Automatic Differentiation (or Differentiable Programming)

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- A brief introduction to AD
- My ongoing work

Vision

Functional programming languages with

- deeply embedded,
- general-purpose

differentiation capability, i.e., **automatic differentiation** (AD) in a functional framework

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differentiation capability, i.e., **automatic differentiation** (AD) in a functional framework

We started calling this **differentiable programming**

Christopher Olah's blog post (September 3, 2015)
`http://colah.github.io/posts/2015-09-NN-Types-FP/`

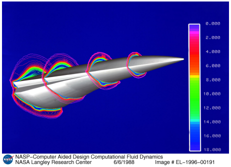
The AD field

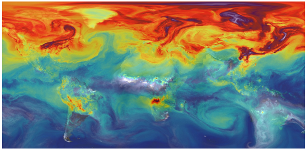
AD is an active research area

`http://www.autodiff.org/`

Traditional application domains of AD in industry and academia (Corliss et al., 2002; Griewank & Walther, 2008) include

- Computational fluid dynamics
- Atmospheric chemistry
- Engineering design optimization
- Computational finance





AD in probabilistic programming

(Wingate, Goodman, Stuhlmüller, Siskind. "Nonstandard interpretations of probabilistic programs for efficient inference." 2011)

- Hamiltonian Monte Carlo (Neal, 1994)
  `http://diffsharp.github.io/DiffSharp/examples-hamiltonianmontecarlo.html`
- No-U-Turn sampler (Hoffman & Gelman, 2011)
- Riemannian manifold HMC (Girolami & Calderhead, 2011)
- Optimization-based inference

Stan (Carpenter et al., 2015)
`http://mc-stan.org/`

What is AD?

Many machine learning frameworks (Theano, Torch, Tensorflow, CNTK) handle derivatives for you

- You build models by defining **computational graphs**
  $\rightarrow$ (constrained) symbolic language
  $\rightarrow$ highly limited control-flow (e.g., Theano's `scan`)
- The framework handles backpropagation
  $\rightarrow$ you don't have to code derivatives
  (unless adding new modules)
- Because derivatives are "automatic", some call it "autodiff" or "automatic differentiation"

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Because "automatic" is a generic (and bad) term, **algorithmic differentiation** is a better name

What is AD?

- AD does not use symbolic graphs
- Gives numeric code that **computes the function AND its derivatives** at a given point

```
f(a, b):                  f'(a, a', b, b'):
   c = a * b        ⟶       (c, c') = (a*b, a'*b + a*b')
   d = sin c                 (d, d') = (sin c, c' * cos c)
   return d                  return (d, d')
```

- Derivatives propagated at the elementary operation level, as a side effect, at the same time when the function itself is computed
  $\rightarrow$ Prevents the "expression swell" of symbolic derivatives
- Full expressive capability of the host language
  $\rightarrow$ **Including conditionals, looping, branching**

Function evaluation traces

All **numeric evaluations** are sequences of elementary operations: a **“trace,”** also called a **“Wengert list”** (Wengert, 1964)

```
f(a, b):
   c = a * b
   if c > 0
     d = log c
   else
     d = sin c
   return d
```

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```

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```

```
a = 2

b = 3

c = a * b = 6

d = log c = 1.791

return 1.791
```

(primal)

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(primal)

```
a  = 2
a’ = 1
b  = 3
b’ = 0
c  = a * b = 6
c’ = a’ * b + a * b’ = 3
d  = log c = 1.791
d’ = c’ * (1 / c) = 0.5
return 1.791, 0.5
```

(tangent)

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return 1.791, 0.5
```

i.e., a Jacobian-vector product $\mathbf{J}_f\,(1,0)\big|_{(2,3)} = \frac{\partial}{\partial a} f(a,b)\big|_{(2,3)} = 0.5$

This is called the **forward (tangent) mode** of AD

Function evaluation traces

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f(a, b):
   c = a * b
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(primal)

```
a  = 2
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c  = a * b = 6
d  = log c = 1.791
d’ = 1
c’ = d’ * (1 / c) = 0.166
b’ = c’ * a = 0.333
a’ = c’ * b = 0.5
return 1.791, 0.5, 0.333
```

(adjoint)

Function evaluation traces

```
f(a, b):
  c = a * b
  if c > 0
    d = log c
  else
    d = sin c
  return d

f(2, 3)
```

```
a = 2
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c = a * b = 6
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```

(primal)

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b’ = c’ * a = 0.333
a’ = c’ * b = 0.5
return 1.791, 0.5, 0.333
```

(adjoint)

i.e., a transposed Jacobian-vector product
$\mathbf{J}_f^T(1)\big|_{(2,3)} = \nabla f\big|_{(2,3)} = (0.5, 0.333)$

This is called the **reverse (adjoint) mode** of AD

Backpropagation is just a special case of the reverse mode: code a neural network objective computation, apply reverse AD

AD in a functional framework

AD has been around since the 1960s
(Wengert, 1964; Speelpenning, 1980; Griewank, 1989)

The foundations for AD in a functional framework
(Siskind & Pearlmutter, 2008; Pearlmutter & Siskind, 2008)

With research implementations

- R6RS-AD
  `https://github.com/qobi/R6RS-AD`
- Stalingrad
  `http://www.bcl.hamilton.ie/~qobi/stalingrad/`
- Alexey Radul's DVL
  `https://github.com/axch/dysvunctional-language`
- Recently, my DiffSharp library
  `http://diffsharp.github.io/DiffSharp/`

AD in a functional framework

"Generalized AD as a first-class function in an augmented λ-calculus" (Pearlmutter & Siskind, 2008)

Forward, reverse, and **any nested combination** thereof, instantiated according to usage scenario

Nested lambda expressions with free-variable references

$$\min\left(\lambda x\ .\ (f\ x) + \min\left(\lambda y\ .\ g\ x\ y\right)\right)$$

($\min$: gradient descent)

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Nested lambda expressions with free-variable references

$$\min\left(\lambda x \,.\, (f\ x) + \min\left(\lambda y \,.\, g\ x\ y\right)\right)$$

$$(\min\text{: gradient descent})$$

Must handle "perturbation confusion" (Manzyuk et al., 2012)

$$D\left(\lambda x \,.\, x \times \left(D\left(\lambda y \,.\, x + y\right) 1\right)\right) 1$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(x\left(\frac{\mathrm{d}}{\mathrm{d}y}x + y\right)\bigg|_{y=1}\right)\bigg|_{x=1} \stackrel{?}{=} 1$$

DiffSharp

`http://diffsharp.github.io/DiffSharp/`

- implemented in F#
- generalizes functional AD to high-performance linear algebra primitives
- arbitrary nesting of forward/reverse AD
- a comprehensive higher-order API
- gradients, Hessians, Jacobians, directional derivatives, matrix-free Hessian- and Jacobian-vector products
- F#'s “code quotations” (Syme, 2006) has great potential for deeply embedding transformation-based AD

DiffSharp

Higher-order differentiation API

	Op.	Value	Type signature	AD	Num.	Sym.
$f : \mathbb{R} \to \mathbb{R}$	`diff`	f'	$(\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to \mathbb{R}$	X, F	A	X
	`diff'`	(f, f')	$(\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to (\mathbb{R} \times \mathbb{R})$	X, F	A	X
	`diff2`	f''	$(\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to \mathbb{R}$	X, F	A	X
	`diff2'`	(f, f'')	$(\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to (\mathbb{R} \times \mathbb{R})$	X, F	A	X
	`diff2''`	(f, f', f'')	$(\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to (\mathbb{R} \times \mathbb{R} \times \mathbb{R})$	X, F	A	X
	`diffn`	$f^{(n)}$	$\mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to \mathbb{R}$	X, F		X
	`diffn'`	$(f, f^{(n)})$	$\mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to (\mathbb{R} \times \mathbb{R})$	X, F		X
$f : \mathbb{R}^n \to \mathbb{R}$	`grad`	∇f	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^n$	X, R	A	X
	`grad'`	$(f, \nabla f)$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R}^n)$	X, R	A	X
	`gradv`	$\nabla f \cdot \mathbf{v}$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^n \to \mathbb{R}$	X, F	A	
	`gradv'`	$(f, \nabla f \cdot \mathbf{v})$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R})$	X, F	A	
	`hessian`	$\mathbf{H}_f$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^{n \times n}$	X, R-F	A	X
	`hessian'`	$(f, \mathbf{H}_f)$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R}^{n \times n})$	X, R-F	A	X
	`hessianv`	$\mathbf{H}_f \mathbf{v}$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^n \to \mathbb{R}^n$	X, F-R	A	
	`hessianv'`	$(f, \mathbf{H}_f \mathbf{v})$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R}^n)$	X, F-R	A	
	`gradhessian`	$(\nabla f, \mathbf{H}_f)$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to (\mathbb{R}^n \times \mathbb{R}^{n \times n})$	X, R-F	A	X
	`gradhessian'`	$(f, \nabla f, \mathbf{H}_f)$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^{n \times n})$	X, R-F	A	X
	`gradhessianv`	$(\nabla f \cdot \mathbf{v}, \mathbf{H}_f \mathbf{v})$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R}^n)$	X, F-R	A	
	`gradhessianv'`	$(f, \nabla f \cdot \mathbf{v}, \mathbf{H}_f \mathbf{v})$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R} \times \mathbb{R}^n)$	X, F-R	A	
	`laplacian`	$\mathrm{tr}(\mathbf{H}_f)$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to \mathbb{R}$	X, R-F	A	X
	`laplacian'`	$(f, \mathrm{tr}(\mathbf{H}_f))$	$(\mathbb{R}^n \to \mathbb{R}) \to \mathbb{R}^n \to (\mathbb{R} \times \mathbb{R})$	X, R-F	A	X
$\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$	`jacobian`	$\mathbf{J}_\mathbf{f}$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^{m \times n}$	X, F/R	A	X
	`jacobian'`	$(\mathbf{f}, \mathbf{J}_\mathbf{f})$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to (\mathbb{R}^m \times \mathbb{R}^{m \times n})$	X, F/R	A	X
	`jacobianv`	$\mathbf{J}_\mathbf{f} \mathbf{v}$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^n \to \mathbb{R}^m$	X, F	A	
	`jacobianv'`	$(\mathbf{f}, \mathbf{J}_\mathbf{f} \mathbf{v})$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^n \to (\mathbb{R}^m \times \mathbb{R}^m)$	X, F	A	
	`jacobianT`	$\mathbf{J}_\mathbf{f}^T$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^{n \times m}$	X, F/R	A	X
	`jacobianT'`	$(\mathbf{f}, \mathbf{J}_\mathbf{f}^T)$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to (\mathbb{R}^m \times \mathbb{R}^{n \times m})$	X, F/R	A	X
	`jacobianTv`	$\mathbf{J}_\mathbf{f}^T \mathbf{v}$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^m \to \mathbb{R}^n$	X, R		
	`jacobianTv'`	$(\mathbf{f}, \mathbf{J}_\mathbf{f}^T \mathbf{v})$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^m \to (\mathbb{R}^m \times \mathbb{R}^n)$	X, R		
	`jacobianTv''`	$(\mathbf{f}, \mathbf{J}_\mathbf{f}^T(\cdot))$	$(\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to (\mathbb{R}^m \times (\mathbb{R}^m \to \mathbb{R}^n))$	X, R		
	`curl`	$\nabla \times \mathbf{f}$	$(\mathbb{R}^3 \to \mathbb{R}^3) \to \mathbb{R}^3 \to \mathbb{R}^3$	X, F	A	X
	`curl'`	$(\mathbf{f}, \nabla \times \mathbf{f})$	$(\mathbb{R}^3 \to \mathbb{R}^3) \to \mathbb{R}^3 \to (\mathbb{R}^3 \times \mathbb{R}^3)$	X, F	A	X
	`div`	$\nabla \cdot \mathbf{f}$	$(\mathbb{R}^n \to \mathbb{R}^n) \to \mathbb{R}^n \to \mathbb{R}$	X, F	A	X
	`div'`	$(\mathbf{f}, \nabla \cdot \mathbf{f})$	$(\mathbb{R}^n \to \mathbb{R}^n) \to \mathbb{R}^n \to (\mathbb{R}^n \times \mathbb{R})$	X, F	A	X
	`curldiv`	$(\nabla \times \mathbf{f}, \nabla \cdot \mathbf{f})$	$(\mathbb{R}^3 \to \mathbb{R}^3) \to \mathbb{R}^3 \to (\mathbb{R}^3 \times \mathbb{R})$	X, F	A	X
	`curldiv'`	$(\mathbf{f}, \nabla \times \mathbf{f}, \nabla \cdot \mathbf{f})$	$(\mathbb{R}^3 \to \mathbb{R}^3) \to \mathbb{R}^3 \to (\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R})$	X, F	A	X

DiffSharp

Matrix operations
`http://diffsharp.github.io/DiffSharp/api-overview.html`

High-performance OpenBLAS backend by default,
currently working on a CUDA-based GPU backend

Support for 64- and 32-bit floats (faster on many systems)

Benchmarking tool
`http://diffsharp.github.io/DiffSharp/benchmarks.html`

A growing collection of tutorials: gradient-based optimization algorithms, clustering, Hamiltonian Monte Carlo, neural networks, inverse kinematics

Hype

`http://hypelib.github.io/Hype/`

An experimental library for “compositional machine learning and **hype**rparameter optimization”, built on DiffSharp

A robust optimization core

- highly configurable functional modules
- SGD, conjugate gradient, Nesterov, AdaGrad, RMSProp, Newton’s method
- Use nested AD for gradient-based hyperparameter optimization (Maclaurin et al., 2015)

Hype

Extracts from Hype neural network code,
freely use F# and higher-order functions, don't think about gradients or backpropagation

https://github.com/hypelib/Hype/blob/master/src/Hype/Neural.fs

```
// Use mixed mode nested AD
open DiffSharp.AD.Float32

type FeedForward() =
    inherit Layer()
    // Feedforward layers executed as "fold", DM -> DM
    override n.Run(x:DM) = Array.fold Layer.run x layers

type GRU(inputs:int, memcells:int) =
    inherit Layer()
    // RNN many-to-many execution as "map", DM -> DM
    override l.Run (x:DM) =
        x |> DM.mapCols
            (fun x ->
                let z = sigmoid(l.Wxz * x + l.Whz * l.h + l.bz)
                let r = sigmoid(l.Wxr * x + l.Whr * l.h + l.br)
                let h' = tanh(l.Wxh * x + l.Whh * (l.h .* r))
                l.h <- (1.f - z) .* h' + z .* l.h
                l.h)
```

Hype

Derivatives are instantiated within the optimization code

```
type Method
    | CG -> // Conjugate gradient
        fun w f g p gradclip ->
            let v', g' = grad' f w // gradient
            let g' = gradclip g'
            let y = g' - g
            let b = (g' * y) / (p * y)
            let p' = -g' + b * p
            v', g', p'
    | NewtonCG -> // Newton conjugate gradient
        fun w f _ p gradclip ->
            let v', g' = grad' f w  // gradient
            let g' = gradclip g'
            let hv = hessianv f w p // Hessian-vector product
            let b = (g' * hv) / (p * hv)
            let p' = -g' + b * p
            v', g', p'
    | Newton -> // Newton's method
        fun w f _ _ gradclip ->
            let v', g', h' = gradhessian' f w // gradient, Hessian
            let g' = gradclip g'
            let p' = -DM.solveSymmetric h' g'
            v', g', p'
```

Hamiltonian Monte Carlo with DiffSharp

Try it on your system: `http://diffsharp.github.io/DiffSharp/examples-hamiltonianmontecarlo.html`

```
let leapFrog (u:DV->D) (k:DV->D) (d:D) steps (x0, p0) =
    let hd = d / 2.
    [1..steps]
    |> List.fold (fun (x, p) _ ->
        let p' = p - hd * grad u x
        let x' = x + d * grad k p'
        x', p' - hd * grad u x') (x0, p0)

let hmc n hdelta hsteps (x0:DV) (f:DV->D) =
    let u x = -log (f x) // potential energy
    let k p = (p * p) / D 2. // kinetic energy
    let hamilton x p = u x + k p
    let x = ref x0
    [|for i in 1..n do
        let p = DV.init x0.Length (fun _ -> rndn())
        let x', p' = leapFrog u k hdelta hsteps (!x, p)
        if rnd() < float (exp ((hamilton !x p) - (hamilton x' p'))) then x := x'
        yield !x|]
```

Thank You!

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