SciencesPo Computational Economics
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1 Computational Economics: Optimization I

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- 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 Proceedure:
    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* proceedure.
- 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:

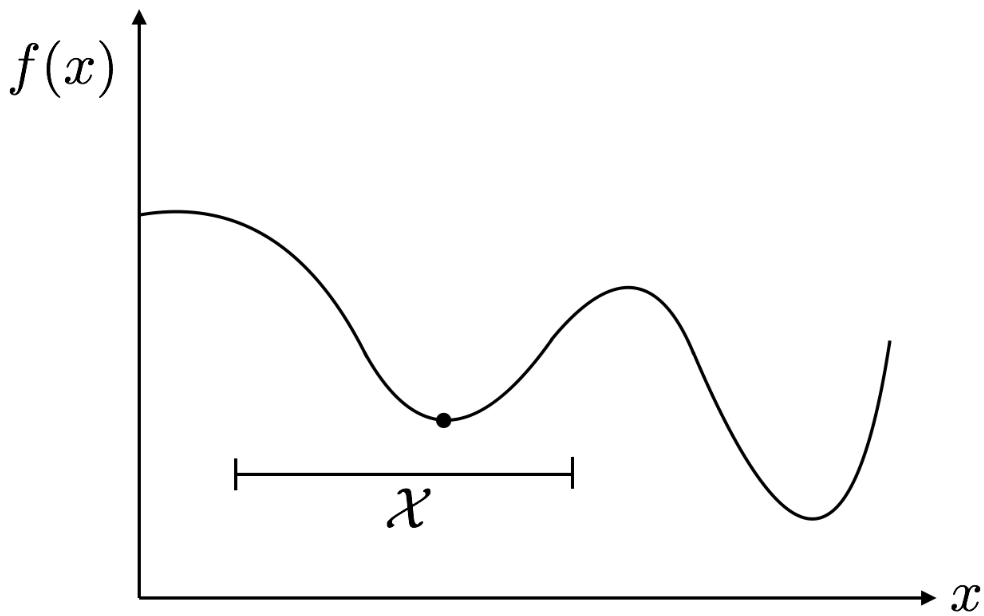
$$\min_{x \in \mathbb{R}^n} f(x) \text{ s.t. } x \in \mathcal{X}$$

- 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

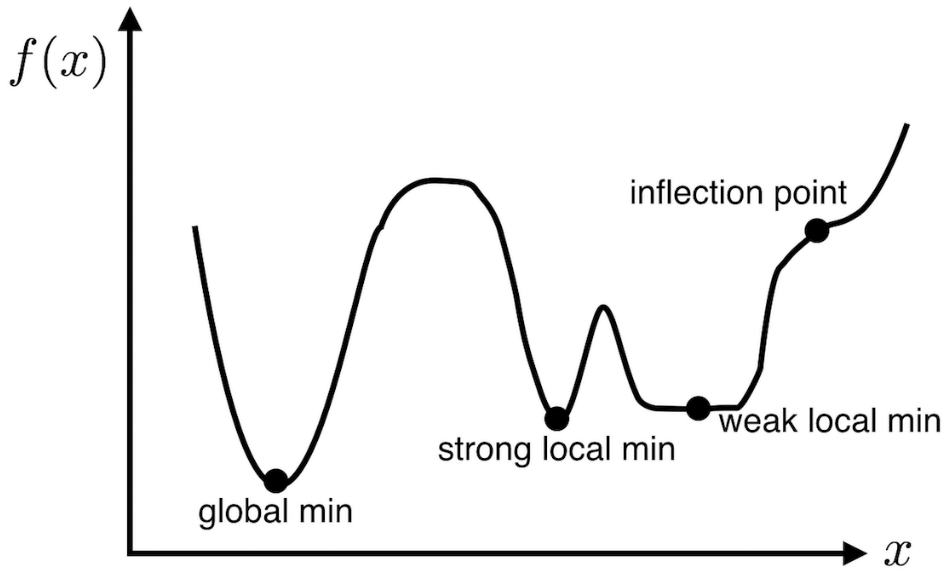
- We often have constraints on problems in economics.

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

- 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))  #ăvalues
        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
WARNING: Method definition midpoints(AbstractArray{T, 1} where T) in module Base at deprecated
```

```
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]  #ăf evaluations

        # plotting
        wireframe(x,y,f,linecolor=: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:

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

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

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

- 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

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

- 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 similiar defintion

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

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

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

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

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

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

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 preferrable
- 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:

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

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 $h = \sqrt{\texttt{eps()}}$

```
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) ,π/2,:forward))")
        println("central = $(Calculus.finite_difference( x->sin(x^2) ,π/2,:central))")
        println("complex = $(Calculus.finite_difference( x->sin(x^2) ,π/2,:complex))")
```

```
forward = 2.000000014901161
central = 1.9999999999829379
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]: 2×2 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
```

Automatic Differentiation (AD)

- Breaks down the actual `code` that defines a function and performs elementary differentiation rules, after disecting 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:

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

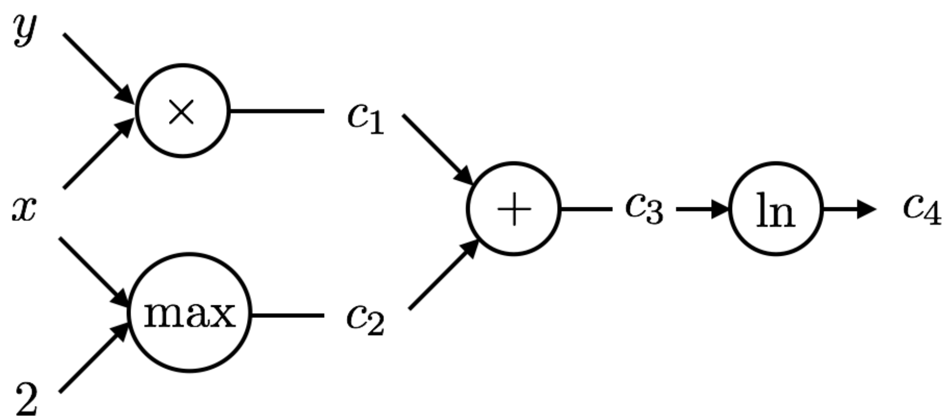
where the indicator function $\mathbf{1}(r) = 1$ if r evaluates to *true*, 0 otherwise.

- 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:

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



1.14.3 Accumulating *forwards* along the call graph

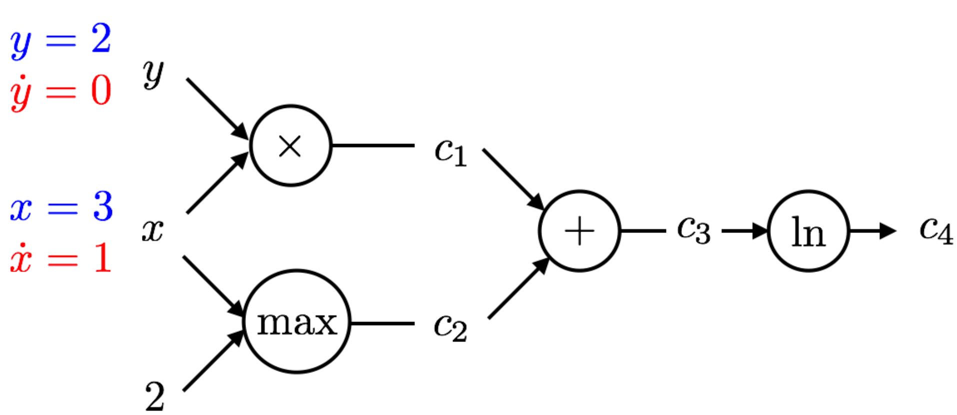
- Let's illustrate how AD in forward mode works for $x = 3, y = 2$ and the example at hand. Remember that

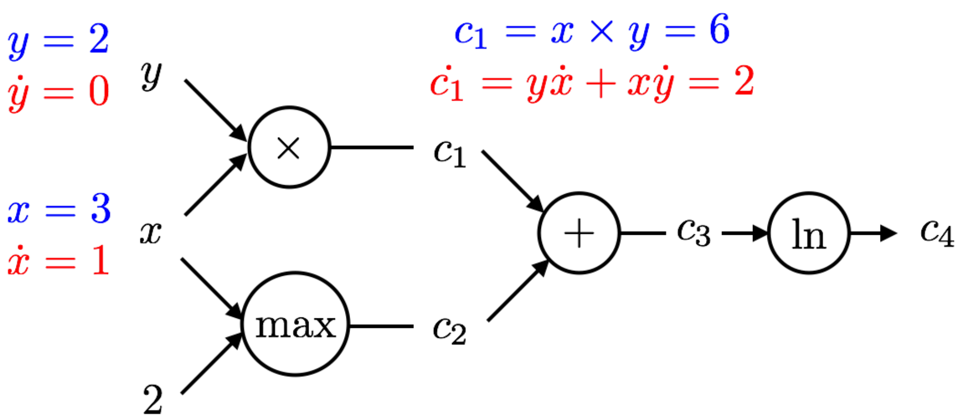
$$f(x, y) = \ln(xy + \max(x, 2))$$

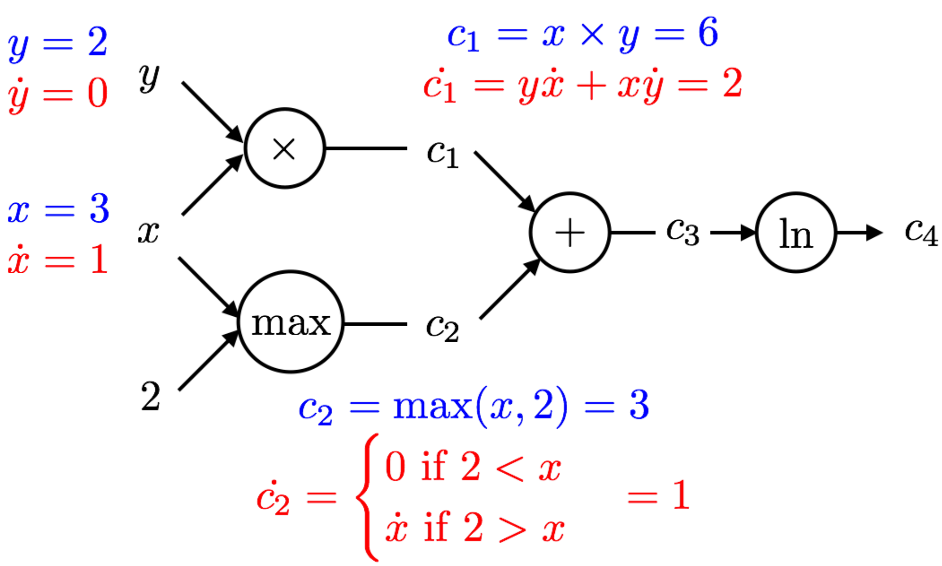
  and, hence

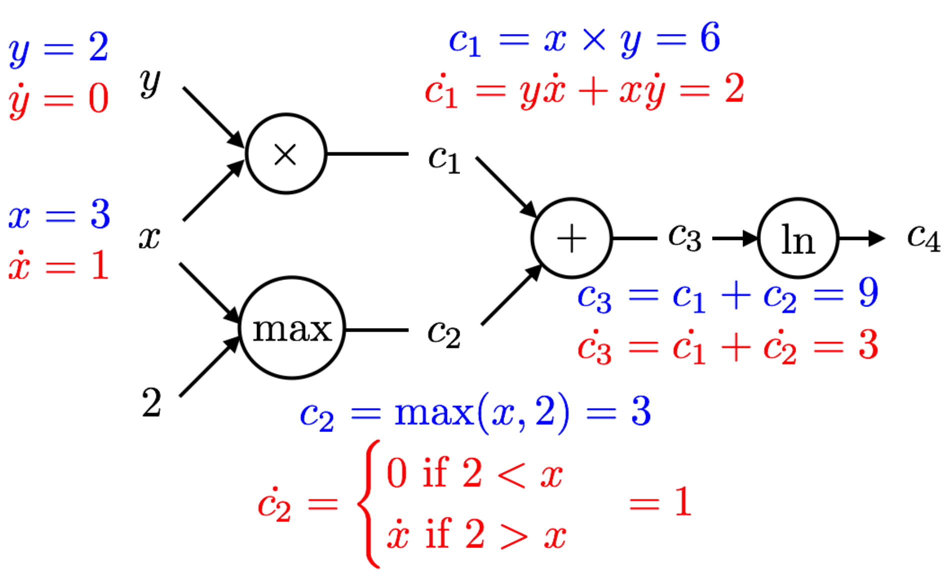
$$f(3, 2) = \ln(6 + 3) = \ln 9 \text{ and } \frac{\partial f}{\partial x} = \frac{1}{6+3}(2+1) = \frac{1}{3}$$

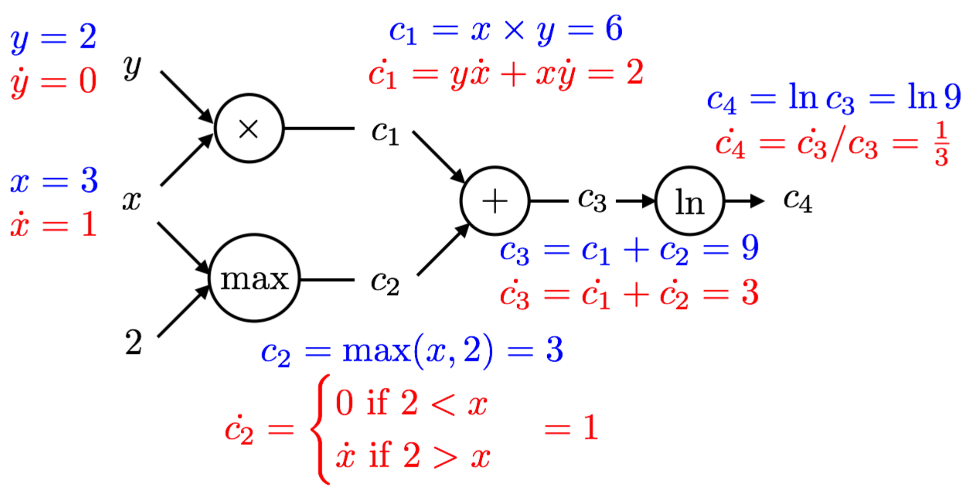
- We start at the left side of this graph with the inputs.
- The key is for each quantity to compute both the value **and** it's partial derivative wrt x in this case.




$y = 2$
$\dot{y} = 0$
$x = 3$
$\dot{x} = 1$
y
x
2
$\times$
max
c_1
c_2
$+$
c_3
ln
c_4
$c_1 = x \times y = 6$
$\dot{c_1} = y\dot{x} + x\dot{y} = 2$


$y = 2$
$\dot{y} = 0$
$x = 3$
$\dot{x} = 1$
y
x
2
$\times$
max
c_1
c_2
$+$
c_3
ln
c_4
$c_1 = x \times y = 6$
$\dot{c_1} = y\dot{x} + x\dot{y} = 2$
$c_2 = \max(x, 2) = 3$
$\dot{c_2} = \begin{cases} 0 \text{ if } 2 < x \\ \dot{x} \text{ if } 2 > x \end{cases} = 1$


$y = 2$
$\dot{y} = 0$
$x = 3$
$\dot{x} = 1$
y
x
2
$\times$
max
c_1
c_2
$+$
c_3
ln
c_4
$c_1 = x \times y = 6$
$\dot{c_1} = y\dot{x} + x\dot{y} = 2$
$c_3 = c_1 + c_2 = 9$
$\dot{c_3} = \dot{c_1} + \dot{c_2} = 3$
$c_2 = \max(x, 2) = 3$
$\dot{c_2} = \begin{cases} 0 \text{ if } 2 < x \\ \dot{x} \text{ if } 2 > x \end{cases} = 1$



- Reverse mode works very similarly.
- So, we saw that AD yields both a function value (c_4) as well as a derivative ($\dot{c_4}$)
- 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.**

1.14.4 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*.

1.14.5 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 Au

Out[11]: (0.3333333333333333, 0.3333333333333333)
```

1.14.6 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)))
#ăwe 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
```

1.15 (Unconstrained) Optimization in `Julia`

- Umbrella Organisation: `http://www.juliaopt.org`
  - We will make ample use of this when we talk about constrained optimsation.
  - 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`

1.16 Introducing `Optim.jl`

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