Mixed-Mode Automatic Differentiation in

Jarrett Revels, Miles Lubin & Juan Pablo Vielma (MIT)

Hi, I’m Jarrett

- Started writing Julia code in 2013, working on AD in Julia since 2015
- Downstream packages: *JuMP*, *Celeste*, *Optim*, *DifferentialEquations*, *RigidBodyDynamics*, *ValidatedNumerics*, etc...
- Previously worked in the Julia Group @ CSAIL under Alan Edelman
- Authored Julia's performance regressions testing facilities (*BenchmarkTools*)
- Recently started an engineering position under Juan Pablo Vielma
- Continuing to work on AD, transitioning to direct JuMP development in the fall

Last Year's Talk: ForwardDiff.jl

- Implements multidimensional dual numbers
- Fully stack-allocated and aggressively inlined, plays well with SIMD
- Tagging system prevents perturbation confusion and drives nested differentiation
- Provides a differentiation API instead of exposing dual numbers
- Used by JuMP for calculating Hessian-vector products

Reverse-Mode AD

Compared to Forward-Mode AD

- Propagating input perturbation forward ⟶ propagate output sensitivity backwards
  - Forward-mode AD evaluates chain rule from right (inner function) to left (outer function)
  - Reverse-mode AD evaluates chain rule from left (outer function) to right (inner function)

- Main hurdle: requires a reverse-traversable computation graph
  - Graph can be defined declaratively via special objects/syntax (JuMP, TensorFlow)
  - ...or by running code + intercepting operations (ReverseDiff, Autograd, PyTorch)

- Which mode should I use?
  - `output_dimension > input_dimension && input_dimension << code_size` ⟶ Use forward mode
  - `output_dimension < input_dimension && input_dimension >> code_size` ⟶ Use reverse mode
  - `output_dimension ≈ input_dimension` ⟶ That's tough

Code Representation

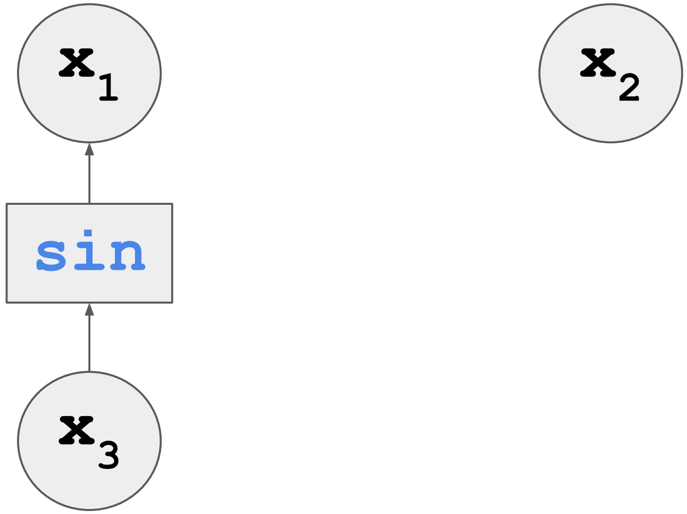
```
function f(x_1, x_2)
    # ?
end
```

Graph Representation

Code Representation

```
function f(x₁, x₂)
    x₃ = sin(x₁)
    # ?
end
```

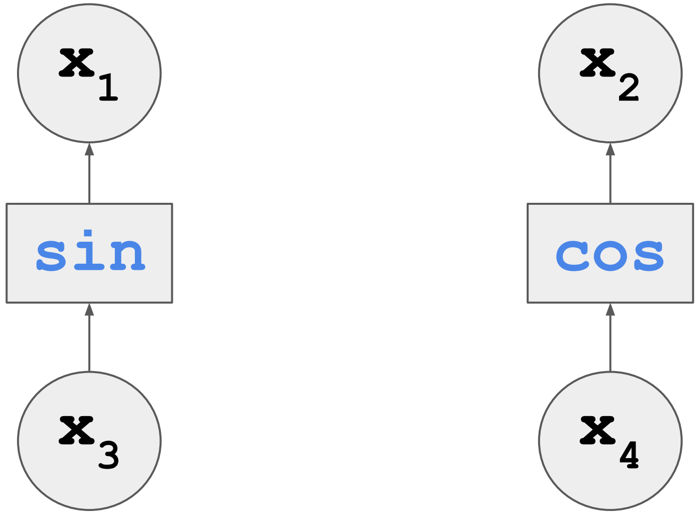
Graph Representation



Code Representation

```
function f(x₁, x₂)
    x₃ = sin(x₁)
    x₄ = cos(x₂)
    # ?
end
```

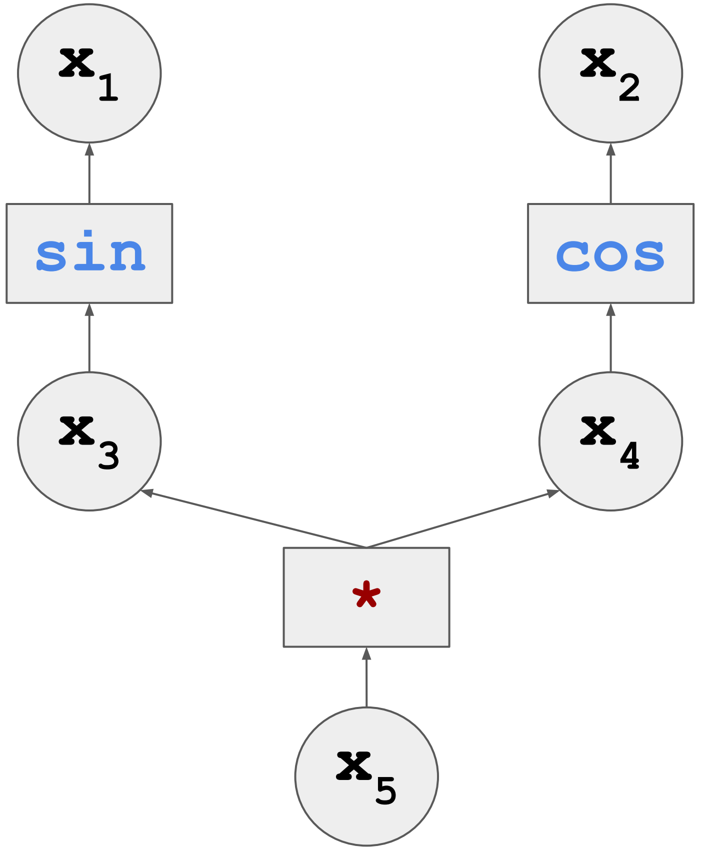
Graph Representation



Code Representation

```
function f(x₁, x₂)
    x₃ = sin(x₁)
    x₄ = cos(x₂)
    x₅ = x₃ * x₄
    # ?
end
```

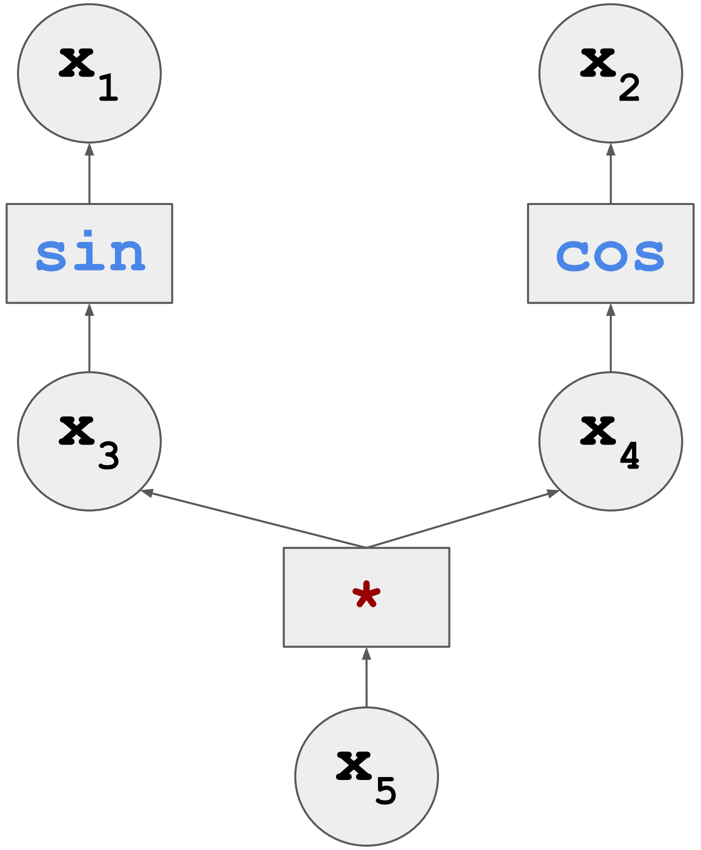
Graph Representation

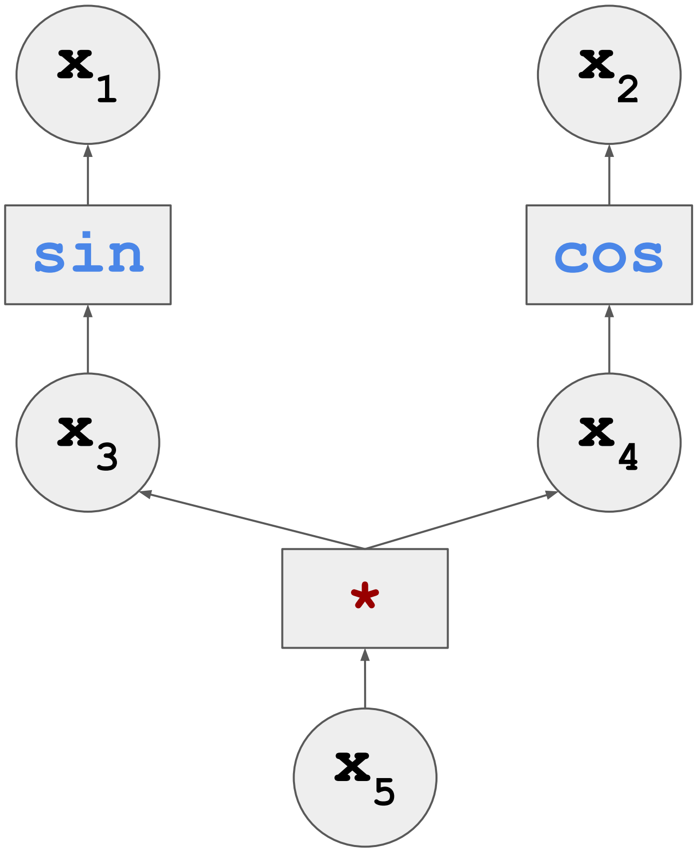


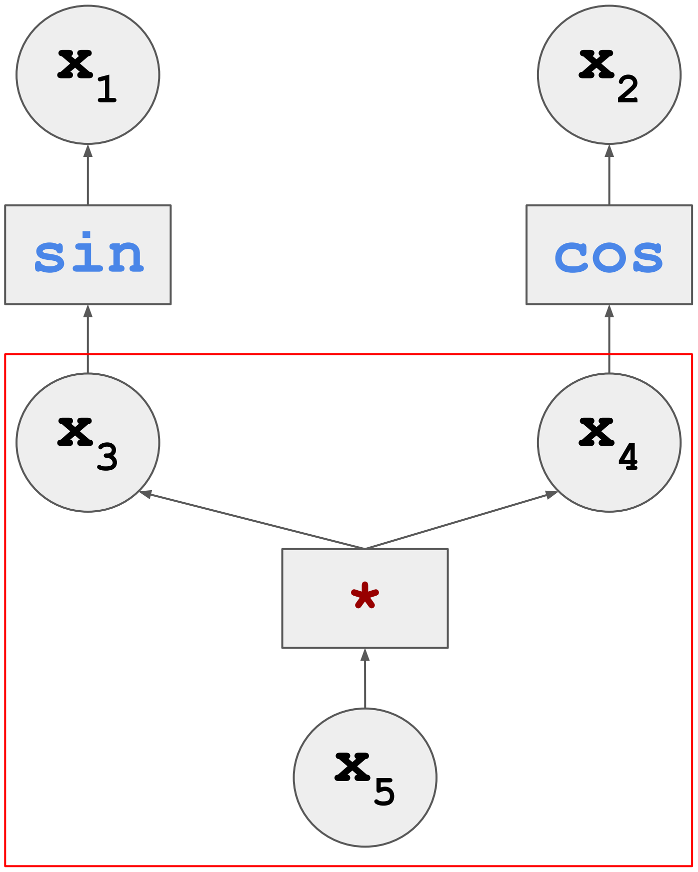
Code Representation

```
function f(x₁, x₂)
    x₃ = sin(x₁)
    x₄ = cos(x₂)
    x₅ = x₃ * x₄
    return x₅
end
```

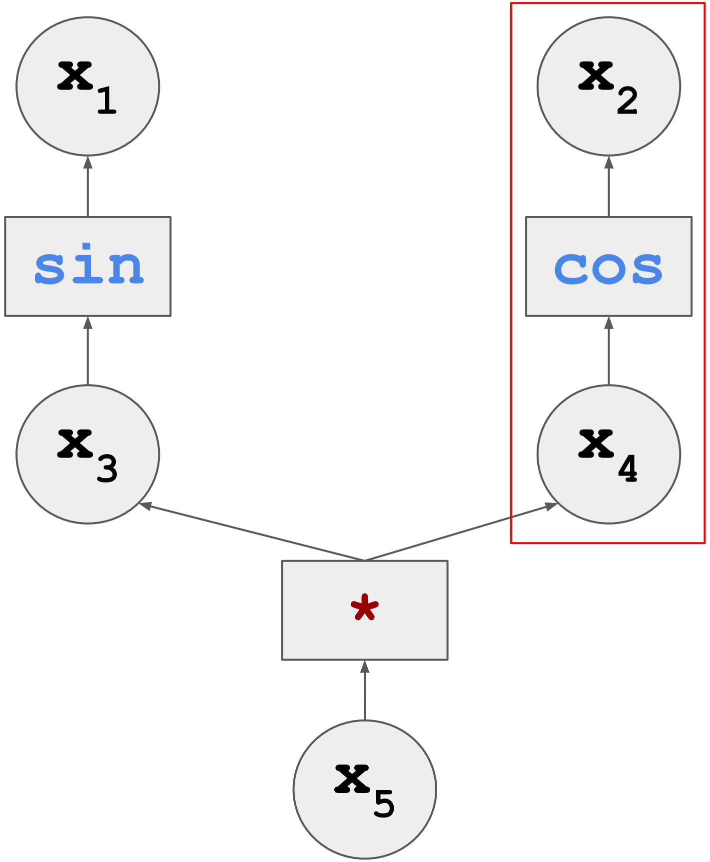
Graph Representation




x1
sin
x2
cos
x3
x4
*
x5

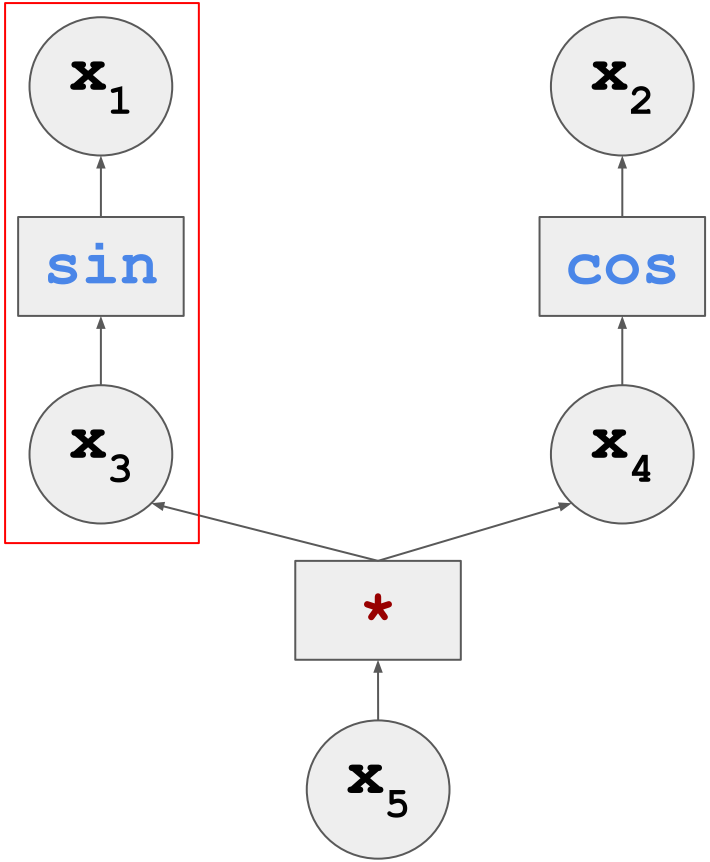


$$x_5 = x_3 * x_4$$



$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$



$x_3 = \sin(x_1)$

$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$

Multivariable Chain Rule

$y_i = \partial x_5/\partial x_i$

$= \text{sum}(y_j * \partial x_j/\partial x_i \text{ for } j \text{ in parents}(i))$

Derivative Outputs

$\partial f(x_1,x_2)/\partial x_1 = \partial x_5/\partial x_1$
$= y_1$

$\partial f(x_1,x_2)/\partial x_2 = \partial x_5/\partial x_2$
$= y_2$

Numerical Results

$x_1 = 1.0$	$y_1 = 0.0$
$x_2 = 1.0$	$y_2 = 0.0$
$x_3 = 0.0$	$y_3 = 0.0$
$x_4 = 0.0$	$y_4 = 0.0$
$x_5 = 0.0$	$y_5 = 0.0$

$x_3 = \sin(x_1)$

$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$

Multivariable Chain Rule

$y_i = \partial x_5 / \partial x_i$

$= \text{sum}(y_j * \partial x_j / \partial x_i \text{ for } j \text{ in parents}(i))$

Derivative Outputs

$\partial f(x_1, x_2) / \partial x_1 = \partial x_5 / \partial x_1$
$= y_1$

$\partial f(x_1, x_2) / \partial x_2 = \partial x_5 / \partial x_2$
$= y_2$

Numerical Results

$x_1 = 1.0$ $y_1 = 0.0$
$x_2 = 1.0$ $y_2 = 0.0$
$x_3 = 0.8$ $y_3 = 0.0$
$x_4 = 0.0$ $y_4 = 0.0$
$x_5 = 0.0$ $y_5 = 0.0$

$x_3 = \sin(x_1)$

$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$

Multivariable Chain Rule

$y_i = \partial x_5/\partial x_i$

$= \text{sum}(y_j * \partial x_j/\partial x_i \text{ for } j \text{ in parents}(i))$

Derivative Outputs

$\partial f(x_1,x_2)/\partial x_1 = \partial x_5/\partial x_1$
$= y_1$

$\partial f(x_1,x_2)/\partial x_2 = \partial x_5/\partial x_2$
$= y_2$

Numerical Results

$x_1 = 1.0$	$y_1 = 0.0$
$x_2 = 1.0$	$y_2 = 0.0$
$x_3 = 0.8$	$y_3 = 0.0$
$x_4 = 0.5$	$y_4 = 0.0$
$x_5 = 0.0$	$y_5 = 0.0$

$x_3 = \sin(x_1)$

$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$

Multivariable Chain Rule

$y_i = \partial x_5/\partial x_i$

$= \text{sum}(y_j * \partial x_j/\partial x_i \text{ for } j \text{ in parents}(i))$

Derivative Outputs

$\partial f(x_1,x_2)/\partial x_1 = \partial x_5/\partial x_1$
$= y_1$

$\partial f(x_1,x_2)/\partial x_2 = \partial x_5/\partial x_2$
$= y_2$

Numerical Results

$x_1 = 1.0$	$y_1 = 0.0$
$x_2 = 1.0$	$y_2 = 0.0$
$x_3 = 0.8$	$y_3 = 0.0$
$x_4 = 0.5$	$y_4 = 0.0$
$x_5 = 0.4$	$y_5 = 0.0$

$x_3 = \sin(x_1)$

$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$

Multivariable Chain Rule

$y_i = \partial x_5/\partial x_i$

$= \text{sum}(y_j * \partial x_j/\partial x_i \text{ for } j \text{ in } \text{parents}(i))$

Derivative Outputs

$\partial f(x_1,x_2)/\partial x_1 = \partial x_5/\partial x_1$
$= y_1$

$\partial f(x_1,x_2)/\partial x_2 = \partial x_5/\partial x_2$
$= y_2$

Numerical Results

$x_1 = 1.0$	$y_1 = 0.0$
$x_2 = 1.0$	$y_2 = 0.0$
$x_3 = 0.8$	$y_3 = 0.0$
$x_4 = 0.5$	$y_4 = 0.0$
$x_5 = 0.4$	$y_5 = 1.0$

$x_3 = \sin(x_1)$

$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$

Multivariable Chain Rule

$y_i = \partial x_5/\partial x_i$

$\quad = \mathrm{sum}(y_j * \partial x_j/\partial x_i \ \mathbf{for}\ j\ \mathbf{in}\ \mathrm{parents}(i))$

Derivative Outputs

$\partial f(x_1,x_2)/\partial x_1 = \partial x_5/\partial x_1$
$\qquad = y_1$

$\partial f(x_1,x_2)/\partial x_2 = \partial x_5/\partial x_2$
$\qquad = y_2$

Numerical Results

$x_1 = 1.0$	$y_1 = 0.0$
$x_2 = 1.0$	$y_2 = 0.0$
$x_3 = 0.8$	$y_3 = 0.5$
$x_4 = 0.5$	$y_4 = 0.8$
$x_5 = 0.4$	$y_5 = 1.0$

$x_3 = \sin(x_1)$

$x_4 = \cos(x_2)$

$x_5 = x_3 * x_4$

$y_3 \mathrel{+}= y_5 * x_4$

$y_4 \mathrel{+}= y_5 * x_3$

Multivariable Chain Rule

```
y_i = ∂x_5/∂x_i

    = sum(y_j * ∂x_j/∂x_i for j in parents(i))
```

Derivative Outputs

```
∂f(x_1,x_2)/∂x_1 = ∂x_5/∂x_1
                 = y_1

∂f(x_1,x_2)/∂x_2 = ∂x_5/∂x_2
                 = y_2 = -0.7
```

Numerical Results

x_1 = 1.0	y_1 = 0.0
x_2 = 1.0	y_2 = -0.7
x_3 = 0.8	y_3 = 0.5
x_4 = 0.5	y_4 = 0.8
x_5 = 0.4	y_5 = 1.0

```
x_3 = sin(x_1)
--------------------
```

```
x_4 = cos(x_2)
--------------------
y_2 += y_4 * -(sin(x_2))
```

```
x_5 = x_3 * x_4
--------------------
y_3 += y_5 * x_4
y_4 += y_5 * x_3
```

Multivariable Chain Rule

```
y_i = ∂x_5/∂x_i

    = sum(y_j * ∂x_j/∂x_i for j in parents(i))
```

Derivative Outputs

$\partial f(x_1, x_2)/\partial x_1 = \partial x_5/\partial x_1$
$= y_1 = 0.2$

$\partial f(x_1, x_2)/\partial x_2 = \partial x_5/\partial x_2$
$= y_2 = -0.7$

Numerical Results

$x_1 = 1.0$	$y_1 = 0.2$
$x_2 = 1.0$	$y_2 = -0.7$
$x_3 = 0.8$	$y_3 = 0.5$
$x_4 = 0.5$	$y_4 = 0.8$
$x_5 = 0.4$	$y_5 = 1.0$

```
x_3 = sin(x_1)
-----------------------
y_1 += y_3 * cos(x_1)
```

```
x_4 = cos(x_2)
-----------------------
y_2 += y_4 * -(sin(x_2))
```

```
x_5 = x_3 * x_4
-----------------------
y_3 += y_5 * x_4

y_4 += y_5 * x_3
```

ReverseDiff.jl

- ❏ Uses operator overloading to dynamically intercept and record native Julia code to an instruction tape
- ❏ Multiple dispatch + JIT + run-time type information enables compiled, specialized primitives
- ❏ Supports array primitives, linear algebraic derivative definitions, and most **`AbstractArray`** types
- ❏ Supports dynamic forward pass (re-recording allows for complex control flow - loops, recursion, etc.)
- ❏ Supports static forward/reverse passes over tape (precomputed dispatch + preallocated instruction caches)
- ❏ Mixed-mode AD! Scalar subgraphs automatically differentiated via ForwardDiff. Includes scalar kernels of elementwise functions (e.g. map/broadcast).

A Few Realizations

"He must be a thorough fool who can learn nothing from his own folly."
- A.W. Hare

Julia Is Pretty Good At This Stuff

- ❏ Seamless/precise operator overloading with no performance penalty
- ❏ Target code can be mostly “AD-unaware”; just needs to be numerically type-generic.
- ❏ Primitives defined via normal Julia code - no magic for creation/extension
- ❏ Writing data-flow semantics in Julia over a Julia-represented DAG means grants efficient nested data-flow semantics for “free”.
- ❏ Heterogeneous device support for "free" (e.g. GPUArrays)

ReverseDiff For JuMP?

- Cons vs. ReverseDiffSparse:
  - ReverseDiffSparse, as the name implies, does indeed exploit Hessian sparsity
  - ReverseDiffSparse has better variable storage locality for scalar operations

- Pros vs. ReverseDiffSparse:
  - ReverseDiffSparse doesn’t support array primitives
  - ReverseDiffSparse doesn’t support dynamic graphs
  - ReverseDiffSparse doesn’t directly support native Julia code
  - ReverseDiffSparse isn’t numerically type-generic
  - ReverseDiffSparse can’t easily handle nested differentiation

- Takeaway: ReverseDiff is more versatile and extensible, but ReverseDiffSparse has some important performance optimizations for tackling large-scale problems

ReverseDiff For Deep Learning?

- ReverseDiff’s API doesn’t expose variable construction directly
  - ...though internal utilities are similar to PyTorch’s/TensorFlow’s exposed APIs

- ReverseDiff’s dynamic recording mechanism writes to a static graph representation
  - ...great for recording traditional optimization graphs
  - ...not so great for recording dynamic graphs in deep learning

- Different Graph Regimes
  - Optimization: Many nodes, computationally cheap scalar operations
  - Deep Learning: Fewer nodes, computationally expensive array operations
  - This is why ML people are cool with fully dynamic taping methods - traversal overhead is negligible

ReverseDiff For…Not AD?

- A native-Julia trace-to-DAG package would be generally useful outside of AD
  - Dynamic code analysis/optimization
  - Parallel operation scheduling
  - Automatic pre-allocation/memory management
  - Interval constraint programming
  - Serialization of Julia code to other DAG frameworks
- It would require generalizing ReverseDiff's taping/execution mechanisms
- It could also enable better AD anyway (e.g. edge-pushing algorithm for sparse Hessians)

Enter *Cassette.jl*

"Multiple dispatch is dead, long live multiple dispatch!"

- Anonymous

What is Cassette?

- A native Julia execution tracer + data flow package for propagating values and arbitrary metadata through pure-Julia computation graphs.
- Inspired by both traditional optimization and deep learning worlds - different representations are supported for static and dynamic graphs
- Exposes trace interception mechanisms to downstream library authors as a hijackable processing pipeline.
- The next version of ReverseDiff is Cassette’s prototypical application
- ***Doesn’t rely on argument type propagation to intercept function calls!***

Multiple Dispatch Is Dead…

```
# we'll define primitives for this on the next slide
struct Interceptor{T,N} <: AbstractArray{T,N}
    data::AbstractArray{T,N}
end
```

Multiple Dispatch Is Dead...

```
# we'll define primitives for this on the next slide
struct Interceptor{T,N} <: AbstractArray{T,N}
     data::AbstractArray{T,N}
end

# primitives defined on `Interceptor` will just call this
struct Intercepted{F} <: Function
     func::F
end

unwrap(x) = x
unwrap(i::Interceptor) = i.data
unwrap(i::Intercepted) = i.func

(i::Intercepted{F})(args...) = (println("called $F");  unwrap(i)(unwrap.(args)...))
```

Multiple Dispatch Is Dead...

```
const AMBIGUOUS_TYPES = [subtypes(AbstractArray)...]

#### 1-arg primitive --> 1 method ################################
Base.f(x::Interceptor) = Intercepted(f)(x)
```

Multiple Dispatch Is Dead...

```julia
const AMBIGUOUS_TYPES = [subtypes(AbstractArray)...]

#### 1-arg primitive --> 1 method ################################
Base.f(x::Interceptor) = Intercepted(f)(x)

#### 2-arg primitive --> ~50 methods! ###########################
Base.f(x::Interceptor, y::Interceptor) = Intercepted(f)(x, y)
for T in AMBIGUOUS_TYPES
     Base.f(x::Interceptor, y::T) = Intercepted(f)(x, y)
     Base.f(x::T, y::Interceptor) = Intercepted(f)(x, y)
end
```

Multiple Dispatch Is Dead...

```julia
const AMBIGUOUS_TYPES = [subtypes(AbstractArray)...]

#### 1-arg primitive --> 1 method ################################
Base.f(x::Interceptor) = Intercepted(f)(x)

#### 2-arg primitive --> ~50 methods ##############################
Base.f(x::Interceptor, y::Interceptor) = Intercepted(f)(x, y)
for T in AMBIGUOUS_TYPES
     Base.f(x::Interceptor, y::T) = Intercepted(f)(x, y)
     Base.f(x::T, y::Interceptor) = Intercepted(f)(x, y)
end

#### 3-arg primitive --> ~2000 methods!!! ######################
Base.f(x::Interceptor, y::Interceptor, z::Interceptor) = Intercepted(f)(x, y, z)
for T in AMBIGUOUS_TYPES
     Base.f(x::Interceptor, y::Interceptor, z::T) = Intercepted(f)(x, y, z)
     Base.f(x::Interceptor, y::T, z::Interceptor) = Intercepted(f)(x, y, z)
     Base.f(x::T, y::Interceptor, z::Interceptor) = Intercepted(f)(x, y, z)
     for S in AMBIGUOUS_TYPES
          Base.f(x::Interceptor, y::T, z::S) = Intercepted(f)(x, y, z)
          Base.f(x::T, y::Interceptor, z::S) = Intercepted(f)(x, y, z)
          Base.f(x::T, y::S, z::Interceptor) = Intercepted(f)(x, y)
     end
end
```

Multiple Dispatch Is Dead...

```julia
const AMBIGUOUS_TYPES = [subtypes(AbstractArray)...]

#### 1-arg primitive --> 1 method ################################
Base.f(x::Interceptor) = Intercepted(f)(x)

#### 2-arg primitive --> ~50 methods #############################
Base.f(x::Interceptor, y::Interceptor) = Intercepted(f)(x, y)
for T in AMBIGUOUS_TYPES
    Base.f(x::Interceptor, y::T) = Intercepted(f)(x, y)
    Base.f(x::T, y::Interceptor) = Intercepted(f)(x, y)
end

#### 3-arg primitive --> ~2000 methods ###########################
Base.f(x::Interceptor, y::Interceptor, z::Interceptor) = Intercepted(f)(x, y, z)
for T in AMBIGUOUS_TYPES
    Base.f(x::Interceptor, y::Interceptor, z::T) = Intercepted(f)(x, y, z)
    Base.f(x::Interceptor, y::T, z::Interceptor) = Intercepted(f)(x, y, z)
    Base.f(x::T, y::Interceptor, z::Interceptor) = Intercepted(f)(x, y, z)
    for S in AMBIGUOUS_TYPES
        Base.f(x::Interceptor, y::T, z::S) = Intercepted(f)(x, y, z)
        Base.f(x::T, y::Interceptor, z::S) = Intercepted(f)(x, y, z)
        Base.f(x::T, y::S, z::Interceptor) = Intercepted(f)(x, y)
    end
end
```

GROSS

...Long Live Multiple Dispatch!

```julia
#### AST pruning pseudocode ##############################

function code_info_with_intercepted_calls(Tuple{F,A,B,C...})
     # 1. Get `CodeInfo` for signature `Tuple{F,A,B,C}`
     # 2. Walk through SSA-form AST and wrap all calls with `Intercepted`
     # 3. Return the modified `CodeInfo`
end

#### `Trace` function wrapper ############################

struct Trace{F,world} <: Function
     func::F
     Trace(func::F) where {F} = new{F,get_world_counter()}(func)
end

@generated function (t::Trace{F,world})(args...) where {F,world}
     return code_info_with_intercepted_calls(F, args...)
end
```

...Long Live Multiple Dispatch!

```
function f(x)
    a = one(eltype(x))
    b = 100 * a
    result = zero(eltype(x))
    for i in 1:length(x)
        result += b * (a - x[i])
    end
    return result
end

# ↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓

function (::Trace{typeof(f)})(x)
    a = Intercepted(one)(Intercepted(eltype)(x))
    b = Intercepted(*)(100, a)
    result = Intercepted(zero)(Intercepted(eltype)(x))
    for i in Intercepted(UnitRange)(1, Intercepted(length)(x))
        result = Intercepted(+)(result, Intercepted(*)(b, Intercepted(-)(a,
                    Intercepted(getindex)(x, i))))
    end
    return result
end
```

…Long Live Multiple Dispatch!

- ❑ No need for target functions to be type generic
- ❑ No need to define an ungodly number of methods per primitive
- ❑ No need to define new number/array/etc. types just to propagate metadata or hijack execution flow
- ❑ Hijack behavior can be overloaded via normal Julia dispatch of downstream function wrappers
- ❑ In the future, we can also wrap SSA-form control flow instructions

The Future

- ❑ Finish + document + test + release Cassette (targeting Julia v0.7)
- ❑ Replace ForwardDiff/ReverseDiff with new Cassette-based packages
- ❑ Replace ReverseDiffSparse → new backend for JuMP
  - ❑ Locality + sparse Hessian optimizations for Cassette graphs
- ❑ Evangelize Cassette for other regimes

Acknowledgements

- *Juan Pablo Vielma, Miles Lubin* @ MIT Operations Research Center
- *Cosmin Petra* @ Lawrence Livermore National Lab
- The Julia Group @ MIT CSAIL: *Alan Edelman*, *Andreas Noack*, *Peter Ahrens*
- *Jameson Nash, Mike Innes* @ Julia Computing (...and everybody else there as well!)
- *Simon Danisch* @ GPUArrays, Inc
- *Robin Deits* @ MIT CSAIL