Most materials in the discussion here follow from the paper (Baydin et al., 2018)

Derivative Calculation I

- From Baydin et al. (2018) there are four types of methods
  - Deriving the explicit form
    Example: consider

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

    We calculate

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = \frac{1}{x_1} + x_2$$

Derivative Calculation II

- Numerical way by finite difference

  $$\frac{f(x+h)-f(x)}{h}$$

  with a small h
- Symbolic way: using tools to get an explicit form
- Automatic differentiation (AD): topic of this set of slides

- Back-propagation is a special case of automatic differentiation

Derivative Calculation III

- So you can roughly guess that in automatic differentiation, chain rules are repeated applied

Forward Mode of AD I

- Consider the function

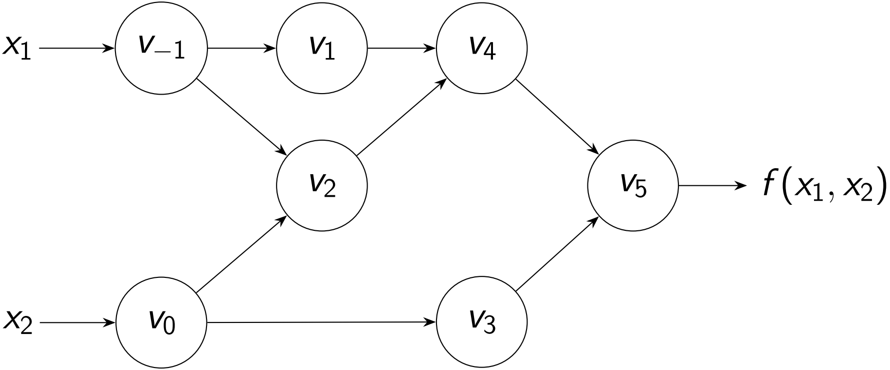
$$f(x_1, x_2) = \ln x_1 + x_1 x_2 - \sin x_2$$

- Forward mode to compute the function value

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

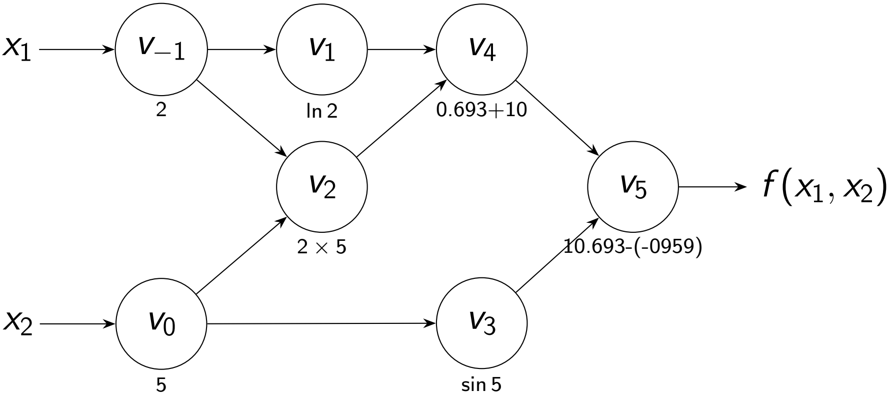
Forward Mode of AD II

- See also the computational graph



Forward Mode of AD III

- Example of Forward Primal Trace (to be discussed)



Forward Mode of AD IV

- Each v_i comes from a simple operation
- For computing
$$\frac{\partial f}{\partial x_1}$$
  we let
$$\dot{v}_i = \frac{\partial v_i}{\partial x_1}$$
  and apply the chain rule
- Forward derivative calculation:

Forward Mode of AD V

$$
\begin{array}{lll}
\dot{v}_{-1} & = \dot{x}_1 & = 1 \\
\dot{v}_0 & = \dot{x}_2 & = 0 \\
\hline
\dot{v}_1 & = \dot{v}_{-1}/v_{-1} & = 1/2 \\
\dot{v}_2 & = \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1} & = 1 \times 5 + 0 \times 2 \\
\dot{v}_3 & = \dot{v}_0 \times \cos v_0 & = 0 \times \cos 5 \\
\dot{v}_4 & = \dot{v}_1 + \dot{v}_2 & = 0.5 + 5 \\
\dot{v}_5 & = \dot{v}_4 - \dot{v}_3 & = 5.5 - 0 \\
\hline
\dot{y} & = \dot{v}_5 & = 5.5
\end{array}
$$

Forward Mode of AD VI

- For example,

$$
\begin{aligned}
v_1 &= \ln v_{-1} \\
\frac{\partial v_1}{\partial x_1} &= \frac{1}{v_{-1}} \times \frac{\partial v_{-1}}{\partial x_1} \\
&= \frac{\dot{v}_{-1}}{v_{-1}}
\end{aligned}
$$

Jacobian Calculation by Forward Mode I

- Consider

$$f : R^n \rightarrow R^m$$

so that

$$\begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} = f(x_1, \ldots, x_n)$$

- The Jacobian is

$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ & \ddots & \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

Jacobian Calculation by Forward Mode II

- If we initialize

$$\dot{x} = [\underbrace{0, \ldots, 0}_{i-1}, 1, 0, \ldots, 0]^T$$

then

$$\begin{bmatrix} \frac{\partial y_1}{\partial x_i} \\ \vdots \\ \frac{\partial y_m}{\partial x_i} \end{bmatrix}$$

can be calculated in one forward pass

Jacobian Calculation by Forward Mode III

- But this means we need n forward passes for the whole Jacobian
- In many optimization methods we do not need the whole Jacobian. Instead we need

  Jacobian-vector products

- That is,

$$J\boldsymbol{r} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ & \ddots & \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix} \begin{bmatrix} r_1 \\ \vdots \\ r_n \end{bmatrix}$$

Jacobian Calculation by Forward Mode IV

- This can be calculated in one pass by initializing with $\dot{\boldsymbol{x}} = \boldsymbol{r}$
- Now $\dot{v}_i$ is changed from

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

to

$$\dot{v}_i = \frac{\partial v_i}{\partial x_1} r_1 + \cdots + \frac{\partial v_i}{\partial x_n} r_n$$

Jacobian Calculation by Forward Mode V

- For example, if

$$v_2 = v_{-1} \times v_0,$$

then we still have

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

- We will see examples of using Jacobian-vector products later in discussing Newton methods

Jacobian Calculation by Forward Mode VI

- The discussion shows that the forward mode is efficient for

$$f : R \to R^m$$

  by one pass
- But for the other extreme

$$f : R^n \to R,$$

  to calculate the gradient

$$\nabla f = \begin{bmatrix} \frac{\partial y}{\partial x_1} & \cdots & \frac{\partial y}{\partial x_n} \end{bmatrix}^T$$

  we need n passes

Jacobian Calculation by Forward Mode VII

- This is not efficient
- Subsequently we will consider another way for AD: reverse mode

References I

A. G. Baydin, B. A. Pearlmutter, A. A. Radul, and J. M. Siskind. Automatic differentiation in machine learning: a survey. *Journal of Machine Learning Research*, 18(153):1–43, 2018.

Acknowledgments

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