

# SciencesPo Computational Economics Spring 2017

Florian Oswald

March 15, 2018

## 1 Computational Economics: Optimization I

Florian Oswald Sciences Po, 2018

- This lecture reminds you of some optimization theory.
- The focus here is to illustrate use cases with julia.
- We barely scratch the surface of optimization, and I refer you to Nocedal and Wright for a more thorough exposition.

This is a 2 part lecture.

### 1.0.1 Optimization I: Basics

1. Intro
2. Conditions for Optima
3. Derivatives and Gradients
4. Numerical Differentiation
5. JuliaOpt

### 1.0.2 Optimization II: Algorithms

1. Bracketing
2. Local Descent
3. First/Second Order and Direct Methods
4. Constraints

## 1.1 The Optimization Process

1. Problem Specification
2. Initial Design
3. Optimization Procedure:
  - a) Evaluate Performance
  - b) Good?
    - i. yes: final design
    - ii. no:
      - \* Change design
      - \* go back to a)

We want to automate step 3.

## 1.2 Optimization Algorithms

- All of the algorithms we are going to see employ some kind of *iterative* procedure.
- They try to improve the value of the objective function over successive steps.
- The way the algorithm goes about generating the next step is what distinguishes algorithms from one another.
  - Some algos only use the objective function
  - Some use both objective and gradients
  - Some add the Hessian
  - and many variants more

## 1.3 Desirable Features of any Algorithm

- Robustness: We want good performance on a wide variety of problems in their class, and starting from *all* reasonable starting points.
- Efficiency: They should be fast and not use an excessive amount of memory.
- Accuracy: They should identify the solution with high precision.

## 1.4 A Word of Caution

- You should **not** normally attempt to write a numerical optimizer for yourself.
- Entire generations of Applied Mathematicians and other numerical pro's have worked on those topics before you, so you should use their work.
  - Any optimizer you could come up with is probably going to perform below par, and be highly likely to contain mistakes.
  - Don't reinvent the wheel.
- That said, it's very important that we understand some basics about the main algorithms, because your task is **to choose from the wide array of available ones**.

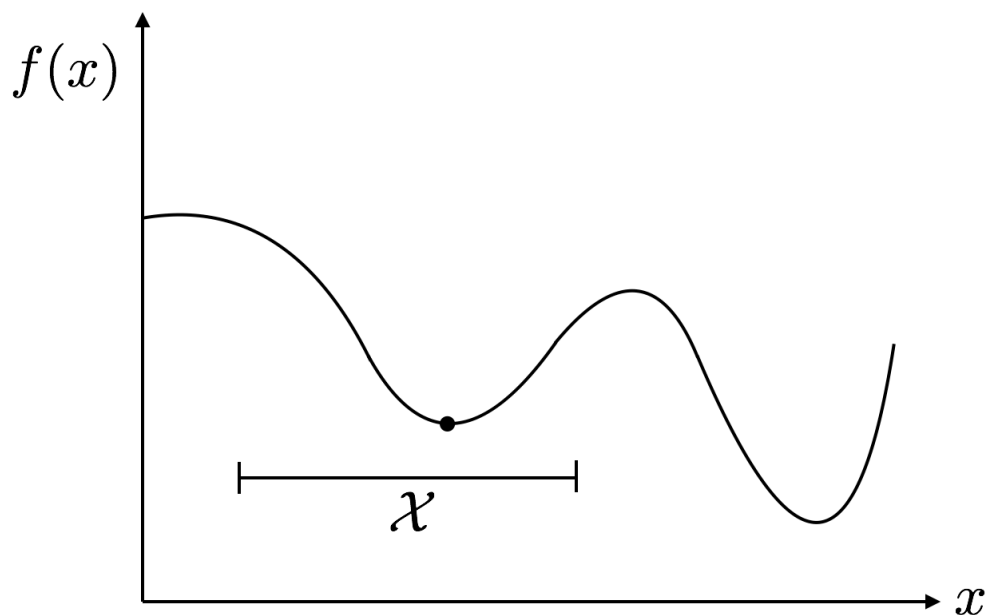
## 1.5 Optimisation Basics

- Recall our generic definition of an optimization problem:

$$\min_{x \in \mathbb{R}^n} f(x) \text{ s.t. } x \in \mathcal{X}$$

- $x$  is our *choice variable* or a *design point*.
- $\mathcal{X}$  is the feasible set.
- $f$  is the *objective function*
- A vector  $x^*$  is a *solution* or a *minimizer* to this problem if  $x^*$  is *feasible* and  $x^*$  minimizes  $f$ .
- Maximization is just minimizing  $(-1)f$ :

$$\min_{x \in \mathbb{R}^n} f(x) \text{ s.t. } x \in \mathcal{X} \equiv \max_{x \in \mathbb{R}^n} -f(x) \text{ s.t. } x \in \mathcal{X}$$



## 1.6 Local Solutions

- Keep in mind that there may be other (better!) solutions outside of your interval of attention.

## 1.7 Constraints

- We often have constraints on problems in economics.

$$\max_{x_1, x_2} u(x_1, x_2) \text{ s.t. } p_1 x_1 + p_2 x_2 \leq y$$

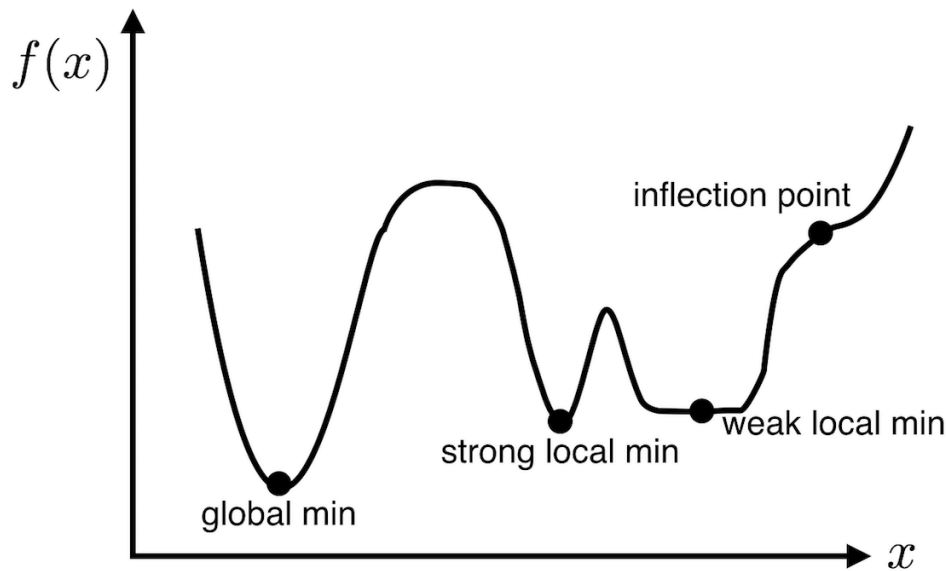
- Constraints define the feasible set  $\mathcal{X}$ .
- It's better to write *weak inequalities* (i.e.  $\leq$ ) rather than strict ones ( $<$ ).

## 1.8 Critical Points

- A given univariate function can exhibit several *critical points* i.e. points where the derivative is zero (as we'll see).
- Ideally we would like to find a *global minimum*. However, that's not always straightforward to do.
- Most of the times, the best we can do is check for a *local minimum*

## 1.9 Conditions for Local Minima

We can define *first and second order necessary conditions*, FONC and SONC. This definition is to point out that those conditions are not sufficient for optimality (only necessary).



### 1.9.1 Univariate $f$

1. **FONC:**  $f'(x^*) = 0$
2. **SONC**  $f''(x^*) \geq 0$  (and  $f''(x^*) \leq 0$  for local maxima)
3. **(SOSC**  $f''(x^*) > 0$  (and  $f''(x^*) < 0$  for local maxima))

### 1.9.2 Multivariate $f$

1. **FONC:**  $\nabla f(x^*) = 0$
2. **SONC**  $\nabla^2 f(x^*)$  is positive semidefinite (negative semidefinite for local maxima)
3. **(SOSC**  $\nabla^2 f(x^*)$  is positive definite (negative definite for local maxima))

```
In [1]: using Plots
        plotlyjs() # choose plotlyjs backend
        v=collect(linspace(-2,2,30)) #avalues
        mini = [x^2 + y^2 for x in v, y in v]
        maxi = -mini
        saddle = [x^2 + y^3 for x in v, y in v];
```

WARNING: Method definition midpoints(Base.Range{T} where T) in module Base at deprecated.jl:56 o  
 WARNING: Method definition midpoints(AbstractArray{T, 1} where T) in module Base at deprecated.j

```
In [2]: surface(v,v,maxi,title="local max",fillalpha=0.8,leg=false,fillcolor=:heat)
```

```
In [3]: surface(v,v,mini,title="local min",fillalpha=0.7,leg=false,fillcolor=:heat)
```

```
In [4]: surface(v,v,saddle,title="saddle",fillalpha=0.7,leg=false,fillcolor=:heat)
```

## 1.10 Example Time: Rosenbrock's Banana Function

A well-known test function for numerical optimization algorithms is the Rosenbrock banana function developed by Rosenbrock in 1960. it is defined by

$$f(\mathbf{x}) = (1 - x_1)^2 + 5(x_2 - x_1^2)^2$$

```
In [5]: # let's get a picture of this
        rosenbrock(x; a=1, b=5) = (a-x[1])^2 + b*(x[2] - x[1]^2)^2
        x=y=collect(linspace(-2,2,100)) # x and y axis
        f = [rosenbrock([ix,iy]) for ix in x, iy in y] #f evaluations

        # plotting
        wireframe(x,y,f,linewidth=:grey)
        surface!(x,y,f,fillcolor=:darkrainbow,colorbar=false)
```

### 1.10.1 Analysing the Rosenbrock function

$$f(\mathbf{x}) = (1 - x_1)^2 + 5(x_2 - x_1^2)^2$$

- Is the point (1,1) satisfying FONC and SONC?
- Let's write down gradient and hessian to find out!

## 1.11 Derivatives and Gradients

- The derivative of a univariate function  $f$  at point  $x$ ,  $f'(x)$  gives the rate at which  $f$  changes at  $x$ .
- Think of a tangent line to a curve.
- There are three different ways to present  $f'$ : forward difference, central difference, and backward difference:

$$f'(x) \equiv \underbrace{\lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}}_{\text{forward diff}} = \underbrace{\lim_{h \rightarrow 0} \frac{f(x+h/2) - f(x-h/2)}{h}}_{\text{central diff}} = \underbrace{\lim_{h \rightarrow 0} \frac{f(x) - f(x-h)}{h}}_{\text{backward diff}}$$

## 1.12 Symbolic Differentiation on a Computer

- If you can write down an analytic form of  $f$ , there are ways to *symbolically* differentiate it.
- This is as if you would do the derivation on paper.
- While this works well, most of the times we don't have an analytic  $f$ .

```
In [6]: using SymEngine
        x = symbols("x");
        f = x^2 + x/2 - sin(x)/x; diff(f, x)
```

```
Out [6]: 1/2 + 2*x + sin(x)/x^2 - cos(x)/x
```

### 1.13 Multiple Dimensions: Gradients

- Unless otherwise noted, we have  $x \in \mathbb{R}^n$  as an  $n$  element vector.
- The **gradient** of a function  $f : \mathbb{R}^n \mapsto \mathbb{R}$  is denoted  $\nabla f : \mathbb{R}^n \mapsto \mathbb{R}^n$  and it returns a vector

$$\nabla f(x) = \left( \frac{\partial f}{\partial x_1}(x), \frac{\partial f}{\partial x_2}(x), \dots, \frac{\partial f}{\partial x_n}(x) \right)$$

- It's **hessian** is a function denoted  $\nabla^2 f(x)$  or  $H_f : \mathbb{R}^n \mapsto \mathbb{R}^{n \times n}$  and returns an  $(n, n)$  matrix given by

$$H_f(x) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_1}(x) & \dots & \frac{\partial^2 f}{\partial x_n \partial x_1}(x) \\ \frac{\partial^2 f}{\partial x_1 \partial x_2}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_2}(x) & \dots & \frac{\partial^2 f}{\partial x_n \partial x_2}(x) \\ \vdots & \vdots & \dots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_n}(x) & \dots & \frac{\partial^2 f}{\partial x_n \partial x_n}(x) \end{pmatrix}$$

- The **directional derivative**  $\nabla_s f(\mathbf{x})$  is an important concept that we will re-encounter when talking about *gradient descent*.
- $\nabla_s f(\mathbf{x})$  tells us the rate of change in  $f$  as  $\mathbf{x}$  is moved at *velocity*  $\mathbf{s}$
- It has similar definition

$$\nabla_s f(\mathbf{x}) \equiv \underbrace{\lim_{h \rightarrow 0} \frac{f(\mathbf{x} + h\mathbf{s}) - f(\mathbf{x})}{h}}_{\text{forward diff}} = \underbrace{\lim_{h \rightarrow 0} \frac{f(\mathbf{x} + h/2\mathbf{s}) - f(\mathbf{x} - h/2\mathbf{s})}{h}}_{\text{central diff}} = \underbrace{\lim_{h \rightarrow 0} \frac{f(\mathbf{x}) - f(\mathbf{x} - h\mathbf{s})}{h}}_{\text{backward diff}}$$

- We can use the gradient  $\nabla f(\mathbf{x})$  to compute it:

$$\nabla_s f(\mathbf{x}) = \nabla f(\mathbf{x})^\top \mathbf{s}$$

- For example, let's compute it for  $f(\mathbf{x}) = x_1 x_2$  at  $\mathbf{x} = [2, 0]$  in direction  $\mathbf{x} = [-1, -1]$

$$\nabla f(\mathbf{x}) = \left[ \frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2} \right] = [x_2, x_1]$$

$$\nabla_s f(\mathbf{x}) = \nabla f(\mathbf{x})^\top \mathbf{s} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \end{bmatrix} = -1$$

### 1.14 Numerical Differentiation

- In most cases we have to compute the derivative numerically. There are 2 strategies:
  1. Finite Differences
  2. Automatic Differentiation

### 1.14.1 Finite Differences

The idea here is to literally take our definition for a derivative from above, and compute it for small  $h$ :

$$f'(x) \approx \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{forward diff}} = \underbrace{\frac{f(x+h/2) - f(x-h/2)}{h}}_{\text{central diff}} = \underbrace{\frac{f(x) - f(x-h)}{h}}_{\text{backward diff}}$$

- The central difference has a quadratic error, as opposed to the forward difference method, hence it's often preferable
- There is however the problem of numerical instability due to a *too small*  $h$ .
- The *complex step method* takes a step in an imaginary direction to bypass this:

$$f'(x) = \frac{\text{Im}(f(x + ih))}{h} + O(h^2) \text{ as } h \rightarrow \infty$$

### 1.14.2 Finite Differences: what's the right step size $h$ ?

- Theoretically, we would like to have  $h$  as small as possible, since we want to approximate the limit at zero.
- In practice, on a computer, there is a limit to this. There is a smallest representable number, as we know.
- `eps()`.
- One can show that the optimal step size is  $h = \sqrt{\text{eps}()}$

```
In [7]: # the Calculus.jl package implements finite differences
using Calculus
```

```
derivative(x->x^2,1.0) # standard signature of function
println("forward = $(Calculus.finite_difference(x->x^2,1.0,:forward))")
println("central = $(Calculus.finite_difference(x->x^2,1.0,:central))")
println("complex = $(Calculus.finite_difference(x->x^2,1.0,:complex))")
println("")
println("forward = $(Calculus.finite_difference( x->sin(x^2) ,/2,:forward))")
println("central = $(Calculus.finite_difference( x->sin(x^2) ,/2,:central))")
println("complex = $(Calculus.finite_difference( x->sin(x^2) ,/2,:complex))")
```

```
forward = 2.000000014901161
central = 1.999999999829379
complex = 2.0
```

```
forward = -2.45424963163794
central = -2.4542495409833656
complex = -2.4542495411512917
```

```
In [8]: # also can compute gradients for multidim functions
Calculus.gradient(x->x[1]^2 * exp(3x[2]),ones(2))
Calculus.hessian(x->x[1]^2 * exp(3x[2]),ones(2))
```

```
Out[8]: 2E2 Array{Float64,2}:
      40.171  120.513
      120.513  180.77
```

```
In [9]: # there is another problem apart from numerical issues with small h:
```

```
f1 = function(x)
    println("evaluation of f1")
    x[1]^2 * exp(3x[2])
end
Calculus.gradient(f1,ones(2))
```

```
# for an f that is expensive to compute, this method quickly becomes infeasible.
```

```
evaluation of f1
evaluation of f1
evaluation of f1
evaluation of f1
```

```
Out[9]: 2-element Array{Float64,1}:
      40.1711
      60.2566
```

## 1.15 Automatic Differentiation (AD)

- Breaks down the actual code that defines a function and performs elementary differentiation rules, after dissecting expressions via the chain rule:

$$\frac{d}{dx}f(g(x)) = \frac{df}{dg} \frac{dg}{dx}$$

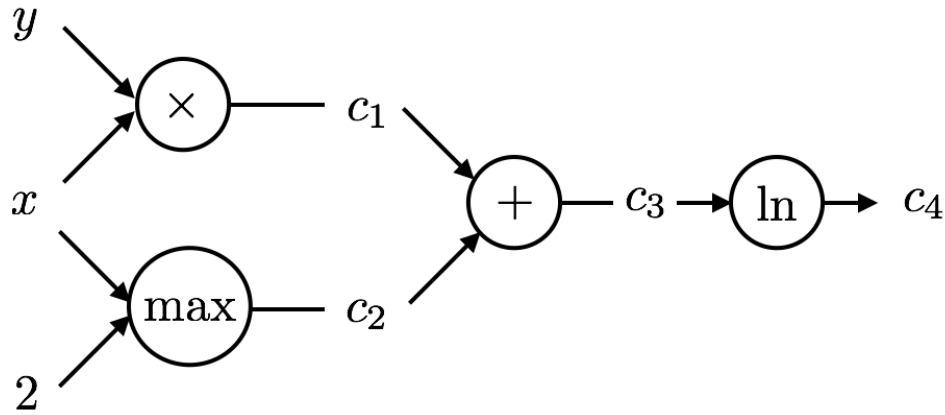
- This produces **analytic** derivatives, i.e. there is **no** approximation error.
- Very accurate, very fast.
- The idea is to be able to *unpick* **expressions** in your code.
- Let's look at an example

Consider the function  $f(x, y) = \ln(xy + \max(x, 2))$ . Let's get the partial derivative wrt  $x$ :

$$\begin{aligned} \frac{\partial f}{\partial x} &= \frac{1}{xy + \max(x, 2)} \frac{\partial}{\partial x}(xy + \max(x, 2)) \\ &= \frac{1}{xy + \max(x, 2)} \left[ \frac{\partial(xy)}{\partial x} + \frac{\partial \max(x, 2)}{\partial x} \right] \\ &= \frac{1}{xy + \max(x, 2)} \left[ \left( y \frac{\partial(x)}{\partial x} + x \frac{\partial(y)}{\partial x} \right) + \left( \mathbf{1}(2 > x) \frac{\partial 2}{\partial x} + \mathbf{1}(2 < x) \frac{\partial x}{\partial x} \right) \right] \\ &= \frac{1}{xy + \max(x, 2)} [y + \mathbf{1}(2 < x)] \end{aligned}$$

where the indicator function  $\mathbf{1}(r) = 1$  if  $r$  evaluates to *true*, 0 otherwise.





- What we just did here, i.e. unpacking the mathematical operation  $\frac{\partial f}{\partial x}$  can be achieved by a computer using a *computational graph*.
- Automatic Differentiation traverses the computational graph of an *expression* either forwards (in *forward accumulation* mode), or backwards (in *reverse accumulation* mode).

This can be illustrated in a **call graph** as below: \* circles denote operators \* arrows are input/output \* We want to unpack the expression by successively applying the chain rule:

$$\frac{df}{dx} = \frac{df}{dc_4} \frac{dc_4}{dx} = \frac{df}{dc_4} \left( \frac{dc_4}{dc_3} \frac{dc_3}{dx} \right) = \frac{df}{dc_4} \left( \frac{dc_4}{dc_3} \left( \frac{dc_3}{dc_2} \frac{dc_2}{dx} \right) \right) = \dots$$

### 1.15.1 Accumulating *forwards* along the call graph

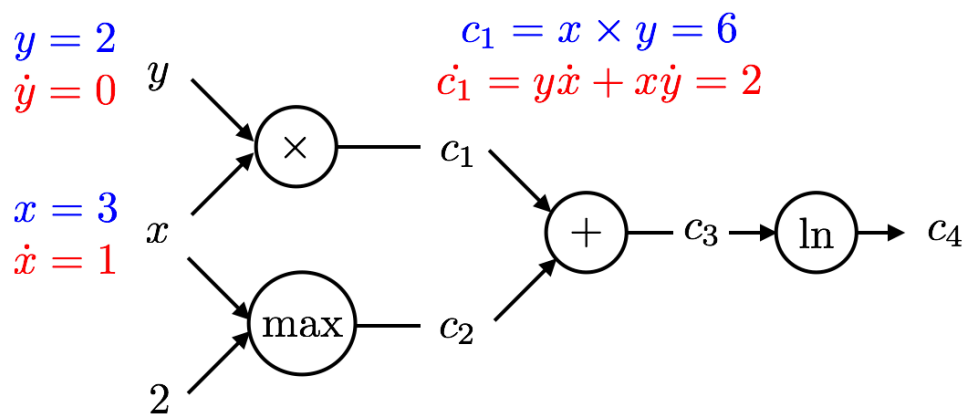
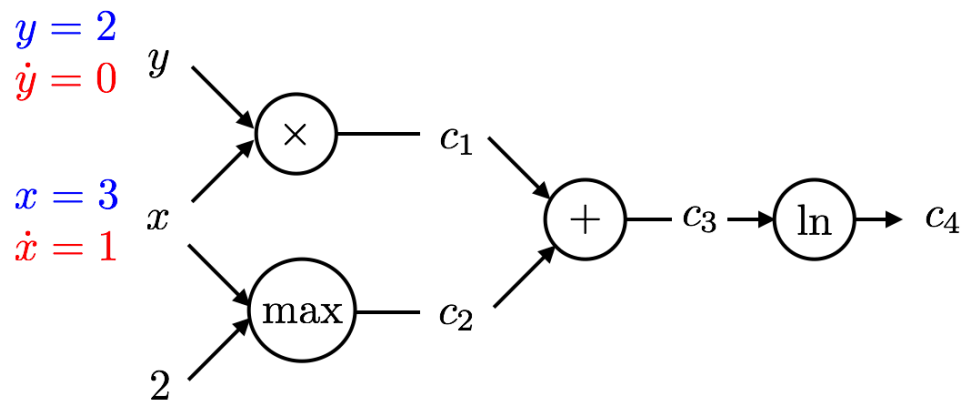
- Let's illustrate how AD in forward mode works for  $x = 3, y = 2$  and the example at hand. Remember that

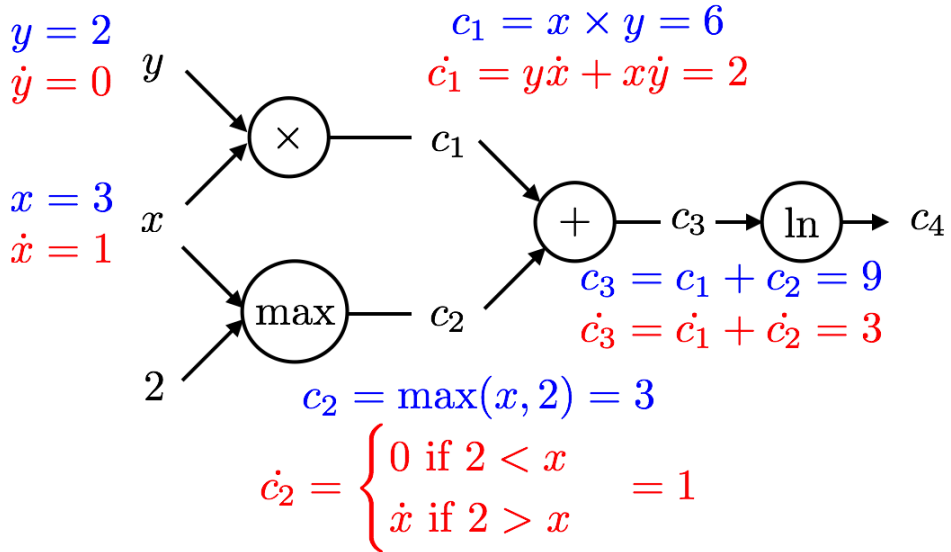
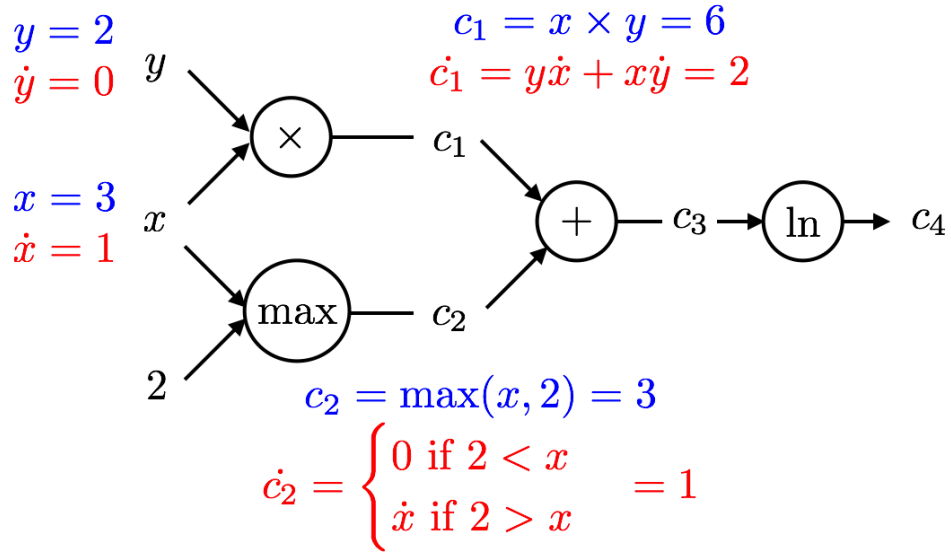
$$f(x, y) = \ln(xy + \max(x, 2))$$

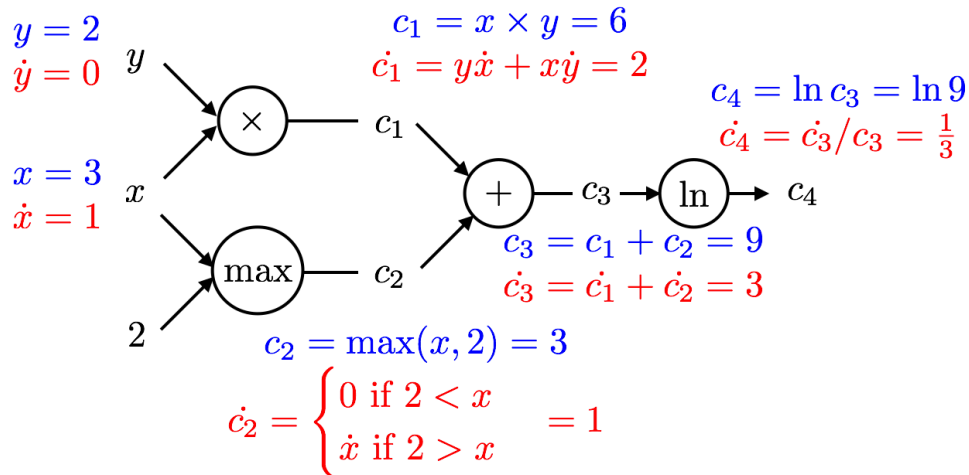
and, hence

$$f(3, 2) = \ln(6 + 3) = \ln 9 \text{ and } \frac{\partial f}{\partial x} = \frac{1}{6 + 3}(2 + 1) = \frac{1}{3}$$

- We start at the left side of this graph with the inputs.
- The key is for each quantity to compute both the value **and** its partial derivative wrt  $x$  in this case.
- Reverse mode works very similarly.
- So, we saw that AD yields both a function value ( $c_4$ ) as well as a derivative ( $c_4$ )
- They have the correct values.
- This procedure required a *single* pass forward over the computational graph.
- Notice that the **exact same amount of computation** needs to be performed by any program trying to evaluate merely the *function value*  $f(3, 2)$ :







1. multiply 2 numbers
2. max of 2 numbers
3. add 2 numbers
4. natural logarithm of a number

QUESTION: WHY HAVE WE NOT BEEN DOING THIS FOR EVER?! ANSWER: **Because it was tedious.**

### 1.15.2 Implementing AD

- What do you need to implement AD?
1. We need what is called *dual numbers*. This is similar to complex numbers, in that each number has 2 components: a standard *value*, and a *derivative*
    - In other words, if  $x$  is a dual number,  $x = a + b\epsilon$  with  $a, b \in \mathbb{R}$ .
    - For our example, we need to know how to do *addition*, *multiplication*, *log* and *max* for such a number type:

$$(a + b\epsilon) + (c + d\epsilon) = (a + c) + (b + d)\epsilon$$

$$(a + b\epsilon) \times (c + d\epsilon) = (ac) + (ad + bd\epsilon)$$

2. You need a programming language where *analyzing expressions* is not too difficult to do. you need a language that can do *introspection*.

### 1.15.3 Implementing Dual Numbers in Julia

This is what it takes to define a Dual number type in julia:

```
struct Dual
    v
```

```

end

Base.:+(a::Dual, b::Dual) = Dual(a.v + b.v, a. + b.)
Base.:*(a::Dual, b::Dual) = Dual(a.v * b.v, a.v*b. + b.v*a.)
Base.log(a::Dual) = Dual(log(a.v), a./a.v)
function Base.max(a::Dual, b::Dual)
    v = max(a.v, b.v)
    = a.v > b.v ? a. : a.v < b.v ? b. : NaN
    return Dual(v, )
end
function Base.max(a::Dual, b::Int)
    v = max(a.v, b)
    = a.v > b ? a. : a.v < b ? 1 : NaN
    return Dual(v, )
end

```

```

In [10]: # ForwardDiff.jl is a julia package for ... Forward AD
using ForwardDiff
x = ForwardDiff.Dual(3,1);
y = ForwardDiff.Dual(2,0);
log(x*y + max(x,2))

```

```

Out[10]: Dual{Void}(2.1972245773362196,0.3333333333333333)

```

```

In [11]: # AutoDiffSource.jl is for reverse mode
using AutoDiffSource
@g(x, y) = log(x*y + max(x,2));
y, = g(3,2);
y
x, y = ()

```

```

INFO: Recompiling stale cache file /Users/74097/.julia/lib/v0.6/AutoDiffSource.ji for module AutoDiffSource

```

```

Out[11]: (0.3333333333333333, 0.3333333333333333)

```

### 1.15.4 Analyzing Expressions

- Everything you type into julia is an Expression:

```
mutable struct Expr <: Any
```

Fields:

```

head :: Symbol
args :: Array{Any,1}
typ  :: Any

```

```

In [12]: println("create an explicit expression by `quoting` it with `:`")
expr = :(x + y)

```

```
println("typeof(expr)=$(typeof(expr))")
```

```
println("\ncan evaluate an expression")
```

```
x = 2;y=3
```

```
println(eval(expr))
```

```
println("\nand we can pick it apart:")
```

```
println("expr.head=$(expr.head)")
```

```
println("expr.args=$(expr.args)")
```

create an explicit expression by `quoting` it with `:`  
typeof(expr)=Expr

can evaluate an expression

5

and we can pick it apart:

```
expr.head=call
```

```
expr.args=Any[:+, :x, :y]
```

In [13]: *# our example was*

```
ex = :(log(x*y + max(x,2)))
```

*#we can access every piece of the call graph, e.g.*  
println(ex.args[1])

*# entire call graph:*  
dump(ex)

log

Expr

```
head: Symbol call
```

```
args: Array{Any}((2,))
```

```
1: Symbol log
```

```
2: Expr
```

```
head: Symbol call
```

```
args: Array{Any}((3,))
```

```
1: Symbol +
```

```
2: Expr
```

```
head: Symbol call
```

```
args: Array{Any}((3,))
```

```
1: Symbol *
```

```
2: Symbol x
```

```
3: Symbol y
```

```
typ: Any
```

```
3: Expr
```

```
head: Symbol call
```

```
args: Array{Any}((3,))
```

```
1: Symbol max
2: Symbol x
3: Int64 2
typ: Any
typ: Any
typ: Any
```

## 1.16 (Unconstrained) Optimization in Julia

- Umbrella Organisation: <http://www.juliaopt.org>
  - We will make ample use of this when we talk about constrained optimisation.
  - The Julia Interface to the very well established C-Library `NLopt` is called `NLopt.jl`. One could use `NLopt` without constraints in an unconstrained problem.
- `Roots.jl`: Simple algorithms that find the zeros of a univariate function.
- Baseline Collection of unconstrained optimization algorithms: `Optim.jl`

## 1.17 Introducing `Optim.jl`

- Multipurpose unconstrained optimization package
  - provides 8 different algorithms with/without derivatives
  - univariate optimization without derivatives