Automatic Differentiation

CSC412/2506
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Later modified by: Xuechen Li, lxuechen@cs.toronto.edu

Based on:

- Baydin, A. G., Pearlmutter, B. A., Radul, A. A., & Siskind, J. M. (2015). *Automatic differentiation in machine learning: a survey.*
- Maclaurin, D. (2016). Modeling, inference and optimization with composable differentiable procedures (Doctoral dissertation).
- Slides on Automatic Differentiation from CSC321/421

What is AD?

“A family of techniques similar to but more general than back propagation for efficiently and accurately evaluating derivatives of numeric functions expressed as computer programs.”

All numerical computations are composed of a finite set of elementary operations.
These elementary operations have known derivatives.
Systematically apply the **chain rule** of differential calculus.

4 Categories of Derivatives for Computer Programs

1. Manual Differentiation

   (compute by hand and code the result)

2. Numerical Differentiation

   (e.g. finite differences approx.)

3. Symbolic Differentiation

   (directly manipulates expressions, e.g. Mathematica, Maple…)

4. Automatic Differentiation

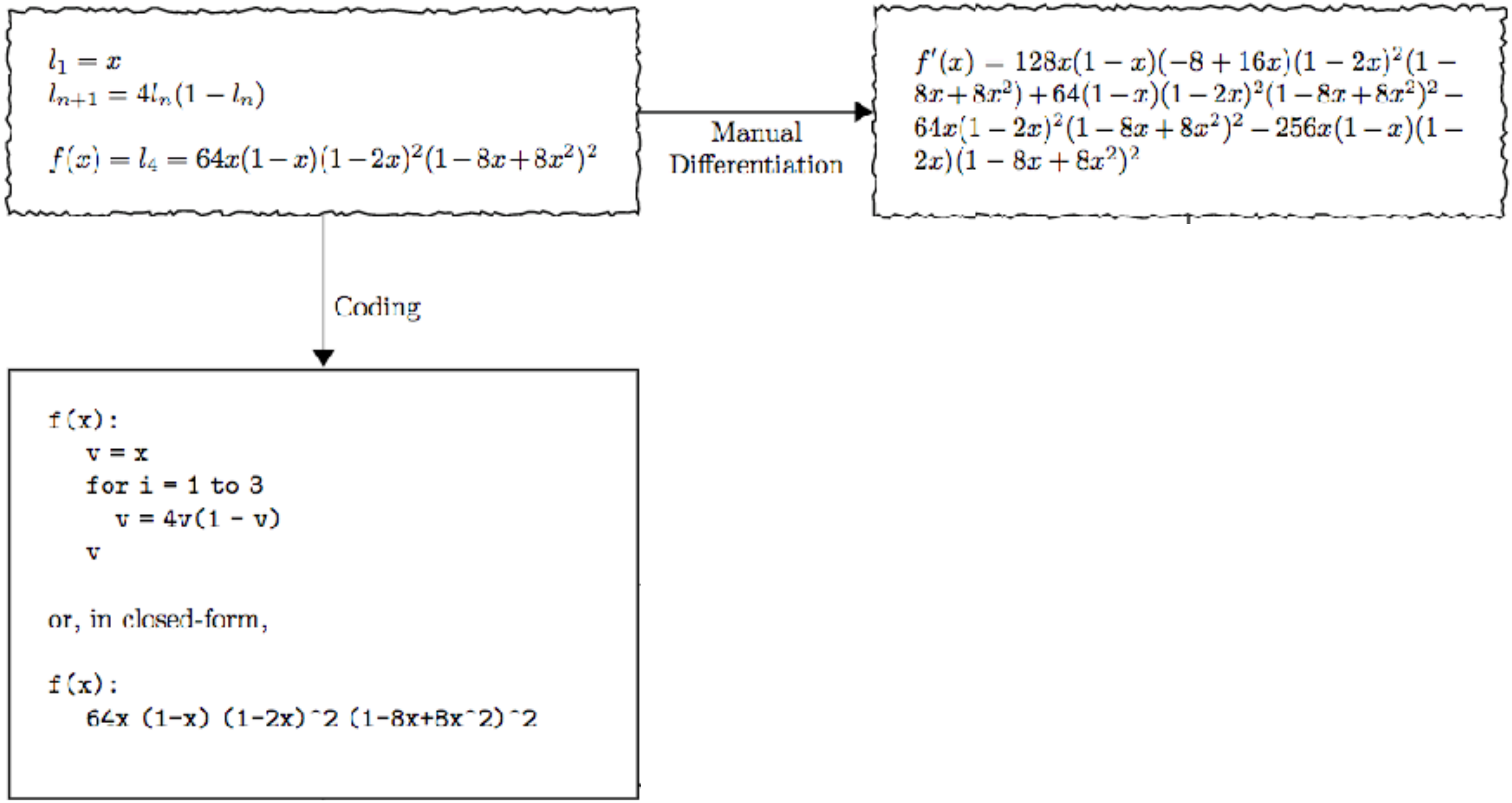
   (fancy ways of using the chain rule; subject of this tutorial)

Why do we need AD?

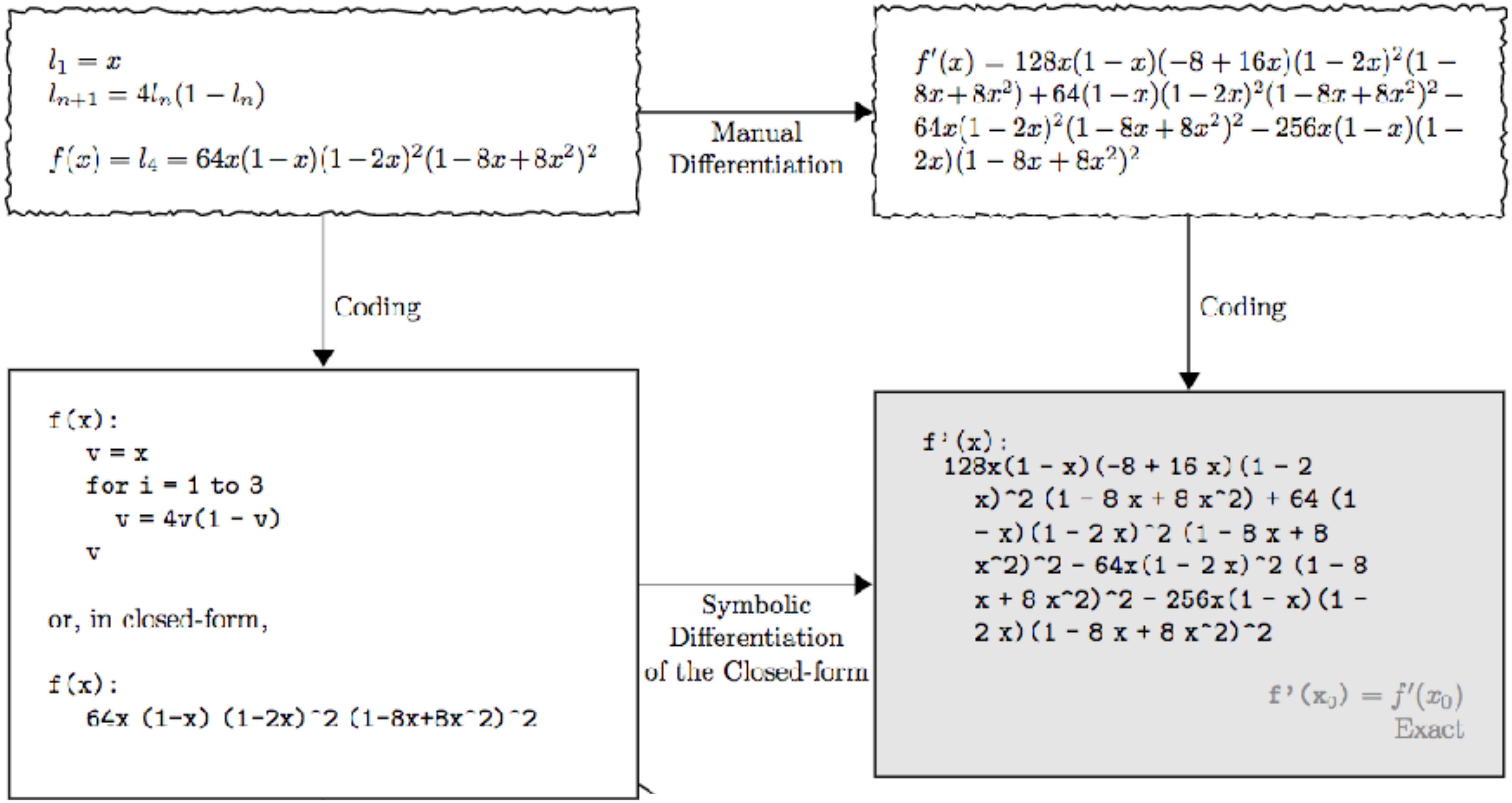
Manual Differentiation is time consuming and error prone.

Numerical Differentiation scales linearly in input dimensionality and is susceptible to roundoff errors. Mostly used for gradient checking and debugging.

Symbolic Differentiation ‘swells’ quickly as derivative expressions become very complex.



$l_1 = x$
$l_{n+1} = 4l_n(1 - l_n)$
$f(x) = l_4 = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$
Manual Differentiation
$f'(x) = 128x(1-x)(-8+16x)(1-2x)^2(1-8x+8x^2)+64(1-x)(1-2x)^2(1-8x+8x^2)^2-64x(1-2x)^2(1-8x+8x^2)^2-256x(1-x)(1-2x)(1-8x+8x^2)^2$
Coding
f(x):
v = x
for i = 1 to 3
v = 4v(1 - v)
v
or, in closed-form,
f(x):
64x (1-x) (1-2x)^2 (1-8x+8x^2)^2



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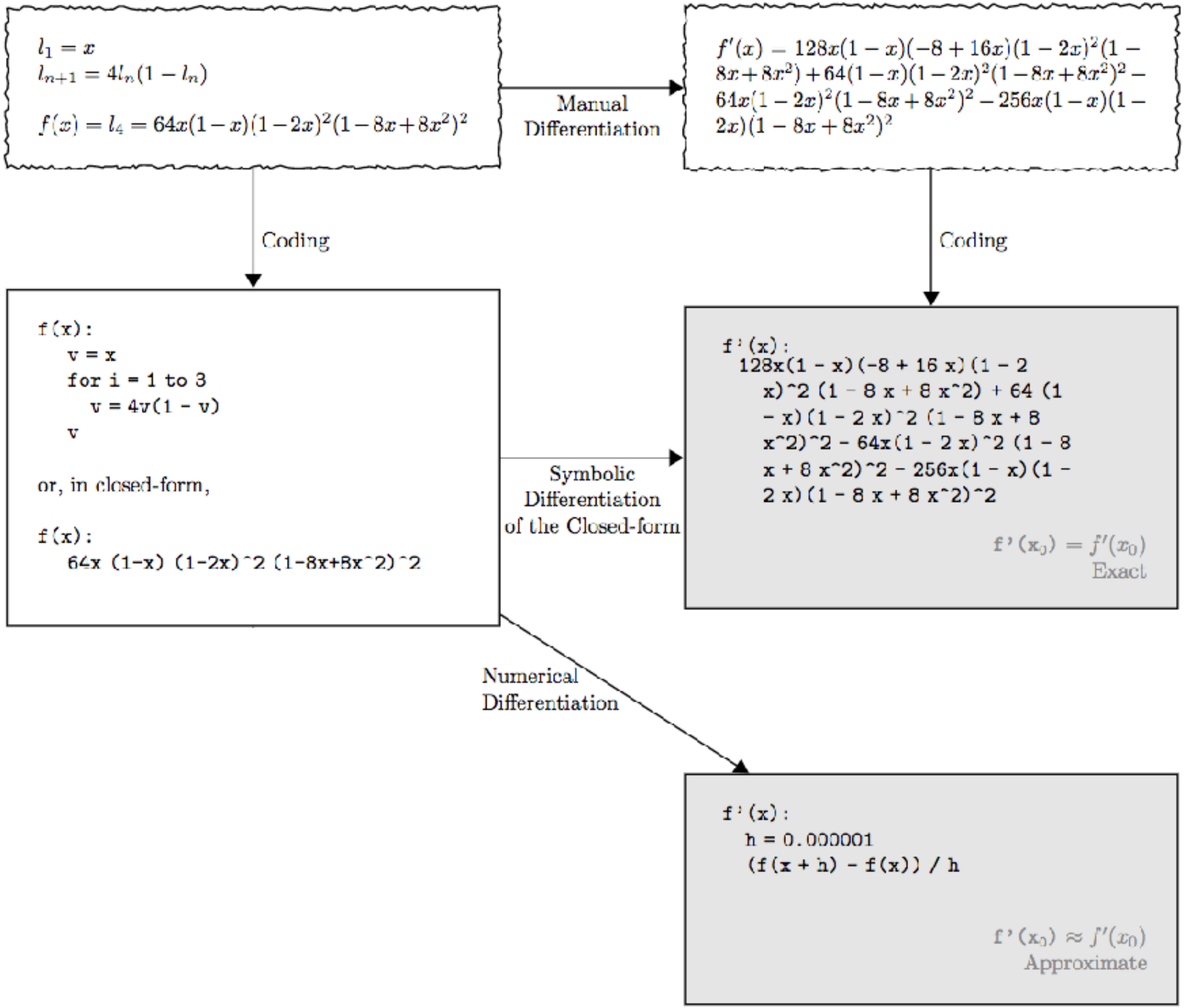
f(x):
64x (1-x) (1-2x)^2 (1-8x+8x^2)^2
Symbolic Differentiation of the Closed-form
f'(x):
128x(1 - x)(-8 + 16 x)(1 - 2 x)^2 (1 - 8 x + 8 x^2) + 64 (1 - x)(1 - 2 x)^2 (1 - 8 x + 8 x^2)^2 - 64x(1 - 2 x)^2 (1 - 8 x + 8 x^2)^2 - 256x(1 - x)(1 - 2 x)(1 - 8 x + 8 x^2)^2
f'(x0) = $f'(x_0)$
Exact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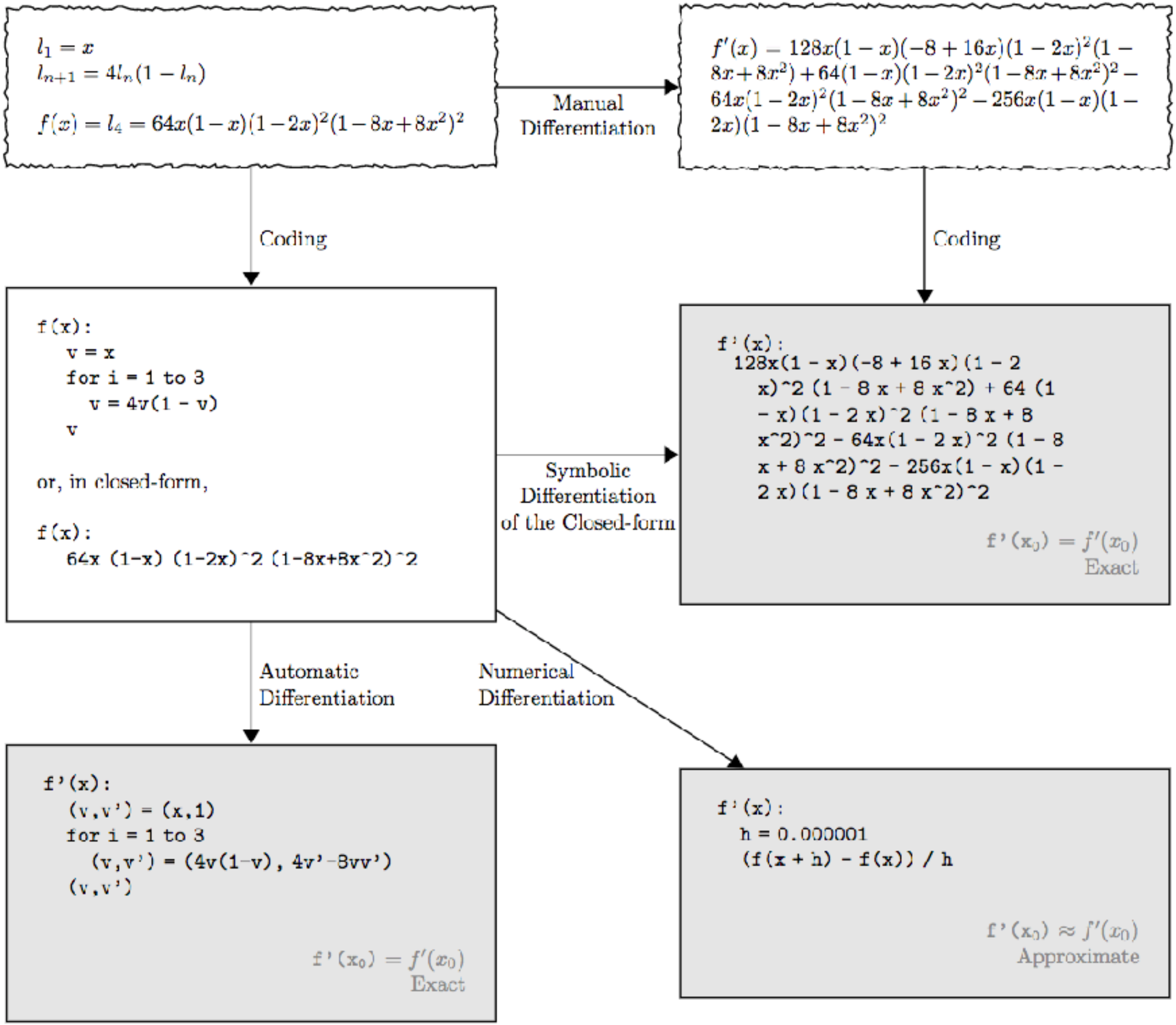
f'(x0) = $f'(x_0)$
Exact
Numerical Differentiation
f'(x):
h = 0.000001
(f(x + h) - f(x)) / h
f'(x0) ≈ $f'(x_0)$
Approximate



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f'(x0) = f'(x0)
Exact
Automatic Differentiation
Numerical Differentiation
f'(x):
(v,v') = (x,1)
for i = 1 to 3
(v,v') = (4v(1-v), 4v'-8vv')
(v,v')
f'(x0) = f'(x0)
Exact
f'(x):
h = 0.000001
(f(x + h) - f(x)) / h
f'(x0) ≈ f'(x0)
Approximate

What is Automatic Differentiation?

2 Modes of AD

$$y = f(g(h(x))) = f(g(h(w_0))) = f(g(w_1)) = f(w_2) = w_3$$

$$\frac{dy}{dx} = \frac{dy}{dw_2}\frac{dw_2}{dw_1}\frac{dw_1}{dx}$$

Forward Accumulation Mode: chain rule inside to outside

$$dw_1/dx \longrightarrow dw_2/dx \longrightarrow dy/dx$$

2 Modes of AD

$$y = f(g(h(x))) = f(g(h(w_0))) = f(g(w_1)) = f(w_2) = w_3$$

$$\frac{dy}{dx} = \frac{dy}{dw_2}\frac{dw_2}{dw_1}\frac{dw_1}{dx}$$

Reverse Accumulation Mode: chain rule outside to inside

$$dy/dw_2 \longrightarrow dy/dw_1 \longrightarrow dy/dx$$

Exercise: Forward Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\dot{x}_1 = 1 \longrightarrow \frac{\delta y}{\delta x_1}$$

Exercise: Forward Mode

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Forward Primal Trace	Forward Tangent (Derivative) Trace

Exercise: Forward Mode

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Forward Primal Trace			Forward Tangent (Derivative) Trace		
v_{-1}	$= x_1$	$= 2$	$\dot{v}_{-1}$	$= \dot{x}_1$	$= 1$
v_0	$= x_2$	$= 5$	$\dot{v}_0$	$= \dot{x}_2$	$= 0$

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v_1	$= \ln v_{-1}$	$= \ln 2$	$\dot{v}_1$	$= \dot{v}_{-1}/v_{-1}$	$= 1/2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2?$		

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v_2	$= v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$

Exercise: Forward Mode

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

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v_2	$= v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
v_3	$= \sin v_0$	$= \sin 5$	$\dot{v}_3$?		

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v_3	$= \sin v_0$	$= \sin 5$	$\dot{v}_3$	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$

Exercise: Forward Mode

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v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$

Forward Tangent (Derivative) Trace		
$\dot{v}_{-1}$	$= \dot{x}_1$	$= 1$
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$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$\dot{v}_3$	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$
$\dot{v}_4?$		

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Forward Tangent (Derivative) Trace		
$\dot{v}_{-1}$	$= \dot{x}_1$	$= 1$
$\dot{v}_0$	$= \dot{x}_2$	$= 0$
$\dot{v}_1$	$= \dot{v}_{-1} / v_{-1}$	$= 1/2$
$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$\dot{v}_3$	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$
$\dot{v}_4$	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$

Exercise: Forward Mode

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v_4	$= v_1 + v_2$	$= 0.693 + 10$	$\dot{v}_4$	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$	$\dot{v}_5$?		

Exercise: Forward Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\dot{x}_1 = 1 \longrightarrow \frac{\delta y}{\delta x_1}$$

Forward Primal Trace		
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$\dot{v}_3$	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$
$\dot{v}_4$	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$\dot{v}_5$	$= \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$

Exercise: Forward Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

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v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Forward Tangent (Derivative) Trace		
$\dot{v}_{-1}$	$= \dot{x}_1$	$= 1$
$\dot{v}_0$	$= \dot{x}_2$	$= 0$
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$\dot{v}_4$	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$\dot{v}_5$	$= \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
$\dot{\boldsymbol{y}}$	$= \dot{\boldsymbol{v}}_5$	$= \mathbf{5.5}$

Which one is faster in Forward Mode?

$$f : \mathbb{R} \rightarrow \mathbb{R}^m \qquad \frac{\delta y_i}{\delta x}$$

$$f : \mathbb{R}^n \rightarrow \mathbb{R} \qquad \nabla f = (\frac{\delta y}{\delta x_1}, \ldots, \frac{\delta y}{\delta x_n})$$

Functions in ML

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

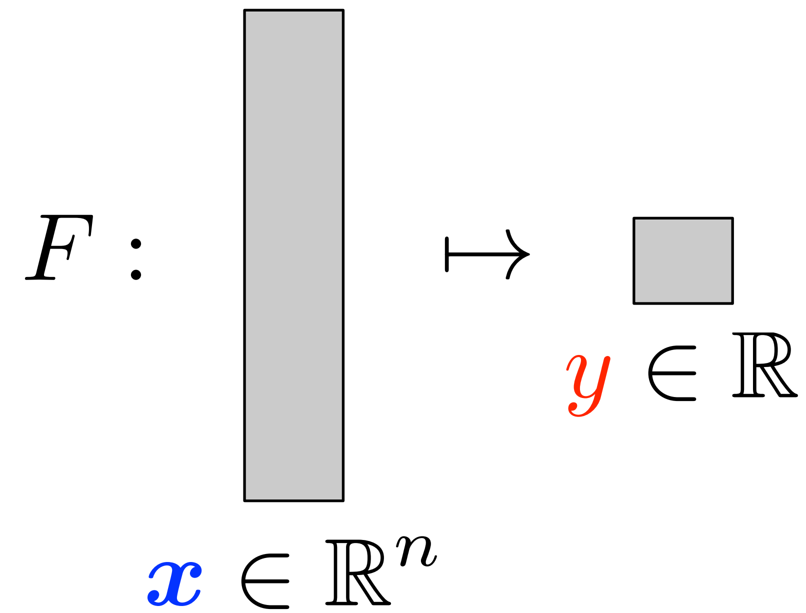
$$n \gg m$$

Forward mode AD is not scalable to input dimensionality

Functions in ML

even more extreme, m=1

$$F : \mathbb{R}^n \to \mathbb{R}$$



$$F = D \circ C \circ B \circ A$$

$$y = F(\boldsymbol{x}) = D(C(B(A(\boldsymbol{x}))))$$

$$y = D(\boldsymbol{c}), \quad \boldsymbol{c} = C(\boldsymbol{b}), \quad \boldsymbol{b} = B(\boldsymbol{a}), \quad \boldsymbol{a} = A(\boldsymbol{x})$$

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$$F'(\boldsymbol{x}) = \frac{\partial y}{\partial \boldsymbol{x}} = \left[\frac{\partial y}{\partial x_1} \quad \cdots \quad \frac{\partial y}{\partial x_n} \right]$$

$$F'(\boldsymbol{x}) = \quad \frac{\partial y}{\partial \boldsymbol{c}} \; \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \; \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \; \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}$$

$$y = D(\boldsymbol{c}), \quad \boldsymbol{c} = C(\boldsymbol{b}), \quad \boldsymbol{b} = B(\boldsymbol{a}), \quad \boldsymbol{a} = A(\boldsymbol{x})$$

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$$F'(\boldsymbol{x}) = \frac{\partial y}{\partial \boldsymbol{c}} \; \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \; \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \; \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}$$

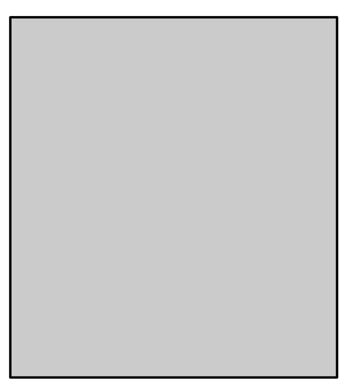
$$\frac{\partial y}{\partial \boldsymbol{c}} = D'(\boldsymbol{c})$$

$$y = D(\boldsymbol{c}), \quad \boldsymbol{c} = C(\boldsymbol{b}), \quad \boldsymbol{b} = B(\boldsymbol{a}), \quad \boldsymbol{a} = A(\boldsymbol{x})$$

$$F'(\boldsymbol{x}) = \frac{\partial y}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} & \cdots & \frac{\partial y}{\partial x_n} \end{bmatrix}$$

$$F'(\boldsymbol{x}) = \quad \frac{\partial y}{\partial \boldsymbol{c}} \; \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \; \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \; \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}$$

$$\frac{\partial y}{\partial \boldsymbol{c}} = D'(\boldsymbol{c}) \qquad \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} = C'(\boldsymbol{b})$$



$$y = D(\boldsymbol{c}), \quad \boldsymbol{c} = C(\boldsymbol{b}), \quad \boldsymbol{b} = B(\boldsymbol{a}), \quad \boldsymbol{a} = A(\boldsymbol{x})$$

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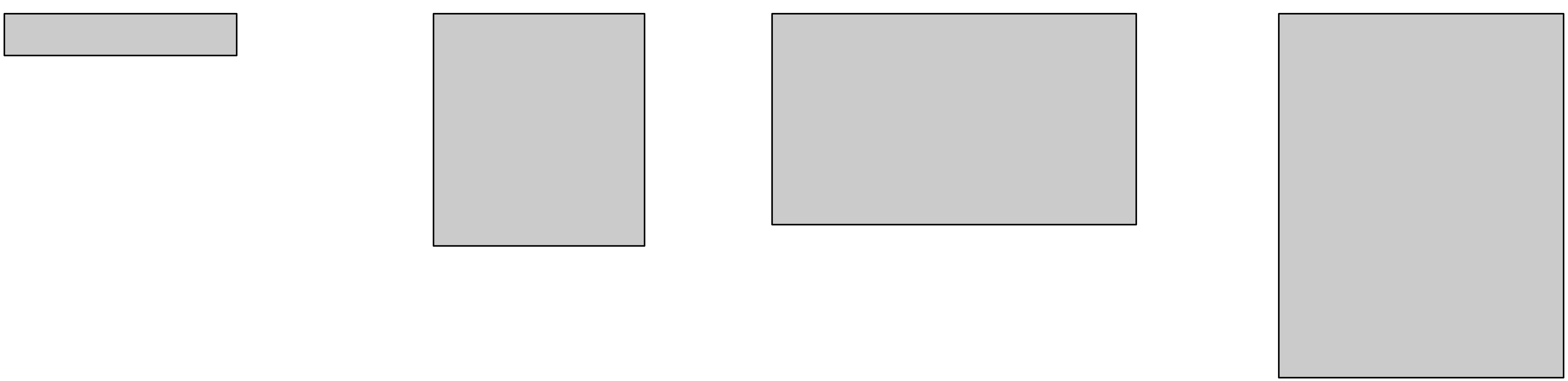
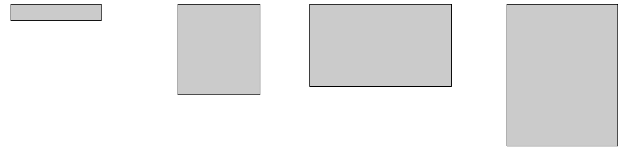
$$F'(\boldsymbol{x}) = \frac{\partial y}{\partial \boldsymbol{c}} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}$$

$$\frac{\partial y}{\partial \boldsymbol{c}} = D'(\boldsymbol{c}) \qquad \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} = C'(\boldsymbol{b}) \qquad \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} = B'(\boldsymbol{a}) \qquad \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} = A'(\boldsymbol{x})$$

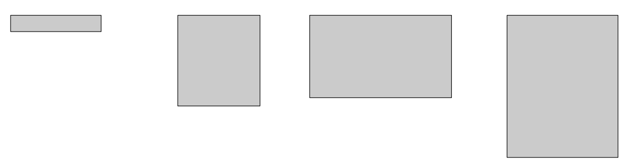




$$F'(\boldsymbol{x}) = \frac{\partial y}{\partial \boldsymbol{c}} \left(\frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \underbrace{\left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} \right)} \right)$$

$$\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial b_1}{\partial x_1} & \cdots & \frac{\partial b_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial b_m}{\partial x_1} & \cdots & \frac{\partial b_m}{\partial x_n} \end{bmatrix}$$

Forward accumulation



$$F'(\boldsymbol{x}) = \left(\underbrace{\left(\frac{\partial y}{\partial \boldsymbol{c}} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \right)} \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \right) \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}$$

$$\frac{\partial y}{\partial \boldsymbol{b}} = \begin{bmatrix} \frac{\partial y}{\partial b_1} & \cdots & \frac{\partial y}{\partial b_m} \end{bmatrix}$$

Reverse accumulation

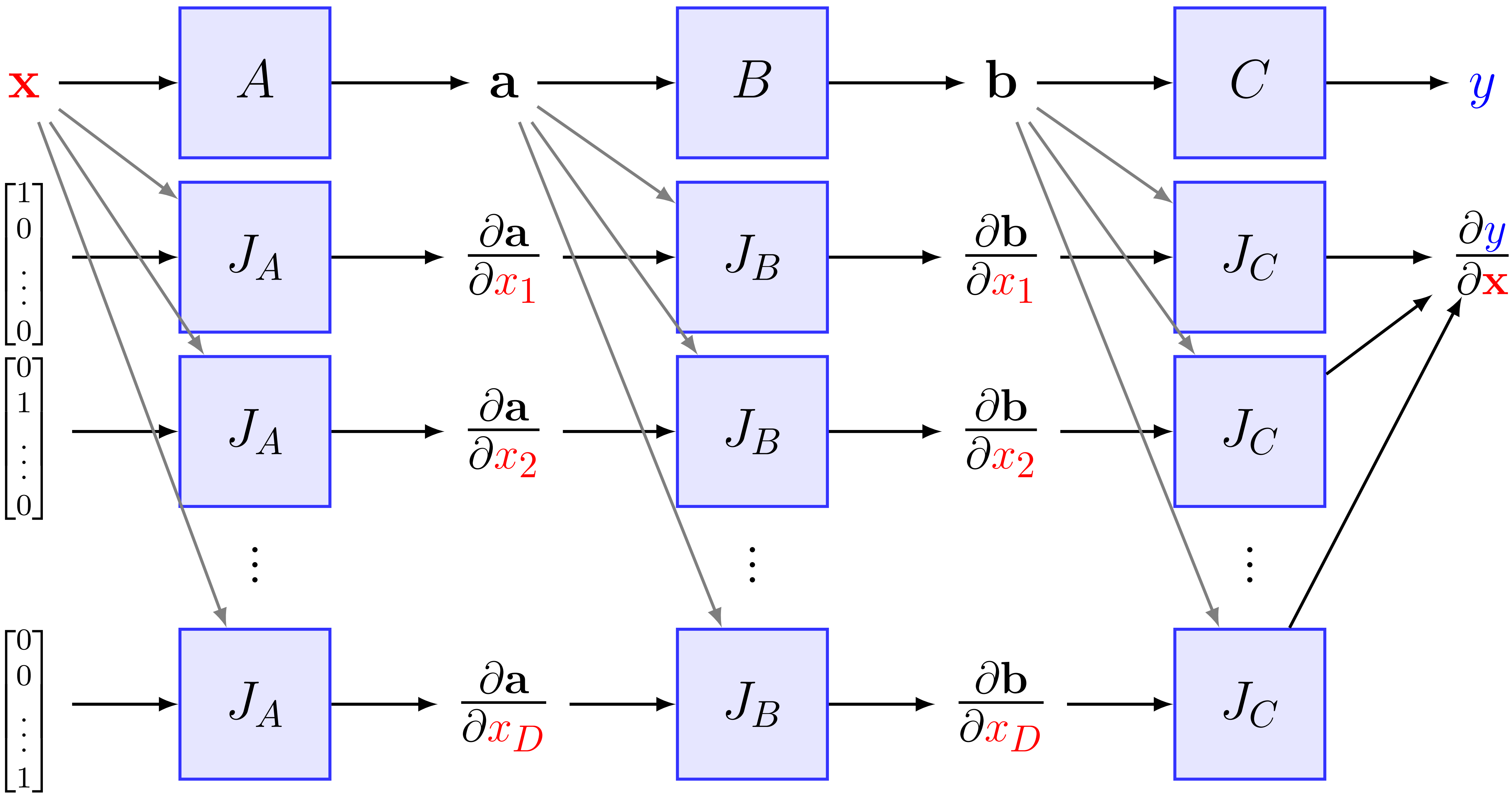
$$F'(\boldsymbol{x})\,\boldsymbol{v} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{c}} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}\,\boldsymbol{v}$$

$$F'(\boldsymbol{x})\,\boldsymbol{v} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{c}} \left(\frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \left(\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}\,\boldsymbol{v} \right) \right) \right)$$

Forward accumulation $\leftrightarrow$ Jacobian-vector products

$$F'(\boldsymbol{x}) = \frac{\partial y}{\partial \boldsymbol{c}} \left(\frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \left(\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{x}} \right) \right) \right)$$

Forward accumulation mode differentiation



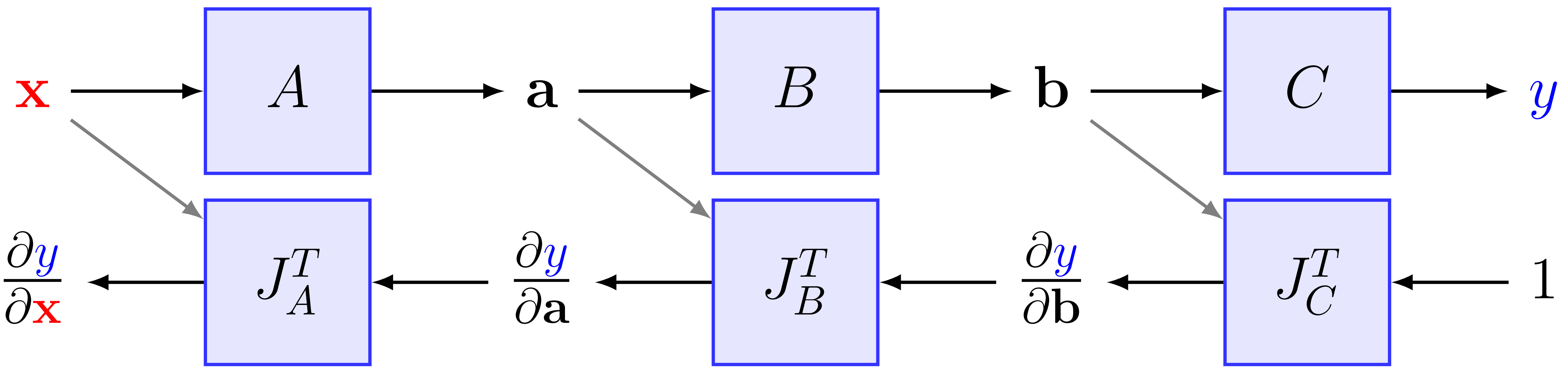
$$\boldsymbol{v}^{\mathsf{T}} F'(\boldsymbol{x}) = \qquad \boldsymbol{v}^{\mathsf{T}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{c}} \quad \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \quad \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \quad \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}$$

$$\boldsymbol{v}^{\mathsf{T}} F'(\boldsymbol{x}) = \left(\left(\left(\boldsymbol{v}^{\mathsf{T}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{c}} \right) \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \right) \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \right) \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} \Bigg) \Bigg) \Bigg)$$

Reverse accumulation $\leftrightarrow$ vector-Jacobian products

$$F'(\boldsymbol{x}) = \left(\left(\left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{y}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{c}} \right) \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \right) \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \right) \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} \Bigg) \Bigg) \Bigg)$$

Reverse accumulation mode differentiation



Efficient for many-to-one functions, but memory intensive

Recent research has explored ways to perform memory-efficient reverse-mode autodiff (Reversible architecture, checkpointing, etc):

- Gomez, A. N., Ren, M., Urtasun, R., & Grosse, R. B. (2017). The reversible residual network: Backpropagation without storing activations. In *Advances in Neural Information Processing Systems* (pp. 2214-2224).
- Jacobsen, J. H., Smeulders, A., & Oyallon, E. (2018). i-RevNet: Deep Invertible Networks. *arXiv preprint arXiv:1802.07088*.
- Martens, J., & Sutskever, I. (2012). Training deep and recurrent networks with hessian-free optimization. In *Neural networks: Tricks of the trade* (pp. 479-535). Springer, Berlin Heidelberg.

Another memory-efficient training schemes using the Adjoint-sensitivity method:

Chen, T. Q., Rubanova, Y., Bettencourt, J., & Duvenaud, D. (2018). Neural Ordinary Differential Equations. *arXiv preprint arXiv:1806.07366*.

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace			Reverse Adjoint Trace
v_{-1}	$= x_1$	$= 2$	
v_0	$= x_2$	$= 5$	
v_1	$= \ln v_{-1}$	$= \ln 2$	
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$	
v_3	$= \sin v_0$	$= \sin 5$	
v_4	$= v_1 + v_2$	$= 0.693 + 10$	
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$	
y	$= v_5$	$= 11.652$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace			Reverse Adjoint Trace			
v_{-1}	$= x_1$	$= 2$				
v_0	$= x_2$	$= 5$				
v_1	$= \ln v_{-1}$	$= \ln 2$				
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$				
v_3	$= \sin v_0$	$= \sin 5$				
v_4	$= v_1 + v_2$	$= 0.693 + 10$				
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$				
y	$= v_5$	$= 11.652$	$\bar{v}_5$	$= \bar{y}$	$= 1$	$(\partial y / \partial y)$

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint Trace			
$\bar{v}_3 ?$			
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint Trace			
$\bar{v}_1$?			
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace		
$v_{-1} = x_1$		$= 2$
$v_0 = x_2$		$= 5$
$v_1 = \ln v_{-1}$		$= \ln 2$
$v_2 = v_{-1} \times v_0$		$= 2 \times 5$
$v_3 = \sin v_0$		$= \sin 5$
$v_4 = v_1 + v_2$		$= 0.693 + 10$
$v_5 = v_4 - v_3$		$= 10.693 + 0.959$
$y = v_5$		$= 11.652$

Reverse Adjoint Trace		
$\bar{v}_2$?		
$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5 = \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace		
$v_{-1} = x_1$		$= 2$
$v_0 = x_2$		$= 5$
$v_1 = \ln v_{-1}$		$= \ln 2$
$v_2 = v_{-1} \times v_0$		$= 2 \times 5$
$v_3 = \sin v_0$		$= \sin 5$
$v_4 = v_1 + v_2$		$= 0.693 + 10$
$v_5 = v_4 - v_3$		$= 10.693 + 0.959$
$y = v_5$		$= 11.652$

Reverse Adjoint Trace		
$\bar{v}_0$?		
$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5 = \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint Trace

$\bar{v}_{-1}$?

$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint Trace

$\bar{v}_0$?

$\bar{v}_{-1}$	$= \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint Trace			
$\bar{v}_{-1}$?			
$\bar{v}_0$	$= \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1}$	$= \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1}, \frac{\delta y}{\delta x_2}$$

both in one reverse pass!

Forward Evaluation Trace

v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint Trace

$\bar{v}_{-1}$	$= \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$	$= \bar{v}_{-1} + \bar{v}_1 / v_{-1}$	$= 5.5$
$\bar{v}_0$	$= \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1}$	$= \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Exercise: Reverse Mode

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

Solve at point $(x_1, x_2) = (2, 5)$

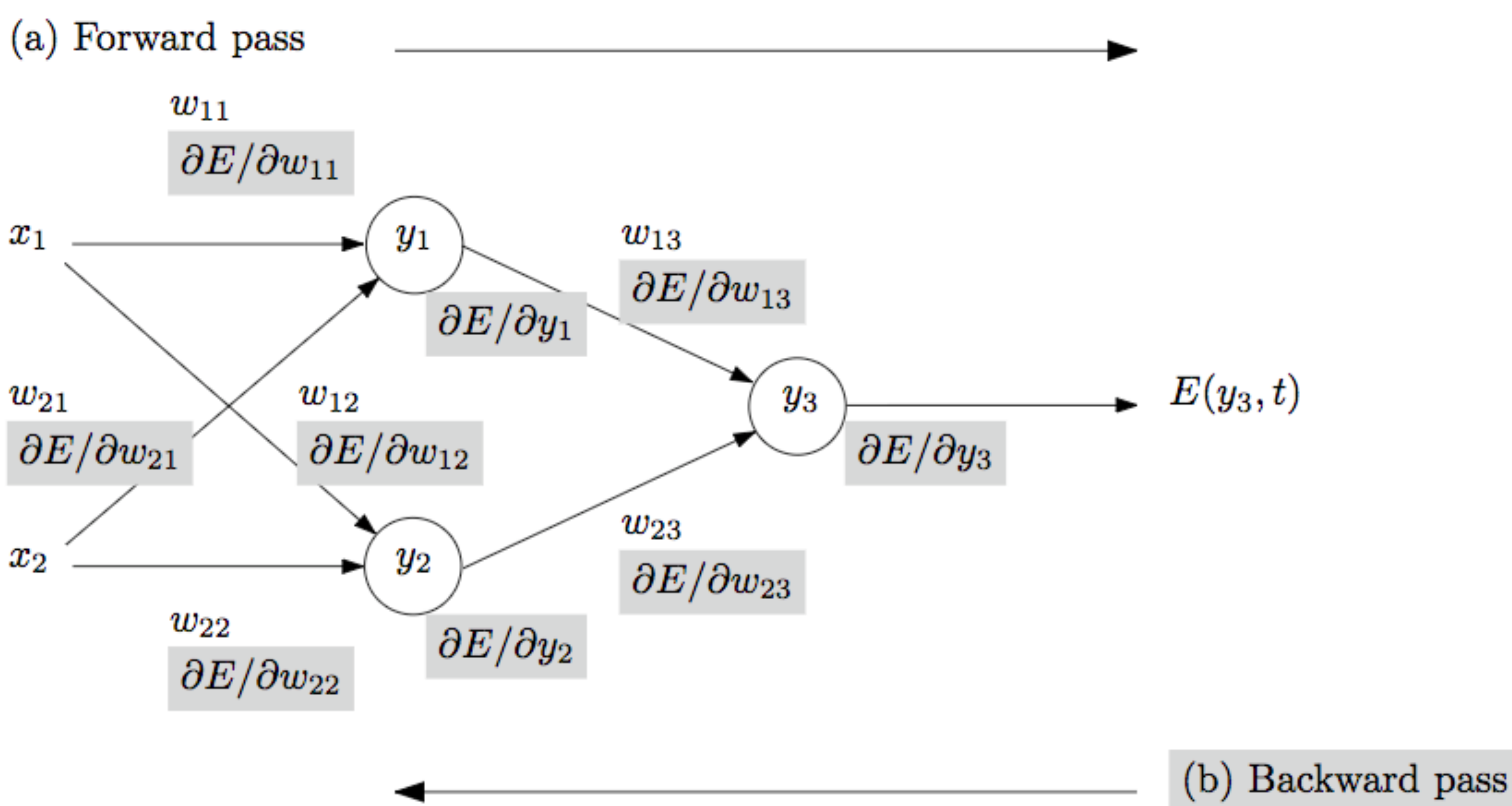
$$\bar{y} = \frac{\delta y}{\delta y} = 1 \longrightarrow \frac{\delta y}{\delta x_1} \, (\bar{x}_1), \quad \frac{\delta y}{\delta x_2} \, (\bar{x}_2)$$

both in one reverse pass!

Forward Evaluation Trace		
$v_{-1} = x_1$		$= 2$
$v_0 = x_2$		$= 5$
$v_1 = \ln v_{-1}$		$= \ln 2$
$v_2 = v_{-1} \times v_0$		$= 2 \times 5$
$v_3 = \sin v_0$		$= \sin 5$
$v_4 = v_1 + v_2$		$= 0.693 + 10$
$v_5 = v_4 - v_3$		$= 10.693 + 0.959$
$y = v_5$		$= 11.652$

Reverse Adjoint Trace		
$\bar{x}_1 = \bar{v}_{-1}$		$= 5.5$
$\bar{x}_2 = \bar{v}_0$		$= 1.716$
$\bar{v}_{-1} = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$	$= \bar{v}_{-1} + \bar{v}_1 / v_{-1}$	$= 5.5$
$\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1} = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5 = \bar{y}$	$= 1$	

Backpropagation is a special case of Reverse Mode AD



Summary

- Numerical Differentiation
  - sensitive to roundoff error; scales poorly with input dimensionality
- Symbolic Differentiation
  - formulas become complicated
- Automatic Differentiation
  - Forward-mode
    - memory saving, but scales poorly for functions in ML
  - Reverse-mode
    - memory intensive, scales well for functions in ML

Question:

- How do the following frameworks compute derivatives?
  - Autograd
  - Theano
  - TensorFlow
  - Chainer
  - PyTorch

	Derivative Computation	Graph	Programming Paradigm
Autograd	Reverse-mode autodiff	Dynamic	Functional
Theano	Reverse-mode autodiff	Static	/
Tensorflow	Reverse-mode autodiff	Static	/
Chainer	Reverse-mode autodiff	Dynamic	OO
PyTorch	Reverse-mode autodiff	Dynamic	OO

1. TensorFlow eager execution is based on dynamic computation graph construction
2. PyTorch recently (late 2018) introduced tracing (e.g. `torch.jit.trace`) to produce static graphs; this is for better deployment