Backpropagation

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CS231n Discussion Section

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Agenda

- Motivation
- Backprop Tips & Tricks
- Matrix calculus primer

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- **Motivation**
- Backprop Tips & Tricks
- Matrix calculus primer

Motivation

Recall: Optimization objective is minimize loss

$$Loss = f(x, y; \theta)$$

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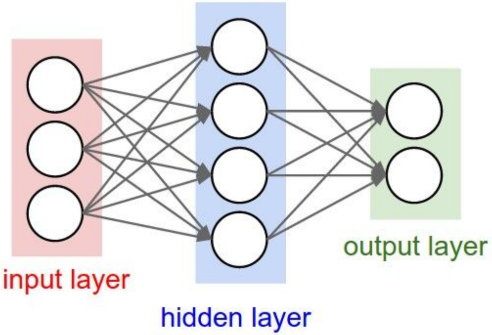
$$Loss = f(x, y; \theta)$$

Goal: how should we tweak the parameters to decrease the loss?



Agenda

- Motivation
- **Backprop Tips & Tricks**
- Matrix calculus primer

A Simple Example

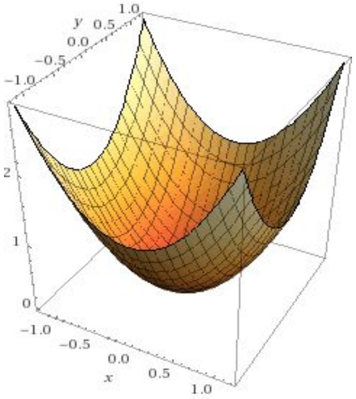
Loss $Loss = f(x, y; \theta)$

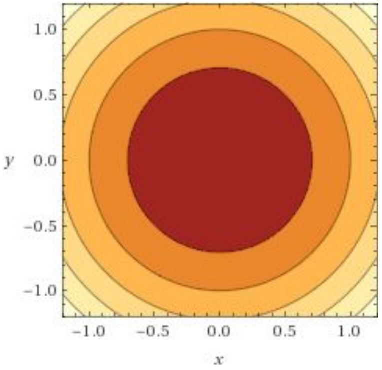
Goal: Tweak the parameters to minimize loss

=> **minimize a multivariable function** in parameter space

A Simple Example

=> **minimize a multivariable function**





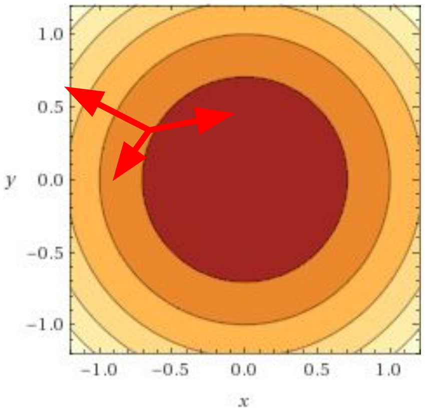
$$f(x, y) = x^2 + y^2$$

Plotted on WolframAlpha

Approach #1: Random Search

Intuition: the *step* we take in the domain of function

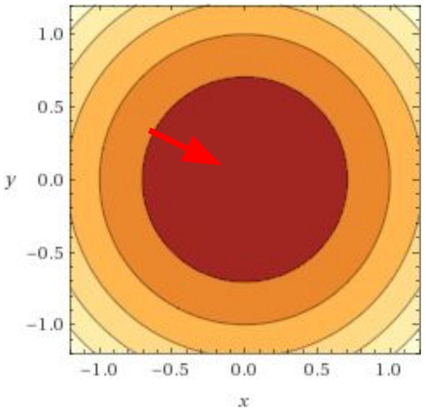
$$f(x, y) = x^2 + y^2$$



Approach #2: Numerical Gradient

Intuition: rate of change of a function with respect to a variable surrounding a small region

$$f(x, y) = x^2 + y^2$$



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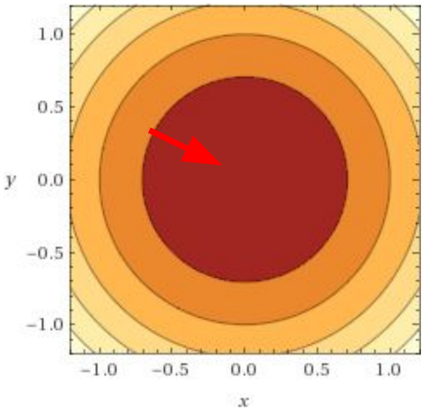


Finite Differences:

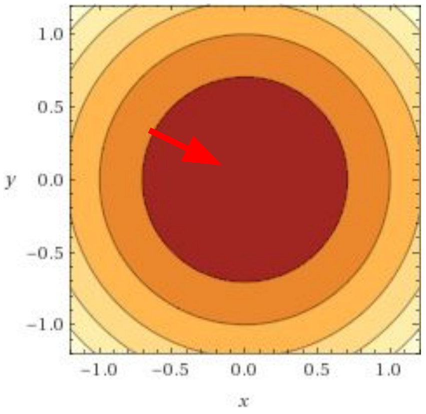
$$\frac{f(x+h, y) - f(x, y)}{h}$$

Approach #3: Analytical Gradient

Recall: partial derivative by limit definition

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

$f(x, y) = x^2 + y^2$



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Recall: chain rule $$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}.$$

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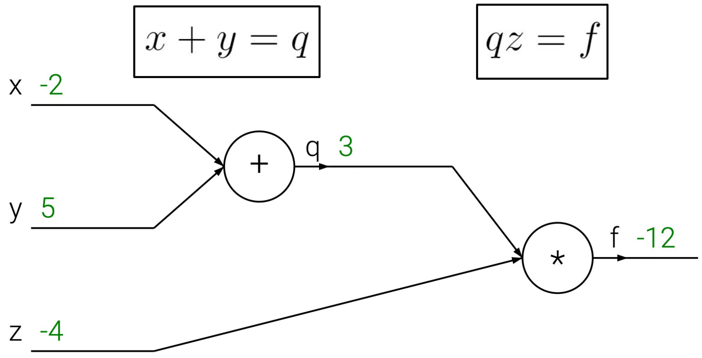
E.g. $f(x, y, z) = (x + y)z$

$$\frac{\partial f}{\partial x} =$$

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

$$\frac{\partial f}{\partial z} =$$



Approach #3: Analytical Gradient

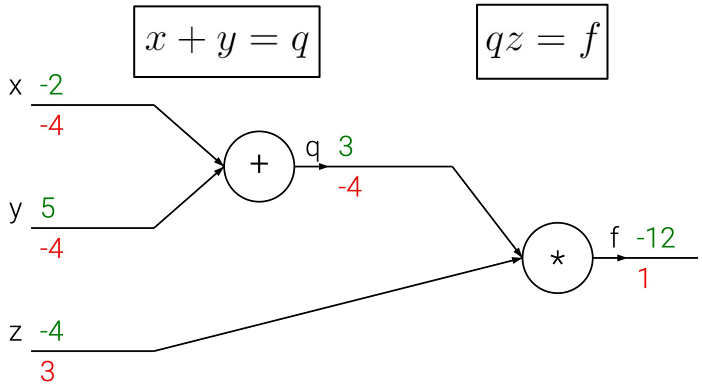
Recall: chain rule $\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}.$

E.g. $f(x, y, z) = (x + y)z$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x} = z \cdot 1 = z = -4$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y} = z \cdot 1 = z = -4$$

$$\frac{\partial f}{\partial z} = q = x + y = -2 + 5 = 3$$



Approach #3: Analytical Gradient

Recall: chain rule $$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}.$$

Intuition: upstream gradient values propagate backwards -- we can reuse them!

Gradient

$$f : R^n \to R$$

$$\nabla f : R^n \to R^n$$

$$\mathbf{x} = [x_1, \cdots, x_n]^T \in R^n$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\mathbf{x}) \end{bmatrix}$$

“direction and rate of fastest increase”

Numerical Gradient vs Analytical Gradient

What about Autograd?

- Deep learning frameworks can automatically perform backprop!

- Problems might surface related to underlying gradients when debugging your models

"Yes You Should Understand Backprop"

https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b

Problem Statement: Backpropagation

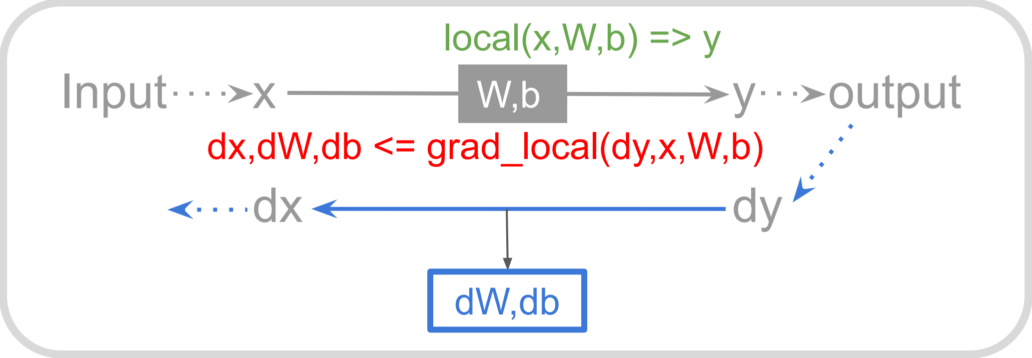
$$Loss = \frac{1}{N}\sum_i L_i(f(x_i,\ \theta\ ), y_i)$$

Given a function ***f*** with respect to inputs ***x***, labels ***y***, and parameters ***θ***
compute the gradient of ***Loss*** with respect to ***θ***

Problem Statement: Backpropagation

An algorithm for computing the gradient of a **compound** function as a series of **local, intermediate gradients**:

1. Identify intermediate functions (forward prop)
2. Compute local gradients (chain rule)
3. Combine with upstream error signal to get full gradient



Modularity: Previous Example

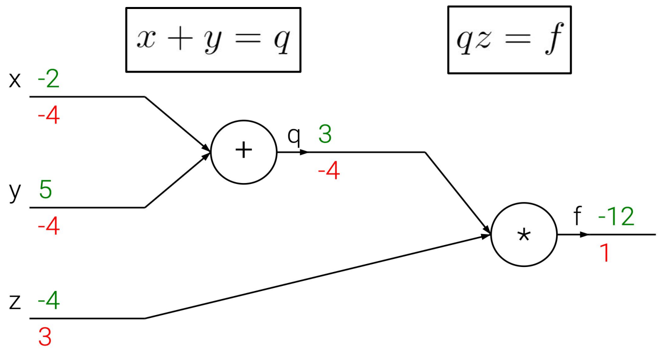
Compound function

$$f(x, y, z) = (x + y)z$$

Intermediate Variables
(forward propagation)

$$q = x + y$$

$$f = qz$$



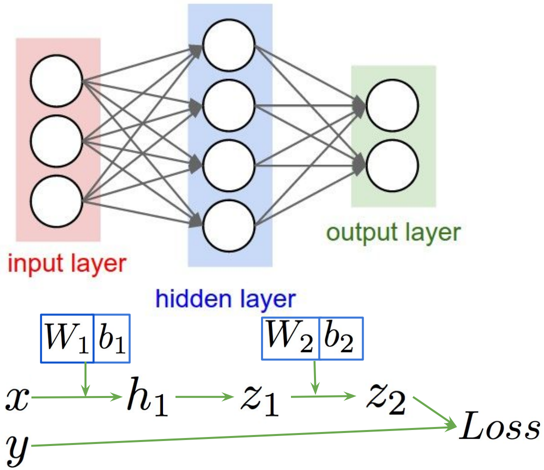
Modularity: 2-Layer Neural Network

Compound function

$$Loss = L\Big(\sigma(xW_1 + b_1)W_2 + b_2, y\Big)$$

Intermediate Variables
(forward propagation)

$$h_1 = xW_1 + b_1$$
$$z_1 = \sigma(h_1)$$
$$z_2 = z_1W_2 + b_2$$



$Loss$ => Squared Euclidean Distance between z_2 and y

Intermediate **Variables**

(forward propagation)

$$h_1 = xW_1 + b_1$$

$$z_1 = \sigma(h_1)$$

$$z_2 = z_1W_2 + b_2$$

? f(x;W,b) = Wx + b ?

(↑ lecture note) Input one feature **vector**

(← here) Input a batch of data (**matrix**)

Intermediate **Variables**

(forward propagation)

1. intermediate functions
2. local gradients
3. full gradients

Intermediate **Gradients**

(backward propagation)

$$h_1 = xW_1 + b_1$$

$$z_1 = \sigma(h_1)$$

$$z_2 = z_1 W_2 + b_2$$

$$Loss = \frac{1}{N}||z_2 - y||_F^2$$

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2}$$

$$\frac{\partial h_1}{\partial W_1}, \frac{\partial h_1}{\partial b_1} \qquad \frac{\partial h_1}{\partial x} \; ? \; ? \; ? \; W_1$$

$$\frac{\partial z_1}{\partial h_1} \; ? \; ? \; ? \; z_1(1 - z_1)$$

$$\frac{\partial z_2}{\partial W_2}, \frac{\partial z_2}{\partial b_2} \qquad \frac{\partial z_2}{\partial z_1} \; ? \; ? \; ? \; W_2$$

$$\frac{\partial Loss}{\partial z_2} = \frac{2}{N}(z_2 - y)$$

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Derivative w.r.t. Vector

Scalar-by-Vector

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} & \frac{\partial y}{\partial x_2} \cdots \frac{\partial y}{\partial x_n} \end{bmatrix}$$

Vector-by-Vector

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

Derivative w.r.t. Vector: Chain Rule

1. intermediate functions
2. local gradients
3. full gradients

$$\begin{tikzcd}
\mathbf{x} \arrow[d, shift left] \\
\mathbf{y} \arrow[d, shift left] \arrow[u, shift left, "\frac{\partial \mathbf{y}}{\partial \mathbf{x}}"'] \\
J \arrow[u, shift left, "\frac{\partial J}{\partial \mathbf{y}}"'] \arrow[uu, bend right, "\frac{\partial J}{\partial \mathbf{x}}"']
\end{tikzcd}$$

$$\frac{\partial J}{\partial \mathbf{x}} = ?$$

$$\frac{\partial J}{\partial x_j} = \sum_i \frac{\partial J}{\partial y_i} \frac{\partial y_i}{\partial x_j}$$

$$= \sum_i \left(\frac{\partial J}{\partial \mathbf{y}}\right)_{1i} \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)_{ij}$$

$$\boxed{\frac{\partial J}{\partial \mathbf{x}} = \frac{\partial J}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{x}}}$$

Derivative w.r.t. Vector: Takeaway

$$\mathbf{y} = A_{m\times n}\mathbf{x}$$

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

$$\frac{\partial J}{\partial \mathbf{x}} = \frac{\partial J}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial J}{\partial \mathbf{y}}A$$

$$\mathbf{y} = \omega(\mathbf{x})$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \omega'(x_1) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \omega'(x_n) \end{bmatrix}$$

$$\frac{\partial J}{\partial \mathbf{x}} = \frac{\partial J}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \left[\frac{\partial J}{\partial y_1}\omega'(x_1), \cdots, \frac{\partial J}{\partial y_n}\omega'(x_n)\right] = \frac{\partial J}{\partial \mathbf{y}} \circ \omega'(\mathbf{x})^T$$

Derivative w.r.t. Matrix

Scalar-by-Matrix

$$\frac{\partial y}{\partial A} = \begin{bmatrix} \frac{\partial y}{\partial A_{11}} & \frac{\partial y}{\partial A_{12}} & \cdots & \frac{\partial y}{\partial A_{1n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial A_{m1}} & \frac{\partial y}{\partial A_{m2}} & \cdots & \frac{\partial y}{\partial A_{mn}} \end{bmatrix}$$

Vector-by-Matrix

?

Derivative w.r.t. Matrix: Dimension Balancing

When you take **scalar-by-matrix** gradients

↓

The gradient has **shape of denominator**

- Dimension balancing is the “cheap” but **efficient** approach to gradient calculations in most practical settings

Derivative w.r.t. Matrix: Takeaway

$$Y_{m\times l} = A_{m\times n}X_{n\times l}$$

$$\frac{\partial J}{\partial X} = A^T\frac{\partial J}{\partial Y}$$

$$\frac{\partial J}{\partial A} = \frac{\partial J}{\partial Y}X^T$$

$$Y_{m\times n} = \omega(X_{m\times n})$$

$$\frac{\partial J}{\partial X} = \frac{\partial J}{\partial Y}\circ\omega'(X)$$

Intermediate **Variables**

(forward propagation)

1. intermediate functions
2. local gradients
3. full gradients

Intermediate **Gradients**

(backward propagation)

$$h_1 = xW_1 + b_1$$

$$z_1 = \sigma(h_1)$$

$$z_2 = z_1 W_2 + b_2$$

$$Loss = \frac{1}{N}\|z_2 - y\|_F^2$$

$$\boxed{\frac{\partial Loss}{\partial W_1}, \frac{\partial Loss}{\partial b_1}} \quad \frac{\partial Loss}{\partial x}$$

$$\frac{\partial Loss}{\partial h_1}$$

$$\boxed{\frac{\partial Loss}{\partial W_2}, \frac{\partial Loss}{\partial b_2}} \quad \frac{\partial Loss}{\partial z_1}$$

$$\frac{\partial Loss}{\partial z_2}$$

Backprop Menu for Success

1. Write down variable graph
2. Keep track of error signals
3. Compute derivative of loss function
4. Enforce shape rule on error signals, especially when deriving over a linear transformation

Vector-by-vector

$$\boxed{\mathbf{y} = A_{m \times n}\mathbf{x}}$$

$$y_i = \sum_{j=1}^{n} A_{ij} x_j$$

$$\frac{\partial y_i}{\partial x_j} = A_{ij}$$

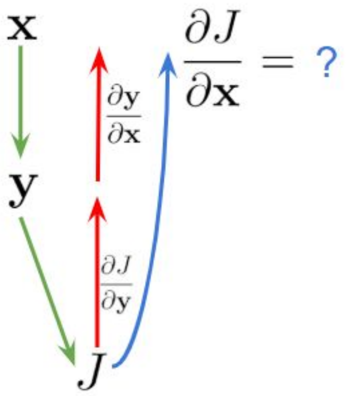
$$\boxed{\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = A}$$

Vector-by-vector

$$\boxed{\begin{aligned}\mathbf{y} &= A_{m\times n}\mathbf{x} \\ \lambda^T &= \frac{\partial J}{\partial \mathbf{y}}\end{aligned}}$$

$$y_i = \sum_{j=1}^{n} A_{ij} x_j \qquad \frac{\partial y_i}{\partial x_j} = A_{ij}$$

$$\lambda_i = \frac{\partial J}{\partial y_i}$$



$$\frac{\partial J}{\partial x_j} = \sum_i \frac{\partial J}{\partial y_i}\frac{\partial y_i}{\partial x_j} = \sum_{i=1}^{m} \lambda_i A_{ij}$$

$$\boxed{\frac{\partial J}{\partial \mathbf{x}} = \lambda^T A = \frac{\partial J}{\partial \mathbf{y}} A}$$

Vector-by-vector

$$\boxed{\mathbf{y} = \omega(\mathbf{x})}$$

$$y_i = \omega(x_i)$$

$$\frac{\partial y_i}{\partial x_i} = \omega'(x_i)$$

$$\frac{\partial y_i}{\partial x_j} = 0 \qquad (i \neq j)$$

$$\boxed{\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \omega'(x_1) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \omega'(x_n) \end{bmatrix}}$$

Vector-by-vector

$$\boxed{\begin{aligned}\mathbf{y} &= \omega(\mathbf{x}) \\ \lambda^T &= \frac{\partial J}{\partial \mathbf{y}}\end{aligned}}$$

$$y_i = \omega(x_i)$$

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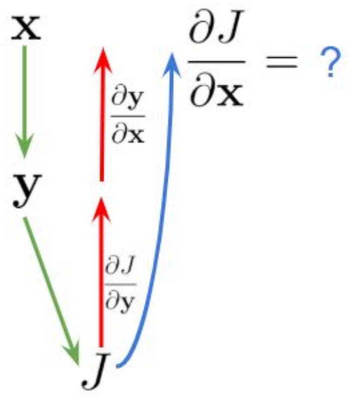


$$\frac{\partial J}{\partial x_j} = \sum_i \frac{\partial J}{\partial y_i} \frac{\partial y_i}{\partial x_j} = \frac{\partial J}{\partial y_j} \frac{\partial y_j}{\partial x_j} = \lambda_j \omega'(x_j)$$

$$\boxed{\frac{\partial J}{\partial \mathbf{x}} = \lambda^T \circ \omega'(\mathbf{x})^T = \frac{\partial J}{\partial \mathbf{y}} \circ \omega'(\mathbf{x})^T}$$

$$\mathbf{y} = A_{m\times n}\mathbf{x} \qquad \frac{\partial J}{\partial \mathbf{x}} = \frac{\partial J}{\partial \mathbf{y}} A$$

$$\frac{\partial J}{\partial \mathbf{x}}^T = A^T \frac{\partial J}{\partial \mathbf{y}}^T$$

Matrix multiplication [Backprop]

$$\boxed{\begin{aligned} Y_{m\times l} &= A_{m\times n} X_{n\times l} \\ \frac{\partial J}{\partial Y} &= \Lambda_{m\times l} \end{aligned}}$$

$$Y_{ij} = \sum_{k=1}^{n} A_{ik} X_{kj}$$

$$\Lambda_{ij} = \frac{\partial J}{\partial Y_{ij}}$$

$$\frac{\partial J}{\partial X_{ij}} = \sum_{i',j'} \frac{\partial J}{\partial Y_{i'j'}} \frac{\partial Y_{i'j'}}{\partial X_{ij}} \qquad = \sum_{i'=1}^{m} \frac{\partial J}{\partial Y_{i'j}} \frac{\partial Y_{i'j}}{\partial X_{ij}}$$

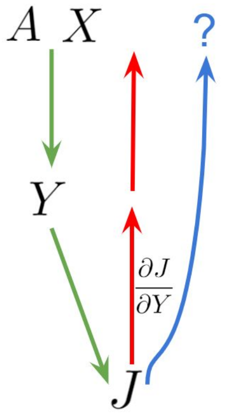
$$= \sum_{i'=1}^{m} A_{i'i} \Lambda_{i'j} \qquad = \sum_{k=1}^{m} A_{ki} \Lambda_{kj}$$

$$\boxed{\frac{\partial J}{\partial X} = A^T \Lambda = A^T \frac{\partial J}{\partial Y}}$$

$$\frac{\partial J}{\partial A_{ij}} = \sum_{i',j'} \frac{\partial J}{\partial Y_{i'j'}} \frac{\partial Y_{i'j'}}{\partial A_{ij}} \qquad = \sum_{j'=1}^{l} \frac{\partial J}{\partial Y_{ij'}} \frac{\partial Y_{ij'}}{\partial A_{ij}}$$

$$= \sum_{j'=1}^{l} \Lambda_{ij'} X_{jj'} \qquad = \sum_{k=1}^{l} \Lambda_{ik} X_{jk}$$

$$\boxed{\frac{\partial J}{\partial A} = \Lambda X^T = \frac{\partial J}{\partial Y} X^T}$$



$$\mathbf{y} = \omega(\mathbf{x}) \qquad \frac{\partial J}{\partial \mathbf{x}} = \frac{\partial J}{\partial \mathbf{y}} \circ \omega'(\mathbf{x})^T$$

$$\frac{\partial J}{\partial \mathbf{x}}^T = \frac{\partial J}{\partial \mathbf{y}}^T \circ \omega'(\mathbf{x})$$

Elementwise function [Backprop]

$$\boxed{\begin{aligned} Y_{m\times n} &= \omega(X_{m\times n}) \\ \frac{\partial J}{\partial Y} &= \Lambda_{m\times n} \end{aligned}}$$

$$Y_{ij} = \omega(X_{ij})$$

$$\Lambda_{ij} = \frac{\partial J}{\partial Y_{ij}}$$

$$\frac{\partial J}{\partial X_{ij}} = \sum_{i',j'} \frac{\partial J}{\partial Y_{i'j'}} \frac{\partial Y_{i'j'}}{\partial X_{ij}}$$

$$= \frac{\partial J}{\partial Y_{ij}} \frac{\partial Y_{ij}}{\partial X_{ij}} = \Lambda_{ij}\omega'(X_{ij})$$

$$\boxed{\frac{\partial J}{\partial X} = \Lambda \circ \omega'(X) = \frac{\partial J}{\partial Y} \circ \omega'(X)}$$