Zygote

Bridging Machine Learning and Scientific Computing

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A powerful, high level language with high performance.

Pythonic, mathematical syntax that looks like notation.

Performance consistently within 2x of tuned C code.

Most of Julia is written in Julia!

```julia
function mandel(z)
    c = z
    maxiter = 80
    for n = 1:maxiter
        if abs(z) > 2
            return n-1
        end
        z = z^2 + c
    end
    return maxiter
end
```

Scientific Computing

JUMP

FEDERAL RESERVE BANK OF NEW YORK • INCORPORATED MAY 18, 1914 •

DSGE.jl

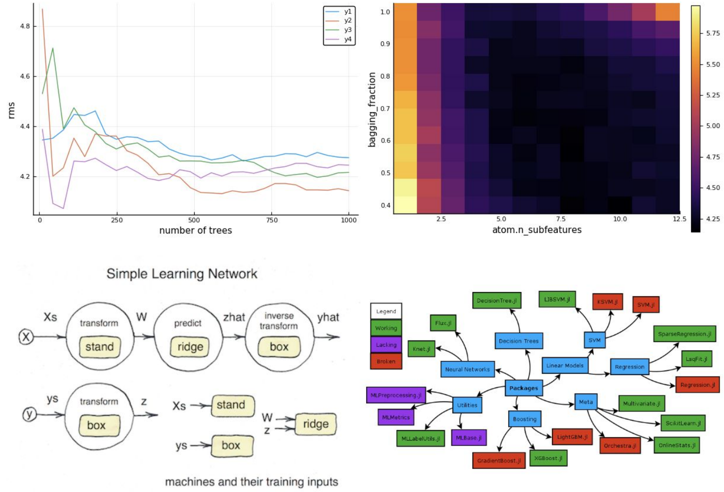
DifferentialEquations.jl

Cori

Machine Learning

flux

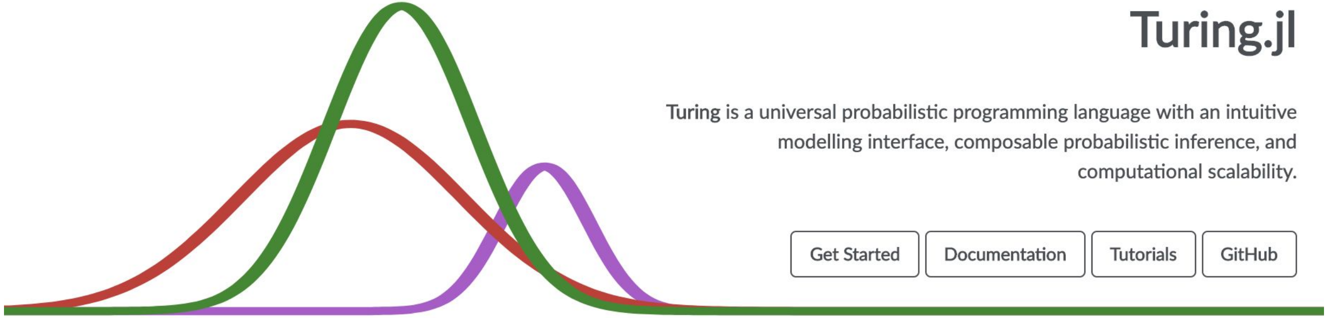
MLJ



Turing.jl

Turing is a universal probabilistic programming language with an intuitive modelling interface, composable probabilistic inference, and computational scalability.

Get Started | Documentation | Tutorials | GitHub



Machine Learning	Scientific Computing
High-level and flexible (Python)	Low-level and manual (Fortran)
High overhead, focus on tensor operations and manual vectorisation	Low overhead, focus on scalar operations
Relatively simple programs (network architectures)	Regularly run over millions of lines of code.
Mutation support considered advanced/unusual.	Research on auto-vectorisation, shared memory parallelism, checkpointing etc.


AD
SCIENTIFIC COMPUTING
MACHINE LEARNING
imgflip.com

Tapenade → Ruthless pragmatism and scalability. Output can be highly optimised using existing optimising compilers.

λ the Ultimate Backpropagator → Elegant recursive formalism, including nested AD (closure), convenience (callee-derives) and bags of expressive power.

```
(v1.2) pkg> add Zygote
 Resolving package versions...
  Updating `~/.julia/environments/v1.2/Project.toml`
  [e88e6eb3] + Zygote v0.3.2
  Updating `~/.julia/environments/v1.2/Manifest.toml`
  [1a297f60] + FillArrays v0.6.3
  [7869d1d1] + IRTools v0.2.2
  [e88e6eb3] + Zygote v0.3.2

julia> using Zygote

julia> function pow(x, n)
           r = 1
           while n > 0
               n -= 1
               r *= x
           end
           return r
       end
pow (generic function with 1 method)

julia> pow(5, 3)
125

julia> gradient(x -> pow(x, 3), 5)
(75,)

julia>
```

User Function

```
function pow(x, n)
  r = 1
  while n > 0
    n -= 1
    r *= x
  end
  return r
end
```

Primal

```
1: (%2, %3)
  br 2 (%3, 1)
2: (%4, %5)
  %6 = %4 > 0
  br 4 unless %6
  br 3
3:
  %7 = %4 - 1
  %8 = %5 * %2
  br 2 (%7, %8)
4:
  return %5
```

Adjoint

```
1: (%1)
  br 2 (%1, 0)
2: (%2, %4)
  br 4 unless @6
  br 3
3:
  %10 = %2 * @2
  %11 = %2 * @5
  %14 = %4 + %11
  br 2 (%10, %14)
4:
  return (%4, 0)
```

```
pow(5, 3) == 125
gradient(pow, 5, 3) == (75, 0)
```

```
julia> y, back = J(pow, 5, 3);

julia> back(1)
(75, nothing)
```

$$y = f(x_1, x_2, \ldots)$$

$$y, \mathcal{B} = \mathcal{J}(f, x_1, x_2, \ldots)$$

$$\bar{x}_1, \bar{x}_2, \ldots = \mathcal{B}(\bar{y})$$

```julia
function foo(x)
  a = bar(x)
  b = baz(a)
  return b
end
```

```julia
function J(::typeof(foo), x)
  a, da = J(bar, x)
  b, db = J(baz, a)
  return b, function(b̄)
    ā = db(b̄)
    x̄ = da(ā)
    return x̄
  end
end
```

```
➜  ~ j
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.2.0-rc1.2 (2019-05-31)
 _/ |\__'_|_|_|\__'_|  |  release-1.2/3fcb168ceb (fork: 74 commits, 81 days)
|__/                   |

julia> fs = Dict("sin" => sin, "cos" => cos, "tan" => tan);

julia> f(x) = fs[readline()](x)
f (generic function with 1 method)

julia> f(1)
sin
0.8414709848078965

julia> gradient(f, 1)
sin
(0.5403023058681398,)

julia> 
```

```
J(::typeof(sin), x) = sin(x), ȳ -> ȳ*cos(x)
```

```
@adjoint sin(x) = sin(x), ȳ -> ȳ*cos(x)
```

Core compiler pass is ~200 lines of code

All semantics added via custom adjoints –
mutation, data structures, checkpointing, etc.

```julia
nestlevel() = 0

@adjoint nestlevel() = nestlevel()+1, _ -> nothing
```

```julia
julia> function f(x)
         println(nestlevel(), " levels of nesting")
         return x
       end

julia> f(1);
0 levels of nesting

julia> grad(f, 1);
1 levels of nesting

julia> grad(x -> x*grad(f, x), 1);
2 levels of nesting
```

```julia
@adjoint hook(f, x) = x, Δ -> (f(Δ),)

hook(-, x) # reverse the gradient of x

@adjoint checkpoint(f, x...) =
  f(x...), Δ -> J(f, x...)[2](Δ)

@adjoint function forwarddiff(f, x)
  y, J = forward_jacobian(f, x)
  y, Δ -> (J'Δ,)
end
```

```julia
julia> hook(f, x) = x
hook (generic function with 1 method)

julia> @adjoint hook(f, x) = x, Δ -> (nothing, f(Δ),)

julia> gradient(2, 3) do a, b
         a*b
       end
(3, 2)

julia> gradient(2, 3) do a, b
         hook(-, a) * b
       end
(-3, 2)

julia> gradient(2, 3) do a, b
         hook(ā -> @show(ā), a) * b
       end
ā = 3
(3, 2)
```

Differentiation á la Carte

- Mixed-mode AD (forward, reverse, Taylor series, …)
- Forward-over-reverse (Hessians)
- Cross-language AD
- Support for Complex and other number types
- Easy custom gradients
- Checkpointing
- Gradient hooks
- Custom types (colours!)
- Hardware backends: CPU, CUDA, TPU, …
- ~~Deeply nested AD~~ (WIP)

```julia
dense(W, b, σ = identity) =
  x → σ.(W * x .+ b)

chain(f ... ) = foldl(∘, reverse(f))

mlp = chain(
  dense(randn(5, 10), randn(5), tanh),
  dense(randn(2, 5), randn(2)))

x = rand(10)

mlp(x)        ⌄ Float64[2]
                0.646…
                2.51…

m̄ = gradient(mlp) do m
  sum(m(x))
end  ((f = (W = [-0.9909137325976834 0.11388709497399903 … -0.7210152885786678 0.9901

m -= η * m̄ # Gradient descent
```

Deep learning in 5 lines.

Data Structures & Mutation

```julia
julia> using Colors

julia> a, b = RGB(1, 0, 0), RGB(0, 1, 0)
(RGB{N0f8}(1.0,0.0,0.0), RGB{N0f8}(0.0,1.0,0.0))

julia> a.r^2
1.0N0f8

julia> gradient(c -> c.r^2, a)
((r = 2.0f0, g = nothing, b = nothing),)

julia> colordiff(a, b)
86.6082357376344

julia> gradient(a -> colordiff(a, b), a)
((r = 0.4590887719632896, g = -9.598786801605689, b = 14.181383399012862),)
```

```julia
julia> vars = Dict(:r => 0, :n => 0)
Dict{Symbol,Int64} with 2 entries:
  :n => 0
  :r => 0

julia> function pow(x, n)
         vars[:r] = 1
         vars[:n] = n
         while vars[:n] > 0
           vars[:n] -= 1
           vars[:r] *= x
         end
       end
pow (generic function with 1 method)

julia> pow(5, 3); vars[:r]
125

julia> gradient(x -> (pow(x, 3); vars[:r]), 5)
(75,)

julia> vars[:r]
125
```

```
py"""
  import torch.nn.functional as F
  def foo(W, b, x):
    return F.sigmoid(W@x + b)
  """

W = randn(2, 5)
b = randn(2)
x = rand(5)

foo(W, b, x)
```

```
Float64[2]
0.207…
0.499…
```

```
dW, db = gradient(W, b) do W, b
  sum((foo(W, b, x) .- [0, 1]).^2)
end
```

```
(2×5 Array{Float64,2}:, Float64[2])
```

```julia
@adjoint function pycall(f, x...; kw...)
 x = map(py, x)
 y = pycall(f, x...; kw...)
 y.detach().numpy(), function (ȳ)
   y.backward(gradient = py(ȳ))
   (nothing, map(x -> x.grad.numpy(), x)...)
 end
end
```

Some Bonus Features

```julia
@grad function (a::Real * b::Real)
  c = a*b
  function back(Δ)
    0//0
  end
  c, back
end  > _forward

function pow(x, n)
  r = one(x)
  while n > 0
    r *= x
    n -= 1
  end
  return r
end  > pow

gradient(pow, 2, 3)
```

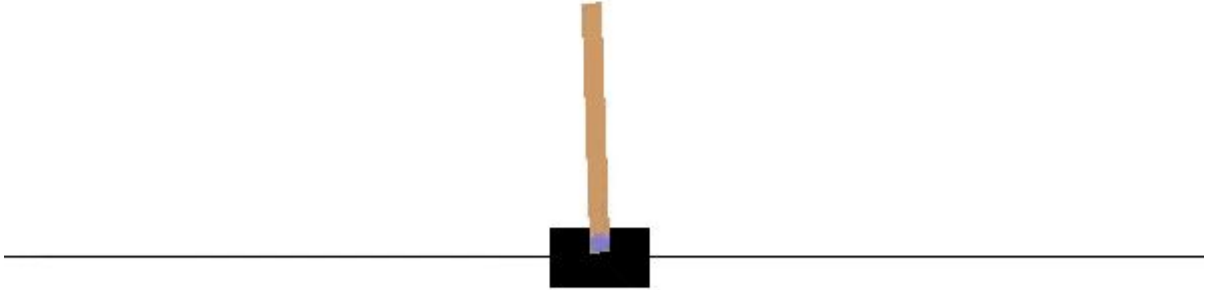
```
ArgumentError: invalid rational: zero(Int64)//zero(Int64)
in top-level scope at base/none
in gradient at Zygote/src/compiler/interface.jl:34
in  at Zygote/src/compiler/interface.jl:28
in  at Zygote/src/compiler/interface2.jl
in pow at test.jl:17
in  at Zygote/src/lib/lib.jl:33
in  at test.jl:9
in // at base/rational.jl:13
```

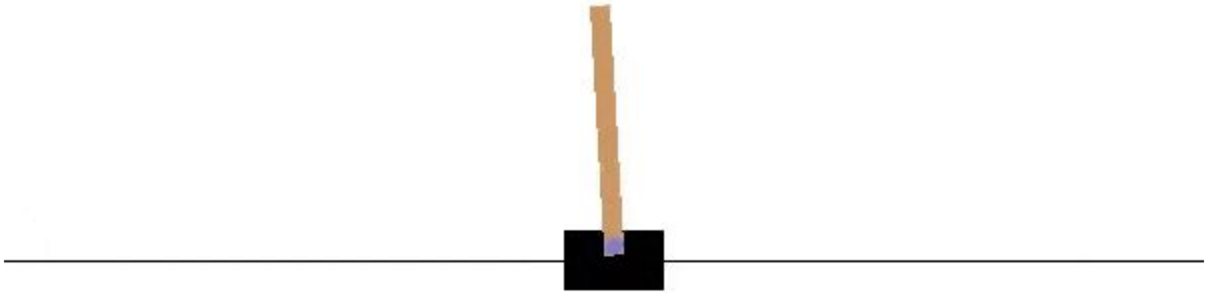
```julia
using Zygote

function f(x)
  for i = 1:5
    x = sin(cos(x))
  end
  return x
end

function loop(x, n)
  r = x/x
  for i = 1:n
    r *= f(x)
  end
  return sin(cos(r))
end

gradient(loop, 2, 3)

Zygote.@profile loop(2, 3)

function logsumexp(x::Array{Float64,1})
```

Future Challenges

- Mutation of values is hard
- Need adjoints to cover the entire standard library
- Compiler improvements
    - More functional-style optimisations
    - Better heuristics for AD-generated code
- Fast code vs. dynamic semantics
- Differentiating Julia’s concurrency and parallelism constructs
- Reducing overheads: currently ~50ns per operation
    - Great compared to ML frameworks but far from optimal

Differentiating CartPole





CartPole Controller

CartPole State

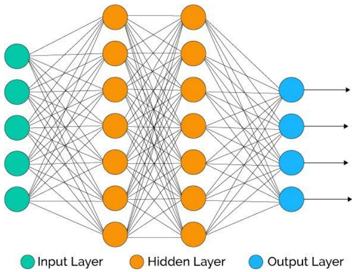
Control Parameters

Loss

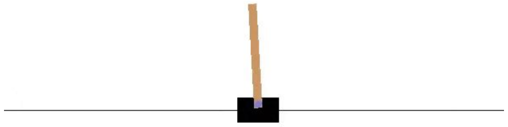
Neural Network

Environment

angle = -3°
velocity = 0.5°/s



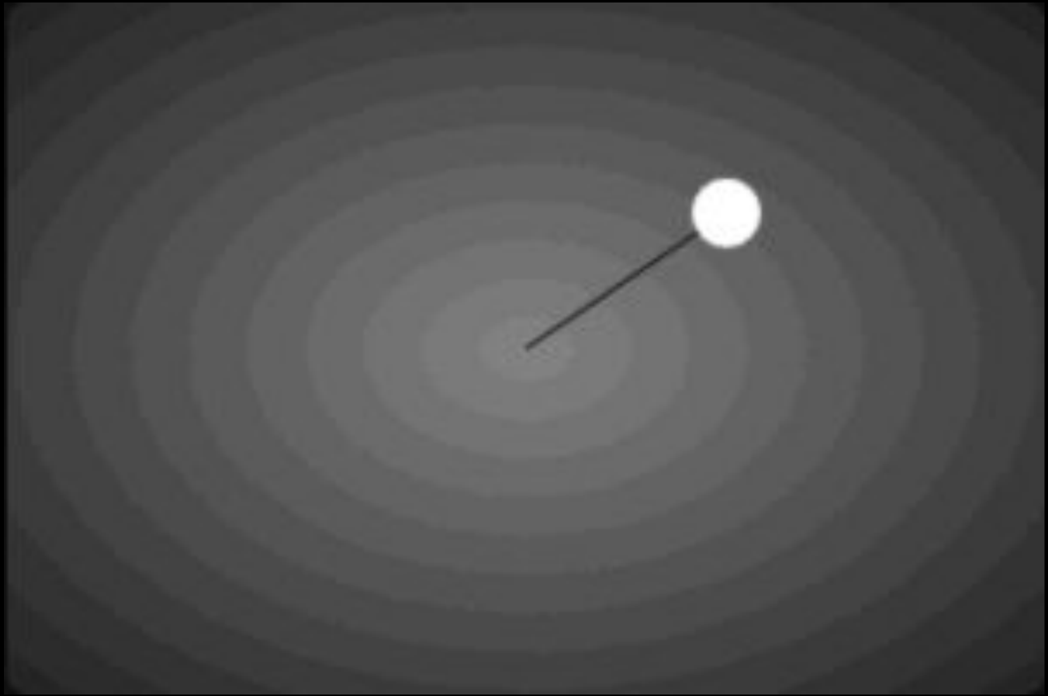
{left, right}



angle^2

Backpropagation

Model-free RL	Differentiable Programming
~400	6
episodes to solve	episodes to solve



pumas.ai

Pharmacokinetics/Pharmacodynamics

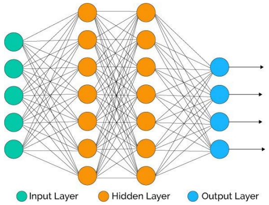
Patient Data
(e.g. X-ray scans)

Simulation parameters
(e.g. drug half-life)

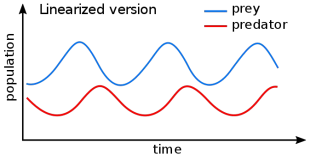
Treatment Outcome

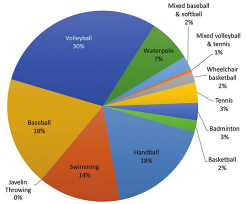
Neural Network

ODE Solver



$\beta = 0.56$





Backpropagation

Is Differentiable Programming a Thing?

Bona fide programming paradigm, or yet another rebranding of neural networks?

Programming Paradigms

A collection of design patterns and organising principles, built on a common abstraction. Answers questions like: how do I manage complexity, implement data structures, build abstractions, represent a domain, or encourage code reuse?

- Procedural programming – imperative procedures
- Object-oriented programming – objects
- Functional programming – pure functions
- Logic programming – predicates
- Concurrent programming – communicating processes
- Symbolic programming – rewrite rules
- Stack-oriented programming – stack operations
- Differentiable programming – ???

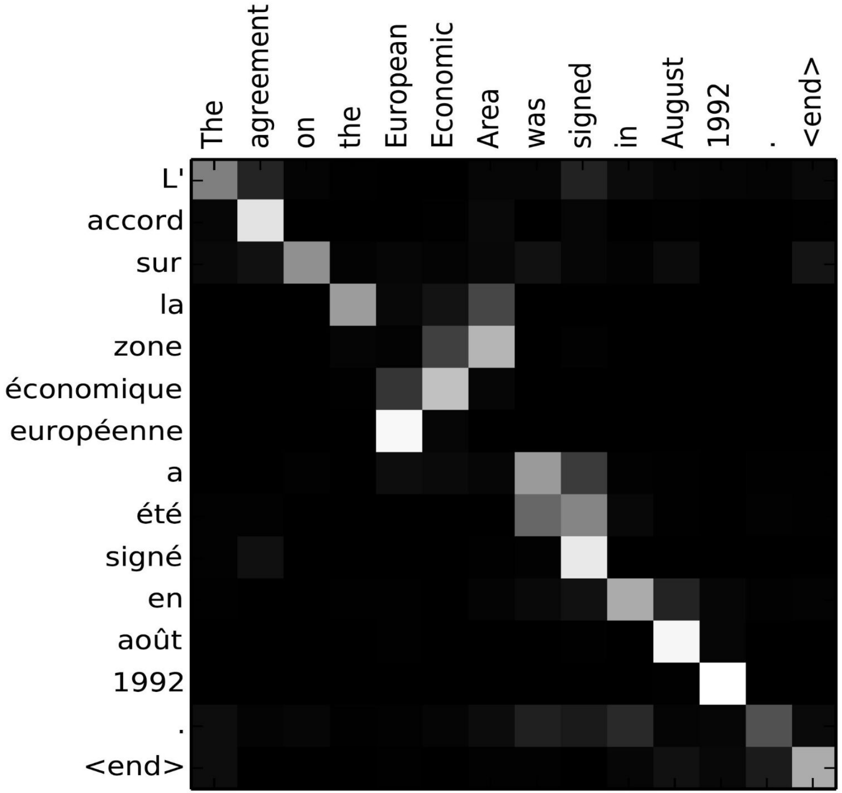
Layers

A lambda that closes over numerical parameters.

```
dense(W, b, σ = identity) =
  x → σ.(W * x .+ b)

chain(f ...) = foldl(∘, reverse(f))

mlp = chain(
  dense(randn(5, 10), randn(5), tanh),
  dense(randn(2, 5), randn(2)))

x = rand(10)

mlp(x)
```

```
Float64[2]
0.646…
```

Data Structures: Attention



See also: Neural Turing Machine

Resources

- Julia Language: julialang.org
- Flux ML library: fluxml.ai
- Zygote AD: github.com/FluxML/Zygote.jl
- Differentiable Control fluxml.ai/blog/2019/03/05/dp-vs-rl.html
- Google Scholar for more papers and technical introductions