Automatic differentiation From Functional Analysis to Functional Programming

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Automatic differentation: What?

- One-shot AD:
  - Input:
    - Procedure p implementing function $f : \mathbb{R}^m \to \mathbb{R}^n$
    - Vector $x \in \mathbb{R}^m$ (point)
    - Input vector $\Delta x \in \mathbb{R}^m$ (offset)
  - Output:
  - $f'(x)(\Delta x)$ where $f'(x) : B(\mathbb{R}^m, \mathbb{R}^n)$ is derivative of f at x.

  $B(\mathbb{R}^m, \mathbb{R}^n)$ = bounded linear functions from $\mathbb{R}^m$ to $\mathbb{R}^n$.
- Staged AD:
  Compute (code for) f' and a neighborhood of x where $f'(x')$ is derivative of (the function implemented by) p at x'.

Automatic differentiation: What for?

- Machine learning (backpropagation of constraints, ...)
- Quantitative finance (sensitivities, "Greeks")
- Atmospheric chemistry
- Breast cancer biostatistical analysis
- Computational fluid dynamics
- Chemical kinetics
- Climate and weather modeling
- Semiconductor device simulation
- Water reservoir simulation
- Mechanical engineering (design optimization)
- ...

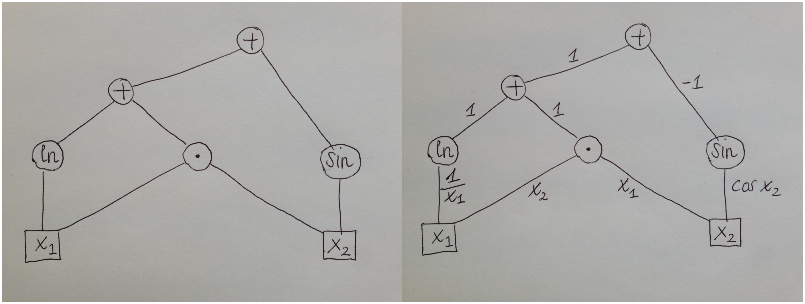
Automatic differentiation: How?

Conceptually:

1. Run p on x with uninterpreted $\mathbb{R}$-primitives, building a computation graph ($= f$ represented as data dependency dag).
2. Annotate edges with derivatives of primitives in nodes above ($= f'$).
3. Compute $y = f(x)$ by evaluating the nodes.
4. Compute $\frac{\partial y}{\partial x}$ as the sum of edge products of all paths from x to y.

Automatic differentiation: Example

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



$$\begin{aligned} \frac{\partial y}{\partial x_1} &= 1 \cdot 1 \cdot \frac{1}{x_1} + 1 \cdot 1 \cdot x_2 &= \frac{1}{x_1} + x_2 \\ \frac{\partial y}{\partial x_2} &= 1 \cdot 1 \cdot x_1 + (-1) \cdot \cos x_2 &= x_1 - \cos x_2 \end{aligned}$$

Automatic differentiation: Basic methods

- Forward-mode AD (1964):
  - Evaluation of $f'(x)(\Delta x)$ by forward (bottom-up) traversal of computation graph.
  - computation graph need not be materialized.
- Reverse-mode AD (1970):
  - Evaluation of $f(x)$ by forward traversal and $f(x)(\Delta x)$ by backward traversal;
  - computation graph ("tape") is materialized.
- Mixed-mode AD: A bit forward, a bit backward.

Jakobian

Definition (Jakobian at x)

$f'(x)$ as $n \times m$-matrix.

Compute Jakobian at x. Basic strategy:

- If $n > m$, use forward mode: For each source (input), compute reachable nodes/traverse whole graph.
- If $m >> n$, use reverse mode: For each sink (output), compute reverse reachable nodes/traverse whole graph.

Theorem (Naumann 2006)

Minimal number of elementary operations required to compute Jakobian from computation graph is NP-complete.

Observations

- AD usually focuses on *scalar* computations:

$$
\begin{array}{l}
\textbf{let } \Delta\bar{v}_4 = \Delta y \cdot 1 \textbf{ in} \\
\textbf{let } \Delta\bar{v}_3 = \Delta y \cdot 1 \textbf{ in} \\
\textbf{let } \Delta\bar{v}_2 = \Delta\bar{v}_4 \cdot 1 \textbf{ in} \\
\textbf{let } \Delta\bar{v}_1 = \Delta\bar{v}_4 \cdot 1 \textbf{ in} \\
\textbf{let } \Delta\bar{x}_2 = \Delta\bar{v}_3 \cdot (-\cos x_2) \textbf{ in} \\
\textbf{let } \Delta v_2 = x_2 \cdot \Delta x_1 + x_1 \cdot \Delta x_2 \textbf{ in} \\
\textbf{let } \Delta\bar{x}_2 = \Delta\bar{v}_2 \cdot x_1 + \Delta\bar{x}_2 \textbf{ in} \\
\textbf{let } \Delta\bar{x}_1 = \Delta\bar{v}_1 \cdot \frac{1}{x_1} + \Delta\bar{v}_2 \cdot x_2 \textbf{ in} \\
\Delta\bar{x}_1 \cdot \Delta x_1 + \Delta\bar{x}_2 \cdot \Delta x_2
\end{array}
$$

  - Obscures computation graph
  - Conflates computation graph with evaluation order
- Derivative represented as Jakobian matrix:
  - For $f : \mathbb{R}^{10000000} \to \mathbb{R}^{10000}$, 10000000×10000 matrix; entries $\mathbb{R}$-expressions with 10000000 free scalar variables
  - What if $f : \mathbb{R}^{\infty} \to \mathbb{R}$?

Fréchet derivative

Definition (Fréchet derivative)

Let V, W be Banach spaces, let $U \subseteq V$ be open, and $f : |U| \to |W|$ a function. $A \in B(V, W)$ is the Fréchet derivative of f at $x \in |V|$, written $f'(x)$, if

$$\lim_{h \to 0} \frac{\|f(x+h) - f(x) - |A|(h)\|}{\|h\|} = 0.$$

f is differentiable at x if it has a Fréchet derivative at x.

(Banach space = vector space + norm + limits)

Chain rule

Theorem (Chain rule)

If $f : U \to V$ *and* $g : V \to W$ *sufficiently differentiable then*

$$(g \circ f)' \quad = \quad (g' \circ f) \mathbin{\hat{\bullet}} f' \tag{1}$$

where

$\circ$ = *function composition;*

$\bullet$ = *linear function composition;*

$\hat{\bullet}$ *lifted linear function composition:* $(g \mathbin{\hat{\bullet}} f)(x) = g(x) \bullet f(x)$.

Bilinear functions

Definition (Bilinear function, tensor product)

$\diamond : U \times V \to W$ is bilinear if it is linear in each argument: for all x, y both $(x\diamond)$ and $(\diamond y)$ are linear maps.

Bilinear functions behave like products: They distribute over addition. Examples:

- Multiplication,
- tensor product,
- linear function composition;
- If $\diamond$ is bilinear, so is $\hat{\diamond}$.

Derivative calculus

Theorem (Linear function derivatives)

If f is linear, then $f'(x) = f$. Equivalently, $f' = K(f)$ where $K(f)(x) = f$.

Theorem (Generalized product rule)

If $\diamond$ is bilinear, then

$$(f \mathbin{\hat{\diamond}} g)'(x)(u) = (f'(x)(u) \diamond g(x)) + (f(x) \diamond g'(x)(u))$$

Equivalently,

$$\begin{aligned}(f \mathbin{\hat{\diamond}} g)'(x) &= (f'(x) \mathbin{\hat{\diamond}} K(g(x))) + (K(f(x)) \mathbin{\hat{\diamond}} g'(x)) \\ (f \mathbin{\hat{\diamond}} g)' &= (f' \mathbin{\hat{\hat{\diamond}}} (K \circ g)) + ((K \circ f) \mathbin{\hat{\hat{\diamond}}} g')\end{aligned}$$

Generalizes product rule of differentiation.

Higher-order derivatives

Using derivatives for primitive functions, the chain rule, rule for linear functions and the generalized product rule, higher-order derivatives can be derived combinatorially.

Corollary

$$
\begin{aligned}
(g \circ f)'' &= ((g' \circ f) \,\hat{\bullet}\, f')' \\
&= (g' \circ f)' \,\hat{\hat{\bullet}}\, (K \circ f') + (K \circ g' \circ f) \,\hat{\hat{\bullet}}\, f'' \\
&= ((g'' \circ f) \,\hat{\bullet}\, f') \,\hat{\hat{\bullet}}\, (K \circ f') + (K \circ g' \circ f) \,\hat{\hat{\bullet}}\, f''
\end{aligned}
$$

Observations

- Linear function representations with explicit composition:
  - Can be much more compact than (normalized) matrix representation. With sharing, linear-sized in function expression differentiated.
  - Embody opportunity for data-parallel computation
  - Optimization of f by linear algebra
  - Optimization of f-generation from p by slicing.
- Extends to towers of derivatives

Benchmarks

In progress. Goal: functions such as

The Gaussian mixture model with Wishart prior has log-posterior function $\log\left(p(\boldsymbol{x};\boldsymbol{w},\boldsymbol{\mu},\boldsymbol{\Sigma})\right) =$

$$\log\left(\prod_{i=1}^{N}\sum_{k=1}^{K} w_k \det\left(2\pi\Sigma_k\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}_i-\boldsymbol{\mu}_k)^T\Sigma_k^{-1}(\boldsymbol{x}_i-\boldsymbol{\mu}_k)\right)\prod_{k=1}^{K} C(D,m)|\Sigma_k|^m \exp\left(-\frac{1}{2}\operatorname{trace}(\Sigma_k)\right)\right)$$
$$\text{s.t.} \sum_{k=1}^{K} w_k = 1 \text{ and } \Sigma_k \text{ is positive-semidefinite } \forall k \in \{1,\dots,K\} \tag{1}$$

and generating code for derivatives that is sequentially competitive with hand-written (C++/C) code for derivatives and superior on GPUs.

What does this have to do with Tom?

- Tensor product
- Slicing
- ...

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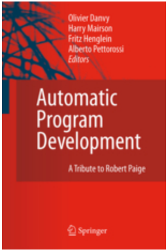
- ...
- Computational divided differencing: Generalization of automatic differentiation



- Tom Reps, Computational divided differencing, US Patent App. 10/161,461, 2002
- Tom Reps, Louis Rall, Computational Divided Differencing and Divided-Difference Arithmetics, in Automatic Program Development, A Tribute to Robert Paige, 2008

Happy Birthday!

From Neil Jones, Jakob Rehof and the Programming Languages Group at DIKU!