Automatic differentiation

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

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,

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

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

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

Finite difference approximations (II)

```python
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 $l_n = 4l_n(1-l_n)$, $l_1 = x$.

Symplify with Mathematica

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

Out[40]= $16 (1-2x)^2 (1-x) - 16 (1-2x)^2 x - 64 (1-2x)(1-x)x$

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]= $-16 \left(-1 + 10x - 24x^2 + 16x^3\right)$

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

Out[41]= $128 (1-2x)^2 (1-x) x (-8+16x) \left(1-8x+8x^2\right) + 64 (1-2x)^2 (1-x) \left(1-8x+8x^2\right)^2 - 64 (1-2x)^2 x \left(1-8x+8x^2\right)^2 - 256 (1-2x)(1-x) x \left(1-8x+8x^2\right)^2$

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]= $-64 \left(-1 + 42x - 504x^2 + 2640x^3 - 7040x^4 + 9984x^5 - 7168x^6 + 2048x^7\right)$

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

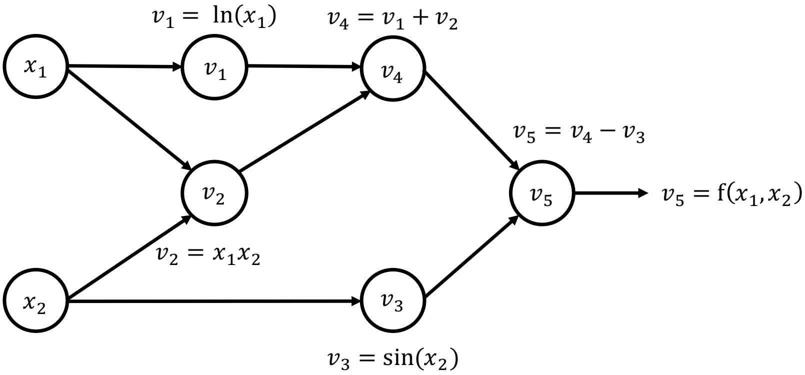
- *Evaluation trace*: composition of elementary operations that lead to a full expression.
- As an example, let us consider the function

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

.

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

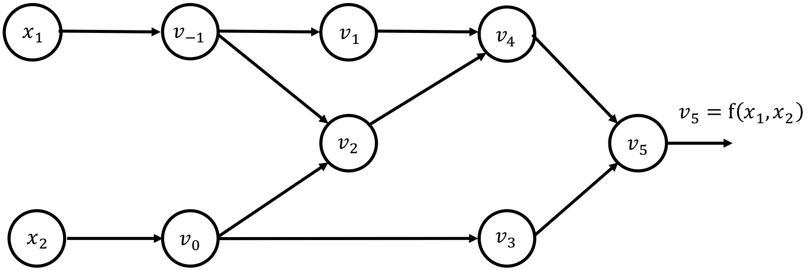
Computational graph



General notation

- Let $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$.
- Variables $v_{i-n} = x_i$, where $i = 1, \cdots, n$ are the input variables.
- Variables v_i, with $i = 1, \cdots, l$ are the intermediate variables.
- Variables $y_{m-i} = v_{l-i}$, with $i = m-1, \cdots, 0$ are the output variables.

New computational graph



Jacobian

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

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

- 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

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

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

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

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

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 $x_1 = 2, x_2 = 5$.

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

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	$= \ln v_{-1}$	$= \ln 2$	$\dot{v}_1$	$= \frac{1}{v_{-1}} \dot{v}_{-1}$	$= \frac{1}{2}(1)$
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)

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	$= \ln v_{-1}$	$= \ln 2$	$\dot{v}_1$	$= \frac{1}{v_{-1}} \dot{v}_{-1}$	$= \frac{1}{2}(1)$
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	$= v_5$	$= 11.652$	$\dot{y}$	$= \dot{v}_5$	$= 5.5$

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	$= \ln v_{-1}$	$= \ln 2$	$\dot{v}_1$	$= \frac{1}{v_{-1}} \dot{v}_{-1}$	$= \frac{1}{2}(1)$
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

- 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 $j = 1, \dots, m$ 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)

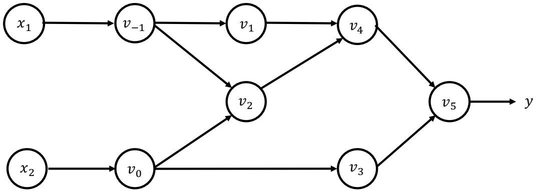
- Let us go back to the example we saw before

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

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

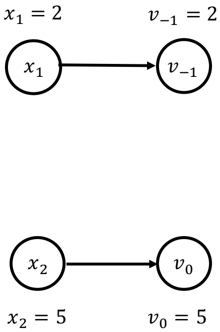
$$\frac{\partial y}{\partial v_0} = \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_0} + \frac{\partial y}{\partial v_3}\frac{\partial v_3}{\partial v_0}.$$

- 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

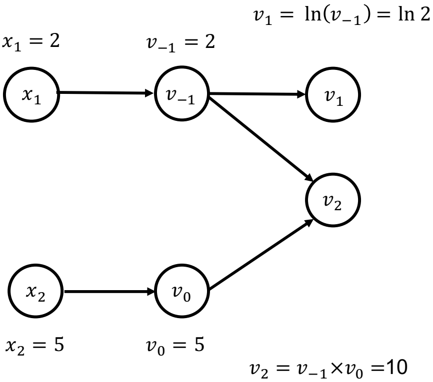
$$\bar{v}_0 = \bar{v}_2\frac{\partial v_2}{\partial v_0} + \bar{v}_3\frac{\partial v_3}{\partial v_0}.$$

- 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.

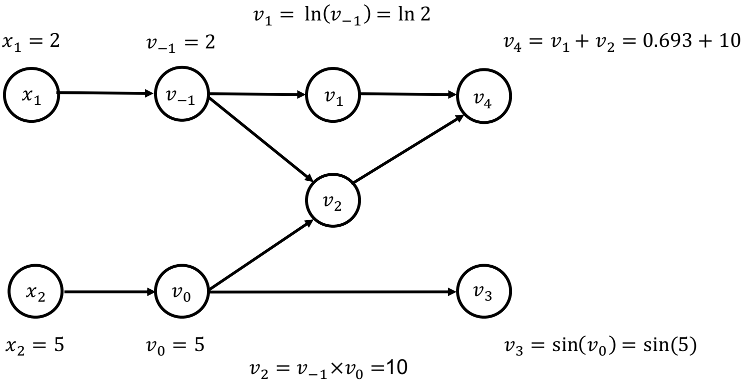
Forward primal trace (forward pass)



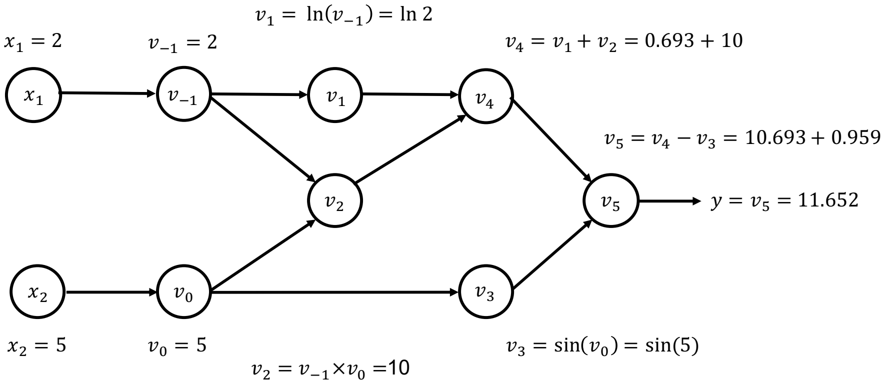
Forward primal trace (forward pass)



Forward primal trace (forward pass)

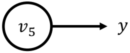


Forward primal trace (forward pass)

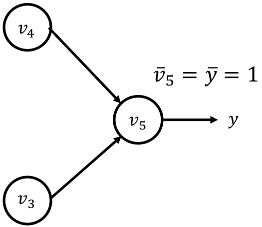


Reverse adjoint (derivative) trace (reverse pass)

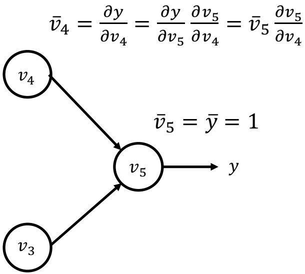
$$\bar{v}_5 = \bar{y} = 1$$



Reverse adjoint (derivative) trace (reverse pass)

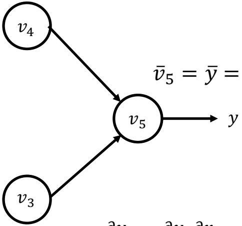


Reverse adjoint (derivative) trace (reverse pass)



Reverse adjoint (derivative) trace (reverse pass)

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

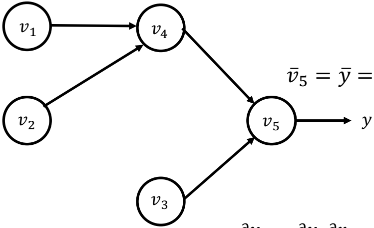


$$\bar{v}_3 = \frac{\partial y}{\partial v_3} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_3} = \bar{v}_5\frac{\partial v_5}{\partial v_3}$$

Reverse adjoint (derivative) trace (reverse pass)

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

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



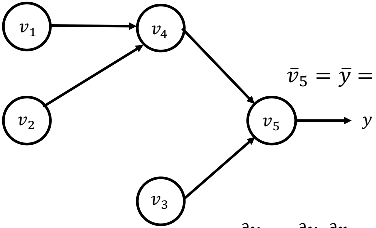
$$\bar{v}_5 = \bar{y} = 1$$

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

Reverse adjoint (derivative) trace (reverse pass)

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

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



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

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

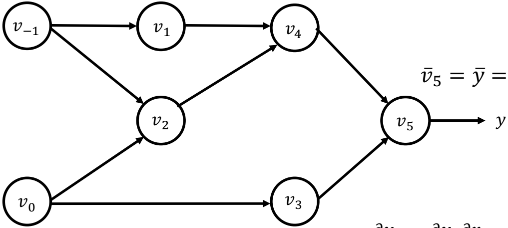
$$\bar{v}_2 = \frac{\partial y}{\partial v_2} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_2} = \bar{v}_4\frac{\partial v_4}{\partial v_2}$$

Reverse adjoint (derivative) trace (reverse pass)

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

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

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



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

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

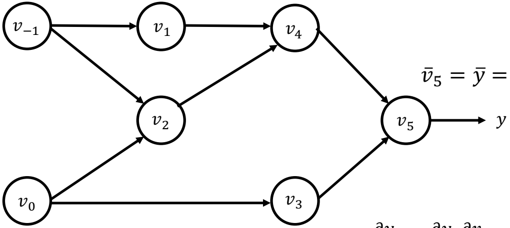
$$\bar{v}_2 = \frac{\partial y}{\partial v_2} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_2} = \bar{v}_4 \frac{\partial v_4}{\partial v_2}$$

Reverse adjoint (derivative) trace (reverse pass)

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

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

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



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

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

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

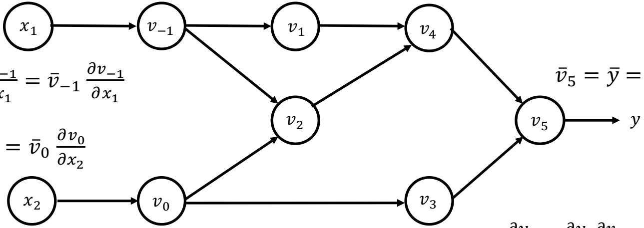
$$\bar{v}_2 = \frac{\partial y}{\partial v_2} = \frac{\partial y}{\partial v_5}\frac{\partial v_5}{\partial v_4}\frac{\partial v_4}{\partial v_2} = \bar{v}_4\frac{\partial v_4}{\partial v_2}$$

Reverse adjoint (derivative) trace (reverse pass)

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

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

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



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

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

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

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

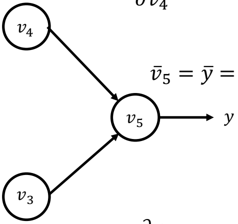
$$\bar{v}_0 = \frac{\partial y}{\partial v_0} = \frac{\partial y}{\partial v_2}\frac{\partial v_2}{\partial v_0} + \frac{\partial y}{\partial v_3}\frac{\partial v_3}{\partial v_0} = \bar{v}_2 \frac{\partial v_2}{\partial v_0} + \bar{v}_3 \frac{\partial v_3}{\partial v_0}$$

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

Numerical evaluation of the reverse adjoint trace

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

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

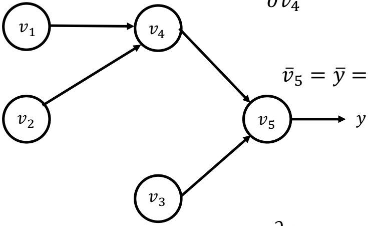


$$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \times (-1) = -1$$

Numerical evaluation of the reverse adjoint trace

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

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



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

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

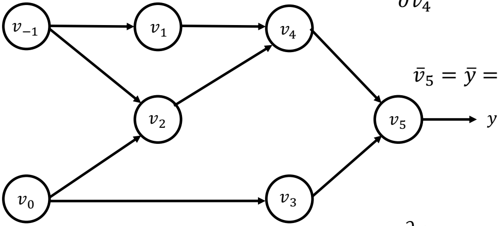
$$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$$

Numerical evaluation of the reverse adjoint trace

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

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

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



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

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

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

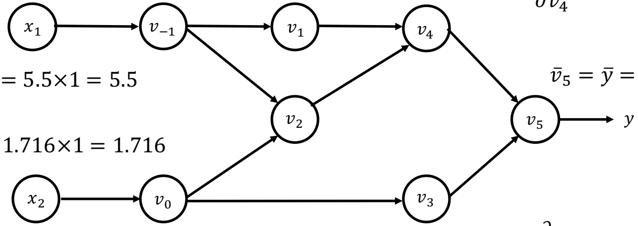
$$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2} = \bar{v}_4 \times 1 = 1$$

Numerical evaluation of the reverse adjoint trace

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

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

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



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

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

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

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

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

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

Complexity

- Reverse mode AD performs better when $n \gg m$.
- The downside is the cost of increased storage, since we need to save intermediate values for v_i in the evaluation trace.

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 $n \gg m$.

- 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/

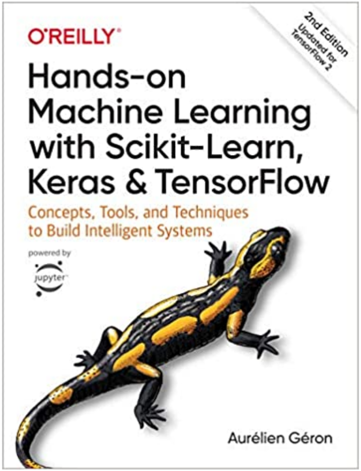
F: Forward, R: Reverse; COM: Compiler, INT: Interpreter, LIB: Library, OO: Operator overloading, ST: Source transformation

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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Automatic Differentiation in Machine Learning: a Survey

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