# Automatic Differentiation <br> <br> CSC412/2506 <br> <br> CSC412/2506 <br> <br> Winter 2018 

 <br> <br> Winter 2018}

Slides based on the excellent review:
Baydin, A. G., Pearlmutter, B. A., Radul, A. A., \& Siskind, J. M. (2015). Automatic differentiation in machine learning: a survey. http://arxiv.org/abs/1502.05767

## 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
(computing by hand and coding the result)
2. Numerical Differentiation
(e.g. finite differences approx.)
3. Symbolic Differentiation
(Mathematica, Maple...)
4. Automatic Differentiation
(subject of this tutorial)

## Why do we need AD?

Manual Differentiation is time consuming and error prone.
Numerical Differentiation scales poorly and highly susceptible to roundoff/truncation errors.

Symbolic Differentiation 'swells' quickly as derivative expressions become very complex.

Also, both Manual and Symbolic require closed-form mathematical expression.





## What is Automatic Differentiation?

## 2 Modes of AD

$$
y=f(g(h(x)))=f\left(g\left(h\left(w_{0}\right)\right)\right)=f\left(g\left(w_{1}\right)\right)=f\left(w_{2}\right)=w_{3}
$$

$$
\frac{d y}{d x}=\frac{d y}{d w_{2}} \frac{\frac{d w_{2}}{d w_{1}}}{\frac{d w_{1}}{d x}}
$$

Forward Accumulation Mode: chain rule inside to outside

$$
d w_{1} / d x \longrightarrow d w_{2} / d x \longrightarrow d y / d x
$$

## 2 Modes of AD

$$
y=f(g(h(x)))=f\left(g\left(h\left(w_{0}\right)\right)\right)=f\left(g\left(w_{1}\right)\right)=f\left(w_{2}\right)=w_{3}
$$

$$
\frac{d y}{d x}=\operatorname{ld}^{\frac{d y}{d w_{2}}} \frac{d w_{2}}{d w_{1}} \frac{d}{d w_{1}}
$$

Reverse Accumulation Mode: chain rule outside to inside

$$
d y / d w_{2} \longrightarrow d y / d w_{1} \longrightarrow d y / d x
$$

## Exercise: Forward Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\dot{x}_{1}=1 \longrightarrow \frac{\delta y}{\delta x_{1}}
$$

## Exercise: Forward Mode

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y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
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$$
\dot{x}_{1}=1 \longrightarrow \frac{\delta y}{\delta x_{1}}
$$

| Forward Primal Trace | Forward Tangent (Derivative) Trace |
| :---: | :---: |
| $v_{-1}=x_{1} \quad=2$ | $\dot{v}_{-1}=\dot{x}_{1} \quad=1$ |
| $v_{0}=x_{2} \quad=5$ | $\dot{v}_{0}=\dot{x}_{2} \quad=0$ |
| $v_{1}=\ln v_{-1} \quad=\ln 2$ | $\dot{v}_{1}=\dot{v}_{-1} / v_{-1} \quad=1 / 2$ |

## Exercise: Forward Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
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| $v_{0}=x_{2} \quad=5$ | $\dot{v}_{0}=\dot{x}_{2} \quad=0$ |
| $\begin{array}{lll}v_{1}=\ln v_{-1} & =\ln 2 \\ v_{2}=v_{-1} \times v_{0} & =2 \times 5\end{array}$ | $\begin{array}{lll}\dot{v}_{1}=\dot{v}_{-1} / v_{-1} & =1 / 2 \\ \dot{v}_{2}=\dot{v}_{-1} \times v_{0}+\dot{v}_{0} \times v_{-1} & =1 \times 5+0 \times 2\end{array}$ |
| $\checkmark$ | $\downarrow$ |

## Exercise: Forward Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
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## Exercise: Forward Mode

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y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
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| Forward Primal Trace |  | Forward Tangent (Derivative) Trace |  |
| :---: | :---: | :---: | :---: |
| $v_{-1}=x_{1}$ | $=2$ | $\dot{v}_{-1}=\dot{x}_{1}$ | $=1$ |
| $v_{0}=x_{2}$ | $=5$ | $\dot{v}_{0}=\dot{x}_{2}$ | $=0$ |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ | $\dot{v}_{1}=\dot{v}_{-1} / v_{-1}$ | $=1 / 2$ |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ | $\dot{v}_{2}=\dot{v}_{-1} \times v_{0}+\dot{v}_{0} \times v_{-1}$ | $=1 \times 5+0 \times 2$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ | $\dot{v}_{3}=\dot{v}_{0} \times \cos v_{0}$ | $=0 \times \cos 5$ |
| $v_{4}=v_{1}+v_{2}$ | $=0.693+10$ | $\dot{v}_{4}=\dot{v}_{1}+\dot{v}_{2}$ | $=0.5+5$ |
| $\downarrow v_{5}=v_{4}-v_{3}$ | $=10.693+0.959$ | - $\dot{v}_{5}$ ? |  |

## Exercise: Forward Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\dot{x}_{1}=1 \longrightarrow \frac{\delta y}{\delta x_{1}}
$$

Forward Primal Trace

\[\)| $v_{-1}=x_{1}$ | $=2$ |
| :--- | :--- |
| $v_{0}=x_{2}$ | $=5$ |

\]

| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| :--- | :--- |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
| $v_{4}=v_{1}+v_{2}$ | $=0.693+10$ |
| $v_{5}=v_{4}-v_{3}$ | $=10.693+0.959$ |


| Forward Tangent (Derivative) |
| :--- |
| $\dot{v}_{-1}=\dot{x}_{1}$ $=1$ <br> $\dot{v}_{0}=\dot{x}_{2}$ $=0$ |
| $\dot{v}_{1}=\dot{v}_{-1} / v-1$ |
| $\dot{v}_{2}=\dot{v}_{-1} \times v_{0}+\dot{v}_{0} \times v_{-1}$ |
| $\dot{v}_{3}=\dot{v}_{0} \times \cos v_{0}$ |
| $\dot{v}_{4}=\dot{v}_{1}+\dot{v}_{2}$ |
| $\dot{v}_{5}=\dot{v}_{4}-\dot{v}_{3}$ |

## Exercise: Forward Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\dot{x}_{1}=1 \longrightarrow \frac{\delta y}{\delta x_{1}}
$$



## Forward Mode for ML?

$$
f: \mathbb{R} \rightarrow \mathbb{R}^{m}
$$

$$
\frac{\delta y_{i}}{\delta x}
$$

can be computed in one forward pass!
$f: \mathbb{R}^{n} \rightarrow \mathbb{R}$

$$
\nabla f=\left(\frac{\delta y}{\delta x_{1}}, \ldots, \frac{\delta y}{\delta x_{n}}\right)
$$

needs n forward passes!

## Functions in ML

$$
\begin{gathered}
f: \mathbb{R}^{n} \rightarrow \mathbb{R}^{m} \\
n \gg m
\end{gathered}
$$

Forward mode AD is not scalable to input dimensionality

## Functions in ML

$$
\begin{gathered}
\text { even more extreme, } \mathbf{m}=\mathbf{1} \\
\boldsymbol{F}: \mathbb{R}^{n} \rightarrow \mathbb{R} \quad F: \\
F=D \circ C \circ B \circ A \quad \mapsto \in \mathbb{R}^{n} \\
y \in \mathbb{R} \\
y=D(\boldsymbol{c}), \quad \boldsymbol{c}=C(\boldsymbol{b}), \quad \boldsymbol{b}=B(\boldsymbol{a}), \quad \boldsymbol{a}=A(\boldsymbol{x})
\end{gathered}
$$

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

$$
F^{\prime}(\boldsymbol{x})=\frac{\partial y}{\partial \boldsymbol{x}}=\left[\begin{array}{lll}
\frac{\partial y}{\partial x_{1}} & \cdots & \frac{\partial y}{\partial x_{n}}
\end{array}\right]
$$

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

$$
\left.\begin{array}{c}
y=D(\boldsymbol{c}), \quad \boldsymbol{c}=C(\boldsymbol{b}), \quad \boldsymbol{b}=B(\boldsymbol{a}), \quad \boldsymbol{a}=A(\boldsymbol{x}) \\
F^{\prime}(\boldsymbol{x})=\frac{\partial y}{\partial \boldsymbol{x}}=\left[\begin{array}{lll}
\frac{\partial y}{\partial x_{1}} & \cdots & \frac{\partial y}{\partial x_{n}}
\end{array}\right] \\
F^{\prime}(x)=\quad \frac{\partial y}{\partial \boldsymbol{c}} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}}
\end{array} \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \quad \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}\right]
$$

$$
\square
$$



Forward
accumulation

Reverse accumulation

$$
\begin{aligned}
& F^{\prime}(x)=\frac{\partial y}{\partial \boldsymbol{c}}\left(\frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}}\left(\begin{array}{ll}
\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} & \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}
\end{array}\right)\right) \\
& \underbrace{2 a} \\
& \frac{\partial \boldsymbol{b}}{\partial x}=\left[\begin{array}{ccc}
\frac{\partial b_{1}}{\partial x_{1}} & \cdots & \frac{\partial b_{1}}{\partial x_{n}} \\
\vdots & \ddots & \vdots \\
\frac{\partial b_{m}}{\partial x_{1}} & \cdots & \frac{\partial b_{m}}{\partial x_{n}}
\end{array}\right] \\
& F^{\prime}(x)=(\underbrace{\left(\frac{\partial y}{\partial \boldsymbol{c}} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}}\right.}) \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}}) \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} \\
& \frac{\partial y}{\partial \boldsymbol{b}}=\left[\begin{array}{lll}
\frac{\partial y}{\partial b_{1}} & \cdots & \frac{\partial y}{\partial b_{m}}
\end{array}\right]
\end{aligned}
$$

$$
\begin{aligned}
F^{\prime}(x) v & =\frac{\partial y}{\partial \boldsymbol{c}} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} v \\
F^{\prime}(x) v & =\frac{\partial y}{\partial \boldsymbol{c}}\left(\frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}}\left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}}\left(\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} v\right)\right)\right)
\end{aligned}
$$

Forward accumulation $\leftrightarrow$ Jacobian-vector products
Build Jacobian one column at a time

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

Forward accumulation mode differentiation


$$
\begin{aligned}
& v^{\top} F^{\prime}(x)=v^{\top} \frac{\partial y}{\partial \boldsymbol{c}} \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}} \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} \\
& \left.\left.\left.v^{\top} F^{\prime}(x)=\left(\left(\left(v^{\top} \frac{\partial y}{\partial \boldsymbol{c}}\right) \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{b}}\right) \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{a}}\right) \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}\right)\right)\right)
\end{aligned}
$$

Reverse accumulation $\leftrightarrow$ vector-Jacobian products
Build Jacobian one row at a time

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

Reverse accumulation mode differentiation


## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\delta x_{2}} \begin{gathered}
\text { both in one } \\
\text { reverse pass! }
\end{gathered}
$$

| Forward Evaluation Trace |
| :--- |
| $v_{-1}=x_{1}$ $=2$ <br> $v_{0}=x_{2}$ $=5$ <br> $v_{1}=\ln v_{-1}$ $=\ln 2$ <br> $v_{2}=v_{-1} \times v_{0}$ $=2 \times 5$ <br> $v_{3}=\sin v_{0}$ $=\sin 5$ <br> $v_{4}=v_{1}+v_{2}$ $=0.693+10$ <br> $v_{5}=v_{4}-v_{3}$ $=10.693+0.959$ <br> $y=v_{5}$ $=11.652$ |

Reverse Adjoint Trace

## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\delta x_{2}} \begin{gathered}
\text { both in one } \\
\text { reverse pass! }
\end{gathered}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ | $=2$ |
| :--- | :--- |
| $v_{0}=x_{2}$ | $=5$ |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
| $v_{4}=v_{1}+v_{2}$ | $=0.693+10$ |
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\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\delta x_{2}} \begin{gathered}
\text { both in one } \\
\text { reverse pass! }
\end{gathered}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ $=2$ <br> $v_{0}=x_{2}$ $=5$ |  |
| :--- | :--- |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
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| $y=v_{5}$ | $=11.652$ |


| Reverse Adjoint Trace |  |  |
| :--- | :--- | :--- |
|  |  |  |
|  |  |  |
|  |  |  |
| $\bar{\vartheta}_{3} ?$ | $=\bar{v}_{5} \times 1$ |  |
| $\bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}}$ | $=1$ |  |
| $\bar{v}_{5}=\bar{y}$ | $=1$ |  |

## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \quad \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\delta x_{2}} \begin{gathered}
\text { both in one } \\
\text { reverse pass! }
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$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ | $=2$ |
| :--- | :--- |
| $v_{0}=x_{2}$ | $=5$ |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
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| Reverse Adjoint Trace |  |  |
| :--- | :--- | :--- |
|  |  |  |
|  |  |  |
|  |  |  |
| $\bar{U}_{1} ?$ | $=\bar{v}_{5} \times(-1)$ | $=-1$ |
| $\bar{v}_{3}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{3}}$ | $=\bar{v}_{5} \times 1$ | $=1$ |
| $\bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}}$ | $=1$ |  |
| $\bar{v}_{5}=\bar{y}$ |  |  |

## Exercise: Reverse Mode

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\end{gathered}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ $=2$ <br> $v_{0}=x_{2}$ $=5$ |  |
| :--- | :--- |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
| $v_{4}=v_{1}+v_{2}$ | $=0.693+10$ |
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> Reverse Adjoint Trace


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Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

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\text { both in one } \\
\text { reverse pass! }
\end{gathered}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ | $=2$ |
| :--- | :--- |
| $v_{0}=x_{2}$ | $=5$ |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
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| $v_{5}=v_{4}-v_{3}$ | $=10.693+0.959$ |
| $y=v_{5}$ | $=11.652$ |

$$
\begin{array}{lll}
\text { Reverse Adjoint Trace } & \\
& \\
& \\
\\
\bar{v}_{0} ? & & \\
\bar{v}_{2}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{2}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{1}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{1}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{3}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{3}} & =\bar{v}_{5} \times(-1) & =-1 \\
\bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}} & =\bar{v}_{5} \times 1 & =1 \\
\hline \bar{v}_{5}=\bar{y} & =1 &
\end{array}
$$

## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
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\text { both in one } \\
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| $v_{0}=x_{2}$ | $=5$ |
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| $y=v_{5}$ | $=11.652$ |

$$
\begin{array}{lll}
\text { Reverse Adjoint Trace } & \\
\\
& \\
\bar{v}_{2} ? ? & & \\
\bar{v}_{0}=\bar{v}_{3} \frac{\partial v_{3}}{\partial v_{0}} & =\bar{v}_{3} \times \cos v_{0} & =-0.284 \\
\bar{v}_{2}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{2}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{1}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{1}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{3}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{3}} & =\bar{v}_{5} \times(-1) & =-1 \\
\bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}} & =\bar{v}_{5} \times 1 & =1 \\
\hline
\end{array}
$$

## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\delta x_{2}} \begin{gathered}
\text { both in one } \\
\text { reverse pass! }
\end{gathered}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ | $=2$ |
| :--- | :--- |
| $v_{0}=x_{2}$ | $=5$ |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
| $v_{4}=v_{1}+v_{2}$ | $=0.693+10$ |
| $v_{5}=v_{4}-v_{3}$ | $=10.693+0.959$ |
| $y=v_{5}$ | $=11.652$ |

$$
\begin{aligned}
& \text { Reverse Adjoint Trace } \\
& \qquad \begin{array}{lll} 
\\
\bar{v}_{0} ? & & \\
\bar{v}_{-1}=\bar{v}_{2} \frac{\partial v_{2}}{\partial v_{-1}} & =\bar{v}_{2} \times v_{0} & =5 \\
\bar{v}_{0}=\bar{v}_{3} \frac{\partial v_{3}}{\partial v_{0}} & =\bar{v}_{3} \times \cos v_{0} & =-0.284 \\
\bar{v}_{2}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{2}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{1}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{1}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{3}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{3}} & =\bar{v}_{5} \times(-1) & =-1 \\
\bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}} & =\bar{v}_{5} \times 1 & =1
\end{array}
\end{aligned}
$$

$$
\bar{v}_{5}=\bar{y} \quad=1
$$

## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\delta x_{2}} \begin{gathered}
\text { both in one } \\
\text { reverse pass! }
\end{gathered}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ | $=2$ |
| :--- | :--- |
| $v_{0}=x_{2}$ | $=5$ |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| $v_{2}=\sqrt{v_{-1} \times v_{0}}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
| $v_{4}=v_{1}+v_{2}$ | $=0.693+10$ |
| $v_{5}=v_{4}-v_{3}$ | $=10.693+0.959$ |
| $y=v_{5}$ | $=11.652$ |

$$
\begin{array}{lll}
\text { Reverse Adjoint Trace } & \\
\\
\bar{v}-1 ? & & \\
\bar{v} \text { ? } & & \\
\bar{v}_{0}=\bar{v}_{0}+\bar{v}_{2} \frac{\partial v_{2}}{\partial v_{0}} & =\bar{v}_{0}+\bar{v}_{2} \times v_{-1} & =1.716 \\
\bar{v}_{-1}=\bar{v}_{2} \frac{\partial v_{2}}{\partial v_{-1}} & =\bar{v}_{2} \times v_{0} & =5 \\
\bar{v}_{0}=\bar{v}_{3} \frac{\partial v_{3}}{\partial v_{0}} & =\bar{v}_{3} \times \cos v_{0} & =-0.284 \\
\bar{v}_{2}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{2}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{1}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{1}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{3}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{3}} & =\bar{v}_{5} \times(-1) & =-1 \\
\bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}} & =\bar{v}_{5} \times 1 & =1 \\
\hline
\end{array}
$$

$$
y=v_{5} \quad=11.652
$$

$$
\bar{v}_{5}=\bar{y} \quad=1
$$

## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\delta x_{2}} \begin{gathered}
\text { both in one } \\
\text { reverse pass! }
\end{gathered}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ $=2$ <br> $v_{0}=x_{2}$ $=5$ <br> $v_{1}=\ln v_{-1}$ $=\ln 2$ <br> $v_{2}=v_{-1} \times v_{0}$ $=2 \times 5$ <br> $v_{3}=\sin v_{0}$ $=\sin 5$ <br> $v_{4}=v_{1}+v_{2}$ $=0.693+10$ <br> $v_{5}=v_{4}-v_{3}$ $=10.693+0.959$ <br> $y=v_{5}$ $=11.652$ |
| :--- | :--- |$.$

$$
y=v_{5}
$$

$$
\bar{v}_{5}=\bar{y}
$$

$$
=1
$$

$$
\begin{aligned}
& \text { Reverse Adjoint Trace } \\
& \begin{cases} \\
\bar{v}_{-1}=\bar{v}_{-1}+\bar{v}_{1} \frac{\partial v_{1}}{\partial v_{-1}}=\bar{v}_{-1}+\bar{v}_{1} / v_{-1} & =5.5 \\
\bar{v}_{0}=\bar{v}_{0}+\bar{v}_{2} & =v_{2}\end{cases} \\
& \bar{v}_{0}=\bar{v}_{0}+\bar{v}_{2} \frac{\partial v_{2}}{\partial v_{0}}=\bar{v}_{0}+\bar{v}_{2} \times v_{-1}=1.716 \\
& \bar{v}_{-1}=\bar{v}_{2} \frac{\partial v_{2}}{\partial v_{-1}} \\
& =\bar{v}_{2} \times v \\
& =5 \\
& \bar{v}_{0}=\bar{v}_{3} \frac{\partial v_{3}}{\partial v_{0}} \quad=\bar{v}_{3} \times \cos v_{0} \quad=-0.284 \\
& \bar{v}_{2}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{2}} \\
& =\bar{v}_{4} \times \\
& =1 \\
& \bar{v}_{1}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{1}} \\
& =\bar{v}_{4} \times 1 \quad=1 \\
& \bar{v}_{3}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{3}} \\
& =\bar{v}_{5} \times(-1) \\
& =-1 \\
& \bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}} \quad=\bar{v}_{5} \times 1 \quad=1
\end{aligned}
$$

## Exercise: Reverse Mode

$$
y=f\left(x_{1}, x_{2}\right)=\ln \left(x_{1}\right)+x_{1} x_{2}-\sin \left(x_{2}\right)
$$

Solve at point $\left(x_{1}, x_{2}\right)=(2,5)$

$$
\bar{y}=\frac{\delta y}{\delta y}=1 \quad \longrightarrow \frac{\delta y}{\delta x_{1}}, \frac{\delta y}{\left(\overline{x_{1}}\right)} \frac{\begin{array}{c}
\text { both in one } \\
\text { reverse pass! }
\end{array}}{\delta\left(\bar{x}_{2}\right)}
$$

Forward Evaluation Trace

| $v_{-1}=x_{1}$ | $=2$ |
| :--- | :--- |
| $v_{0}=x_{2}$ | $=5$ |
| $v_{1}=\ln v_{-1}$ | $=\ln 2$ |
| $v_{2}=v_{-1} \times v_{0}$ | $=2 \times 5$ |
| $v_{3}=\sin v_{0}$ | $=\sin 5$ |
| $v_{4}=v_{1}+v_{2}$ | $=0.693+10$ |
| $v_{5}=v_{4}-v_{3}$ | $=10.693+0.959$ |

Reverse Adjoint Trace

$$
\left\{\begin{array}{lll}
\overline{\boldsymbol{x}}_{1}=\overline{\boldsymbol{v}}_{-\mathbf{1}} & =\mathbf{5 . 5} \\
\overline{\boldsymbol{x}}_{\mathbf{2}}=\overline{\boldsymbol{v}}_{0} & =\mathbf{1 . 7 1 6} \\
\hline \bar{v}_{-1}=\bar{v}_{-1}+\bar{v}_{1} \frac{\partial v_{1}}{\partial v_{-1}} & =\bar{v}_{-1}+\bar{v}_{1} / v_{-1} & =5.5 \\
\bar{v}_{0}=\bar{v}_{0}+\bar{v}_{2} \frac{\partial v_{2}}{\partial v_{0}} & =\bar{v}_{0}+\bar{v}_{2} \times v_{-1} & =1.716 \\
\bar{v}_{-1}=\bar{v}_{2} \frac{\partial v_{2}}{\partial v_{-1}} & =\bar{v}_{2} \times v_{0} & =5 \\
\bar{v}_{0}=\bar{v}_{3} \frac{\partial v_{3}}{\partial v_{0}} & =\bar{v}_{3} \times \cos v_{0} & =-0.284 \\
\bar{v}_{2}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{2}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{1}=\bar{v}_{4} \frac{\partial v_{4}}{\partial v_{1}} & =\bar{v}_{4} \times 1 & =1 \\
\bar{v}_{3}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{3}} & =\bar{v}_{5} \times(-1) & =-1 \\
\bar{v}_{4}=\bar{v}_{5} \frac{\partial v_{5}}{\partial v_{4}} & =\bar{v}_{5} \times 1 & =1 \\
\hline \bar{v}_{5}=\bar{y} & =1 &
\end{array}\right.
$$

## Backpropagation is a special case of Reverse Mode AD

(a) Forward pass

(b) Backward pass

