Deep Learning (BEV033DLE)
Lecture 4. Backpropagation

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- ✦ What should it do
  - Geometric understanding
- ✦ How to compute
  - Forward / backward propagation
  - Implementation
  - General DAG, total derivatives
  - Pitfalls

What is Backpropagation?

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D) Rules for computing gradient of a composite function

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

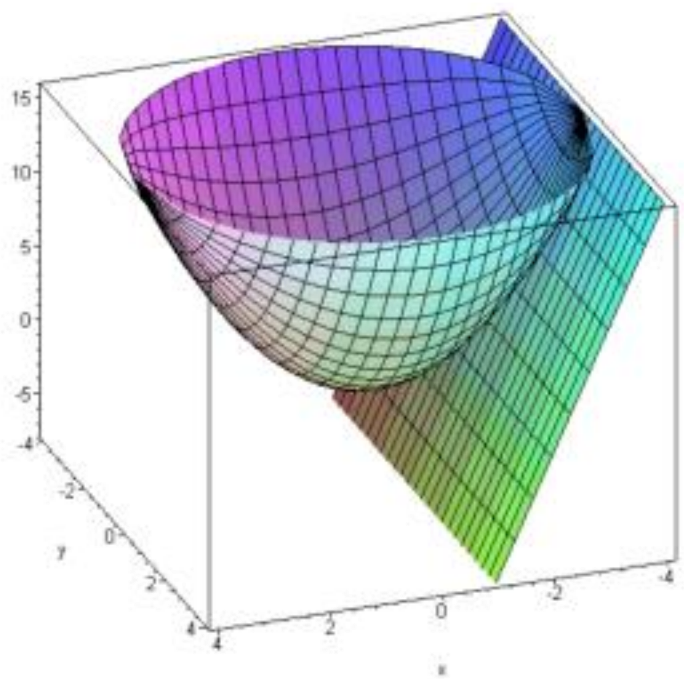
Linear Approximation to a Function

- Function $f\colon \mathbb{R}^m \to \mathbb{R}^n$
- Local linear approximation: $f(x+\Delta x) = f(x) + J(x)\Delta x + o(\|\Delta x\|)$

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

Jacobian (matrix)

$\mathbb{R}^2 \to \mathbb{R}$



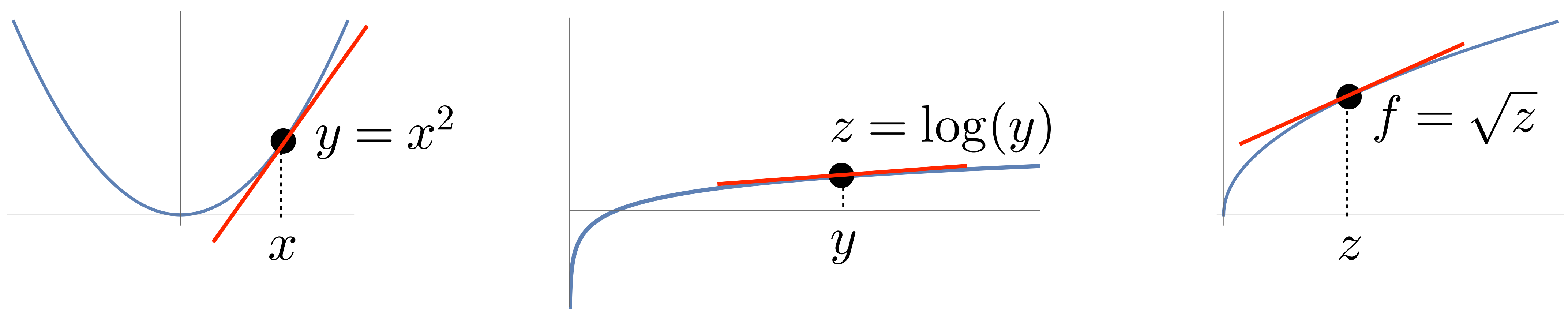
- Linear approximation is sufficient for finding descent directions
  - (Steepest) Gradient Descent, Mirror-Descent
- For a sum of functions their linear approximations add up
  - SGD, Stochastic MD
- For a composition of functions their linear approximations compose

Remark: partial derivatives should be continuous in a neighborhood. If not (e.g. with ReLU) usually it is not a problem, but we will see a pitfall later.

Compositions

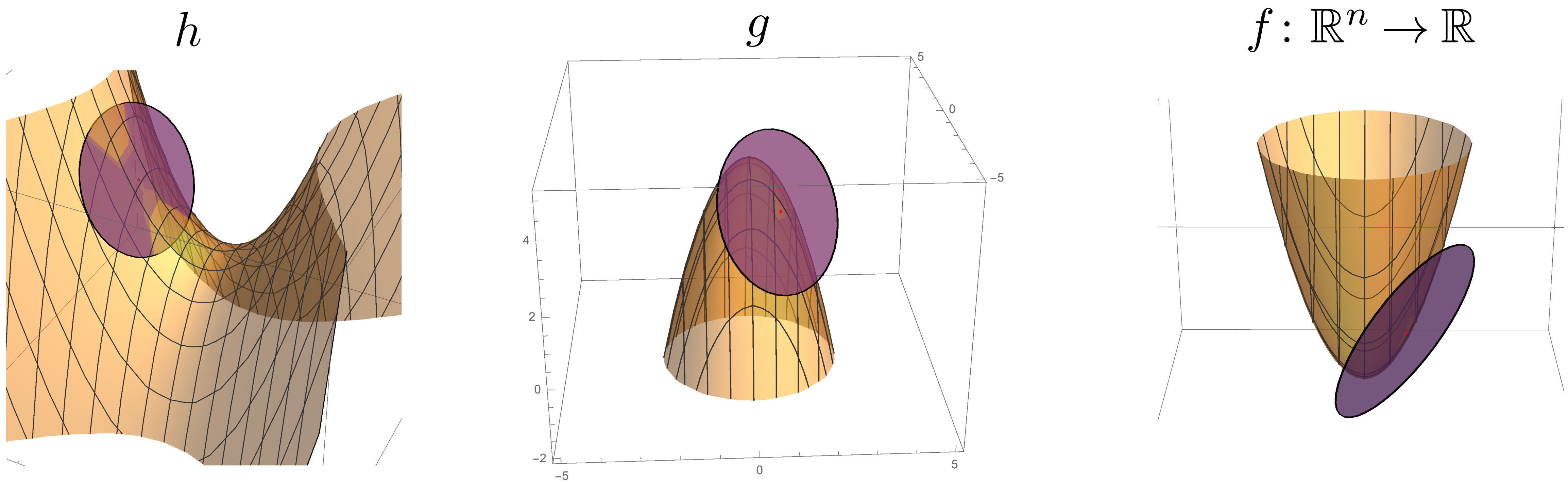
- Linear function: $f(x) = Ax$,
$$J_f = A$$
- Composition of linear functions: $f(x) = (A \circ B)x = ABx$,
$$J_f = AB$$
- Composition of non-linear functions: $f = g \circ h$,
$$J_f = J_g J_h$$
- **Chain Rule**: approximate every function in the composition locally around its argument and compose approximations

Example $f = \sqrt{\log(x^2)}$: Composition: $\sqrt{\ } \circ \log \circ \text{pow}_2$



$$J_f = \left(\frac{\partial \sqrt{z}}{\partial z}\right)_{z=\log(x^2)} \left(\frac{\partial \log y}{\partial y}\right)_{y=x^2} \left(\frac{\partial x^2}{\partial x}\right)_{x} \qquad J_f = \left(z^{-1/2}\right)\left(y^{-1}\right)(2x)$$

Scalar Loss



- Consider composition of functions: $F = f \circ g \circ h$

  Compose linear approximations: $J_F = J_f J_g J_h$

  (Notice the order is the same)

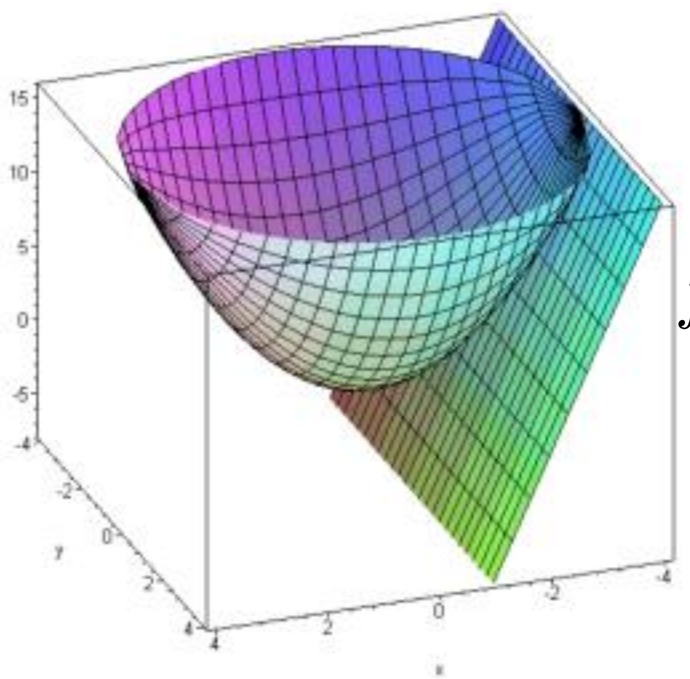
- Let f be a scalar loss: $f : \mathbb{R}^n \to \mathbb{R}$, then

$$J_F = \begin{pmatrix} \frac{\partial f}{\partial g_1} & \frac{\partial f}{\partial g_2} & \dots & \frac{\partial f}{\partial g_n} \end{pmatrix} \begin{pmatrix} \quad & J_g & \quad \end{pmatrix} \begin{pmatrix} \quad & J_h & \quad \end{pmatrix}$$

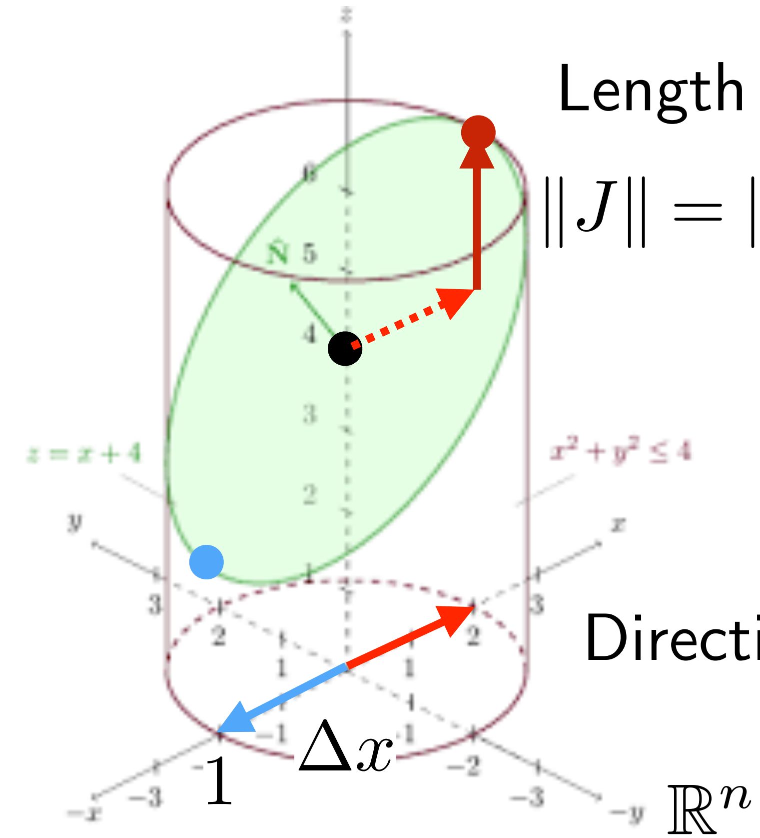
- Matrix product is associative, we can choose how to group multiplications
- Going left-to-right is cheaper: $O(Ln^2)$ *vs.* $O((L-1)n^3 + n^2)$
- Where is backward pass?

Gradient

- Consider scalar-valued function: $f\colon \mathbb{R}^n \to \mathbb{R}$



$$f(x+\Delta x) \approx f(x) + J\Delta x$$



- Jacobian J is a *row* vector $\left(\cdots \frac{\partial f}{\partial x_i} \cdots\right)$
- What is the steepest descent direction for the linear approximation?

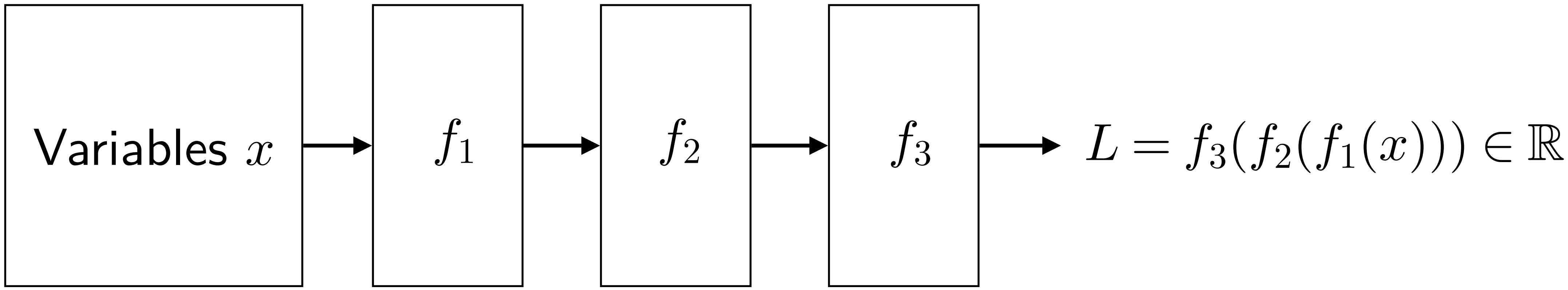
$$\min_{\|\Delta x\|=1} \left(f(x) + J\Delta x\right) \quad \Rightarrow \quad \Delta x = -\frac{J^\mathsf{T}}{\|J\|}$$

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

Backpropagation on a Higher Level

✦ Summary so far:

- Composition of functions — **forward**



- Linear approximation $L(x + \Delta x) \approx L(x) + J_L \Delta x$
- Compose linear approximations: $J_L = J_3 \circ J_2 \circ J_1$
- Transposed for the gradient: $\nabla_x L = J_L^\top = J_1^\top \circ J_2^\top \circ J_3^\top$
- Go in the **backward** order multiplying one matrix-vector at a time (reverse mode automatic differentiation)

Exercise

Let $f\colon \mathbb{R}^n \to \mathbb{R}^m$. Match concepts on the left and explanations on the right.

a) Gradient of f
b) Derivative of f
c) Jacobian of f

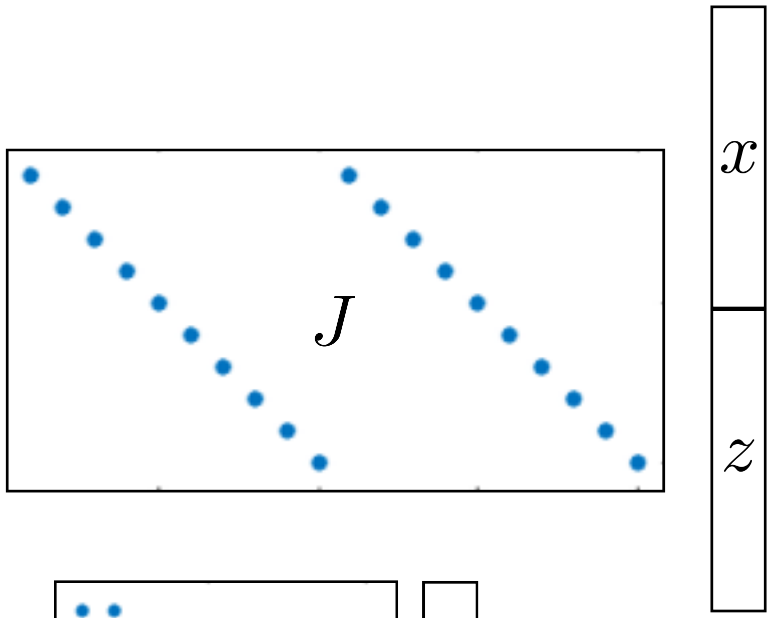
1) A linear mapping approximating f locally around a point.
2) Expression of the derivative in coordinates as a matrix.
3) Column vector of partial (or total) derivatives in case f is scalar-valued, i.e. $m = 1$.

Examples

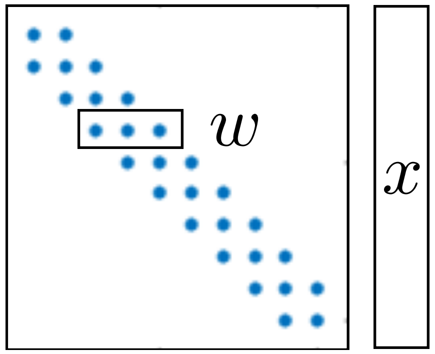
- **General procedure for back-propagating one layer** $y = y(x)$
  - $L = L(y)$ – the loss function of the layer's output (may be composite)
  - Assume already computed gradient $\nabla_y L$
  - We compute $\nabla_x L := (J_y)^\mathsf{T}(\nabla_y L)$, in components: $\nabla_{x_i} L = \sum_j \left(\frac{\partial y_j}{\partial x_i}\right)(\nabla_{y_j} L)$

- $y = Wx$
  - $\nabla_x := W^\mathsf{T} \nabla_y$

- $y = x + z$
  - $\nabla_x := \nabla_y$, $\nabla_z := \nabla_y$



- $y_j = \sum_k w_k x_{j+k} + b_j$
  - $\nabla_b := \nabla_y$
  - $\nabla_{w_k} := \sum_j \frac{\partial y_j}{w_k} \nabla_{y_j} = \sum_j x_{j+k} \nabla_{y_j}$
  - $\nabla_{x_i} := \sum_j \frac{\partial y_j}{x_i} \nabla_{y_j} = \sum_j w_{i-j} \nabla_{y_j}$



Various special cases of linear dependencies can be handled in O(n) instead of O(n^2)

A detailed complete example will follow

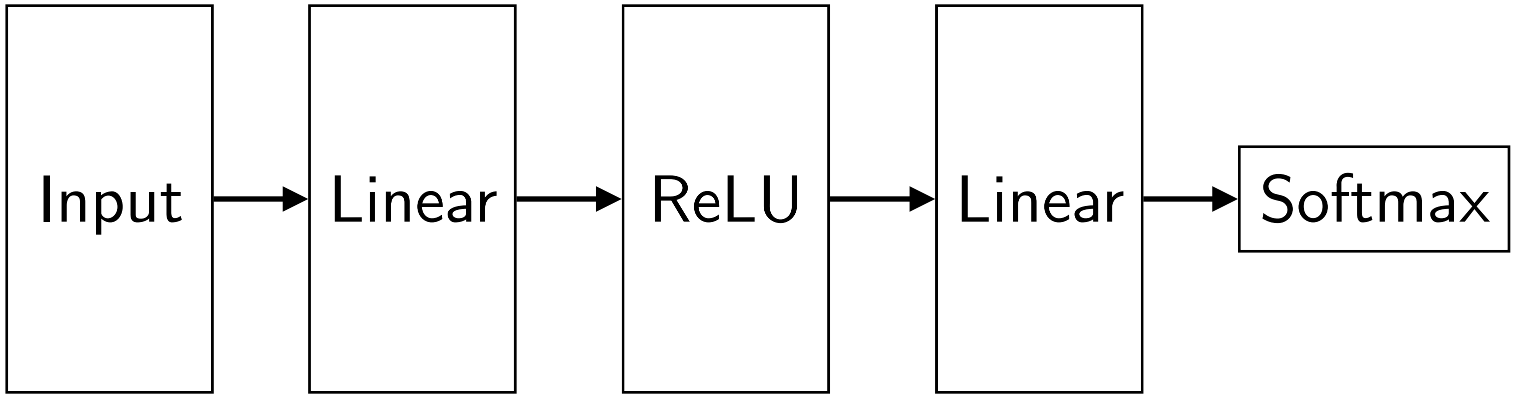
Computation Graph, Forward Propagation

✦ Approach 1:

- Declare

```
import torch
import torch.nn as nn

net = nn.Sequential(
    nn.Linear(748, 200),
    nn.ReLU(),
    nn.Linear(200, 10),
    nn.Softmax(),
)
```



Nothing is computed yet

- Execute it with some input (forward propagation)

```
x = torch.randn(748)
y = net.forward(x)
```

Software already knows the graph (here sequence),

what inputs and parameters each operation has and how to apply it,

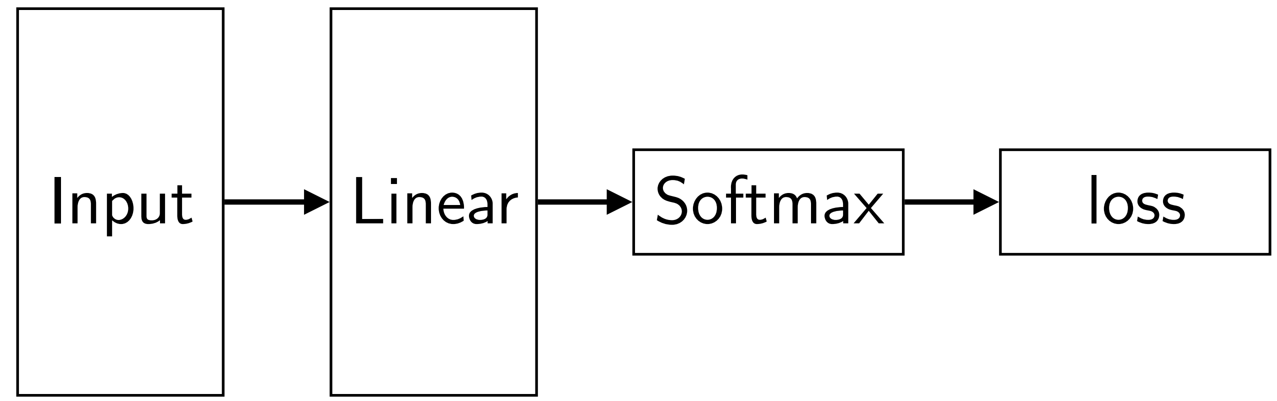
saves the output of each operation,

may optimize the computation.

Computation Graph, Forward Propagation

- Approach 2:
  - Compute what we need

Higher level model graph



Declare and initialize variables

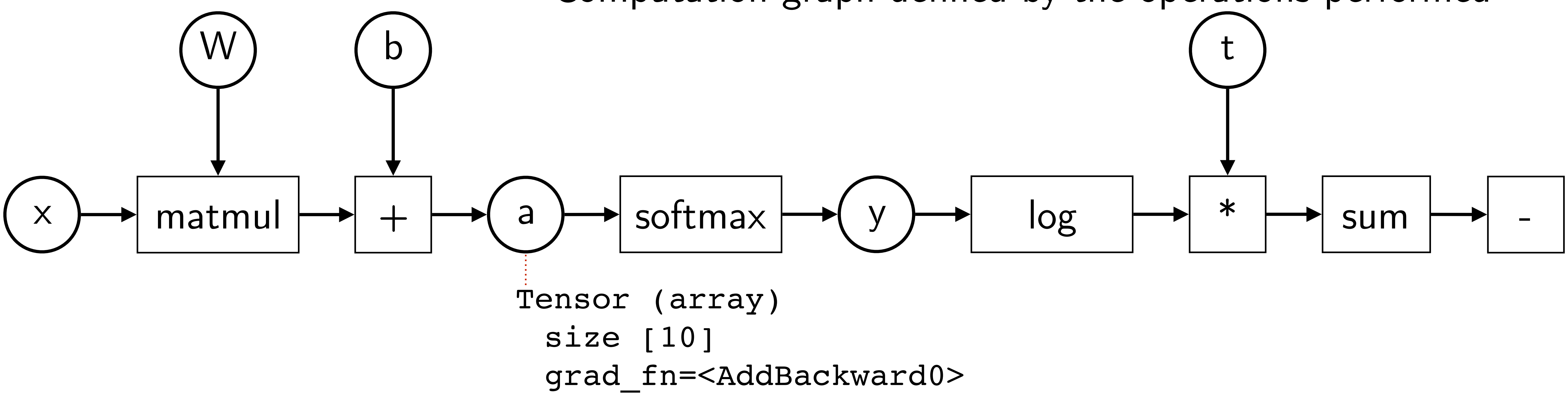
```
from torch.nn import Parameter
import torch.nn.functional as F

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

Perform some operations

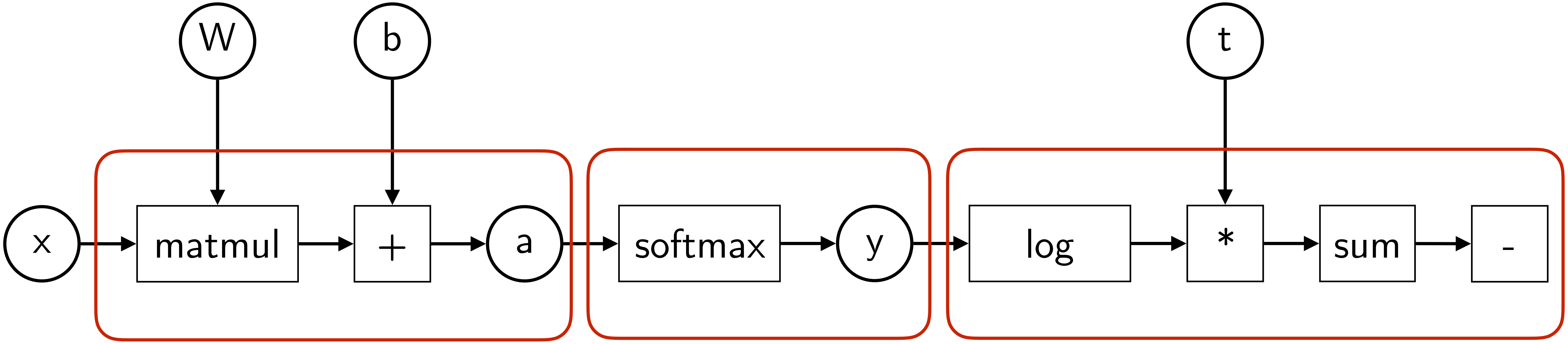
```
a = W.matmul(x) + b
y = F.softmax(a)
loss = -(t * y.log()).sum()
```

Computation graph defined by the operations performed



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

Backward Propagation



$a = \mathrm{linear}(x, W, b)$

$y = \mathrm{softmax}(a)$

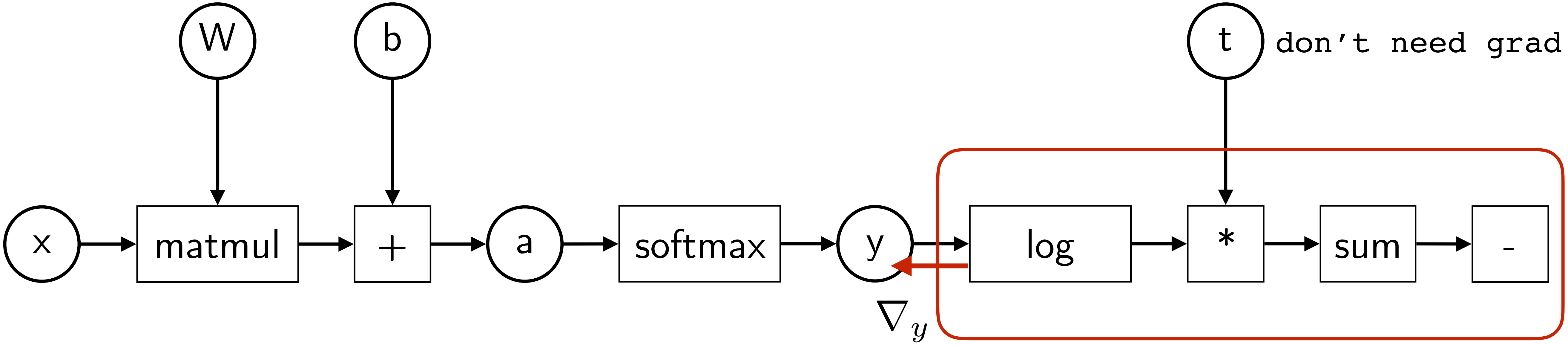
$L = -t^{\mathsf{T}} \log(y)$

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

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

- For the purpose of example we will propagate these larger blocks

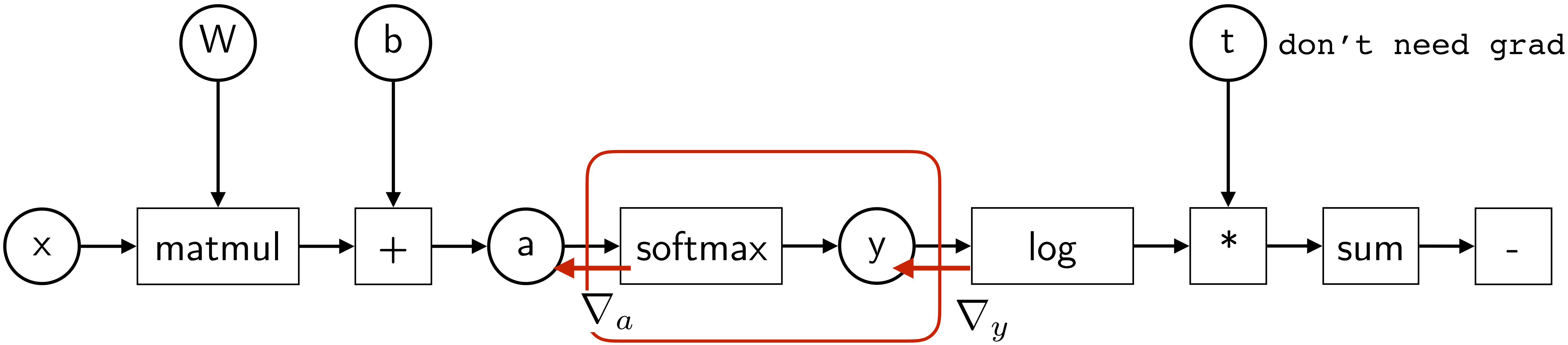
Backward Propagation



$$L = -t^\top \log(y)$$

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

Backward Propagation



Recall: $y_j = \frac{e^{a_j}}{\sum_i e^{a_i}}$

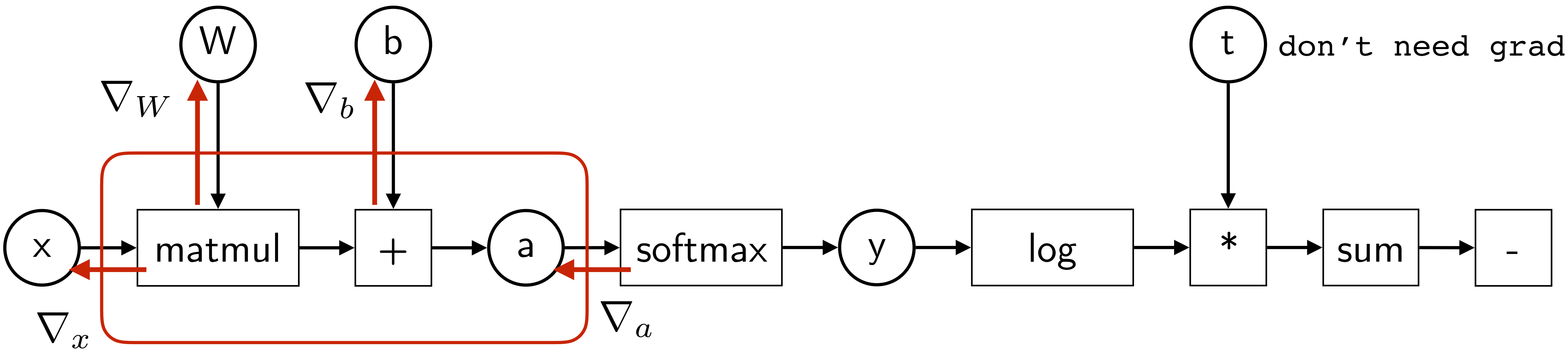
$$\nabla_{a_i} = \sum_j \frac{\partial y_j}{\partial a_i} \nabla_{y_j}$$

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

$$\nabla_a = (\mathrm{Diag}(y) - y y^\mathsf{T}) \nabla_y = y \odot \nabla_y - y (y^\mathsf{T} \nabla_y)$$

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

Backward Propagation



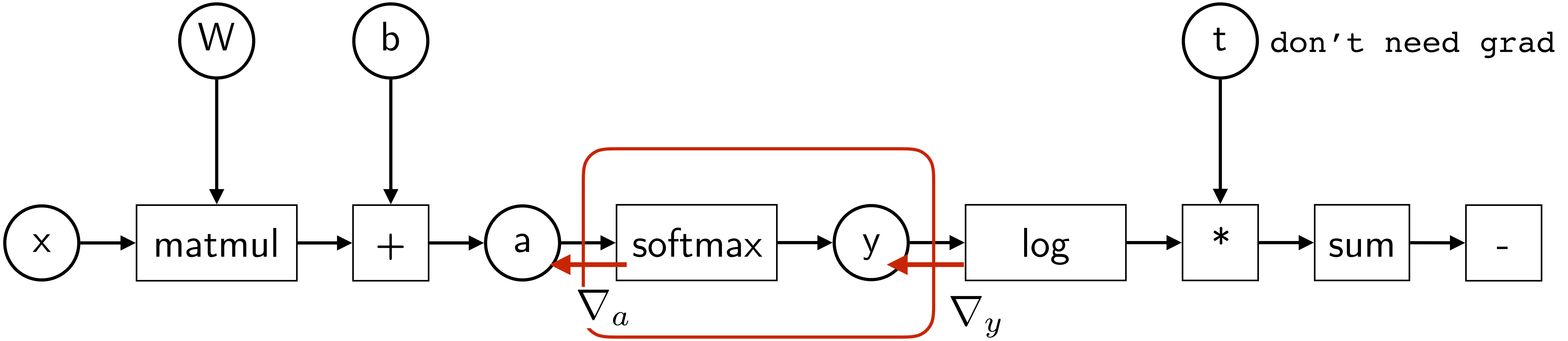
Recall: $a_j = \sum_i W_{ji} x_i + b$

$\nabla_b = \nabla_a$

$\nabla_{x_i} = \sum_j \frac{\partial a_j}{\partial x_i} \nabla_{a_j} = \sum_j W_{ij} \nabla_{a_j}$
$\nabla_x = W^\mathsf{T} \nabla_a$

$\nabla_{W_{ji}} = \sum_j \frac{\partial a_j}{\partial W_{ji}} \nabla_{a_j} = x_i \nabla_{a_j}$
$\nabla_W = (\nabla_a) x^\mathsf{T}$ – outer (column-row) product

Backward Propagation



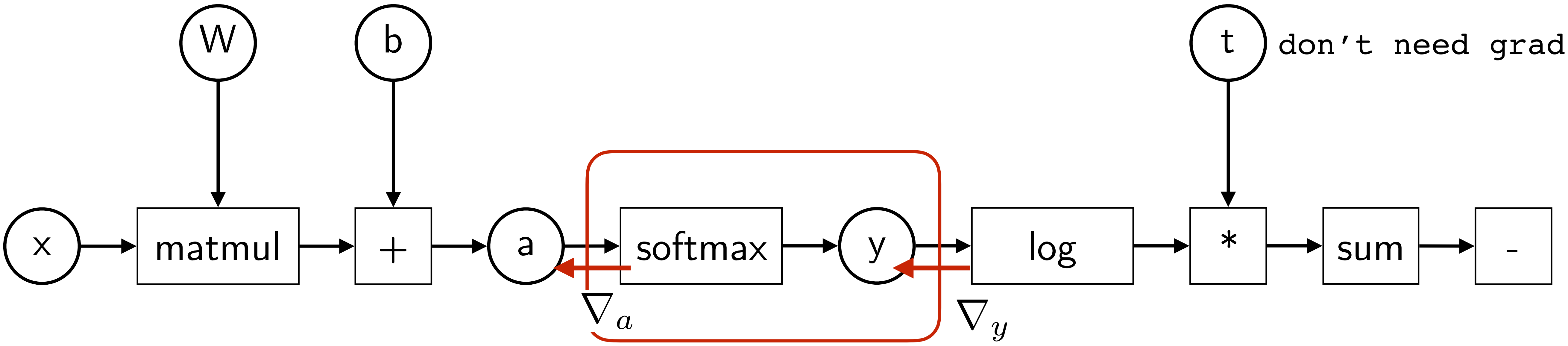
Recall: $y_j = \frac{e^{a_j}}{\sum_i e^{a_i}}$

$$\nabla_a = (\mathrm{Diag}(y) - yy^\mathsf{T})\nabla_y = y \odot \nabla_y - y(y^\mathsf{T}\nabla_y)$$

```python
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
```

Backward Propagation



Recall: $y_j = \frac{e^{a_j}}{\sum_i e^{a_i}}$

$$\nabla_a = (\mathrm{Diag}(y) - yy^\mathsf{T})\nabla_y = y \odot \nabla_y - y(y^\mathsf{T}\nabla_y)$$

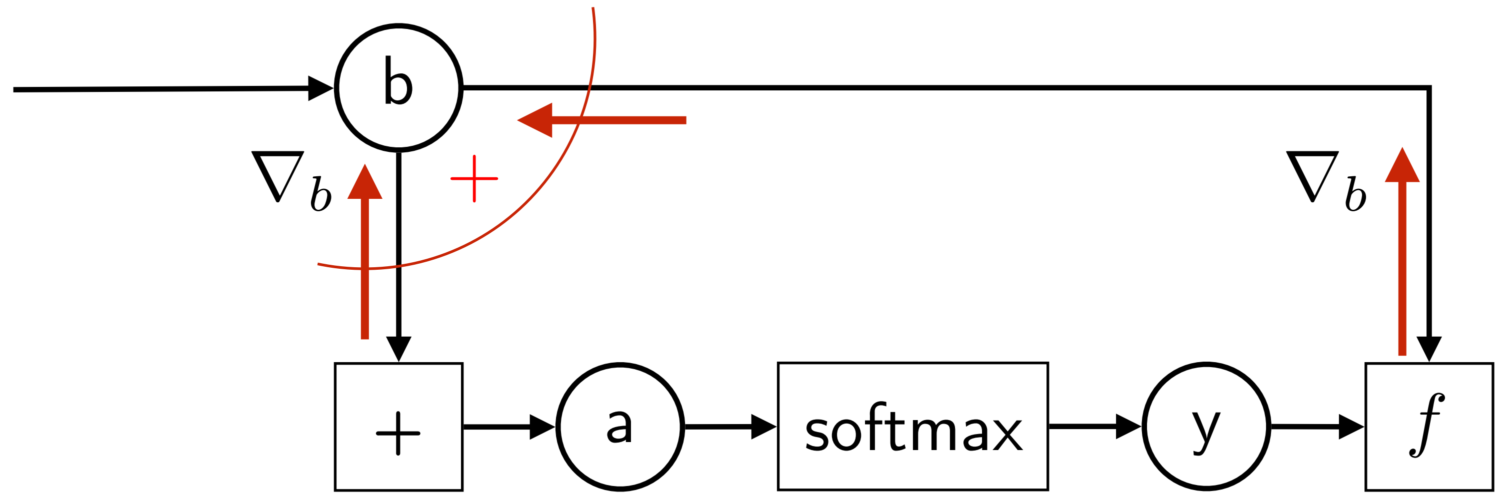
```
class MySoftmax:
    def forward(self, a):
        y = a.exp()
        y /= y.sum()
        self.y = y
        return y

    def backward(self, dy):
        y = self.y
        da = y * dy - y * (y * dy).sum()
        return da

    def cleanup(self):
        del self.y
```

General DAG

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

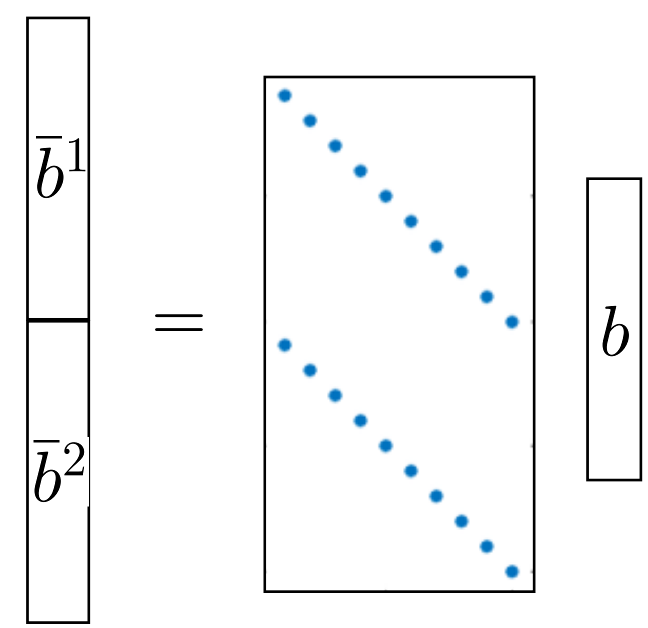


- The total derivative rule emerges:

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

- Follows from the composition:

$$f(\bar{b}) = f(\bar{b}^1, y(\bar{b}^2))$$



$$\nabla_b = \nabla_{\bar{b}^1} + \nabla_{\bar{b}^2}$$

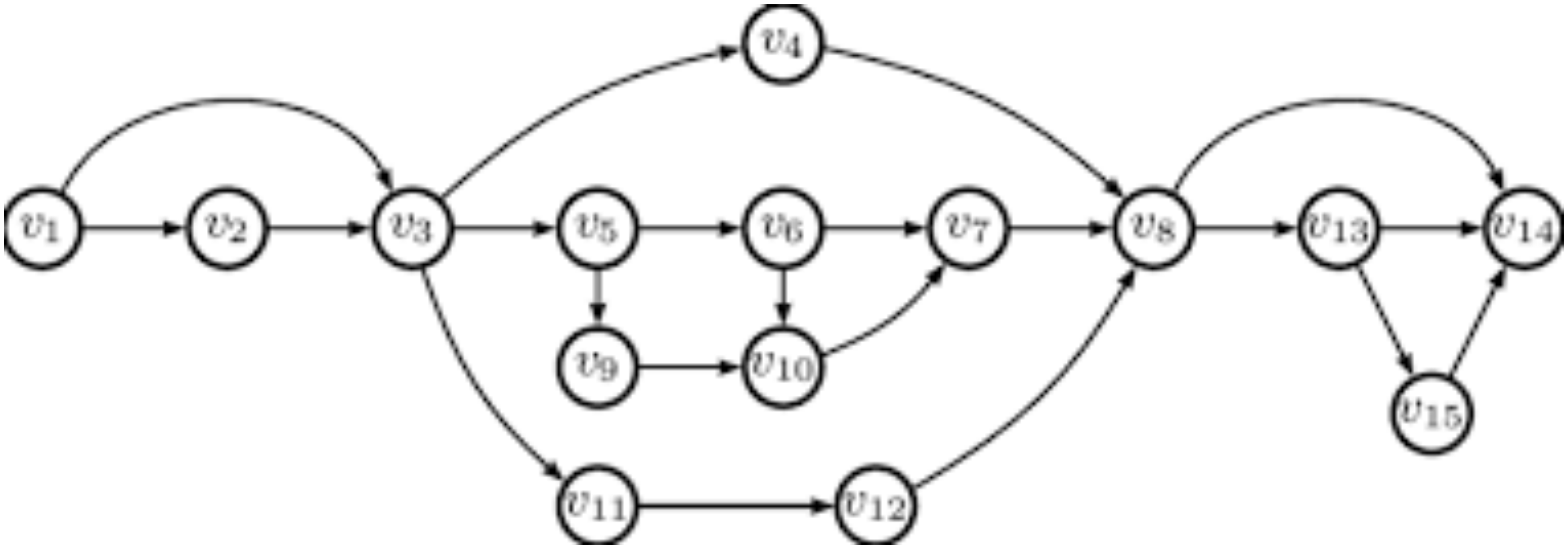
We can say then:

- Jacobian of composition = "total Jacobian"
- Gradient of a composition = "total gradient"

General DAG

✦ Need to find the order of processing

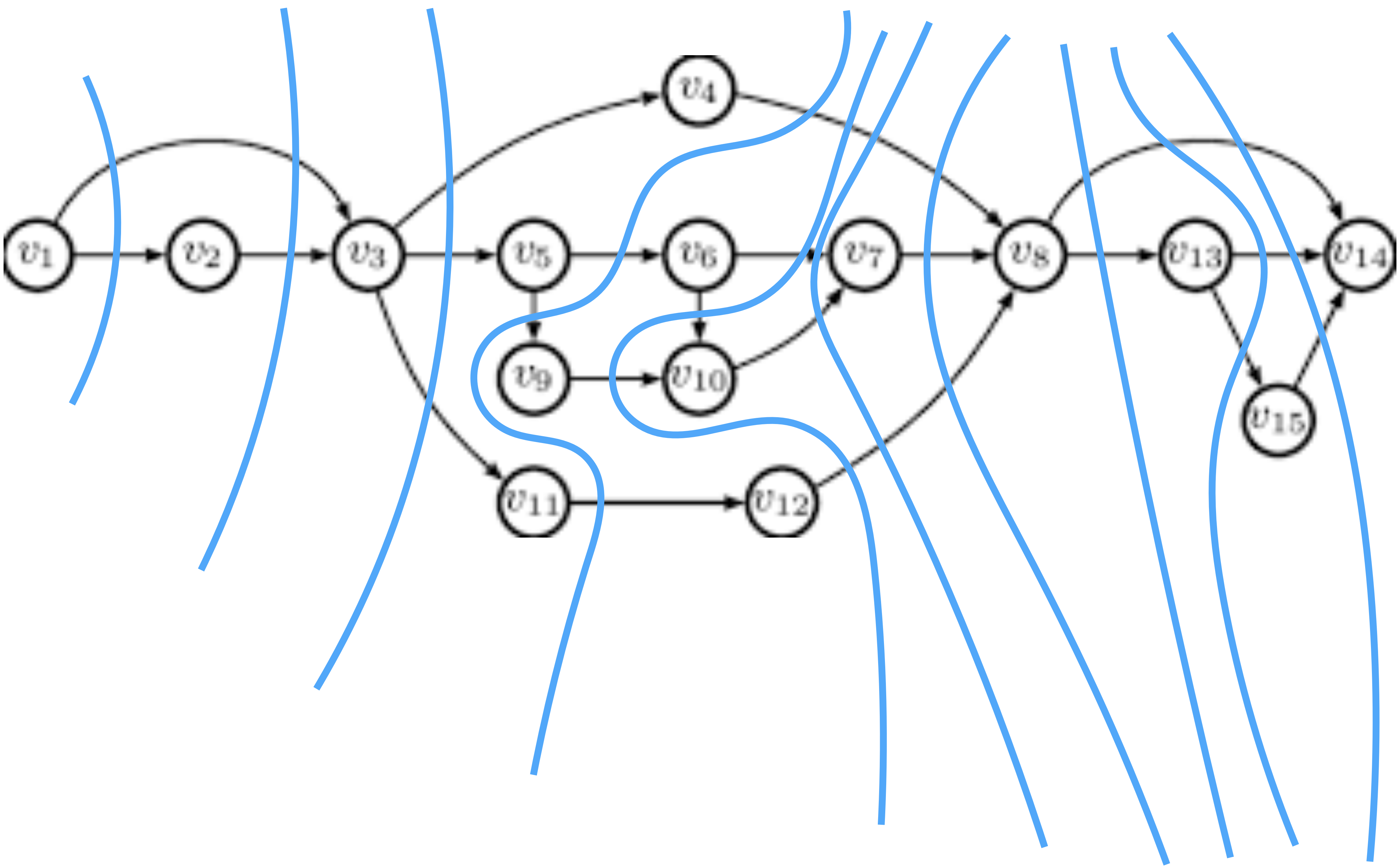
- a node may be processed when all its parents are ready
- some operations can be executed in parallel
- for the backward pass we reverse the edges



General DAG

✦ Any directed acyclic graph can be topologically ordered

- Equivalent to a layered network with skip connections
- Equivalent to a layered network with extended layer outputs



General DAG

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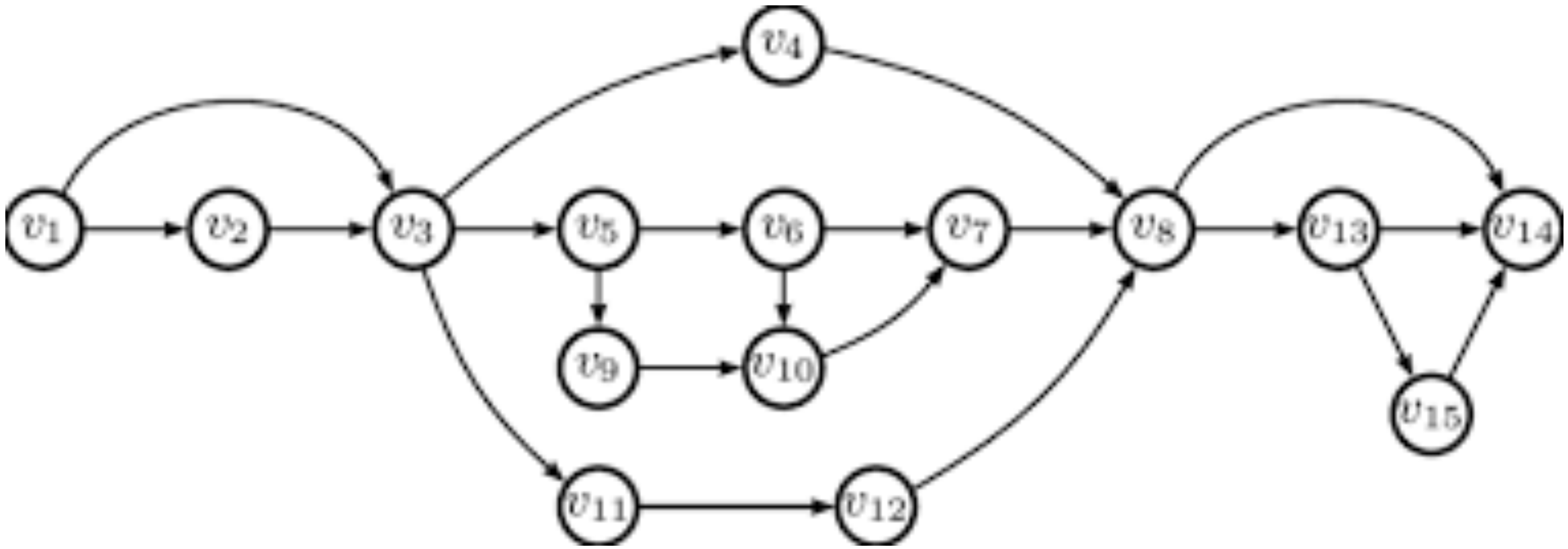
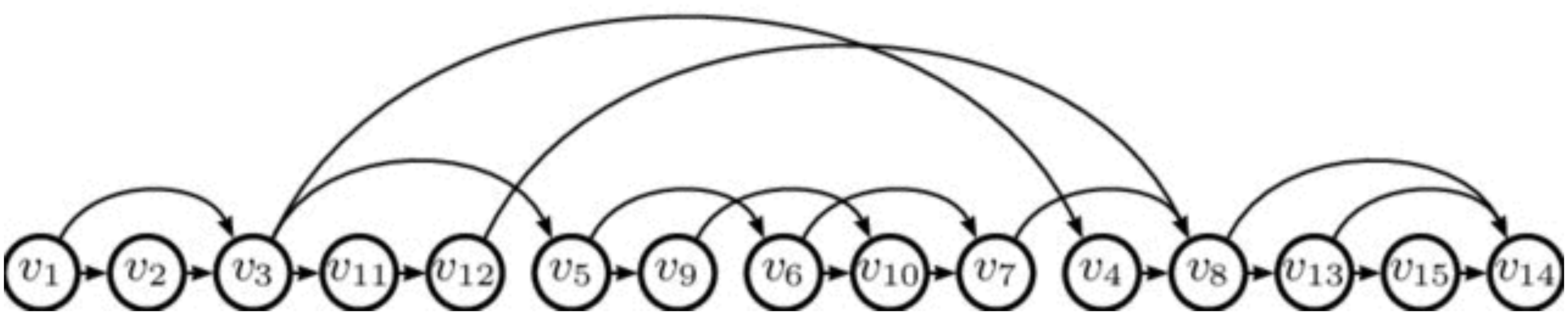


Can be made a total order, but here we do not see what can be executed in parallel



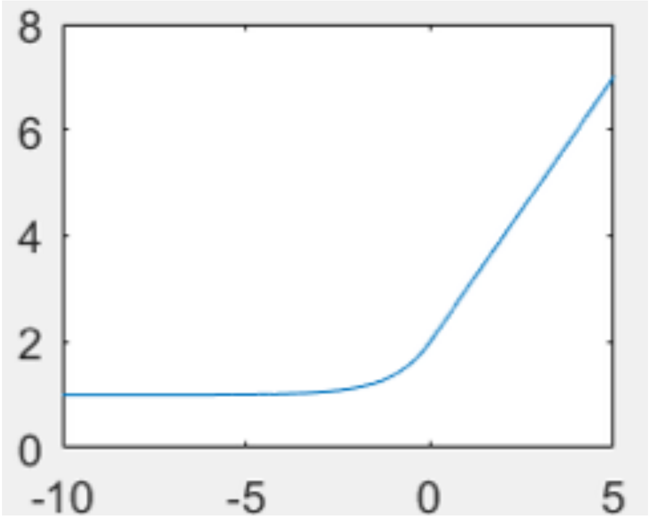
Pitfalls

- Discontinuous Gradients Example

  A nice smooth function: $y = \min(e^x, 1) + \max(x+1, 1)$

  Suppose we initialized with $x = 0$

  Why the gradient is zero?



- Exponents e.g. in the $\mathrm{softmax}(x) = \frac{e_i^x}{\sum_i e^{x_i}}$ will overflow when $x_i > 88.7$
  - may be cancelled in the numerator and denominator in advance

($\star$) $\log\mathrm{softmax}$ is a more friendly function with bounded derivatives

Advanced Variants

- Derivatives of implicit functions
- Derivatives of optimization problems