

Automatic Differentiation

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Introduction

- Automatic Differentiation is a set of techniques to calculate the derivative of a specified function.
 - Capitalizes on the elementary capabilities that computers have (multiplication, subtract, add, divide)
 - Uses the chain run

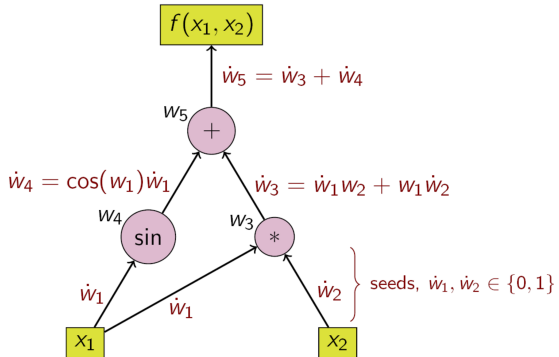
$$(f \circ g)' = (f' \circ g) \cdot g' \quad \text{or} \quad (f(g(x)))' = f'(g(x)) \cdot g'(x)$$

- Automatic Differentiation is not Symbolic Differentiation and it is not Numerical Differentiation
 - Symbolic Differentiation - software developed for the manipulation of mathematical expressions or objects
 - Numerical Differentiation - numerical analysis and algorithms for approximating functions or derivatives of functions
- Automatic Differentiation solves problems for calculating partial derivatives with respect to many inputs quickly
 - Can calculate higher order derivatives with less error than Symbolic/Numerical computation methods.

Forward Accumulation

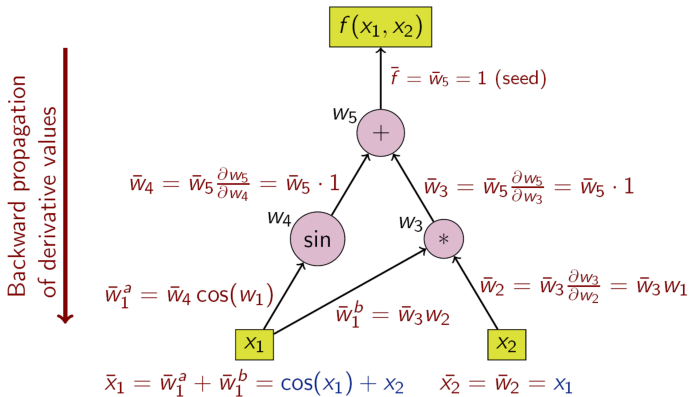
$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial w_1} \frac{\partial w_1}{\partial x} = \frac{\partial y}{\partial w_1} \left(\frac{\partial w_1}{\partial w_2} \frac{\partial w_2}{\partial x} \right) = \frac{\partial y}{\partial w_1} \left(\frac{\partial w_1}{\partial w_2} \left(\frac{\partial w_2}{\partial w_3} \frac{\partial w_3}{\partial x} \right) \right) = \dots$$

Forward propagation
of derivative values



Backward Accumulation

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial w_1} \frac{\partial w_1}{\partial x} = \left(\frac{\partial y}{\partial w_2} \frac{\partial w_2}{\partial w_1} \right) \frac{\partial w_1}{\partial x} = \left(\left(\frac{\partial y}{\partial w_3} \frac{\partial w_3}{\partial w_2} \right) \frac{\partial w_2}{\partial w_1} \right) \frac{\partial w_1}{\partial x} = \dots$$



References

- Safiran, Niloofar; Lotz, Johannes; and Naumann, Uwe. *Algorithmic Differentiation of Numerical Methods: Second-Order Adjoint Solvers for Parameterized Systems of Nonlinear Equations*, Procedia Computer Science 80 (2016): 2231-2235. ScienceDirect. Web. 10 March. 2017.
<http://www.sciencedirect.com/science/article/pii/S187705091630864X>.
- Eberhard, Peter and Bishchof, Christan. *Automatic Differentiation of Numerical Integration Algorithms*. Mathematics of Computation 68.226 (1999): 717-713. AMS. Web. 10 March. 2017.
<http://www.ams.org/journals/mcom/1999-68-226/S0025-5718-99-01027-3>.
- Griewank, Andreas. *On Automatic Differentiation* Mathematics and Computer Science Division - Argonne National Laboratory. November 1988. Web. 10 March. 2017.
<http://softlib.rice.edu/pub/CRPC-TRs/reports/CRPC-TR89003.pdf>.
- "Automatic Differentiation." Wikipedia. Wikimedia Foundation, 23 Feb. 2017. Web. 10 Mar. 2017.
https://en.wikipedia.org/wiki/Automatic_differentiation.