ForwardDiff.jl

Fast Derivatives Made Easy

Overview

Numerical Derivatives 101

Let's say I give you an implementation of a function $f : \mathbb{R} \to \mathbb{R}$ whose code you **didn’t write** and **can’t read**. How do you calculate $f'(x)$?

Finite Difference Method

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h} = \boxed{\frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)}$$

Advantages

- works “out of the box”

Disadvantages

- $\mathcal{O}(h^2)$ truncation error
- h too small $\rightarrow$ subtractive cancellation error
- requires 2 evaluations of f

Complex Step Method

$$f(x+ih) = f(x)+f'(x)hi+\frac{f''(x)}{2!}h^2i^2\ldots = f(x)+f'(x)hi-\frac{f''(x)}{2!}h^2\ldots$$

$$\boxed{f'(x) = \frac{\mathrm{Im}[f(x+hi)]}{h} + \mathcal{O}(h^2)}$$

Advantages

- no subtractive cancellation error
- Doesn't need 2 calls to f
- A lot of languages offer efficient complex number implementations
- truncation error can be close to machine epsilon in practice

Disadvantages

- complex number operations can be much slower than real number operations
- unsafe for programs which already incorporate complex inputs
- requires operator overloading and/or source code transformation

Dual Number Method

$$f(x+y\epsilon) = f(x)+f'(x)y\epsilon+\frac{f''(x)}{2!}y^2\epsilon^2 \ldots \text{ where } \epsilon \neq 0, \epsilon^2 = 0$$

$$= f(x) + f'(x)y\epsilon$$

$$\boxed{f'(x) = \mathrm{Eps}[f(x+\epsilon)]}$$

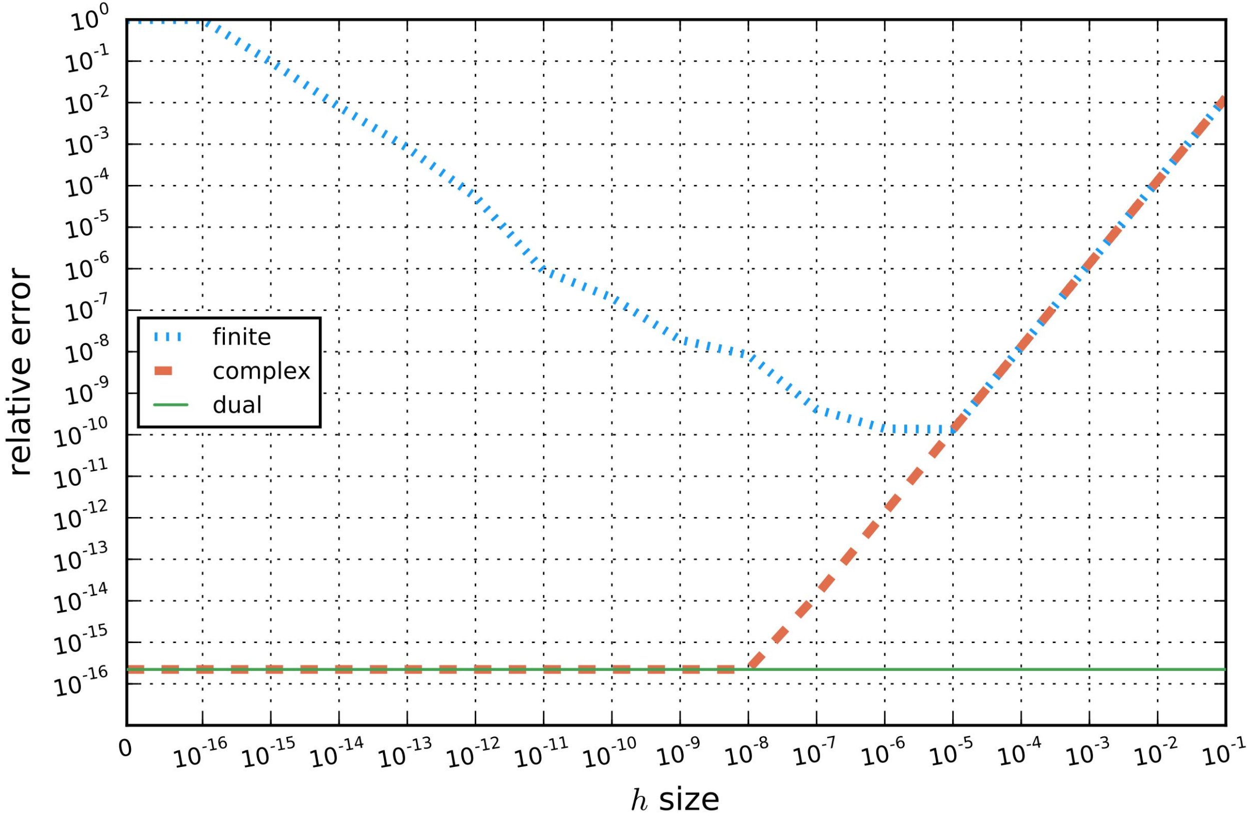
Advantages

- no approximation error

Disadvantages

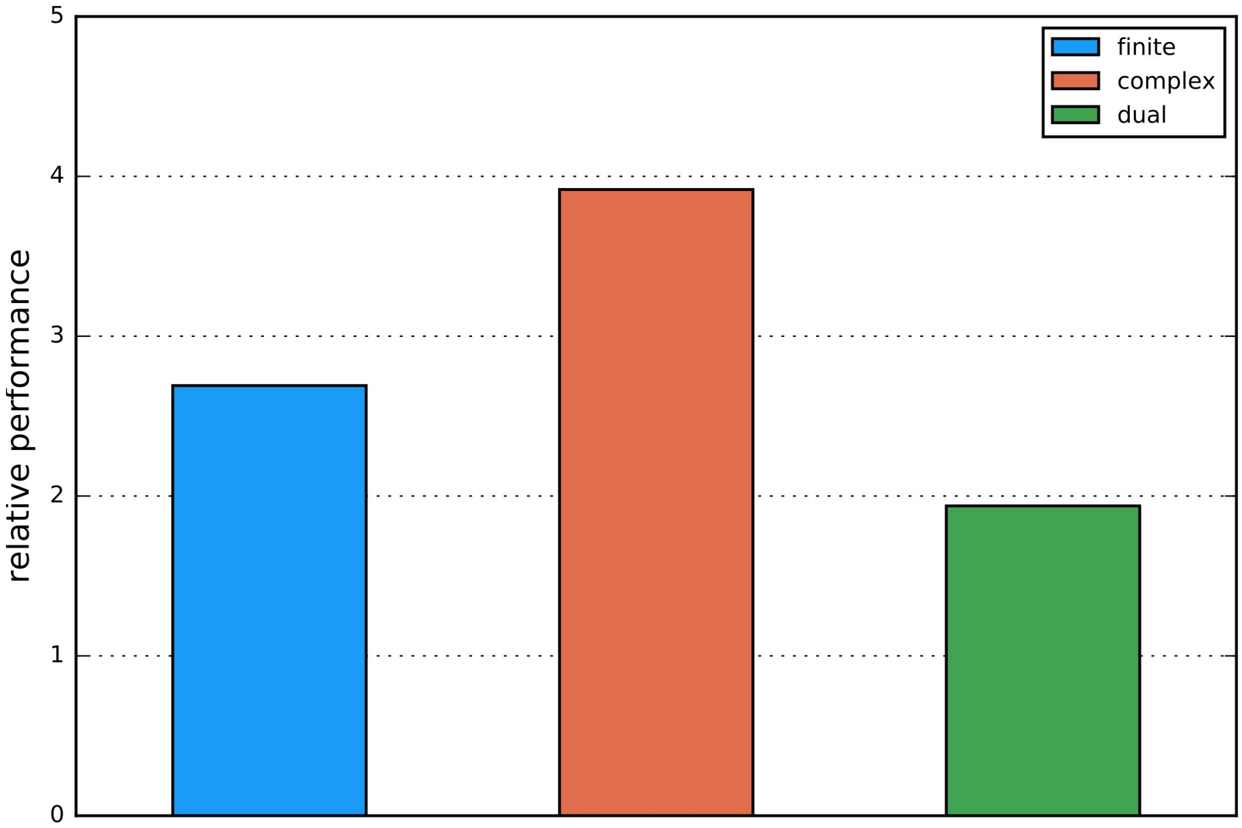
- target program must accept generic number types
- requires operator overloading and/or source code transformation

Error Comparison



Performance Comparison

$$f(x) = \frac{e^x}{\sqrt{\sin^3(x) + \cos^3(x)}}$$



performance is relative to $f(x)$

Going to Higher Dimensions

First-order derivatives of scalar functions are **boring**. What about functions like $g : \mathbb{R}^n \to \mathbb{R}$ or $\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^m$? What about **gradients** and **Jacobians**?

Gradients

$$\boxed{\nabla g(\mathbf{x}) = \begin{bmatrix} \frac{\partial g(\mathbf{x})}{\partial x_1} \\ \vdots \\ \frac{\partial g(\mathbf{x})}{\partial x_i} \\ \vdots \\ \frac{\partial g(\mathbf{x})}{\partial x_n} \end{bmatrix}}$$

Gradients

$$\nabla g(\mathbf{x}) = \begin{bmatrix} \dfrac{\partial g(\mathbf{x})}{\partial x_1} \\ \vdots \\ \dfrac{\partial g(\mathbf{x})}{\partial x_i} \\ \vdots \\ \dfrac{\partial g(\mathbf{x})}{\partial x_n} \end{bmatrix}$$

$$f(x + \epsilon) = f(x) + f'(x)\epsilon$$

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$$f(x+\epsilon) = f(x) + f'(x)\epsilon$$

$$g\left(\begin{bmatrix} x_1 \\ \vdots \\ x_i + \epsilon \\ \vdots \\ x_n \end{bmatrix} \right) = g(\mathbf{x}) + \boxed{\frac{\partial g(\mathbf{x})}{\partial x_i}}\epsilon$$

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$$f(x+\epsilon) = f(x) + f'(x)\epsilon$$

But do we really need n calls to g?

$$g\left(\begin{bmatrix} x_1 \\ \vdots \\ x_i + \epsilon \\ \vdots \\ x_n \end{bmatrix}\right) = g(\mathbf{x}) + \boxed{\frac{\partial g(\mathbf{x})}{\partial x_i}}\epsilon$$

Extending Dual Numbers

$$\boxed{f(x + y\epsilon) = f(x) + f'(x)y\epsilon \text{ where } \epsilon \neq 0, \epsilon^2 = 0}$$

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$$g(\mathbf{x}_\epsilon) = g(\mathbf{x}) + \boxed{\sum_{i=1}^{n} \frac{\partial g(\mathbf{x})}{\partial x_i}}\epsilon_i$$

Jacobians

$$\mathbf{J}(\mathbf{g})(\mathbf{x}) = \begin{bmatrix} \frac{\partial g_1(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial g_1(\mathbf{x})}{\partial x_i} & \cdots & \frac{\partial g_1(\mathbf{x})}{\partial x_n} \\ \vdots & \ddots & \vdots & \ddots & \\ \frac{\partial g_j(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial g_j(\mathbf{x})}{\partial x_i} & \cdots & \frac{\partial g_j(\mathbf{x})}{\partial x_n} \\ \vdots & \ddots & \vdots & \ddots & \\ \frac{\partial g_m(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial g_m(\mathbf{x})}{\partial x_i} & \cdots & \frac{\partial g_m(\mathbf{x})}{\partial x_n} \end{bmatrix}$$

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ForwardDiff In Action

The `Dual` Type

```
# special fixed-sized vector for storing partial derivatives
immutable Partials{N,T}
    values::NTuple{N,T}
end

# type definition of a dual number
immutable Dual{N,T<:Real} <: Real
    value::T
    partials::Partials{N,T}
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# overload math functions to propagate derivatives to `Partials`
Base.sin(d::Dual) = Dual(sin(d.value), cos(d.value) * d.partials)
Base.:*(a::Dual, b::Dual) = Dual(a.value * b.value,
                                 b.value * a.partials + a.value * b.partials)
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# ...and all of the other methods one needs to define for new number types
```

Jacobian of **cumprod**

$$\mathrm{cumprod}\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}\right) = \begin{bmatrix} x_1 \\ x_2 x_1 \\ x_3 x_2 x_1 \\ \vdots \\ x_n x_{n-1} x_{n-2} \dots x_1 \end{bmatrix}$$

```
function cumprod(x)
    y = similar(x)
    if length(x) < 1
        return y
    end
    y[1] = x[1]
    for i in 2:length(y)
        y[i] = y[i-1]*x[i]
    end
    return y
end
```

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$$\mathbf{J}(\text{cumprod})\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) = \begin{bmatrix} x_1 & 0 & 0 \\ x_2 x_1 & x_1 & 0 \\ x_3 x_2 & x_3 x_1 & x_2 x_1 \end{bmatrix}$$

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$$\mathbf{J}(\text{cumprod})\left(\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}\right) = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 6 & 3 & 2 \end{bmatrix}$$

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```
julia> using ForwardDiff: Dual

julia> x = [Dual(1, 1, 0, 0),  # 1 + □1
            Dual(2, 0, 1, 0),  # 2 + □2
            Dual(3, 0, 0, 1)]; # 3 + □3
```

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julia> cumprod(x)
3-element Array{ForwardDiff.Dual{3,Int64},1}:
 Dual(1,1,0,0)
 Dual(2,2,1,0)
 Dual(6,6,3,2)
```

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 Dual(2,2,1,0)
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julia> ForwardDiff.jacobian(cumprod, [1,2,3])
3x3 Array{Int64,2}:
 1  0  0
 2  1  0
 6  3  2
```

Benchmarking vs. `autograd`

The Python package **autograd** is a popular **reverse-mode** automatic differentiation tool. Reverse-mode AD is algorithmically more efficient than Forward-mode AD for taking gradients of functions $g : \mathbb{R}^n \to \mathbb{R}$.

Benchmarking v.s. **`autograd`**

$$\text{Rosenbrock}(\vec{x}) = \sum_{i=1}^{k-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2$$

Function	Input Size	autograd Time (s)	ForwardDiff Time (s)	Ratio
Rosenbrock	10	0.000866	0.000001	866.0
Rosenbrock	100	0.004395	0.000028	156.96
Rosenbrock	1000	0.040702	0.002605	15.62
Rosenbrock	10000	0.411095	0.257495	1.60
Rosenbrock	100000	4.173851	26.596339	0.16

Benchmarking v.s. `autograd`

$$\text{Ackley}(\vec{x}) = -a\exp\left(-b\sqrt{\frac{1}{k}\sum_{i=1}^{k} x_i^2}\right) - \exp\left(\frac{1}{k}\sum_{i=1}^{k}\cos(cx_i)\right) + a + \exp(1)$$

Function	Input Size	autograd Time (s)	ForwardDiff Time (s)	Ratio
Ackley	10	0.001204	0.000001	1204.00
Ackley	100	0.008472	0.000048	176.50
Ackley	1000	0.081499	0.004925	16.55
Ackley	10000	0.835441	0.516848	1.65
Ackley	100000	8.361769	52.337054	0.15

Pitfalls

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2. **The function must accept** `Real` **or** `Array{T<:Real}` **inputs**

3. **The function should be type-stable** (okay, not strictly, but it really should be)

Perturbation Confusion

```
D = (f, x_0) -> df/dx evaluated at x_0

# nested, closed over differentiation
D(x -> x * D(y -> x + y, 1), 1)

# correct answer
d1 = D(x -> x * D(y -> x + y, 1), 1)
d1 = D(x -> x * (y -> 1)(1), 1)
d1 = D(x -> x, 1)
d1 = (x -> 1)(1)
d1 = 1
```

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```

```
const D = ForwardDiff.derivative

# nested, closed over differentiation
D(x -> x * D(y -> x + y, 1), 1)

# what ForwardDiff will compute
d2 = D(x -> x * D(y -> x + y, 1), 1)
d2 = D(x -> x * epsilon(x + (1 + □)), 1)
d2 = epsilon((1 + □) * epsilon((1 + □) + (1 + □)))
d2 = epsilon((1 + □) * epsilon(2 + 2□))
d2 = epsilon((1 + □) * 2)
d2 = epsilon(2 + 2□)
d2 = 2 # != d1
```

Future Work

1. **Fix Perturbation Confusion. Tagging System? Perturbation Interception?**

2. **SIMD for the `Partials` type**

3. **Overload matrix functions, provide API for derivative injection**

4. **Reverse-mode AD?**

Resources

- Presentation repository: https://github.com/jrevels/ForwardDiffPresentation
- ForwardDiff repository: https://github.com/JuliaDiff/ForwardDiff.jl
- AD research web portal: http://www.autodiff.org/
- Complex Step Method: http://www.math.u-psud.fr/~maury/paps/NUM_CompDiff.pdf
- Finite Difference Method: http://ocw.usu.edu/Civil_and_Environmental_Engineering/Numerical_Methods_in_Civil_Engineering/ODEsMatlab.pdf
- Perturbation Confusion: http://www.bcl.hamilton.ie/~barak/papers/ifl2005.pdf

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- **Contributors to ForwardDiff:** Kristoffer Carlsson, Tim Holy, and others
- **JuliaCon Sponsors and Organizers**