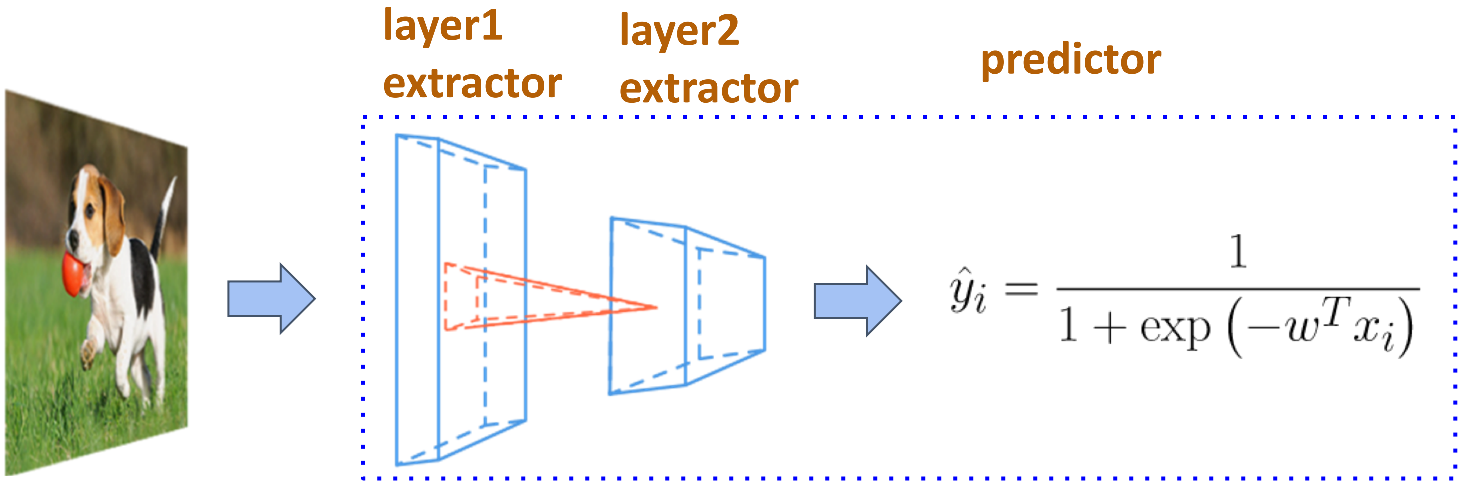
Lecture 4: Backpropagation and Automatic Differentiation

CSE599W: Spring 2018

Announcement

- Assignment 1 is out today, due in 2 weeks (Apr 19th, 5pm)

Model Training Overview



$$\hat{y}_i = \frac{1}{1+\exp\left(-w^T x_i\right)}$$

Objective $$L(w) = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \lambda \|w\|^2$$

Training $$w \leftarrow w - \boxed{\eta \nabla_w L(w)}$$

Symbolic Differentiation

- Input formulae is a symbolic expression tree (computation graph).
- Implement differentiation rules, e.g., sum rule, product rule, chain rule

$$\frac{d(f+g)}{dx} = \frac{df}{dx} + \frac{dg}{dx} \qquad \frac{d(fg)}{dx} = \frac{df}{dx}g + f\frac{dg}{dx} \qquad \frac{d\big(h(x)\big)}{dx} = \frac{df\big(g(x)\big)}{dx} \cdot \frac{dg(x)}{x}$$

✗ For complicated functions, the resultant expression can be exponentially large.

✗ Wasteful to keep around intermediate symbolic expressions if we only need a numeric value of the gradient in the end

✗ Prone to error

Numerical Differentiation

- We can approximate the gradient using

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e_i}) - f(\boldsymbol{x})}{h}$$

$$f(W, x) = \qquad W \qquad \cdot \qquad x$$

$$\begin{bmatrix} -0.8 & 0.3 \end{bmatrix} \cdot \begin{bmatrix} 0.5 \\ -0.2 \end{bmatrix}$$

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$$f(W, x) = \quad W \quad \cdot \quad x \qquad\qquad f(W, x) = \quad W \quad \cdot \quad x$$

$$\begin{bmatrix} -0.8 & 0.3 \end{bmatrix} \cdot \begin{bmatrix} 0.5 \\ -0.2 \end{bmatrix} \qquad\qquad \begin{bmatrix} -0.8 + \varepsilon & 0.3 \end{bmatrix} \cdot \begin{bmatrix} 0.5 \\ -0.2 \end{bmatrix}$$

Numerical Differentiation

- We can approximate the gradient using

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e_i}) - f(\boldsymbol{x})}{h}$$

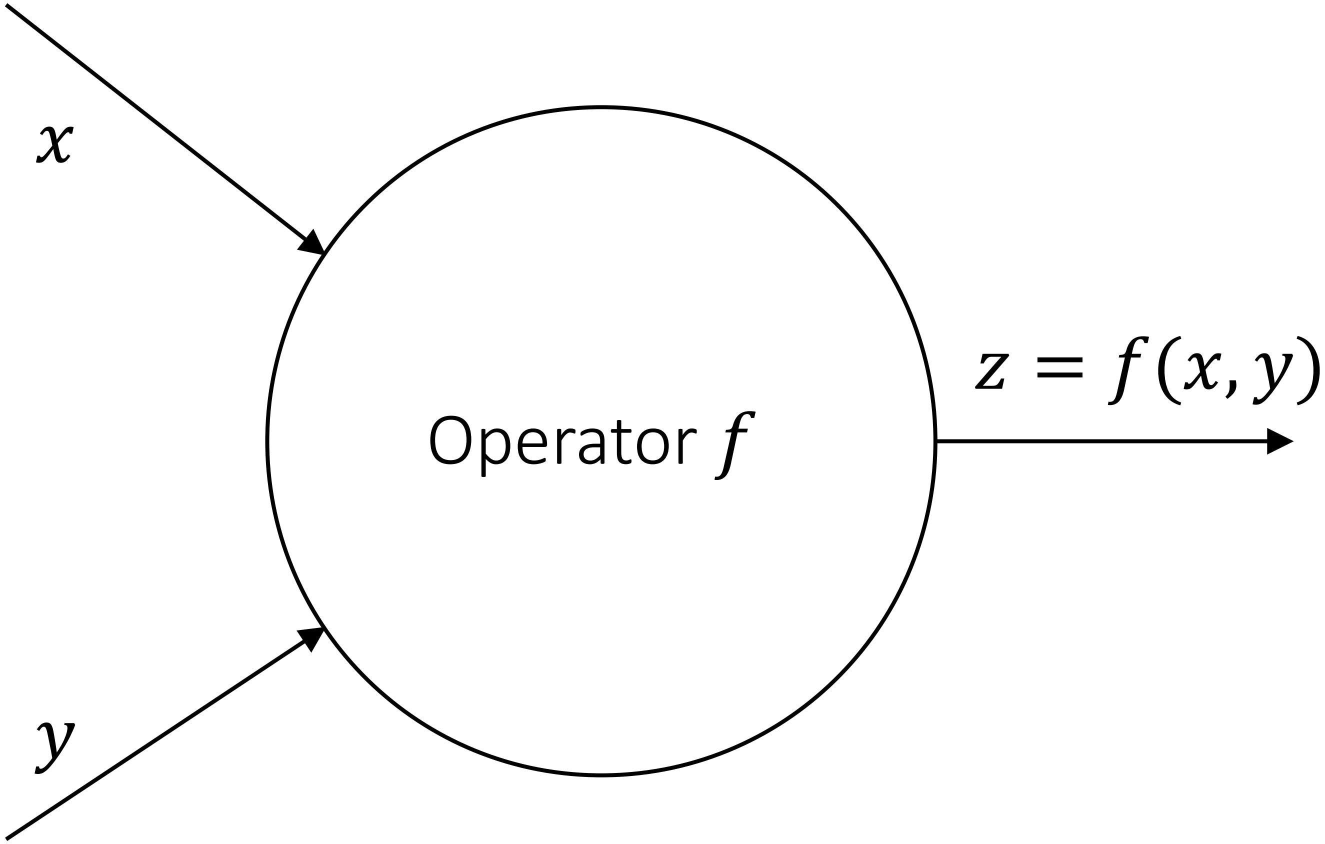
- Reduce the truncation error by using center difference

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e_i}) - f(\boldsymbol{x} - h\boldsymbol{e_i})}{2h}$$

✗ Bad: rounding error, and slow to compute

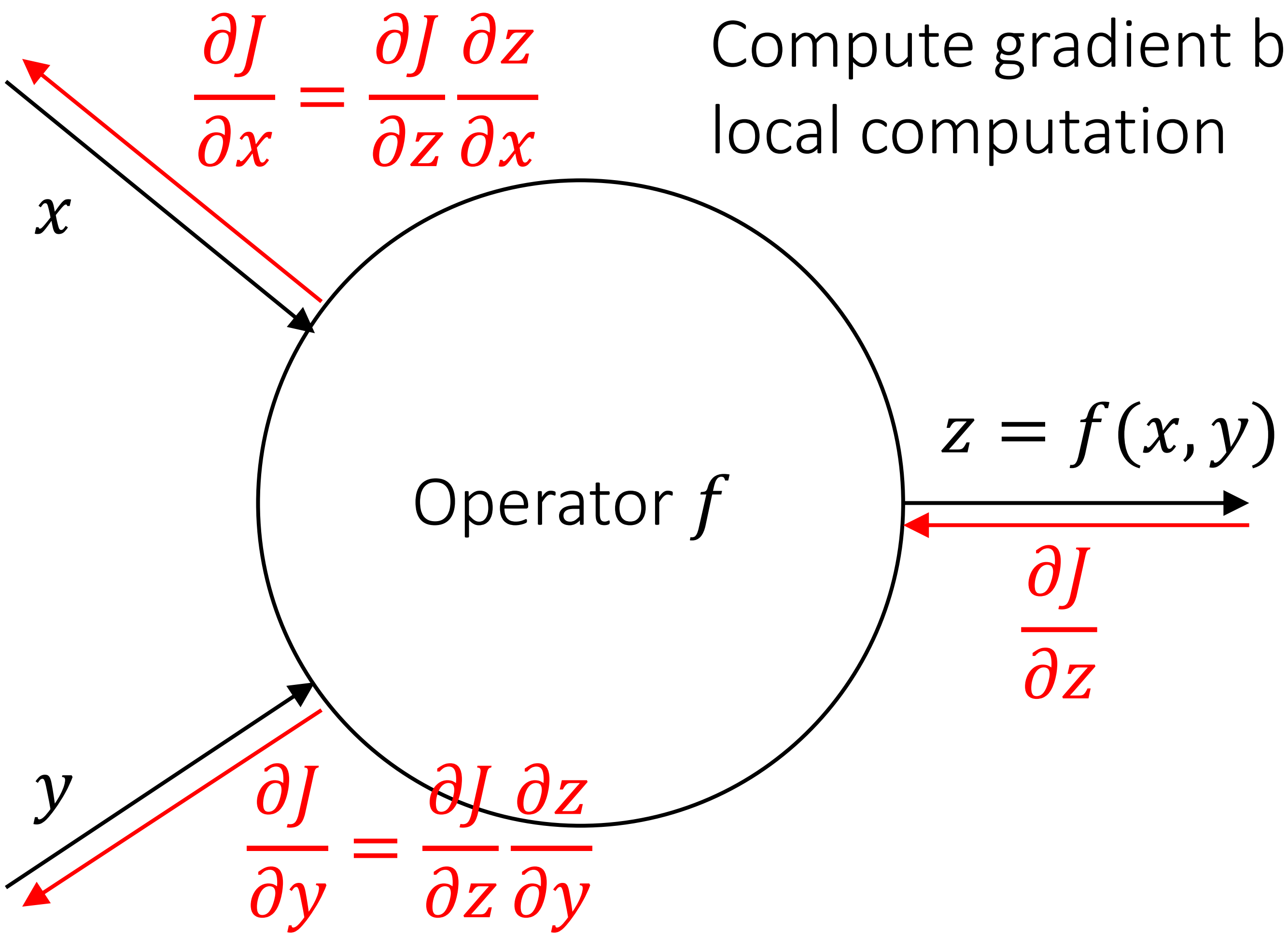
✓ A powerful tool to check the correctness of implementation, usually use h = 1e-6.

Backpropagation



Backpropagation

Compute gradient becomes local computation



$\frac{\partial J}{\partial x} = \frac{\partial J}{\partial z}\frac{\partial z}{\partial x}$
x
Operator f
$z = f(x, y)$
$\frac{\partial J}{\partial z}$
y
$\frac{\partial J}{\partial y} = \frac{\partial J}{\partial z}\frac{\partial z}{\partial y}$

Backpropagation simple example

$$f = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + w_2 x_2)}}$$

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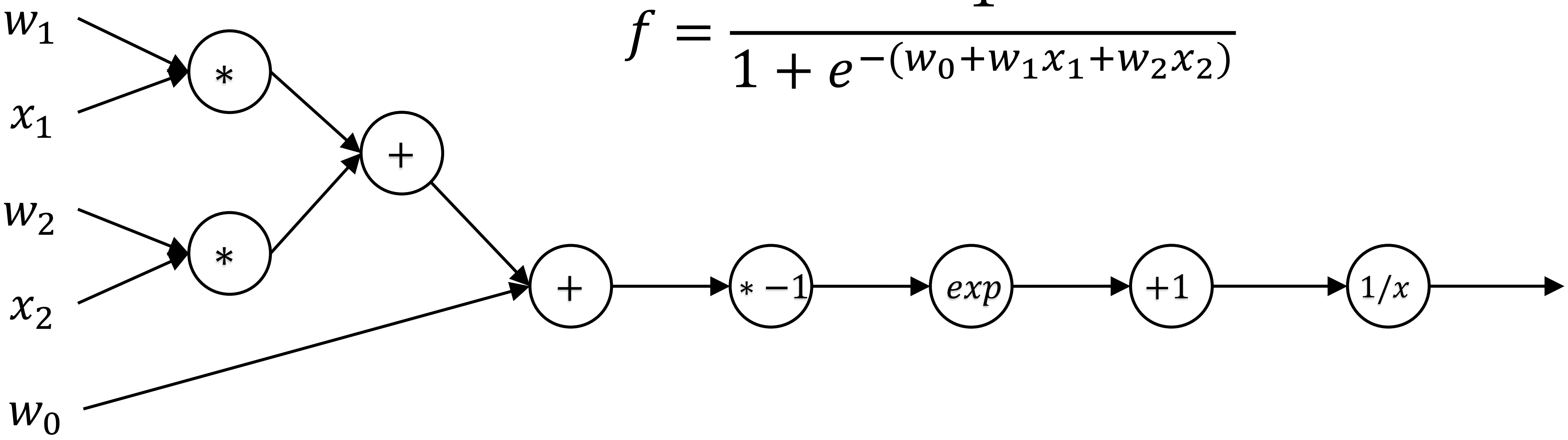

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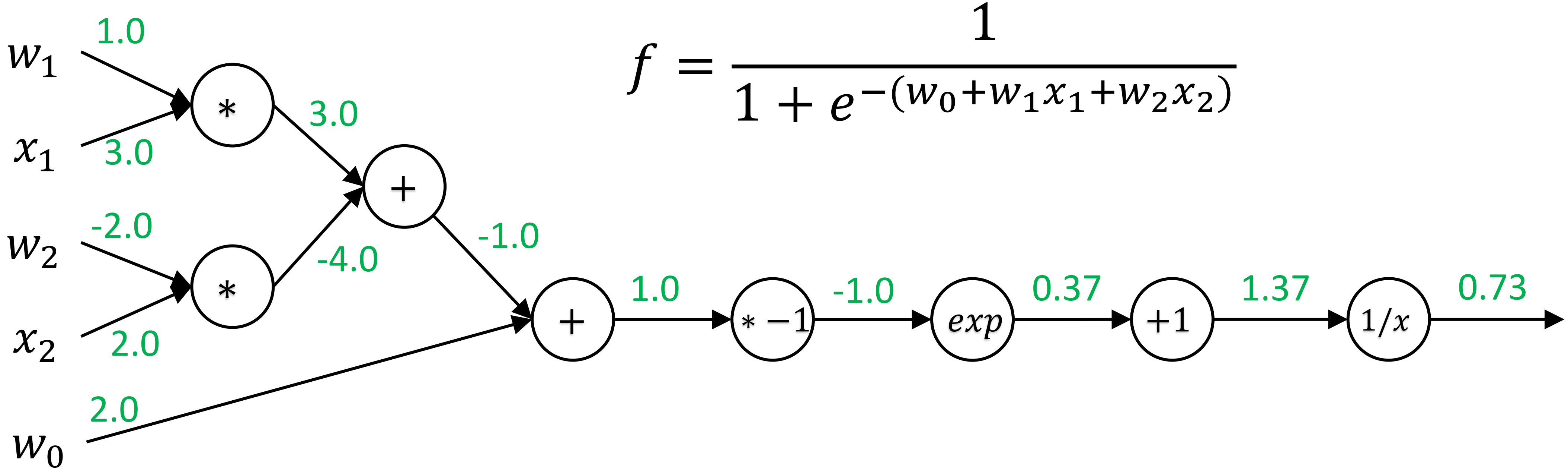

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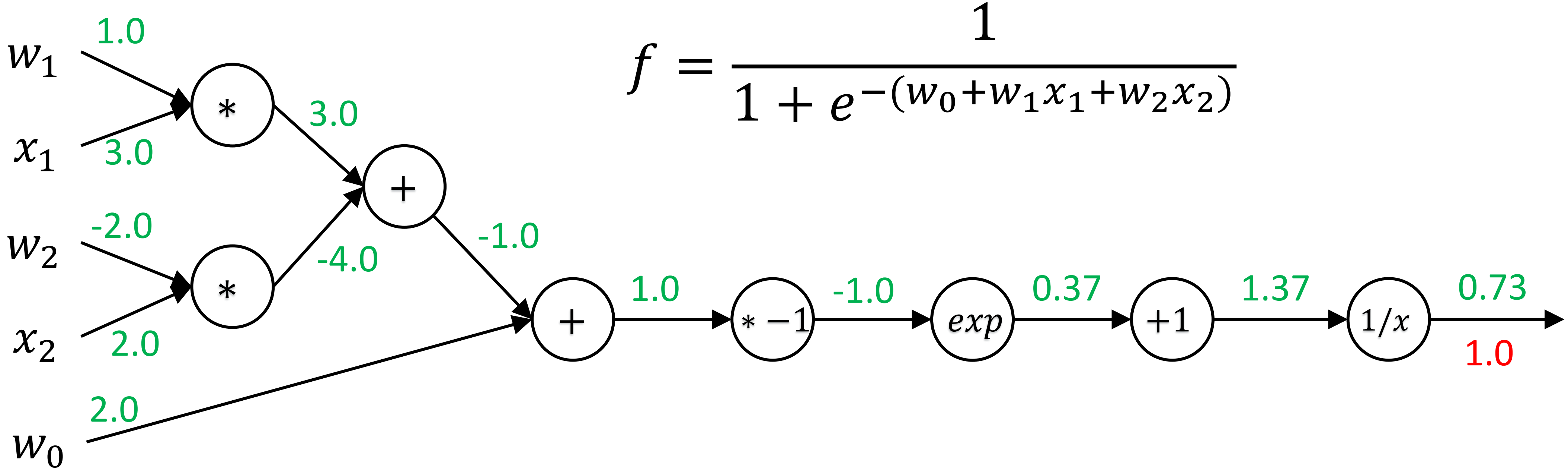

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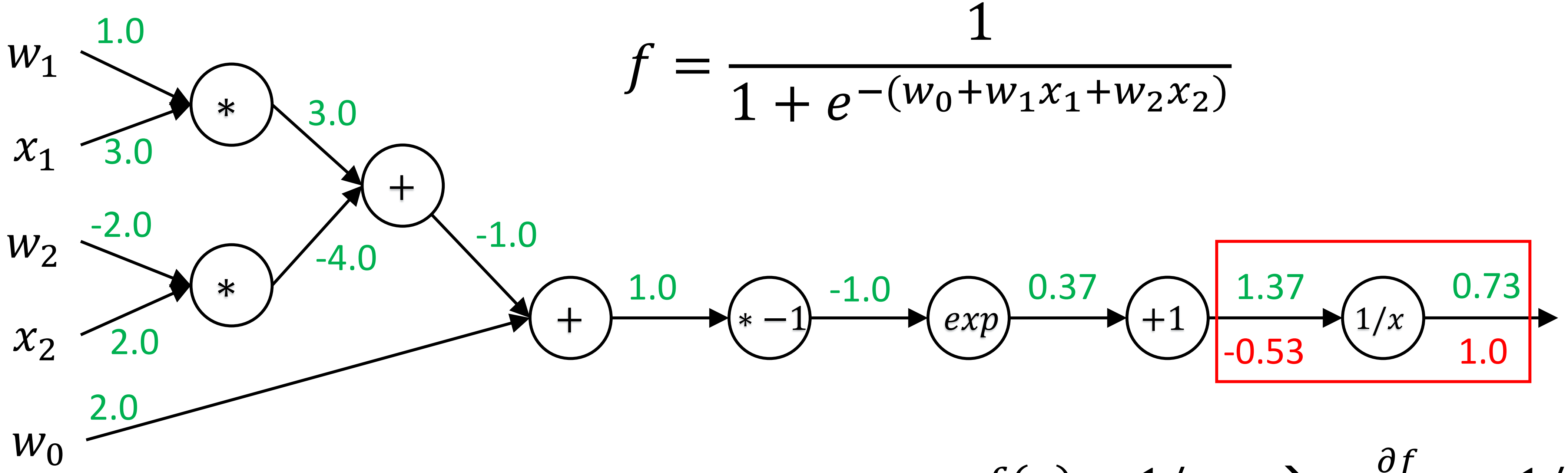

$$f = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + w_2 x_2)}}$$

$$f(x) = 1/x \quad \rightarrow \quad \frac{\partial f}{\partial x} = -1/x^2$$

$$\frac{\partial J}{\partial x} = \frac{\partial J}{\partial f}\frac{\partial f}{\partial x} = -1/x^2$$

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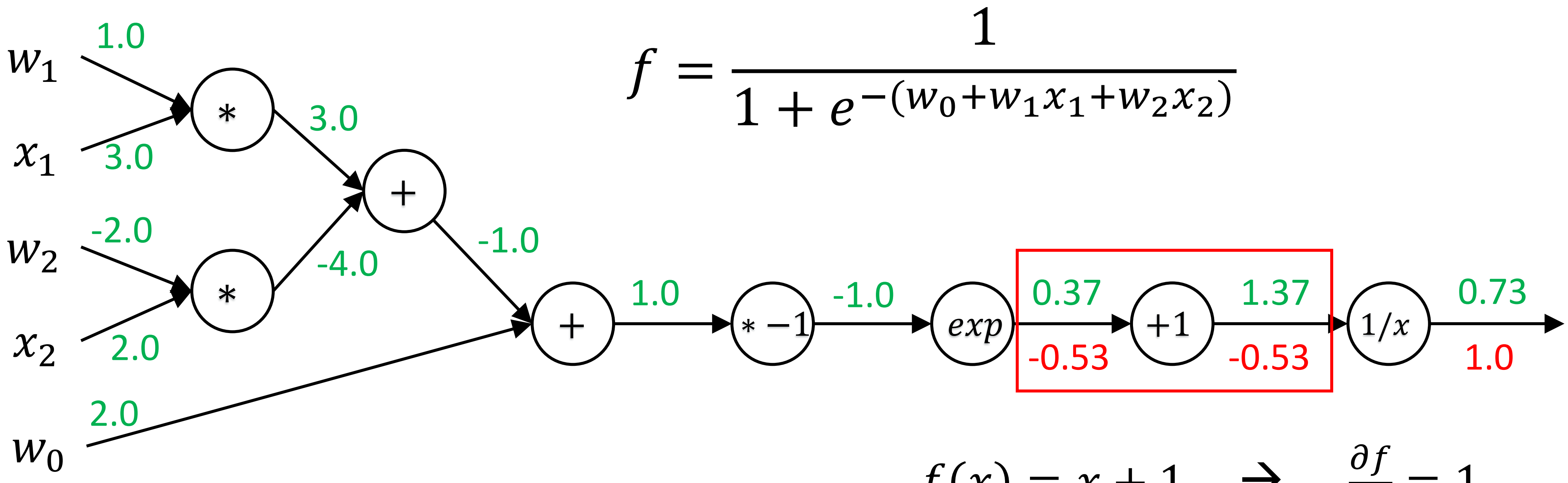
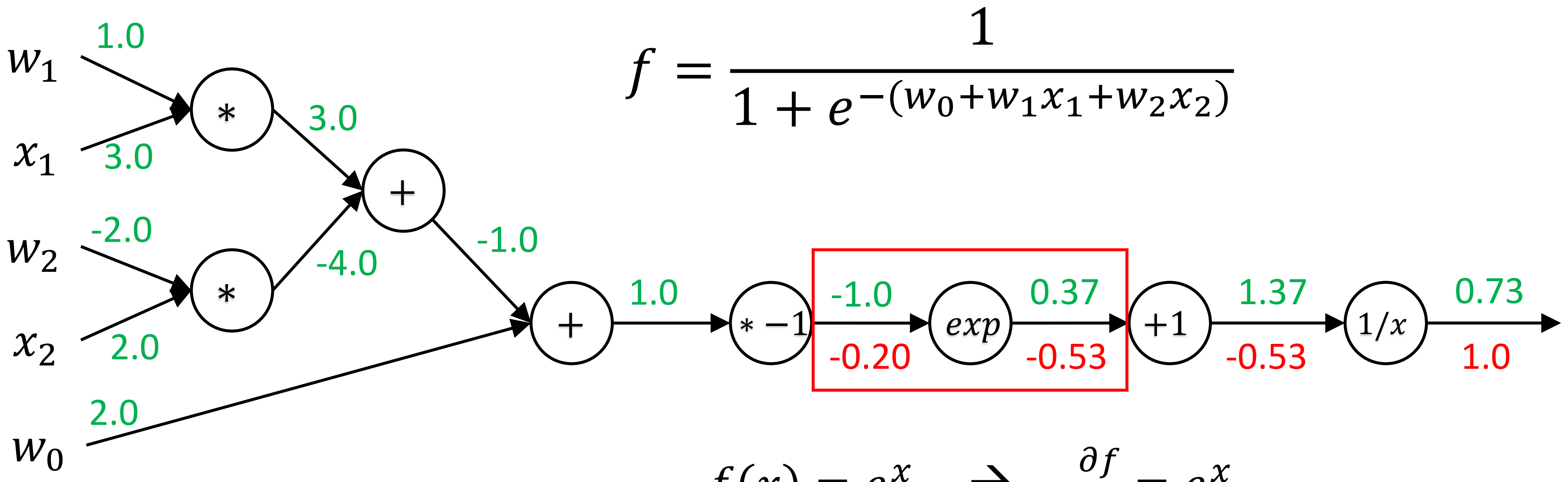
Backpropagation simple example



$$f = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + w_2 x_2)}}$$

$$f(x) = x + 1 \quad \rightarrow \quad \frac{\partial f}{\partial x} = 1$$

Backpropagation simple example



$$f = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + w_2 x_2)}}$$

$$f(x) = e^x \quad \rightarrow \quad \frac{\partial f}{\partial x} = e^x$$

$$\frac{\partial J}{\partial x} = \frac{\partial J}{\partial f}\frac{\partial f}{\partial x} = \frac{\partial J}{\partial f} \cdot e^x$$

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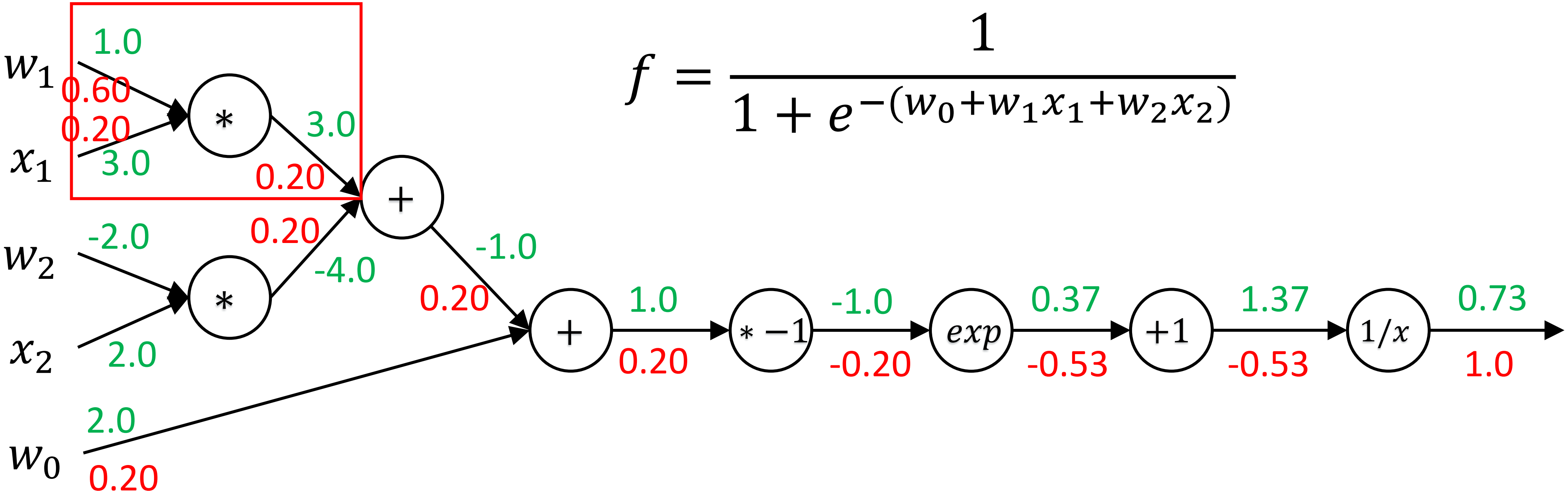
Backpropagation simple example



$$f = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + w_2 x_2)}}$$

$$f(x, w) = xw \quad \rightarrow \quad \frac{\partial f}{\partial x} = w, \ \frac{\partial f}{\partial w} = x$$

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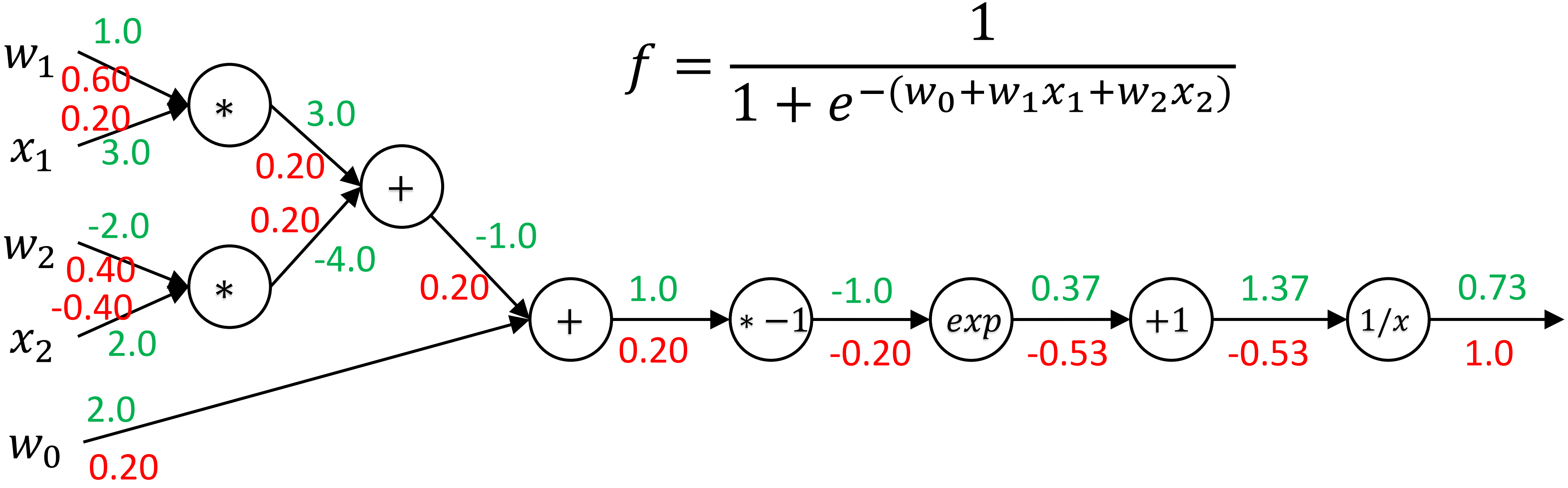
Backpropagation simple example



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Any problem?
Can we do better?

Problems of backpropagation

- You always need to keep intermediate data in the memory during the forward pass in case it will be used in the backpropagation.
- Lack of flexibility, e.g., compute the gradient of gradient.

Automatic Differentiation (autodiff)

- Create computation graph for gradient computation

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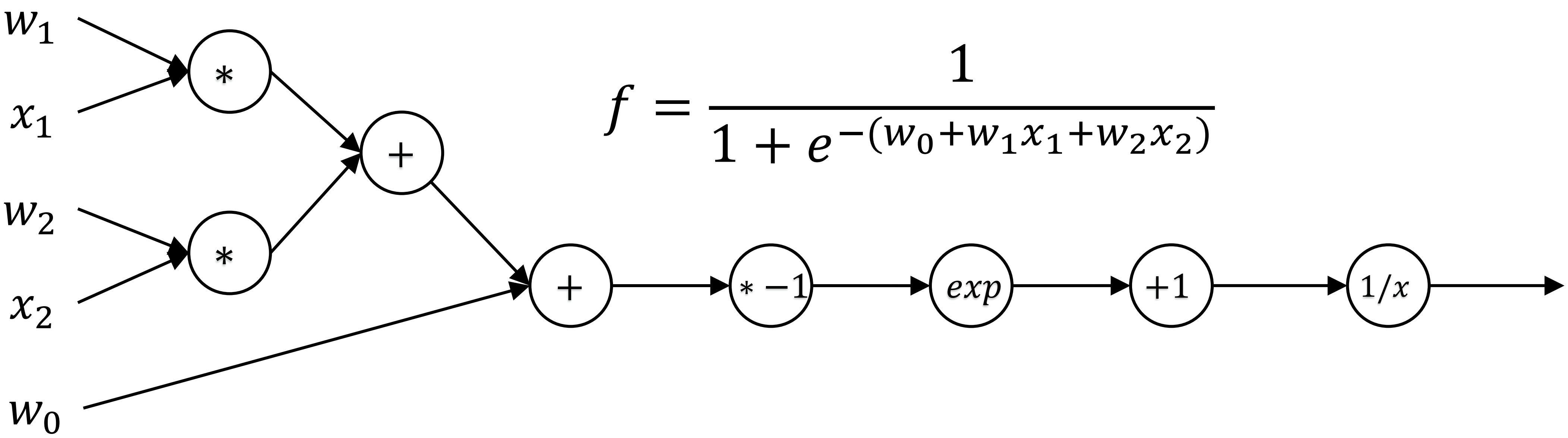

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Automatic Differentiation (autodiff)

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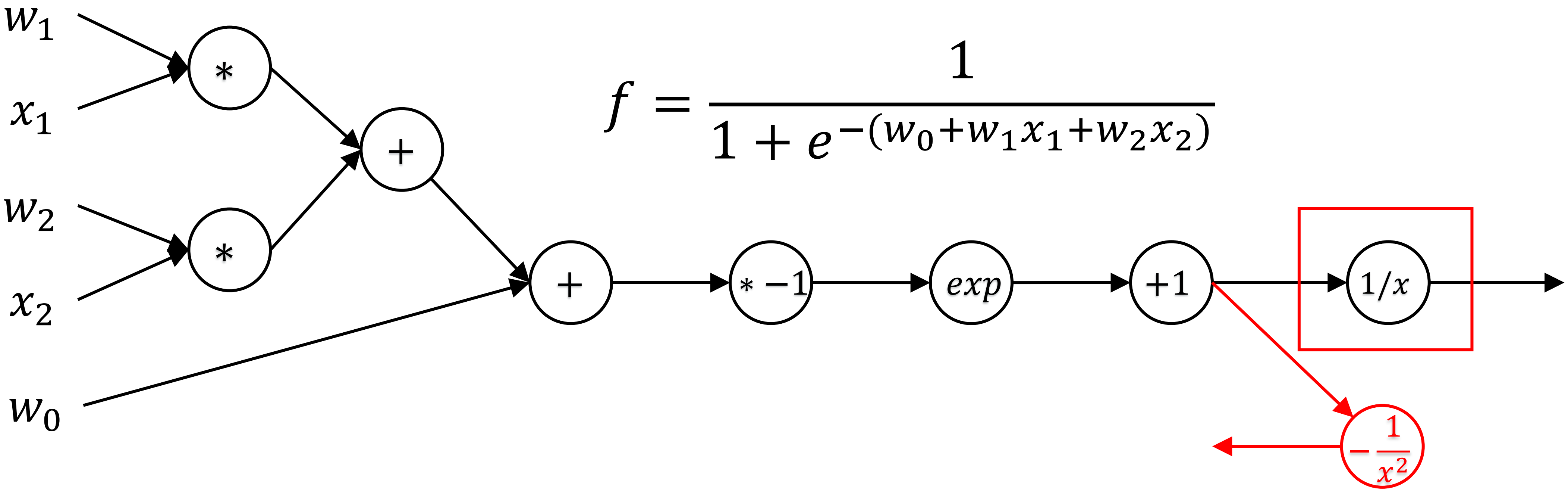

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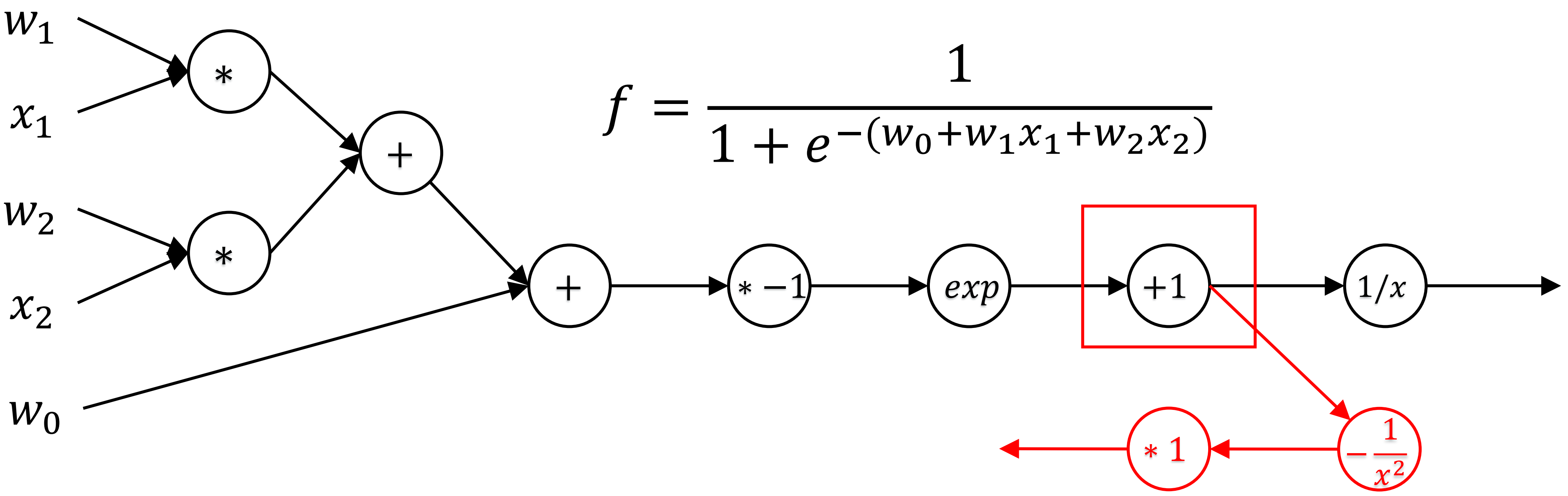

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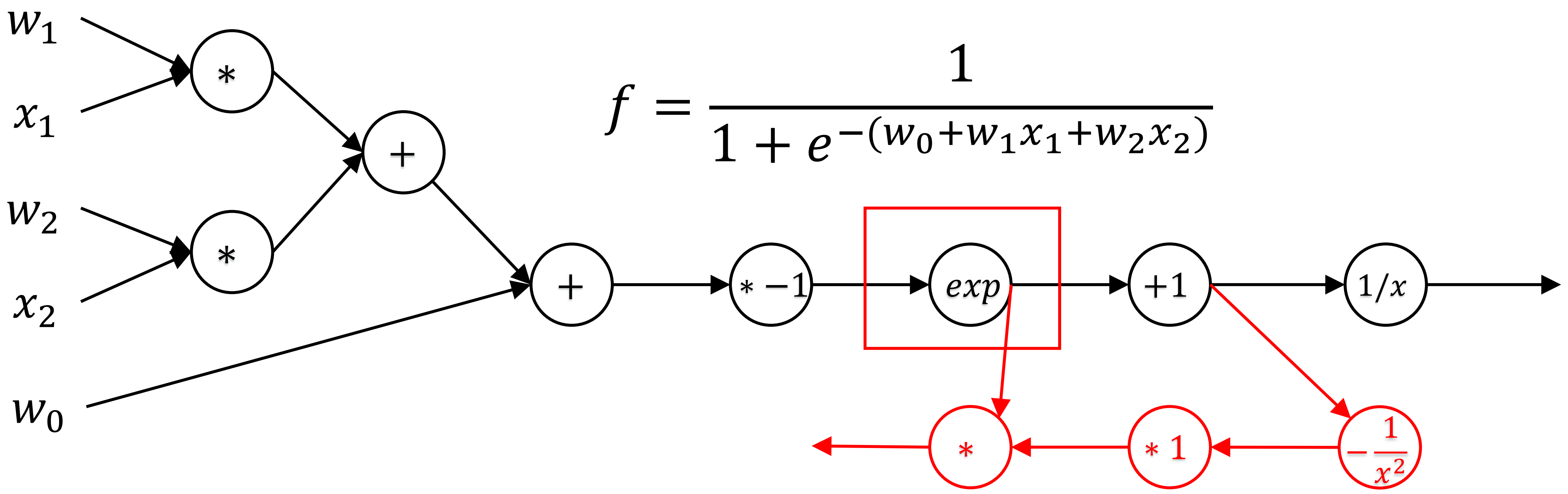

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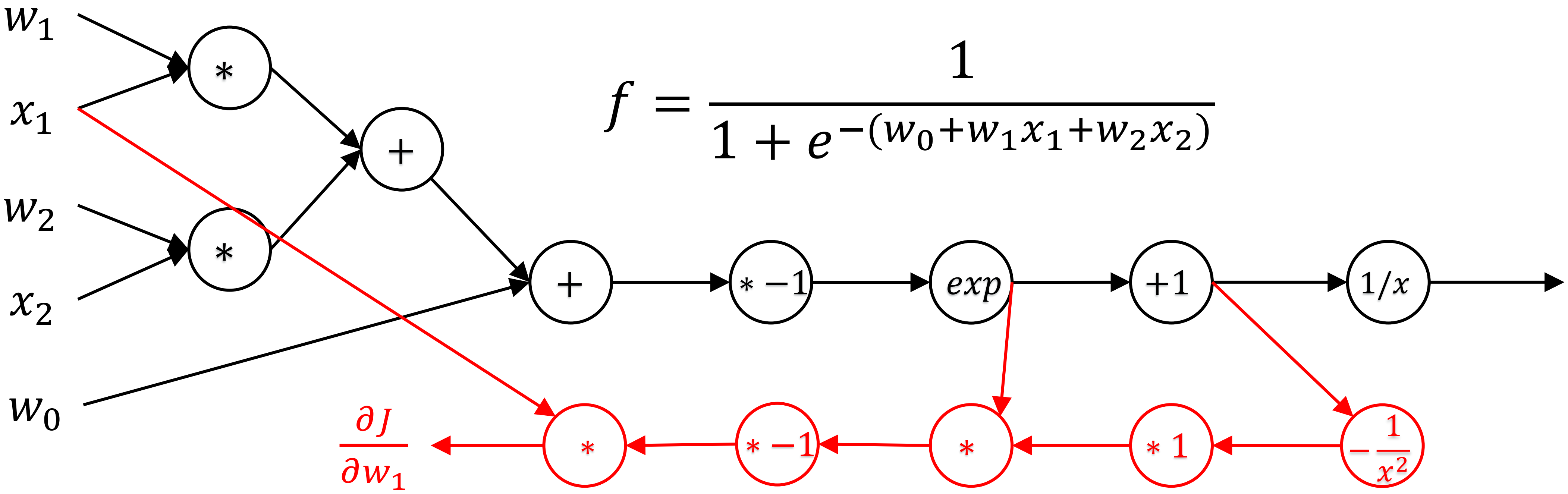

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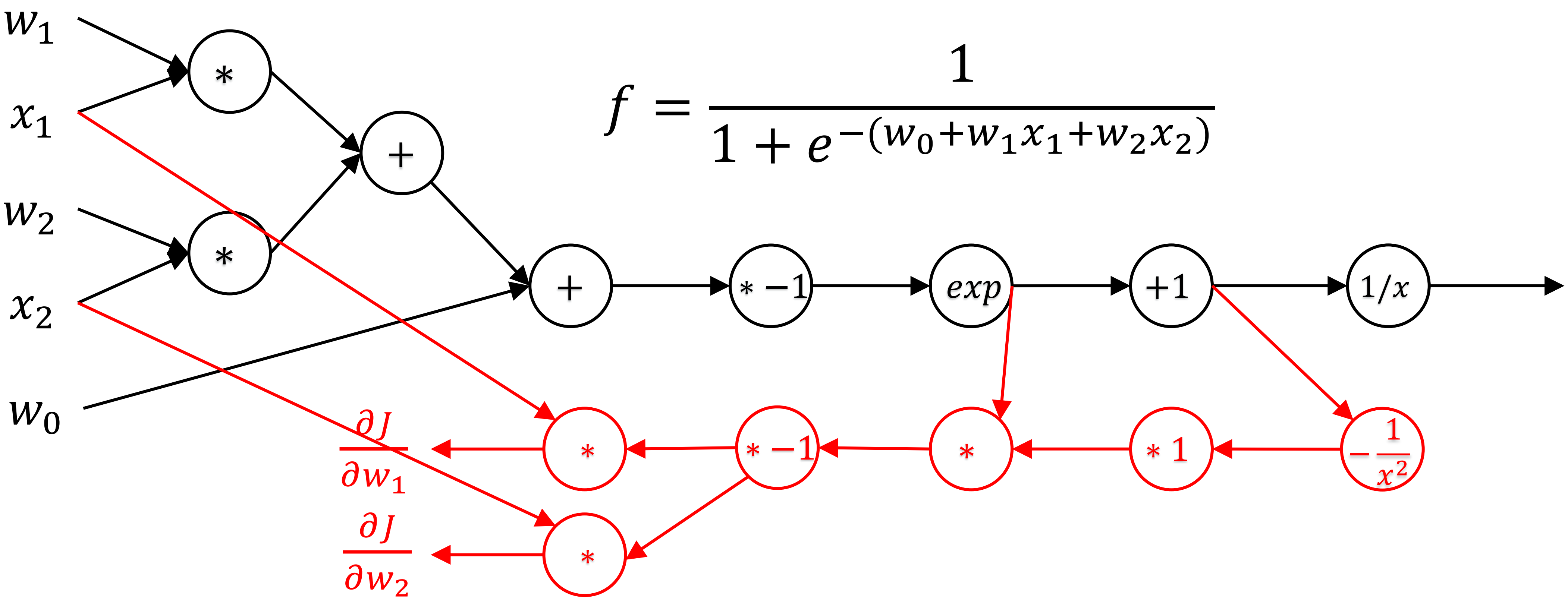

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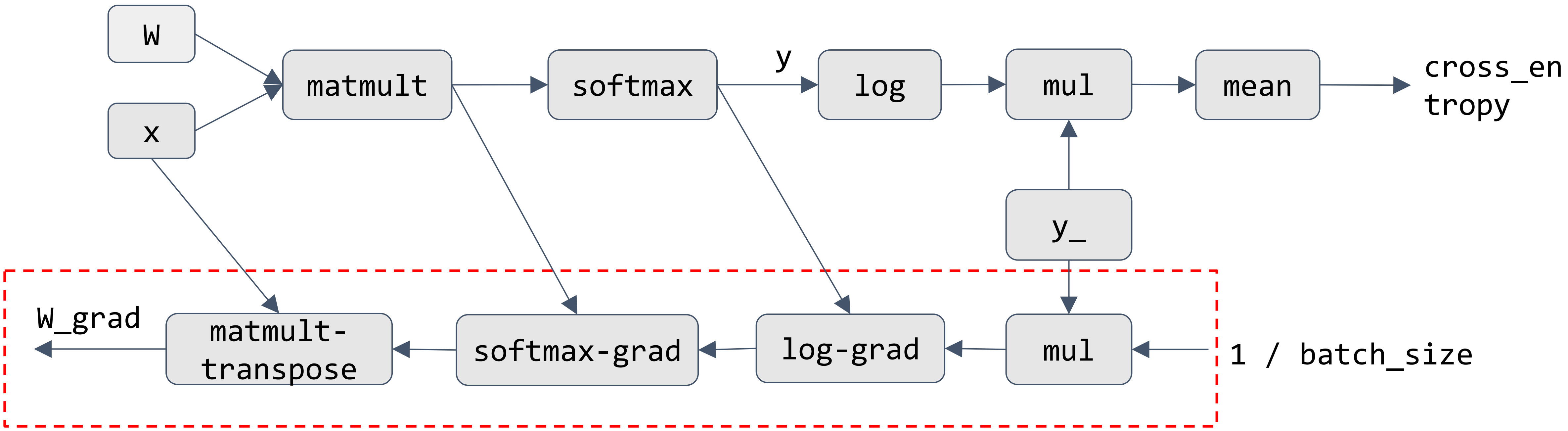
AutoDiff Algorithm



AutoDiff Algorithm

```
⇨ def gradient(out):
    node_to_grad[out] = 1
    nodes = get_node_list(out)
    for node in reverse_topo_order(nodes):
      grad ← sum partial adjoints from output edges
      input_grads ← node.op.gradient(input, grad) for input in node.inputs
      add input_grads to node_to_grad
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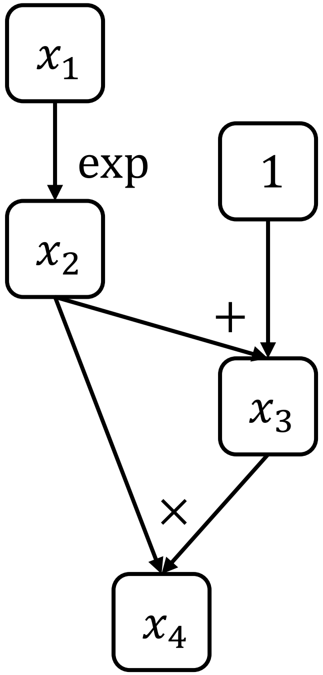

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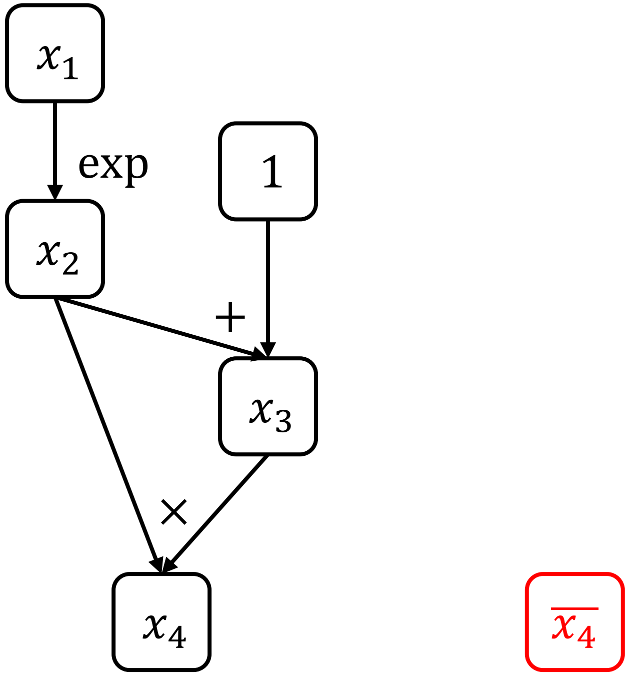
node_to_grad:
  x_4: $\overline{x_4}$



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node_to_grad:
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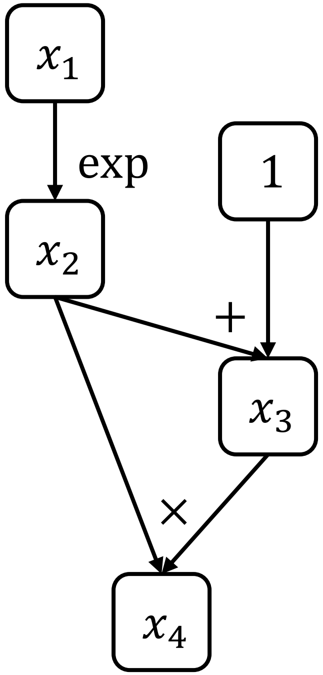
x_4	x_3	x_2	x_1
⇧			



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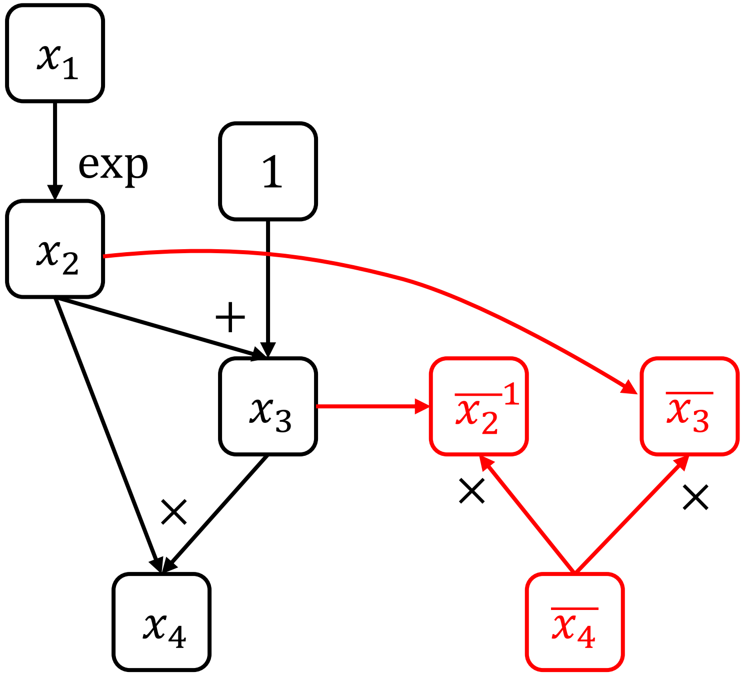

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x_2: $\overline{x_2}^{1}$

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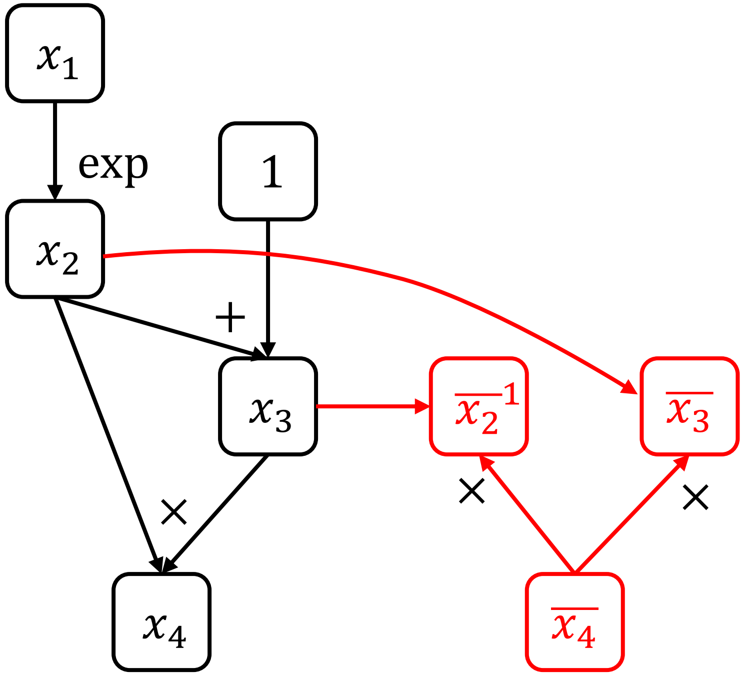

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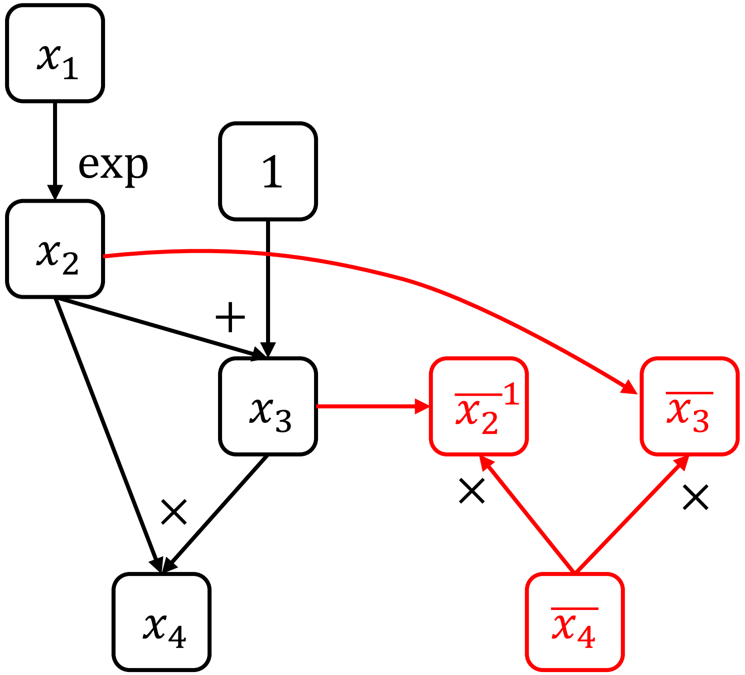

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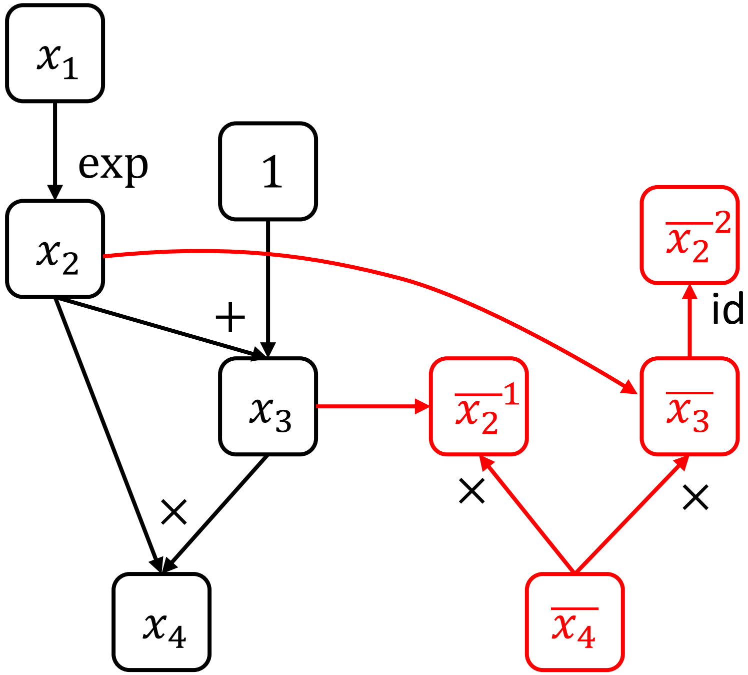

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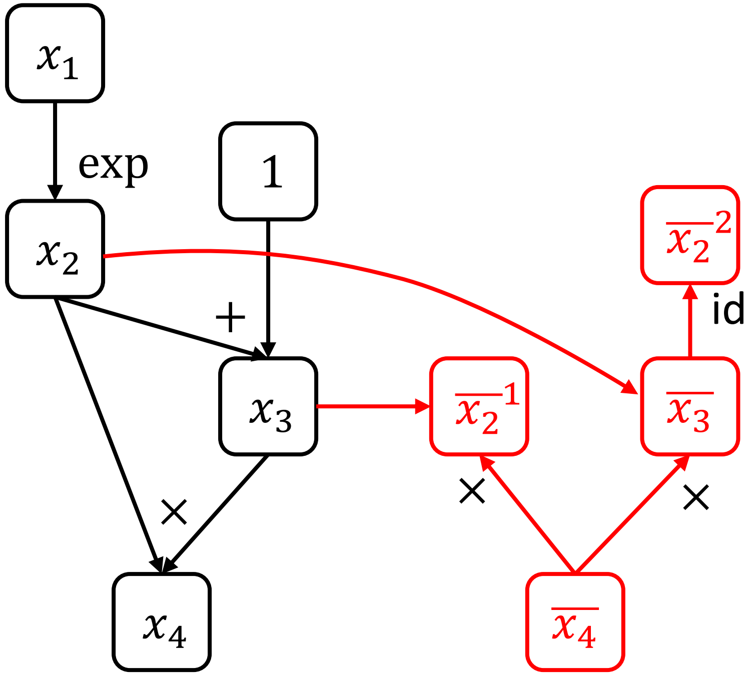

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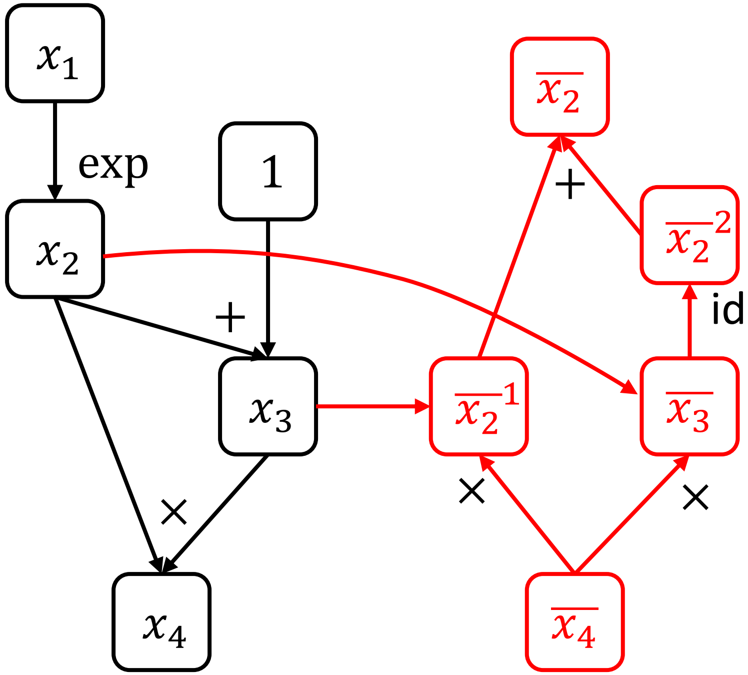

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x_4	x_3	x_2	x_1

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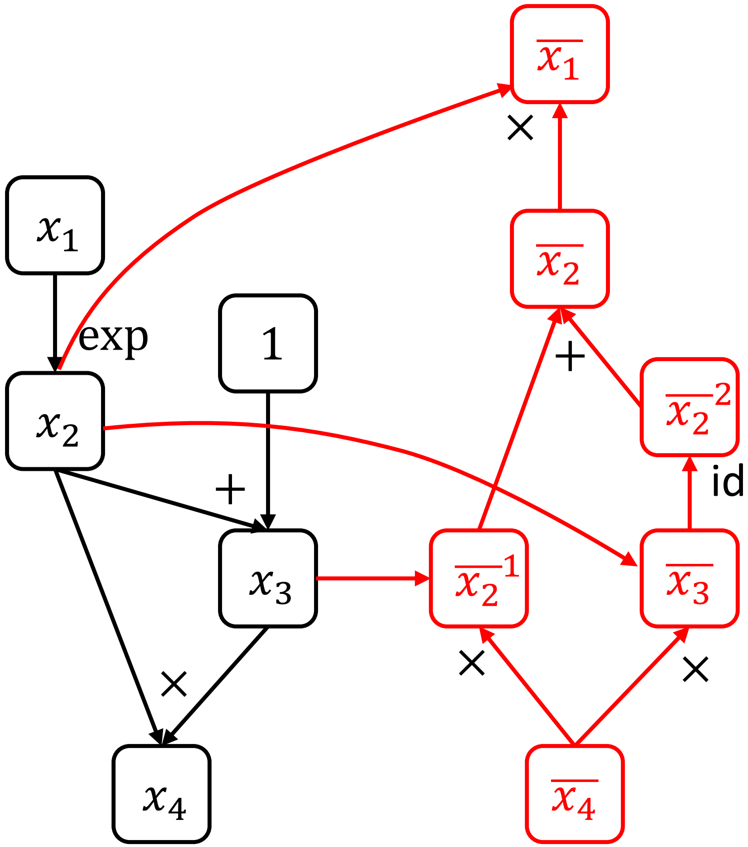

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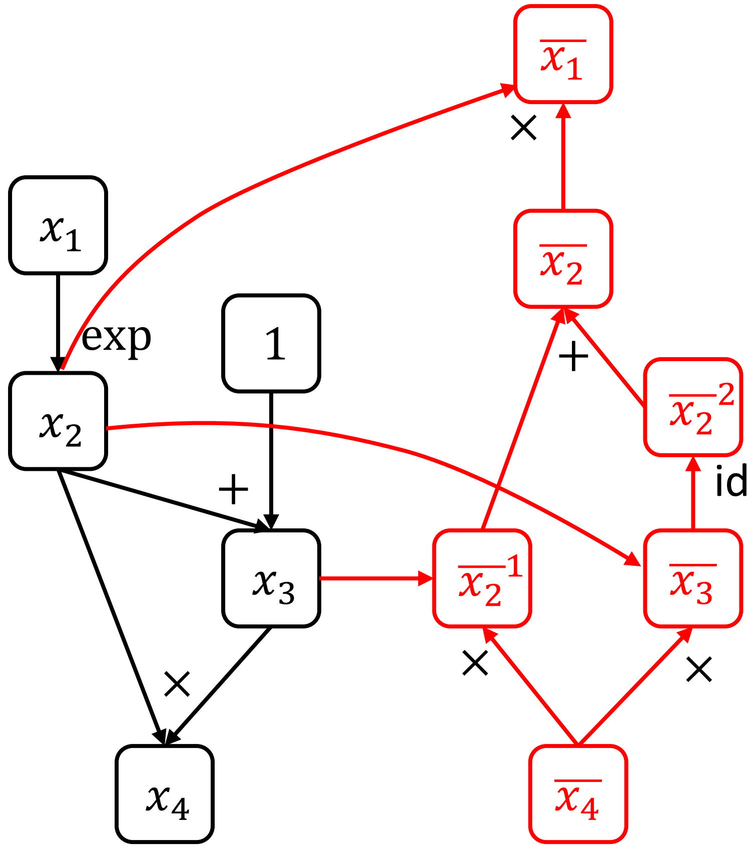

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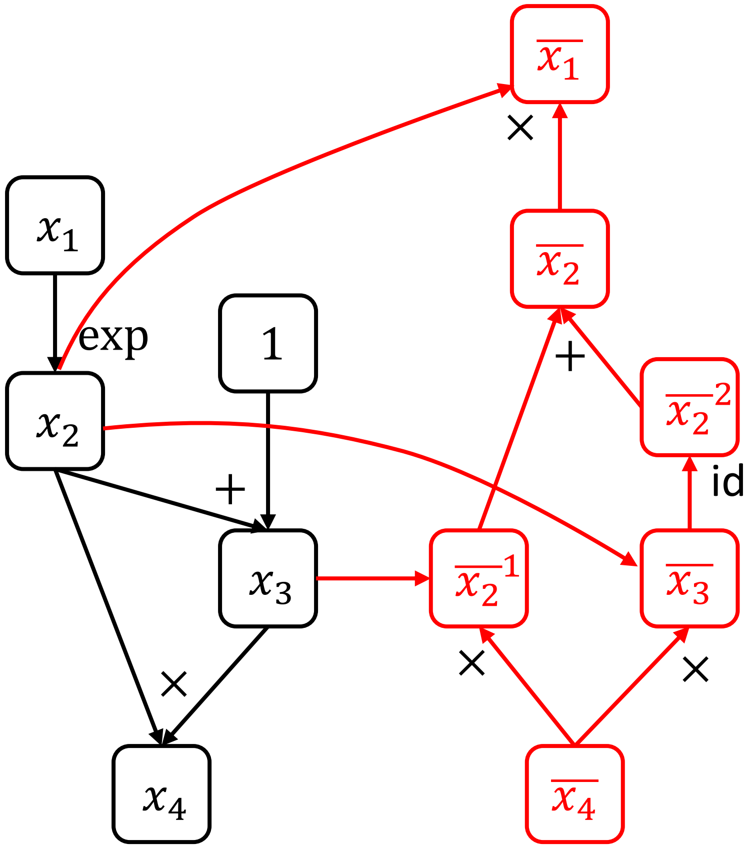
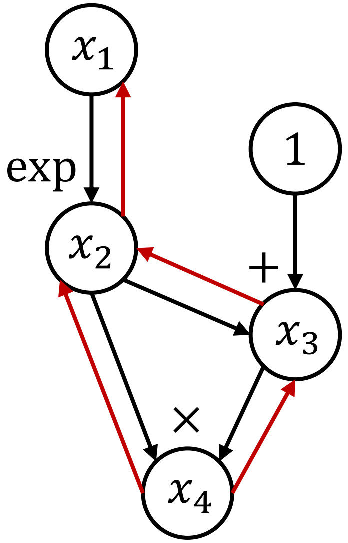
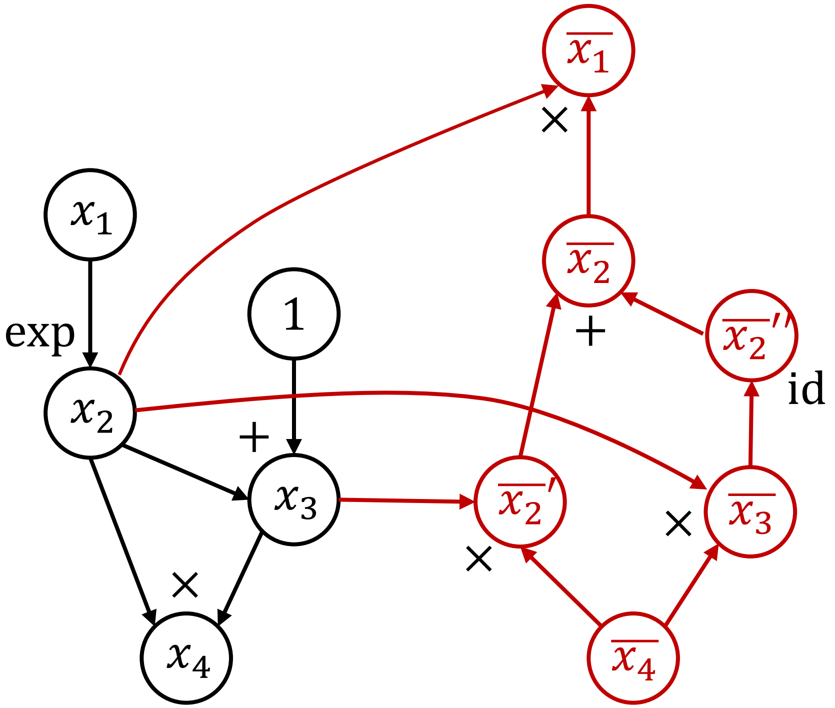


Backpropagation vs AutoDiff

Backpropagation



AutoDiff



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Recap

- Numerical differentiation
  - Tool to check the correctness of implementation
- Backpropagation
  - Easy to understand and implement
  - Bad for memory use and schedule optimization
- Automatic differentiation
  - Generate gradient computation to entire computation graph
  - Better for system optimization

References

- Automatic differentiation in machine learning: a survey https://arxiv.org/abs/1502.05767
- CS231n backpropagation: http://cs231n.github.io/optimization-2/