What happens internally

AD Model Builder foundation

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It is all about minimizing functions

- Want to find the parameters $\theta = (\theta_1, \ldots, \theta_n)$ that makes the observations most likely.
- Equivalent to minimizing the negative log likelihood w.r.t. θ

$$\widehat{\theta} = \underset{\theta}{\text{argmin}}\, \ell(y|\theta)$$

- If the dimension of θ is low (say n less than 5 or 10) any method can be used (grid search, random search, finite difference approximations, ...)
- AD Model Builder is capable of handling much larger problems
- Important for fixed effects models, and even more for random effects models
- AD Model Builder uses a quasi-Newton minimizer aided by automatic differentiation
- Here we will try to explain what that is, and why that is important

Quasi-Newton minimizer

ADMB

Automatic Differentiation Model Builder

- A Newton minimizer is an iterative algorithm
- Each step assumes that the function $\ell(x, \theta)$ can be approximated locally by a quadratic function
- It uses the first ℓ'_θ and second ℓ''_θ derivatives to find the minimum
- Instead of calculating ℓ''_θ at every step, a quasi-Newton minimizer uses successive first derivatives ℓ'_θ to approximate ℓ''_θ.
- Bottom line: We need a fast and accurate way to calculate ℓ'_θ

Finite difference: Simple, inaccurate, and slow

- Algorithm: The i'th element in ℓ'_θ is calculated by
  - Add a small number $\Delta\theta_i$ to the i'th element of θ to get $\tilde{\theta}_i$
  - Calculate $(\ell'_\theta)_i \approx \frac{\ell(\tilde{\theta}_i,x)-\ell(\theta,x)}{\Delta\theta_i}$
- Notice: all that is required is that we can evaluate $\ell(\theta, x)$ at any point
- Notice: it is an approximation
- Notice: it will be expensive if the dimension of θ is high

Analytical: The best thing when possible

- Situations where we can find a nice analytical expression for ℓ'_θ are:
  - Fast
  - Accurate
  - Extremely rare

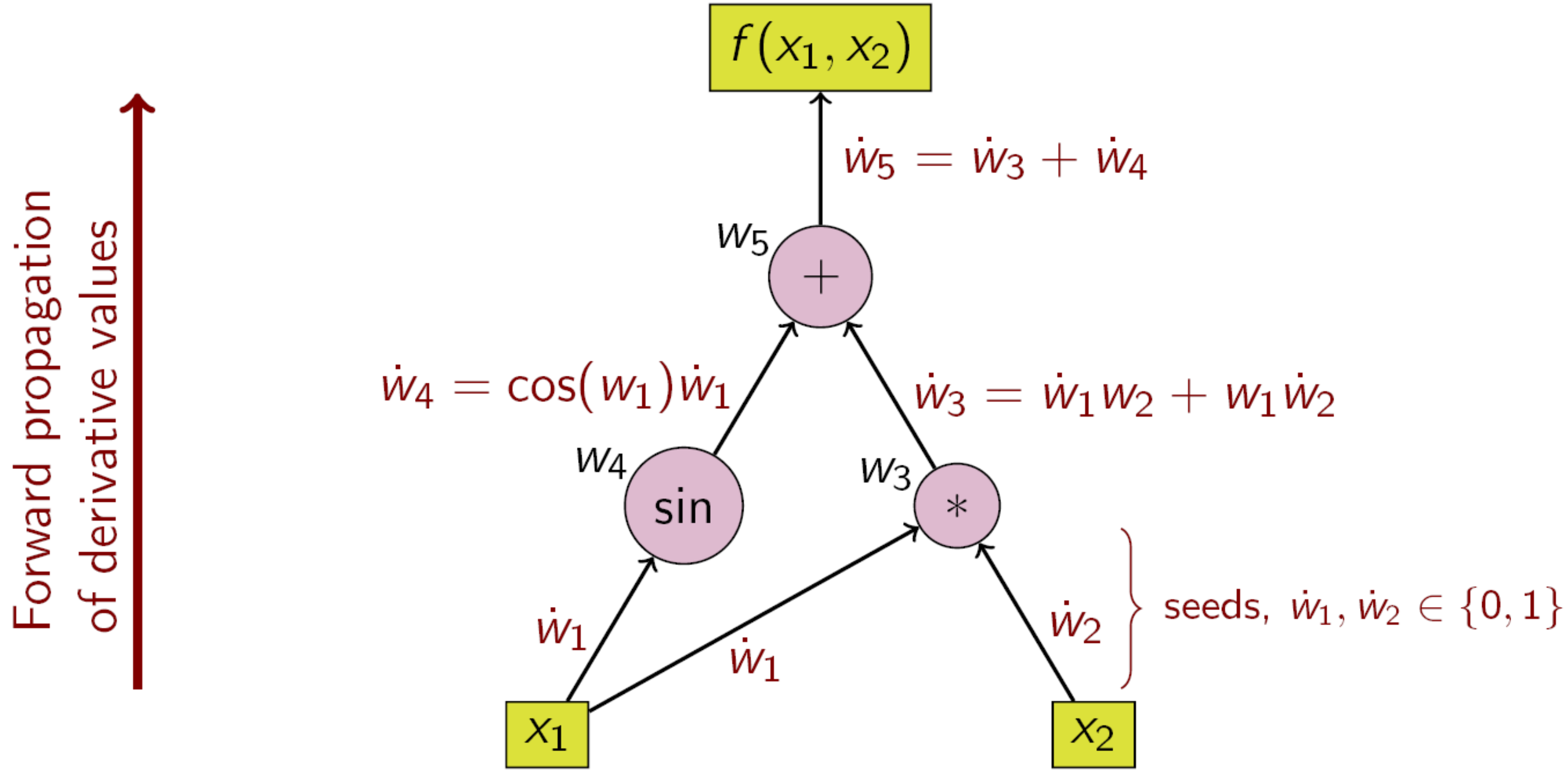
Automatic differentiation: Fast and accurate

- We need to write a program to compute $\ell(\theta, x)$ anyway
- A computer program is a long list of simple operations:
  '$+$', '-', '*', '$/$', 'exp', 'log', 'sin', 'cos', 'tan', 'sqrt', and so on
- We know how to derive each of these operations
- The chain rule tells us how to combine: $(f(g(x)))' = f'(g(x))g'(x)$
- So if the computer is instructed to:
  - keep track of all the simple operations used when calculating $\ell(\theta, x)$
  - use the simple derivative formulas and the chain rule
- Then once $\ell(\theta, x)$ is computed, we also have ℓ'_θ with a minimum of extra calculations
- This is fast and accurate, and the difficult part is built into AD Model Builder(!)
- To get a better understanding consider the following code, wich is modified from a larger example by Uffe Høgsbro Thygesen.

```
#include <math.h>
#include <iostream.h>

class result {
  private: double v,d;
  public: result(){v = 0;d= 0;};
          result(double val){v = val; d = 0;};
          result(double val,double der){v = val; d = der;};
          double Value(){return v;};
          double Deriv(){return d;};
};

class parameter: public result {
  public: parameter(double pval) : result(pval,1.0) {};
          parameter() : result(0.0,1.0) {};
};

result sin(result n){
  return result(sin(n.Value()), cos(n.Value())*n.Deriv());
};

result operator*(result n1,result n2){
  return(result(n1.Value()*n2.Value(), n1.Deriv()*n2.Value() + n2.Deriv()*n1.Value()));
};

ostream& operator<<(ostream& o,result n){
  o << n.Value() << " (Derivative: " << n.Deriv() << ") ";
  return o;
}

int main(int argc, char* argv[]){
  parameter theta(2);
  result y;
  y = sin(theta*theta);
  cout << "The result is " << y << endl;
}
```

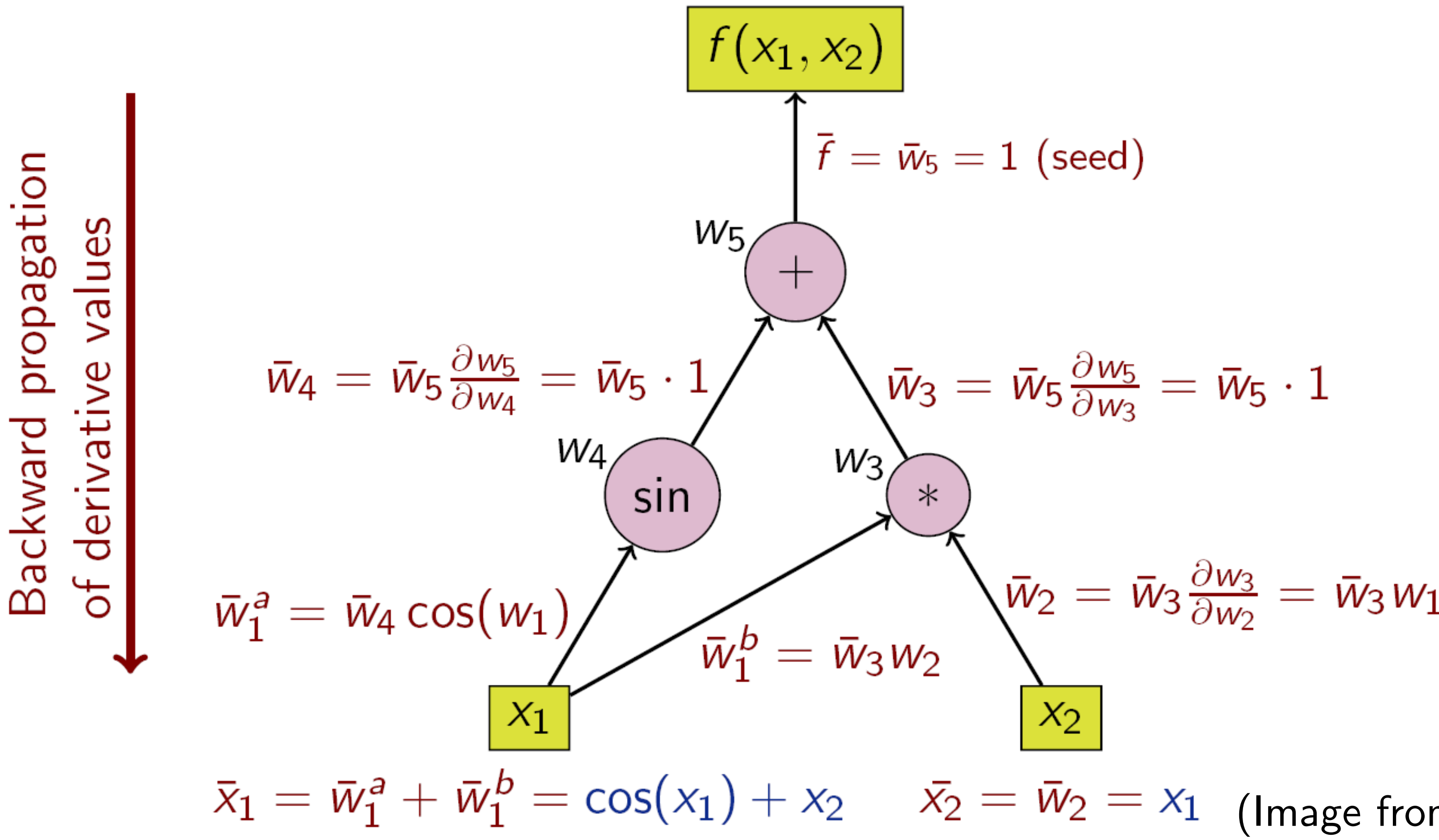
```
The result is -0.756802 (Derivative: -2.61457)
```

Forward and reverse mode



(Image from Wikipedia)

- Forward mode is easy to understand and implement
- Not efficient when θ is high dimensional



(Image from Wikipedia)

- Requires recording a stack of all operations
- Efficient in number of operations
- AD Model Builder uses reverse mode
- Except for random effects models where a combo of forward and reverse mode is used

This should be a help in understanding why ...

- we should careful about statement like:

```
if(theta<7.0){nll=...;}else{nll=...;}
```

- we can sometimes observe the memory requirements growing rather big if do a lot of iterative calculations
- a 'double' is different from a 'dvariable', a 'dvector' is different from a 'dvar_vector', ...
- we cannot do coding like:

```
dvariable x=5; ... double y; y=x; ... x=y;
```

- it is usually better to use the built-in functions in AD Model Builder than coding them yourself

Exercises

Exercise 1: Add the functionality to handle the plus operator, division operator and the cosine function to the program on page 6. Evaluate f'(2), where:

$$f(x) = \frac{\sin(\sin(x^2) + \cos(x))}{x^2}$$

Solution:

```
The result is -0.230474 (Derivative: -0.110843)
```

Exercise 2: AD Model Builder has a facility to check the automatic derivatives by comparing them to the finite difference approximations. It can be started by pressing `ctrl-c` while a minimizer is running, or by starting the program with the flag `progname -dd 1` which will start the derivative checker after the first function evaluation. Verify the derivatives for one of the previous programs (for instance the 1D diffusion model).

Solution:

```
an@ch-pcb-an:~/talks/admbcourse$ ./turbot -dd 1

Initial statistics: 3 variables; iteration 0; function evaluation 0
Function value   1.3294890e+02; maximum gradient component mag  -1.3054e+02
Var   Value    Gradient   |Var   Value    Gradient   |Var   Value    Gradient
  1  0.00000 -2.06761e-03 |  2  6.90776  8.30058e+01 |  3  0.00000 -1.30543e+02

Enter index(1...3) of derivative to check. To check all derivatives, enter 0: To quit enter -1: 0

   Checking all derivatives. Press X to terminate checking.
   Enter step size (to quit derivative checker, enter 0): 1.0e-6

       X           Function     Analytical     Finite Diff;  Index
   1.90075e-08   1.32929e+02  -2.07065e-03  -2.07085e-03 ;     1
   6.90699e+00   1.32929e+02   8.29584e+01   8.29584e+01 ;     2
   1.20007e-03   1.32929e+02  -1.30223e+02  -1.30223e+02 ;     3
an@ch-pcb-an:~/talks/admbcourse$
```