

Sept. 14 2005: Lecture 4:

## Introduction to Mathematica III

### Simplifying and Picking Apart Expression, Calculus, Numerical Evaluation

A great advantage of using a symbolic algebra software package like MATHEMATICA<sup>®</sup> is that it reduces or even eliminates errors that inevitably creep into pencil and paper calculations. However, this advantage does come with a price: what was once a simple task of arranging an expression into a convenient form is something that has to be negotiated with MATHEMATICA<sup>®</sup>. In fact, there are cases where you cannot even coerce MATHEMATICA<sup>®</sup> into representing an expression the way that *you* want it.

A MATHEMATICA<sup>®</sup> session often results in very cumbersome expressions. You can decide to live with them, or use one of MATHEMATICA<sup>®</sup>'s many simplification algorithms. Section 1.4.5 (or Help Browser/The Mathematica Book/A Practical Introduction/Algebraic Calculations/Advanced Topic: Putting Expressions into Different Forms) of the MATHEMATICA<sup>®</sup> book has a good summary of frequently used simplification algorithms. Another method is to identify patterns and replace them with your own definitions.

MATHEMATICA<sup>®</sup> has its own internal representation for rational functions (i.e.,  $\frac{\text{numerator expression}}{\text{denominator expression}}$ ) and has special operations for dealing with these.

MATHEMATICA<sup>®</sup> Example: Lecture-04

#### Operations on Polynomials

*Expand, Factor, Coefficients*

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#### Operations on Rational Expression

*Together, Apart, Numerator*

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MATHEMATICA<sup>®</sup> is very fastidious about simplifying roots of numbers. Unless, it is specified otherwise, MATHEMATICA<sup>®</sup> makes no assumptions about whether a variable is real, complex, positive, or negative.

MATHEMATICA<sup>®</sup> Example: Lecture-04

### Simplifying Roots

*PowerExpand, Simplify with Assumptions*

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“Deep Blue” is a program that is very very good at playing chess, perhaps better than any human. However, it uses an algorithm that is very different from humans to play. Analogously, MATHEMATICA<sup>®</sup> is very very good at doing calculus—and it too uses algorithms that would not be useful for most humans. Nevertheless, it is nice to have a partner who can integrate, differentiate, and perform Taylor expansions on anything that you can—and also quickly and accurately.

MATHEMATICA<sup>®</sup> Example: Lecture-04

### Calculus: Limits, Derivatives, Integrals

*Limit, D, Integrate*

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### Calculus: Series expansions about a value

*Series, Normal, fitting functions*

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MATHEMATICA<sup>®</sup> solves equations and, if possible, for each solution gives you rules that you can apply. It is generally a good idea to name the solution so that you can use it to apply its rules. This is a powerful aspect of MATHEMATICA<sup>®</sup>: it allows you to tackle solutions that would be very onerous otherwise.

MATHEMATICA<sup>®</sup> Example: Lecture-04

### Solving Equations

*Solve[] and its resulting rules*

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Sometimes, no closed form solution is possible. MATHEMATICA<sup>®</sup> will try to give you rules (in perhaps a very strange form) but it really means that you don't have a solution to work with. One usually resorts to a numerical technique when no closed form solution is possible—MATHEMATICA<sup>®</sup> has a large number of built-in numerical techniques to help out. A numerical solution is an approximation to the actual answer. Good numerical algorithms can anticipate where numerical errors creep in and account for them, but it is always a good idea to check a numerical solution to make sure it approximates the solution the original equation.

Of course, to get a numerical solution, the equation in question must evaluate to a number. This means if you want to know the numerical approximate solutions  $x(b)$  that satisfy  $x^6 + 3x^2 + bx = 0$ , you have to iterate over values of  $b$  and “build up” your function  $x(b)$  one  $b$  at a time.

Sections 1.6.1–1.6.7 (or Help Browser/The Mathematica Book/A Practical Introduction/Algebraic Calculations/Numerical Mathematics) of the MATHEMATICA<sup>®</sup> book have an overview of frequently used numerical algorithms.

MATHEMATICA<sup>®</sup> Example: Lecture-04

### Numerical Solutions

*NIntegrate, FindRoot*

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1. You will want to save your work.
2. You will want to modify your old saved work
3. You will want to use your output as input to another program
4. You will want to use the output of another program as input to MATHEMATICA<sup>®</sup>.

You have probably learned that you can save your MATHEMATICA<sup>®</sup> notebook with a menu. This is one way to take care of the first two items above. There are more ways to do this and if you want to do something specialized like the last two items, then you will have to make MATHEMATICA<sup>®</sup> interact with files. Because an operating system has to allow many different kinds of programs interact with its files, the internal operations to do input/output (I/O) seem somewhat more complicated than they should be. MATHEMATICA<sup>®</sup> has a few simple ways to do I/O—and it has some more complex ways to do it as well.

It is useful to have a few working examples that you can modify for your purposes. The examples will serve you well about 90% of the time. For the rest of the 10%, one has to take up the task of learning the guts of I/O—hopefully, beginners can ignore the gory bits.

MATHEMATICA<sup>®</sup> Example: Lecture-04

### Interacting with files

*Redirection, reading, opening, streams, formatting*

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### Using Packages

*Reading Packages*

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There are a number of packages that come with MATHEMATICA<sup>®</sup> (and more that can be bought for special purposes). You should look through the various packages in the help browser to get an idea of what is there—it is also a good idea to take a look at the inside of a package by editing a package file with an editor. By doing this, you will see some of internal structure of MATHEMATICA<sup>®</sup> and good examples of professional programming.