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Preliminary Notions

1.1 Introduction

Mathematica[1] is the brainchild of Stephen Wolfram, born in London in 1959 and educated at Eton, Oxford, and Caltech. He has a PhD in Theoretical Physics from Caltech. He was the youngest recipient of the MacArthur Prize Fellowship. His early works were on particle physics and cosmology. His significant contribution is in the field of cellular automata. He was a professor of physics, mathematics, and computer science at the University of Illinois, where he launched Wolfram Research Inc. and started developing **Mathematica**. He has been the president and CEO of Wolfram Research since its inception. Wolfram Research is one of the world's renowned computer, web, and cloud software companies – as well as a powerhouse of scientific and technical innovation. As a pioneer in computation and computational knowledge, the Wolfram Foundation has pursued a long-term vision to develop the science, technology, and tools to make computation an ever-more-potent force in today's world.

　Mathematica is a very powerful tool for performing high-level mathematical computing. The way to acquaint yourself with **Mathematica** is to play with various operators until their proper usage is understood. **Mathematica** does both symbolic and numerical computing, which is the basis of its real power. It has over three million users around the globe and hundreds of books have already been written on it. There are also several periodicals which are devoted exclusively to **Mathematica**. The Wolfram Research Foundation's **Mathematica** website contains thousands of pages of material, which is constantly updated. The Wolfram Language is the programming language used in **Mathematica**.

1.2 Versions of Mathematica

The first version of **Mathematica** was realized on 23 June 1988. Since then, several versions of **Mathematica** have been developed. The version 12.2 was released

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in December 2020 and expands **Mathematica**'s functionality in biomolecular sequence operations, partial differential equations (PDE) modeling, spatial statistics, and remote batch job evaluation with new notebook interface features and more, by adding 228 new functions. The newer versions[2] of **Mathematica** fully support the earlier versions. Information on this can be obtained from the website www.wolfram.com.

1.3 Getting Started

Mathematica can be run both on WINDOWS or UNIX platforms. It virtually supports almost every computer platform. When you double click on the **Mathematica** icon after installation on your computer, you will briefly see the **Mathematica** logo and then a Mathematica desktop window will appear. **Mathematica** starts with a blank notebook. Type the required operation and then press Shift + Enter (hold down the Shift key and press Enter) to tell the Wolfram Language to evaluate your input. One can also execute the operation by clicking Evaluate Notebook in the Evaluation menu. After performing the required operations, save and exit which are shown in the File menu.

1.4 Simple Calculations

1.4.1 Arithmetic Operations

Once you have opened a blank notebook, you can do some simple calculations as you would do on a pocket calculator. It is important to note that, if your input is an integer, the output of **Mathematica** is also an integer. On the other hand, if the input has an explicit decimal point, then the output will always have a decimal point. Let us look at a few examples.

Example 1.1
Find the sum of 355 and 422.
In the blank notebook type:

In[1] := 355 + 422
Out[1] = 777

The output of **Mathematica** is the solution.

The following standard symbols are used in **Mathematica** to do arithmetic operations (Table 1.1).

It is possible in **Mathematica** to insert comments in the notebook. We are introducing this feature at an early stage as we will be generating all the **Mathematica** outputs with comments in the notebook itself. You can add text at any point in your code simply by enclosing it in parenthesis (*text*).

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2 **Mathematica** 13.0 was released on December 2021, and **Mathematica** 13.1 was released on June 2022 and Mathematica 13.2 was released in December 2022 during the last phase of the development of this book.

Table 1.1 Standard symbols are used in Mathematica to do arithmetic operations.

Standard symbol	Operation
+	Addition
-	Subtraction
* or Space	Multiplication
/	Division
^	Exponentiation

Example 1.2

In[2] := 14.5/12.4 (* Division *)
Out[2] = 1.16935

   Note that whatever is inserted with the (*text*) is for our reference only and it will not be executed.

1.4.2   Approximate Numerical Results

It is possible to obtain the numerical result by ending your input with **//N**, where **N** stands for numerical. The expression **//N** gives an approximate numerical value of the output. We illustrate this with an example.

Example 1.3
Find the numerical value of $\frac{1}{3} + \frac{2}{7} + \frac{9}{12}$

Solution

In[3] := 1/3 + 2/7 + 9/12//N
Out[3] = 1.36905

1.4.3   Algebraic Calculations

It is possible to do both symbolic (symbolic means that computation is done in terms of symbols or variables rather than numbers) and numerical calculations. Here is an example. We will discuss these more as we proceed.

Example 1.4
Simplify $9x^6 - 18x^5 + 12x^5 - 5x^4 + 2x^4 - 2x + x + 9 - 2$.

Solution

In[4] := 9 x^6- 18 x^5+ 12 x^5- 5 x^4+2 x^4-2 x + x + 9-2

   Mathematica simplifies and returns the expression.

Out[4] = 7 - x - 3 x^4 - 6 x^5 + 9 x^6

1.4.4 Defining Variables

One can use the equal sign to assign values to a variable.

Example 1.5
Given $z = 12.34$, find $z^2 + 34.32$

Solution

In[5] := z=12.34
Out[5] = 12.34
In[6] := z^2+34.32
Out[6] = 186.596

Unless the output is suppressed explicitly by using a command, **Mathematica** displays all the executed results. In the above example, 12.34 is the z value. The 186.596 corresponds to the needed output value. It is very important to realize that the values you assign to variables are permanent. Once you have assigned a value to a particular variable, the value will be kept until you explicitly remove it. The value will, of course, disappear if you start a whole new **Mathematica** session. Forgetting earlier definitions that you made is the most common cause of mistake while using **Mathematica**. When we have set $z = 12.34$, **Mathematica** assumes that we always want z to have the value 12.34, until we explicitly tell it otherwise. To avoid mistakes, you should remove values you have defined as soon as you have finished using them. To clear the value of the variable z, type **Clear[z]**. Here is an example.

Example 1.6

In[7] := z = 7.2
Out[7] = 7.2
In[8] := x = z^2
Out[8] = 51.84
In[9] := Clear[z]

Clears all the previously assigned values of z.
Now if we define

In[10] := r = 4z^3 − 3z^2 + 2

and execute the file, the **Mathematica** output is

Out[10] = 2 - 3 z^2 + 4 z^3

Mathematica returns the input and the previously assigned z value has been cleared. If we had not cleared the value of z, **Mathematica** would have substituted $z = 7.2$ in evaluating r.

Below is another example:

Example 1.7

In[11] := k = 2.0;
In[12] := m = 5.2;
In[13] := z1 = k^2 − m^2
Out[13] = −23.04

If we do not clear the values of k and m, subsequent expressions wherever k and m appear are replaced by 2 and 5.2, respectively.

We can clear the assigned values for k and m by using

In[14] := Clear[k, m] or **k = .;** and **m = .;**

Now, if we type

In[15] := z2 = k^2 + m^2

Mathematica returns the input as the previously assigned values of k and m have been cleared.

Out[15] = $k^2 + m^2$

It is important to note the following while doing symbolic calculations.

(i) $x\,y\,z$ (x blank y blank z) means x times y times z, whereas xyz is a new variable.
(ii) If an algebraic quantity is multiplied by a number, even without space, it is taken as multiplication. For example, 76z is the same as 76 z.

1.4.5   Using the Previous Results

In **Mathematica**, it is possible to use already-generated output. Hence, there is no need to retype the output obtained. To use the previous results, you can work with the following list of operations (Table 1.2).

Table 1.2   Ways to refer to previous results.

Command	Meaning
%	The last result generated
% %	The next-to-last result
%% …% (k times)	The kth previous result
% **n**	The result on output line Out[n]

1.4.6 Suppressing the Output

If you end your input with a semicolon, **Mathematica** performs the operations you specify but displays no output. **expr;** does an operation but displays no output. You can use **%** to get the corresponding output or type explicitly the variable. Below is an example.

Example 1.8
Evaluate $e^{|x-y|}$, when $x = 2$ and $y = 3$.

Solution

In[16] := x = 2.0; y = 3.0;
In[17] := z = Exp[Abs[x − y]];

When the file is executed, the outputs x, y, and z will not be displayed because of the semicolon at the end of the input. Now to get the value of say, z, just type z.

In[18]:= z
Out[18]= 2.71828

1.4.7 Sequences of Operations

Sequences of operations can be done by simply separating the pieces of inputs with semicolons. The sequences of operations like $expr_1$; $expr_2$; $expr_3$ do several operations and give the result on the last line. On the other hand, $expr_1$; $expr_2$; $expr_3$; do the operations, but give no output. Below is an example.

Example 1.9
Compute the wavelength of an electron. Given $\lambda = \frac{h}{mv}$ where m is the rest mass of the electron, h is the Planck's constant, and v is the velocity of the electron. Given $h = 6.6 \times 10^{-34}$ J s; $v = 10^6$ m/s; $m = 9.1 \times 10^{-31}$ kg

Solution
$p = mv$ is the momentum of the electron.

In[19] := h = 6.6*10^-34;
In[20] := v = 10^6;
In[21] := m = 9.1*10^-31;
In[22] := p = % * %%
Out[22] = 9.1×10^{-25}

% %% multiples the two previous inputs m and v. Hence, the momentum is 9.1×10^{-25} m/s. The wavelength λ is given by,

In[23] := λ = (% % % %)/%
Out[23] = 7.25275×10^{-10}

Hence, the wavelength of the electron is $7.25\ 275 \times 10^{-10}$ m. There should not be any gap between **%** and the number, i.e. **%n** is a single word. If there is a gap, then **Mathematica** will multiply the previous result and give the output.

1.5   Built-in Functions

Mathematica has several built-in functions. By clicking on the built-in functions in the help browser, one gets the complete list of the built-in functions. In **Mathematica**, it is important to note that all built-in functions begin with capital letters and the arguments of the functions are enclosed in square brackets. Below we list a few elementary built-in functions (Table 1.3).

Notice that the arguments of the trigonometric functions are always in radians. To get the value in degrees, it has to be specified in the input. For this, one can use the built -in constant, **Degree**, whose value is $\pi/180$, i.e. **30Degree** represents 30°. Here is an example.

Example 1.10
Evaluate Cos[60 Degree].

Solution
You can evaluate it in degrees or radians (Table 1.4).

Example 1.11
Find the value of (i) sin(300°) (ii) cos(−600°) (iii) sec(405°)

Table 1.3   List of a few elementary built-in functions.

Mathematical notation	Built-in Mathematica functions
π	π can be directly copied from the Palette
Square root x ($\sqrt{x}$)	**Sqrt[x]**
Natural logarithm ($\ln x$)	**Log[x]**
Logarithm to base b ($\log_b x$)	**Log[b,x]**
Trigonometric functions (with arguments in radians)	**Sin[x], Csc[x], Cos[x], Sec[x]** **Tan[x], Cot[x]**
Inverse trigonometric functions	**ArcSin[x], ArcCsc[x], ArcCos[x], ArcSec[x]** **ArcTan[x], ArcCot[x]**
The hyperbolic functions	**Sinh[x], Csch[x], Cosh[x], Sech[x]** **Tanh[x], Coth[x]**
Inverse hyperbolic functions	**ArcSinh[x], ArcCsch[x], ArcCosh[x]** **ArcSech[x], ArcTanh[x], ArcCoth[x]**
Factorial (product of integers 1,2,…,n)	**n!**
Absolute value	**Abs[x]**
Close integer to x	**Round[x]**
Maximum, Minimum of $x,y,…$	**Max[x,y,…], Min[x,y,…]**

Table 1.4 Evaluation in degrees or radians.

From palettes	Evaluation in radians	Evaluation in degrees
Go to the file menu and click on Basic Math Input	Press the radio button π in the palettes menu $\mathrm{Cos}\left[\frac{\pi}{3}\right]$ Or type $\mathrm{Cos}\left[\frac{Pi}{3}\right]$ $\frac{1}{2}$	Press the radio button $^\circ$ in the palettes menu. $\mathrm{Cos}[60^\circ]$ Or type $\mathrm{Cos}\,[60\ \mathrm{Degree}]$ $\frac{1}{2}$

Solution

(i) **In[24] := Sin[300°]**
    Out[24] $= -\frac{\sqrt{3}}{2}$

(ii) **In[25] := Cos[−600°]**
    Out[25] $= -\frac{1}{2}$

(iii) **In[26] := Sec[405°]**
    Out[26] $= \sqrt{2}$

Example 1.12
Evaluate sinh(120).
We will evaluate it directly and also using the formula for sinh.

Solution

In[27] := Sinh[120]
Out[27] $= 6.5209 \times 10^{51}$

Using the formula, $\sinh x = \frac{e^x - e^{-x}}{2}$,

In[28]:= (Exp[120] - Exp[-120])/2.
Out[28] $= 6.5209 \times 10^{51}$

As expected, both forms give the same result.

Example 1.13
Find $\tan(315^\circ)\cot(-405^\circ) + \cot(495^\circ)\tan(-585^\circ)$.

Solution

In[29] := Tan[315 º] Cot[-405 º] + Cot[495 º] Tan[-585 º]
Out[29] $= 2$

Table 1.5 Illustrations of built-in functions.

Command	Mathematica input and output
Log and factorial Stirling's approximation is valid for large values of n $\log n! = n\log n - n$, Evaluate expression when $n = 10\text{^}5$	**Log[10^5!]//N or Log[Factorial[10^5]]//N** 10.513×10^6 **(10^5Log[10^5] − 10^5)//N** 10.5129×10^6
Inverse hyperbolic functions Built-in Functions: ArcSinh, ArcCosh, etc. Find the value of $\sinh^{-1}(-\sqrt{3}/2)$ and $\sin^{-1}(\sqrt{3}/12)$	**ArcSinh$\left[-\frac{\sqrt{3}}{2}\right]$//N** -0.7834 **ArcSin$\left[-\frac{\sqrt{3}}{12}\right]$//N** -0.144843
Absolute value Built-in Function: **Abs** Find absolute value of $(a + b)$ given $a = 3$ and $b = -5$	**a=3; b=-5;** **Abs[a−b]** 2
Mod value Built-in Function: **Mod[n,m]** (remainder on the division of n by m) Find the reminder when 2^23 is divided by 47	**Mod[2^23, 47]** 1

Example 1.14
Find (i) $\log_{32}256$ (ii) $\ln 0$.

Solution

(i) **In[30] := Log[32, 256]**
    Out[30] = $\frac{8}{5}$
(ii) **In[31] := Log[0]**
    Out[31] = $-\infty$

Illustrations of built-in functions are given below (Table 1.5).

1.6 Additional Features

1.6.1 Arbitrary-Precision Calculations

When we have a numerical result with a large number of digits, rounding it off to a required number of digits is necessary. Rounding off a number to n significant digits can be achieved by using **N[expr,n]**. Below is an example.

Example 1.15
Find the value of $\sqrt{\sinh(134)8!\,\pi}$ to 20 decimal places.

Solution

N[expr,20], gives the numerical result up to 20 decimal points.

In[32] := N[Sqrt[Sinh[134]8! π], 20]
Out[32] = $3.1517407561599210602 \times 10^{31}$

1.6.2 Value for Symbols

It is possible to replace a symbol such as z with a definite "value." The value might be a number or any other expression. To replace z with the value 9, you should create the transformation rule $z \rightarrow 9$. You must type $\rightarrow$ between the pair of characters, with no space in between. You can think of $z \rightarrow 9$ as being a rule in which "z goes to 9." The transformation rule is to type **expr/.** rule. The replacement operator "**/.**" is typed as a pair of characters with no space in between, i.e. **expr/.z** $\rightarrow$ value. More than one replacement can also be done. **expr /.** {y $\rightarrow$ yvalue, z $\rightarrow$ zvalue} performs several replacements.

The following example will illustrate the above:

Example 1.16

Find $\frac{(2x+y)}{1-xy}$ at $x = 1$, $y = -3$

Solution

In[33] := $\frac{2x+y}{1-x\,y}$ **/.{x → 1, y → −3}**
Out[33] = $-\frac{1}{4}$

1.6.3 Defining Naming and Evaluating Functions

Functions, expressions, and graphics can be given a name other than the name of a built-in **Mathematica** function. Sometimes it is necessary to evaluate an expression several times for different input values of a function. In such a situation, it is convenient to define a function. It is important to note that every mathematical expression can be named. For example, the function $f(x) = x^3 - 1$ for values of $x = 3$, 6, and 9 are evaluated in the following way:

In[34] := f [x_] = (x^3-1);

When the function is defined for the first time, the argument of the function has to be enclosed in a square bracket followed by an underline (or blank) "_". To evaluate the function, type the name of the function with an argument and press ENTER. In the above example, if you enter f[3], the output will be,

In[35] := f[3]
Out[35] = 26

Similarly,

In[36] := f[6]
Out[36] = **215**
In[37] := f[9]
Out[37] = **728**

Example 1.17
Given $f[x, y] = \frac{\sqrt{x}}{x^2+xy}$, find (i) $f(2, 3)$ (ii) $f(2+h, 3)$.

Solution
First, we will use the command **Clear** to clear all the existing definitions and then enter the definition of each function.

In[38] := Clear[f, x, y, h]
In[39] := f[x_, y_] = $\frac{\sqrt{x}}{x^2+x\,y}$;
(i) **In[40] := f[2, 3]**
   Or else
   In[41] := f[x, y]/. {x → 2, y → 3}
   Will do the needful
   Out[41] = $\frac{1}{5\sqrt{2}}$
(ii) **In[42] := f[2 + h, 3];**
   Out[42] = $\frac{\sqrt{h+2}}{(h+2)^2+3(h+2)}$

Example 1.18
Given $f(x) = \frac{(1-x)}{(1+x)}$.

Solution

In[43] := f[x_] = $\frac{(1-x)}{(1+x)}$;
In[44] := Simplify $\left[f\left[\frac{(1-x)}{(1+x)} \right] \right]$;
Out[44] = x

Example 1.19
If $f(x) = x^2 + 4x - 3$, find $f(\tan^3 x)$.

Solution

In[45] := f[x_] = x² + 4x − 3;
In[46] := f[Tan[x] ^ 3]
Out[46] = $-3 + 4\text{Tan}[x]^3 + \text{Tan}[x]^6$

1.6.4   Composition of Functions

It is possible to evaluate a function of a function or composite function (for example, $z = g(f(x))$). The composite $[g, f, h, \ldots]$ computes the composite of functions g, f, h. Consider the following example.

Example 1.20

If $f(x) = x^2 + x$ and $g(x) = x^3 + 1$, compute $f(g(x))$.

Solution

In[47] := f[x_]=x²+x;
In[48] := g[x_]=x³+1;
In[49] := f[g[x]]
Out[49] =$1 + x^3 + (1 + x^3)^2$

Composition[f, g][x], also gives the same result.

In[50] := Composition[f, g][x]
Out[50] = $1 + x^3 + (1 + x^3)^2$

Defining a function of the form $f[x\_] = \ldots$ instructs **Mathematica** to define f and then compute $f[x]$. The form $f[x\_] := \ldots$ instructs **Mathematica** to define f. In this case, $f[x]$ is not computed and **Mathematica** returns no output. The form $f[x\_] :=$ is of use when **Mathematica** cannot evaluate $f[x]$ unless the particular value of x is specified. The form $f[x\_] :=$ is very useful while defining piecewise functions. When functions are defined recursively, the $:=$ operator must be used.

For example, the definition $f[x\_] = x^3$ specifies that whenever **Mathematica** encounters an expression that matches the pattern $f[x\_]$, it should replace the expression by x^3. Definitions like $f[x\_] = x^3$ can be compared with definitions like $f[a] = b$ for indexed variables. On the other hand, $f[x\_]:$ is used when the defining function is used recursively. For example, $f[x\_]: = x^3$, when executed will not give any output.

F[4] instructs that in the definition of $f[x\_]:$, x should be replaced by 4 and f[8] instructs that x should be replaced by 8 in the definition of $f[x\_]:$ In the same way functions of two or more variables can also defined in a similar fashion

Example 1.21

Given $e^x + \sin x$, find $f\left(\frac{\pi}{3}\right)$.

Solution

Entering $f[x\_] := \text{Exp}[x] + \text{Sin}[x]$, defines $f[x]$ but it is not computed.

In[51] := f[x_] := Exp[x] + Sin[x]

However, the function can be evaluated for a particular value of x. For example,

In[52] := f$\left[\frac{Pi}{3}\right]$;

The solution is:

Out[52] = $\frac{\sqrt{3}}{2} + e^{\pi/3}$

1.6.5 Conditional Assignment

The command **/;** is a conditional assignment. For example, in $g[x\_] := x^2 /; x \geq 0$, an assignment will be made only if $x \geq 0$.

Example 1.22

If $h(x) = \begin{cases} \ln x, & x \geq 0 \\ e^x, & x < 0 \end{cases}$, evaluate $h(12.2)$, $h(-3.4)$ then

Solution

In[53] := h[x_]:=Log[x]/; x ≥ 0
In[54] := h[x_]:=Exp[x]/; x < 0
In[55] := h[12.2]
Out[55] = 2.50144
In[56] := h[−3.4]
Out[56] = 0.0333733

1.6.6 Warnings and Messages

Mathematica prints an error message if the given input is not displayed according to the format, which has to be followed. The error in expression is pointed out immediately below the input. **Mathematica** prints the error message also. Moreover, **Mathematica** beeps whenever it does not understand your input or cannot perform what you have asked for. You can go to the help menu and click on "**Why the Beep**?" in the Mathematica help menu, which explains why it beeped.

1.6.7 Interrupting Calculations

If **Mathematica** is hung up in a calculation or is just taking too long to perform an operation, you can abort it by pressing Alt and Comma (,) keys simultaneously. The **Mathematica** output is $Aborted. If **Abort Evaluation** does not succeed in stopping the **computation**, you can quit the active kernel.

Example 1.23
Find 1234567!

Solution

In[57] := 1234567! Or Factorial[1234567]

   Mathematica evaluates it (you can try!), but it takes some time. If you want to abort the calculation press Alt-Comma. Now, you can either abort the calculation or continue to evaluate it by clicking on the local kernel interrupt. If you press help, it will go to the help browser, which also lists details about how to interrupt the calculation. But, if you prefer to close or exit from the notebook, you will see on the terminal that the notebook "filename.nb" contains a running evaluation. If you choose to close it now, any results will be placed in the messages window. If you click O.K., **Mathematica** will ask whether you wish to save the file or not. You can choose the relevant option (just copy from the file, but typing the output is better).

1.6.8 Using Symbols to Tag Objects

There are many ways to use symbols in **Mathematica**. So far, we have concentrated on using symbols to store values and represent mathematical variables. It is possible

in **Mathematica** to work out problems and get the results with the proper units. The idea is to use symbols as "tags" for different types of objects. This is achieved by attaching a tag, which serves as the unit for a physical quantity. For example, when you specify the length of an object, you mention not only a number but also the unit in which the length is measured. For example, use meters to indicate the unit of measurement as below.

In[58] := 12 meters;

The symbol meters here acts as a tag, which indicates the unit used. It is possible to add the length.

In[59] := % + 5.3 meters

the output is

Out[59] = 17.3 meters

To get the speed

In[60] := %/25 seconds
Out[60] = 0.692 meters seconds

There is in fact a standard **Mathematica** package that allows you to work with units. The package defines many symbols that represent standard types of units. You have to load the **Mathematica** package for handling units.

<<Miscellaneous'Units'

It is important to check the version of **Mathematica** you are using, as in later versions it may not be necessary to type any command. The package uses standardized names for units. Even without loading the package, you can define your own units and do the calculations. Here is a simple example.

Example 1.24
Two charges of equal magnitude 1.6×10^{-19} C are separated by a distance of 4×10^{-15} m. Find the electrostatic force between the two charges (given $\varepsilon_0 = 8.85\,419 \times 10^{-12}$ C^2/(Nm^2).

Solution

In[61] := $e_1 = 1.6 \times 10^{-19}$ coulomb; $e_2 = 1.6 \times 10^{-19}$ coulomb;
In[62] := $r = 4 \times 10^{-15}$ meter; $\varepsilon_0 = 8.85419 \times 10^{-12}$ coulomb^2/(newton meter^2);
In[63] := $F = \frac{1}{4\pi\varepsilon_0} \frac{e_1 e_2}{r^2}$
Out[63] = 14.3801 newton