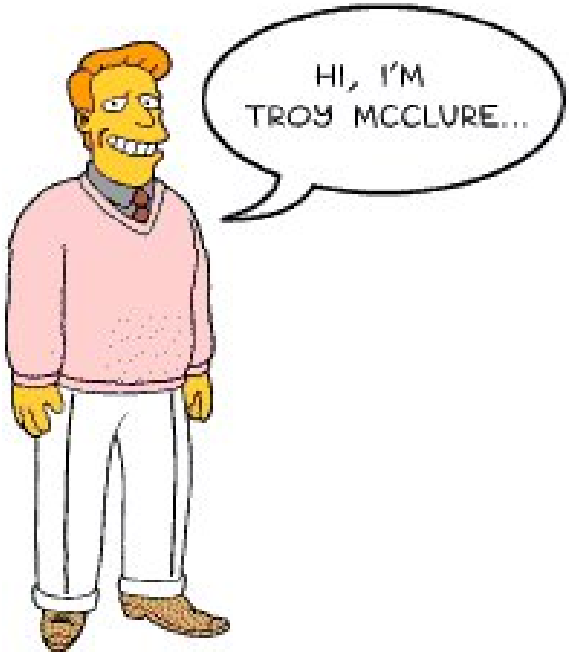
HI, I'M
TROY MCCLURE...

Automatic Differentiation: History and Headroom

Barak A. Pearlmutter

Department of Computer Science, Maynooth University, Co. Kildare, Ireland

Prof Andrei A. Markov

Lev Semenovich Pontryagin P. S. Alexandrov Andrey N. Kolmogorov

The very first computer science PhD dissertation introduced forward accumulation mode automatic differentiation.

The very first computer science PhD dissertation introduced forward accumulation mode automatic differentiation.

Wengert (1964)

Robert Edwin Wengert. *A simple automatic derivative evaluation program*. Communications of the ACM **7***(8)*:463–4, Aug 1964.

A procedure for automatic evaluation of total/partial derivatives of arbitrary algebraic functions is presented. The technique permits computation of numerical values of derivatives without developing analytical expressions for the derivatives. **The key to the method is the decomposition of the given function**, by introduction of intermediate variables, **into a series of elementary functional steps.** A library of elementary function subroutines is provided for the automatic evaluation and differentiation of these new variables. The final step in this process produces the desired function's derivative. The main feature of this approach is its simplicity. It can be used as a quick-reaction tool where the derivation of analytical derivatives is laborious and also as a debugging tool for programs which contain derivatives.

WENGERT'S NUMERICAL METHOD FOR PARTIAL DERIVATIVES, ORBIT DETERMINATION, AND QUASILINEARIZATION

R. Bellman, H. Kagiwada and R. Kalaba

PREPARED FOR:
UNITED STATES AIR FORCE PROJECT RAND

The RAND Corporation
SANTA MONICA • CALIFORNIA

R. E. Bellman, H. Kagiwada, and R. E. Kalaba (1965) *Wengert's numerical method for partial derivatives, orbit determination and quasilinearization*, Communications of the ACM **8***(4)*:231–2, April 1965, doi:10.1145/363831.364886

In a recent article in the Communications of the ACM, R. Wengert suggested a technique for machine evaluation of the partial derivatives of a function given in analytical form. In solving nonlinear boundary-value problems using quasilinearization many partial derivatives must be formed analytically and then evaluated numerically. **Wengert's method** appears very attractive from the programming viewpoint and **permits the treatment of large systems** of differential equations **which might not otherwise be undertaken.**

Automatic Differentiation: a crash course

Automatic Differentiation (AD) mechanically calculates the derivatives (Leibnitz, 1664; Newton, 1704) of functions expressed as computer programs (Turing, 1936), at machine precision (Konrad Zuse, 1941, Z3; Burks, Goldstine, and von Neumann, 1946, §5.3, p14), and with complexity guarantees.

Automatic Differentiation

- Derivative of $f : \mathbb{R}^n \to \mathbb{R}^m$ is $m \times n$ "Jacobian matrix" J.
- AD, forward accumulation mode: Jv (Wengert, 1964)
- AD, reverse accumulation mode: $J^T v$ (Speelpenning, 1980)
- About a zillion other modes and tricks
- Big Iron FORTRAN-77 valve-age implementations
- Vibrant field with regular workshops, conferences, updated community portal (http://autodiff.org)

What is AD?

Automatic Differentiation
aka *Algorithmic Differentiation*
aka *Computational Differentiation*

AD Type I: A calculus for efficiently calculating derivatives of functions specified by a set of equations.

AD Type II: A way of transforming a computer program implementing a numeric function to also efficiently calculate some derivatives.

AD Type III: A computer program which automatically transforms an input computer program specifying a numeric function into one that also efficiently calculates derivatives.

Forward AD

Symmetric Truncated Taylor (1715) Expansion

$$f(x+\epsilon) = \sum_{i=0}^{\infty} \frac{f^{(i)}(x)}{i!}\,\epsilon^i = f(x) + f'(x)\,\epsilon + \mathcal{O}(\epsilon^2)$$

Symmetric Truncated Taylor (1715) Expansion

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$$f(x+\overline{x'}\,\epsilon) = f(x) + f'(x)\,\overline{x'}\,\epsilon + \mathcal{O}(\epsilon^2)$$

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$$f(x+\overline{x'}\,\epsilon + \mathcal{O}(\epsilon^2)) = f(x) + f'(x)\,\overline{x'}\,\epsilon + \mathcal{O}(\epsilon^2)$$

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$$f(x \rhd \overline{x'}) = f(x) \rhd f'(x)\,\overline{x'}$$

$$f(x \triangleright \overrightarrow{x}) = f(x) \triangleright f'(x) \overrightarrow{x}$$

Won't *anyone* think of the ~~children~~ types?

$$f : \mathbb{R} \to \mathbb{R}$$

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$$x,\ \overline{x'},\ f(x) : \mathbb{R}$$

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$$(x \rhd \overrightarrow{x'}) : \mathbb{D}\mathbb{R} \qquad \leftarrow \text{dual number (Clifford, 1873)}$$

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Won't *anyone* think of the ~~children~~ types?

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$$f(x \rhd \overrightarrow{x}) = f(x) \rhd f'(x)\,\overrightarrow{x} \qquad \leftarrow \textit{type error!}$$

$$\overrightarrow{\mathcal{J}} : (\mathbb{R} \to \mathbb{R}) \to (\mathbb{DR} \to \mathbb{DR})$$

$$\overrightarrow{\mathcal{J}} f(x \rhd \overrightarrow{x}) = f(x) \rhd f'(x)\,\overrightarrow{x}$$

$$\overrightarrow{\mathcal{J}} f(x \triangleright \overrightarrow{x}) = f(x) \triangleright f'(x) \overrightarrow{x}$$

Multifaceted Key to Forward AD!

$$\overrightarrow{\mathcal{J}} f(x \triangleright \overline{x'}) = f(x) \triangleright f'(x)\,\overline{x'}$$

Multifaceted Key to Forward AD!

$$\overrightarrow{\mathcal{J}} f\,(x \rhd \overrightarrow{x'}) = f(x) \rhd f'(x)\,\overrightarrow{x'}$$

Generalises beyond dual numbers (Clifford, 1873) and scalars:

$f : \mathbb{R}^n \to \mathbb{R}^m$	(multidimensional)
$x,\ \overrightarrow{x'} : \mathbb{R}^n$	(column vectors)
$x \rhd \overrightarrow{x'} : \mathbb{D}\mathbb{R}^n$	(vector of *dual numbers*)
$f'(x) : \mathbb{R}^{m \times n}$	(Jacobian matrix, **J**)
$\overrightarrow{\mathcal{J}} : (\mathbb{R}^n \to \mathbb{R}^m) \to (\mathbb{D}\mathbb{R}^n \to \mathbb{D}\mathbb{R}^m)$	(Forward AD transform)

Multifaceted Key to Forward AD!

$$\overrightarrow{\mathcal{J}} f(x \rhd \overrightarrow{x'}) = f(x) \rhd f'(x)\, \overrightarrow{x'}$$

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$\overrightarrow{\mathcal{J}} : (\mathbb{R}^n \to \mathbb{R}^m) \to (\mathbb{DR}^n \to \mathbb{DR}^m)$	(Forward AD transform)

1. Compositional: $\overrightarrow{\mathcal{J}}(f \circ g) = \overrightarrow{\mathcal{J}} f \circ \overrightarrow{\mathcal{J}} g$
2. How to "lift" when f is a primop (elt of numeric basis)
3. What such "lifting" delivers when f is a defined function

Example: Application of $\overrightarrow{\mathcal{J}}$ to a Primop

$$v := \sin u$$

$$\Rightarrow \boxed{\overrightarrow{\mathcal{J}}} \Rightarrow$$

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$\Rightarrow$ inline & destructure $\Rightarrow$

$$v \rhd \overrightarrow{v}' := \overrightarrow{\mathcal{J}} \sin (u \rhd \overrightarrow{u}')$$

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$$v \rhd \overrightarrow{v'} := \sin u \rhd (\cos u) * \overrightarrow{u'}$$

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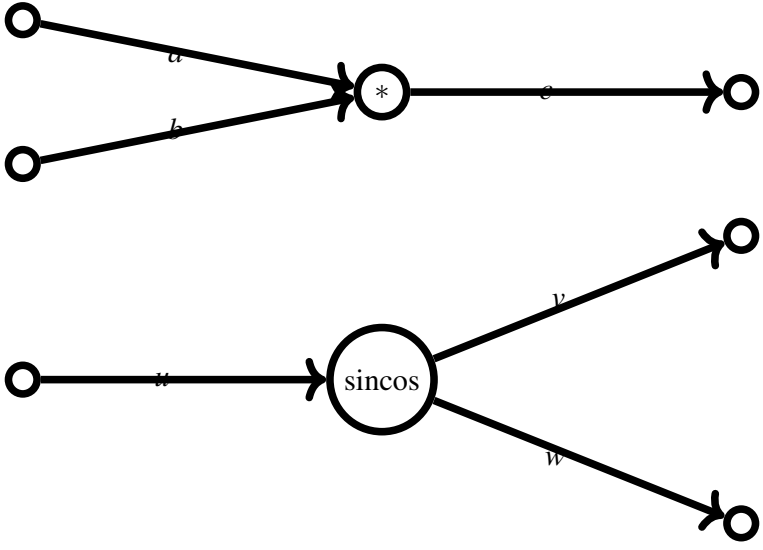
$$v := \sin u$$
$$\overrightarrow{v'} := (\cos u) * \overrightarrow{u'}$$

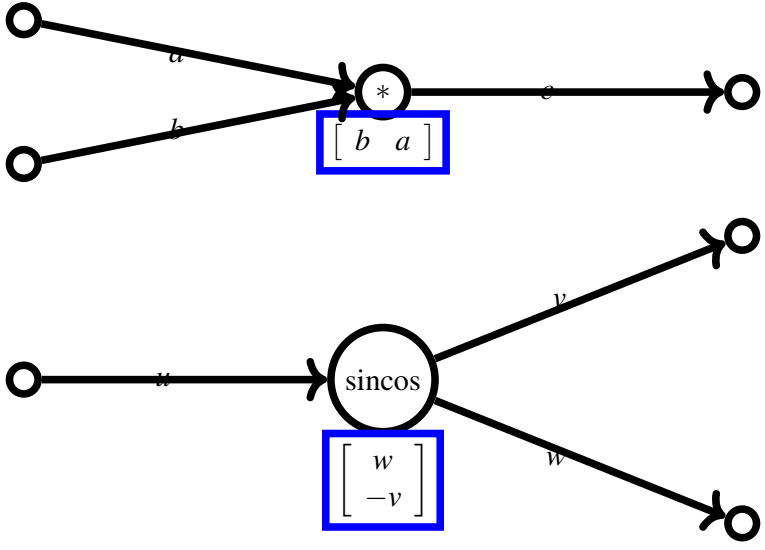
Simple Code

$$c := a * b$$
$$(v, w) := \text{sincos } u$$

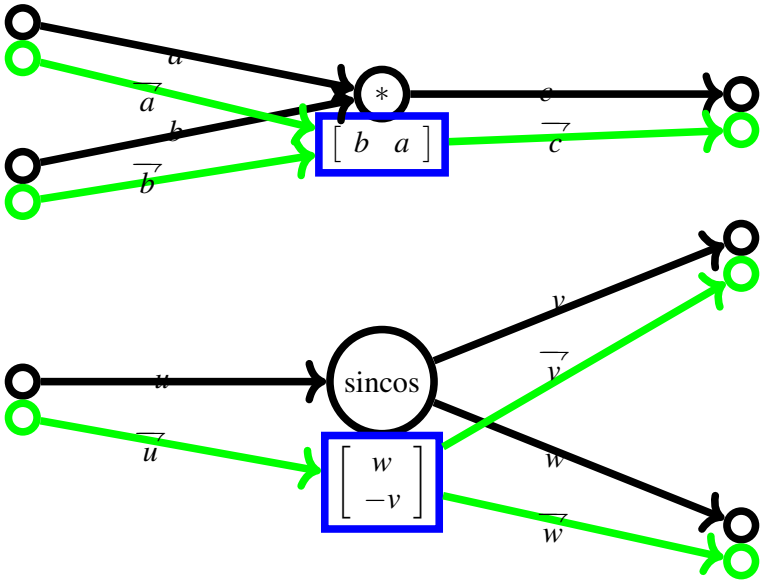
Data Flow Graph



Data Flow Graph



Data Flow Graph



Transform Graph as Netlist, *i.e.*, Code

$$c := a * b \qquad \Rightarrow \boxed{\overrightarrow{\mathcal{J}}} \Rightarrow \qquad c := a * b$$

$$(v, w) := \text{sincos } u \qquad \overline{c}' := a * \overline{b}' + b * \overline{a}'$$

$$(v, w) := \text{sincos } u$$

$$\overline{v}' := w * \overline{u}'$$

$$\overline{w}' := -v * \overline{u}'$$

AKA

- Forward Automatic Differentiation
- Forward Propagation
- Directional Derivative
- Push Forward
- Perturbation Analysis

Reverse AD

(aka backprop)

In the 1970s, tools for automated generation of adjoint codes (aka reverse accumulation mode automatic differentiation, aka backpropagation) were developed.

Type I: Geniuses transforming mathematical systems
(Gauss; Feynman (1939); Rozonoer and Pontryagin (1959))

Type II: Manual transformation of computational processes
(Bryson (1962); Werbos (1974); Le Cun (1985); Rumelhart, Hinton, and Williams (1986))

Type III: Computer programs transform other computer programs
(Speelpenning (1980); LUSH; TAPENADE)

Type IV: First-class AD operators; closure
(STALIN∇; R^{6}RS-AD; AUTOGRAD; DIFFSHARP)

Bert Speelpenning

UIUCDCS-R-80-1002

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COO-2383-0063

COMPILING FAST PARTIAL DERIVATIVES OF FUNCTIONS GIVEN BY ALGORITHMS

by

Bert Speelpenning

January 1980

by arbitrary algorithms.

What is needed is a system as sketched in Figure 1.

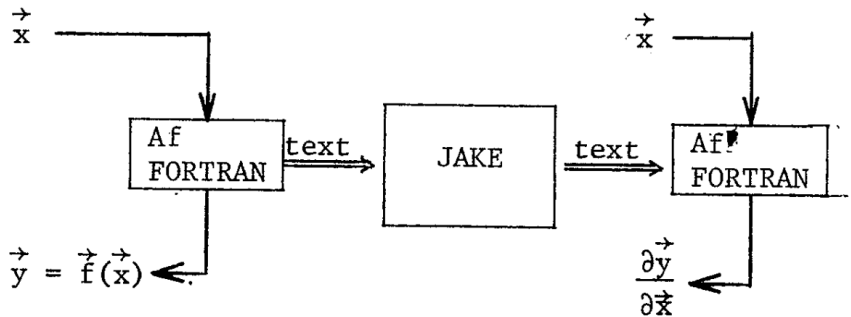


Figure 1. Use of Jake

Such a system will accept the text of an algorithm Af, embodying $y=f(x)$

1.2. Major Results of this Research

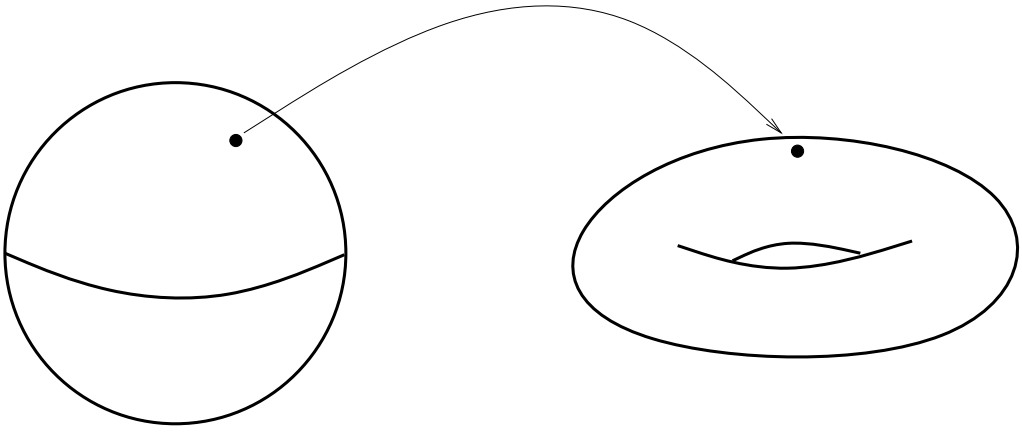
A full solution to the problem of compiling fast gradients has been obtained. For the problem of compiling fast Jacobians of arbitrary shape a partial solution has been found. This thesis describes a method and its implementation capable of producing algorithms Af′ that compute the gradient of a function $f(x_1,\ldots,x_n)$ in an amount of time equivalent to a constant number of function evaluations independent of n. The space requirements of the algorithm Af′ are modest.

specialization occurring within Computer Science. The separation of Numerical Analysis from Software is virtually complete and few people care to bridge the gap between the areas. In Numerical Analysis, the notion of programs that produce programs rather than numbers is largely absent. For most numerical analysts the FORTRAN compiler is completely transparent, as if Created on the same day as the computer. There is little awareness of language processing as a software writing tool in the sense of the products we have come to expect from places like Bell Labs. Notable exceptions include user languages for physical modeling and for statistical computations. Conversely, people involved in writing software tools may have a tendency to write only such software tools that aid in the writing of other software tools, and although this opens fascinating avenues of auto-catalysis, the real usefulness of these tools must ultimately come from application to outside areas. Tools are means to an end, not ends in themselves. What seems required is not merely cooperation between software people and numerical analysts but efforts by people with a certain minimal understanding and interest in both areas. The effort invested in such hetero-catalysis could pay off very handsomely.

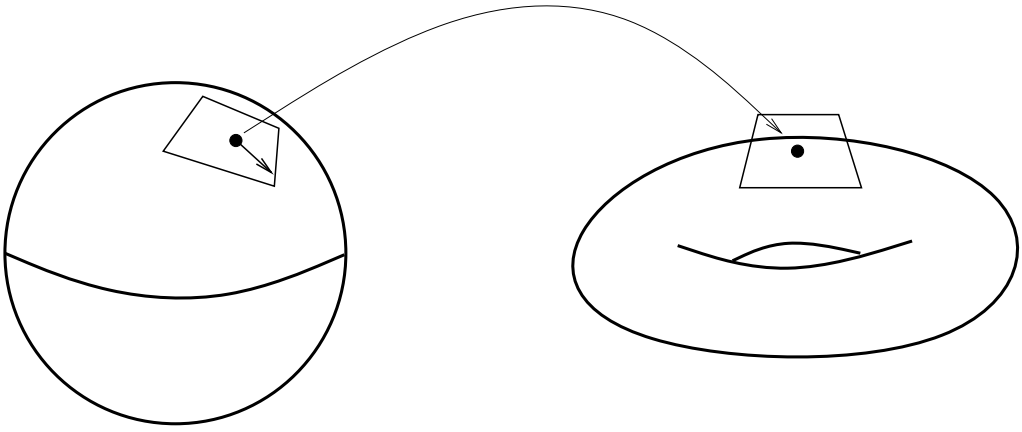
Differential Geometry

(digression)

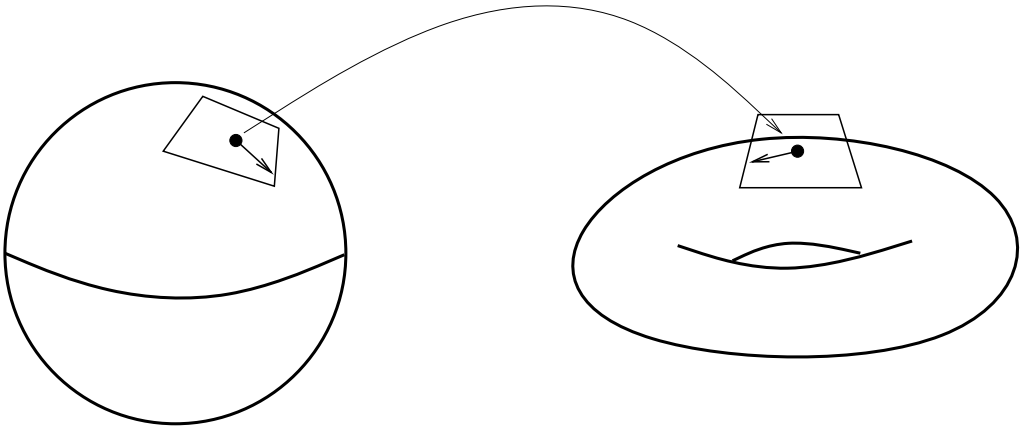
Tangent Space



Tangent Space



Tangent Space



Cotangent Space

$$\overleftarrow{a} : \overleftarrow{\alpha_a}$$

$$\overleftarrow{\alpha_a} = \overrightarrow{\alpha'_a} \xrightarrow{\text{linear}} \mathbb{R}$$

$$(\bullet) : \overleftarrow{\alpha_a} \to \overrightarrow{\alpha'_a} \to \mathbb{R}$$

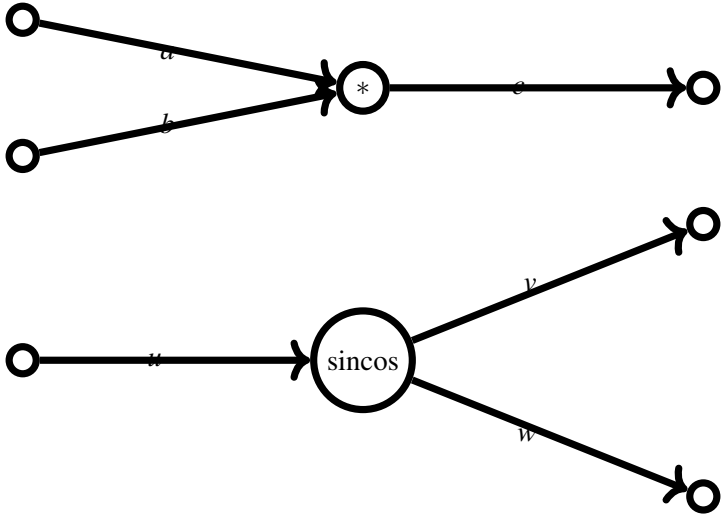
Gradients & Reverse AD are *Dual* to Perturbations & Forward AD

$$\overleftarrow{a} \bullet \overrightarrow{a'} = \overleftarrow{b} \bullet \overrightarrow{b'} \qquad (\bullet) : \overleftarrow{\alpha} \to \overrightarrow{\alpha'} \to \mathbb{R}$$

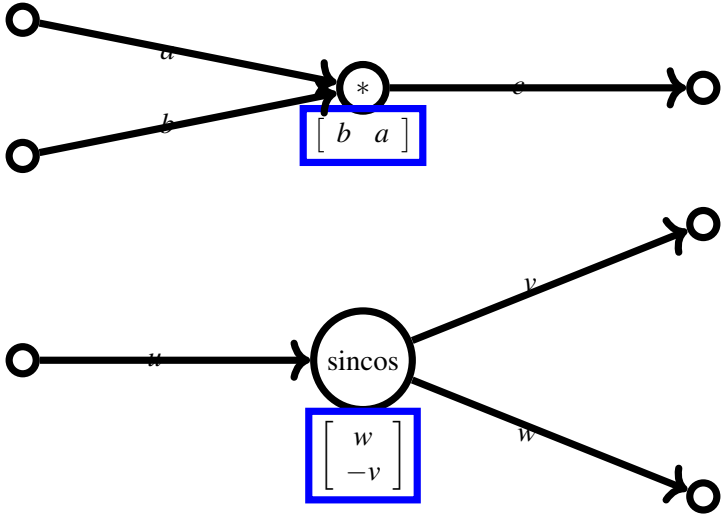
where we let

$$\begin{aligned} b &= f\ a & f &: \alpha \to \beta \\ (b \rhd \overrightarrow{b'}) &= \overrightarrow{\mathcal{J}}\ f\ (a \rhd \overrightarrow{a'}) & \overrightarrow{\mathcal{J}}\ f &: \overrightarrow{\alpha} \to \overrightarrow{\beta} \\ (b, \bar{f}) &= \overleftarrow{\mathcal{J}}\ f\ a & \overleftarrow{\mathcal{J}}\ f &: \alpha \to (\beta \times (\overleftarrow{\beta} \to \overleftarrow{\alpha})) \\ \overleftarrow{a} &= \bar{f}\ \overleftarrow{b} & \bar{f} &: \overleftarrow{\beta} \to \overleftarrow{\alpha} \end{aligned}$$

Data Flow Graph



Data Flow Graph



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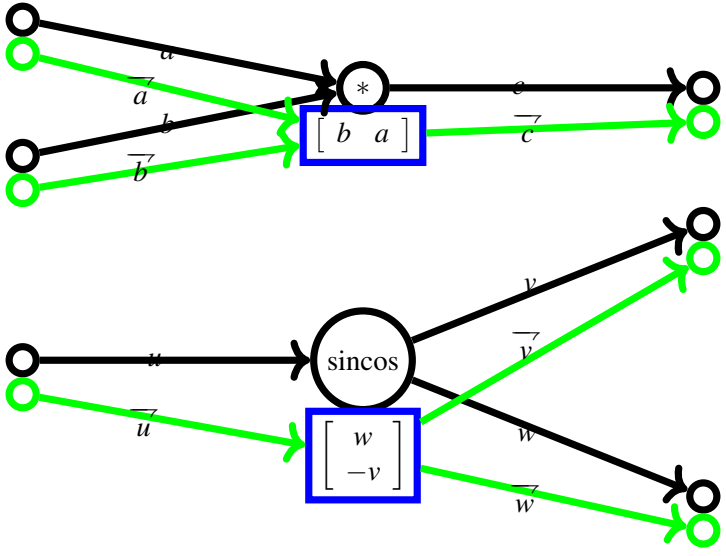

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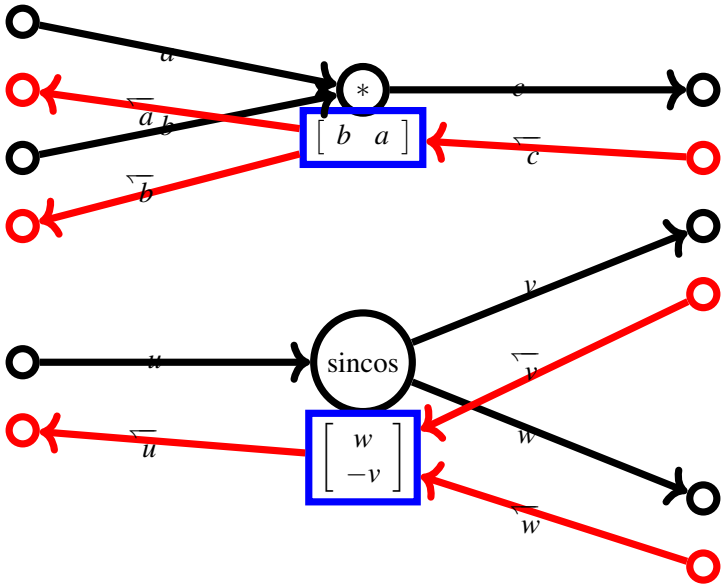
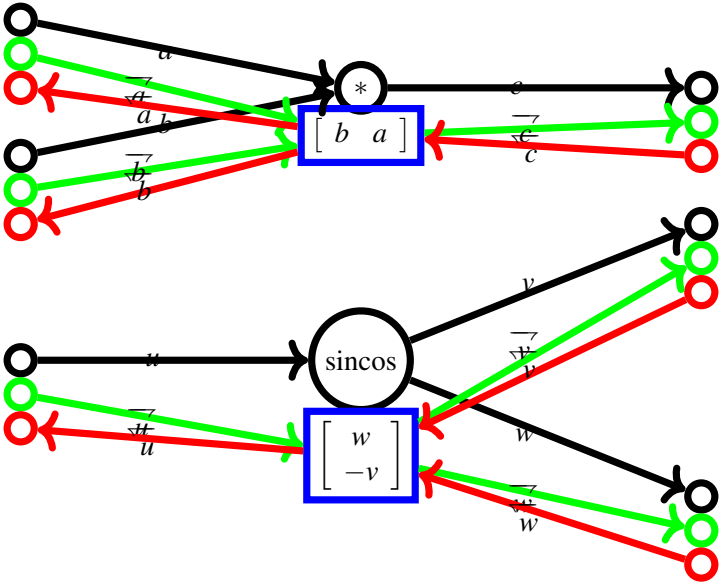


Data Flow Graph



$$
\begin{aligned}
c &:= a * b \\
(v, w) &:= \operatorname{sincos} u
\end{aligned}
\qquad \Rightarrow \boxed{\overrightarrow{\mathcal{F}}} \Rightarrow \qquad
\begin{aligned}
c &:= a * b \\
\overline{c}' &:= a * \overline{b}' + b * \overline{a}' \\
(v, w) &:= \operatorname{sincos} u \\
\overline{v}' &:= w * \overline{u}' \\
\overline{w}' &:= -v * \overline{u}'
\end{aligned}
$$

$$
\begin{aligned}
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\end{aligned}
\quad \Rightarrow \boxed{\overrightarrow{\mathcal{J}}} \Rightarrow \quad
\begin{aligned}
c &:= a * b \\
\overrightarrow{c} &:= a * \overrightarrow{b} + b * \overrightarrow{a} \\
(v, w) &:= \operatorname{sincos} u \\
\overrightarrow{v} &:= w * \overrightarrow{u} \\
\overrightarrow{w} &:= -v * \overrightarrow{u}
\end{aligned}
$$

$$
\Rightarrow \boxed{\overleftarrow{\mathcal{J}}} \Rightarrow \quad
\begin{aligned}
c &:= a * b \\
(v, w) &:= \operatorname{sincos} u \\
&\vdots \\
\overleftarrow{u} &:= w * \overleftarrow{v} - v * \overleftarrow{w} \\
\overleftarrow{a} &:= b * \overleftarrow{c} \\
\overleftarrow{b} &:= a * \overleftarrow{c}
\end{aligned}
$$

Generalise: All Types Are Manifolds

- can be disconnected (e.g., union type)
- components can have varying dimensionality (e.g., list $\mathbb{R}$)
- components can be zero dimensional (e.g., **bool**, enum, $\mathbb{Z}$), in which case tangent space is zero dimensional (**void**)

primary $\overleftarrow{\mathcal{I}}$ technical difficulty:

fanout

even today, our tools for high-performance numeric computations do not support automatic differentiation as a first-class citizen.

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Dominant AD technology for high-performance systems: preprocessors.

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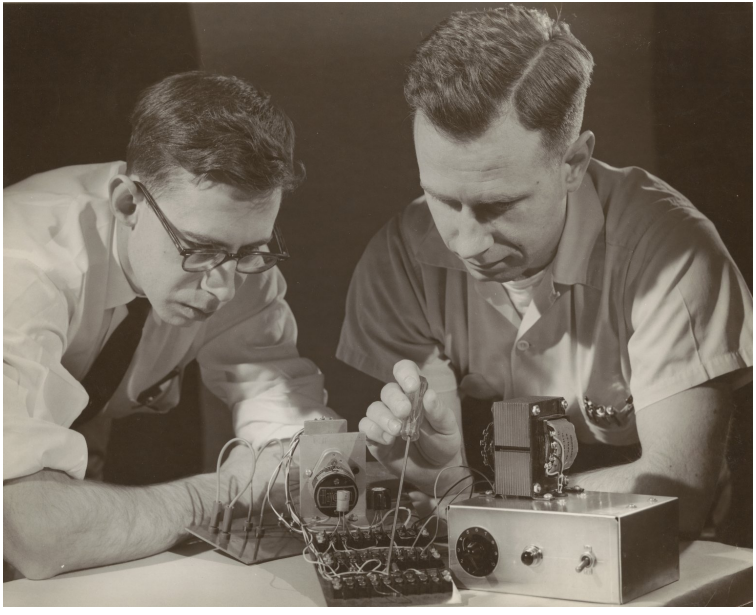
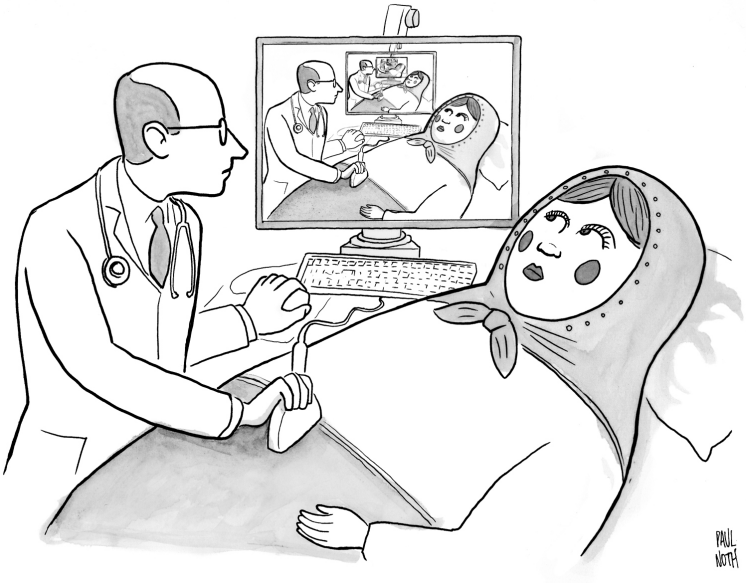
Dominant AD technology for high-performance systems: preprocessors.

- very hard to apply in a nested fashion
- caller-derives API impedes modularity
- brittle and idiosyncratic.



Rosenblatt Wightman



nesting

Uses of Nesting

- Differential objective:

$$\min_w \sum_i \|f(x_i; w) - y_i\|^2 + \| (d/dx) f(x; w)|_{x=x_i} - z_i\|^2$$

- Multilevel optimization (GANs, learn-to-learn, etc. So hot!)
- Optimizing game's rules so rational players exhibit desired behaviour
- Design optimization of "smart" devices, or devices involving PDEs
- Hyperparameter optimization
- Sensitivity/robustness analysis of processes involving AD

Generalise

Generalise $\overrightarrow{\mathcal{J}}$, $\overleftarrow{\mathcal{J}}$ to apply to *all* functions ...

$$\overrightarrow{\mathcal{J}} : (\alpha \to \beta) \to (\overrightarrow{\alpha} \to \overrightarrow{\beta})$$
$$\overleftarrow{\mathcal{J}} : (\alpha \to \beta) \to (\alpha \to (\beta \times (\overleftarrow{\beta} \to \overleftarrow{\alpha})))$$

... to *all* objects ...

$$\overrightarrow{\mathcal{J}} : \alpha \to \overrightarrow{\alpha}$$
$$\overrightarrow{\alpha \to \beta} = \overrightarrow{\alpha} \to \overrightarrow{\beta}$$
$$\overleftarrow{\mathcal{J}} : \alpha \to \overleftarrow{\alpha}$$

Technicalities!

- Tangent space is usually isomorphic to "$\mathbb{R}$ holes" in primal space, since $\mathbb{R}$ is our only non-zero-dimensional primitive type.

  But not always (function types).

- Cotangent space is usually isomorphic to tangent space.

  But not always (function types).

- Due to issues related to this, parts of reverse mode must be "lazy" even if primal & forward AD computations are "eager".

Functions Diff. Geom. Handles

- arithmetic functions
- functions over discrete spaces
- functions over disconnected manifolds of differing dimensionality
- higher-order functions over concrete linear functions
- higher-order functions like `map` and compose (`∘`)
- higher-order functions like `numeric-iterate-to-fixedpoint` (Feynman, 1939; Pineda, 1987; Almeida, 1987)
- higher-order functions like $\overrightarrow{\mathcal{J}}$ and $\overleftarrow{\mathcal{J}}$

delicate dance

fielded systems with first-class AD:

slow

rough edges

headroom for acceleration

research prototype compiler

Benchmarks

		particle				saddle				probabilistic-lambda-calculus		probabilistic-prolog		backprop		
		FF	FR	RF	RR	FF	FR	RF	RR	F	R	F	R	F	Fv	R
VLAD	STALIN∇	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	■	1.00
FORTRAN	ADIFOR	2.05	■	■	■	5.44	■	■	■	■	■	■	■	15.51	3.35	■
	TAPENADE	5.51	■	■	■	8.09	■	■	■	■	■	■	■	14.97	5.97	6.86
C	ADIC	■	■	■	■	■	■	■	■	■	■	■	■	22.75	5.61	■
C++	ADOL–C	■	■	■	■	■	■	■	■	■	■	■	■	12.16	5.79	32.77
	CPPAD	■	■	■	■	■	■	■	■	■	■	■	■	54.74	■	29.24
	FADBAD++	93.32	■	■	■	60.67	■	■	■	■	■	■	■	132.31	46.01	60.71
ML	MLTON	78.13	111.27	45.95	32.57	114.07	146.28	12.27	10.58	129.11	114.88	848.45	507.21	95.20	■	39.90
	OCAML	217.03	415.64	352.06	261.38	291.26	407.67	42.39	50.21	249.40	499.43	1260.83	1542.47	202.01	■	156.93
	SML/NJ	153.01	226.84	270.63	192.13	271.84	299.76	25.66	23.89	234.62	258.53	2505.59	1501.17	181.93	■	102.89
HASKELL	GHC	209.44	■	■	■	247.57	■	■	■	■	■	■	■	■	■	■
SCHEME	BIGLOO	627.78	855.70	275.63	187.39	1004.85	1076.73	105.24	89.23	983.12	1016.50	12832.92	7918.21	743.26	■	360.07
	CHICKEN	1453.06	2501.07	821.37	1360.00	2276.69	2964.02	225.73	252.87	2324.54	3040.44	44891.04	24634.44	1626.73	■	1125.24
	GAMBIT	578.94	879.39	356.47	260.98	958.73	1112.70	89.99	89.23	1033.46	1107.26	26077.48	14262.70	671.54	■	379.63
	IKARUS	266.54	386.21	158.63	116.85	424.75	527.57	41.27	42.34	497.48	517.89	8474.57	4845.10	279.59	■	165.16
	LARCENY	964.18	1308.68	360.68	272.96	1565.53	1508.39	126.44	112.82	1658.27	1606.44	25411.62	14386.61	1203.34	■	511.54
	MIT SCHEME	2025.23	3074.30	790.99	609.63	3501.21	3896.88	315.17	295.67	4130.88	3817.57	87772.39	49814.12	2446.33	■	1113.09
	MZC	1243.08	1944.00	740.31	557.45	2135.92	2434.05	194.49	187.53	2294.93	2346.13	57472.76	31784.38	1318.60	■	754.47
	MZSCHEME	1309.82	1926.77	712.97	555.28	2371.35	2690.64	224.61	219.29	2721.35	2625.21	60269.37	33135.06	1364.14	■	772.10
	SCHEME->C	582.20	743.00	270.83	208.38	910.19	913.66	82.93	69.87	811.37	803.22	10605.32	5935.56	597.67	■	280.93
	SCMUTILS	4462.83	■	■	■	7651.69	■	■	■	7699.14	■	83656.17	■	5889.26	■	■
	STALIN	364.08	547.73	399.39	295.00	543.68	690.64	63.96	52.93	956.47	1994.44	15048.42	16939.28	435.82	■	281.27

Comparative benchmark results for the `particle` and `saddle` examples (Siskind and Pearlmutter, 2008a), the `probabilistic-lambda-calculus` and `probabilistic-prolog` examples (Siskind, 2008) and an implementation of backpropagation in neural networks using AD. Column labels are for AD modes and nesting: F for forward, Fv for forward-vector aka stacked tangents, RF for reverse-over-forward, etc. All run times normalized relative to a unit run time for STALIN∇ on the corresponding example except that run times for `backprop-Fv` are normalized relative to a unit run time for STALIN∇ on `backprop-F`. Pre-existing AD tools are named in blue, others are custom implementations. Key: ■ not implemented but could implement, including FORTRAN, C, and C++; ■ not implemented in pre-existing AD tool; ■ problematic to implement. All code available at http://www.bcl.hamilton.ie/~qobi/ad2016-benchmarks/.

Benchmarks

COME TO JEFF SISKIND'S TALK

		particle				probabilistic-lambda-calculus				probabilistic-prolog		backprop		
		FF	FR	RF	RR	FF	FR	RF	RR	F	R	F	Fv	R
VLAD	STALIN∇	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	■	1.00
FORTRAN	ADIFOR	2.05	■	■	■	1.41	■	■	■	■	■	■	■	■
	TAPENADE	5.51	■	■	■	2.09	■	■	■	■	■	■	■	■
C	ADIC	■	■	■	■	■	■	■	■	■	■	■	■	■
C++	ADOL-C	■	■	■	■	■	■	■	■	■	■	■	■	■
	CPPAD	■	■	■	■	■	■	■	■	■	■	■	■	■
	FADBAD++	93.32	■	■	■	60.67	■	■	■	■	■	■	■	■
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Comparative benchmark results for the particle and puddle examples (Siskind and Pearlmutter, 2008a), the probabilistic-lambda-calculus and probabilistic-prolog examples (Siskind 2008) and an implementation of backpropagation in neural networks using AD. Column labels are for modes and timing: F forward, Fv forward-vector aka stacked tangents, RF for reverse-over-forward, etc. All run times normalized relative to a unit run time for STALIN∇ the corresponding example except that run times for backprop-Fv are normalized relative to a unit run time for STALIN∇ backprop-F. Re-executing AD tools' names in blue, others are custom implementations. Key: ■ not implemented but could implement, including FORTRAN, C, and C++; ■ not implemented in pre-existing AD tool; ■ problematic to implement. All code available at http://www.bcl.hamilton.ie/~qobi/ad2016-benchmarks/.

Functional AD: A Usable System

DiffSharp is a functional automatic differentiation (AD) library in F# for the multiplatform **.NET** framework.

```
let (y, dydx) = grad' f x
```

https://diffsharp.github.io/DiffSharp/

https://github.com/DiffSharp/DiffSharp

DiffSharp-using library shows how nested AD allows succinct implementations of, e.g., optimization of hyperparameters:
https://hypelib.github.io/Hype/

Atılım Güneş Baydin

history of automatic differentiation and of backpropagation

history of automatic differentiation and of backpropagation ✓

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embellishments and variants (backpropagation through time, RTRL, etc)

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embellishments and variants (backpropagation through time, RTRL, etc)

(Pearlmutter, 1994; Williams and Zipser, 1989; Simard et al., 1992)

```
backProp E f w x = ∇ (w↦E(f x)) w

hessianVector f x v = dd (r↦∇ f (x+r*v)) 0

RTRL f w x E =
  map (i↦(dd (w↦E(f w x)) w (e i))) (ι(dim w))

tangentProp E r f x =
  ∇ (w↦E(f x) + sqr(len(dd (θ↦f(r θ x)) 0)))
      w

hyperOpt E R train1 train2 =
  argmin (h↦
   let w0 =
    argmin (w↦R h w + sum(map (t↦E w t) train1))
    in sum(map (t↦E w0 t) train2)
```

Method of Temporal Differences

$$E(w) = \cdots + \lambda \sum_{t=0}^{t_f-2} \|y(t;w) - y(t+1;w)\|^2 + \cdots \qquad \text{TD}(\lambda)$$

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$$\nabla \; E \; w \qquad ?$$

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No!

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$$\nabla\ E\ w \qquad ?$$

$$\nabla\ (w \mapsto \|y(t;w) - y(t+1;w)\|^2)\ w \qquad ?$$

No!

$$\text{let } v = w \text{ in } \nabla\ (w \mapsto \|y(t;w) - y(t+1;v)\|^2)\ w$$

Hooks

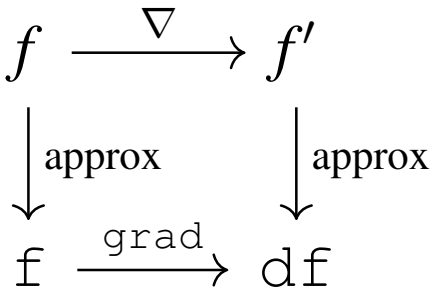
- Do you know what *Checkpoint reverse* is? *Cross-country optimization*?
- Did you know that computing $\partial^n f(x_1, \ldots, x_n)/\partial x_1 \cdots \partial x_n$ is #P-complete?
- Have you heard of Tapenade? FadBad++? ADIFOR/ADIC? Adolc? Stalin∇? ADiMat? DiffSharp? autograd? Haskell ad? http://autodiff.org?

Theoretical Frontier of AD

my idiosyncratic ravings

- Preallocation
- Not-so-simple derivatives (e.g., input vs feature space, natural gradient)
- Storage reduction by clever re-computation
- AD-enabled JIT Compiler
- Nice λ-Calculus Formulation (Correctness Proofs)
- Convergent Loops — Detailed Pragmatics
- Tropical Tangent/Co-Tangent Algebras for HMMs, etc
- Efficient $\nabla(x \mapsto \cdots \sum \cdots)$
- Derivatives and Approximation Do Not Commute

Does Not Commute! Does Not Commute!



Does Not Commute! Does Not Commute!

$$\begin{array}{ccc} f & \xrightarrow{\nabla} & f' \\ \downarrow \text{approx} & & \downarrow \text{approx} \\ \texttt{f} & \xrightarrow{\texttt{grad}} & \texttt{df} \end{array}$$


YOUR COMMUTE OFFICIALLY MAKES YOU MISERABLE

Conclusions

- AD is ancient.
- AD is in its infancy
- “Manual” AD is bug-ridden and scales poorly.
- Existing AD tools are fantastic when they match your needs.
- Better (more general, faster) tools are on the horizon.

Conclusions

- AD is ancient.
- AD is in its infancy
- “Manual” AD is bug-ridden and scales poorly.
- Existing AD tools are fantastic when they match your needs.
- Better (more general, faster) tools are on the horizon.
  If we only had the resources to build them...

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