Mathematica

Symbolic Linear Algebra

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Introduction (1)

This course is NOT going to be easy

But you can get results you can't get otherwise

It is a seriously tricky computational technique

- I can't give you simple recipes, and won't try to
- It will show you how to tackle such problems Don't worry if the details are confusing

You can go back and work through the examples There are more than we shall go through now

Introduction (2)

Prerequisite: Mathematica – Linear Algebra etc. OR: You already know what that course covers

Tou alleauy know what that course covers

It includes nothing on the basic use of Mathematica And little on elementary linear algebra, either

If you don't understand, please interrupt Don't feel afraid to ask any question you want to

Yes, I have to refer to the documentation, too!

Beyond the Course

Mathematica/

http://reference.wolfram.com/mathematica/... .../guide/Mathematica.html

Logging In

• No practicals, as such, but are examples Recommended to try them as I describe the topics Can use cut-and-paste from file Examples_2.txt

If using Microsoft Windows, find mathematica Somewhere in Applications

If not using Microsoft Windows, CTRL-ALT-DEL Select Restart, then Linux and log in Start by mathematica or math

You should also display <a>Examples_2.txt

Symbolic Manipulation

This is an automation of standard mathematics You use formulae with variables, not just values

For simple manipulations, it's almost trivial, but:

- Simplifying (cancelling) formulae isn't
- Avoiding combinatorial explosion isn't

Managing those two is where the difficulties lie

But careful, step-by-step, methodology works Check the effect of each step before proceeding

Trivial Example (1)

$$(x^3 - y^3) / (x - y) // InputForm$$

Well, that doesn't do what we want it to . . .

Cancel [(
$$x^3 - y^3$$
) / ($x - y$)] // InputForm

$$x^{2} + x^{*}y + y^{2}$$

Cancel is a built-in transformation function

Trivial Example (2)

Many built-in functions work on symbolic formulae

Solve
$$[x^3 - a + 1 == 0, x]$$
 // InputForm
{ { x -> (-1 + a) ^ (1/3) },
{ x -> - ((-1) ^ (1/3) * (-1 + a) ^ (1/3)) },
{ x -> (-1) ^ (2/3) * (-1 + a) ^ (1/3) }

Now try the following – do you know why it fails?

Solve
$$[x^5 + a * x^3 + 1 == 0, x]$$
 // InputForm

Simple Matrix Algebra (1)

Let's use the following matrix and vectors

$$a = \{ \{ 4.2, 2.2 + p, -3.9, 9.3, 0.1 \}, \\ \{ 8.6 - p, r, 0.7, -2.3, -0.3 \}, \\ \{ 8.4, -5.9, -8.1 + q, 9.6, 3.8 \}, \\ \{ -0.8, -9.4, -9.9, 9.9, 5.0 - r \}, \\ \{ -1.3, -8.1, 0.6, -9.2 + r, -7.3 \} \}$$

 $b = \{ -6.8, 2.3, 2.7, -7.0, 2.0 \}$

 $c = \{p, 1.0, p+q, 1.0, q\}$

Simple Matrix Algebra (2)

If we want to transform a known vector, it's trivial That's just the most elementary matrix algebra

a.b

You can do exactly the same with a . c

Perturbation Analysis

Error analysis of a numerical solution

Conventional error analysis is in terms of norms This is a well-understood area, with useful results

• Use the formulae for it in books etc.

Mathematica helps with non-standard analyses How specific variations affect the results

Useful for understanding specific points in detail This is easier to show than to explain

Low-Order Approximations

Consider small variations around a solution Ignore (say) all second order terms and above

See how solution will vary with perturbations Can be used to answer questions like:

Is parameter A critical to the result?

What's the best way to change the results?

Does it matter if parameters A and B are linked?

Alternative Approaches

There are a lot of existing results on this E.g. sensitivity analysis in statistics

Where those answer your question, they are better Use this technique when they don't help

The specific examples I use are fairly simple There are other ways, perhaps better ones

An example at the end where only this works

Jumping Ahead

For example: c . MatrixExp[a] . c to second order

```
2
-1486.11 - 3585.23 p + 2150.23 p + 3953.26 q +
2
12339.7 p q + 1800.52 q - 3154.22 r -
2
6192.86 p r + 408.955 q r - 410.955 r
```

Getting there isn't hard, but needs background We shall work up to it slowly, explaining why and how

How Mathematica Works

Mathematica's operation is very simple (even dumb) You need to know how it works for symbolic work

Everything is an expression, stored as a tree

FullForm [1.23 * x + y + 4.56 * z]

Plus [Times [1.23', x], y, Times [4.56', z]]

Everything works by transforming that tree

Assignment (1)

It expands the RHS recursively This is more-or-less literal expansion

It replaces variables with their values Any unset names are left in symbolic form

Remember that values are always expressions

0.12 + 7.89 (4.56 + 1.23 a) + z

Assignment (2)

You can use the LHS variable in the RHS Provided it already has a value

$$x = 1.23 * x + 4.56$$

4.56 + 1.23 (4.56 + 1.23 a)

But this goes into an infinite loop

x =. (* Ensure that x has no value *)
x =
$$1.23 * x + 4.56$$

How To Stay Sane

Keep the following two as separate as possible:

- Symbols you use for physical quantities For example, e, m and c in $e = m c^2$
- Symbols you use for Mathematica variables I.e. ones used for programming language variables

Unfortunately, often need to use one as the other It is very easy to get confused doing that Minimise and localise such uses

Transformations (1)

There are a great many built-in ones Look under "Formula Manipulation" for more

There is an "easy to use" function Simplify Not used here, as it doesn't say what it does

There is almost always something that helps You search the documentation, and then experiment

If not, you can manipulate the tree yourself This course does not cover such advanced use

Transformations (2)

Shall use only the few that we actually need These are the ones used in the examples:

Cancel [expr]: cancels out common factors in the numerator and denominator of expr

CoefficientList [poly, var]: gives a list of coefficients of powers of var in poly, starting with power 0

Collect [expr , var]: collects together terms involving the same powers of objects matching var

Transformations (3)

Expand [expr]: expands out products and positive integer powers in expr

ExpandAll [expr]: expands out all products and integer powers in any part of expr

Together [expr]: puts terms in a sum over a common denominator, and cancels factors in the result

Rules (1)

Rules are user-defined and explicit transformations

Set all powers of x beyond the third to zero

rule =
$$x \wedge k_{, k > 3 -> 0$$

Expand [(1 + x) ^ 7] /. rule

Rules (2)

Now, how does that work? Let's go through it slowly

rule =
$$x \wedge k_{, k > 3 \rightarrow 0$$

", k > 3" is a condition that says k > 3

"-> 0" says replace the pattern by 0

Rules (3)

Expand [
$$(1 + x)^{7}$$
] /. rule

Expand [(1 + x)^7] is an arbitrary expression

". rule" applies the rule to that expression

Remember The Tree?

Everything works on the expression tree If that isn't in the right form, they don't work

x y + x z

Try one rule at once; if it doesn't work, either:

- Change the rule to work better
- Transform the tree so it does

Delayed Rules

The RHS is evaluated during the definition That's not right if it includes a function call

There's a variant syntax for a delayed rule It just replaces the "->" by ":>"

In this case, it makes no difference, of course

Repeated Rules

There's a variant syntax for a repeated rule It applies it repeatedly until there is no change

```
Just replace the "/." by "//."
```

That's all we shall use of rules and patterns Mathematica has quite a lot more features

Worked Example (1)

Let's use the previous matrix and vectors And calculate c.a.a.c to first order

For simplicity, use a single infinitesimal (say 'e') Other values transformed to 'constant \times e'

Then define a rule to kill high powers of e

Worked Example (2)

Well, that doesn't do what we want it to . . . We need to expand the powered expressions

- 1125.78 - 2593.47 e p1 - 1261.99 e q1 + 67.65 e r1

Hey, presto!

Worked Example (3)

We can now restore the original variables Use some rules to convert 'p1 e' to 'p' etc.

Remember to unset the effect of 'p' etc. first!

- 1125.78 - 2593.47 p - 1261.99 q + 67.65 r

Worked Example (4)

Let's try second order – it's much the same

We need a different approach to restoration

Worked Example (5)

- 2 – 1125.78 – 2593.47 p – 2628.74 p – 1261.99 q
- 2 + 9.05 p q + 191.281 q + 67.65 r
- 2 + 120.61 p r – 109.2 q r – 4.7 r

Aside: Syntactic Gotcha

You separate statements by semicolons (";") Usually, omitting them before a newline prints

But not always (especially in function definitions) . . .

Syntax::newl: The newline character after "fred[] := (x = arg[[1]]" is understood as a multiplication operator.

Something Harder

What about c. MatrixExp[a]. c to first order? That's truly horrible (and useless to us)...

Not surprising, given our simplistic approach MatrixExp[a] doesn't have a finite expansion

But matrix exponentiation is just like numeric

$$exponent(A) = \sum_{k \ge 0} A^k/k!$$

What Can We Do?

Solution is to write our own MatrixExp Which clobbers second order terms at each stage

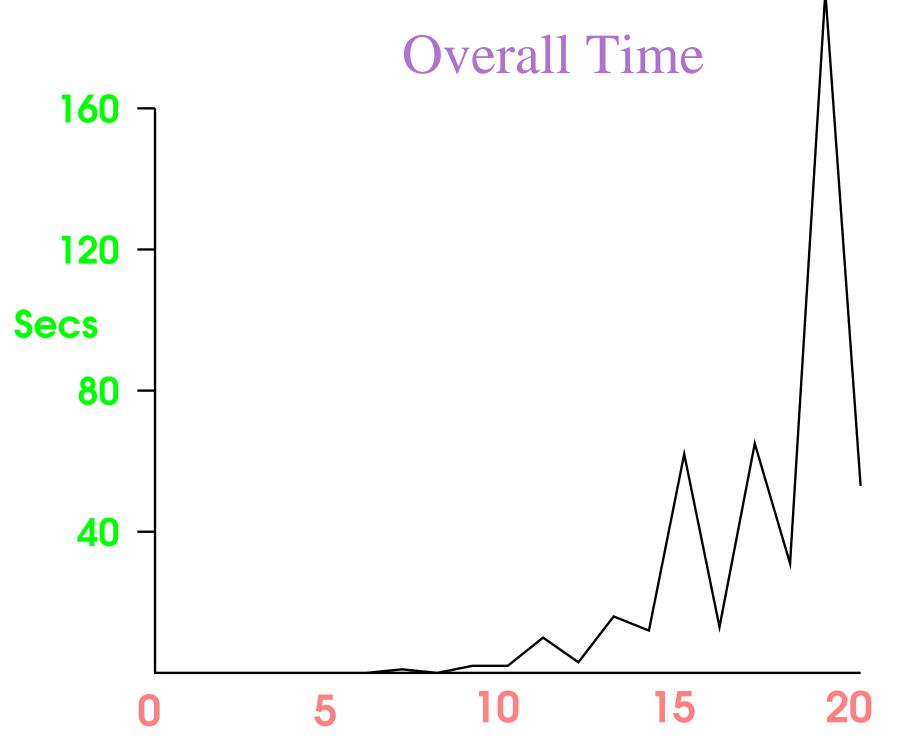
This is a general technique in this area Reduce was the same, 30 years ago

Mathematica is less automatic than Reduce The handouts explain why we can't use MatrixPower

Using MatrixPower

Let's time $A^k/k!$ and its simplification first

]]]



Mathematica - p. 37/??

Back To Basics (1)

How would we do it in Fortran and floating-point?

```
PURE FUNCTION exponent (arg)
```

```
exponent = 1.0 ; value = 1.0

DO k = 1 , HUGE ( k )

value = value * arg / k

temp = exponent + value

IF ( temp == exponent ) EXIT

END DO

END FUNCTION exponent
```

Back To Basics (2)

And this is the Mathematica equivalent:

Timing That

Timing [

$$p = p1 * e; q = q1 * e; r = r1 * e;$$

 $a1 = a; rule = e^k /; k > 1 -> 0;$
 $x = c. matexp [a1, rule].c;$
 $y = Expand [x] /. rule;$
 $p = .; q = .; r = .;$
 $p1 = p/e; q1 = q/e; r1 = r/e;$
 $z = y; p1 = .; q1 = .; r1 = .; z$
]

{ 0.304019 , -1486.11 - 3585.23 p + 3953.26 q - 3154.22 r }

Under 1/3 of a second – that's not too not bad Now let's go back and work through the function

Second order (1)

```
Timing [
     p = p1 * e; q = q1 * e; r = r1 * e;
    a1 = a;
                                        (* Changed *)
    rule = e^{k} /; k > 2 -> 0;
     x = c \cdot matexp[a1, rule] \cdot c;
     y = Expand [x]/.rule;
     p =.; q =.; r =.;
     p1 = p/e; q1 = q/e; r1 = r/e;
     Z = Y;
     p1 =.; q1 =.; r1 =.;
     Ζ
```

Second order (2)

```
2
{ 0.820051 , -1486.11 - 3585.23 p + 2150.23 p +
2
3953.26 q + 12339.7 p q + 1800.52 q - 3154.22 r -
2
6192.86 p r + 408.955 q r - 410.955 r }
```

Which still takes under a second!

MatrixPower

Here is how you would do MatrixPower, incidentally It takes well under 0.1 seconds in each case

Fourier Transforms (1)

Fourier transforms are just matrix multiplication With matrices of a special form, of course

Fourier::fftl: Argument { 0.906, 4.528, <<17>>, -3.463} is not a nonempty list or rectangular array of numeric quantities.

Boring – so we have to do it by hand

Fourier Transforms (2)

See http://en.wikipedia.org/wiki/... .../Discrete_Fourier_transform/

Tedious, but not exactly difficult Now, why can't Mathematica do that?

Solving Equations (1)

Solving linear equations is a little trickier We use the matrix and vector we had earlier

$$a = \{ \{ 4.2, 2.2 + p, -3.9, 9.3, 0.1 \}, \\ \{ 8.6 - p, r, 0.7, -2.3, -0.3 \}, \\ \{ 8.4, -5.9, -8.1 + q, 9.6, 3.8 \}, \\ \{ -0.8, -9.4, -9.9, 9.9, 5.0 - r \}, \\ \{ -1.3, -8.1, 0.6, -9.2 + r, -7.3 \} \}$$

 $c = \{p, 1.0, p+q, 1.0, q\}$

v = LinearSolve [a, c] (* That's not pretty *)

Solving Equations (2)

So let's calculate a first order solution Obviously need to expand powers top and bottom Hence use ExpandAll rather than Expand

Unfortunately, ExpandAll doesn't seem to work There are products of expressions still not expanded

What do we do? We try a slightly different approach

Solving Equations (3)

Let's convert it to a common denominator first

w = ExpandAll [Together [v]] /. rule1

That's a lot better, and worth working from So we shall now work from that expansion, w

This is a very important general technique Try bypassing problems by using a variant approach If it works, it works – don't worry too much why

Solving Equations (4)

We need to convert a/(b+c*e) to (a/b)*(1-(c/b)*e)

Well, that improves things, but doesn't get there We need to apply the rule repeatedly until no change

x = w //. rule2

Hah! We are in sight of victory! Use x from now

Solving Equations (5)

We just need to expand again and apply rule1

$$y = Expand [x]/.rule1$$

And then convert back to our original variables

Solving Equations (6)

Which gives us the final result:

- -0.137433 + 0.211331 p + 0.851368 q + 0.0507513 r
 - 2.19542 2.31209 p 7.83925 q 2.67286 r
- -4.41552 + 4.43115 p + 15.082 q + 5.05721 r
- -2.31043 + 2.17963 p + 7.79656 q + 2.73433 r
 - 0.137312 + 0.145104 p 0.176435 q 0.390099 r

Solving Equations (7)

So our complete program becomes:

Solving Equations (8)

Check that we got it right by reverse substitution:

I.e. c with rounding errors – also try this:

Second Order (1)

Let's try just adding a rule for $a/(b+c*x+d*x^2)$ We need to collect terms in x to do this

```
v = LinearSolve[a, c];
p = p1 * e; q = q1 * e; r = r1 * e;
rule1 = e^{k_{1}}; k > 2 -> 0;
w = ExpandAll [Together [v]]/.rule1;
rule2 = k1_ / ( k2_ + k3_ * e ) ->
    k1 * (1 - (k3 / k2) * e) / k2;
rule3 = k1_ / ( k2_ + k3_ * ( e | e ^ * k4_ ) ->
    k1 * (1 – (k3 / k2) * e –
         ((k3/k2)^2)*e^2-
         (k4/k2) * e ^ 2) / k2;
x = Collect [w, e] //. rule2 //. rule3
```

Second Order (2)

Sigh. Collect applies only at top level

We need to go back a step and write a function We start with $a/(b+c*x+d*x^2)$

And we turn it into $(a/b)*(1-(c/b)*x+((b/c)^2-d)*x^2)$

Second Order (3)

Now use that – note that we need a delayed rule Start from after the w = ExpandAll line

Tidy up by restoring the original variables

Second Order (4)

Check that we got it right by reverse substitution:

Which is c with some rounding errors

Practicalities

How did I work that out? Just as I showed you
Lots of trial and error, step-by-step

As we saw, not everything works as specified The documentation makes it unnecessarily hard

Nothing is specified precisely or completely There is no comprehensive index to a topic The tutorials are almost always too simple

But that can be handled, with care
 And I haven't found anything not documented

User's Guide (1)

- Firstly, work out the next step Make sure it's really, really simple
- Then look in the documentation Remember that there is a search facility
- Look into sections with more information Check all the other useful–looking functions
- Don't forget to look in the tutorials But check the description of what you find

User's Guide (2)

- Run an experiment on each new feature Check that you understand the description
- Then try it for real, and see if it helps Check on what it has done (if anything) Then tweak it, if you can see something to do

If it works, good – if not, iterate!
 Go back and check its description and tutorials
 Or go right back and look for another feature

Yes, it's tedious

User's Guide (3)

But not as tedious as doing it by hand!

Try it if you don't believe me . . .

Performance (1)

The above is OK for for small, simple matrices But the time can build exponentially

Ouch. We need to take a different approach Start by describing the general technique

Performance (2)

As with MatrixExp, you go back to basics Gaussian Elimination solves such equations Lots of Web pages that describe it, including:

http://mathworld.wolfram.com/... .../GaussianElimination.html

Test using floating-point, because it's much easier

You can use Mathematica to generate test results In this case, compare against LinearSolve

Performance (3)

You have a working Gaussian Elimination solver Now start converting it for symbolic work

Create a suitable symbolic test case Add simplification rules, step-by-step

For tricky problems, save values using InputForm Then you can work on just that, in a separate program

Then use the answer in your main code And carry on working on that . . .

Gaussian Elimination (1)

There are some programs that do the first step There's nothing tricky about this, just tedious

NOT how best to code Gaussian Elimination E.g. we shall omit all pivoting, for simplicity

All files are in directory Examples_2

File gaussian_1.math uses LinearSolve File gaussian_2.f90 is Fortran 90 code File gaussian_3.math is Mathematica code

Gaussian Elimination (2)

You have learnt enough to add the simplifications This is left as an exercise, with an answer provided

You should start with file gaussian_3.math

 \Rightarrow File gaussian_4.math is the specimen answer

File worked_1.math uses LinearSolve Just the example worked through above, for reference

Gaussian Elimination (3)

There are also files containing second order solvers

File worked_2.math uses LinearSolve Just the example worked through above, for reference Function invert is a bit more complicated To handle expressions that are not quadratic

You should start with file gaussian_4.math

File gaussian_5.math uses Gaussian Elimination → This is the result you should be aiming for

Eigenvalues etc. (1)

Harder than linear equation solving – why?

Numerical ones are fairly well–understood But applies to real (\mathbb{R}) and complex (\mathbb{C}) ONLY

They are solutions of the characteristic polynomial

CharacteristicPolynomial [HankelMatrix [5], x]

Eigenvalues etc. (2)

You can solve a quartic in radicals (roots) Galois proved you can't solve a general quintic

Eigenvalues of symbolic matrices need a solution So you can't get them, in general, above 4×4

Solve [CharacteristicPolynomial [HankelMatrix [4] , x] == 0 , x]

Solve [CharacteristicPolynomial [HankelMatrix [5], x] == 0, x]

Eigenvalues etc. (3)

But we know that we can get them, numerically!

You would adapt one of the iterative solvers And would start from the numerical solution

Symbolic calculations are very like that Few things are impossible, but many are hard

And you almost always have to go back to basics

Where I Came In (1)

My initial interest in this area was statistics I had some complicated combinatoric distributions Think hypergeometric, only a bit more complicated

$$probability = rac{{\binom{K}{k}\binom{N-K}{n-k}}}{{\binom{N}{K}}}$$

That is asymptotically normal under many conditions I wanted the first 3–4 terms in the approximation

Where I Came In (2)

You expand factorials using Stirling's formula

That's bad enough, and my problem was worse! After 2 terms using pencil and paper, I gave up

Where I Came In (3)

Reduce was painful – but better than by hand! The key to solving my problem was twofold:

- Deal with highest rank terms first $N^N > a^N > N^a$ etc.
- Cancel the highest rank terms Then reduce the residue to the next lower rank

I can no longer remember the details! But please contact me if you have this problem