# Introduction to Deep Learning

## 3. Gradient and Auto Differentiation

## STAT 157, Spring 2019, UC Berkeley


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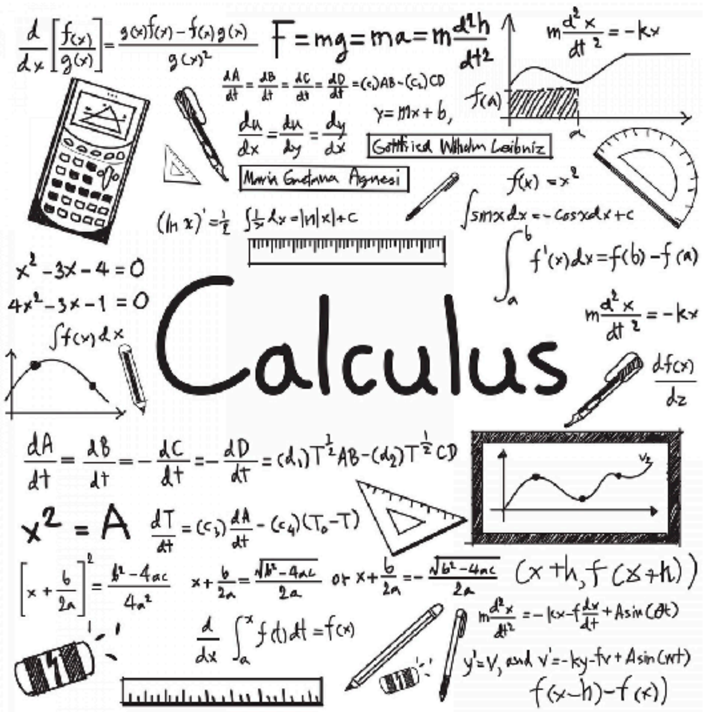
## courses.d2l.ai/berkeley-stat-157

# Matrix



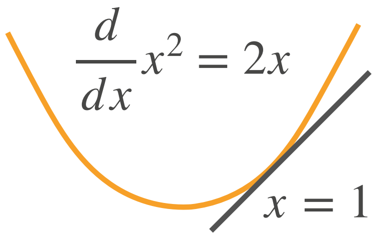
# Review Scalar Derivative

| $y$ | $a$ | $x^n$ | $\exp(x)$ | $\log(x)$ | $\sin(x)$ |
|---|---|---|---|---|---|
| $\frac{dy}{dx}$ | $0$ | $nx^{n-1}$ | $\exp(x)$ | $\frac{1}{x}$ | $\cos(x)$ |

$a$ is not a function of $x$

| $y$ | $u+v$ | $uv$ | $y=f(u),\ u=g(x)$ |
|---|---|---|---|
| $\frac{dy}{dx}$ | $\frac{du}{dx}+\frac{dv}{dx}$ | $\frac{du}{dx}v+\frac{dv}{dx}u$ | $\frac{dy}{du}\frac{du}{dx}$ |

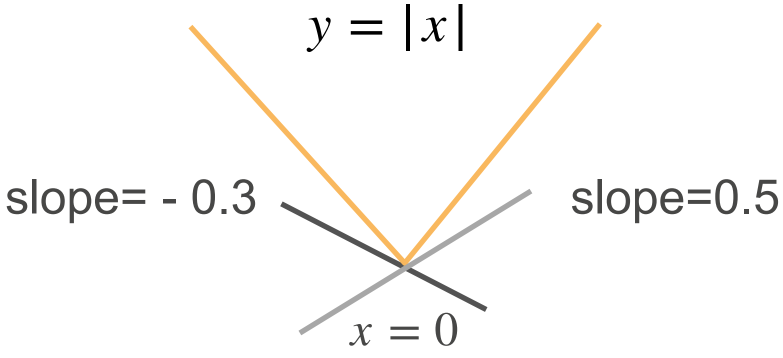
Derivative is the slope of the tangent line




The slope of the tangent line is 2

# Subderivative

- Extend derivative to non-differentiable cases




$$\frac{\partial |x|}{\partial x} = \begin{cases} 1 & \text{if } x > 0 \\ -1 & \text{if } x < 0 \\ a & \text{if } x = 0, \quad a \in [-1,1] \end{cases}$$

Another example:

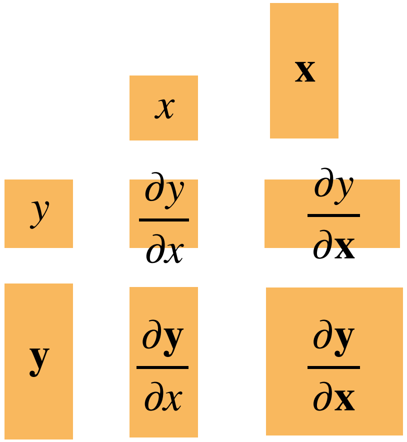
$$\frac{\partial}{\partial x} \max(x,0) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0 \\ a & \text{if } x = 0, \quad a \in [0,1] \end{cases}$$

# Gradients

- Generalize derivatives into vectors

| | | Scalar | Vector |
|---|---|---|---|
| | | $x$ | $\mathbf{x}$ |
| Scalar | $y$ | $\frac{\partial y}{\partial x}$ | $\frac{\partial y}{\partial \mathbf{x}}$ |
| Vector | $\mathbf{y}$ | $\frac{\partial \mathbf{y}}{\partial x}$ | $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$ |

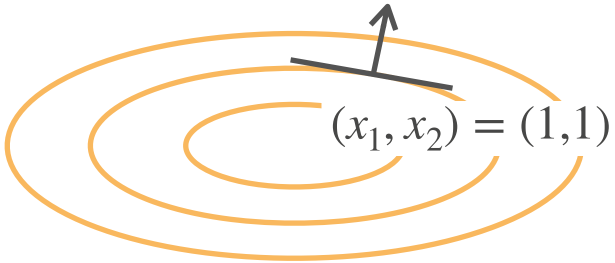
# $\partial y / \partial \mathbf{x}$




$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \frac{\partial y}{\partial \mathbf{x}} = \left[\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \ldots, \frac{\partial y}{\partial x_n}\right]$$

$$\frac{\partial}{\partial \mathbf{x}} x_1^2 + 2x_2^2 = [2x_1, 4x_2]$$

Direction (2, 4), perpendicular to the contour lines



# Examples

| $y$ | $a$ | $au$ | $\text{sum}(\mathbf{x})$ | $\|\mathbf{x}\|^2$ |
|---|---|---|---|---|
| $\frac{\partial y}{\partial \mathbf{x}}$ | $\mathbf{0}^T$ | $a\frac{\partial u}{\partial \mathbf{x}}$ | $\mathbf{1}^T$ | $2\mathbf{x}^T$ |

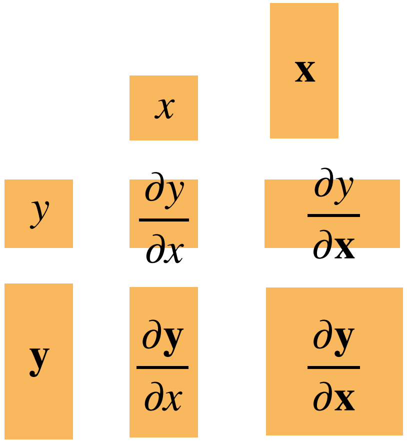
$a$ is not a function of $\mathbf{x}$

$\mathbf{0}$ and $\mathbf{1}$ are vectors

| $y$ | $u+v$ | $uv$ | $\langle \mathbf{u}, \mathbf{v} \rangle$ |
|---|---|---|---|
| $\frac{\partial y}{\partial \mathbf{x}}$ | $\frac{\partial u}{\partial \mathbf{x}} + \frac{\partial v}{\partial \mathbf{x}}$ | $\frac{\partial u}{\partial \mathbf{x}}v + \frac{\partial v}{\partial \mathbf{x}}u$ | $\mathbf{u}^T\frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \mathbf{v}^T\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$ |

# $\partial \mathbf{y}/\partial x$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \qquad \frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} \\ \frac{\partial y_2}{\partial x} \\ \vdots \\ \frac{\partial y_m}{\partial x} \end{bmatrix}$$

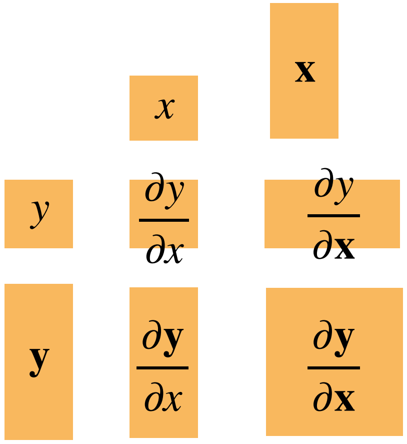



$\partial y/\partial \mathbf{x}$ is a row vector, while $\partial \mathbf{y}/\partial x$ is a column vector

It is called numerator-layout notation. The reversed version is called denominator-layout notation

# $\partial \mathbf{y}/\partial \mathbf{x}$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$




$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial \mathbf{x}} \\ \frac{\partial y_2}{\partial \mathbf{x}} \\ \vdots \\ \frac{\partial y_m}{\partial \mathbf{x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1}, \frac{\partial y_1}{\partial x_2}, \ldots, \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1}, \frac{\partial y_2}{\partial x_2}, \ldots, \frac{\partial y_2}{\partial x_n} \\ \vdots \\ \frac{\partial y_m}{\partial x_1}, \frac{\partial y_m}{\partial x_2}, \ldots, \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

# Examples

| $\mathbf{y}$ | $\mathbf{a}$ | $\mathbf{x}$ | $\mathbf{A}\mathbf{x}$ | $\mathbf{x}^T\mathbf{A}$ |
|---|---|---|---|---|
| $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$ | $\mathbf{0}$ | $\mathbf{I}$ | $\mathbf{A}$ | $\mathbf{A}^T$ |

$$\mathbf{x} \in \mathbb{R}^n, \quad \mathbf{y} \in \mathbb{R}^m, \quad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \in \mathbb{R}^{m \times n}$$

$a$, $\mathbf{a}$ and $\mathbf{A}$ are not functions of $\mathbf{x}$

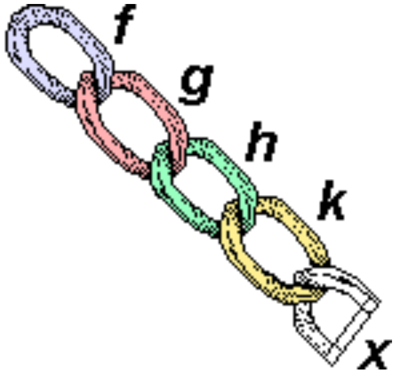
$\mathbf{0}$ and $\mathbf{I}$ are matrices

| $\mathbf{y}$ | $a\mathbf{u}$ | $\mathbf{A}\mathbf{u}$ | $\mathbf{u} + \mathbf{v}$ |
|---|---|---|---|
| $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$ | $a\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$ | $\mathbf{A}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$ | $\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$ |

# Generalize to Matrices

| | | Scalar | Vector | Matrix |
|---|---|---|---|---|
| | | $x$ $(1,)$ | $\mathbf{x}$ $(n,1)$ | $\mathbf{X}$ $(n,k)$ |
| Scalar | $y$ $(1,)$ | $\frac{\partial y}{\partial x}$ $(1,)$ | $\frac{\partial y}{\partial \mathbf{x}}$ $(1,n)$ | $\frac{\partial y}{\partial \mathbf{X}}$ $(k,n)$ |
| Vector | $\mathbf{y}$ $(m,1)$ | $\frac{\partial \mathbf{y}}{\partial x}$ $(m,1)$ | $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$ $(m,n)$ | $\frac{\partial \mathbf{y}}{\partial \mathbf{X}}$ $(m,k,n)$ |
| Matrix | $\mathbf{Y}$ $(m,l)$ | $\frac{\partial \mathbf{Y}}{\partial x}$ $(m,l)$ | $\frac{\partial \mathbf{Y}}{\partial \mathbf{x}}$ $(m,l,n)$ | $\frac{\partial \mathbf{Y}}{\partial \mathbf{X}}$ $(m,l,k,n)$ |

# Chain Rule



# Generalize to Vectors

- Chain rule for scalars:

$$y = f(u),\ u = g(x) \qquad \frac{\partial y}{\partial x} = \frac{\partial y}{\partial u}\frac{\partial u}{\partial x}$$

- Generalize to vectors straightforwardly

$$\underset{(1,n)}{\frac{\partial y}{\partial \mathbf{x}}} = \underset{(1,)}{\frac{\partial y}{\partial u}}\underset{(1,n)}{\frac{\partial u}{\partial \mathbf{x}}} \qquad \underset{(1,n)}{\frac{\partial y}{\partial \mathbf{x}}} = \underset{(1,k)}{\frac{\partial y}{\partial \mathbf{u}}}\underset{(k,n)}{\frac{\partial \mathbf{u}}{\partial \mathbf{x}}} \qquad \underset{(m,n)}{\frac{\partial \mathbf{y}}{\partial \mathbf{x}}} = \underset{(m,k)}{\frac{\partial \mathbf{y}}{\partial \mathbf{u}}}\underset{(k,n)}{\frac{\partial \mathbf{u}}{\partial \mathbf{x}}}$$

# Example 1

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$$

Assume $\mathbf{x}, \mathbf{w} \in \mathbb{R}^n, \quad y \in \mathbb{R}$

$$z = \left( \langle \mathbf{x}, \mathbf{w} \rangle - y \right)^2$$

Compute $\frac{\partial z}{\partial \mathbf{w}}$

Decompose

$$a = \langle \mathbf{x}, \mathbf{w} \rangle$$
$$b = a - y$$
$$z = b^2$$

$$\begin{aligned}
\frac{\partial z}{\partial \mathbf{w}} &= \frac{\partial z}{\partial b} \frac{\partial b}{\partial a} \frac{\partial a}{\partial \mathbf{w}} \\
&= \frac{\partial b^2}{\partial b} \frac{\partial a - y}{\partial a} \frac{\partial \langle \mathbf{x}, \mathbf{w} \rangle}{\partial \mathbf{w}} \\
&= 2b \cdot 1 \cdot \mathbf{x}^T \\
&= 2 \left( \langle \mathbf{x}, \mathbf{w} \rangle - y \right) \mathbf{x}^T
\end{aligned}$$

# Example 2

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$$

Assume $\mathbf{X} \in \mathbb{R}^{m \times n}, \quad \mathbf{w} \in \mathbb{R}^n, \quad \mathbf{y} \in \mathbb{R}^m$

$$z = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

Compute $\dfrac{\partial z}{\partial \mathbf{w}}$

Decompose

$$\mathbf{a} = \mathbf{X}\mathbf{w}$$
$$\mathbf{b} = \mathbf{a} - \mathbf{y}$$
$$z = \|\mathbf{b}\|^2$$

$$\begin{aligned}
\frac{\partial z}{\partial \mathbf{w}} &= \frac{\partial z}{\partial \mathbf{b}} \frac{\partial \mathbf{b}}{\partial \mathbf{a}} \frac{\partial \mathbf{a}}{\partial \mathbf{w}} \\
&= \frac{\partial \|\mathbf{b}\|^2}{\partial \mathbf{b}} \frac{\partial \mathbf{a} - \mathbf{y}}{\partial \mathbf{a}} \frac{\partial \mathbf{X}\mathbf{w}}{\partial \mathbf{w}} \\
&= 2\mathbf{b}^T \times \mathbf{I} \times \mathbf{X} \\
&= 2\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)^T \mathbf{X}
\end{aligned}$$

# Auto Differentiation

# Auto Differentiation (AD)

- AD evaluates gradients of a function specified by a program at given values
- AD differs to
  - Symbolic differentiation

```
In[1]:= D[4 x^3 + x^2 + 3, x]

Out[1]= 2 x + 12 x^2
```

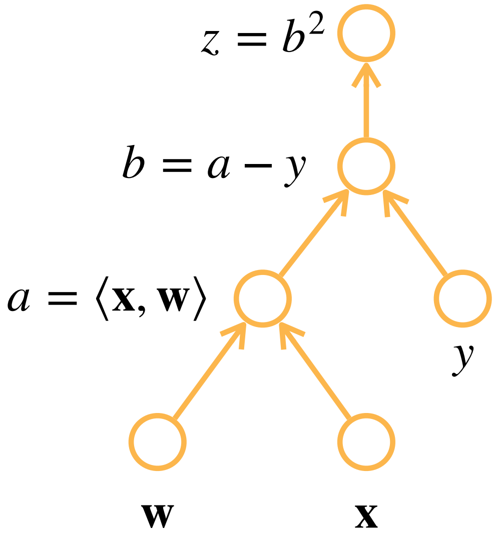
  - Numerical differentiation

$$\frac{\partial f(x)}{\partial x} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

# Computation Graph

Assume $z = \left(\langle \mathbf{x}, \mathbf{w} \rangle - y\right)^2$

- Decompose into primitive operations
- Build a directed acyclic graph to present the computation



# Computation Graph

- Decompose into primitive operations
- Build a directed acyclic graph to present the computation
- Build explicitly
    - Tensorflow/Theano/MXNet

```
from mxnet import sym

a = sym.var()
b = sym.var()
c = 2 * a + b
# bind data into a and b later
```

# Computation Graph

- Decompose into primitive operations
- Build a directed acyclic graph to present the computation
- Build explicitly
  - Tensorflow/Theano/MXNet
- Build implicitly though tracing
  - PyTorch/MXNet

```
from mxnet import autograd, nd

with autograd.record():
    a = nd.ones((2,1))
    b = nd.ones((2,1))
    c = 2 * a + b
```

# Two Modes

- By chain rule $$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u_n}\frac{\partial u_n}{\partial u_{n-1}}\dots\frac{\partial u_2}{\partial u_1}\frac{\partial u_1}{\partial x}$$

- Forward accumulation

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u_n}\left(\frac{\partial u_n}{\partial u_{n-1}}\left(\dots\left(\frac{\partial u_2}{\partial u_1}\frac{\partial u_1}{\partial x}\right)\right)\right)$$

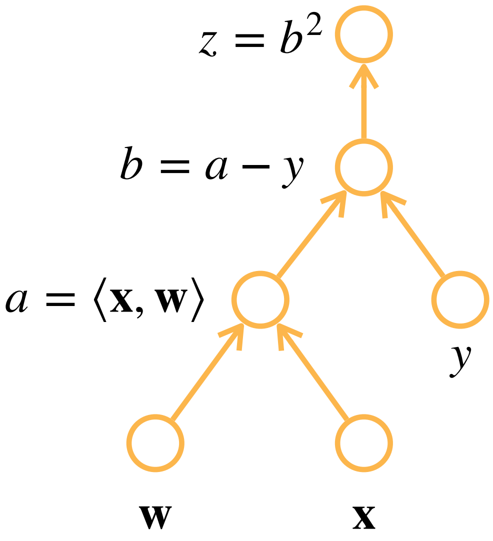
- Reverse accumulation (a.k.a Backpropagation)

$$\frac{\partial y}{\partial x} = \left(\left(\left(\frac{\partial y}{\partial u_n}\frac{\partial u_n}{\partial u_{n-1}}\right)\dots\right)\frac{\partial u_2}{\partial u_1}\right)\frac{\partial u_1}{\partial x}$$

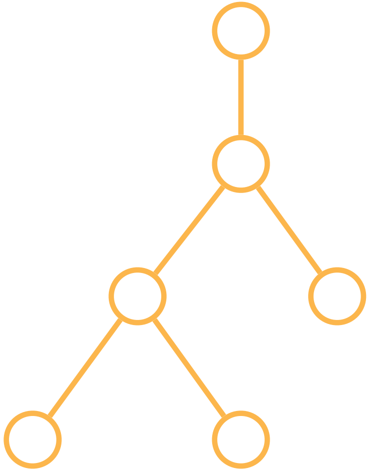
# Reverse Accumulation

Assume $z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$

Forward



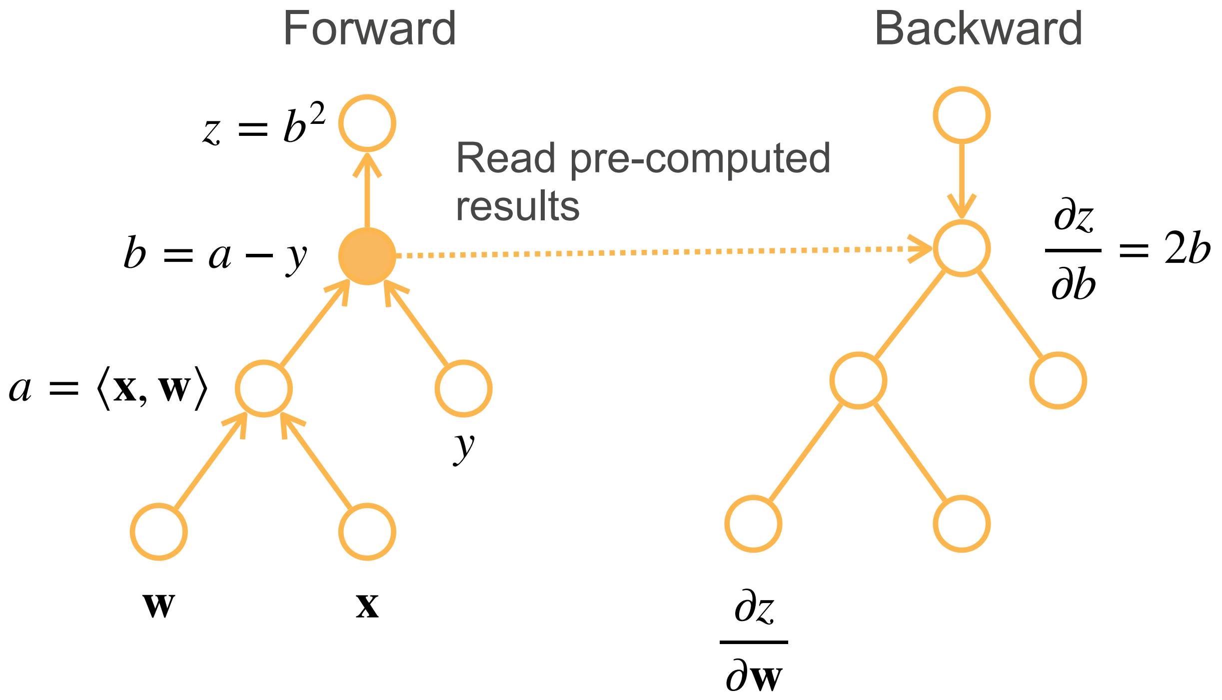

Backward



$$\frac{\partial z}{\partial \mathbf{w}}$$

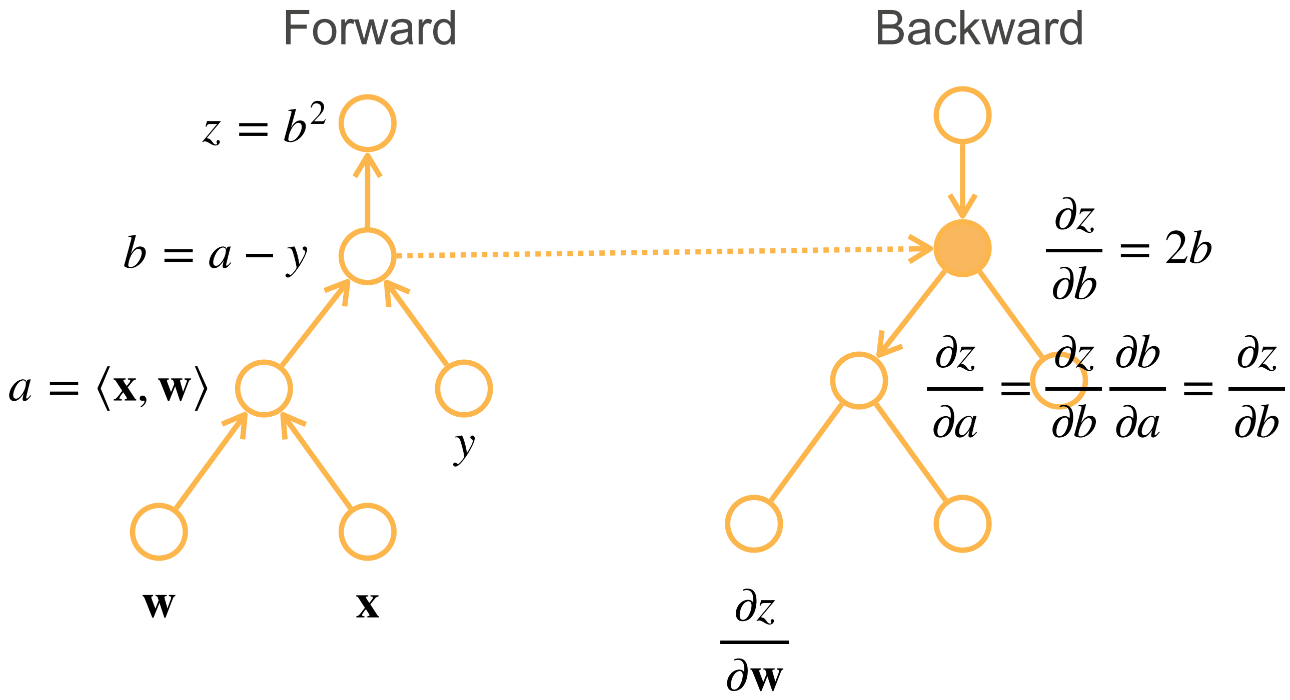
# Reverse Accumulation

Assume $z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$



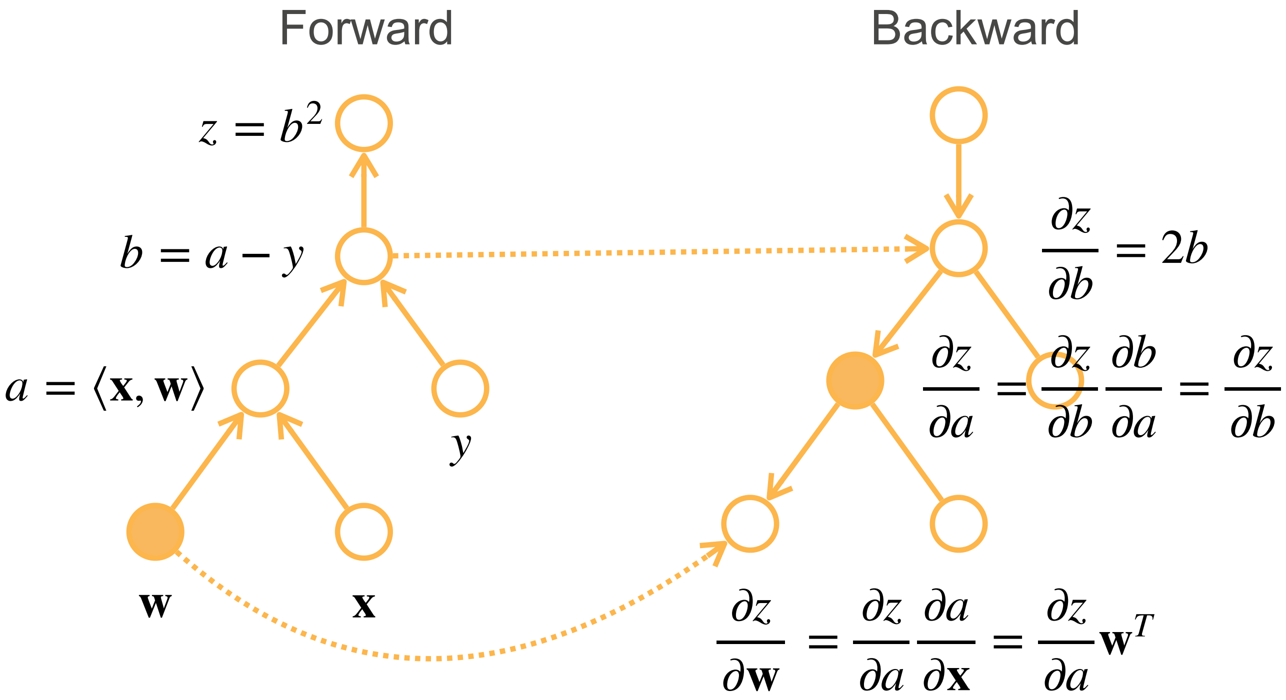
# Reverse Accumulation

Assume $z = (\langle \mathbf{x}, \mathbf{w} \rangle - y)^2$



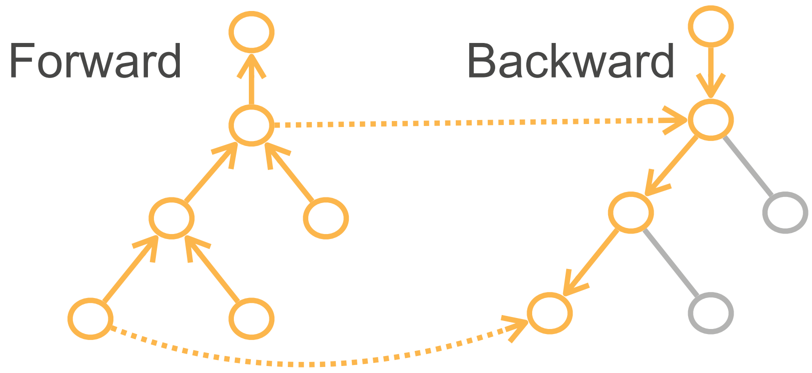
# Reverse Accumulation

Assume $z = \left(\langle \mathbf{x}, \mathbf{w} \rangle - y\right)^2$



# Reverse Accumulation Summary

- Build a computation graph
- Forward: Evaluate the graph, store intermediate results
- Backward: Evaluate the graph in a reversed order
    - Eliminate paths not needed



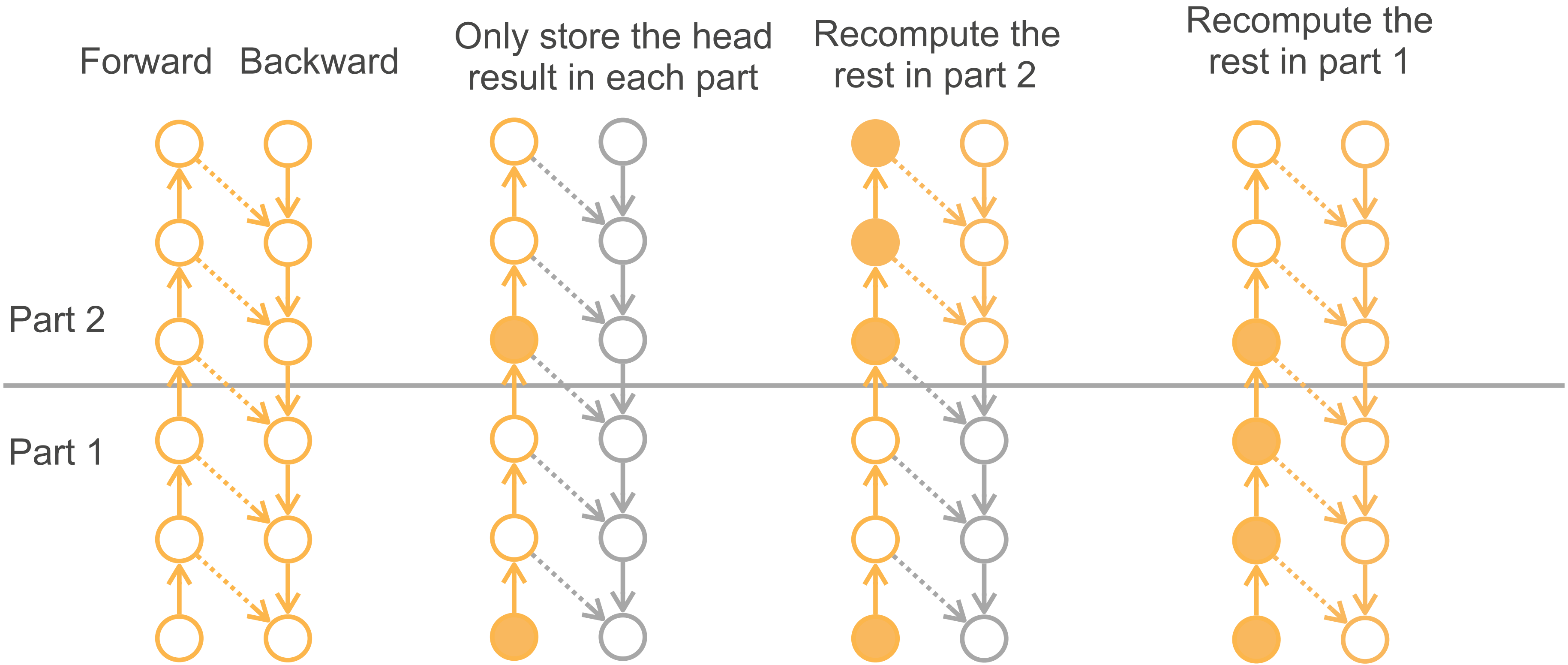
# Complexities

- Computational complexity: *O(n)*, *n* is #operations, to compute all derivatives
  - Often similar to the forward cost
- Memory complexity: O(n), needs to record all intermediate results in the forward pass
- Compare to forward accumulation:
  - O(n) time complexity to compute one gradient, O(n*k) to compute gradients for k variables
  - O(1) memory complexity

# [Advanced] Rematerialization

- Memory is bottleneck for backward accumulation
    - Linear to #layers and batch size
    - Limited GPU memory (32GB max)
- Trade computation for memory
    - Save a part of intermediate results
    - Recompute the rest when needed

# Rematerialization



# Complexities

- An additional forward pass
- Assume *m* parts, then *O(m)* for head results, *O(n/m)* to store one part's results
  - Choose $m = \sqrt{n}$ then the memory complexity is $O\left(\sqrt{n}\right)$
- Applying to deep neural networks
  - Only throw aways simple layers, e.g. activation, often <30% additional overhead
  - Train 10x larger networks, or 10x large batch size

# Autograd in MXNet

https://d2l.ai/chapter_crashcourse/autograd.html

# Limitations

- Does not support every operations
    - Indexing
    - Inplace
- Not smart enough to get numerical stable results
    - Homework