Automatic Differentiation of Functional Programs or Lambda the Ultimate Calculus or How I Learned to Stop Worrying and Love Map-Closure

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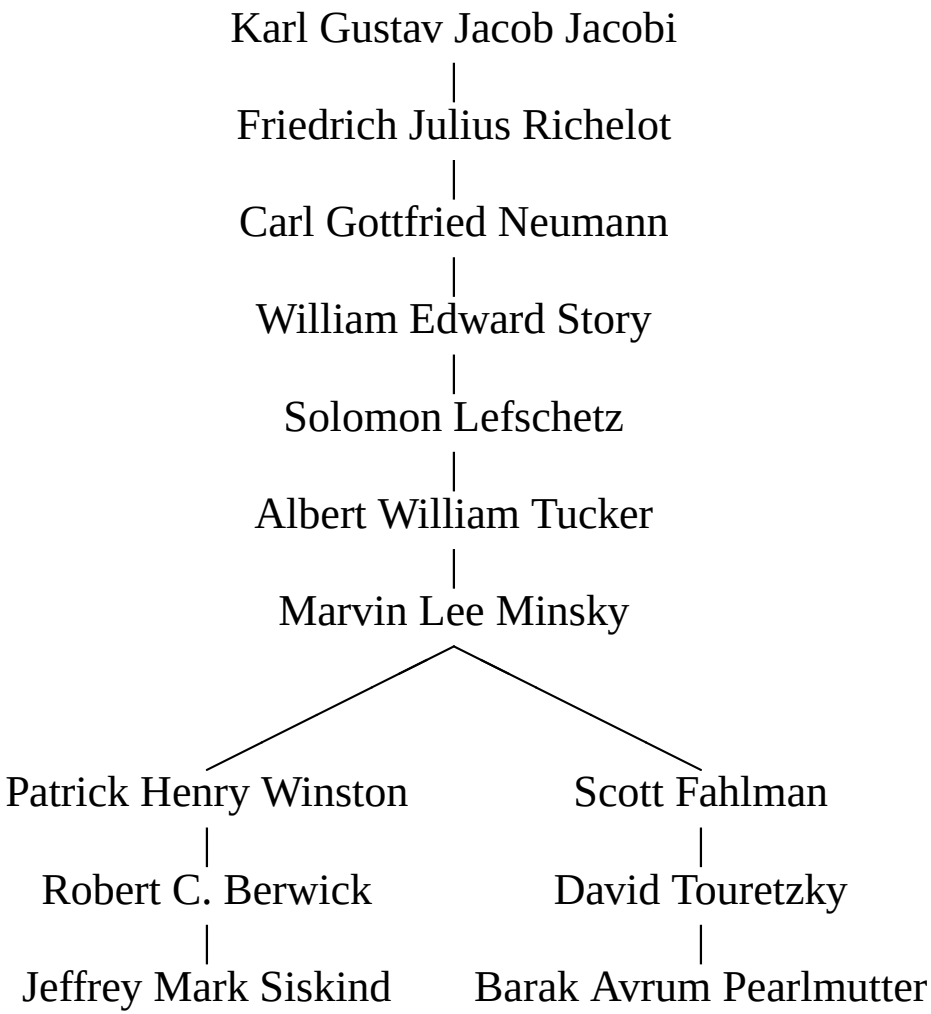
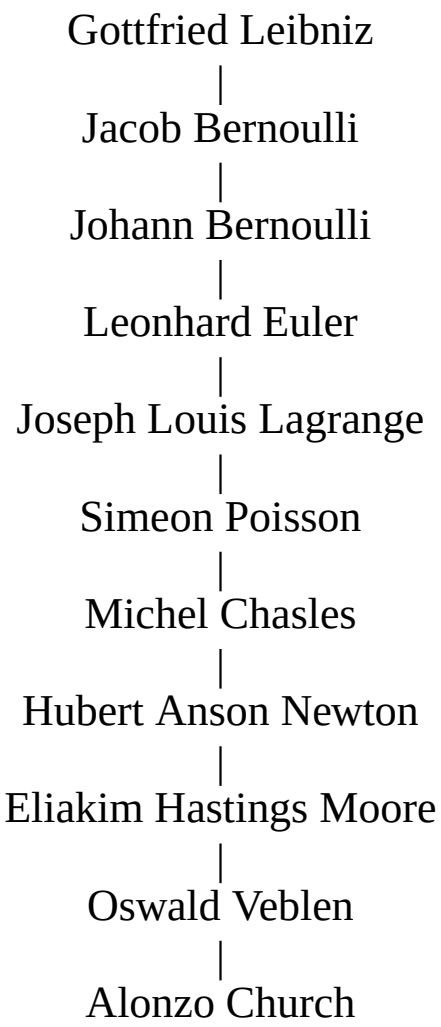
Joint work with Barak A. Pearlmutter.


Karl Gustav Jacob Jacobi
Friedrich Julius Richelot
Carl Gottfried Neumann
William Edward Story
Solomon Lefschetz
Albert William Tucker
Marvin Lee Minsky
Patrick Henry Winston
Scott Fahlman
Robert C. Berwick
David Touretzky
Jeffrey Mark Siskind
Barak Avrum Pearlmutter

It is, of course, not excluded that the range of arguments or range of values of a function should consist wholly or partly of functions. The derivative, as this notion appears in the elementary differential calculus, is a familiar mathematical example of a function for which both ranges consist of functions.

(¶4)

Church, A. (1941). *The Calculi of Lambda Conversion*, Princeton University Press, Princeton, NJ.


Gottfried Leibniz
Jacob Bernoulli
Johann Bernoulli
Leonhard Euler
Joseph Louis Lagrange
Simeon Poisson
Michel Chasles
Hubert Anson Newton
Eliakim Hastings Moore
Oswald Veblen
Alonzo Church

Leibnitz (1664) + Church (1941) = Siskind & Pearlmutter (2007)

Leibnitz, G. W. (1664). A new method for maxima and minima as well as tangents, which is impeded neither by fractional nor irrational quantities, and a remarkable type of calculus for this, *Acta Eruditorum*.

Everything You Always Wanted to Know About the Lambda Calculus*

*But Were Afraid To Ask

Everything You Always Wanted to Know About the Lambda Calculus*

(in 7 slides)

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*But Were Afraid To Ask
(omitted for this audience)

Differential Calculus for Dummies

Differential Calculus for Dummies

(in 6 slides)

Derivatives

$$\frac{\mathrm{d}ax^2}{\mathrm{d}x} \rightsquigarrow 2ax$$

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$$\mathcal{D}\ \lambda x\ ax^2$$

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$$\mathcal{D}_i : (\mathbb{R}^n \to \mathbb{R}) \to (\mathbb{R}^n \to \mathbb{R})$$

Gradients

$$\nabla f\ \mathbf{x} \quad = \quad (\mathcal{D}_1 f\ \mathbf{x}), \ldots, (\mathcal{D}_n f\ \mathbf{x})$$

$$\nabla \quad : \quad (\mathbb{R}^n \to \mathbb{R}) \to (\mathbb{R}^n \to \mathbb{R}^n)$$

Jacobians

$$f : \mathbb{R}^n \to \mathbb{R}^m$$

$$\mathbf{f} : (\mathbb{R}^n \to \mathbb{R})^m$$

$$(\mathcal{J}\ f\ \mathbf{x})[i,j] = (\nabla\ (\mathbf{f}[i]))[j]$$

$$\mathcal{J} : (\mathbb{R}^n \to \mathbb{R}^m) \to (\mathbb{R}^n \to \mathbb{R}^{m \times n})$$

Operators

$\mathcal{D}$, ∇, and $\mathcal{J}$ are traditionally called *operators*.
A more modern term is *higher-order functions*.
Higher-order functions are common in mathematics, physics, and engineering:

> *summations*, *comprehensions*, *quantifications*, *optimizations*, *integrals*, *convolutions*, *filters*, *edge detectors*, *Fourier transforms*, *differential equations*, *Hamiltonians*, . . .

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The Essence of Forward-Mode AD

Taylor expansion:

$$f(c+\varepsilon) = \frac{f(c)}{0!} + \frac{f'(c)}{1!}\varepsilon + \frac{f''(c)}{2!}\varepsilon^2 + \cdots + \frac{f^{(i)}(c)}{i!}\varepsilon^i + \cdots$$

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- evaluate f

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(Analogous to complex numbers $a + b\mathrm{i}$ represented as $\langle a, b \rangle$.)

Taylor Expansions and Dual Numbers

Taylor, B. (1715). *Methodus Incrementorum Directa et Inversa*, London.

Clifford, W. K. (1873). Preliminary Sketch of Bi-quaternions, *Proceedings of the London Mathematical Society*, **4**:381–95.

Arithmetic on Truncated Power Series (i.e. Dual Numbers)

$$(x_0 + x_1\varepsilon + \mathcal{O}(\varepsilon^2)) + (y_0 + y_1\varepsilon + \mathcal{O}(\varepsilon^2)) = (x_0 + y_0) + (x_1 + y_1)\varepsilon + \mathcal{O}(\varepsilon^2)$$

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$$\begin{aligned}(x_0 + x_1\varepsilon + \mathcal{O}(\varepsilon^2)) \times (y_0 + y_1\varepsilon + \mathcal{O}(\varepsilon^2)) \\ = (x_0 \times y_0) + (x_0 \times y_1 + x_1 \times y_0)\varepsilon + \mathcal{O}(\varepsilon^2)\end{aligned}$$

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$$u\ (x_0 + x_1\varepsilon + \mathcal{O}(\varepsilon^2)) = (u\ x_0) + (x_1 \times (u'\ x_0))\varepsilon + \mathcal{O}(\varepsilon^2)$$

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$$\begin{aligned}b\ ((x_0 + x_1\varepsilon + \mathcal{O}(\varepsilon^2)), (y_0 + y_1\varepsilon + \mathcal{O}(\varepsilon^2))) \\ = (b\ (x_0, y_0)) + (x_1 \times (b^{(1,0)}\ (x_0, y_0)) + y_1 \times (b^{(0,1)}\ (x_0, y_0)))\varepsilon + \mathcal{O}(\varepsilon^2)\end{aligned}$$

Traditional Forward-Mode AD

$$\mathbb{R}^n \to \mathbb{R}^m \quad \rightsquigarrow \quad (\mathbb{R}^n \times \mathbb{R}^n) \to (\mathbb{R}^m \times \mathbb{R}^m)$$
$$\mathbb{R}^n \to \mathbb{R}^m \quad \rightsquigarrow \quad (\mathbb{R} \times \mathbb{R})^n \to (\mathbb{R} \times \mathbb{R})^m$$

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

In differential algebra, dual numbers are known as *bundles* of (primal) values x and their *tangents* $\overline{x'}$.

$$x \rhd \overline{x'}$$

```
(define-structure bundle primal tangent)
```

Tangent Spaces

$$
\begin{aligned}
\overline{v'} &\in \mathbb{R} \quad \text{when } v \in \mathbb{R} \\
\overline{v'} &= v \quad \text{when } v \text{ is a discrete scalar} \\
\overline{v \rhd \overline{v'}} &= \overline{v'} \rhd \overline{\overline{v'}} \\
\overline{v_1, v_2'} &= \overline{v_1'}, \overline{v_2'} \\
\overline{\langle \{x_1 \mapsto v_1, \ldots, x_n \mapsto v_n\}, \lambda x\ e \rangle} &= \langle \{x_1 \mapsto \overline{v_1'}, \ldots, x_n \mapsto \overline{v_n'}\}, \lambda x\ e \rangle
\end{aligned}
$$

$$v \blacktriangleright \overline{v'} \stackrel{\triangle}{=} v \rhd \overline{v'} \qquad \text{when } v \text{ is a scalar}$$

$$v \blacktriangleright \overline{v'} \stackrel{\triangle}{=} \overrightarrow{v} \qquad \text{when } v \text{ is a primitive}$$

$$(v \rhd \overline{v'}) \blacktriangleright \overline{(v \rhd \overline{v'})} \stackrel{\triangle}{=} (v \blacktriangleright \overline{v'}) \rhd (\overline{v'} \blacktriangleright \overline{\overline{v'}})$$

$$(v_1, v_2) \blacktriangleright \overline{(v_1, v_2)} \stackrel{\triangle}{=} (v_1 \blacktriangleright \overline{v_1'}), (v_2 \blacktriangleright \overline{v_2'})$$

$$\langle \{x_1 \mapsto v_1, \ldots, x_n \mapsto v_n\}, \lambda x\ e \rangle \blacktriangleright \overline{\langle \{x_1 \mapsto v_1, \ldots, x_n \mapsto v_n\}, \lambda x\ e \rangle} \stackrel{\triangle}{=}$$

$$\langle \{x_1 \mapsto (v_1 \blacktriangleright \overline{v_1'}), \ldots, x_n \mapsto (v_n \blacktriangleright \overline{v_n'})\}, \lambda x\ e \rangle$$

$$\overrightarrow{u} \triangleq \lambda(v \blacktriangleright \overline{v})\ ((u\ v) \blacktriangleright ((\mathcal{D}\ u\ v) \times \overline{v}))$$

$$\overrightarrow{b} \triangleq \lambda((v_1, v_2) \blacktriangleright \overline{(v_1, v_2)})\ (b\ (v_1, v_2)) \blacktriangleright (((\mathcal{D}_1\ b\ (v_1, v_2)) \times \overline{v_1}) + ((\mathcal{D}_2\ b\ (v_1, v_2)) \times \overline{v_2}))$$

$$\overrightarrow{p} \triangleq \lambda(v \blacktriangleright \overline{v})\ \overrightarrow{\mathcal{J}}\ (p\ v)$$

$$\overrightarrow{q} \triangleq \lambda((v_1, v_2) \blacktriangleright \overline{(v_1, v_2)})\ \overrightarrow{\mathcal{J}}\ (q\ (v_1, v_2))$$

```
(define (bundle v v-tangent)
 (cond ((or (and (null? v) (null? v-tangent))
            (and (boolean? v) (eq? v v-tangent))
            (and (real? v) (real? v-tangent)))
        (make-bundle v v-tangent))
       ((and (equal? v +) (equal? v-tangent +))
        (lambda (v-forward)
         (bundle (+ (car (primal v-forward))
                    (cdr (primal v-forward)))
                 (+ (car (tangent v-forward))
                    (cdr (tangent v-forward))))))
       ;; ...
       ((and (bundle? v) (bundle? v-tangent))
        (make-bundle
         (bundle (bundle-primal v) (bundle-primal v-tangent))
         (bundle (bundle-tangent v) (bundle-tangent v-tangent))))
       ((and (pair? v) (pair? v-tangent))
        (cons (bundle (car v) (car v-tangent))
              (bundle (cdr v) (cdr v-tangent))))
       ((and (procedure? v) (procedure? v-tangent))
        (map-closure bundle v v-tangent))
       (else (fuck-up))))
```

$\textsc{Primal}\ \overrightarrow{v} \stackrel{\triangle}{=} v \qquad$ when v is a primitive

$\textsc{Primal}\ (v \rhd \overrightarrow{v'}) \stackrel{\triangle}{=} v$

$\textsc{Primal}\ ((v_1 \blacktriangleright \overrightarrow{v_1'}), (v_2 \blacktriangleright \overrightarrow{v_2'})) \stackrel{\triangle}{=} v_1, v_2$

$\textsc{Primal}\ \langle \{x_1 \mapsto (v_1 \blacktriangleright \overrightarrow{v_1'}), \ldots, x_n \mapsto (v_n \blacktriangleright \overrightarrow{v_n'})\}, \lambda x\ e \rangle \stackrel{\triangle}{=}$
$\langle \{x_1 \mapsto v_1, \ldots, x_n \mapsto v_n\}, \lambda x\ e \rangle$

```
(define (primal v)
 (cond
  ((equal? v (j* +)) +)
  ;; ...
  ((bundle? v) (bundle-primal v))
  ((pair? v)
   (cons (primal (car v)) (primal (cdr v))))
  ((procedure? v) (map-closure primal v))
  (else (fuck-up))))
```

$\textsc{Tangent}\ \overrightarrow{v} \stackrel{\triangle}{=} v \qquad$ when v is a primitive

$\textsc{Tangent}\ (v \rhd \overrightarrow{v'}) \stackrel{\triangle}{=} \overrightarrow{v'}$

$\textsc{Tangent}\ ((v_1 \blacktriangleright \overrightarrow{v_1'}), (v_2 \blacktriangleright \overrightarrow{v_2'})) \stackrel{\triangle}{=} \overrightarrow{v_1'}, \overrightarrow{v_2'}$

$\textsc{Tangent}\ \langle \{x_1 \mapsto (v_1 \blacktriangleright \overrightarrow{v_1'}), \ldots, x_n \mapsto (v_n \blacktriangleright \overrightarrow{v_n'})\}, \lambda x\ e \rangle \stackrel{\triangle}{=}$
$\langle \{x_1 \mapsto \overrightarrow{v_1'}, \ldots, x_n \mapsto \overrightarrow{v_n'}\}, \lambda x\ e \rangle$

```
(define (tangent v)
 (cond
  ((equal? v (j* +)) +)
  ;; ...
  ((bundle? v) (bundle-tangent v))
  ((pair? v)
   (cons (tangent (car v)) (tangent (cdr v))))
  ((procedure? v) (map-closure tangent v))
  (else (fuck-up))))
```

$$\mathbf{0}\ v \stackrel{\triangle}{=} 0 \qquad \text{when } v \in \mathbb{R}$$

$$\mathbf{0}\ v \stackrel{\triangle}{=} v \qquad \text{when } v \text{ is a discrete scalar}$$

$$\mathbf{0}\ (v \rhd \overline{v'}) \stackrel{\triangle}{=} (\mathbf{0}\ v) \rhd (\mathbf{0}\ \overline{v'})$$

$$\mathbf{0}\ (v_1, v_2) \stackrel{\triangle}{=} (\mathbf{0}\ v_1), (\mathbf{0}\ v_2)$$

$$\mathbf{0}\ \langle \{x_1 \mapsto v_1, \ldots, x_n \mapsto v_n\}, \lambda x\ e \rangle \stackrel{\triangle}{=} \langle \{x_1 \mapsto (\mathbf{0}\ v_1), \ldots, x_n \mapsto (\mathbf{0}\ v_n)\}, \lambda x\ e \rangle$$

```
(define (zero v)
 (cond
  ((real? v) 0)
  ((null? v) v)
  ((boolean? v) v)
  ((bundle? v)
   (make-bundle (zero (bundle-primal v))
                (zero (bundle-tangent v))))
  ((pair? v) (cons (zero (car v)) (zero (cdr v))))
  ((procedure? v) (map-closure zero v))
  (else (fuck-up))))
```

$$\overrightarrow{\mathcal{J}}\ v \stackrel{\triangle}{=} v \blacktriangleright (\mathbf{0}\ v)$$

```
(define (j* v) (bundle v (zero v)))
```

A Xillion Implementations of AD

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MAPLE: GRADIENT (Monagan & Neuenschwander, 1993)

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FORTRAN: ADIFOR (Bischof *et al.*, 1996)

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	⋮

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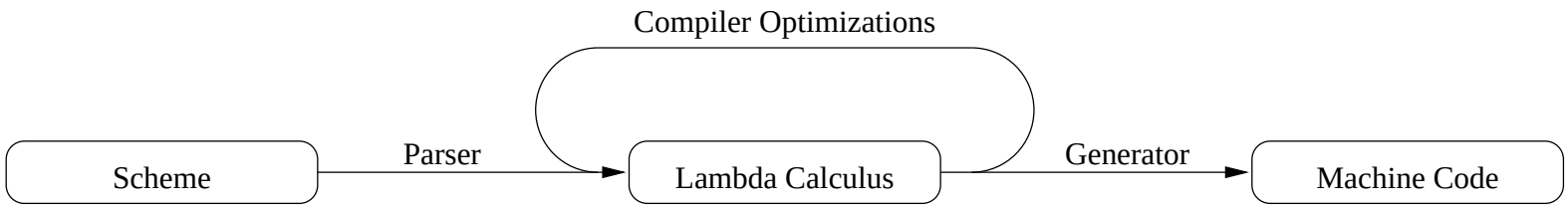
SCHEME: SCMUTILS (Sussman *et al.*, 2001)

MATLAB: ADIMAT (Bischof *et al.*, 2003)

⋮

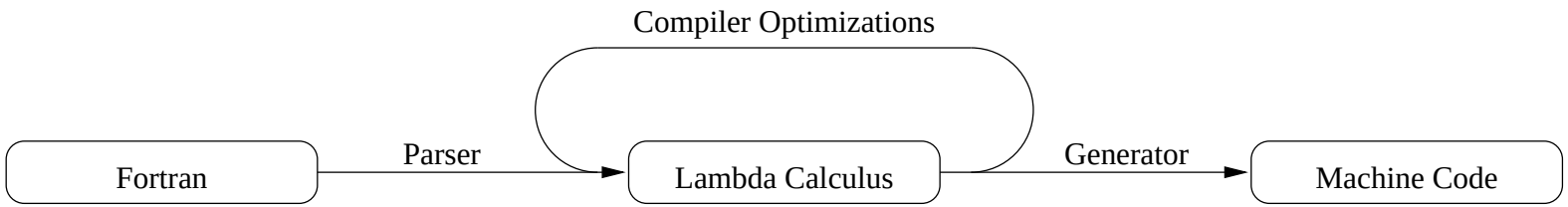
`http://www.autodiff.org`

Lambda the Ultimate Intermediate Language



Steele, Jr., G. L. and Sussman, G. J. (1976). *Lambda, the Ultimate Imperative*, MIT AI memo 353.

Lambda the Ultimate Intermediate Language



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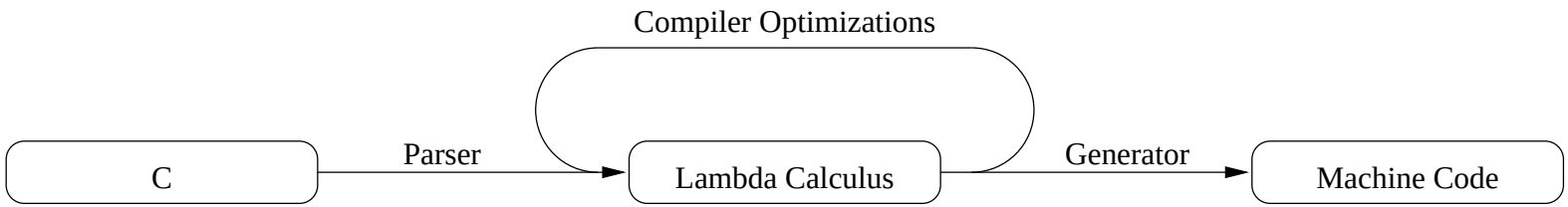

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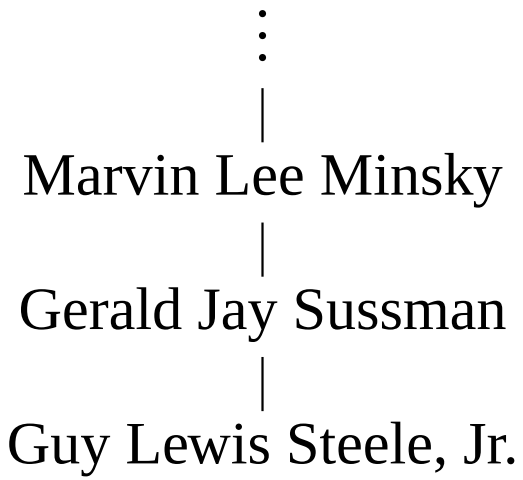
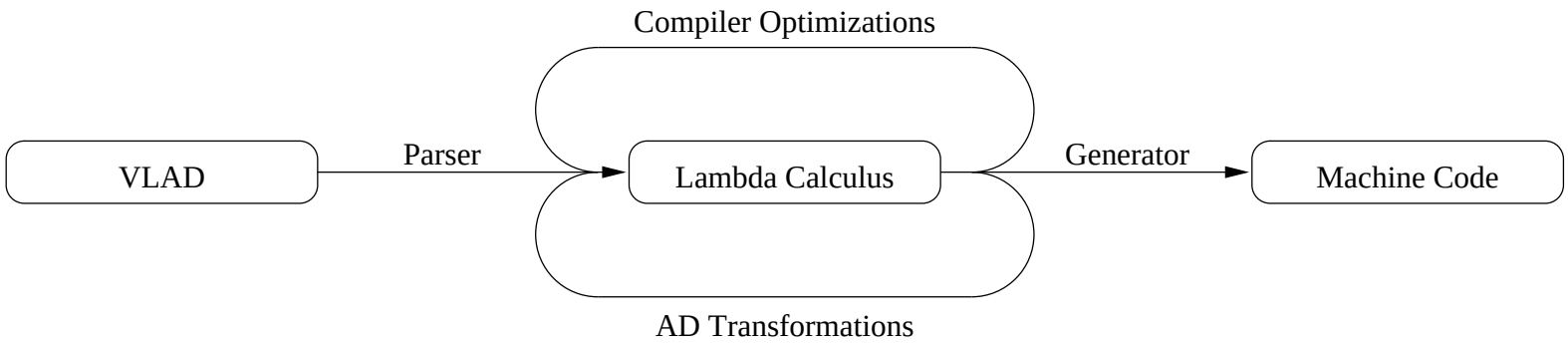
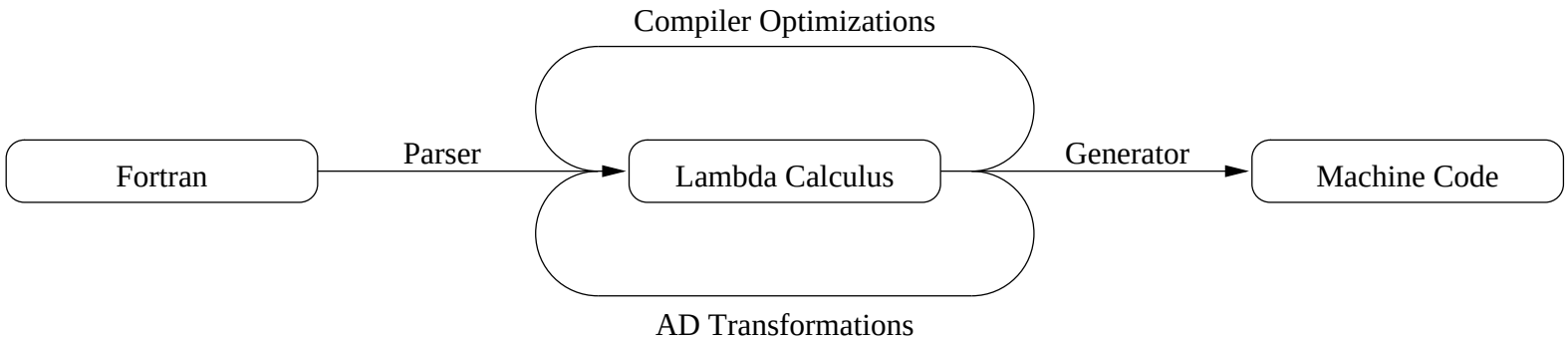

Marvin Lee Minsky
Gerald Jay Sussman
Guy Lewis Steele, Jr.

Lambda the Ultimate Intermediate Language *for AD*



Lambda the Ultimate Intermediate Language *for AD*



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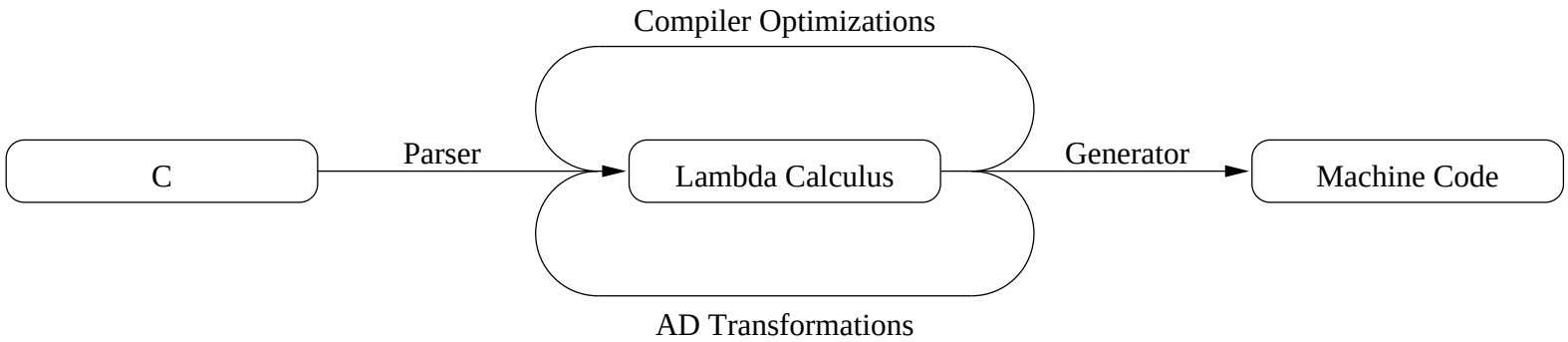

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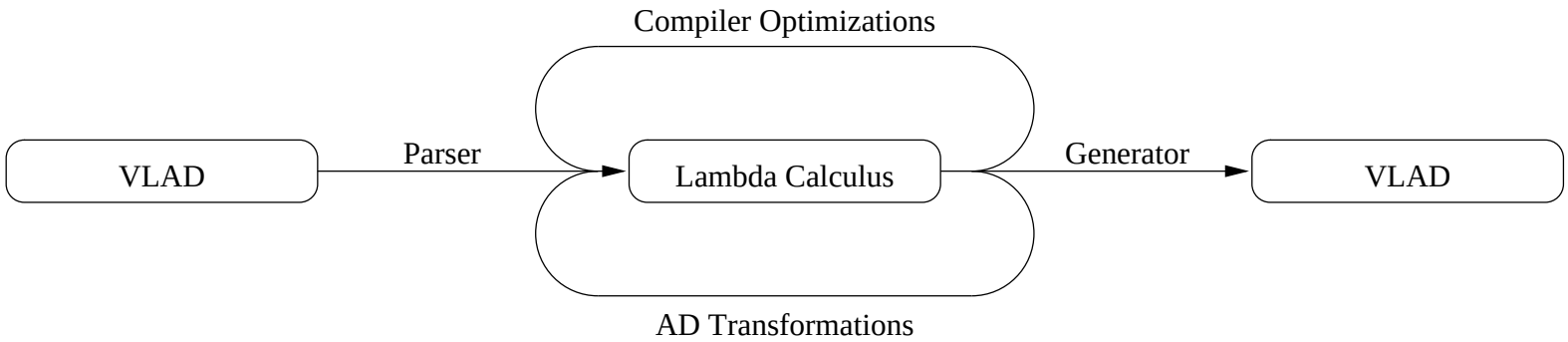
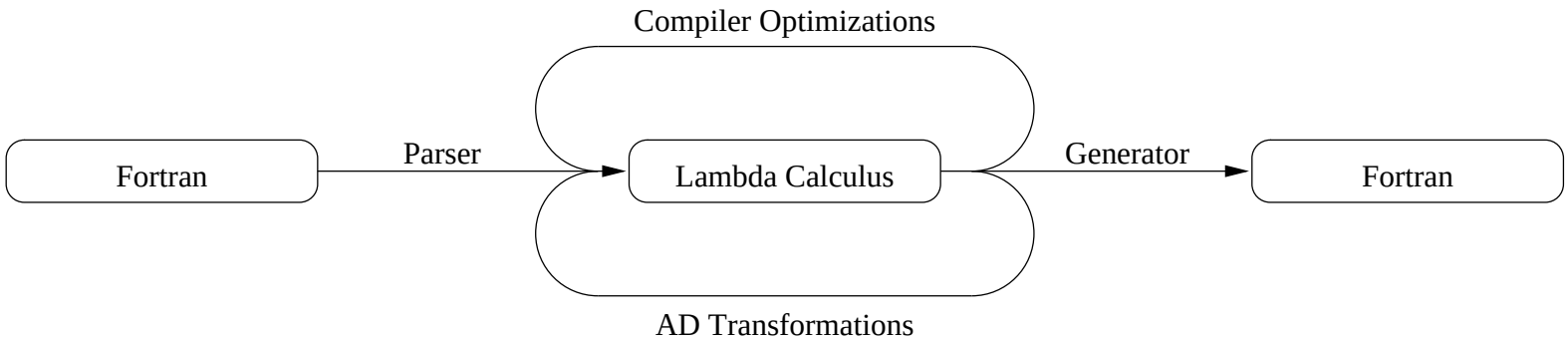
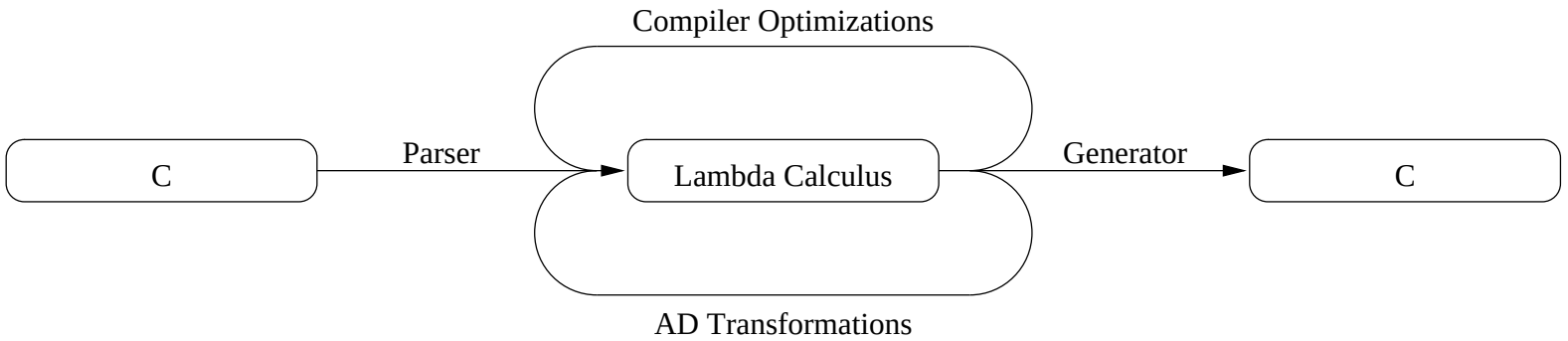


Lambda the Ultimate Intermediate Language *for AD*

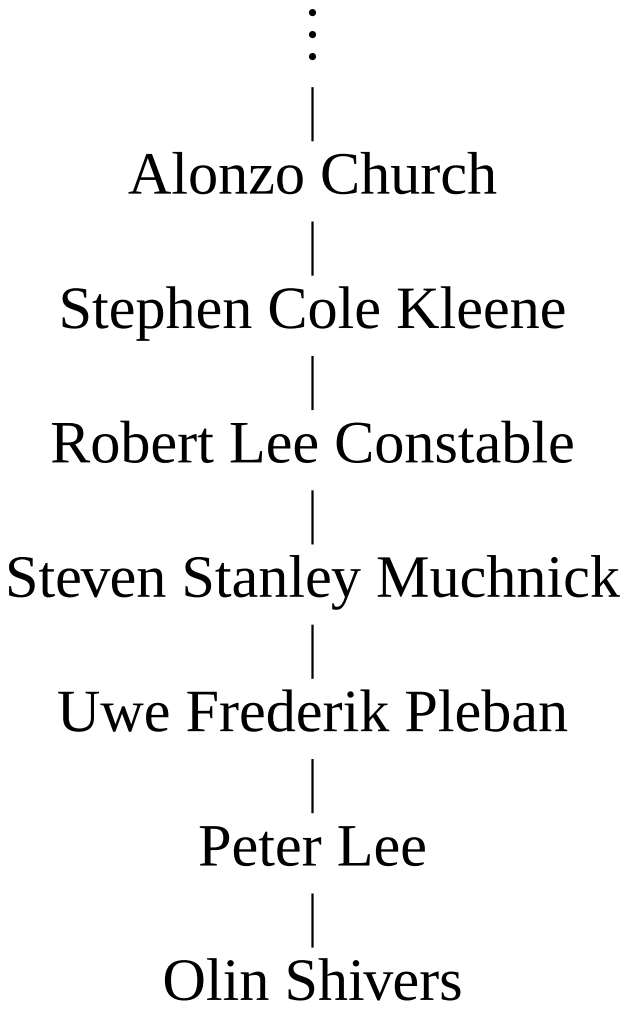


Lambda the Ultimate Intermediate Language *for AD*



Polyvariant flow analysis can (in most cases) eliminate run-time invocation of `map-closure` in `bundle`, `primal`, `tangent`, and `zero`.

Shivers, III, O. G. (1991). *Control-Flow Analysis of Higher-Order Languages* ***or*** *Taming Lambda*, Ph.D. thesis, CMU.


Alonzo Church
Stephen Cole Kleene
Robert Lee Constable
Steven Stanley Muchnick
Uwe Frederik Pleban
Peter Lee
Olin Shivers

Derivatives

$$\mathcal{D}\ f\ x \stackrel{\triangle}{=} \textsc{Tangent}\ ((\overrightarrow{\mathcal{J}}\ f)\ (x \blacktriangleright 1))$$

Roots using Newton-Raphson

$$\text{ROOT}\ f\ x_0\ \epsilon \stackrel{\triangle}{=} \textbf{let}\ x' \stackrel{\triangle}{=} x_0 - \frac{f\ x_0}{\mathcal{D}\ f\ x_0}$$
$$\textbf{in if}\ |x_0 - x'| \leq \epsilon\ \textbf{then}\ x_0\ \textbf{else}\ \text{ROOT}\ f\ x'\ \epsilon$$

Univariate Minimizer

Line Search

$$\textsc{LineSearch}\ f\ x_0\ \epsilon \stackrel{\triangle}{=} \textsc{Root}\ (\mathcal{D}\ f)\ x_0\ \epsilon$$

Gradients

$$\nabla f\ x \stackrel{\triangle}{=} \textbf{let}\ n \stackrel{\triangle}{=} \textsc{Length}\ x$$
$$\textbf{in}\ \textsc{Map}\ (\lambda i\ \textsc{Tangent}\ ((\overrightarrow{\mathcal{J}}\ f)\ (x \blacktriangleright e_{i,n})))\ (\iota\ n)$$

Multivariate Minimizer

Gradient Descent

$$\begin{array}{l}
\textsc{GradientDescent}\ f\ x_0\ \epsilon \stackrel{\triangle}{=} \\
\quad \textbf{let}\ g \stackrel{\triangle}{=} \nabla f\ x_0 \\
\quad \textbf{in if}\ \|g\| \leq \epsilon \\
\qquad \textbf{then}\ x_0 \\
\qquad \textbf{else}\ \textsc{GradientDescent} \\
\qquad\quad f\ (x_0 + ((\textsc{LineSearch}\ (\lambda k\ f\ (x_0 + (k \times g)))\ 0\ \epsilon) \times g))\ \epsilon
\end{array}$$

Saddle Points

Continuous Two-Person Zero Sum Games

$$\mathbf{x} : \mathbb{R}^m$$
$$\mathbf{y} : \mathbb{R}^n$$
$$\textsc{Payoff} : \mathbb{R}^m \times \mathbb{R}^n \rightarrow \mathbb{R}$$
$$\min_{\mathbf{x}} \max_{\mathbf{y}} \textsc{Payoff}\ (\mathbf{x}, \mathbf{y})$$

$$(\mathbf{x}^*, \mathbf{y}^*) = \textbf{let}\ \mathbf{x}^* \stackrel{\triangle}{=} \textsc{GradientDescent}\ (\lambda \mathbf{x}\ \textsc{GradientDescent}\ (\lambda \mathbf{y}\ (-\textsc{Payoff}\ (\mathbf{x}, \mathbf{y})))\ \mathbf{y}_0\ \epsilon)\ \mathbf{x}_0\ \epsilon$$
$$\textbf{in}\ (\mathbf{x}^*, (\textsc{GradientDescent}\ (\lambda \mathbf{y}\ (-\textsc{Payoff}\ (\mathbf{x}^*, \mathbf{y})))\ \mathbf{y}_0\ \epsilon))$$

von Neumann, J. and Morgenstern, O. (1944). *Theory of Games and Economic Behavior*. Princeton University Press, Princeton, NJ.

Carl Gauss

|

Christoph Gudermann

|

Karl Weierstrass

|

Hermann Schwarz

|

Leopold Fejér

|

John von Neumann

Neural Nets

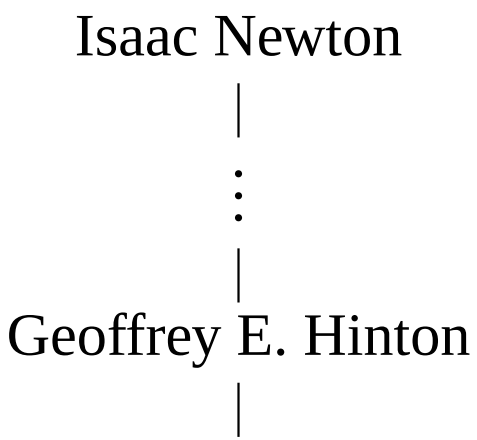
$$\textsc{Neuron}\ \mathbf{w}\ \mathbf{x} \stackrel{\triangle}{=} \textsc{Sigmoid}\ (\mathbf{w} \cdot \mathbf{x})$$

$$\textsc{NeuralNet}\ [\mathbf{w}, \mathbf{w}_1, \ldots, \mathbf{w}_m]\ \mathbf{x} \stackrel{\triangle}{=}$$
$$\quad \textsc{Neuron}\ \mathbf{w}\ [(\textsc{Neuron}\ \mathbf{w}_1\ \mathbf{x}), \ldots, (\textsc{Neuron}\ \mathbf{w}_m\ \mathbf{x})]$$

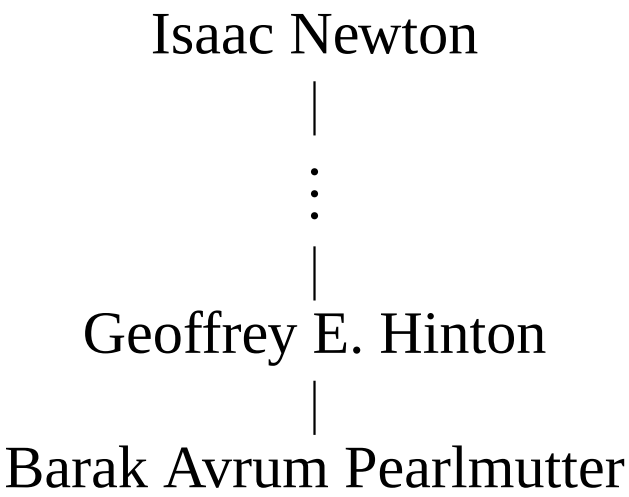
$$\textsc{Error}\ \mathbf{w} \stackrel{\triangle}{=}$$
$$\quad \|[y_1, \ldots, y_n] - [(\textsc{NeuralNet}\ \mathbf{w}\ \mathbf{x}_1), \ldots, (\textsc{NeuralNet}\ \mathbf{w}\ \mathbf{x}_n)]\|$$

$$\textsc{GradientDescent}\ \textsc{Error}\ \mathbf{w}_0\ \epsilon$$

Rumelhart, D. E., Hinton, G. E., and Williams, R. J. (1986). Learning representations by back-propagating errors, *Nature*, **323**:533–6.



Newton, I. (1704). De quadratura curvarum, In *Optiks*, 1704 edition, appendix.



Newton, I. (1704). De quadratura curvarum, In *Optiks*, 1704 edition, appendix.

Work in Progress

Lambda: the ultimate calculus

Part of larger project to combine λ-calculus and AD.

Work in Progress

Lambda: the ultimate calculus

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- include both forward-mode and reverse-mode operators

Work in Progress

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- include both forward-mode and reverse-mode operators
- get numerically correct answers
- via correct transformation (time/space complexity)

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- get numerically correct answers
- via correct transformation (time/space complexity)
- make $\overrightarrow{\mathcal{J}}$ and $\overleftarrow{\mathcal{J}}$ first class
- make them apply to *all* (differentiable) programs
- handle nested application (self-application of $\overrightarrow{\mathcal{J}}$ and $\overleftarrow{\mathcal{J}}$)

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- good puns
  - programming language: Voice for FP + AD
    Functional Language for AD

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    Functional Language for AD

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    Functional Language for AD
  - implementation: high-performance SCHEME + AD

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    Functional Language for AD
  - implementation: STALIN + AD

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    Functional Language for AD
  - implementation: STALIN + gradients

Work in Progress

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- good puns
  - programming language: VLAD
    Functional Language for AD
  - implementation: STALIN $+ \nabla$

Work in Progress

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  - programming language: VLAD
    Functional Language for AD
  - implementation: STALIN∇

Work in Progress

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- handle nested application (self-application of $\overrightarrow{\mathcal{J}}$ and $\overleftarrow{\mathcal{J}}$)
- good puns
  - programming language: VLAD
    Functional Language for AD
  - implementation: STALIN∇
- manuscripts and code:
  `http://www.bcl.hamilton.ie/~qobi/stalingrad/`