Deep Learning (BEV033DLA)
Lecture 2. Backpropagation

Czech Technical University in Prague

- Theory and Intuition
  - Linear approximation
  - Derivative of Composite Function
- Practice
  - Forward / backward propagation
  - Efficient Implementation, Computation Graph

What is Backpropagation?

A) Method to learn neural networks

B) Method to optimize training loss

C) Defines the step direction for gradient descent

D) Rules for computing gradient of a composite function

E) Computationally efficient automatic differentiation for scalar-valued composite functions

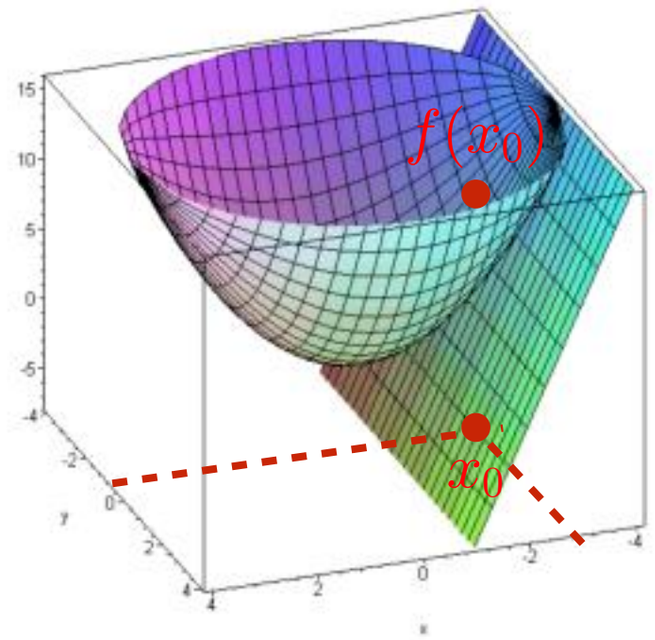
Automatic Differentiation


```
""" From karpathy/microgpt.py, (abbreviated for illustration purposes)"""
# Let there be Autograd to recursively apply the chain rule through a computation graph
class Value:
    def __init__(self, data, children=(), local_grads=()):
        self.data = data                # scalar value of this node calculated during forward pass
        self.grad = 0                   # derivative of the loss w.r.t. this node, calculated in backward pass
        self._children = children       # children of this node in the computation graph
        self._local_grads = local_grads # local derivative of this node w.r.t. its children

    def __add__(self, other):
        other = other if isinstance(other, Value) else Value(other)
        return Value(self.data + other.data, (self, other), (1, 1))

    def __mul__(self, other):
        other = other if isinstance(other, Value) else Value(other)
        return Value(self.data * other.data, (self, other), (other.data, self.data))

    def __pow__(self, other): return Value(self.data**other, (self,), (other * self.data**(other-1),))

    ...

    def backward(self):
        topo = build_topo(self) # order of processing, will be explained later
        self.grad = 1
        for v in reversed(topo):
            for child, local_grad in zip(v._children, v._local_grads):
                child.grad += local_grad * v.grad
```

Derivative

- Function $f\colon \mathbb{R}^m \to \mathbb{R}^n$ (from domain $\mathbb{R}^m$ to codomain $\mathbb{R}^n$)
- Local linear approximation: $f(x_0+\Delta x) = f(x_0) + J\Delta x + o(\|\Delta x\|)$
- When such J exists, it is unique and called **derivative**
- Expressed in coordinates J is called the **Jacobian (matrix) (at x_0):** $\mathbb{R}^2 \to \mathbb{R}$

$$f(x+\Delta x) \approx f(x) + \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \dots & \frac{\partial f_n}{\partial x_m} \end{pmatrix} \begin{pmatrix} \Delta x_1 \\ \Delta x_2 \\ \vdots \\ \Delta x_m \end{pmatrix}$$



$\frac{\partial f_i}{\partial x_j}$ – speed of growth (slope) of f_i along x_j

✦ Linear approximations form a closed class under addition and composition:

- sum of linear functions is linear -- can approximate sum of log-likelihoods over many data points
- composition of linear functions is linear -- can approximate a deep feed-forward network

Finite Difference

- Given **scalar-valued** function: $\mathcal{L}\colon \mathbb{R}^n \to \mathbb{R}$

$$\mathcal{L}(x_0 + \Delta x) \approx \mathcal{L}(x_0) + \sum_i \frac{\partial L(x)}{\partial x_i} \Delta x_i$$

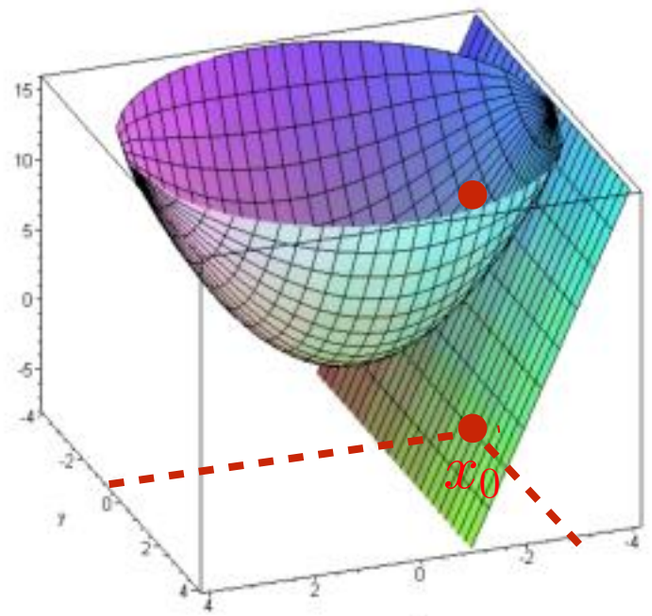
$$\frac{\partial L(x)}{\partial x_i} = \lim_{\varepsilon \to 0} \frac{L(x_0 + \varepsilon e^i) - L(x_0)}{\varepsilon}$$

Finite difference approximation:

$$\frac{\partial L(x)}{\partial x_i} = \frac{L(x_0 + \varepsilon e^i) - L(x_0)}{\varepsilon} + O(\varepsilon)$$

For a twice differentiable function symmetric difference is more accurate:

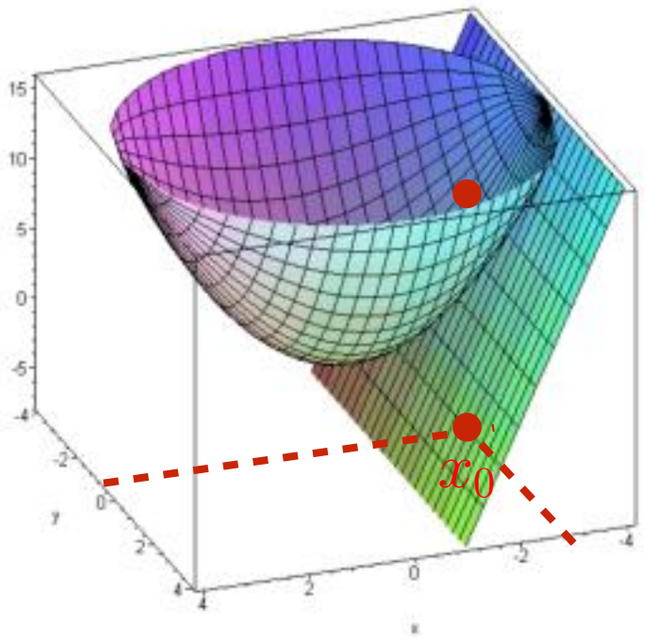
$$\frac{\partial L(x)}{\partial x_i} = \frac{L(x_0 + \varepsilon e^i) - L(x_0 - \varepsilon e^i)}{2\varepsilon} + O(\varepsilon^2)$$



- Can be used for numerical verification
- Can be used with some complex functions that depend on few variables (e.g. solver for the camera pose from 4 correspondences)

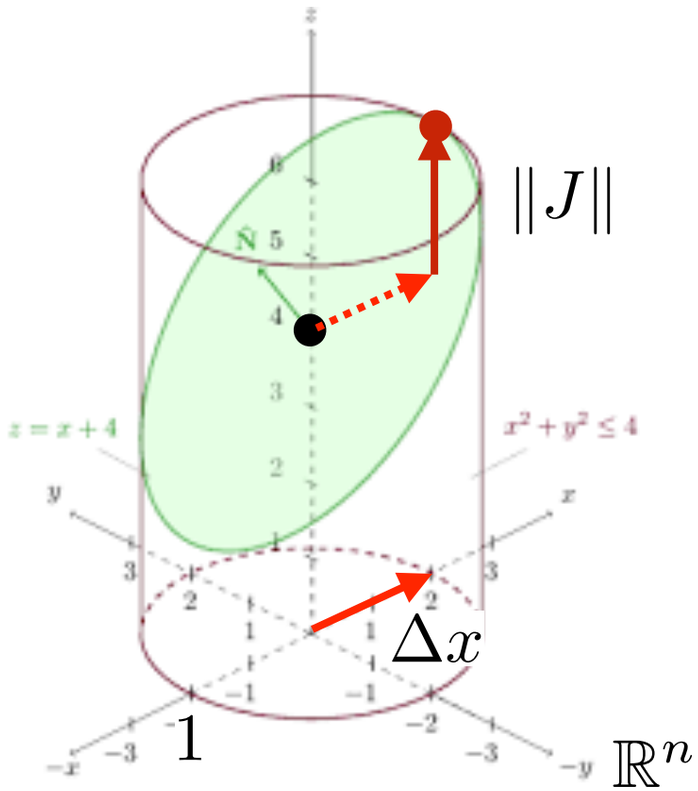
Steepest Ascent

- Given **scalar-valued** function: $\mathcal{L}\colon \mathbb{R}^n \to \mathbb{R}$



$$\mathcal{L}(x_0 + \Delta x) \approx \mathcal{L}(x_0) + J\Delta x$$

J is a *row* vector $\left(\cdots \frac{\partial f}{\partial x_i} \cdots\right)$



- What is the steepest ascent direction to maximize the linear approximation?

$$\max_{\Delta x\colon \|\Delta x\|_2 = 1} \left(f(x^0) + J\Delta x\right) \quad \Rightarrow \quad \Delta x = \frac{J^\mathsf{T}}{\|J\|}$$

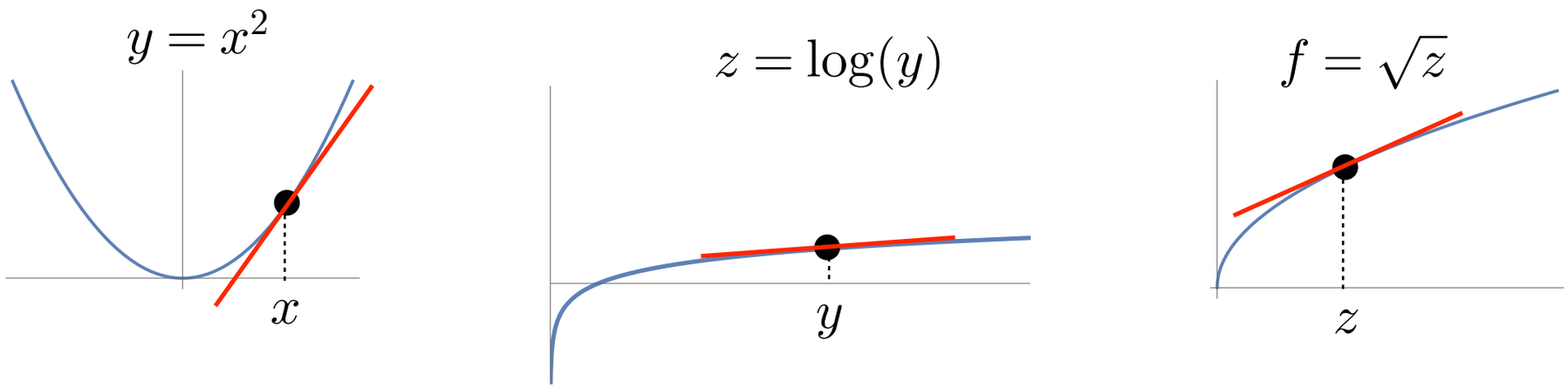
- **Gradient** $\nabla_x f$ is the *column* vector of partial derivatives $\begin{pmatrix} \vdots \\ \frac{\partial f}{\partial x_i} \\ \vdots \end{pmatrix} = J^\mathsf{T}$

- (Steepest) gradient descent: $x^{t+1} = x^t - \varepsilon \nabla_x f(x^t)$

Compositions

- **Our notation** J_x^f – derivative of f in x.
- Linear function: $f(x) = Ax$, then $J_x^f = A$
- Composition of linear functions: $f(x) = ABx \qquad J_x^f = AB$
- Non-linear composition: make a linear approximation to all steps and compose

  Example $f = \sqrt{\log(x^2)} = \sqrt{\ } \circ \log \circ x^2$



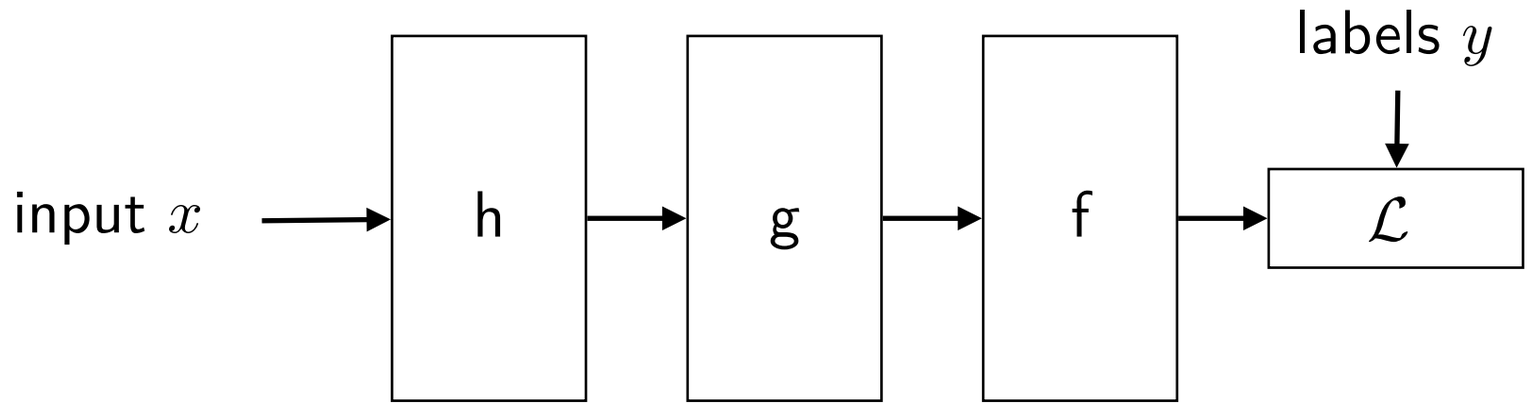
$$J_x^f = \left.\frac{\partial\sqrt{z}}{\partial z}\right|_{z=\log(y)} \left.\frac{\partial \log y}{\partial y}\right|_{y=x^2} \left.\frac{\partial x^2}{\partial x}\right|_{x} = (\tfrac{1}{2}z^{-1/2})(y^{-1})(2x)$$

- General case, $f(g(x)) = (f \circ g)(x)$:

$$J_x^f = J_g^f J_x^g$$

$$\frac{\mathrm{d}f_i}{\mathrm{d}x_j} = \sum_k \frac{\partial f_i}{\partial g_k}\frac{\partial g_k}{\partial x_j}$$ (chain / total derivative rule)

In Neural Networks



Loss $\mathcal{L}(f(g(h(x))))$

- We will need derivatives of the loss in different parameters. Shorthand: $J_x \equiv J_x^{\mathcal{L}} \equiv \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}x}$.
- In order to compute J_x we need to multiply all Jacobians:

Loss: $\mathcal{L} \circ f \circ g \circ h \circ x$

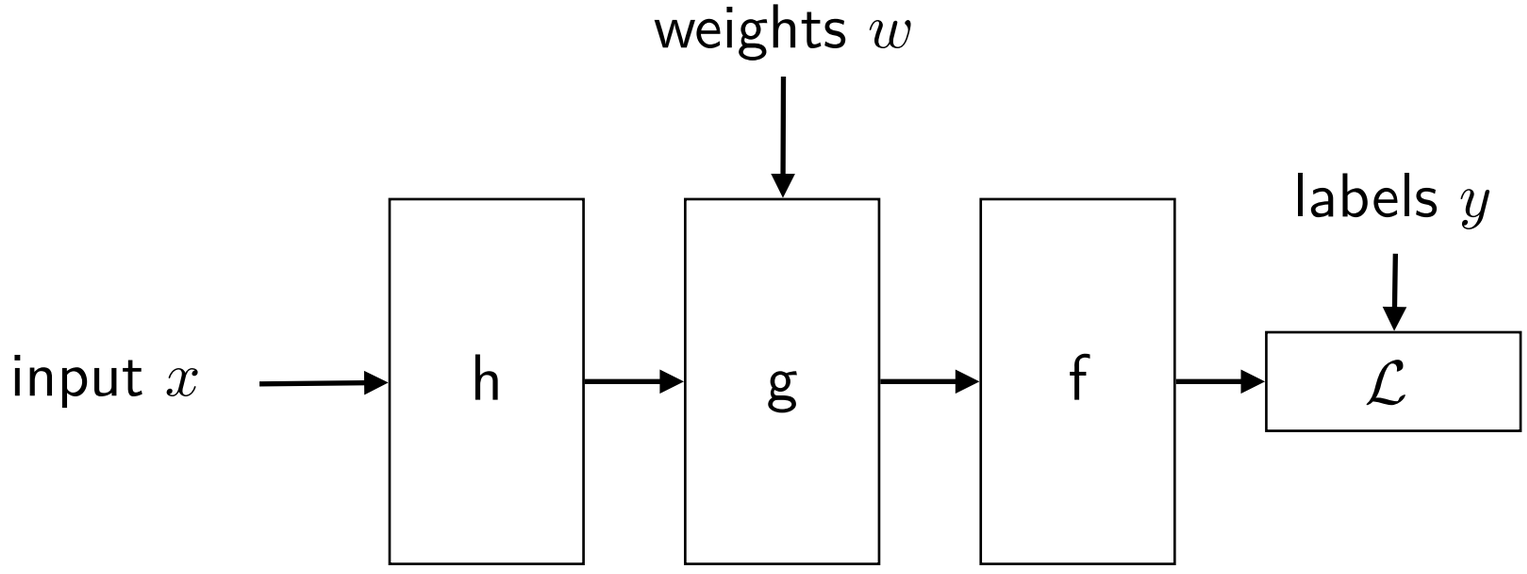
Derivative: $J_x = J_f^{\mathcal{L}} \; J_g^f \; J_h^g \; J_x^h$

Expanded: $J_x = \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial f_1} & \frac{\partial \mathcal{L}}{\partial f_2} & \cdots & \frac{\partial \mathcal{L}}{\partial f_n} \end{pmatrix} \begin{pmatrix} \\ J_g^f \\ \\ \end{pmatrix} \begin{pmatrix} \\ J_h^g \\ \\ \end{pmatrix} \begin{pmatrix} \\ J_x^h \\ \\ \end{pmatrix}$

- Matrix product is associative
- Going left-to-right is cheaper: $O(Ln^2)$ *vs.* $O((L-1)n^3 + n^2)$,
  for L fully connected layers with n input-output units (except the loss)

Backpropagation

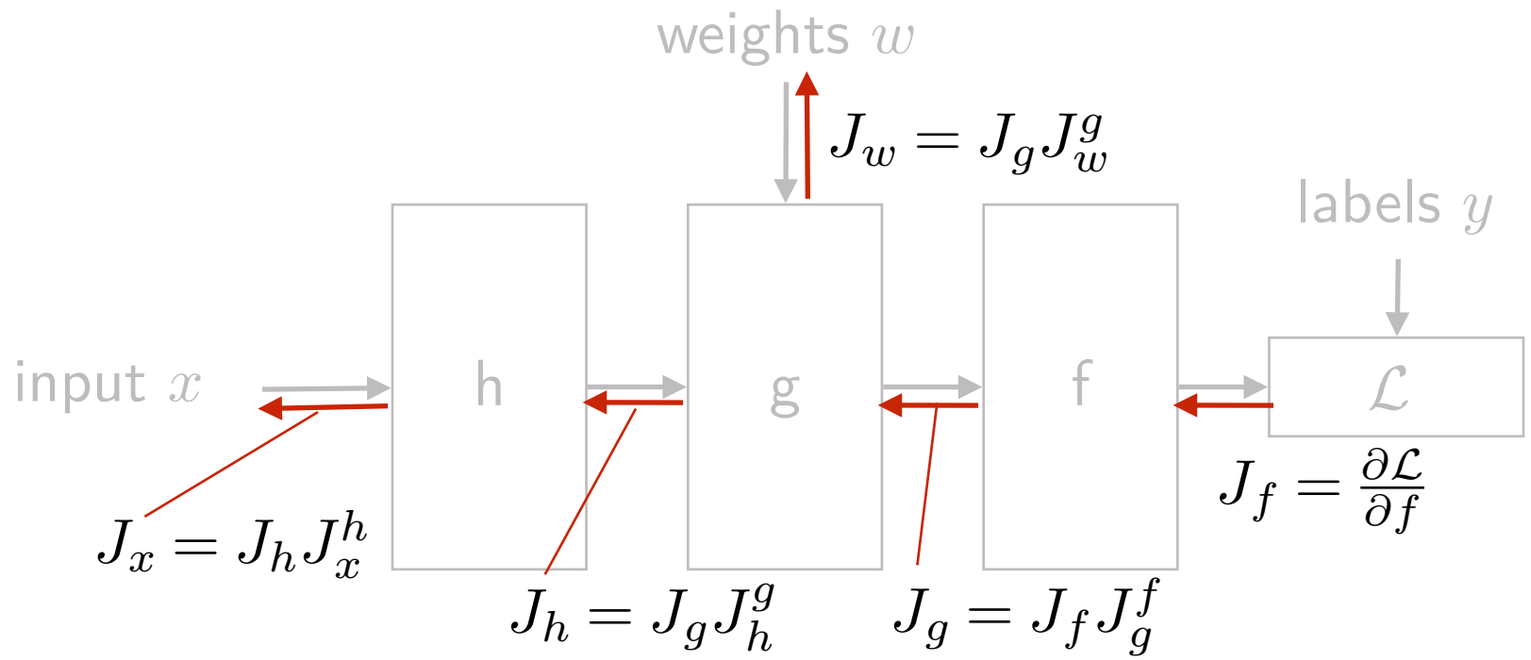
✦ **Forward** — composition of functions



Loss $\mathcal{L}(f(\,g(h(x), w)\,), y)$

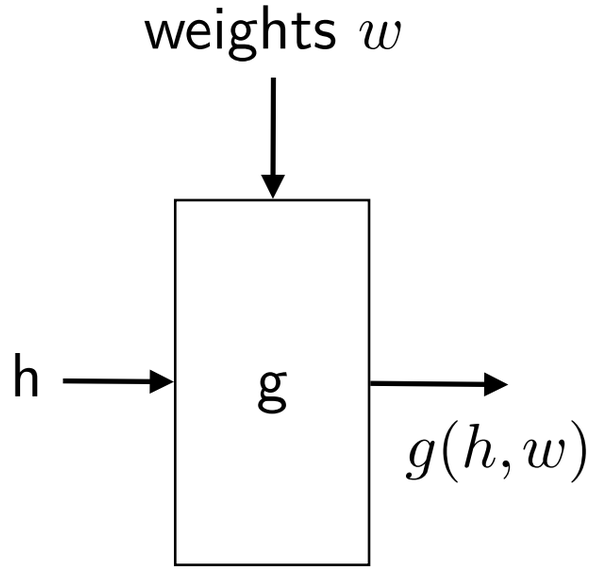
- Feed-forward network $\Rightarrow$ computation graph is a DAG
- Composition ($\circ$) notation possible when fixing all but one inputs

✦ **Backward:**

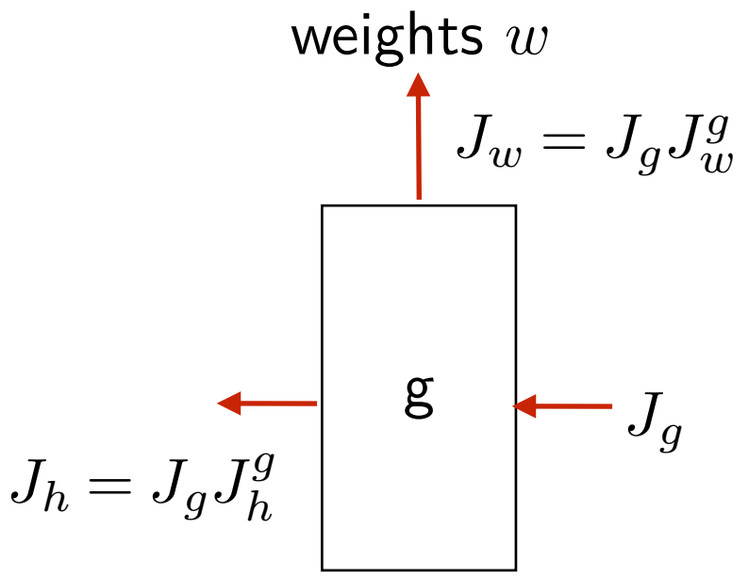


Both Forward and Backward are Modular

- **Forward:**

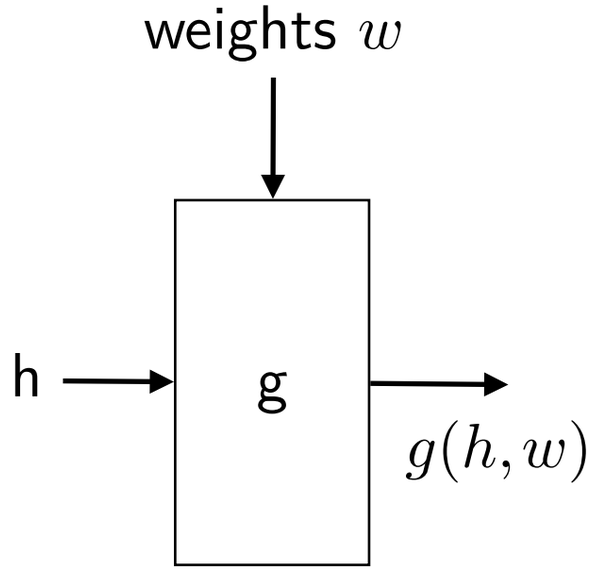


- **Backward:**

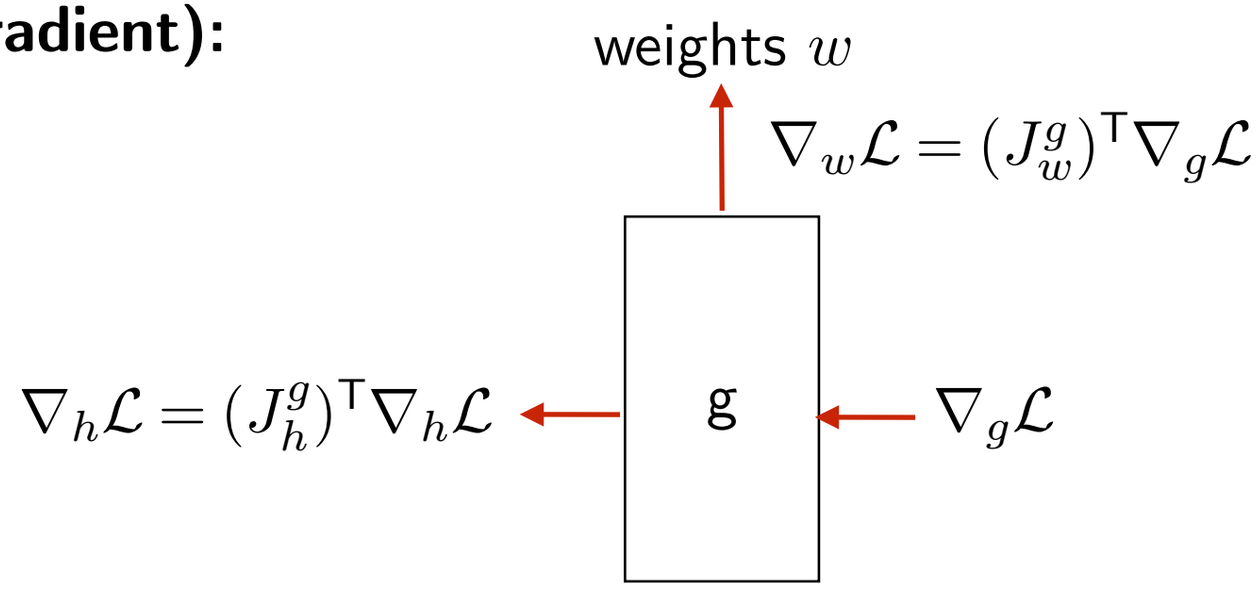


Both Forward and Backward are Modular

- **Forward:**



- **Backward (gradient):**



Example

- Correlation layer with inputs x and weights w: $y_j = \sum_k w_k x_{j+k} + b_j$
  - Backward input: $g_j = \frac{d\mathcal{L}}{dy_j}$
  - Need $\frac{d\mathcal{L}}{dx_i}$, $\frac{d\mathcal{L}}{dw_k}$, $\frac{d\mathcal{L}}{db_j}$
  - Total derivative (chain) rule:

$$\begin{aligned}
\frac{d\mathcal{L}}{dx_i} &= \sum_j \frac{d\mathcal{L}}{dy_j}\frac{\partial y_j}{\partial x_i} \\
&= \sum_j g_j \frac{\partial}{\partial x_i}\left(\sum_k w_k x_{j+k} + b_j\right) \\
&= \sum_j g_j \sum_k w_k \frac{\partial}{\partial x_i} x_{j+k} \\
&= \sum_j g_j \sum_k w_k [\![j+k{=}i]\!] \\
&= \sum_j g_j w_{i-j}
\end{aligned}$$

Various special cases of linear dependencies can be handled in O(n) instead of O(n²)

Computation Graph, Forward Propagation

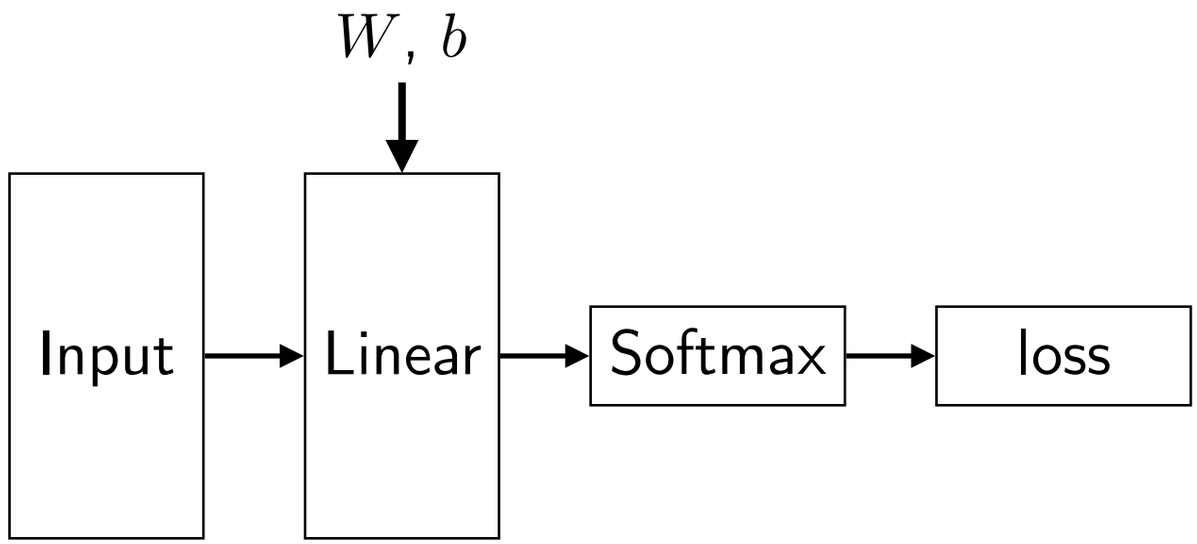
- Dynamic Graph (Eager Execution): just compute what we need

Declare and initialize variables

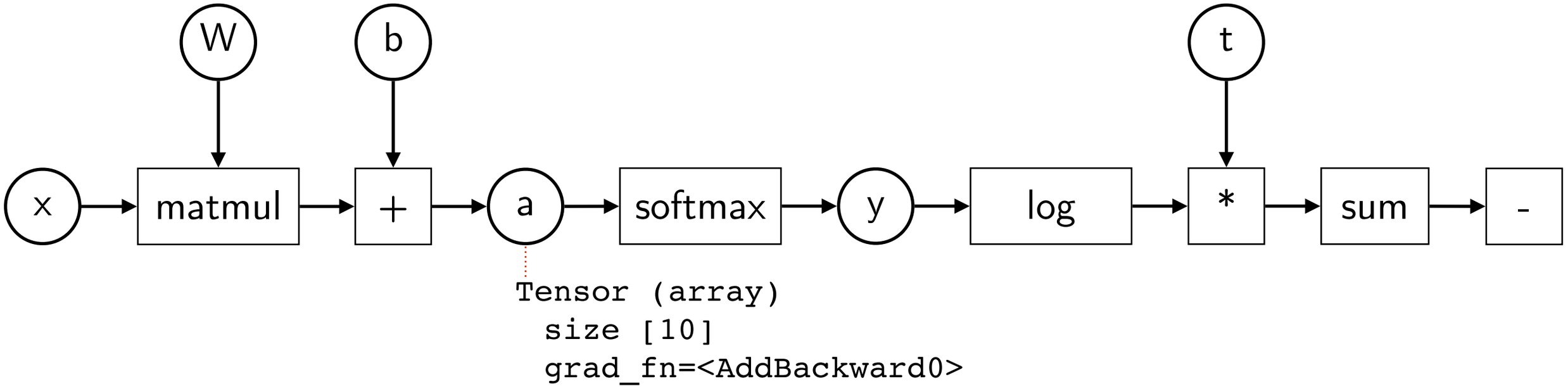
```
from torch.nn import Parameter
import torch.nn.functional as F

W = Parameter(torch.randn(10, 748))
b = Parameter(torch.randn(10))
```

Perform some operations

```
x = torch.randn(748)
t = torch.ones(10)
a = W @ x + b
y = F.softmax(a)
loss = -(t * y.log()).sum()
```

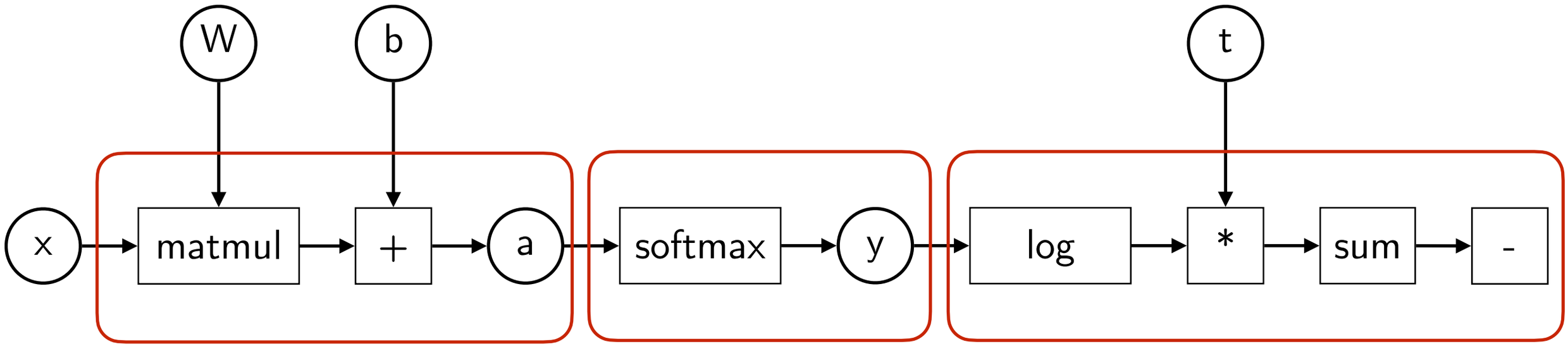


Computation graph defined by the operations performed:



- Wow! Any computation can be made a part of a neural network

Backward Propagation

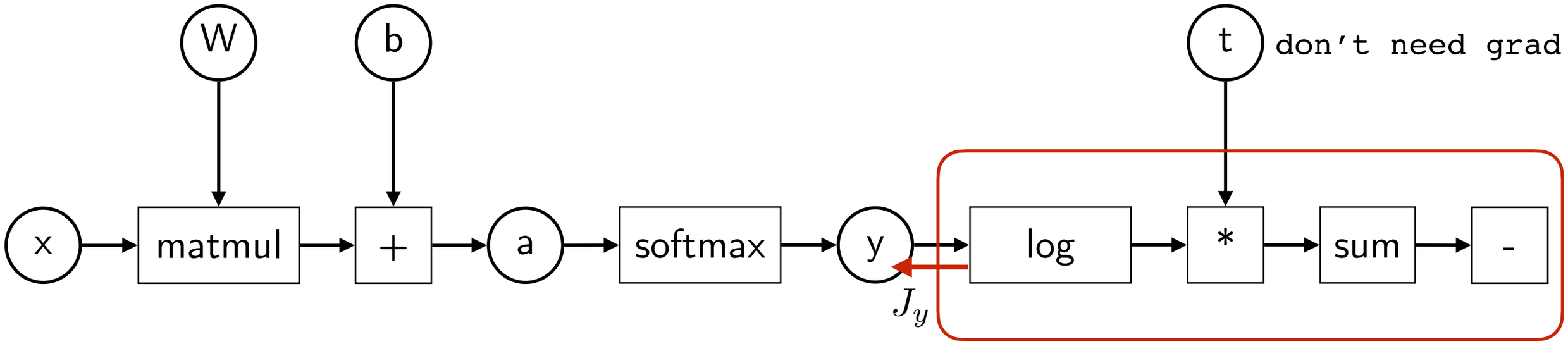


$a = \text{linear}(x, W, b)$ $y = \text{softmax}(a)$ $L = -t^{\mathsf{T}} \log(y)$

```
a = F.linear(x,W,b)        y = F.softmax(a)
```

- Computationally more efficient to compute backward for larger blocks.
  Also convenient for this example.

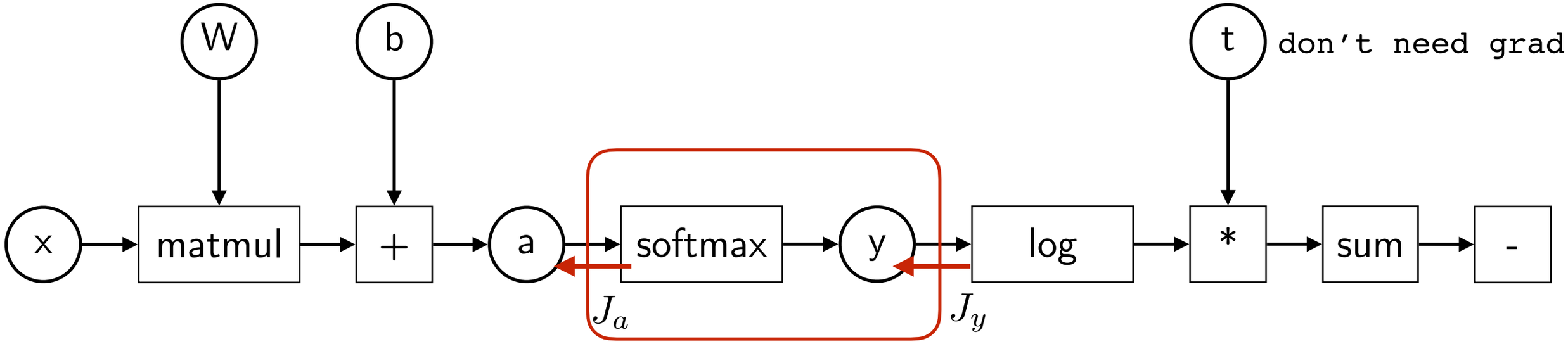
Backward Propagation



$$\mathcal{L} = -t^\mathsf{T} \log(y)$$

$$J_{y_i} = \frac{\partial \mathcal{L}}{\partial y_i} = -\frac{\partial}{\partial y_i} \sum_j t_j \log(y_j) = -\frac{1}{y_i} t_i$$

Backward Propagation



$$y_j = \text{softmax}(a)_j = \frac{e^{a_j}}{\sum_i e^{a_i}}$$

$$J_{a_i} = J_y J_a^y = \sum_j J_{y_j} \frac{\partial y_j}{\partial a_i}$$

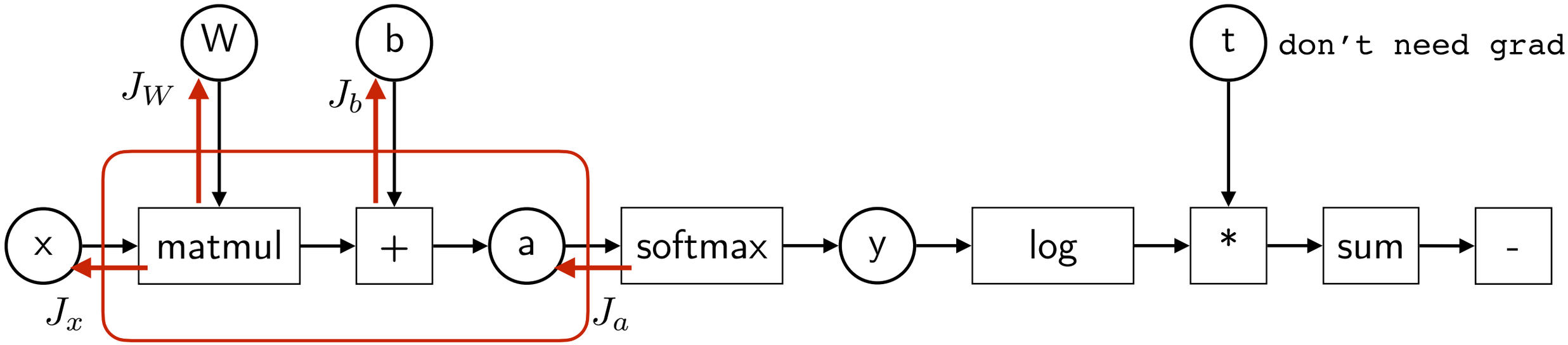
$$= \sum_j J_{y_j} (y_i [\![i{=}j]\!] - y_i y_j) = y_i \big(J_{y_i} - \sum_j y_j J_{y_j} \big)$$

$$J_a = J_y(\text{Diag}(y) - yy^\mathsf{T}) = J_y \odot y - (J_y y) y^\mathsf{T}$$

(need to remember either input a or directly the output y)

Notice: forward and backward are both linear complexity

Backward Propagation



$$a_j = \sum_i W_{ji} x_i + b$$

$$J_b = J_a \quad (\star)$$

$$J_{x_k} = \sum_j J_{a_j} \frac{\partial a_j}{\partial x_i} = \sum_j J_{a_j} W_{i,j} [\![i{=}k]\!] = \sum_j J_{a_j} W_{k,j}$$

$$J_x = J_a W$$

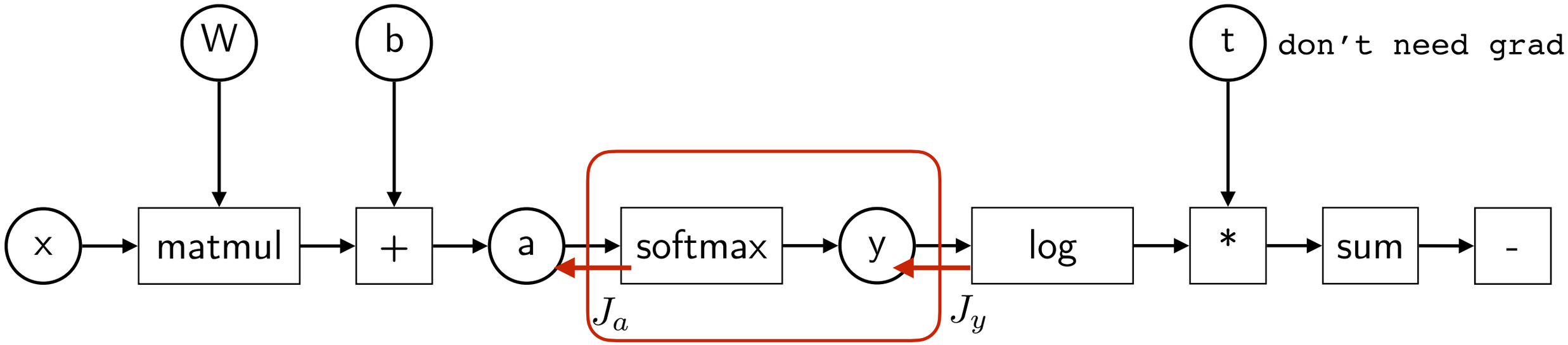
$$\nabla_x \mathcal{L} = W^\mathsf{T} \nabla_a \mathcal{L}$$

Note: a transposed product in comparison with Wx

$$J_{W_{ij}} = \sum_j J_{a_j} \frac{\partial a_j}{\partial W_{ij}} = x_i J_j$$

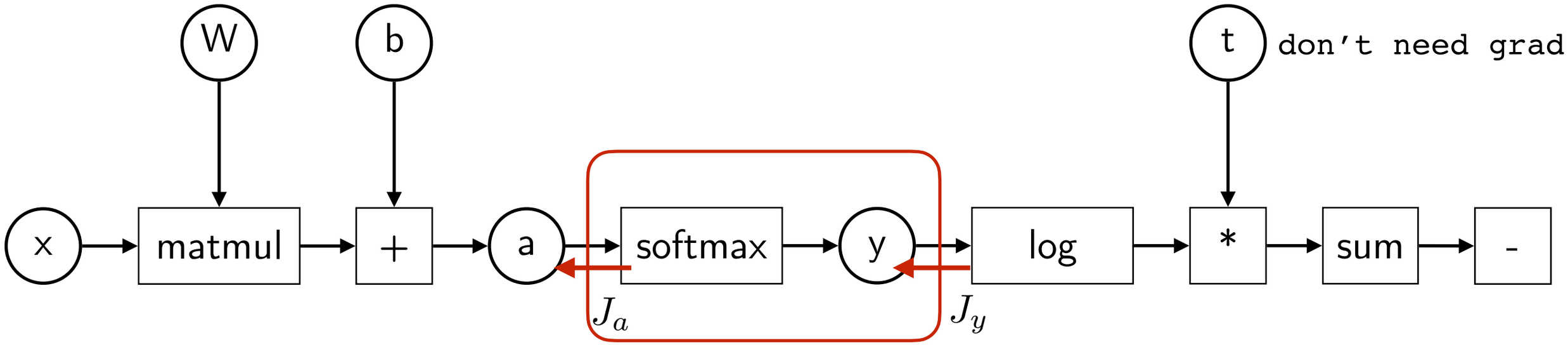
$J_W = xJ$ – outer (column-row) product

Backward Propagation



- What we have learned towards practical implementation:
  - Do not need to explicitly compute the Jacobian of each layer, only need to "backpropagate" through the layer
  - The granularity is up to the implementation: flexibility vs. efficiency
  - Need to store the input (point at which the Jacobian is evaluated) or recompute it
  - In real applications gradients are often shaped as higher dimensional tensors:
    E.g. convolution with weights w [in, out, k_h, k_w]
    - gradient in w is shaped as [in, out, k_h, k_w]
    - special efficient implementation for forward
    - special efficient implementation for backward (transposed convolution)

Backward Propagation



$$y_j = \text{softmax}(a)_j = \frac{e^{a_j}}{\sum_i e^{a_i}}$$

$$J_a = J_y(\text{Diag}(y) - yy^\mathsf{T}) = J_y \odot y - (J_y y)y^\mathsf{T}$$

1)

```
y = a.softmax()
```

2)

```
class MySoftmax(torch.nn.Module):
    def forward(self, a):
        y = a.exp()
        y = y / y.sum()
        return y
```

```
y = MySoftmax().forward(a)
```

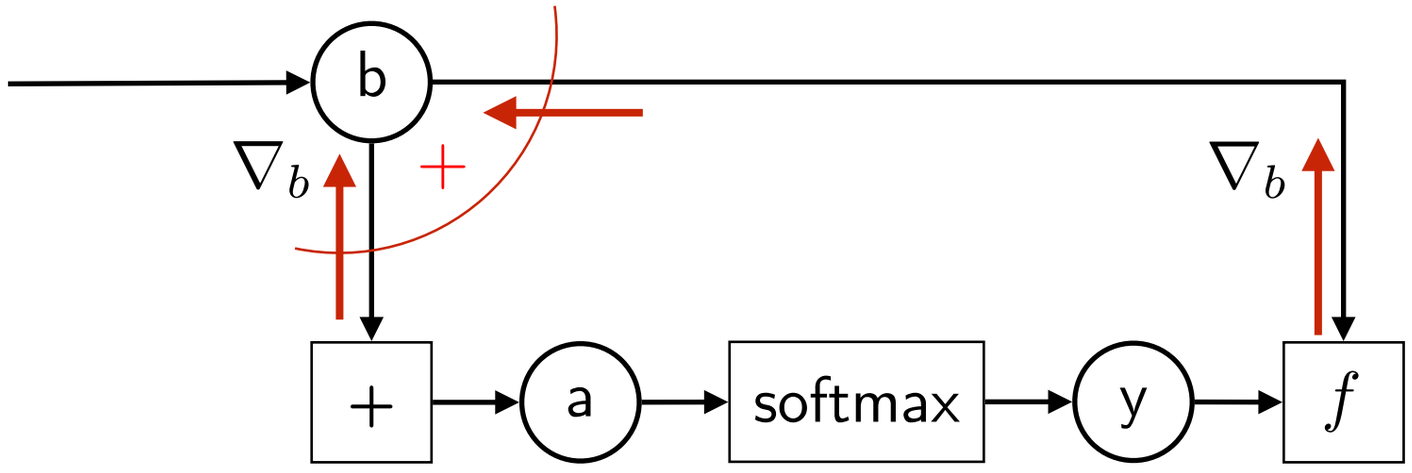
3)

```
class MySoftmax(torch.autograd.Function):
    @staticmethod
    def forward(ctx, a):
        y = a.exp()
        y /= y.sum()
        ctx.save_for_backward(y)
        return y

    @staticmethod
    def backward(ctx, dy):
        y, = ctx.saved_tensors
        da = y * dy - y * (y * dy).sum()
        return da
```

```
y = MySoftmax.apply(a)
```

General DAG

- Consider the case when some of the inputs are used in several places



- The total derivative rule:

$$\frac{\mathrm{d}}{\mathrm{d}b} f(b, y(b)) = \frac{\partial f}{\partial b} + \frac{\partial f}{\partial y} \frac{\mathrm{d}y}{\mathrm{d}b}$$

- The copy operation:

$$\bar{b}^1 = b$$

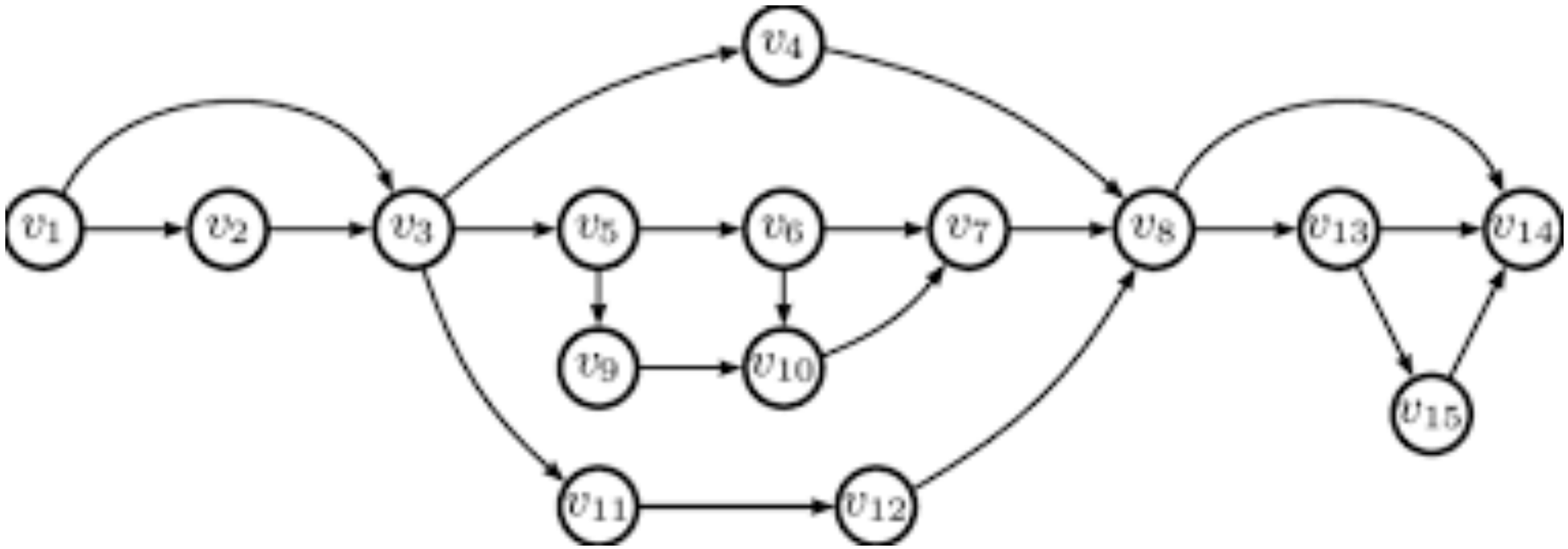
$$\bar{b}^2 = b$$

$$\begin{bmatrix} \bar{b}^1 \\ \bar{b}^2 \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \\ \\ \end{bmatrix} b$$

$$J_b = J_{\bar{b}^1} + J_{\bar{b}^2}$$

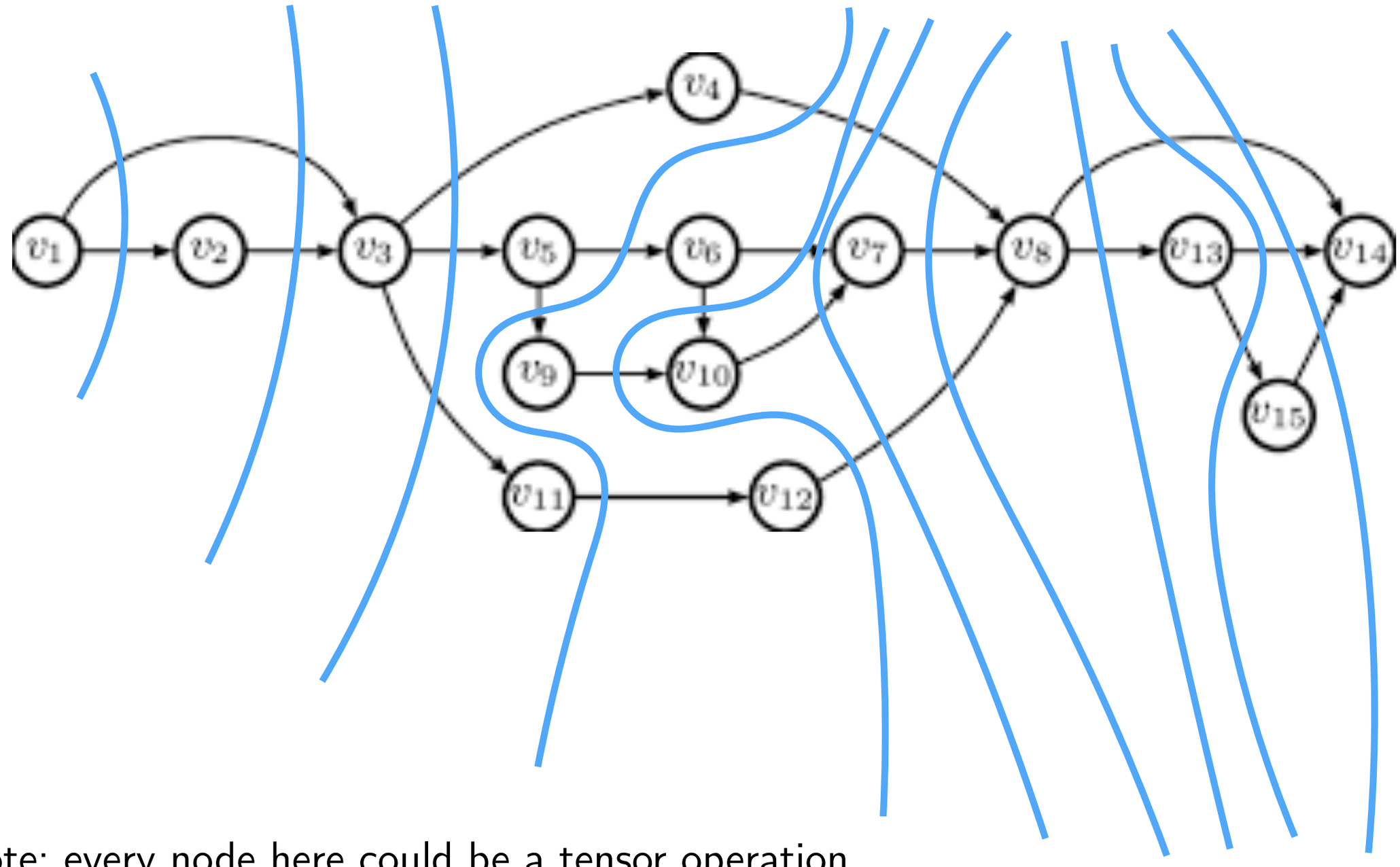
General DAG

- Need to find the order of processing
  - a node may be processed when all its parents are ready
  - some operations can be executed in parallel
  - reverse the edges for the backward pass



General DAG

- Any directed acyclic graph can be topologically ordered
  - Equivalent to a layered network with skip connections



Note: every node here could be a tensor operation

Implicit Layers

- Explicit layer: $z = f(x)$
- Implicit Layer: $g(x, z) = 0$

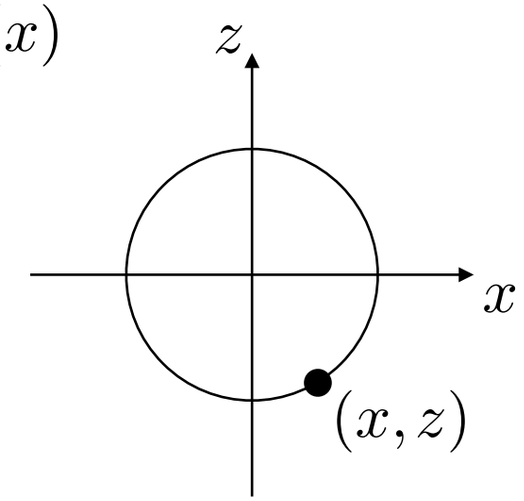
  Examples:
  - Eigenvalue decomposition: input X output (U, S) such that $X = USU^T$.
  - Finding camera pose from correspondences (system of algebraic equations)
  - Limit of fixed point iteration: $z^* = f(x, z^*)$
  - Optimization problems: $z^* = \operatorname{argmin}_z f(z, x)$
  - Differential equations

- Deep Equilibrium Model: $z^* = f(Wz^* + Ux + b)$
  - Can represent any feed-forward NN, with the same number of parameters

Implicit Layers

- Implicit Layer
  - Let $g\colon \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$. Consider vector equation $g(x, z) = \mathbf{0}$
  - Suppose we can compute a solution (x, z)
  - Under some conditions z is locally a function of x, let's call it $z(x)$

$$x^2 + z^2 = 1$$



$$g(x, z(x)) = 0$$

$$\frac{\mathrm{d}g(x, z(x))}{dx} = 0$$

$$\frac{\partial g(x, z(x))}{\partial x} + \frac{\partial g(x, z)}{\partial z}\Big|_{z=z(x)} \frac{\partial z(x)}{\partial x} = 0$$

$$\frac{\partial z(x)}{\partial x} = \left(\frac{\partial g(x, z)}{\partial z}\right)^{-1} \frac{\partial g(x, z)}{\partial x}.$$

- Backprop of $\mathcal{L}(z)$:
  - $J_z^{\mathcal{L}} \left(\frac{\partial g(x,z)}{\partial z}\right)^{-1} \left(\frac{\partial g(x,z)}{\partial x}\right)$
  - Need to solve a linear system on backward