

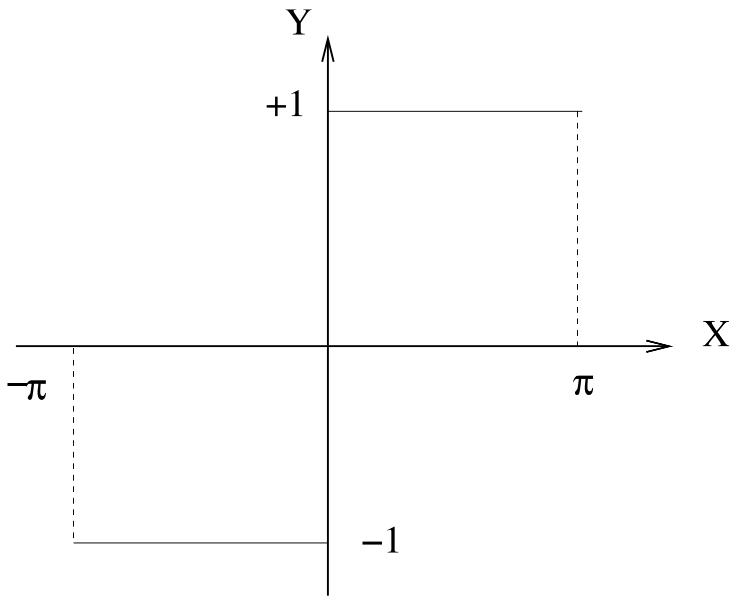
Solution

From the figure, we can see that the function is *odd* - this mean that its Fourier series must consist of purely *odd functions.* That is, there can be no cosine terms in the expansion. Generally, it is enough just to say this, but we shall also show it analytically here.
We have

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\,dx = \frac{1}{\pi}\int_{-\pi}^{0}(-1)\,dx + \frac{1}{\pi}\int_0^{\pi} 1\,dx = \frac{1}{\pi}(-\pi) + 1 = 0$$

Similarly, a_m is given by

$$\begin{aligned} a_m &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos mx\,dx = -\frac{1}{\pi}\int_{-\pi}^{0}\cos mx\,dx + \frac{1}{\pi}\int_0^{\pi}\cos mx\,dx \\ &= -\frac{1}{\pi}\left[\frac{\sin mx}{m}\right]_{-\pi}^{0} + \frac{1}{\pi}\left[\frac{\sin mx}{m}\right]_0^{\pi} = 0 \end{aligned}$$



Thus, as stated, $a_m = 0, \;\; m = 0, 1, 2, ...$

For the $b_m$terms we have

$$\begin{aligned} b_m &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\sin mx\,dx = -\frac{1}{\pi}\int_{-\pi}^{0}\sin mx\,dx + \frac{1}{\pi}\int_{0}^{\pi}\sin mx\,dx \\ &= \frac{1}{\pi}\left[\frac{\cos mx}{m}\right]_{-\pi}^{0} + \frac{1}{\pi}\left[-\frac{\cos mx}{m}\right]_{0}^{\pi} \\ &= \frac{1}{m\pi}\left[1-(-1)^m\right] + \frac{1}{m\pi}\left[-(-1)^m+1\right] \\ &= \frac{2}{m\pi}\left[1-(-1)^m\right] \end{aligned}$$

Hence,

$$\begin{aligned} f(x) &= \sum_{n=1}^{\infty}\frac{2}{n\pi}(1-(-1)^n)\sin nx \\ &= \frac{4}{\pi}\left(\sin x + \frac{1}{3}\sin 3x + \frac{1}{5}\sin 5x + ...\right) \end{aligned}$$

AMA252 Lecture 6: Fourier Series 2

16 Odd and Even Functions

Even Functions

A function $f(x)$, defined on $-\pi \leq x \leq \pi$ is an *even function* of x if, for x in the range, then $f(x) = f(-x)$. For example, x^2 is an even function since $(3)^2 = (-3)^2 = 9$.

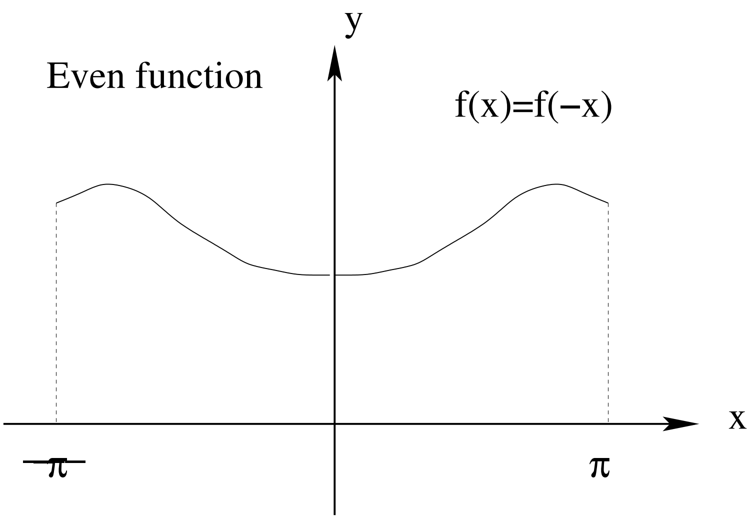


Figure 4:

Also, x^4, $\cos x$,... and figure 4.

Odd Functions

A function $f(x)$, defined on $-\pi \leq x \leq \pi$ is an *odd function* of x if, for x in the range, then $f(x) = -f(-x)$. For example, x^3 is an odd function since $(3)^3 = -(-3)^3 = 27$.

Also x, $\sin x$,... and figure 4

Comments

- Even function $\times$ Even function =Even function
- Odd function $\times$ Odd function =Even function
- Odd function $\times$ Even function =Odd function
- $\cos nx$ is an *even* function
- $\sin nx$ is an *odd* function

16.1 Fourier Series for an Even Function

The Fourier series for an *even function* $f(x)$ defined on $-\pi \leq x \leq \pi$ is a pure *cosine* series.

Proof

For a_n we have:

$$\begin{aligned} a_n &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos nx\,dx \\ \text{Now use fact that } f(x)\cos nx \text{ is even} & \\ &= \frac{2}{\pi}\int_{0}^{\pi} f(x)\cos nx\,dx \end{aligned}$$

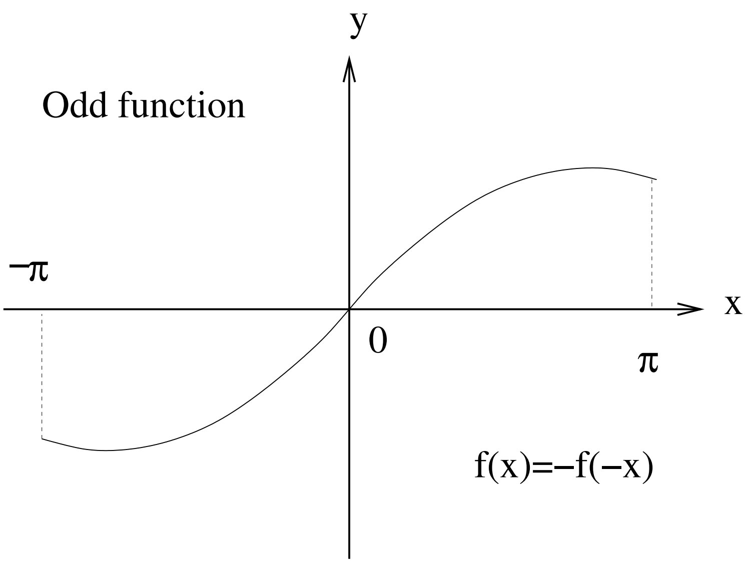


Figure 5:

For b_n we have:

$$\begin{aligned} b_n &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\sin nx\,dx \\ \text{Now use fact that } f(x)\sin nx \text{ is odd} & \\ &= 0 \end{aligned}$$

Hence, we finally get, for an *even* function $f(x)$

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos nx$$

This is called a *Fourier cosine series*.

16.2 Fourier Series for an Odd Function

The Fourier series for an *odd function* $f(x)$ defined on $-\pi \le x \le \pi$ is a pure *sine* series.

Proof

For a_n we have:

$$\begin{aligned} a_n &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos nx\,dx \\ \text{Now use fact that } f(x)\cos nx \text{ is odd} & \\ &= 0 \end{aligned}$$

For b_n we have:

$$\begin{aligned} b_n &= \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\sin nx\,dx \\ \text{Now use fact that } f(x)\sin nx \text{ is even} & \\ &= \frac{2}{\pi}\int_{0}^{+\pi} f(x)\sin nx\,dx \end{aligned}$$

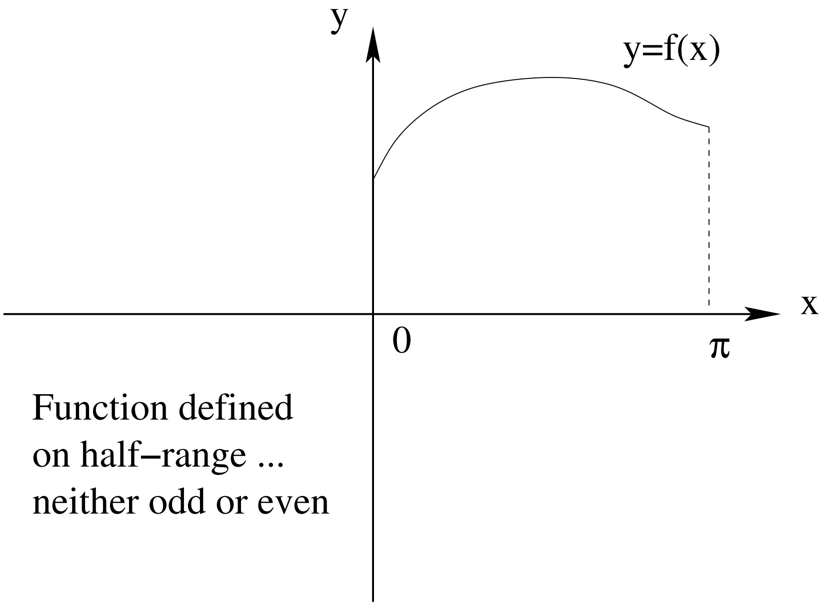


Figure 6:

Hence, we finally get, for an *odd* function $f(x)$

$$f(x) = \sum_{n=1}^{\infty} b_n \sin nx$$

This is called a *Fourier sine series*.

17 Special Cases

Suppose a function $g(x)$ is defined for $0 \leq x \leq \pi$ (see figure 6) rather than on the whole range $-\pi \leq x \leq +\pi$, then it can be represented as *either* a Fourier cosine series, or as a Fourier sine series ...

17.1 The Sine Series Form of $g(x)$

The function $g(x)$ defined on $0 \leq x \leq \pi$ is neither even or odd. To get the sine-series representation of it, we simply *extend* the definition of it to the full range $-\pi \leq x \leq +\pi$ making it an *odd* function: that is

$$G(x) = \begin{cases} +g(x), & 0 \leq x \leq \pi \\ -g(-x), & -\pi \leq x \leq 0 \end{cases}$$

Now we see that $G(x)$ is an *odd* function which equals $g(x)$ over the range on which $g(x)$ is defined. See figure 7. Using the results of §16.2 we immediately get

$$G(x) = \sum_{n=1}^{\infty} b_n \sin nx$$

where

$$b_n = \frac{2}{\pi} \int_0^{+\pi} G(x) \sin nx \, dx, \quad n = 1, 2, ...$$

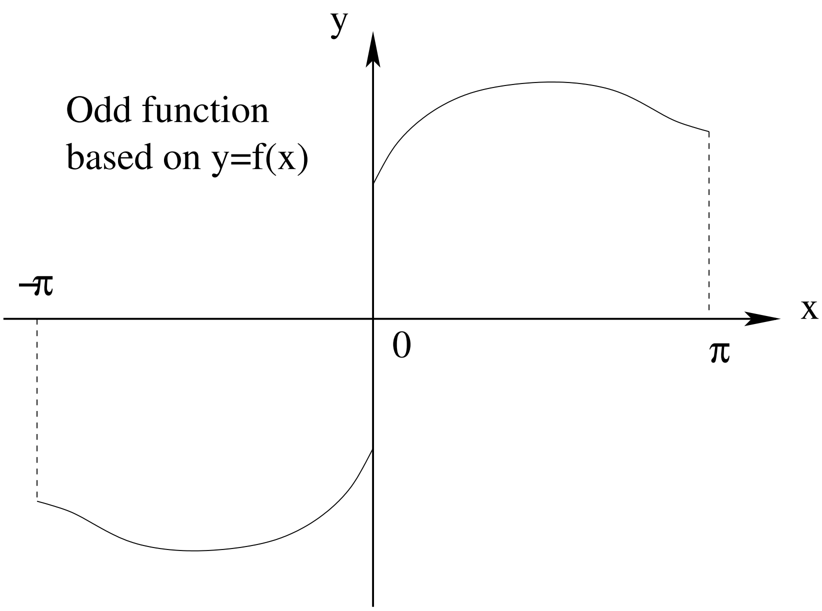


Figure 7:

17.2 The Cosine Series Form of $g(x)$

To get the cosine-series representation of $g(x)$, we simply *extend* the definition of it to the full range $-\pi \leq x \leq +\pi$ making it an *even* function (see figure 8): that is

$$G(x) = \begin{cases} +g(x), & 0 \leq x \leq \pi \\ +g(-x), & -\pi \leq x \leq 0 \end{cases}$$

Now we see that $G(x)$ is an *even* function which equals $g(x)$ over the range on which $g(x)$ is defined. Using the results of §16.1 we immediately get

$$G(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos nx$$

where

$$a_n = \frac{2}{\pi}\int_0^{+\pi} G(x)\cos nx\,dx, \quad n = 0, 1, 2, ...$$

Example 3

Find the Fourier sine and cosine series for $g(x) = 1,\ 0 \leq x \leq \pi.$

Solution Sine Series

$$\begin{aligned} b_m &= \frac{2}{\pi}\int_0^{\pi} \sin mx\,dx = -\frac{2}{m\pi}\left[\cos mx\right]_0^{\pi} \\ &= \frac{2}{m\pi}\left[1 - (-1)^m\right] \\ &\downarrow \\ g(x) &= \sum_{m=1}^{\infty} \frac{2}{m\pi}\left[1 - (-1)^m\right]\sin mx \end{aligned}$$

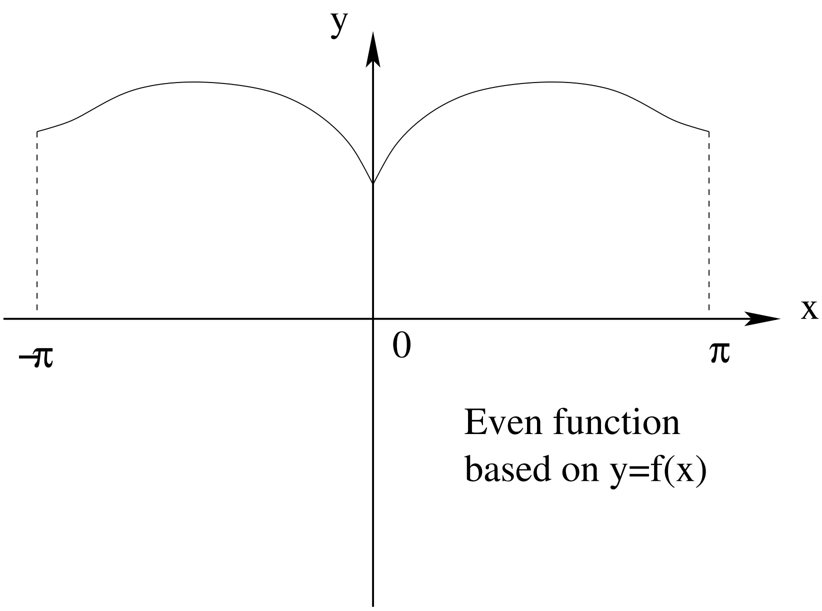


Figure 8:

Solution Cosine Series

$$
\begin{aligned}
a_0 &= \frac{2}{\pi}\int_0^{\pi} 1\,dx = 2 \\
a_m &= \frac{2}{\pi}\int_0^{\pi} \cos mx\,dx = \frac{2}{m\pi}\left(\sin mx\right)_0^{\pi} = 0, \quad m > 0 \\
&\downarrow \\
g(x) &= 1
\end{aligned}
$$

18 Convergence

We have seen how to express a function $f(x)$ as an infinite series of sine and/or cosine terms. The question now arises *Under what conditions will such a series actually CONVERGE to the function $f(x)$ over the range of its definition?*

Dirichlet's Conditions (1829)

Suppose $f(x)$ is defined on $-\pi \leq x \leq +\pi$ and

- $f(x)$ has only a finite number of max and min
- $f(x)$ has only a finite number of *finite* discontinuities in the range

then the F-S converges to the sum

$$\frac{1}{2}\left[f(x+0^+) + f(x+0^-)\right]$$

at x. Thus, if at a point x_0 the function $f(x)$ is continuous, then the value of the Fourier series (F-S) is $f(x_0)$. But, if $f(x)$ has a jump at x_0 then the value of the F-S is the value of the mid-point of the jump at x_0(see figure 9):

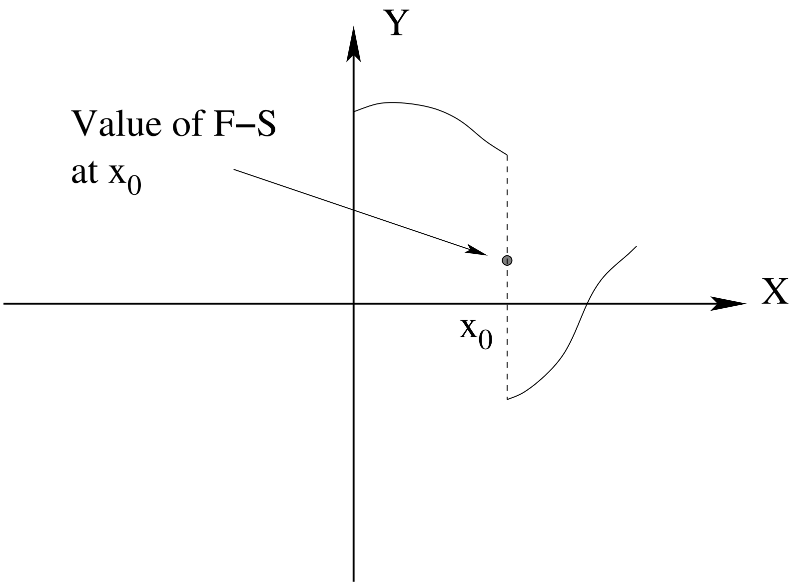


Figure 9:

Notes

- The function $(4-x^2)^{-1}$ does *not* satisfy the Dirichlet condition in $-\pi \le x \le +\pi$ - the discontinuity at $x=2$ is *infinite;*
- The function $\sin[1/(x-1)]$ does *not* satisfy the Dirichlet condition in $-\pi \le x \le +\pi$- the function has an *infinite* number of max/min near $x=1$.

Example 4

From example 1 of the previous lecture, the F-S for the function shown in figure 10 is given by

$$f(x) = \frac{\pi}{4} + \sum_{n=1}^{\infty}\left[\left(\frac{(-1)^n - 1}{n^2\pi}\right)\cos nx + \frac{(-1)^{n+1}}{n}\sin nx\right]$$

The function $f(x)$ is continuous everywhere so that F-S $= f(x)$ on $-\pi \le x \le +\pi$. At $x=0$ we therefore can say

$$0 = \frac{\pi}{4} + \sum_{n=1}^{\infty}\left[\left(\frac{(-1)^n - 1}{n^2\pi}\right).1 + 0\right] \rightarrow \frac{\pi^2}{4} = \sum_{n=1}^{\infty}\left[\left(\frac{1-(-1)^n}{n^2}\right)\right]$$

Fourier series are very useful at getting this kind of interesting identity.

Example 5

From example 2 of the previous lecture, the F-S for the function shown in figure 11 is given by

$$f(x) = \sum_{n=1}^{\infty}\frac{2}{n\pi}(1-(-1)^n)\sin nx$$

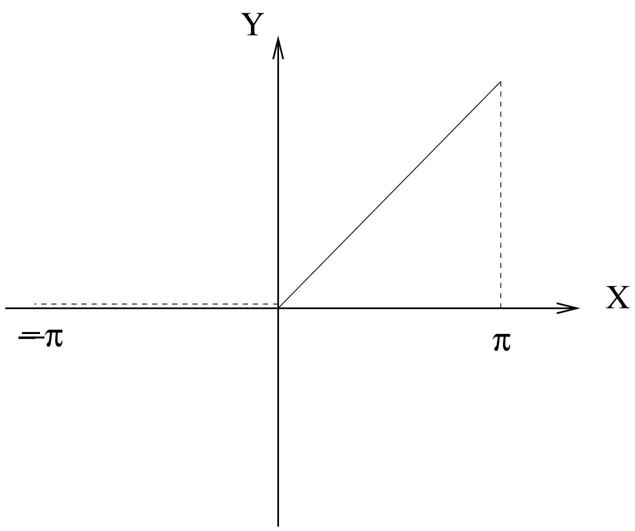


Figure 10:

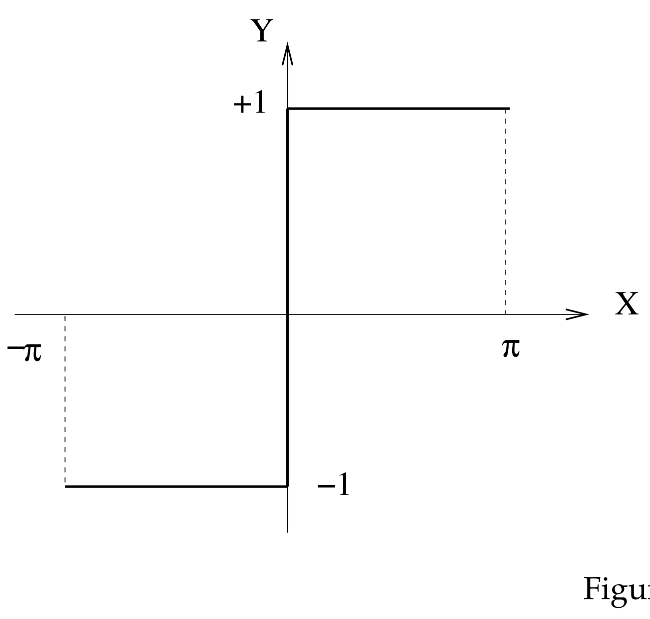


Figure 11:

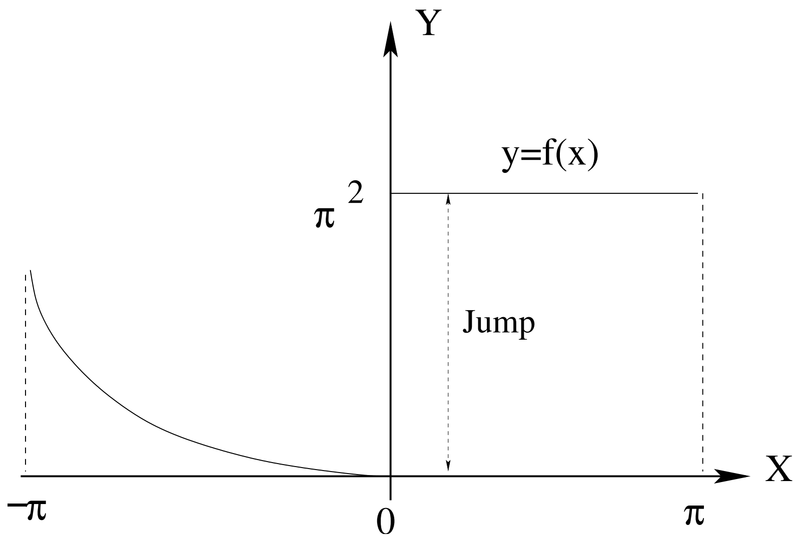


Figure 12:

The function $f(x)$ is continuous at $x = 0$. Hence, at $x = 0$ the F-S takes the value

$$\frac{1}{2}(-1+1) = 0.$$

For another interesting identity, consider the case of $x = \pi/2$ when $f(x) = 1$: The F-S gives

$$\begin{aligned} 1 &= \frac{4}{\pi}\left[\sin\frac{\pi}{2} + \frac{1}{3}\sin\frac{3\pi}{2} + \frac{1}{5}\sin\frac{5\pi}{2} + ...\right] \\ &= \frac{4}{\pi}\left[1 + \frac{1}{3}(-1) + \frac{1}{5}(1) + ...\right] = \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1} \end{aligned}$$

so that, finally:

$$\frac{\pi}{4} = \sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}$$

Example 6

Consider the function

$$f(x) = \begin{cases} x^2 & -\pi \le x < 0 \\ \pi^2 & 0 < x \le +\pi \end{cases}$$

also shown in figure 12 The F-S is given by

$$\frac{2\pi^2}{3} + \sum_{n=1}^{\infty}\left\{\frac{2(-1)^n}{n^2}\cos nx + \left[\frac{\pi}{n} + \frac{2(1-(-1)^n}{n^3\pi}\right]\sin nx\right\}$$

The F-S converges to $f(x)$ on $-\pi \le x < 0$ and $0 < x \le \pi$ and therefore to the value $\pi^2/2$ at $x = 0$. Thus:

$$\frac{\pi^2}{2} = \frac{2\pi^2}{3} + \sum_{n=1}^{\infty}\frac{2(-1)^n}{n^2}$$

$$\begin{aligned} &\downarrow \\ -\frac{\pi^2}{12} &= \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \\ &\downarrow \\ \frac{\pi^2}{12} &= \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2} \end{aligned}$$

Example 7

For the function above, the F-S converges at $x = \pi$. Hence

$$\begin{aligned} \pi^2 &= \frac{2\pi^2}{3} + \sum_{n=1}^{\infty} \frac{2(-1)^n}{n^2}(-1)^n \\ &= \frac{2\pi^2}{3} + \sum_{n=1}^{\infty} \frac{2}{n^2} \\ &\downarrow \\ \frac{\pi^2}{6} &= \sum_{n=1}^{\infty} \frac{1}{n^2} \end{aligned}$$

19 Ranges other than $(-\pi, +\pi)$

1. If the range has length 2π then then only change to the foregoing is the limits on the integration: that is, if the range is $(\alpha,\, \alpha + 2\pi)$ then the integration limits $(-\pi,\, \pi)$ get replaced by $(\alpha,\, \alpha + 2\pi)$. Thus, suppose $f(x)$ is defined for $0 \le x \le 2\pi$, then everything is as before except that we have
$$\frac{1}{\pi}\int_0^{2\pi} \cdots$$
throughout.

2. If the range is defined for $-l \le x \le +l$, then refer to formulae sheet.

3. If the range is defined for $0 \le x \le 2l$, then exactly as above, but range of integration is $0 \le x \le 2l$ throughout.

4. Ex 6 on the problem sheet has $f(t)$ defined for $0 \le t \le 2\pi/\omega$. Here, set $l = \pi/\omega$ and follow above.

5. Half-range series: here $f(x)$ defined on $0 \le x \le l$. See formulae sheet - we will use these later in course.

Example 9

Consider the function

$$f(x) = \begin{cases} -x/2 + 1 & 0 \le x \le 2 \\ +x/2 + 1 & -2 \le x \le 0 \end{cases}$$

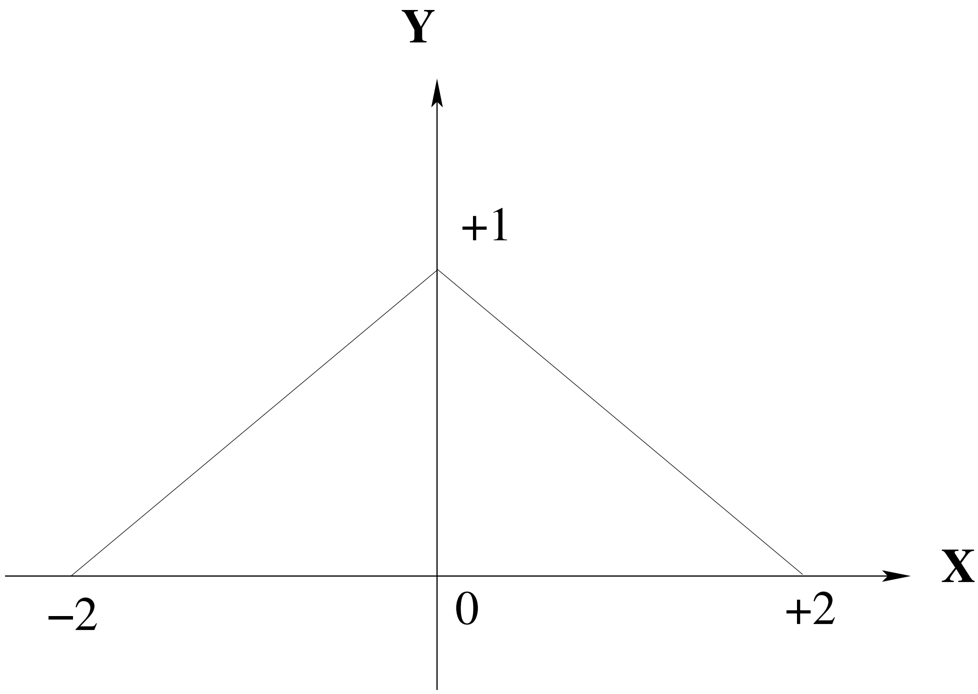


Figure 13:

which is also shown in figure 13. This is an *even* function so that $b_n = 0$, and we must have a cosine series defined on $-2 \leq x \leq 2$. Thus, we use $l = 2$ and use formulae sheet:

$$
\begin{aligned}
a_0 &= \frac{1}{2}\int_{-2}^{+2} f(x)\,dx = \frac{2}{2}\int_0^2 f(x)\,dx \\
&= \int_0^2 \left(-\frac{1}{2}x + 1\right)\,dx = \left(-\frac{1}{4}x^2 + x\right)_0^2 = 1 \\
a_n &= \frac{1}{2}\int_{-2}^{+2} f(x)\cos\frac{n\pi x}{2}\,dx = \frac{2}{2}\int_0^2 \left(-\frac{1}{2}x + 1\right)\cos\frac{n\pi x}{2}\,dx \\
&= \int_0^2 -\frac{1}{2}x\cos\frac{n\pi x}{2}\,dx + \int_0^2 \cos\frac{n\pi x}{2}\,dx \\
&= -\frac{1}{2}\left\{\left[\frac{2}{n\pi}x\sin\frac{n\pi x}{2}\right]_0^2 - \int_0^2 \frac{2}{n\pi}\sin\frac{n\pi x}{2}\,dx\right\} + \left[\frac{2}{n\pi}\sin\frac{n\pi x}{2}\right]_0^2 \\
&= \frac{1}{n\pi}\int_0^2 \sin\frac{n\pi x}{2}\,dx = -\frac{2}{n^2\pi^2}\left[\cos\frac{n\pi x}{2}\right]_0^2 = -\frac{2}{n^2\pi^2}\left[(-1)^n - 1\right]
\end{aligned}
$$

Hence, finally, the F-S is given by

$$f(x) = \frac{1}{2} + \sum_{n=1}^{\infty}\frac{2}{n^2\pi^2}\left[1 - (-1)^n\right]\cos\frac{n\pi x}{2}.$$

20 Introduction: Separation of Variables

Example 1

Find a solution of

$$x\frac{\partial\phi}{\partial x} = 3\phi + \frac{\partial\phi}{\partial y} \qquad (\text{Notation note: Same as } \; x\phi_x = 3\phi + \phi_y$$

where $\phi \equiv \phi(x, y)$.

Solution 1

Look for a solution of the form $\phi(x, y) \equiv X(x)\,Y(y)$ ... with this assumption, we expect the original PDE to reduce to a couple of simple ODEs:

$$\begin{aligned}\frac{\partial\phi}{\partial x} &= \frac{dX}{dx}Y = X'Y \\ \frac{\partial\phi}{\partial y} &= X\frac{dY}{dy} = XY'\end{aligned}$$

Hence, from the original eqn

$$xX'Y = 3XY + XY'$$

Now divide by XY to get:

$$x\frac{X'}{X} = 3 + \frac{Y'}{Y}$$

The lhs is purely a function of x and the rhs is purely a function of y - but x and y are *independent*. The only possibility is that each side of the eqn equals a constant: that is

$$x\frac{X'}{X} = 3 + \frac{Y'}{Y} = \alpha$$

where α is *constant*. Hence, we get

$$\begin{aligned}\frac{X'}{X} &= \frac{\alpha}{x} \rightarrow \ln X = \alpha \ln x + A \rightarrow X = Bx^{\alpha} \\ \frac{Y'}{Y} &= \alpha - 3 \rightarrow \ln Y = (\alpha - 3)y + C \rightarrow Y = D\mathrm{e}^{(\alpha-3)y}\end{aligned}$$

Hence

$$\phi(x, y) \equiv X(x)\,Y(y) = Ex^{\alpha}\mathrm{e}^{(\alpha-3)y} \tag{25}$$

Note: in the above A, B, C, D, E are purely undetermined constants of integration.

Solution 2

Now suppose that the same eqn is specified, but with the additional information that $\phi = x^2$ along the line $y = 0$. In this case, we can use (25) to say that

$$\phi(x, 0) = Ex^{\alpha} \cdot 1 = x^2$$

Hence, $\alpha = 2$ and $E = 1$ so that the solution satisfying the given condition is:

$$\phi(x, y) = x^2\mathrm{e}^{-y}$$

20.1 The Diffusion Equation

The PDEs which arise from physical problems are commonly 2nd order - that is, they involve 2nd order derivatives (but not higher order ones!). One such equation which commonly arises in some form or other is the *heat conduction equation*:

$$\frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial x^2} \tag{26}$$

where k is some constant. This equation describes many quite distinct physical processes. For example:

- The temperature distribution, θ, along a long thin rod of homogeneous material in which there is no variation across any section of the rod (this corresponds, for example, to a thin rod being insulated along its length): in this case, x denotes spatial displacement, t denotes time and k denotes the thermal diffusivity.
- The concentration of chloride salts along a long thin concrete section in which the concentration across any section is uniform (corresponds to a thin rod with an impervious coating along its length).

The equation is the most simple example of *parabolic equation.* To solve it, we proceed as above: Let $\theta(x,t) = X(x)T(t)$. Hence the PDE becomes

$$\begin{aligned} XT' &= kX''T \\ &\downarrow \\ \frac{T'}{kT} &= \frac{X''}{X} = \alpha \text{ (constant)} \end{aligned}$$

Note that the lhs is a function of t only whilst the rhs is a function of x only. Hence

$$X'' = \alpha X, \quad T' = \alpha k T \tag{27}$$

The general behaviour of the solution varies according to whether α is *positive* or *negative* with $\alpha = 0$ being a special case. It turns out that, for most cases, the $\alpha > 0$ case is non-physical (to see why, solve $T' = \omega^2 T,\ \ \omega^2 > 0$) so that we need only consider $\alpha \leq 0$.

Case $\alpha = 0$

Putting $\alpha = 0$ in (27) we get

$$\begin{aligned} X'' = 0 \quad &\rightarrow \quad X = b_1 x + c_1 \\ \text{and}& \\ T' = 0 \quad &\rightarrow \quad T = d_1 \\ &\downarrow \\ \theta(x,t) = X(x)T(t) \quad &\rightarrow \quad \theta(x,t) = d_1(b_1 x + c_1) = bx + c \end{aligned}$$

Case $\alpha < 0$

To emphasize negativity of the constant, we write $\alpha = -s^2$ so that the second of (27) gives directly

$$T = C\mathrm{e}^{-s^2kt}$$

For the first of (27), we now have

$$X'' = -s^2X \to X'' + s^2X = 0$$

This last eqn we recognize as the SHM equation (*Simple Harmonic Motion*) which has the general solution

$$X = A_0 \cos sx + B_0 \sin sx$$

Hence, we get

$$\theta(x,t) = X(x)T(t) = (A\cos sx + B\sin sx)\,\mathrm{e}^{-s^2kt} \tag{28}$$

where we have absorbed all the constants into A and B.

Since the original equation, (26) is *linear* then we can add separate solutions together to get more general solutions - thus

$$\theta(x,t) = bx + c + (A\cos sx + B\sin sx)\mathrm{e}^{-s^2kt} \tag{29}$$

is a more general solution. However, we can go much further.

20.2 Boundary Conditions and Unique Solutions

To get unique solutions for any given problem, we need extra information - *the boundary conditions and the initial conditions.* For example, suppose a steel rod, of length l and insulated along its length, has been heated in some way, and we are interested in the temperature distribution, $\theta(x,t),\ 0 < x < l,\ 0 < t < \infty$, throughout the rod at any time during the cooling process - the rod cools through the uninsulated ends. Then, clearly, we would need to know:

- the *initial* temperature distribution of the heated rod. This would be the *initial condition,* $\theta(x,0)$.
- since the cooling is taking place via heat transfer at the two ends of the rod, we need information about these end conditions - *the boundary conditions.*
  - Typically, we might assume that the rod ends are at room temperature so that $\theta(0,t)$ and $\theta(l,t)$ are specified.
  - Or we might have that the end $x = 0$ is perfectly insulated, so that no heat flows ($\partial\theta(0,t)/\partial t = 0$) whilst the other end is held at a fixed temperature ($\theta(l,t) = const$).

20.2.1 The End Conditions

For the moment, we ignore the *initial condition* $\theta(x,0)$, and consider two possible cases for the *end conditions.*

Case 1: $\theta(0,t) = 0^oC,\ \ \theta(l,t) = 50^oC$

From (29), we have, immediately:

$$0 = c + A\mathrm{e}^{-s^2kt}$$

$$50 = bl + c + (A\cos sl + B\sin sl)\mathrm{e}^{-s^2kt}$$

Since the first of these two equations must be true for all t then we can immediately deduce that $A = 0$ and $c = 0$. Thus, the second equation becomes

$$50 = bl + B\,\mathrm{e}^{-s^2kt}\,\sin sl$$

which also must be true for all t. The only way this can be true is if either $B = 0$ or $\sin sl = 0$ and $b = 50/l$. However, since $A = 0$ necessarily, then we *cannot* have $B = 0$ - since otherwise the solution (29) would be completely independent of t and this is *non-physical.* So, we *must* have $b = 50/l$ and $\sin sl = 0$. This can only be the case if

$$sl = m\pi,\ \ m = 0, 1, 2, ... \rightarrow s = \frac{m\pi}{l},\ \ m = 0, 1, 2, ...$$

Thus (29) becomes

$$\theta(x,t) = \frac{50}{l}x + B\,\mathrm{e}^{-m^2\pi^2kt/l^2}\sin\left(\frac{m\pi x}{l}\right),\ \ m = 0, 1, 2, ...$$

But this satisfies the end conditions $\theta(0,t) = 0$ and $\theta(l,t) = 50$ for *any* value of m ... consequently, the most *general* solution satisfying these end conditions is given by

$$\theta(x,t) = \frac{50}{l}x + \sum_{m=1}^{\infty} B_m\,\mathrm{e}^{-m^2\pi^2kt/l^2}\sin\left(\frac{m\pi x}{l}\right) \tag{30}$$

where B_m, $m = 1, 2, ...$ are undetermined constants (to be determined by the ***initial conditions)***.

Case 2: $\partial\theta(0,t)/\partial x = 0,\ \ \theta(l,t) = 50^oC$

This case corresponds to an perfectly insulated end at $x = 0$. From (29) we have

$$\frac{\partial\theta}{\partial x} = b + s(-A\sin sx + B\cos sx)\mathrm{e}^{-s^2kt}$$

so that when $x = 0$ we have

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0} = b + Bs\mathrm{e}^{-s^2t} = 0$$

which must be true for *all* t. The only way this can happen is if $B = 0$ so that, necessarily, $b = 0$. Hence, from (29) the solution has the form

$$\theta(x,t) = c + A\cos sx\,\mathrm{e}^{-s^2kt}$$

We now apply the condition $\theta(l,t) = 50$:

$$50 = c + A\cos ls\,\mathrm{e}^{-s^2kt}$$

Again, since this must be true for all t then $c = 50$ and *either* $A = 0$ *or* $ls = (2m+1)\pi/2,\ m = 0, 1, 2, ...$ Since we already have $B = 0$ then choosing $A = 0$ also would make the solution independent of t and therefore *non-physical.* We must therefore choose

$$s = \frac{(2m+1)\pi}{2l},\ m = 0, 1, 2, ...$$

so that the solution becomes

$$\theta(x,t) = 50 + A\cos\frac{(2m+1)\pi x}{2l}\,\mathrm{e}^{-(2m+1)^2\pi^2 kt/4l^2},\ \ m = 0, 1, 2, ...$$

As before, this solution satisfies the end-conditions for *any* value of m. Hence, the most general solution is given by

$$\theta(x,t) = 50 + \sum_{m=0}^{\infty} A_m \cos\frac{(2m+1)\pi x}{2l}\,\mathrm{e}^{-s^2 kt} \tag{31}$$

where A_m are undertermined constants (to be determined by the ***initial conditions).***

20.2.2 The Initial Conditions

The solutions (30) and (31) each satisfy particular *end conditions* - but they each contain an infinite number of *undetermined* constants, $B_m,\ m = 1, 2, ...$ and $A_m,\ m = 0, 1, 2, ...$ which must be determined before we can say we have unique solutions. To finally fix the solutions, we need to use the *initial conditions,* $\theta(x, 0) = \theta_0(x),\ 0 \le x \le l$ for some specified intial temperature distribution $\theta_0(x)$ along the rod.

To illustrate the process, let us consider **Case 1** above. Putting $t = 0$ in (30) gives

$$\theta_0(x) = \frac{50}{l}x + \sum_{m=1}^{\infty} B_m \sin\left(\frac{m\pi x}{l}\right)$$

which is simply a Fourier sine series for $\theta_0(x) - 50x/l$. Thus

$$B_m = \frac{2}{l}\int_0^l \left[\theta_0(x) - \frac{50}{l}x\right] \sin\left(\frac{m\pi x}{l}\right),\ \ m = 1, 2, ...$$

For example, if $\theta_0(x) \equiv V_0 x$ for some given constant V_0, then we could evaluate the B_m explicitly using

$$B_m = \frac{2}{l}\left[V_0 - \frac{50}{l}\right]\int_0^l x\,\sin\left(\frac{m\pi x}{l}\right),\ \ m = 1, 2, ...$$

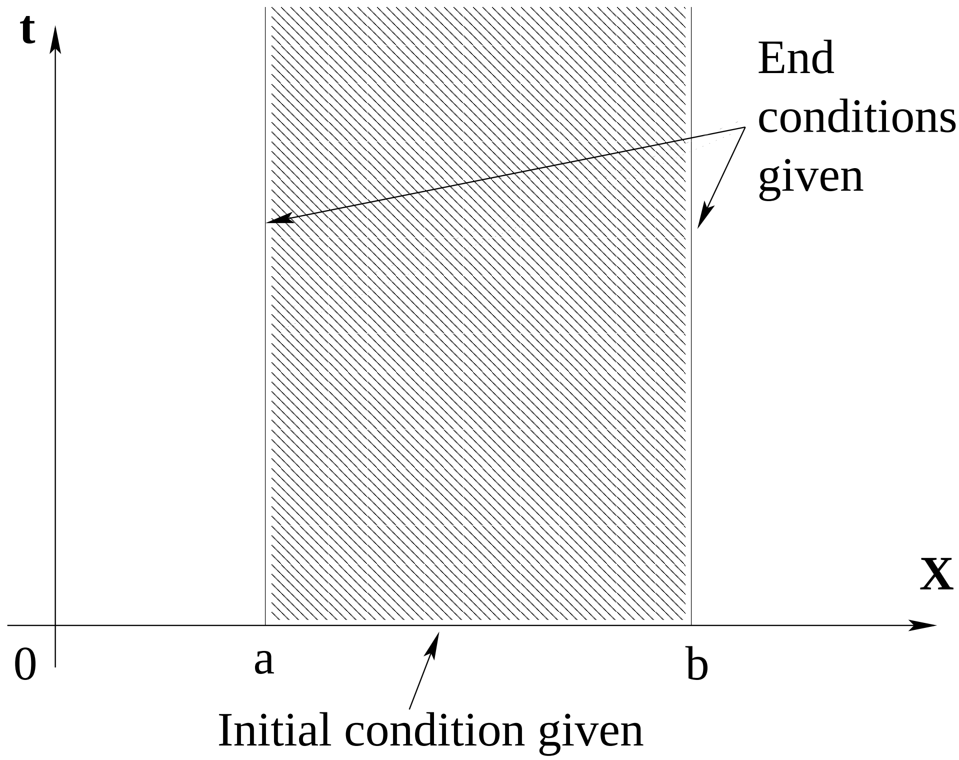


Figure 14:

21 Numerical Techniques

21.1 Setting the problem up

In practice, only very simple problems can be solved using the exact methods discussed above. For more realistic problems, it becomes necessary to use *numerical methods.* We develop these by reference to the basic parabolic problem:

$$\frac{\partial U}{\partial t} = D\,\frac{\partial^2 U}{\partial x^2} \tag{32}$$

where $D > 0$ is some constant - in heat conduction problems, it is *thermal diffusivity.* We require to solve (32) in the shaded region shown in figure 14. We shall approximate the equation by *finite difference* formulae defined over the shaded region, and shall obtain an *approximate* solution at a finite set of grid-points, indicated in figure 15 The grid-points are labelled (x_i, t_j) where

$$\begin{aligned} x_i &= a + ih, \;\; i = 0, 1, 2, ..., N+1, \;\; h = \frac{b-a}{N+1} \\ t_j &= jk, \;\; j = 0, 1, 2, ... \end{aligned}$$

Here, h is the spatial grid (or mesh) step, whilst k is the time-step. Note that, in this notation, $x_{N+1} = a + (N+1)h = b$.

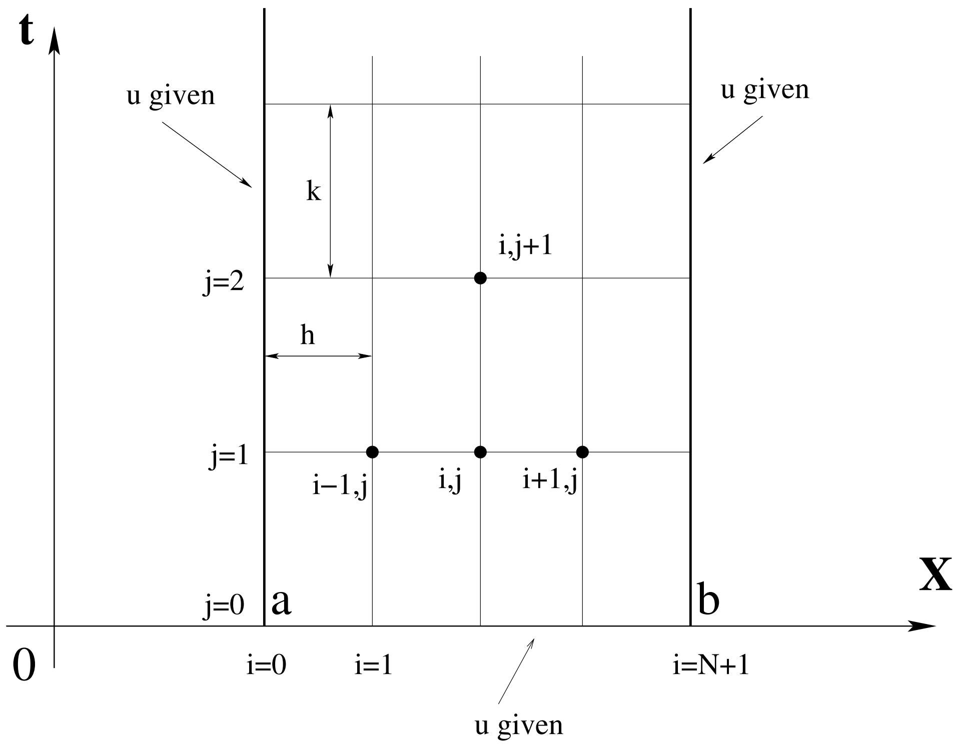


Figure 15:

Since u is given on $j = 0$ $(t = 0)$ (ie, the *initial condition)* and we are assuming that u is given on $x = a$ and $x = b$ (the *end conditions*), then we need to calculate $U_{i,j} \equiv U(x_i, t_j)$ for the spatial points $i = 1, 2, ..., N$ (also called the *internal* points) at $j = 1, 2, ...$ (the *time* steps). There are many ways of doing this, but first we must introduce the idea of the *finite difference approximation.*

21.2 Finite Difference (FD) Approximations

The basic formulae we use are the following Taylor series expansions of $F(x)$ about the point x:

$$F(x+h) = F(x) + hF'(x) + \frac{h^2}{2!}F''(x) + ... \tag{33}$$

$$F(x-h) = F(x) - hF'(x) + \frac{h^2}{2!}F''(x) - ... \tag{34}$$

Note that the second can be obtained from the first by replacing h by $-h$.

21.2.1 Finite Difference Approximations to $F'(x)$

From (33), we can say

$$F(x+h) - F(x) = hF'(x) + O(h^2)$$

where $O(h^2)$ indicates that the ignored term is approximately proportional to h^2. Hence, we get

$$F'(x) = \frac{F(x+h) - F(x)}{h} + O(h) \tag{35}$$

Or, we could use (34) to get

$$F'(x) = \frac{F(x) - F(x-h)}{h} + O(h) \tag{36}$$

Or, we could *subtract* (33) and (34) to get, after some algebra:

$$F'(x) = \frac{F(x+h) - F(x-h)}{2h} + O(h^2) \tag{37}$$

When we neglect the $O(h)$ errors, relations (35), (36) are called the *forward difference, backward difference* approximations to $F'(x)$respectively, whilst if we ignore the $O(h^2)$ error, relation (37) is called *central difference* approximation to $F'(x)$.

21.2.2 Finite Difference Approximations to $F''(x)$

If we *add* (33) and (34) we get

$$F(x+h) + F(x-h) = 2F(x) + h^2 F''(x) + O(h^4)$$

so that, after a bit of algebra,

$$F''(x) = \frac{F(x+h) - 2F(x) + F(x-h)}{h^2} + O(h^2) \tag{38}$$

Ignoring the $O(h^2)$ error gives a *central difference* approximation to $F''(x)$.

21.2.3 Summary of Finite Difference Formulae

The basic finite difference approximations we shall actually use are obtained from (35), (36) and (38) respectively:

$$\begin{aligned} F'(x) &\approx \frac{F(x+h) - F(x)}{h} \\ F'(x) &\approx \frac{F(x) - F(x-h)}{h} \\ F''(x) &\approx \frac{F(x+h) - 2F(x) + F(x-h)}{h^2} \end{aligned} \tag{39}$$

21.2.4 Generalization to funtions $U(x,t)$.

We illustrate by finding FD approximations for $\partial U/\partial t$: Using the notation of §21.1, we have $U_{ij} \equiv U(x_i, t_j)$ so that

$$U(x_i, t_j + k) = U(x_i, t_j) + k\frac{\partial}{\partial t}U(x_i, t_j) + \frac{k^2}{2!}\frac{\partial^2}{\partial t^2}U(x_i, t_j) + ...$$

$$
\begin{aligned}
&\downarrow \\
U_{i,j+1} &= U_{i,j} + k\left(\frac{\partial U}{\partial t}\right)_{ij} + \frac{k^2}{2!}\left(\frac{\partial^2 U}{\partial t^2}\right)_{ij} + \ldots \\
&\downarrow \\
\left(\frac{\partial U}{\partial t}\right)_{ij} &= \frac{U_{i,j+1} - U_{i,j}}{k} + O(k) \qquad (40)
\end{aligned}
$$

which we see is a direct generalization of the first formulae of (39). All the other formulae generalize in the same way.

21.3 Using the FD Approximations for a $U(x,t)$ problem

We are typically interested in solving PDEs like (32) so that we need approximations for $\partial U/\partial t$ and $\partial^2 U/\partial x^2$. Using the notation of (40), and generalizing the FD formulae of (39) we could have any of

$$
\begin{aligned}
\frac{\partial U}{\partial t} &\approx \frac{U_{i,j+1} - U_{i,j}}{k} \\
\frac{\partial U}{\partial t} &\approx \frac{U_{i,j} - U_{i,j-1}}{k} \\
\frac{\partial U}{\partial t} &\approx \frac{U_{i,j+1} - U_{i,j-1}}{2k}
\end{aligned}
$$

together with

$$
\frac{\partial^2 U}{\partial x^2} \approx \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2}.
$$

In practice, the central difference approximation for $\partial U/\partial t$ is never used - it leads to ***unstable*** schemes.

21.3.1 The Explicit Scheme for the Heat Conduction Equation

We wish to solve

$$
\frac{\partial U}{\partial t} = D\,\frac{\partial^2 U}{\partial x^2}
$$

subject to some initial and boundary conditions. The ***explicit scheme*** centered on the point (i,j) uses the ***forward*** difference approximation for $\partial U/\partial t$ and the standard scheme for $\partial^2 U/\partial x^2$ to get

$$
\frac{U_{ij+1} - U_{ij}}{k} = D\,\frac{U_{i+1j} - 2U_{ij} + U_{i-1j}}{h^2}
$$

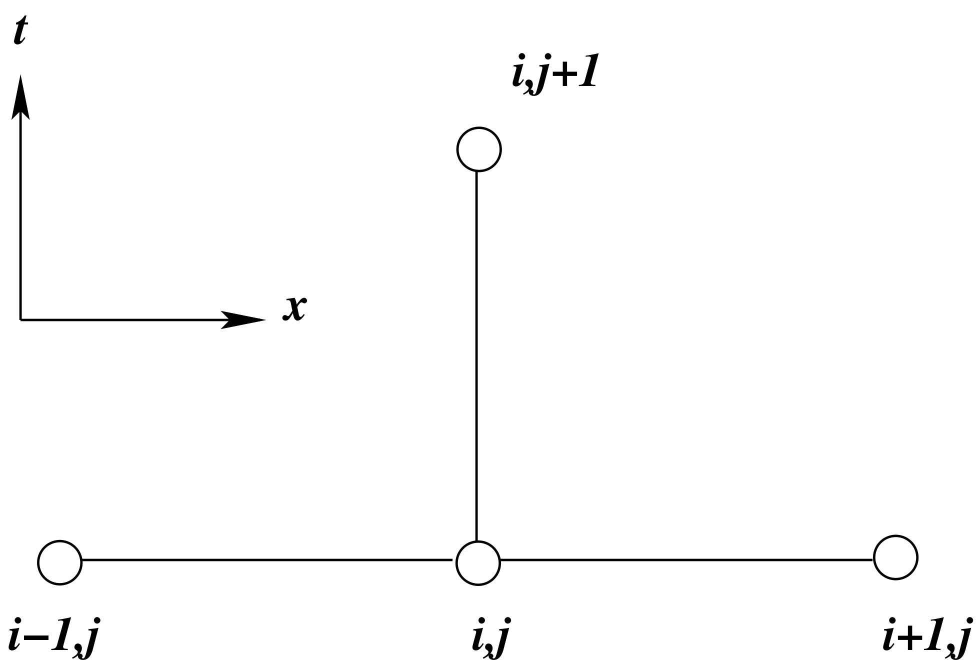


Figure 16:

Writing $r = D\,k/h^2$ in this, and rearranging, gives

$$\begin{aligned} U_{ij+1} &= U_{ij} + r(U_{i+1j} - 2U_{ij} + U_{i-1j})\,, \quad i = 1...N,\ j = 0, 1, ... \\ &\downarrow \\ U_{ij+1} &= rU_{i+1j} + (1-2r)U_{ij} + rU_{i-1j}\,, \quad i = 1...N,\ j = 0, 1, ... \end{aligned}$$

which is the required ***explicit scheme.*** It is conveniently represented using the ***finite difference molecule,*** shown in 16. The molecule show that the solution at node $(i, j+1)$ is given purely in terms of the solution at the nodes $(i-1, j)$, (i, j), $(i+1, j)$. If we consider the case $j = 0$, the formula becomes

$$U_{i,1} = rU_{i+1,0} + (1-2r)U_{i,0} + rU_{i-1,0}\,, i = 1...N$$

- We now see that the solution at $t = t_1$ is given purely in terms of the solution at $t = 0$ - which is the known ***initial condition;***
- In general, this formula gives the solution at $t = t_j$ purely in terms of the solution at the previous time, $t = t_{j-1}$, which will ***always*** be known;
- We can now see why the scheme is called the ***explicit scheme.***

Example 1

The exact solution of

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} \quad \text{given} \quad U(x,0) = \begin{cases} 2x & 0 \le x \le 1/2 \\ 2(1-x) & 1/2 \le x \le 1 \end{cases}$$

$$\text{with} \qquad U(0,t) = U(1,t) = 0$$

is given by:

$$u(x,t) = \frac{8}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\sin\left(\frac{n\pi}{2}\right)\sin\left(n\pi x\right)\mathrm{e}^{-n^2\pi^2 t}$$

Investigate the numerical solution arising from the explicit method for the following three cases:

- **Case 1:** $h = 0.1, \;\; k = 0.001$ so that $r = 0.1$;
- **Case 2:** $h = 0.1, \;\; k = 0.005$ so that $r = 0.5$;
- **Case 3:** $h = 0.1, \;\; k = 0.01$ so that $r = 1$.

Case 1:			$h = 0.1$	$k = 0.001$	$r = 0.1$		
		$m = 0$	1	2	3	4	5
		$x = 0$	0.1	0.2	0.3	0.4	0.5
$n = 0$	$t = 0.000$	0	0.2000	0.4000	0.6000	0.8000	1.0000
$n = 1$	$t = 0.001$	0	0.2000	0.4000	0.6000	0.8000	0.9600
$n = 2$	$t = 0.002$	0	0.2000	0.4000	0.6000	0.7960	0.9280
$n = 3$	$t = 0.003$	0	0.2000	0.4000	0.5996	0.7896	0.9016
$n = 4$	$t = 0.004$	0	0.2000	0.4000	0.5986	0.7818	0.8792
$n = 5$	$t = 0.005$	0	0.2000	0.3999	0.5971	0.7732	0.8597
...	...	...	...	...	...	...	...
$n = 10$	$t = 0.010$	0	0.1996	0.3968	0.5822	0.7281	0.7867
$n = 20$	$t = 0.020$	0	0.1938	0.3781	0.5373	0.6486	0.6891

Case 1:		FD soln	Exact Soln		
		$x = 0.3$	$x = 0.3$	Difference	% error
$n = 5$	$t = 0.005$	0.5971	0.5966	0.0005	0.08
$n = 10$	$t = 0.010$	0.5822	0.5799	0.0023	0.40
$n = 20$	$t = 0.020$	0.5373	0.5334	0.0039	0.70
$n = 100$	$t = 0.100$	0.2472	0.2444	0.0028	1.10

Case 2:			$h = 0.1$	$k = 0.005$	$r = 0.5$		
		$m = 0$	1	2	3	4	5
		$x = 0$	0.1	0.2	0.3	0.4	0.5
$n = 0$	$t = 0.000$	0	0.2000	0.4000	0.6000	0.8000	1.0000
$n = 1$	$t = 0.005$	0	0.2000	0.4000	0.6000	0.8000	0.8000
$n = 2$	$t = 0.010$	0	0.2000	0.4000	0.6000	0.7000	0.8000
$n = 3$	$t = 0.015$	0	0.2000	0.4000	0.5500	0.7000	0.7000
$n = 4$	$t = 0.020$	0	0.2000	0.3750	0.5500	0.6250	0.7000
...	...	...	...	...	...	...	...
$n = 20$	$t = 0.100$	0	0.0949	0.1717	0.2484	0.2778	0.3071

Case 2:		FD soln	Exact Soln		
		$x = 0.3$	$x = 0.3$	Difference	% error
$n = 1$	$t = 0.005$	0.6000	0.5966	0.0034	0.57
$n = 2$	$t = 0.010$	0.6000	0.5799	0.0201	3.50
$n = 4$	$t = 0.020$	0.5500	0.5334	0.0166	3.10
$n = 20$	$t = 0.100$	0.2484	0.2444	0.0040	1.60

Case 3:			$h = 0.1$	$k = 0.010$	$r = 1.0$		
		$m = 0$	1	2	3	4	5
		$x = 0$	0.1	0.2	0.3	0.4	0.5
$n = 0$	$t = 0.00$	0	0.2	0.4	0.6	0.8	1.0
$n = 1$	$t = 0.01$	0	0.2	0.4	0.6	0.8	0.6
$n = 2$	$t = 0.02$	0	0.2	0.4	0.6	0.4	1.0
$n = 3$	$t = 0.03$	0	0.2	0.4	0.2	1.2	-0.2
$n = 4$	$t = 0.04$	0	0.2	0.0	1.4	-1.2	2.6

We see that the **case 3** calculation becomes ***unstable!!***

21.4 The Treatment of Derivative Boundary Conditions

We now consider problems of the type: Solve

$$\frac{\partial U}{\partial t} = D\,\frac{\partial^2 U}{\partial x^2}$$

subject to the ***initial condition***

$$U(x,0) = f(x),\ \ 0 \le x \le 1$$

together with the ***boundary conditions***

$$\begin{aligned} U(0,t) &= C_0 \ \ \text{(a given value)} \\ \left.\frac{\partial U}{\partial x}\right|_{x=1} &= C_1 \ \ \text{(a given value)} \end{aligned}$$

The new thing here is the ***derivative condition*** at $x = 1$.

Method

As before, the spatial range $0 \le x \le 1$ is divided into $N+1$ intervals each of length $h = 1/(N+1)$, and the temporal range $0 \le t < \infty$ is made discrete with time-step $\Delta t = k$. Thus, we compute solutions at (x_i, t_j) where $i = 1..N+1$ and $j = 0, 1, 2, ...$

We shall illustrate the method using the ***explicit scheme:***

$$U_{ij+1} = rU_{i+1j} + (1-2r)U_{ij} + rU_{i-1j}\,, \quad i = 1...N,\ \ j = 0, 1, .. \tag{41}$$

where we remember that $U_{0j} \equiv U(0,t)$ and $U_{N+1j} \equiv U(1,t)$.

- We know $U_{00}, U_{10}, U_{20}, ..., U_{N+1,0}$
- the eqn can be used to get U_{i1} for $i = 1..N$
- we cannot use it to calculate $U_{N+1,1}$
- set $j = 1$ and, since we do not know $U_{N+1,1}$ then we cannot calculate $U_{N,2}$ etc
- There is a problem at the $x = 1$ boundary - we ***need*** to calculate $U_{N+1,j}$ somehow.

But, we do know that

$$\left.\frac{\partial U}{\partial x}\right|_{x=1} = C_1 \to \frac{U_{N+2j} - U_{N,j}}{2h} = C_1 \tag{42}$$

However, this introduces the unknown value $U_{N+2,j} \equiv U(1+h,t)$ which is ***outside*** the spatial domain on which the problem is defined. See figure 17, in which $(N+2, j)$ has been labelled as a ***fictitious point !*** We need more information ... this is provided by applying (41) on the boundary $x = 1 \equiv i = N+1$:

$$U_{N+1j+1} = rU_{N+2j} + (1-2r)U_{N+1j} + rU_{Nj} \tag{43}$$

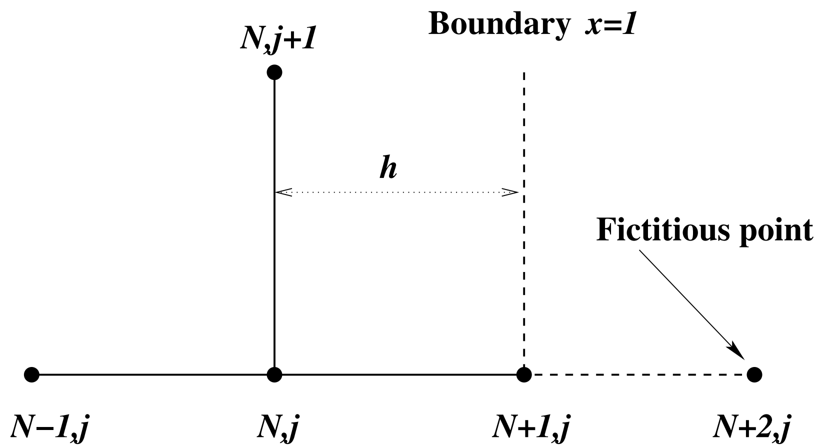


Figure 17:

Comparing (42) and (43) we see that the fictitious value U_{N+2j} can be elimated between them: that is, from (42) we have

$$U_{N+2j} = 2hC_1 + U_{Nj}$$

so that (43) becomes

$$U_{N+1j+1} = r(2hC_1 + U_{Nj}) + (1-2r)U_{N+1j} + rU_{Nj}$$

$$\downarrow$$

$$U_{N+1j+1} = 2rU_{Nj} + (1-2r)U_{N+1j} + 2rhC_1 \ , j = 0, 1, ... \qquad (44)$$

Since we know everything on the intitial $j = 0$ line for $i = 0, 1, ..., N+1$, this last formula allows us to calculate $U(1,t) \equiv U_{N+1j}$.

Example 2

Use $h = 0.2$, and $k = 0.03$ to find an approximate solution of

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} \quad \text{given} \quad U(x,0) = 1-(x-1)^2 \ \ 0 \le x \le 1$$

$$\text{with} \qquad U(0,t) = 0, \ \left.\frac{\partial U}{\partial x}\right|_{x=1} = 0$$

at $t = 0.03$ over $0 \le x \le 1$.

Solution

Since $h = 0.2$, then $0 \le x \le 1 \to i = 0..5$. Now use $r = k/h^2 = 0.03/0.04 = 0.75$ so that explicit scheme (41) for $j = 0$ becomes

$$U_{i1} = rU_{i+1,0} + (1-2r)U_{i0} + rU_{i-1,0} \ , i = 1..4 \ \ \text{(the internal points)}$$

$$\downarrow$$

$$U_{i1} = 0.75U_{i+1,0} - 0.5U_{i0} + 0.75U_{i-1,0} \ \ i = 1, 2, 3, 4$$

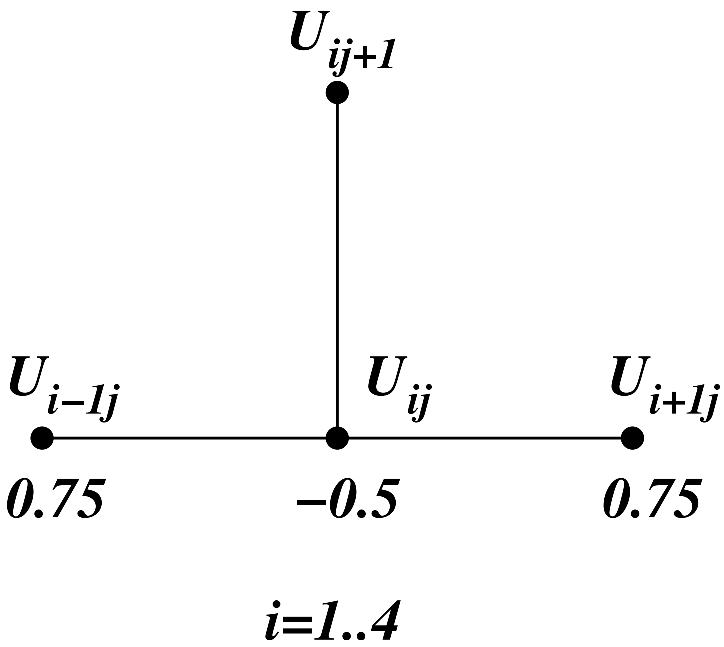


Figure 18:

and (44) becomes

$$U_{N+1j+1} = 2rU_{Nj} + (1-2r)U_{N+1j} + 2rhC_1$$

$$\downarrow$$

$$U_{5,1} = 1.5U_{4,0} - 0.5U_{5,0}$$

Hence, we get the finite-difference molecules of figures 18 and 19. Hence, finally, we get the results of the table

$U(t=0.03)$	0.0	0.30	0.58	0.78	0.90	0.94
$U(t=0.00)$	0.0	0.36	0.64	0.84	0.96	1.00
i	0	1	2	3	4	5
x	0.0	0.2	0.4	0.6	0.8	1.0

AMA252 Lecture 8: PDEs 2

22 Laplace's Equation

Laplace's equation, given by

$$\nabla^2\Phi \equiv \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + \frac{\partial^2\Phi}{\partial z^2} = 0$$

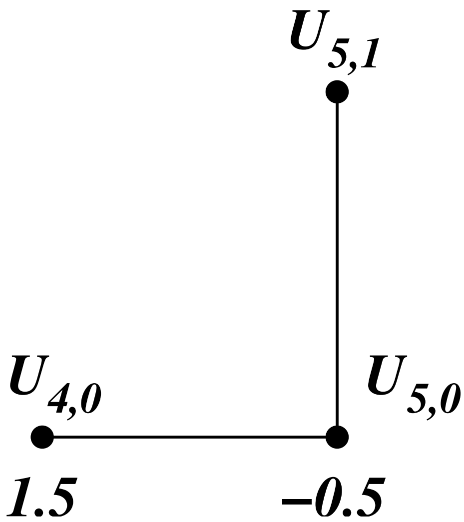


Figure 19:

in its three-dimensional form, and by

$$\nabla^2 \Phi \equiv \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = 0 \tag{45}$$

in its two-dimensional form, is the architypical ***elliptic partial differential equation.*** In all cases, information must be given on ***completely closed*** boundaries. It is of fundamental importance in physics and engineering. It usually arises in the context of ***steady-state*** problems to be solved over some ***finite spatial domain***. Two specific applications are

- Modelling the ***steady state*** temperature distribution a three dimensional object.
- Modelling ***steady state*** ground water flows in a porous medium.

Usually it is necessary to use numerical techniques to obtain solutions for practical problems but, sometimes, analytical solutions are possible.

Example 1

Write down a general solution of (45) over some finite region in the (x, y) plane. The ***separation of variables*** technique does the job: Assume $\Phi(x, y) = X(x)Y(y)$ so that the pde gives

$$X''Y + XY'' = 0$$

$$\downarrow$$

$$\frac{X''}{X} = -\frac{Y''}{Y} = \alpha$$

where α is an arbitrary constant. - ***NOTE α can be zero, real, imaginary or complex!*** From these we get

$$X'' - \alpha X = 0 \tag{46}$$

$$Y'' + \alpha Y = 0 \tag{47}$$

In the ***heat conduction*** eqn case, we knew that the parameter was negative for all dissipation problems - because as $t \to \infty$, we knew the soln had to remain finite. Here, the solution is to be found over a finite region in the (x, y) space - therefore, we do not have any restrictions of this kind on α - it can be positive, zero or negative according to circumstances.

Case $\alpha = 0$

The equations become $X'' = 0,\ Y'' = 0$ so that $X(x) = Ax + B$ and $Y(y) = Cy + D$. Thus, for this case, the solution is

$$\Phi(x, y) = X(x)Y(y) = (Ax + B)(Cy + D).$$

Case $\alpha \neq 0$

We can easily show that the two equations now have the general solutions

$$\begin{aligned} X(x) &= A\mathrm{e}^{\sqrt{\alpha}x} + B\mathrm{e}^{-\sqrt{\alpha}x} \\ Y(y) &= C\mathrm{e}^{j\sqrt{\alpha}y} + D\mathrm{e}^{-j\sqrt{\alpha}y} \end{aligned}$$

Student: Check this! Note that if α is ***positive***, then $X(x)$ has ***exponential*** behaviour and $Y(y)$ has ***sinusoidal*** behaviour, whilst if α is ***negative***, it is the other way around. Putting these together, we get

$$\Phi(x, y) = X(x)Y(y) = (A\mathrm{e}^{\sqrt{\alpha}x} + B\mathrm{e}^{-\sqrt{\alpha}x})(C\mathrm{e}^{j\sqrt{\alpha}y} + D\mathrm{e}^{-j\sqrt{\alpha}y})$$

for any α!

The General Solution

The general solution is just the sum of ***all possible*** combinations of these solutions. Thus, it can be expressed ***symbolically*** as

$$\Phi(x, y) = (ax + b)(cy + d) + \sum_{\alpha}(A\mathrm{e}^{\sqrt{\alpha}x} + B\mathrm{e}^{-\sqrt{\alpha}x})(C\mathrm{e}^{j\sqrt{\alpha}y} + D\mathrm{e}^{-j\sqrt{\alpha}y})$$

When we consider particular examples, we find that the possible values of α are constrained by the ***boundary conditions.*** The following example makes the discussion a bit more concrete!

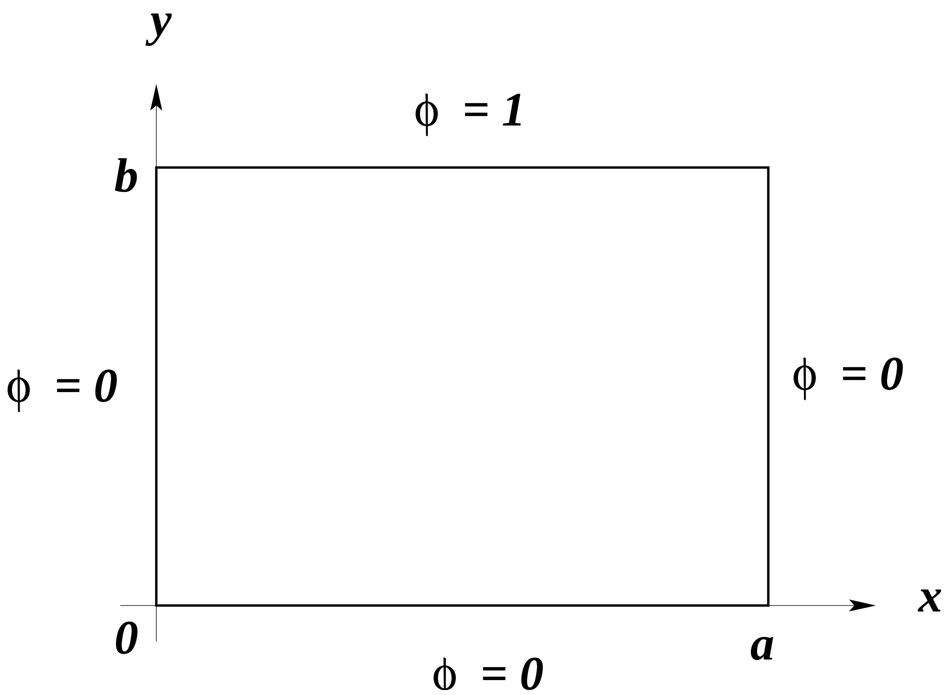


Figure 20:

Example 2

The following example requires $\alpha \leq 0$ always! Solve the equation

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = 0 \tag{48}$$

over the region shown in figure 20 with the indicated boundary conditions.

Solution

The simplicity of the geometry and the boundary conditions means that we can solve this problem exactly. Let $\Phi(x, y) = X(x)\, Y(y)$. Hence (48) becomes

$$X''Y + X\,Y'' = 0$$

$$\downarrow$$

$$\frac{X''}{X} = -\frac{Y''}{Y} = \alpha$$

from which we get

$$X'' - \alpha X = 0 \tag{49}$$

$$Y'' + \alpha Y = 0 \tag{50}$$

The Boundary Conditions

- Since $\Phi(0, y) \equiv X(0)Y(y) = 0$ then we ***must*** have $X(0) = 0$;
- Since $\Phi(a, y) \equiv X(a)Y(y) = 0$ then we ***must*** have $X(a) = 0$;
- Since $\Phi(x, 0) \equiv X(x)Y(0) = 0$ then we ***must*** have $Y(0) = 0$;
- The remaining condition is $\Phi(x, b) \equiv X(x)Y(b) = 1$. All we can say about this at the moment is that we must have $X(x) = const$.

Thus, for now, we can only be definite about (49) since we have the conditions $X(0) = 0,\ X(a) = 0$. We have three cases to consider: $\alpha > 0,\ \alpha = 0,\ \alpha < 0$.

Case $\alpha > 0$ **Eqn (49)**

Put $\alpha \equiv p^2$ so that (49) becomes

$$X'' - p^2 X = 0.$$

This has solution

$$X(x) = A\,\mathrm{e}^{px} + B\,\mathrm{e}^{-px} \tag{51}$$

Since $X(0) = X(a) = 0$ then we get

$$\begin{aligned} A + B &= 0 \\ A\,\mathrm{e}^{pa} + B\,\mathrm{e}^{-pa} &= 0 \end{aligned}$$

Thus, $A = B = 0$. Hence, we ***reject*** solution (51).

Case $\alpha = 0$ **Eqn (49)**

Put $\alpha = 0$ so that (49) becomes

$$X'' = 0.$$

This has solution

$$X(x) = A\,x + B \tag{52}$$

Since $X(0) = X(a) = 0$ then we get $A = B = 0$ directly.. Hence, we ***reject*** solution (52).

Case $\alpha < 0$ **Eqn (49)**

Put $\alpha \equiv -s^2$ so that (49) becomes

$$X'' + s^2 X = 0.$$

This has solution

$$X(x) = A\,\cos sx + B\,\sin sx \tag{53}$$

Since $X(0) = 0,\ X(a) = 0$ then we get

$$\begin{aligned} A &= 0 \\ B\,\sin sa &= 0 \end{aligned}$$

respectively. From the second of these, ***either*** $B = 0$ ***or*** $sa = m\pi,\ m = 1, 2, ...$. Choosing $B = 0$ would mean that $X(x) = 0$ always - no good. Hence we choose $sa = m\pi,\ m = 1, 2, ...$ so that, remembering $A = 0$, we get:

$$X(x) = B\ \sin\frac{m\pi x}{a}\,, \quad m = 1, 2, ...$$

Now we consider (50): Since the cases $\alpha = 0,\ \alpha > 0$ have been rejected, we need only consider:

Case $\alpha < 0$ Eqn (50)

Equation (50) becomes

$$Y'' - s^2 Y = 0$$

where we know that $s = m\pi/a$. The solution is

$$\begin{aligned} Y(y) &= C_0\, e^{sy} + D_0\, e^{-sy} \\ &\downarrow \\ Y(y) &= C\ \cosh\frac{m\pi y}{a} + D\ \sinh\frac{m\pi y}{a} \end{aligned}$$

Note: it is more convenient (but not necessary) to work with $\cosh$ ***and*** $\sinh$ ***here.*** The boundary condition $Y(0) = 0$ gives directly that $C = 0$. Hence $Y(y) = D\ \sinh m\pi y/a$. The solution so far can therefore be written as

$$\Phi(x, y) = X(x)Y(y) \equiv BD\ \sin\frac{m\pi x}{a}\ \sinh\frac{m\pi y}{a}\,, \ \ m = 1, 2, ...$$

These solutions satisfy Laplace's eqn ***and*** the ***zero*** boundary conditions for ***any*** value of $m = 1, 2, ...$ Hence, any linear combination of these solutions does the same ... we can therefore say the most general solution so far is given by

$$\Phi(x, y) = \sum_{m=1}^{\infty} B_m\ \sin\frac{m\pi x}{a}\ \sinh\frac{m\pi y}{a}$$

where the B_m are constants to be determined. They are used to fix the boundary condition $\Phi(x, b) = 1$:

$$\begin{aligned} \Phi(x, b) &= 1 = \sum_{m=1}^{\infty} B_m\ \sin\frac{m\pi x}{a}\ \sinh\frac{m\pi b}{a} \\ &\downarrow \\ 1 &= \sum_{m=1}^{\infty} C_m\ \sin\frac{m\pi x}{a} \qquad \text{where} \ \ C_m \equiv B_m \sinh\frac{m\pi b}{a} \end{aligned}$$

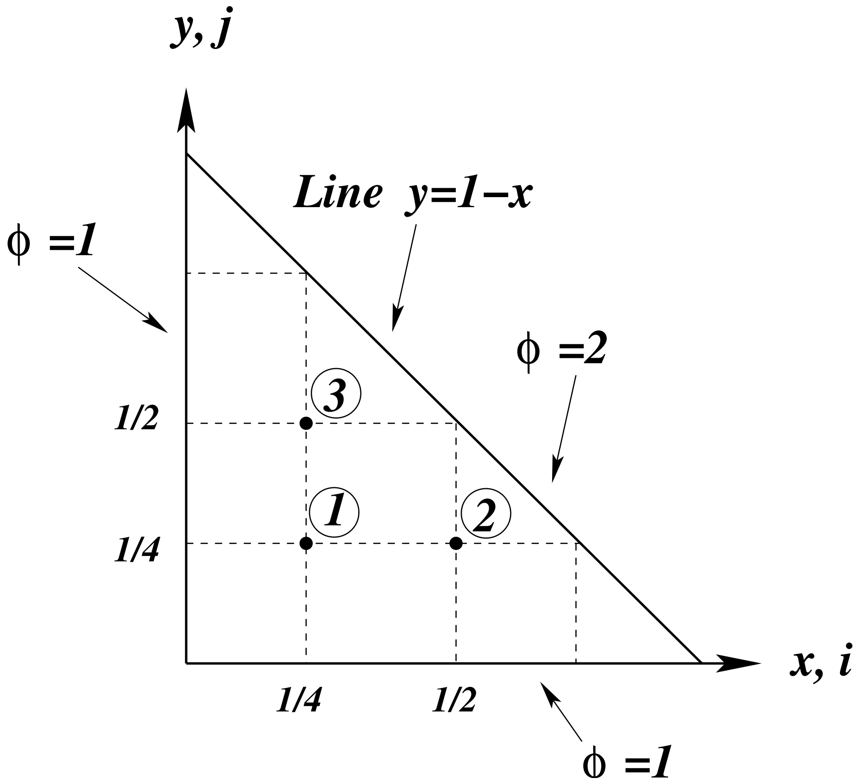


Figure 21:

The coefficients C_m can now be determined by a standard Fourier Sine-series analysis on the range $0 \leq x \leq a$:

$$
\begin{aligned}
C_m &= \frac{2}{a}\int_0^a (1)\sin\frac{m\pi}{a}\,dx = \ldots = \frac{2\{1+(-1)^{m+1}\}}{m\pi} \\
&\downarrow \\
B_m &= \frac{2\{1+(-1)^{m+1}\}}{m\pi\sinh m\pi b/a}
\end{aligned}
$$

Hence, the final complete solution to the original boundary value problem is given by

$$
\Phi(x,y) = \sum_{m=1}^{\infty} \frac{2\{1+(-1)^{m+1}\}}{m\pi\sinh m\pi b/a}\,\sin\frac{m\pi x}{a}\,\sinh\frac{m\pi y}{b}
$$

23 Numerical Methods: Finite Differences

We illustrate using a very simple example: Solve

$$
\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = -16 \tag{54}
$$

in the triangular region shown in figure 21, which has a square grid with $h = 1/4$. The values of Φ on the boundary are indicated in the figure.

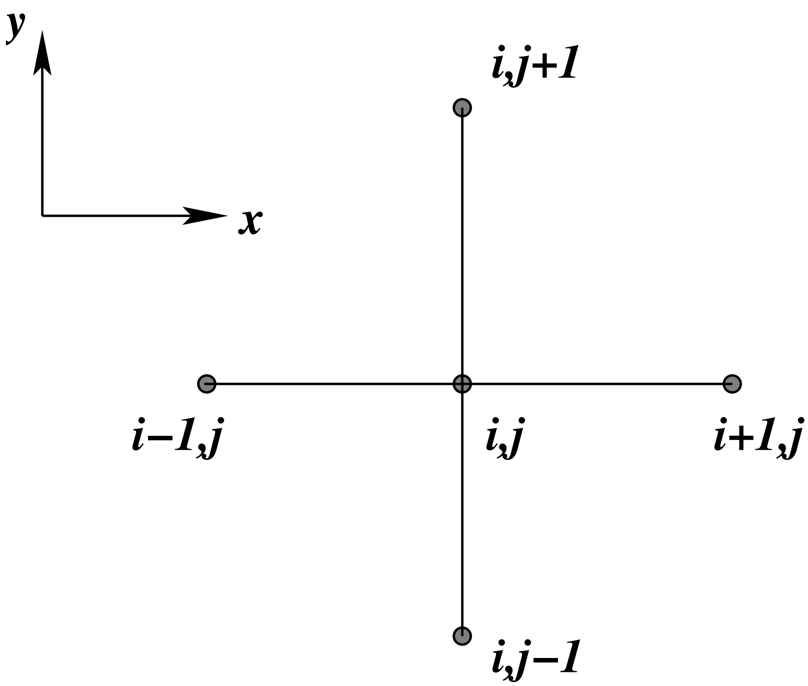


Figure 22:

Method

We use the approximations

$$\frac{\partial^2 \Phi}{\partial x^2} \approx \frac{\Phi_{i+1,j} - 2\Phi_{ij} + \Phi_{i-1,j}}{h^2}$$

$$\frac{\partial^2 \Phi}{\partial y^2} \approx \frac{\Phi_{i,j+1} - 2\Phi_{ij} + \Phi_{i,j-1}}{h^2}$$

in (54) so that, after slight rearrangement, we get:

$$\Phi_{i-1,j} + \Phi_{i+1,j} + \Phi_{i,j-1} + \Phi_{i,j+1} - 4\Phi_{ij} = -16\, h^2 \tag{55}$$

This is known as a ***five-point*** formula, and has a finite difference molecule show in figure 22 Since Φ is given everywhere on the boundary, we need to solve the pde ***within*** the boundary - that is, using the numbering indicated in figure 21, we need to calculate Φ_1, Φ_2 and Φ_3:

$$\text{At point1 :} \qquad 1 + \Phi_2 + 1 + \Phi_3 - 4\Phi_1 = -1$$

$$\text{At point 2 :} \qquad \Phi_1 + 2 + 1 + 2 - 4\Phi_2 = -1$$

$$\text{At point 3 :} \qquad 1 + 2 + \Phi_1 + 2 - 4\Phi_3 = -1$$

or, in matrix form

$$\begin{pmatrix} -4 & 1 & 1 \\ 1 & -4 & 0 \\ 1 & 0 & -4 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix} = \begin{pmatrix} -1-2 \\ -1-5 \\ -1-5 \end{pmatrix} = - \begin{pmatrix} 3 \\ 6 \\ 6 \end{pmatrix}$$

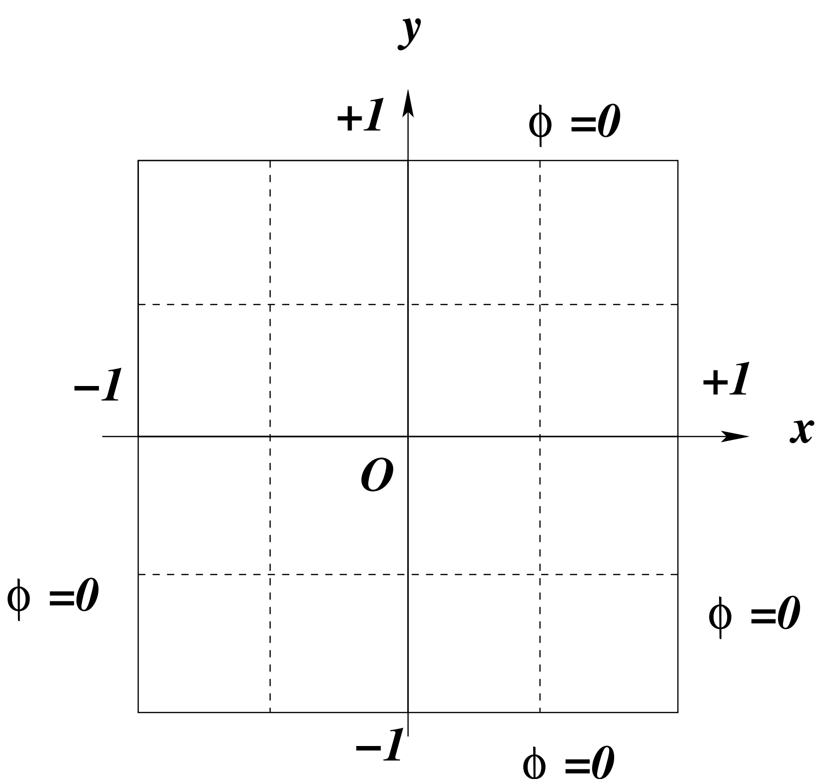


Figure 23:

This is a linear system of the form $A\mathbf{\Phi} = \mathbf{b}$ which can be solved to give

$$\begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{pmatrix} = \begin{pmatrix} 12/7 \\ 27/14 \\ 27/14 \end{pmatrix}$$

Notice that there is symmetry in ***this particular problem*** about the line $y = x$ ... thus, we could have deduced that $\Phi_3 = \Phi_2$ at the outset, and hence we could have solved a smaller problem. With $\Phi_3 = \Phi_2$, we see that, in fact, the third equation is ***redundant*** so that we need only have solved the 2×2 problem

$$\begin{pmatrix} -4 & 2 \\ 1 & -4 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = -\begin{pmatrix} 3 \\ 6 \end{pmatrix} \rightarrow \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \begin{pmatrix} 12/7 \\ 27/14 \end{pmatrix}$$

etc.

Example 2

Solve

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = -2 \tag{56}$$

in the region shown in figure 23.

Solution

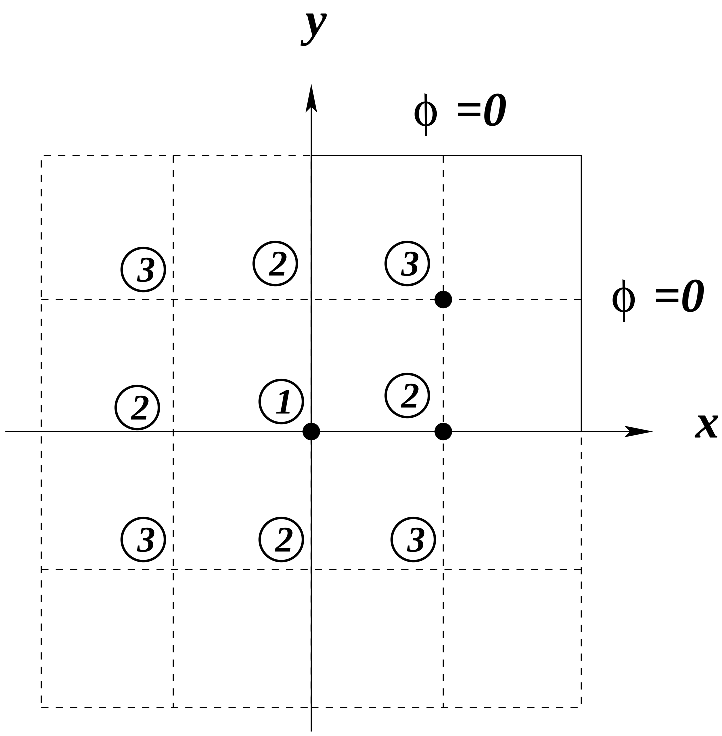


Figure 24:

We firstly note the symmetries of this problem:

- There is symmetry about Oy;
- There is symmetry about Ox
- There is symmetry about $y = x$ and $y = -x$

Using these, we see that it is only necessary to solve at points $1, 2, 3$ marked by solid circles in the bold-box of figure 24 . From the figure, we see that $h = 0.5$ so that the equation (56) can be approximated as:

$$\Phi_{i-1,j} + \Phi_{i+1,j} + \Phi_{i,j-1} + \Phi_{i,j+1} - 4\Phi_{ij} = -2\,h^2 = -\frac{1}{2}$$

Applying this at points $1, 2$ and 3, we get:

$$\text{Point 1} \qquad \Phi_2 + \Phi_2 + \Phi_2 + \Phi_2 - 4\Phi_1 = -\frac{1}{2}$$

$$\text{Point 2} \qquad \Phi_1 + 0 + \Phi_3 + \Phi_3 - 4\Phi_2 = -\frac{1}{2}$$

$$\text{Point 3} \qquad \Phi_2 + 0 + \Phi_2 + 0 - 4\Phi_3 = -\frac{1}{2}$$

Example 3

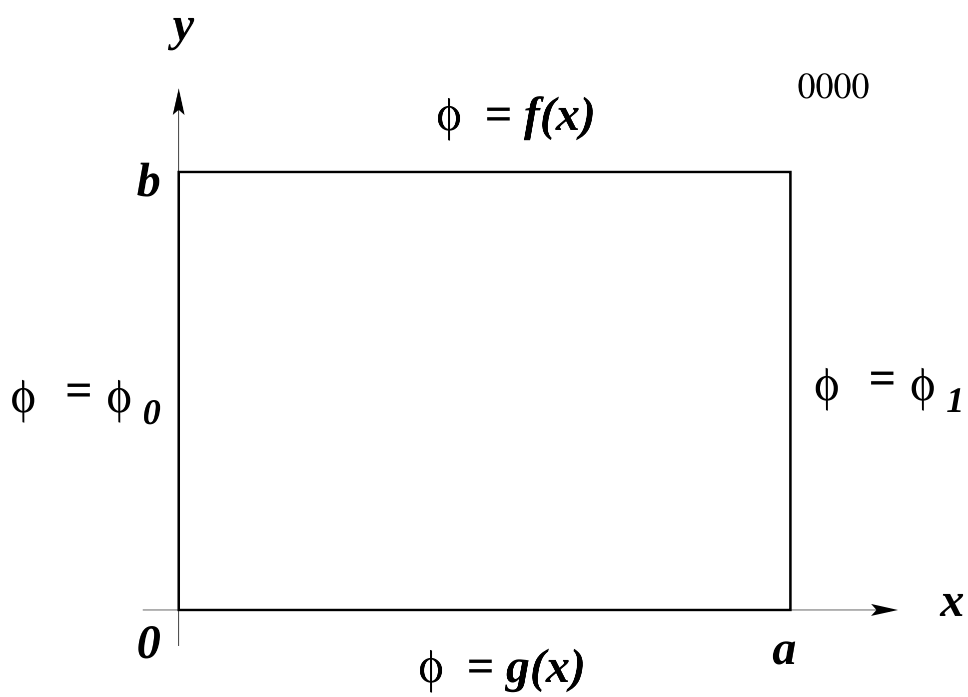


Figure 25:

Solve

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = 0 \tag{57}$$

over the region shown in figure 25 with the indicated boundary conditions.

Solution

Seperation of variables: Put $\Phi = X(x)\,Y(y)$ so that (57) becomes

$$\begin{aligned} X'' - \alpha X &= 0 \\ Y'' + \alpha Y &= 0 \end{aligned}$$

For the case $\alpha = 0$ we get

$$X'' = 0\,, \quad Y'' = 0$$

$$X = Ax + B, \qquad Y = Cy + D$$

for arbitrary constants A, B, C, D. Thus, solution has the form

$$\Phi(x,y) = (Ax + B)(Cy + D) \tag{58}$$

Now use the boundary condition on $x = 0$: Here, we have $\Phi = \Phi_0$ so that $\Phi_0 = B(Cy + D)$ for all y. Hence, we *must* have $C = 0$ and $BD = \Phi_0$. Hence, (58) becomes

$$\Phi(x,y) = ADx + BD = Ex + \Phi_0$$

for arbitrary constant E.
Now use the boundary condition on $x = 1$: Here, we have $\Phi = \Phi_1$ so that the above gives $\Phi_1 = Ea + \Phi_0$. Thus, $E = (\Phi_1 - \Phi_0)/a$ so that the solution so far can be written as

$$\Phi(x, y) = \Phi_0 + \frac{\Phi_1 - \Phi_0}{a} x \tag{59}$$

This solution satisfies the pde (57) and the boundary conditions on $x = 0$ and $x = a$. It ***does not*** satisfy the boundary conditions on $y = 0$ and $y = b$. Thus, the solution is not yet complete.