CS6216 Advanced Topics in Machine Learning (Systems)

Automatic Differentiation

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Paper reading & discussion

TensorFlow: A System for Large-Scale Machine Learning   OSDI 2016

- What are TensorFlow's core design principles? What are the pros & cons of using dataflow graphs?
- How to evaluate the proposed system?

Discuss in groups & submit your answers **with names.**

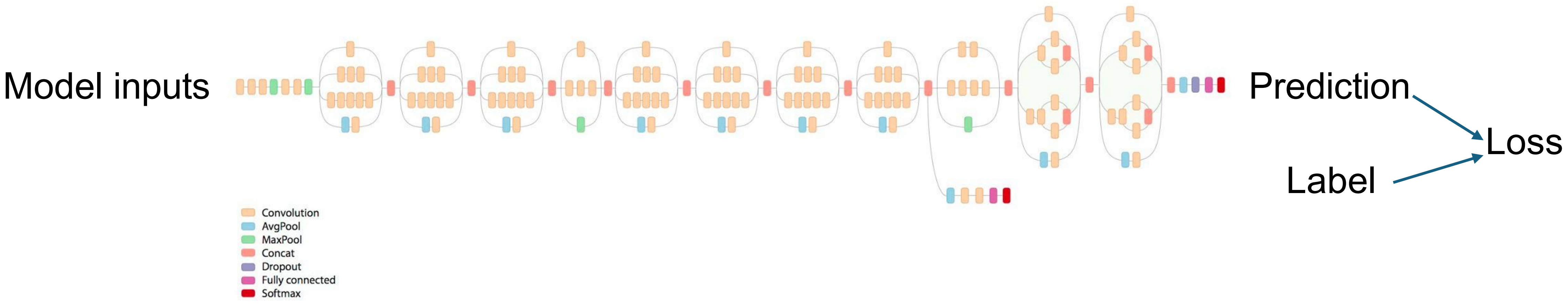
pe.app/yaolu1

Recap: algorithmic workflows

Stochastic Gradient Descent (SGD)

Train ML models through many iterations of 3 stages

1. **Forward propagation**: apply model to a batch of input samples and run calculation through operators to produce a prediction
2. **Backward propagation**: run the model in reverse to produce partial gradients / errors for each trainable weight
3. **Weight update**: use the loss value to update model weights $w \leftarrow w - \eta \nabla_w L(w)$



Ways to compute gradients

- Numerical differentiation
- Symbolic differentiation
- Forward mode automatic differentiation
- Backward mode automatic differentiation

Numerical Differentiation

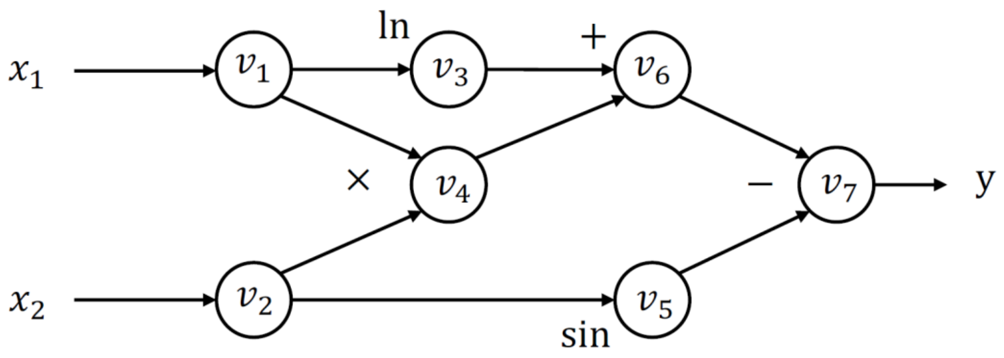
- Directly compute the partial gradient by symbolic definitions

$$\frac{\partial f(\theta)}{\partial \theta_i} = \lim_{\epsilon \to 0} \frac{f(\theta + \epsilon e_i) - f(\theta)}{\epsilon}$$

⇒Hard to work correctly due to precision / numerical errors

Recap: compute graph

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



- Each node represents an (intermediate) value in the computation. Edges present input/output relations.

Forward propagation steps

$v_1 = x_1 = 2$

$v_2 = x_2 = 5$

$v_3 =$

$v_4 =$

$v_5 =$

$v_6 =$

$v_7 =$

$y =$

Recap: compute graph

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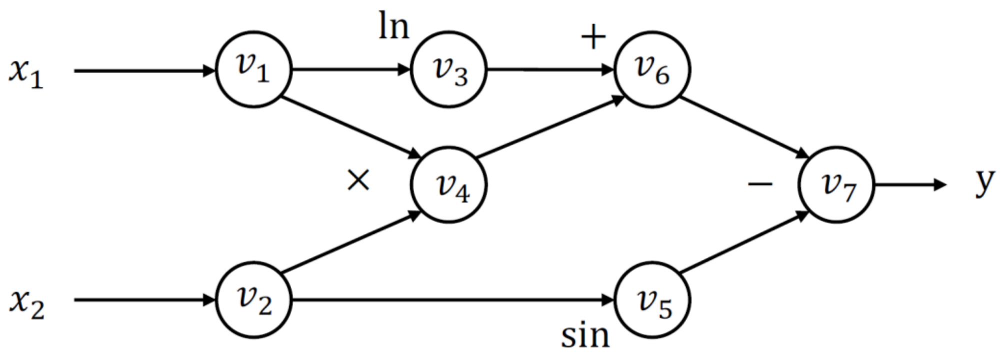


- Each node represents an (intermediate) value in the computation. Edges present input/output relations.

Forward propagation steps

$v_1 = x_1 = 2$

$v_2 = x_2 = 5$

$v_3 = \ln v_1 = \ln 2 = 0.692$

$v_4 = v_1 \times v_2 = 10$

$v_5 = \sin v_2 = \sin 5 = -0.959$

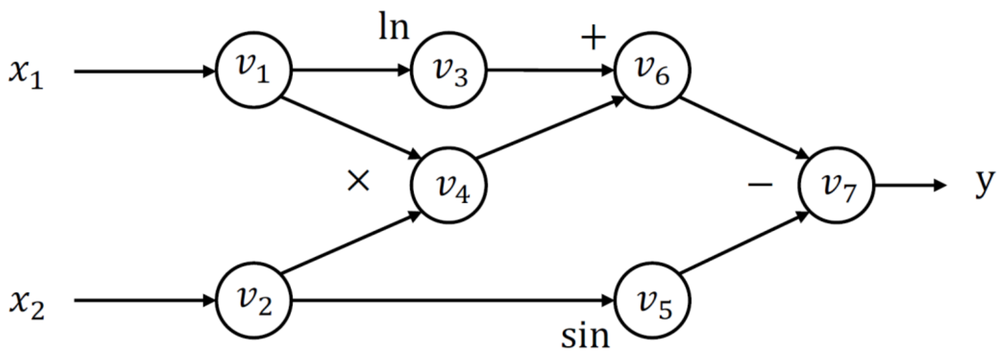
$v_6 = v_3 + v_4 = 10.693$

$v_7 = v_6 - v_5 = 11.652$

$y = v_7 = 11.652$

Forward Mode Automatic Differentiation (AutoDiff)

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



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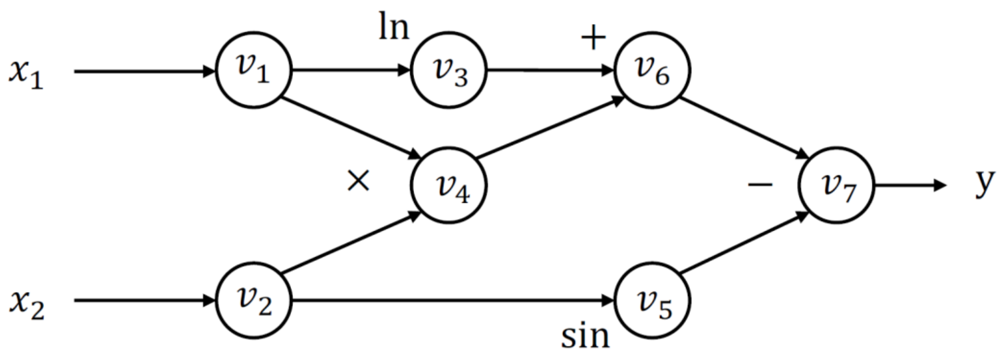
- Tweak the input and watch how the output changes

- **How much do you have?**
- **$100?**
- **$50?**

- **Guess**
- **Too much**
- **Too few**

Forward Mode Automatic Differentiation (AutoDiff)

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



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$y = v_7 = 11.652$

Let $\Delta v_i = \frac{\partial v_i}{\partial x_1}$,

we can compute Δv_i by tweaking the inputs and perform forward propagation:

$\Delta v_1 = 1$

$\Delta v_2 = 0$

$\Delta v_3 =$

$\Delta v_4 =$

$\Delta v_5 =$

$\Delta v_6 =$

$\Delta v_7 =$

$$\frac{\partial y}{\partial x_1} =$$

Forward Mode Automatic Differentiation (AutoDiff)

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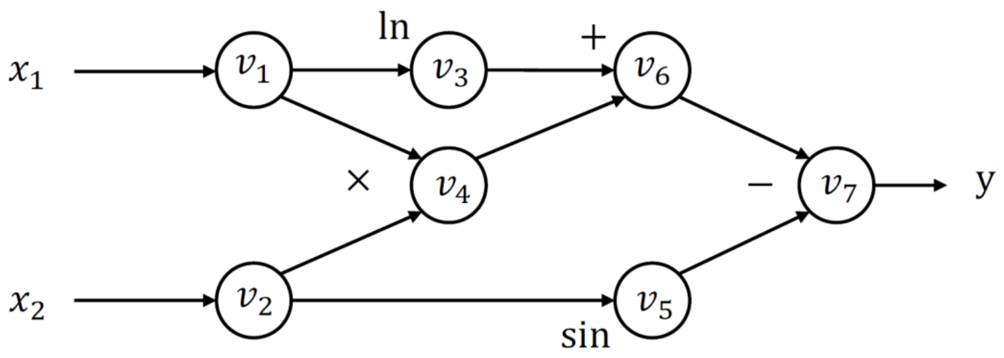

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Let $\Delta v_i = \frac{\partial v_i}{\partial x_1}$,

we can compute Δv_i by tweaking the inputs and perform forward propagation:

$\Delta v_1 = 1$

$\Delta v_2 = 0$

$$\Delta v_3 = \frac{\Delta v_1}{v_1} = 0.5$$

$\Delta v_4 = \Delta v_1 v_2 + \Delta v_2 v_1 = 1 \times 5 + 0 \times 2 = 5$

$\Delta v_5 = \Delta v_2 \cos v_2 = 0 \times \cos 5 = 0$

$\Delta v_6 = \Delta v_3 + \Delta v_4 = 0.5 + 5 = 5.5$

$\Delta v_7 = \Delta v_6 - \Delta v_5 = 5.5 - 0 = 5.5$

$$\frac{\partial y}{\partial x_1} = \Delta v_7 = 5.5$$

Forward Mode Automatic Differentiation (AutoDiff)

- However, each input x_i needs a whole forward propagation.
- Pros & Cons?

⇒Very expensive

⇒Hard to set proper Δx, know Δy only

⇒Often used to check the correctness of coding

Symbolic Differentiation

- Use the model formula to derive gradients by sum, product and chain rules
  - $\frac{\partial\left(f(\theta)+g(\theta)\right)}{\partial(\theta)} =$
  - $\frac{\partial\left(f(\theta)g(\theta)\right)}{\partial(\theta)} =$
  - $\frac{\partial f(g(\theta))}{\partial(\theta)} =$

$\Rightarrow$ Lots of repeated compute: $f(\theta) = \prod_{i=1}^{n} \theta_i$, $\frac{f(\theta)}{\partial \theta_k} = \prod_{j \neq k}^{n} \theta_j$

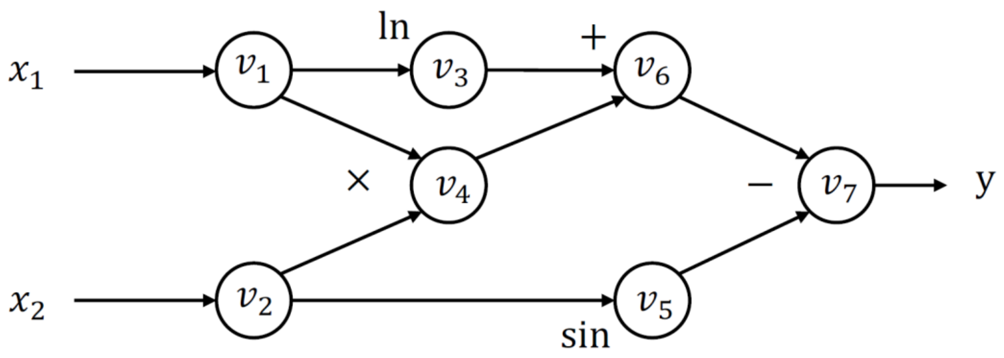
Symbolic Differentiation

- Use the model formula to derive gradients by sum, product and chain rules
  - $\frac{\partial(f(\theta)+g(\theta))}{\partial(\theta)} = \frac{\partial f(\theta)}{\partial\theta} + \frac{\partial g(\theta)}{\partial\theta}$
  - $\frac{\partial(f(\theta)g(\theta))}{\partial(\theta)} = g(\theta) \times \frac{\partial f(\theta)}{\partial\theta} + f(\theta) \times \frac{\partial g(\theta)}{\partial\theta}$
  - $\frac{\partial f(g(\theta))}{\partial(\theta)} = \frac{\partial f(g(\theta))}{\partial g(\theta)} \times \frac{\partial g(\theta)}{\partial\theta}$

$\Rightarrow$ Lots of repeated compute: $f(\theta) = \prod_{i=1}^{n} \theta_i$, $\frac{f(\theta)}{\partial\theta_k} = \prod_{j\neq k}^{n} \theta_j$

Reverse Mode Automatic Differentiation (AutoDiff)

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



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Let $\Delta v_i = \frac{\partial y}{\partial v_i}$,

we can compute Δv_i in a reverse order of the graph

$\Delta v_7 = \frac{\partial y}{\partial v_7} = 1$

$\Delta v_6 =$

$\Delta v_5 =$

$\Delta v_4 =$

$\Delta v_3 =$

$\Delta v_2 =$

$\Delta v_1 =$

Reverse Mode Automatic Differentiation (AutoDiff)

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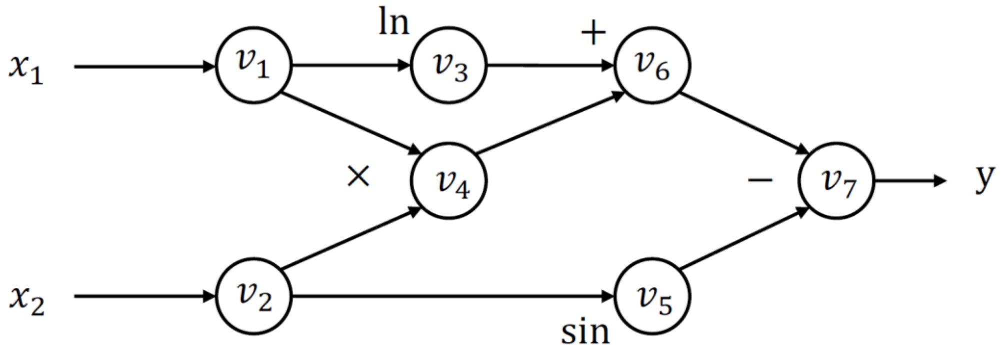

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Let $\Delta v_i = \frac{\partial y}{\partial v_i}$,

we can compute Δv_i in a reverse order of the graph

$$\Delta v_7 = \frac{\partial y}{\partial v_7} = 1$$

$$\Delta v_6 = \Delta v_7 \times \frac{\partial v_7}{\partial v_6} = \Delta v_7 \times 1 = 1$$

$$\Delta v_5 = \Delta v_7 \times \frac{\partial v_7}{\partial v_5} = \Delta v_7 \times (-1) = -1$$

$$\Delta v_4 = \Delta v_6 \times \frac{\partial v_6}{\partial v_4} = \Delta v_6 \times 1 = 1$$

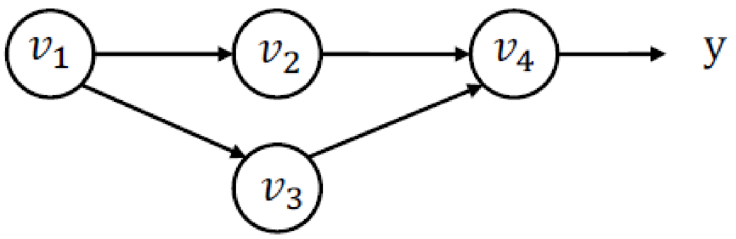
$$\Delta v_3 = \Delta v_6 \times \frac{\partial v_6}{\partial v_3} = \Delta v_6 \times 1 = 1$$

$$\Delta v_2 = \Delta v_5 \times \frac{\partial v_5}{\partial v_2} + \Delta v_4 \times \frac{\partial v_4}{\partial v_2} = \Delta v_5 \times \cos v_2 + \Delta v_4 \times v_1 = -\cos 5 + 2$$

$$\Delta v_1 = \Delta v_4 \times \frac{\partial v_4}{\partial v_1} + \Delta v_3 \times \frac{\partial v_3}{\partial v_1} = \Delta v_4 \times v_2 + \Delta v_3 \times \frac{1}{v_1} = 5 + \frac{1}{2} = 5.5$$

Derivation for branches

- In reverse model AutoDiff, gradients are summed up from branches



$$\Delta v_1 = \frac{\partial y}{\partial v_1} = \frac{\partial f(v_2, v_3)}{\partial v_2} \times \frac{\partial v_2}{\partial v_1} + \frac{\partial f(v_2, v_3)}{\partial v_3} \times \frac{\partial v_3}{\partial v_1}$$
$$= \Delta v_2 \times \frac{\partial v_2}{\partial v_1} + \Delta v_3 \times \frac{\partial v_3}{\partial v_1}$$

- Define partial adjoint $\Delta v_{i \to j} = \Delta v_j \times \frac{\partial v_j}{\partial v_i}$ for each pair of adjacent node i, j

- Then for a node with multiple outbound pathways,

$$\Delta v_i = \sum_{j \in \text{adj}(i)} \Delta v_{i \to j}$$

We can compute partial adjoints, and then sum them together.

Reverse Model AutoDiff Algorithm

```
def gradient(out):
  node_to_grad = {out: [1]}
  for i in reverse_topo_order(out):
    Δv_i = Σ_j Δv_{i→j} = sum(node_to_grad[i])
    for k ∈ inputs(i):
        compute Δv_{k→i} = Δv_i ∂v_i/∂v_k
        append Δv_{k→i} to node_to_grad[k]
  return adjoint of input Δv_input
```

Reverse Model AutoDiff Algorithm

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```

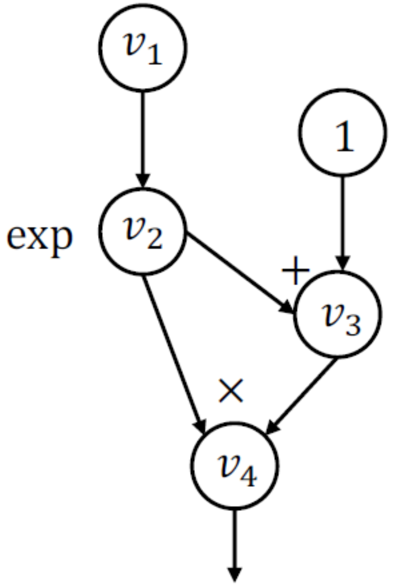
out: dictionary to record a list of partial adjoints for each node

Propagates partial adjoint to its input node

Key is to compute the adjoint values for each node and construct the graph on the fly.

Reverse Model AutoDiff Algorithm

def gradient(out):
  node_to_grad = {out: [1]}
  for i in reverse_topo_order(out):
    $\Delta v_i = \sum_j \Delta v_{i \to j}$ = sum(node_to_grad[i])
    for $k \in inputs(i)$:
      compute $\Delta v_{k \to i} = \Delta v_i \dfrac{\partial v_i}{\partial v_k}$
      append $\Delta v_{k \to i}$ to node_to_grad[k]
    return adjoint of input Δv_{input}



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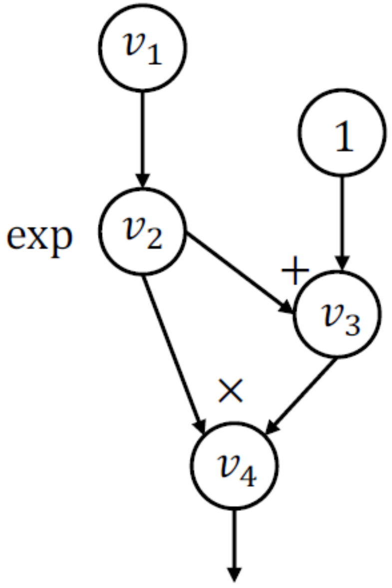
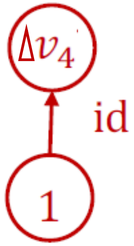
      append $\Delta v_{k \to i}$ to node_to_grad[k]
  return adjoint of input Δv_{input}

$i = 4$
node_to_grad: {
  4: [Δv_4]
}





id = identity function

Reverse Model AutoDiff Algorithm

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```
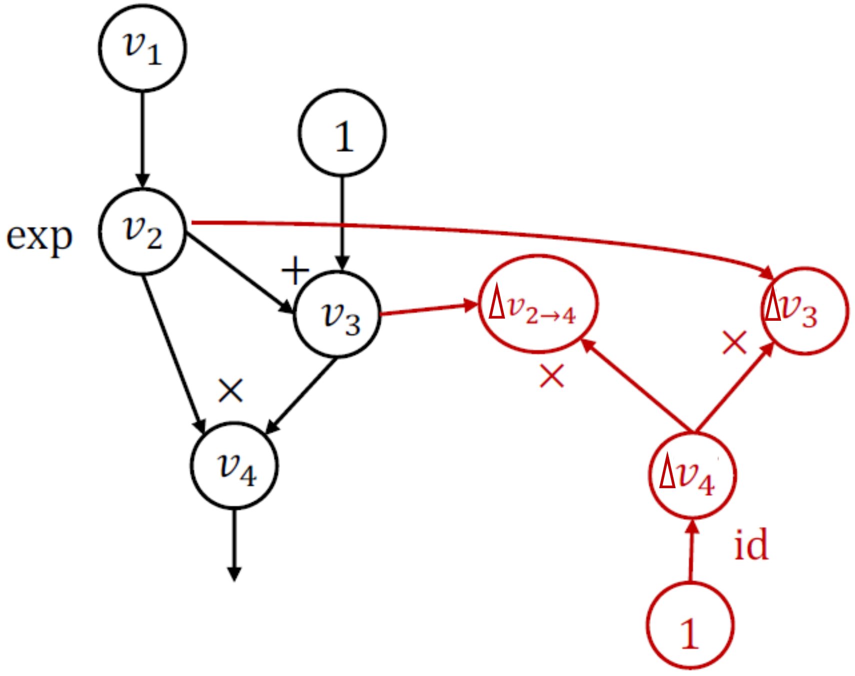

$i = 4$

node_to_grad: {
  2: [$\Delta v_{2\to 4}$]
  3: [Δv_3]
  4: [Δv_4]
}



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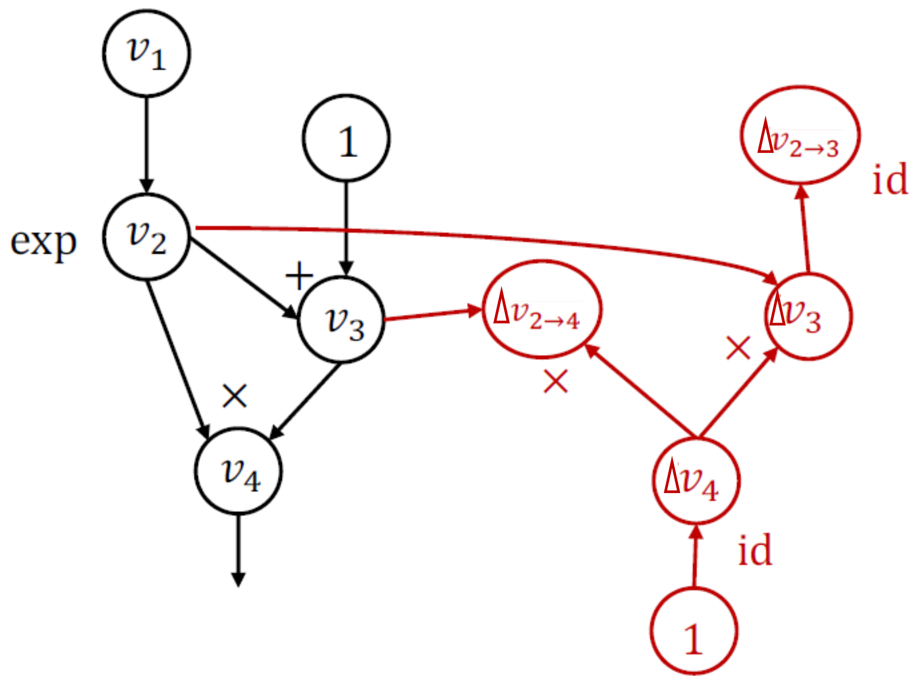
  return adjoint of input Δv_input
```

$i = 3$

```
node_to_grad: {
  2: [Δv_{2→4}, Δv_{2→3}]
  3: [Δv_3]
  4: [Δv_4]
}
```



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Reverse Model AutoDiff Algorithm

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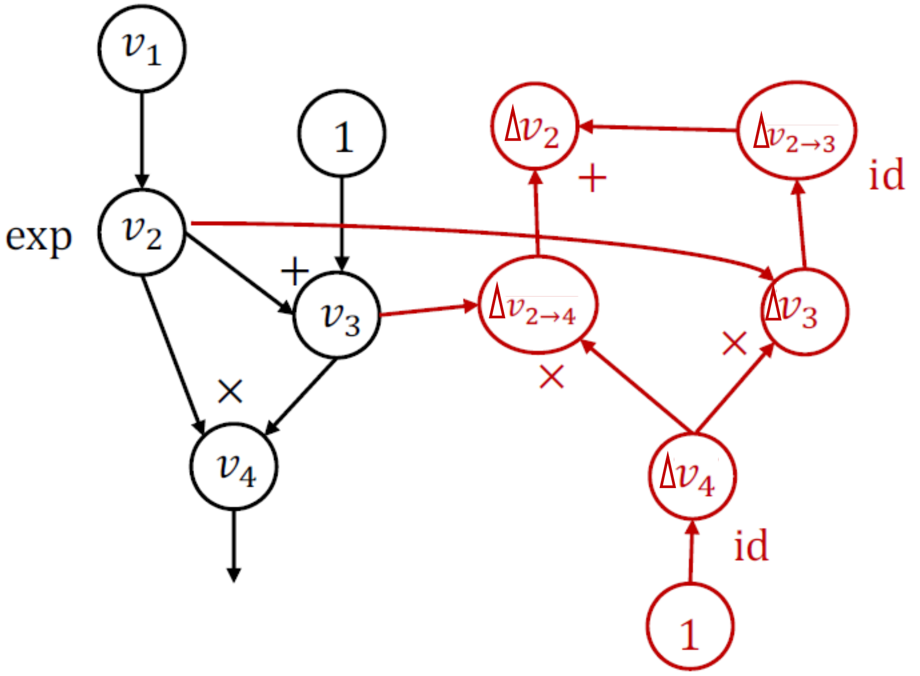

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```
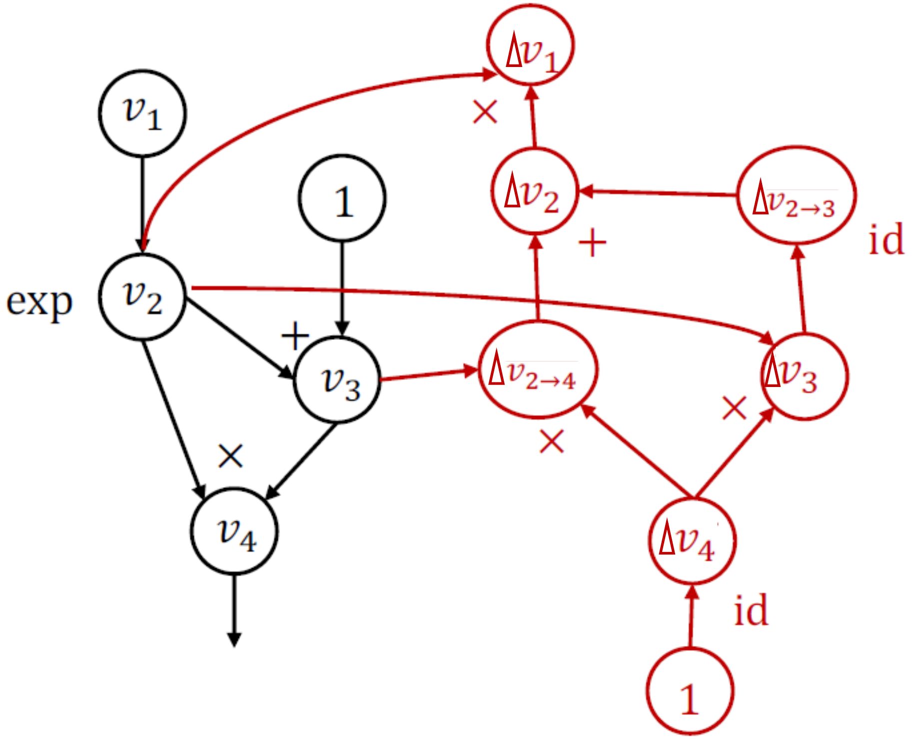

```
i = 2
node_to_grad: {
  1: [Δv_1]
  2: [Δv_{2→4}, Δv_{2→3}]
  3: [Δv_3]
  4: [Δv_4]
}
```



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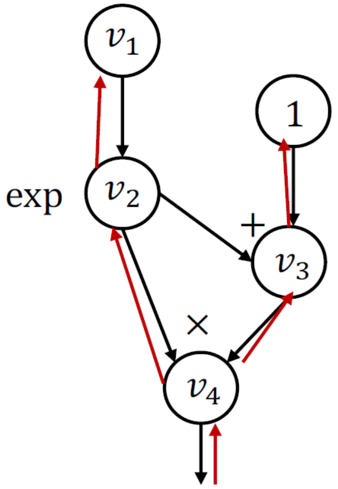
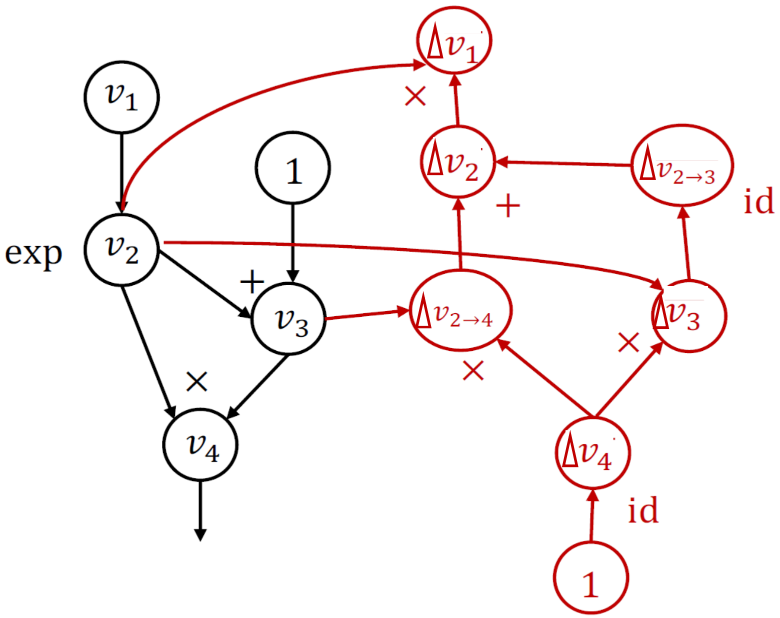
Compute in-place vs. Reverse Model AutoDiff

Compute in-place



- Run backprop on the forward graph
- Used in earlier frameworks (caffe etc.)

Reverse mode AutoDiff w/ compute graph



- Construct separate graph nodes for adjoints
- Used in modern frameworks (Pytorch etc.)

Ways to compute gradients

	Pros	Cons
Numerical differentiation		
Symbolic differentiation		
Forward model AutoDiff		
Backward model AutoDiff		

Ways to compute gradients

	Pros	Cons
Numerical differentiation	Intuitive & easy to compute	Numerical error
Symbolic differentiation		Repeated compute
Forward model AutoDiff		Repeated compute
Backward model AutoDiff	Scalable & saves compute	Memory consumption

Paper reading & discussion

[Why Deep Learning Models Run Faster on GPUs: A Brief Introduction to CUDA Programming]

[NVIDIA Blackwell Architecture Technical Brief - Built for the Age of AI Reasoning]