Automatic differentiation

Mauricio A. Álvarez

Machine Learning and Adaptive Intelligence
The University of Sheffield

The University Of Sheffield.

Contents

Derivatives

- Derivatives are required to perform optimisation in several ML algorithms.
- For example, computing the gradient is necessary for batch gradient descent and SGD.
- Derivatives are also necessary for computing Hessians which are used in second-order optimisation methods.

Methods to compute derivatives in computer programs

- Manually working out derivatives and coding them.
- Numeric differentiation using finite difference approximations.
- Symbolic differentiation.
- Automatic differentiation (or algorithmic differentiation).

Example

- Suppose we have the following function

$$f(x, y) = x^2 y + y + 2.$$

- We require to compute the gradient of this function, for example, because we want to use it in gradient descent,

$$\frac{df(x, y)}{d\mathbf{z}} = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{bmatrix},$$

where $\mathbf{z} = [x \; y]^\top$.

$z = \begin{bmatrix} x \\ y \end{bmatrix}$ $\quad \frac{df(x,y)}{dz}$: derivatives for $f(x,y)$ wrt z: $z = \begin{bmatrix} x \\ y \end{bmatrix}$

Manual differentiation (I)

- We use our calculus knowledge to derive the proper equation.

- For the function we saw before, we need to apply the following rules of calculus
  - The derivative of a constant is 0.
  - The derivative of ax with respect to x is a, where a is a constant.
  - The derivative of x^a is ax^{a-1}.
  - The derivative is a linear operation so, the derivative of the sum of two functions is the sum of the derivatives.
  - The derivative of a constant times a function, is equal to the constant times the derivative of that function.

- Using these rules we get the following partial derivatives,

Manual differentiation (II)

- Partial derivative of $f(x, y)$ with respect to x

$$\frac{\partial}{\partial x} f(x, y) = \frac{\partial}{\partial x} \left(x^2 y + y + 2 \right) = 2xy.$$

- Partial derivative of $f(x, y)$ with respect to y

$$\frac{\partial}{\partial y} f(x, y) = \frac{\partial}{\partial y} \left(x^2 y + y + 2 \right) = x^2 + 1.$$

- We can then write

$$\frac{df(x, y)}{d\mathbf{z}} = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{bmatrix} = \begin{bmatrix} 2xy \\ x^2 + 1 \end{bmatrix}$$

Problems with manual differentiation

When a function $f(\cdot)$ depends on many variables or is a rather complicated expression, manual differentiation is tedious and prone to mistakes.

Finite difference approximations (I)

- Remember the definition of a derivative of a function $h(x)$ at a point x_0,

$$\frac{dh(x_0)}{dx} = \lim_{x \to x_0} \frac{h(x) - h(x_0)}{x - x_0}$$
$$= \lim_{\epsilon \to 0} \frac{h(x_0 + \epsilon) - h(x_0)}{\epsilon}$$

- The partial derivative of $h(x, y)$ at point (x_0, y_0) is defined as

$$\frac{\partial h(x_0, y_0)}{\partial x} = \lim_{\epsilon \to 0} \frac{h(x_0 + \epsilon, y_0) - h(x_0, y_0)}{\epsilon}$$
$$\frac{\partial h(x_0, y_0)}{\partial y} = \lim_{\epsilon \to 0} \frac{h(x_0, y_0 + \epsilon) - h(x_0, y_0)}{\epsilon}$$

Finite difference approximations (II)

easy to implement

$x^2y + y + 2$

$\frac{df}{dx} = 2xy \; ; \; \frac{df}{dy} = x^2 + 1$

$\frac{f(3+10^{-6}, 2) - f(3,2)}{10^{-6}}$

$\frac{f(3, 2+10^{-6}) - f(3,2)}{10^{-6}}$

```
def f(x, y):
    return x**2*y + y + 2

x_0 = 3
y_0 = 2
epsilon = 1e-6
dfdx_numerical = (f(x_0+epsilon, y_0) - f(x_0, y_0))/epsilon
dfdy_numerical = (f(x_0, y_0+epsilon) - f(x_0, y_0))/epsilon

dfdx_analytical  = 2*x_0*y_0
dfdy_analytical = x_0**2 + 1
```

Script in python for the finite differences

```
In [22]: dfdx_numerical
Out[22]: 12.000002001855137

In [23]: dfdx_analytical
Out[23]: 12
```

$\frac{\partial f(x,y)}{\partial dx}$

```
In [24]: dfdy_numerical
Out[24]: 10.000000003174137

In [25]: dfdy_analytical
Out[25]: 10
```

$\frac{\partial f(x,y)}{\partial dy}$

Problems with finite difference approximation

- The result is imprecise and gets worse with more complicated functions.
- We need to call the function at least twice. For big parametric models, we'd need to call the function several times becoming very inefficient.
- The method is easy to implement, so one can use it to test whether the manual implementation is correct.

Symbolic differentiation (I)

- Symbolic differentiation performs an automatic manipulation of expressions to obtain the corresponding derivative expressions.
- The mathematical expression is represented using data structures (e.g. trees, lists, etc.).
- It is then possible to follow a mechanistic process to obtain the derivatives.

Symbolic differentiation (II)

Mathematica

Maxima

Maple

Symbolic differentiation with Mathematica

```
In[33]:= D[x, x]
Out[33]= 1

In[34]:= D[4 x (1 - x), x]
Out[34]= 4 (1 - x) - 4 x

In[35]:= D[16 x (1 - x) ((1 - 2 x) ^ 2), x]
Out[35]= 16 (1 - 2 x)^2 (1 - x) - 16 (1 - 2 x)^2 x - 64 (1 - 2 x) (1 - x) x

In[36]:= D[64 x (1 - x) ((1 - 2 x) ^ 2) ((1 - 8 x + 8 x ^ 2) ^ 2), x]
Out[36]= 128 (1 - 2 x)^2 (1 - x) x (-8 + 16 x) (1 - 8 x + 8 x^2) +
  64 (1 - 2 x)^2 (1 - x) (1 - 8 x + 8 x^2)^2 - 64 (1 - 2 x)^2 x (1 - 8 x + 8 x^2)^2 -
  256 (1 - 2 x) (1 - x) x (1 - 8 x + 8 x^2)^2
```

Problems with symbolic differentiation

- Due to the mechanistic approach, there is usually a lot of redundancy in the expressions generated.
- If not handled properly, it produces unneccesary long expressions difficult to makes sense of and to evaluate.
- Such behavior is known as *expression swell*.

Example of *expression swell*

n	l_n	$\frac{dl_n}{dx}$
1	x	1
2	$4x(1-x)$	$4(1-x)-4x$
3	$16x(1-x)(1-2x)^2$	$16(1-2x)^2(1-x)-16(1-2x)^2x-64(1-2x)(1-x)x$
4	$64x(1-x)(1-2x)^2(8x^2-8x+1)^2$	$128(1-2x)^2(1-x)x(-8+16x)(1-8x+8x^2)+64(1-2x)^2(1-x)(1-8x+8x^2)^2-64(1-2x)^2x(1-8x+8x^2)^2-256(1-2x)(1-x)x(1-8x+8x^2)^2$

Logistic map $l_n = 4l_n(1-l_n)$, $l_1 = x$.

Expression swell

↳ can be simplified

Symplify with Mathematica

```
In[40]:= D[16 x (1 - x) ((1 - 2 x) ^ 2), x]
Out[40]= 16 (1 - 2 x)^2 (1 - x) - 16 (1 - 2 x)^2 x - 64 (1 - 2 x) (1 - x) x

In[39]:= Simplify[16 (1 - 2 x)^2 (1 - x) - 16 (1 - 2 x)^2 x - 64 (1 - 2 x) (1 - x) x]
Out[39]= -16 (-1 + 10 x - 24 x^2 + 16 x^3)

In[41]:= D[64 x (1 - x) ((1 - 2 x) ^ 2) ((1 - 8 x + 8 x ^ 2) ^ 2), x]
```

Expression swell

```
Out[41]= 128 (1 - 2 x)^2 (1 - x) x (-8 + 16 x) (1 - 8 x + 8 x^2) +
  64 (1 - 2 x)^2 (1 - x) (1 - 8 x + 8 x^2)^2 - 64 (1 - 2 x)^2 x (1 - 8 x + 8 x^2)^2 -
  256 (1 - 2 x) (1 - x) x (1 - 8 x + 8 x^2)^2

In[42]:= Simplify[128 (1 - 2 x)^2 (1 - x) x (-8 + 16 x) (1 - 8 x + 8 x^2) +
  64 (1 - 2 x)^2 (1 - x) (1 - 8 x + 8 x^2)^2 - 64 (1 - 2 x)^2 x (1 - 8 x + 8 x^2)^2 -
  256 (1 - 2 x) (1 - x) x (1 - 8 x + 8 x^2)^2]
Out[42]= -64 (-1 + 42 x - 504 x^2 + 2640 x^3 - 7040 x^4 + 9984 x^5 - 7168 x^6 + 2048 x^7)
```

Automatic differentiation

- AD is concerned about exact numerical computation of the derivatives, rather than their actual symbolic form.
- It computes the derivative by only storing the values of intermediate sub-expressions.
- It uses a combination of: symbolic differentiation at the elementary operation level and keeping intermediate numerical results.

Contents

Evaluation trace

- *Evaluation trace*: composition of elementary operations that lead to a full expression.
- As an example, let us consider the function

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

- The inputs are x_1 and x_2.
- The elementary operations include
  - $v_1 = \ln(x_1)$
  - $v_2 = x_1 x_2$
  - $v_3 = \sin(x_2)$
  - $v_4 = v_1 + v_2$
  - $v_5 = v_4 - v_3$
  - $f(x_1, x_2) = v_5$.

$v_1 = \ln(x_1)$

$v_2 = x_1 x_2$

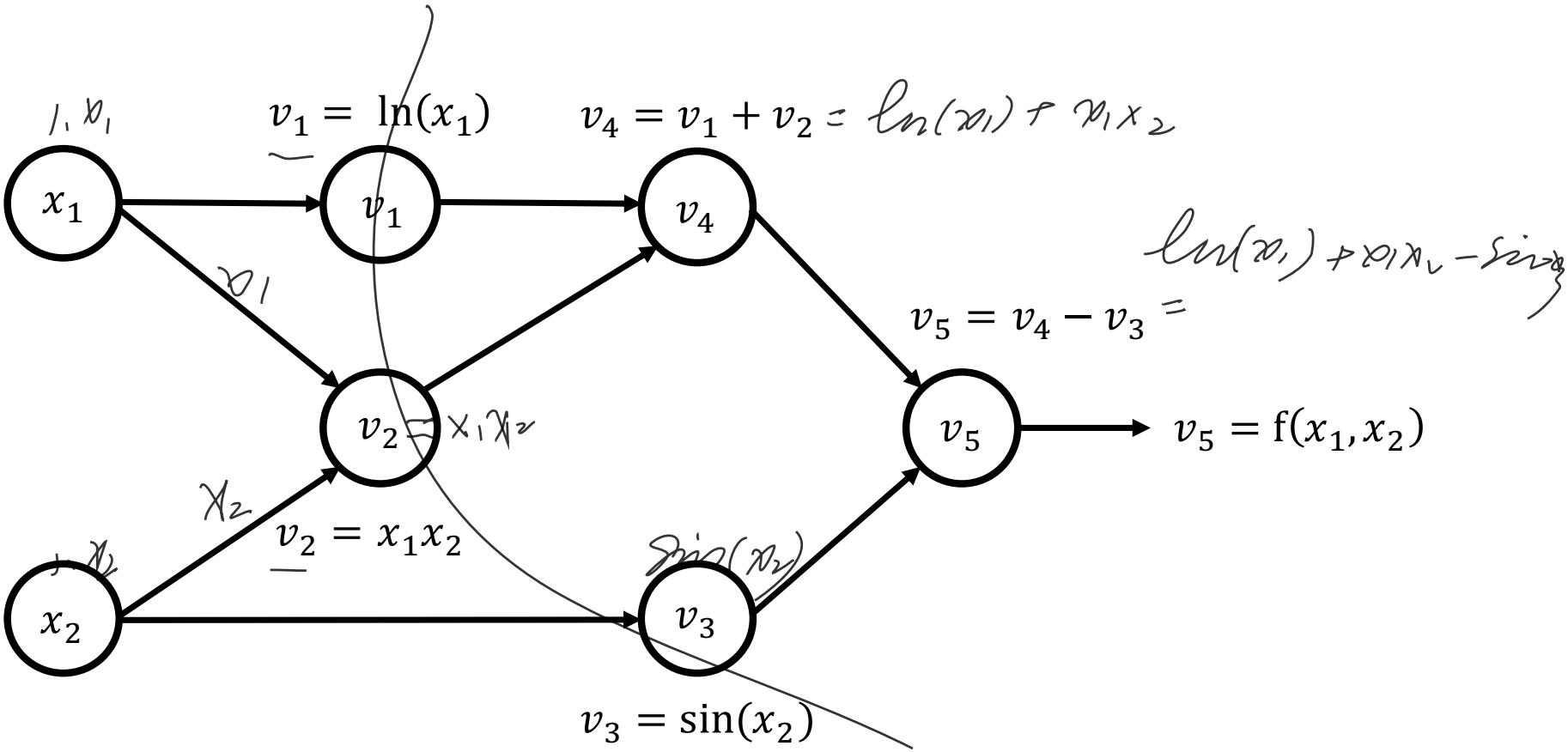
$v_1 = \sin(x_2)$

$v_4 = v_1 + v_2$

$v_8 = v_4 - v_3$

$f(x_1, x_2) = v_5$

Computational graph



General notation

$x_1 \in \mathbb{R}^n$, $x_2 \in \mathbb{R}^n$

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

for example:

In this case: $n = 2$, $i = \{1, 2\}$

- Let $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$.

$v_{1-2} = v_{-1} = x_1$, $v_{2-2} = v_0 = x_2$ } are input var

- Variables $v_{i-n} = x_i$, where $i = 1, \cdots, n$ are the input variables.

$v_{-1} = x_1$, $v_0 = x_2$ } inputs

$v_1 = \ln(x_1) \Rightarrow$ is an intermediate variable.

- Variables v_i, with $i = 1, \cdots, l$ are the intermediate variables.

$v_1 = \ln(x_1)$, $v_2 = x_1 x_2$, $v_3 = \sin(x_2)$ } intermediate

$l = ?$ $\quad i = 1, 2, 3, \Rightarrow l = 3$

- Variables $y_{m-i} = v_{l-i}$, with $i = m-1, \cdots, 0$ are the output variables.

how many output?

$l = 3$, $v_5 : f = y_{-(-2)}$ $\quad m = m - 1 = -2 \Rightarrow m = -1$.

$i = -2, -1, 0$.

will there be more than one ?

it can be negative : $i < 0$.

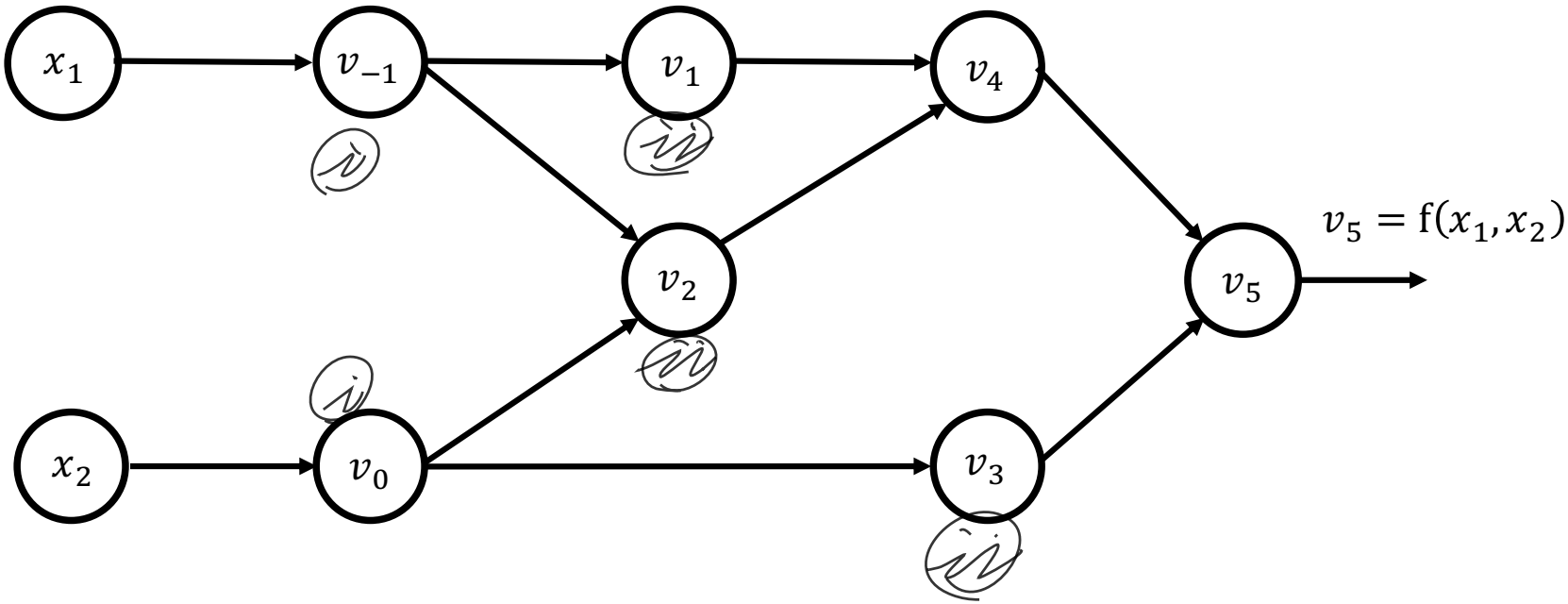
if i is 0, and $v_{l-2} = v_{3-2} = v_5$: $y_{-1-0} = y_{-1} = v_5$ is the output variable?

$i = 0$: $v_{l-i} = v_{3-0} = v_3$ $\quad y_{-1-(-1)} = y_0 = v_1 + v_0$ is output variables!

$i = -2$: $v_{3-(-2)} = v_5$ $\quad y_{-1-(-2)} = y_{-1} = v_5$ $\quad y_0 = v_5$

New computational graph

which of these are ...
i) input variables ?
ii) intermediate variables
iii) output variables



Jacobian

a function depend on several vars $f(x_1, x_2, \cdots x_n)$

- Say that we have several functions $y_i = f_i(\cdot)$ for $i = 1, \ldots, m$ that depend on several input variables $x_1, x_2, \cdots, x_n$,

$$\begin{aligned} y_1 &= f_1(x_1, \ldots, x_n) \\ y_2 &= f_2(x_1, \ldots, x_n) \\ &\vdots \qquad\qquad \vdots \\ y_m &= f_m(x_1, \ldots, x_n) \end{aligned}$$

- The Jacobian $\mathbf{J}$ of dimensions $m \times n$ is a matrix with entries $\mathbf{J}_{ij} = \frac{\partial f_i}{\partial x_j}$ given as

what does the sign mean?

$$J_{ij} = \frac{\partial f_i}{\partial x_j}$$

$$\mathbf{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

why not use $\left(\frac{df_i}{dx_i}\right)$?

$\frac{df_i}{dx_i}$ → get the derivative of f_i, with respect to x_i

Contents

Forward accumulation mode

- Forward accumulation mode or tangent linear mode.

- To compute the derivative of f with respect to x_1, each intermediate variable v_i has a derivative, and calculate the derivative of functions (intermediate)

$$\dot{v}_i = \frac{\partial v_i}{\partial x_1}$$

- For each evaluation (or forward primal) trace, it builds a forward *derivative* (or tangent) trace.

- Essentially, this forward derivative trace is just implementing the *chain rule of differentiation*

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dz}\frac{dz}{dx}.$$

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (I)

- Let us compute the forward tangent trace $\frac{\partial y}{\partial x_1}$ for the function we had before

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

- The following table shows both the forward primal trace and the forward tangent trace

Forward primal trace	Forward tangent trace
$v_{-1} = x_1$	$\dot{v}_{-1} = \dot{x}_1$
$v_0 = x_2$	$\dot{v}_0 = \dot{x}_2$
$v_1 = \ln v_{-1}$	$\dot{v}_1 = \frac{1}{v_{-1}} \dot{v}_{-1}$
$v_2 = v_{-1} \times v_0$	$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$
$v_3 = \sin(v_0)$	$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$
$v_4 = v_1 + v_2$	$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$
$v_5 = v_4 - v_3$	$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$
$y = v_5$	$\dot{y} = \dot{v}_5$

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

We now compute the derivative $\frac{\partial y}{\partial x_1}$ at $x_1 = 2, x_2 = 5$.

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

We now compute the derivative $\frac{\partial y}{\partial x_1}$ at $x_1 = 2, x_2 = 5$.

Forward primal trace	Forward tangent trace
$v_{-1} = x_1 \quad = 2$	$\dot{v}_{-1} = \dot{x}_1$
$v_0 = x_2 \quad = 5$	$\dot{v}_0 = \dot{x}_2$
$v_1 = \ln v_{-1}$	$\dot{v}_1 = \frac{1}{v_{-1}} \dot{v}_{-1}$
$v_2 = v_{-1} \times v_0$	$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$
$v_3 = \sin(v_0)$	$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$
$v_4 = v_1 + v_2$	$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$
$v_5 = v_4 - v_3$	$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$
$y = v_5$	$\dot{y} = \dot{v}_5$

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

We now compute the derivative $\frac{\partial y}{\partial x_1}$ at $x_1 = 2, x_2 = 5$.

Forward primal trace		Forward tangent trace	
$v_{-1} = x_1$	$= 2$	$\dot{v}_{-1} = \dot{x}_1$	$= 1$
$v_0 = x_2$	$= 5$	$\dot{v}_0 = \dot{x}_2$	$= 0$
$v_1 = \ln v_{-1}$		$\dot{v}_1 = \frac{1}{v_{-1}} \dot{v}_{-1}$	
$v_2 = v_{-1} \times v_0$		$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	
$v_3 = \sin(v_0)$		$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	
$v_4 = v_1 + v_2$		$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	
$v_5 = v_4 - v_3$		$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	
$y = v_5$		$\dot{y} = \dot{v}_5$	

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

We now compute the derivative $\frac{\partial y}{\partial x_1}$ at $x_1 = 2, x_2 = 5$.

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$v_{-1} = x_1$	$= 2$	$\dot{v}_{-1} = \dot{x}_1$	$= 1$
$v_0 = x_2$	$= 5$	$\dot{v}_0 = \dot{x}_2$	$= 0$
$v_1 = \ln v_{-1}$	$= \ln 2$	$\dot{v}_1 = \frac{1}{v_{-1}} \dot{v}_{-1}$	$= \frac{1}{2}(1)$
$v_2 = v_{-1} \times v_0$		$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	
$v_3 = \sin(v_0)$		$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	
$v_4 = v_1 + v_2$		$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	
$v_5 = v_4 - v_3$		$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	
$y = v_5$		$\dot{y} = \dot{v}_5$	

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

We now compute the derivative $\frac{\partial y}{\partial x_1}$ at $x_1 = 2, x_2 = 5$.

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$v_2 = v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$v_3 = \sin(v_0)$		$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	
$v_4 = v_1 + v_2$		$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	
$v_5 = v_4 - v_3$		$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	
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$v_3 = \sin(v_0)$	$= \sin(5)$	$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	$= 0 \times \cos(5)$
$v_4 = v_1 + v_2$		$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	
$v_5 = v_4 - v_3$		$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	
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$v_1 = \ln v_{-1}$	$= \ln 2$	$\dot{v}_1 = \frac{1}{v_{-1}} \dot{v}_{-1}$	$= \frac{1}{2}(1)$
$v_2 = v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$v_3 = \sin(v_0)$	$= \sin(5)$	$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	$= 0 \times \cos(5)$
$v_4 = v_1 + v_2$	$= 0.693 + 10$	$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$v_5 = v_4 - v_3$		$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	
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Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

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$v_1 = \ln v_{-1}$	$= \ln 2$	$\dot{v}_1 = \frac{1}{v_{-1}} \dot{v}_{-1}$	$= \frac{1}{2}(1)$
$v_2 = v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$v_3 = \sin(v_0)$	$= \sin(5)$	$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	$= 0 \times \cos(5)$
$v_4 = v_1 + v_2$	$= 0.693 + 10$	$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$v_5 = v_4 - v_3$	$= 10.693 + 0.959$	$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
$y = v_5$		$\dot{y} = \dot{v}_5$	

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

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$v_2 = v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$v_3 = \sin(v_0)$	$= \sin(5)$	$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	$= 0 \times \cos(5)$
$v_4 = v_1 + v_2$	$= 0.693 + 10$	$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$v_5 = v_4 - v_3$	$= 10.693 + 0.959$	$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
$y = v_5$	$= 11.652$	$\dot{y} = \dot{v}_5$	$= 5.5$

Forward primal trace and tangent trace for $\frac{\partial y}{\partial x_1}$ (II)

We now compute the derivative $\frac{\partial y}{\partial x_1}$ at $x_1 = 2, x_2 = 5$.

which also means that to calculate the derivatives wrt x_1

Forward primal trace		Forward tangent trace	
$v_{-1} = x_1$	$= 2$	$\dot{v}_{-1} = \dot{x}_1$	$= 1$
$v_0 = x_2$	$= 5$	$\dot{v}_0 = \dot{x}_2$	$= 0$
$v_1 = \ln v_{-1}$	$= \ln 2$	$\dot{v}_1 = \frac{1}{v_{-1}} \dot{v}_{-1}$	$= \frac{1}{2}(1)$
$v_2 = v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2 = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$v_3 = \sin(v_0)$	$= \sin(5)$	$\dot{v}_3 = \dot{v}_0 \times \cos(v_0)$	$= 0 \times \cos(5)$
$v_4 = v_1 + v_2$	$= 0.693 + 10$	$\dot{v}_4 = \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$v_5 = v_4 - v_3$	$= 10.693 + 0.959$	$\dot{v}_5 = \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
$y = v_5$	$= 11.652$	$\dot{y} = \dot{v}_5$	$= 5.5$

If we want to compute $\frac{\partial y}{\partial x_2}$ instead, we set $\dot{v}_{-1} = 0$ and $\dot{v}_0 = 1$.

Generalisation to the Jacobian of a function

- Let $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ be a function with n independent variables x_i and m dependent variables y_j.

- The derivatives in the Jacobian, $\frac{\partial y_j}{\partial x_i}$, are computed by making $\dot{x}_i = 1$ initially in the forward pass and all the other derivatives $\dot{x}_k = 0$ for $k \neq i$.

- The values of the derivatives at $\mathbf{x} = \mathbf{a}$,

$$\dot{y}_j = \left.\frac{\partial y_j}{\partial x_i}\right|_{\mathbf{x}=\mathbf{a}}.$$

  are obtained by a forward pass of AD.

- Notice that for a specific x_i, we can compute all the derivatives $\frac{\partial y_j}{\partial x_i}$ for $j = 1, \ldots, m$, which corresponds to the column i in the Jacobian.

- To compute the whole Jacobian, we need n forward passes, one per input variable.

Complexity

Expensive when computing
choose reverse mode of AD

- AD with forward mode is efficient for functions like $\mathbf{f} : \mathbb{R} \to \mathbb{R}^m$.
- The reason, as we saw before, is because we can compute all the derivatives $\frac{\partial y_j}{\partial x}$ for $j = 1, \ldots, m$ in one pass.
- In the other extreme, $f : \mathbb{R}^n \to \mathbb{R}$, it needs n forward passes and it can become computationally expensive when n is large.
- In general, when $n \gg m$, the reverse mode of AD is preferred.

Contents

Backpropagate

- AD in reverse mode propagates derivatives backwards from a given output.

- It is done by computing intermediate variables for v_i known as *adjoints*,

$$\bar{v}_i = \frac{\partial y_j}{\partial v_i},$$

representing the sensitivity of output y_j to input v_i.

- AD in reverse mode uses two-phases
  - a *forward* step to compute the variables v_i and to book-keep dependencies in the computational graph.
  - a *backward* or *reverse* step, in which the adjoints are used to compute the derivatives, starting from the outputs and going back to the inputs.

Example (I)

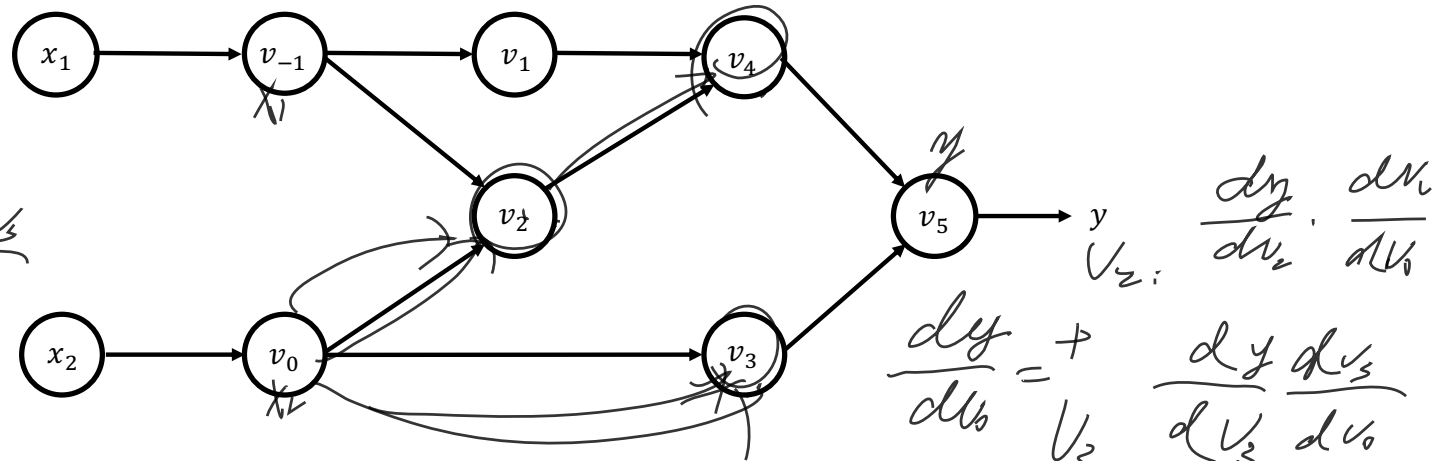
- Let us go back to the example we saw before

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

  and focus on v_0 ($v_0 = x_2$).

- We want to compute the adjoint $\bar{v}_0 = \frac{\partial y}{\partial v_0}$, this is, how the change in v_0 affects the output y.

- From the computational graph, we see that v_0 affects y through v_2 and v_3,



Example (II)

- So the contribution of v_0 to y is given as

$$\frac{\partial y}{\partial v_0} = \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_0} + \frac{\partial y}{\partial v_3}\frac{\partial v_3}{\partial v_0}.$$

direct way

Total Gradient

- By definition $\frac{\partial y}{\partial v_2} = \bar{v}_2$ and $\frac{\partial y}{\partial v_3} = \bar{v}_3$, so we can write the expression above as

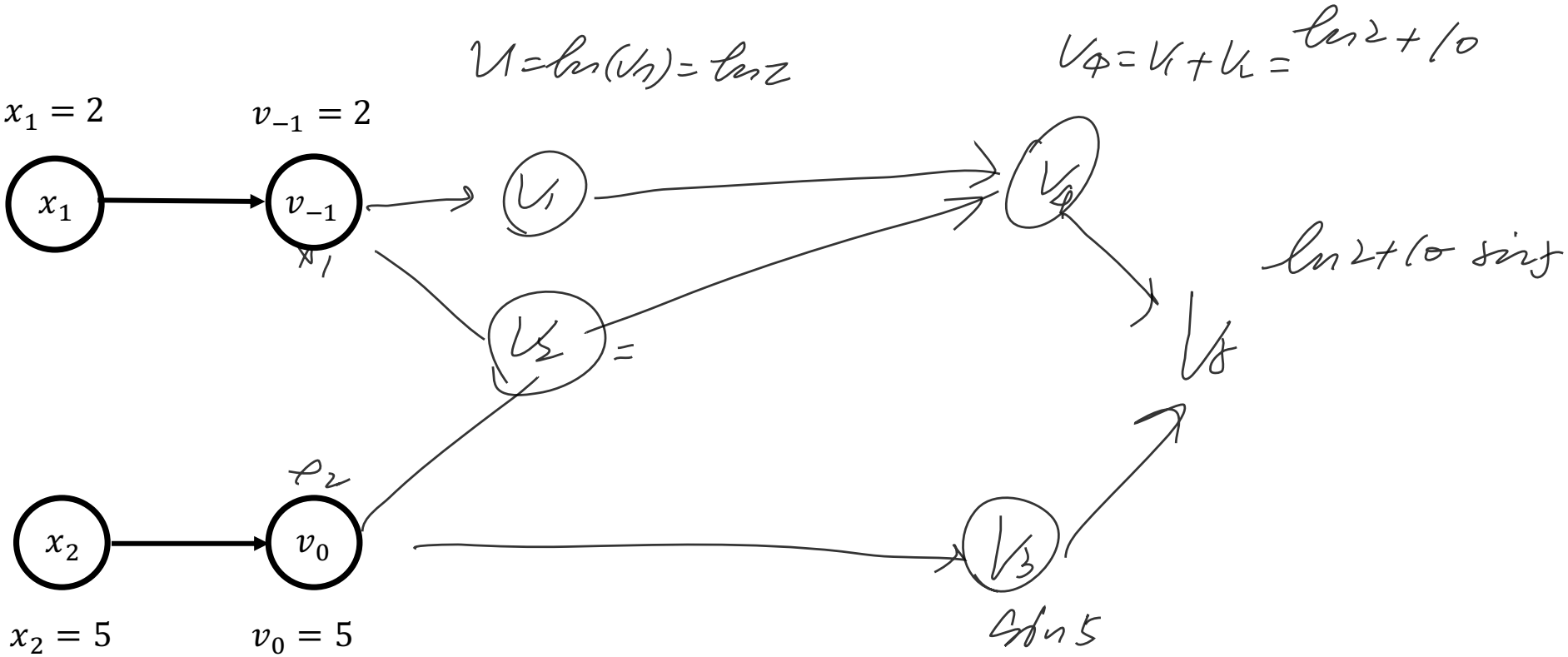
adjoint for v_2:

$$\bar{v}_0 = \bar{v}_2\frac{\partial v_2}{\partial v_0} + \bar{v}_3\frac{\partial v_3}{\partial v_0}.$$

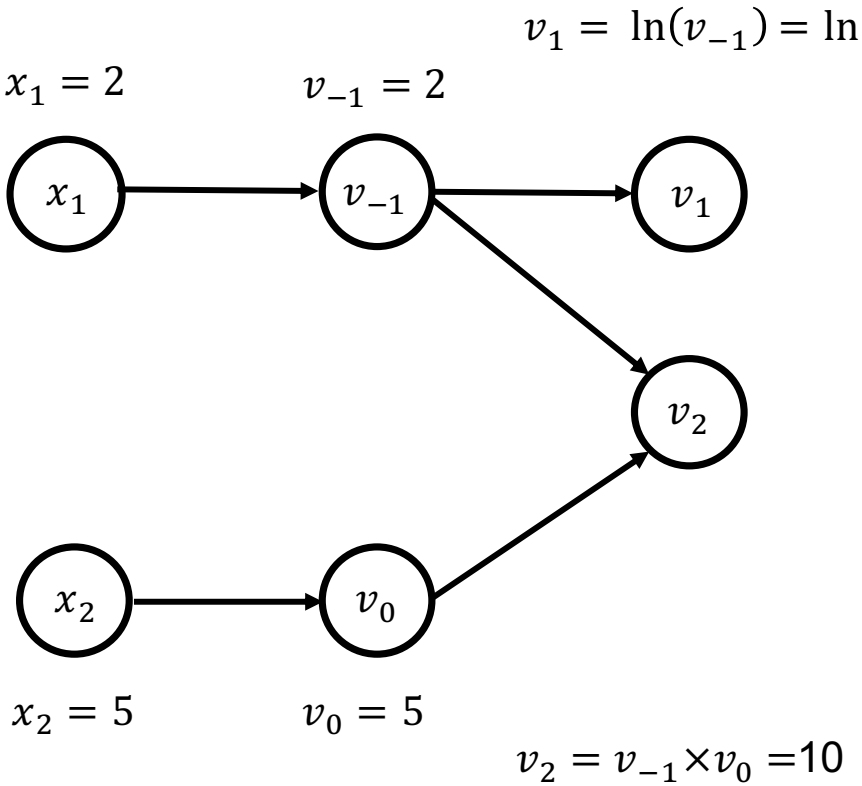
- After the forward pass to compute v_i, the reverse pass computes the adjoints, starting with $\bar{v}_5 = \bar{y} = \frac{\partial y}{\partial y} = 1$, and computing $\frac{\partial y}{\partial x_1} = \bar{x}_1$ and $\frac{\partial y}{\partial x_2} = \bar{x}_2$ at the end.

reverse mode

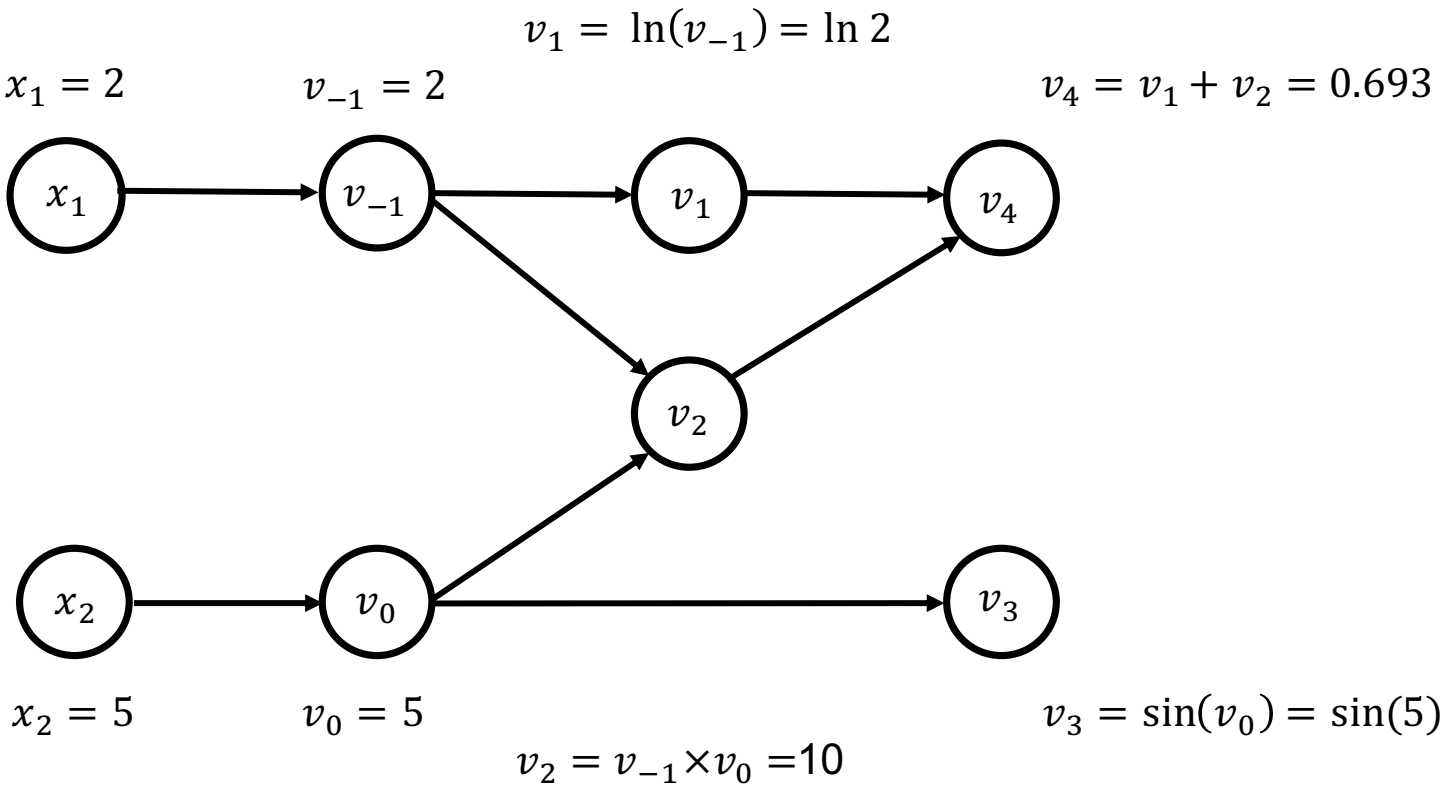
Forward primal trace (forward pass)



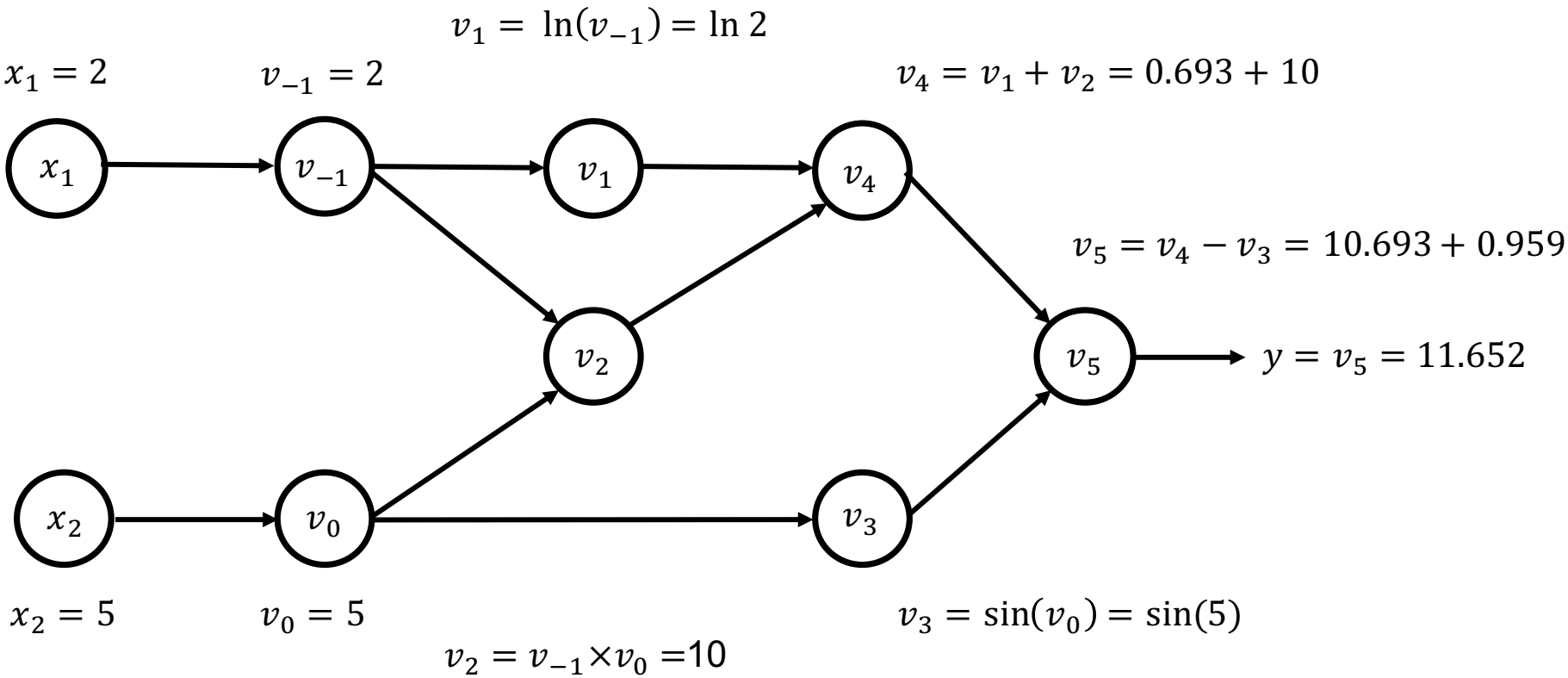
Forward primal trace (forward pass)



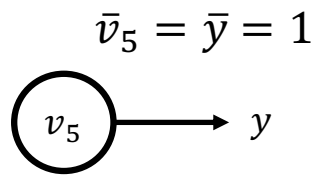
Forward primal trace (forward pass)



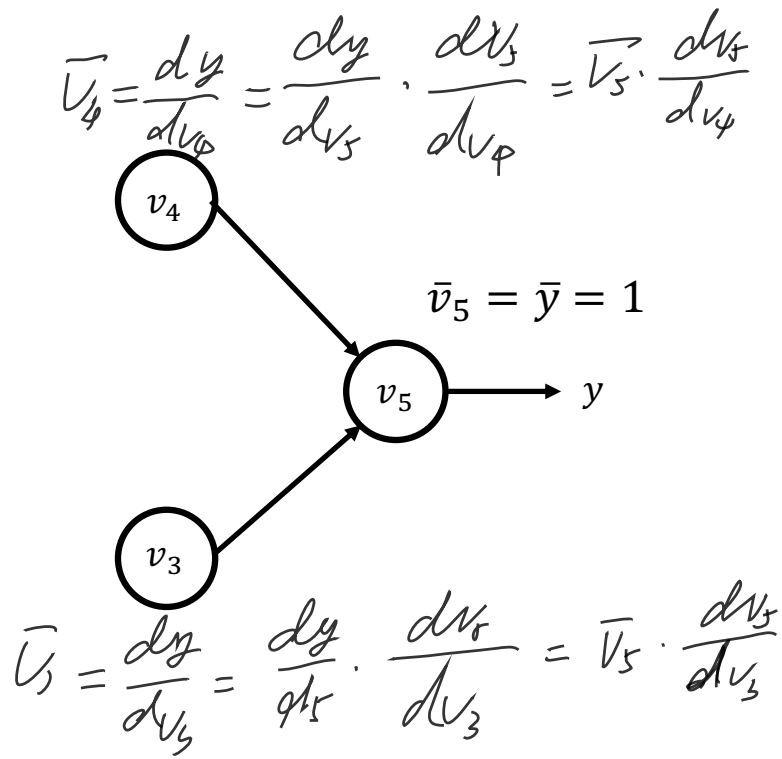
Forward primal trace (forward pass)



Reverse adjoint (derivative) trace (reverse pass)

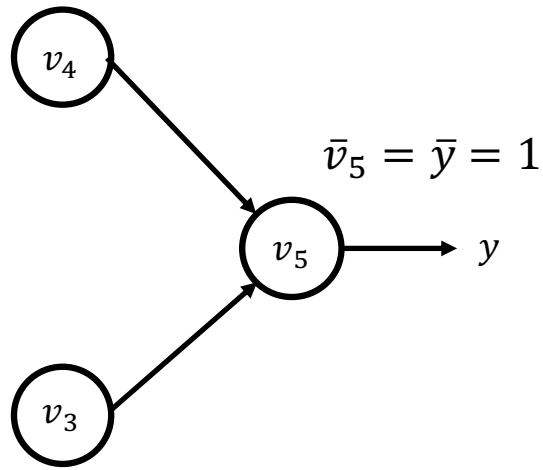


Reverse adjoint (derivative) trace (reverse pass)



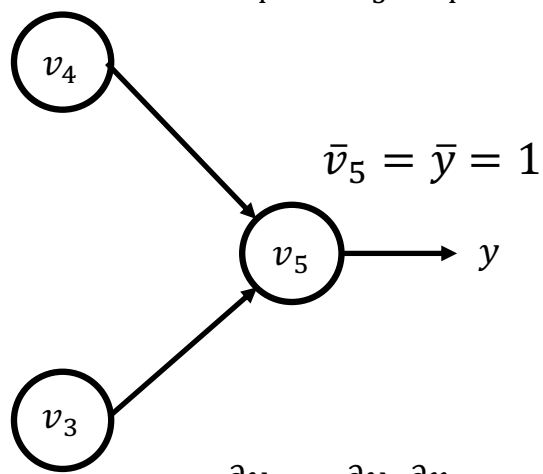
Reverse adjoint (derivative) trace (reverse pass)

$$\bar{v}_4 = \frac{\partial y}{\partial v_4} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4} = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$$



Reverse adjoint (derivative) trace (reverse pass)

$$\bar{v}_4 = \frac{\partial y}{\partial v_4} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4} = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$$

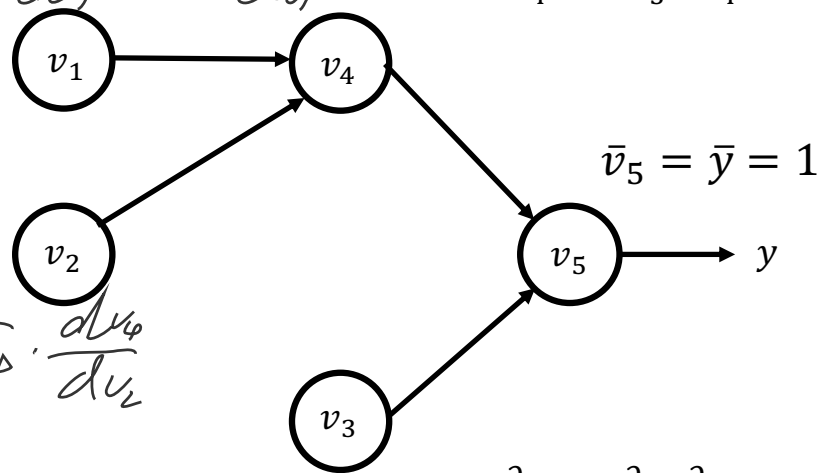


$$\bar{v}_3 = \frac{\partial y}{\partial v_3} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_3} = \bar{v}_5 \frac{\partial v_5}{\partial v_3}$$

Reverse adjoint (derivative) trace (reverse pass)

$$\bar{v}_1 = \frac{\partial y}{\partial v_1} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_1} = \bar{v}_4 \frac{\partial v_4}{\partial v_1}$$

$$\bar{v}_4 = \frac{\partial y}{\partial v_4} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4} = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$$



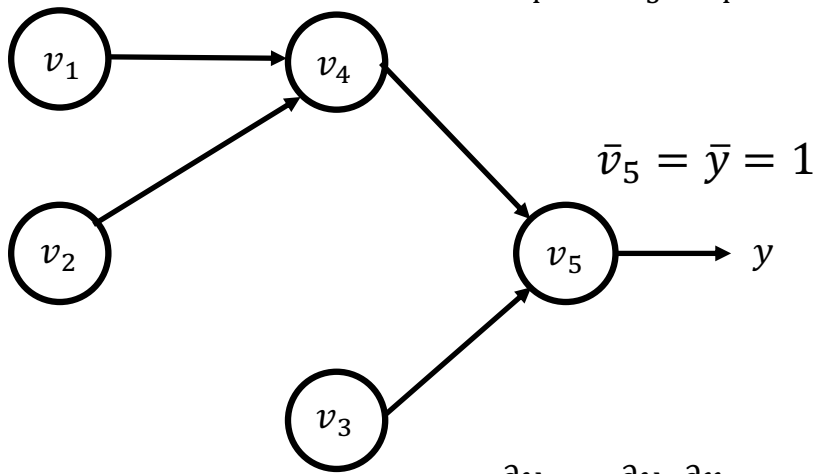
$$\bar{v}_5 = \bar{y} = 1$$

$$\bar{v}_3 = \frac{\partial y}{\partial v_3} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_3} = \bar{v}_5 \frac{\partial v_5}{\partial v_3}$$

Reverse adjoint (derivative) trace (reverse pass)

$$\bar{v}_1 = \frac{\partial y}{\partial v_1} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_1} = \bar{v}_4\frac{\partial v_4}{\partial v_1}$$

$$\bar{v}_4 = \frac{\partial y}{\partial v_4} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4} = \bar{v}_5\frac{\partial v_5}{\partial v_4}$$



$$\bar{v}_5 = \bar{y} = 1$$

$$\bar{v}_3 = \frac{\partial y}{\partial v_3} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_3} = \bar{v}_5\frac{\partial v_5}{\partial v_3}$$

$$\bar{v}_2 = \frac{\partial y}{\partial v_2} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_2} = \bar{v}_4\frac{\partial v_4}{\partial v_2}$$

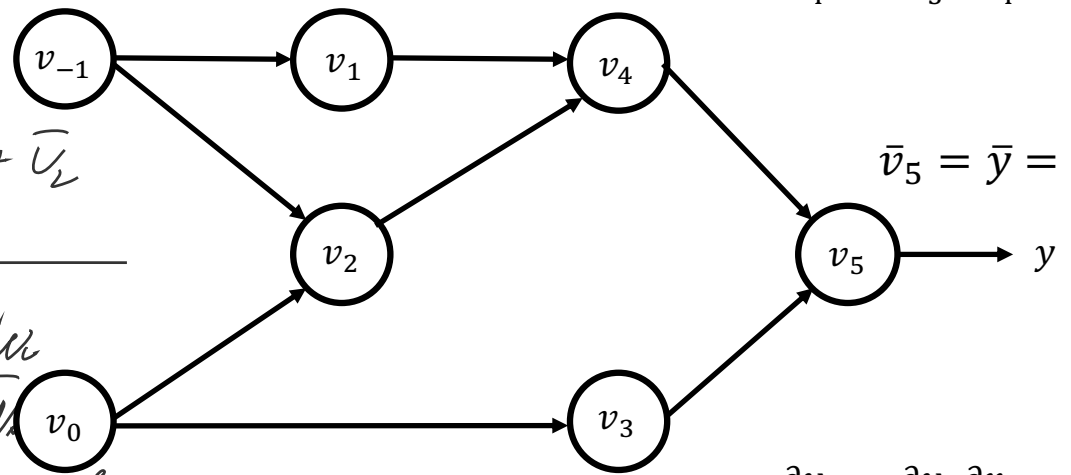
Reverse adjoint (derivative) trace (reverse pass)

$$\bar{v}_i = \frac{dy}{dv_i}$$

$$\bar{v}_1 = \frac{\partial y}{\partial v_1} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_1} = \bar{v}_4\frac{\partial v_4}{\partial v_1}$$

$$\bar{v}_{-1} = \frac{\partial y}{\partial v_{-1}} = \frac{\partial y}{\partial v_1}\frac{\partial v_1}{\partial v_{-1}} + \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_{-1}} = \bar{v}_1\frac{\partial v_1}{\partial v_{-1}} + \bar{v}_2\frac{\partial v_2}{\partial v_{-1}}$$

$$\bar{v}_4 = \frac{\partial y}{\partial v_4} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4} = \bar{v}_5\frac{\partial v_5}{\partial v_4}$$



$$\bar{v}_5 = \bar{y} = 1$$

different places

$$\bar{v}_3 = \frac{\partial y}{\partial v_3} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_3} = \bar{v}_5\frac{\partial v_5}{\partial v_3}$$

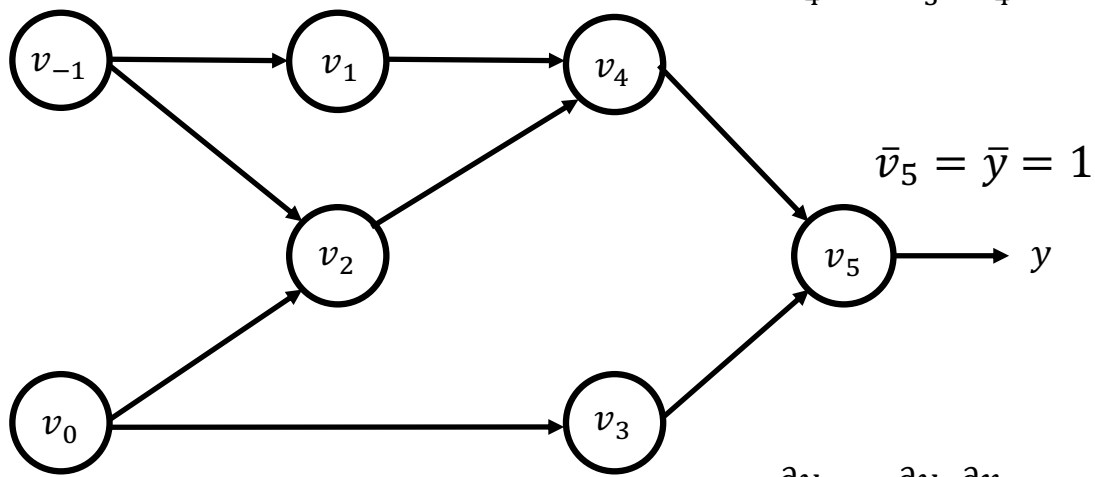
$$\bar{v}_2 = \frac{\partial y}{\partial v_2} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_2} = \bar{v}_4\frac{\partial v_4}{\partial v_2}$$

Reverse adjoint (derivative) trace (reverse pass)

$$\bar{v}_1 = \frac{\partial y}{\partial v_1} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_1} = \bar{v}_4\frac{\partial v_4}{\partial v_1}$$

$$\bar{v}_{-1} = \frac{\partial y}{\partial v_{-1}} = \frac{\partial y}{\partial v_1}\frac{\partial v_1}{\partial v_{-1}} + \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_{-1}} = \bar{v}_1\frac{\partial v_1}{\partial v_{-1}} + \bar{v}_2\frac{\partial v_2}{\partial v_{-1}}$$

$$\bar{v}_4 = \frac{\partial y}{\partial v_4} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4} = \bar{v}_5\frac{\partial v_5}{\partial v_4}$$



$$\bar{v}_0 = \frac{\partial y}{\partial v_0} = \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_0} + \frac{\partial y}{\partial v_3}\frac{\partial v_3}{\partial v_0} = \bar{v}_2\frac{\partial v_2}{\partial v_0} + \bar{v}_3\frac{\partial v_3}{\partial v_0}$$

$$\bar{v}_3 = \frac{\partial y}{\partial v_3} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_3} = \bar{v}_5\frac{\partial v_5}{\partial v_3}$$

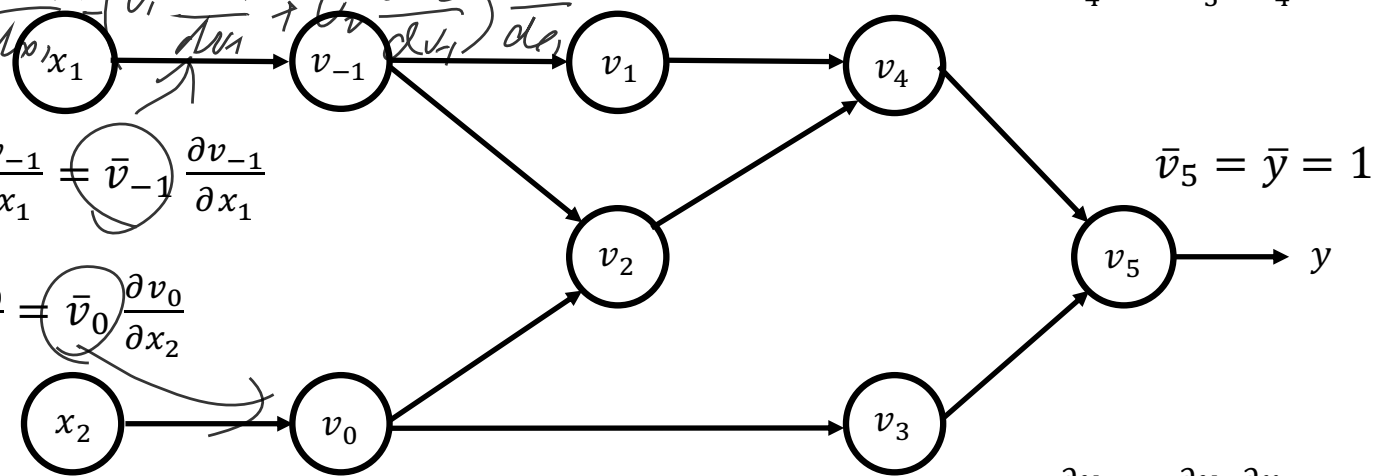
$$\bar{v}_2 = \frac{\partial y}{\partial v_2} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_2} = \bar{v}_4\frac{\partial v_4}{\partial v_2}$$

Reverse adjoint (derivative) trace (reverse pass)

$$\bar{v}_1 = \frac{\partial y}{\partial v_1} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_1} = \bar{v}_4\frac{\partial v_4}{\partial v_1}$$

$$\bar{v}_{-1} = \frac{\partial y}{\partial v_{-1}} = \frac{\partial y}{\partial v_1}\frac{\partial v_1}{\partial v_{-1}} + \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_{-1}} = \bar{v}_1\frac{\partial v_1}{\partial v_{-1}} + \bar{v}_2\frac{\partial v_2}{\partial v_{-1}}$$

$$\bar{v}_4 = \frac{\partial y}{\partial v_4} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4} = \bar{v}_5\frac{\partial v_5}{\partial v_4}$$



$$\bar{x}_1 = \frac{\partial y}{\partial x_1} = \frac{\partial y}{\partial v_{-1}}\frac{\partial v_{-1}}{\partial x_1} = \bar{v}_{-1}\frac{\partial v_{-1}}{\partial x_1}$$

$$\bar{v}_5 = \bar{y} = 1$$

$$\bar{x}_2 = \frac{\partial y}{\partial x_2} = \frac{\partial y}{\partial v_0}\frac{\partial v_0}{\partial x_2} = \bar{v}_0\frac{\partial v_0}{\partial x_2}$$

$$\bar{v}_0 = \frac{\partial y}{\partial v_0} = \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_0} + \frac{\partial y}{\partial v_3}\frac{\partial v_3}{\partial v_0} = \bar{v}_2\frac{\partial v_2}{\partial v_0} + \bar{v}_3\frac{\partial v_3}{\partial v_0}$$

$$\bar{v}_3 = \frac{\partial y}{\partial v_3} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_3} = \bar{v}_5\frac{\partial v_5}{\partial v_3}$$

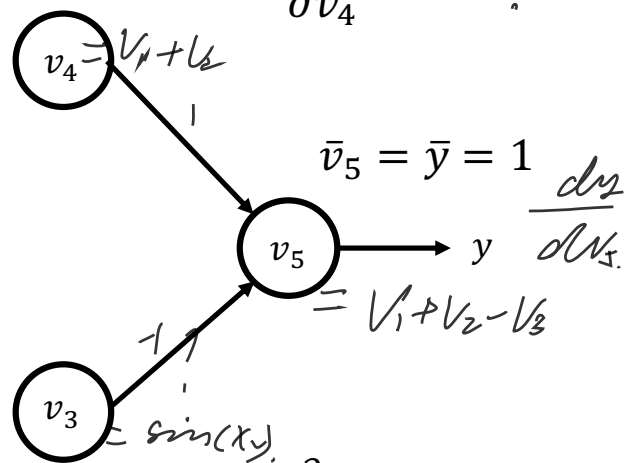
$$\bar{v}_2 = \frac{\partial y}{\partial v_2} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_2} = \bar{v}_4\frac{\partial v_4}{\partial v_2}$$

Numerical evaluation of the reverse adjoint trace

reverse adjoint trace

why? $\frac{dv_5}{dv_4} = 1$?

$$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4} = \bar{v}_5 \times 1 = 1$$



$$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$$

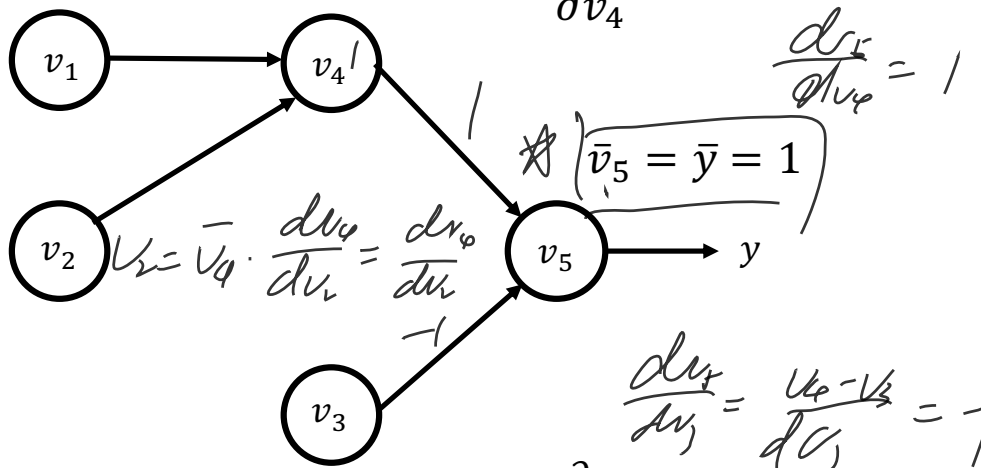
why $\frac{dv_5}{dv_3} = -1$

If you don't know something just follow more steps.

Numerical evaluation of the reverse adjoint trace

$$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_4 \times 1 = 1$$

$$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4} = \bar{v}_5 \times 1 = 1$$



$$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$$

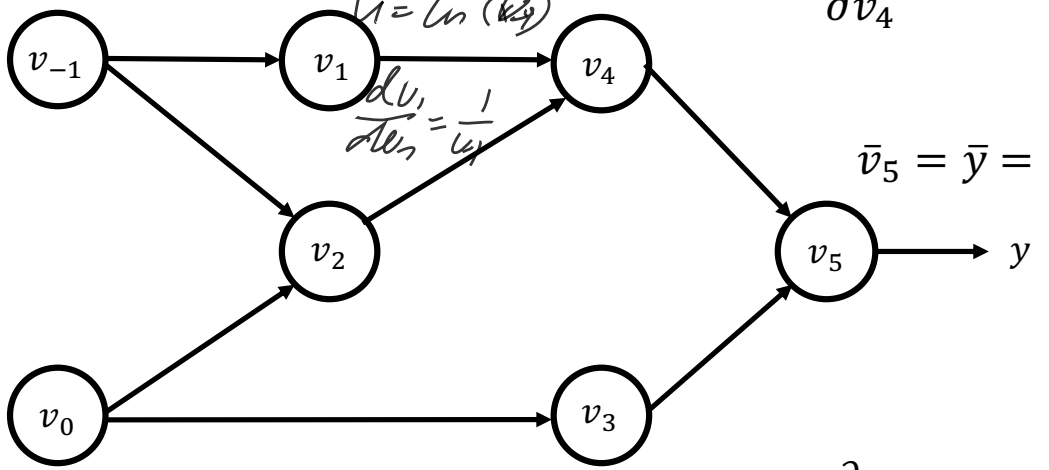
$$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$$

Numerical evaluation of the reverse adjoint trace

$$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_4 \times 1 = 1$$

$$\bar{v}_{-1} = \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} + \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} = \bar{v}_1 \times \frac{1}{v_{-1}} + \bar{v}_2 \times v_0 = 5.5$$

$$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4} = \bar{v}_5 \times 1 = 1$$



$$\bar{v}_5 = \bar{y} = 1$$

$$\bar{v}_0 = \bar{v}_2 \frac{\partial v_2}{\partial v_0} + \bar{v}_3 \frac{\partial v_3}{\partial v_0} = \bar{v}_2 \times v_{-1} + \bar{v}_3 \cos(v_0) = 1.716$$

$$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$$

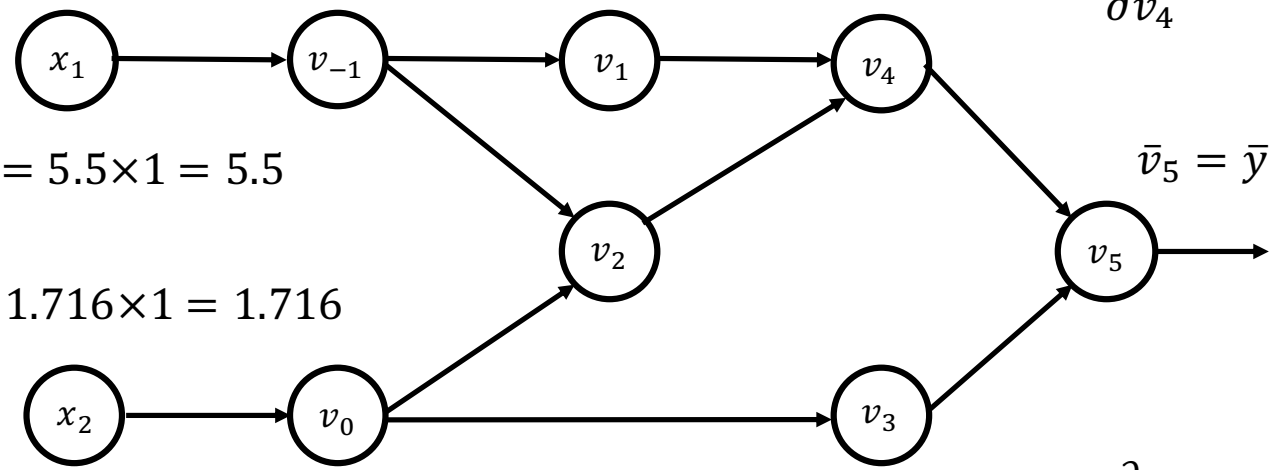
$$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$$

Numerical evaluation of the reverse adjoint trace

$$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_4 \times 1 = 1$$

$$\bar{v}_{-1} = \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} + \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} = \bar{v}_1 \times \frac{1}{v_{-1}} + \bar{v}_2 \times v_0 = 5.5$$

$$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4} = \bar{v}_5 \times 1 = 1$$



$$\bar{x}_1 = \bar{v}_{-1} \frac{\partial v_{-1}}{\partial x_1} = 5.5 \times 1 = 5.5$$

$$\bar{v}_5 = \bar{y} = 1$$

$$\bar{x}_2 = \bar{v}_0 \frac{\partial v_0}{\partial x_2} = 1.716 \times 1 = 1.716$$

$$\bar{v}_0 = \bar{v}_2 \frac{\partial v_2}{\partial v_0} + \bar{v}_3 \frac{\partial v_3}{\partial v_0} = \bar{v}_2 \times v_{-1} + \bar{v}_3 \cos(v_0) = 1.716$$

$$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$$

$$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$$

Complexity

why? why it performs better.

- Reverse mode AD performs better when $n \gg m$.

Because it starts at the end

- The downside is the cost of increased storage, since we need to save intermediate values for v_i in the evaluation trace.

↔ For forward trace, do not need to save the intermediate values. → just calculate is good enough to get results.

Reverse mode AD and backpropagation

- Reverse mode AD is the algorithm used to train neural networks and deep learning models.

- To train a neural network model, we optimise an objective function, $E(\mathbf{w}) : \mathbb{R}^n \to \mathbb{R}^m$ that usually depends on a high-dimensional input vector of parameters $\mathbf{w} \in \mathbb{R}^n$, with $n \gg m$.

really high dimensional input vector → a relatively small number of results.
we consider several factors. (A-LOT-OF)

- In the machine learning community, reverse mode AD goes by the name of *backpropagation*, which you will see again in the session on neural networks.

Contents

AD implementations

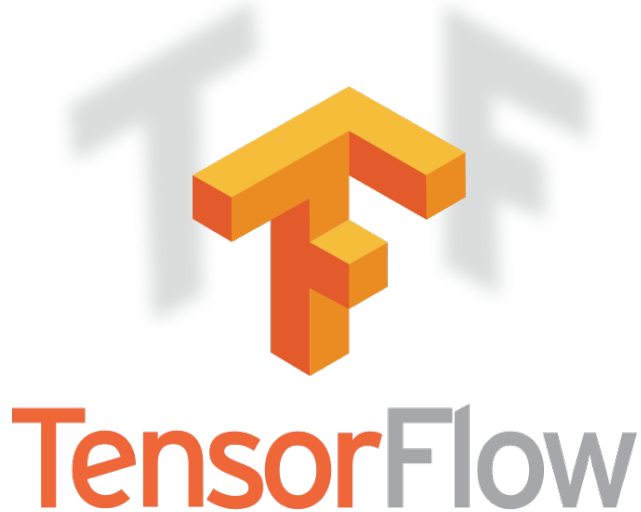
Table 5: Survey of AD implementations. Tools developed primarily for machine learning are highlighted in bold.

Language	Tool	Type	Mode	Institution / Project	Reference	URL
AMPL	AMPL	INT	F, R	Bell Laboratories	Fourer et al. (2002)	http://www.ampl.com/
C, C++	ADIC	ST	F, R	Argonne National Laboratory	Bischof et al. (1997)	http://www.mcs.anl.gov/research/projects/adic/
	ADOL-C	OO	F, R	Computational Infrastructure for Operations Research	Walther and Griewank (2012)	https://projects.coin-or.org/ADOL-C
C++	Ceres Solver	LIB	F	Google		http://ceres-solver.org/
	CppAD	OO	F, R	Computational Infrastructure for Operations Research	Bell and Burke (2008)	http://www.coin-or.org/CppAD/
	FADBAD++	OO	F, R	Technical University of Denmark	Bendtsen and Stauning (1996)	http://www.fadbad.com/fadbad.html
	Mxyzptlk	OO	F	Fermi National Accelerator Laboratory	Ostiguy and Michelotti (2007)	
C#	AutoDiff	LIB	R	George Mason Univ., Dept. of Computer Science	Shtof et al. (2013)	http://autodiff.codeplex.com/
F#, C#	**DiffSharp**	OO	F, R	Maynooth University, Microsoft Research Cambridge	Baydin et al. (2016a)	http://diffsharp.github.io
Fortran	ADIFOR	ST	F, R	Argonne National Laboratory	Bischof et al. (1996)	http://www.mcs.anl.gov/research/projects/adifor/
	NAGWare	COM	F, R	Numerical Algorithms Group	Naumann and Riehme (2005)	http://www.nag.co.uk/nagware/Research/ad_overview.asp
	TAMC	ST	R	Max Planck Institute for Meteorology	Giering and Kaminski (1998)	http://autodiff.com/tamc/
Fortran, C	COSY	INT	F	Michigan State Univ., Biomedical and Physical Sci.	Berz et al. (1996)	http://www.bt.pa.msu.edu/index_cosy.htm
	Tapenade	ST	F, R	INRIA Sophia-Antipolis	Hascoët and Pascual (2013)	http://www-sop.inria.fr/tropics/tapenade.html
Haskell	ad	OO	F, R	Haskell package		http://hackage.haskell.org/package/ad
Java	ADiJaC	ST	F, R	University Politehnica of Bucharest	Slusanschi and Dumitrel (2016)	http://adijac.cs.pub.ro
	Deriva	LIB	R	Java & Clojure library		https://github.com/lambder/Deriva
Julia	JuliaDiff	OO	F, R	Julia packages	Revels et al. (2016a)	http://www.juliadiff.org/
Lua	**torch-autograd**	OO	R	Twitter Cortex		https://github.com/twitter/torch-autograd
MATLAB	ADiMat	ST	F, R	Technical University of Darmstadt, Scientific Comp.	Willkomm and Vehreschild (2013)	http://adimat.sc.informatik.tu-darmstadt.de/
	INTLab	OO	F	Hamburg Univ. of Technology, Inst. for Reliable Comp.	Rump (1999)	http://www.ti3.tu-harburg.de/rump/intlab/
	TOMLAB/MAD	OO	F	Cranfield University & Tomlab Optimization Inc.	Forth (2006)	http://tomlab.biz/products/mad
Python	ad	OO	R	Python package		https://pypi.python.org/pypi/ad
	autograd	OO	F, R	Harvard Intelligent Probabilistic Systems Group	Maclaurin (2016)	https://github.com/HIPS/autograd
	Chainer	OO	R	Preferred Networks	Tokui et al. (2015)	https://chainer.org/
	PyTorch	OO	R	PyTorch core team	Paszke et al. (2017)	http://pytorch.org/
	Tangent	ST	F, R	Google Brain	van Merriënboer et al. (2017)	https://github.com/google/tangent
Scheme	R6RS-AD	OO	F, R	Purdue Univ., School of Electrical and Computer Eng.		https://github.com/qobi/R6RS-AD
	Scmutils	OO	F	MIT Computer Science and Artificial Intelligence Lab.	Sussman and Wisdom (2001)	http://groups.csail.mit.edu/mac/users/gjs/6946/refman.txt
	Stalingrad	COM	F, R	Purdue Univ., School of Electrical and Computer Eng.	Pearlmutter and Siskind (2008)	http://www.bcl.hamilton.ie/~qobi/stalingrad/

F: Forward, R: Reverse; COM: Compiler, INT: Interpreter, LIB: Library, OO: Operator overloading, ST: Source transformation

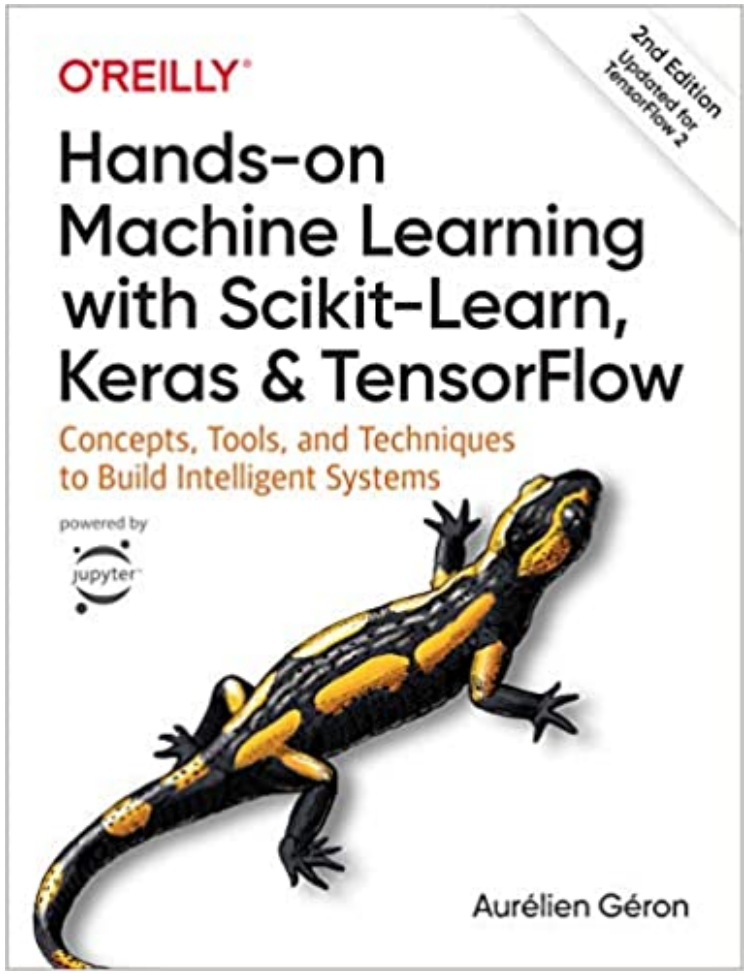
Two popular implementations in the ML community

PyTorch



TensorFlow

References



Appendix D of “Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow”

References

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Atılım Güneş Baydin GUNES@ROBOTS.OX.AC.UK
Department of Engineering Science
University of Oxford
Oxford OX1 3PJ, United Kingdom

Barak A. Pearlmutter BARAK@PEARLMUTTER.NET
Department of Computer Science
National University of Ireland Maynooth
Maynooth, Co. Kildare, Ireland

Alexey Andreyevich Radul AXCH@MIT.EDU
Department of Brain and Cognitive Sciences
Massachusetts Institute of Technology
Cambridge, MA 02139, United States

Jeffrey Mark Siskind QOBI@PURDUE.EDU
School of Electrical and Computer Engineering
Purdue University
West Lafayette, IN 47907, United States