Autograd

Computational graphs, backpropagation and the automatic gradient computation

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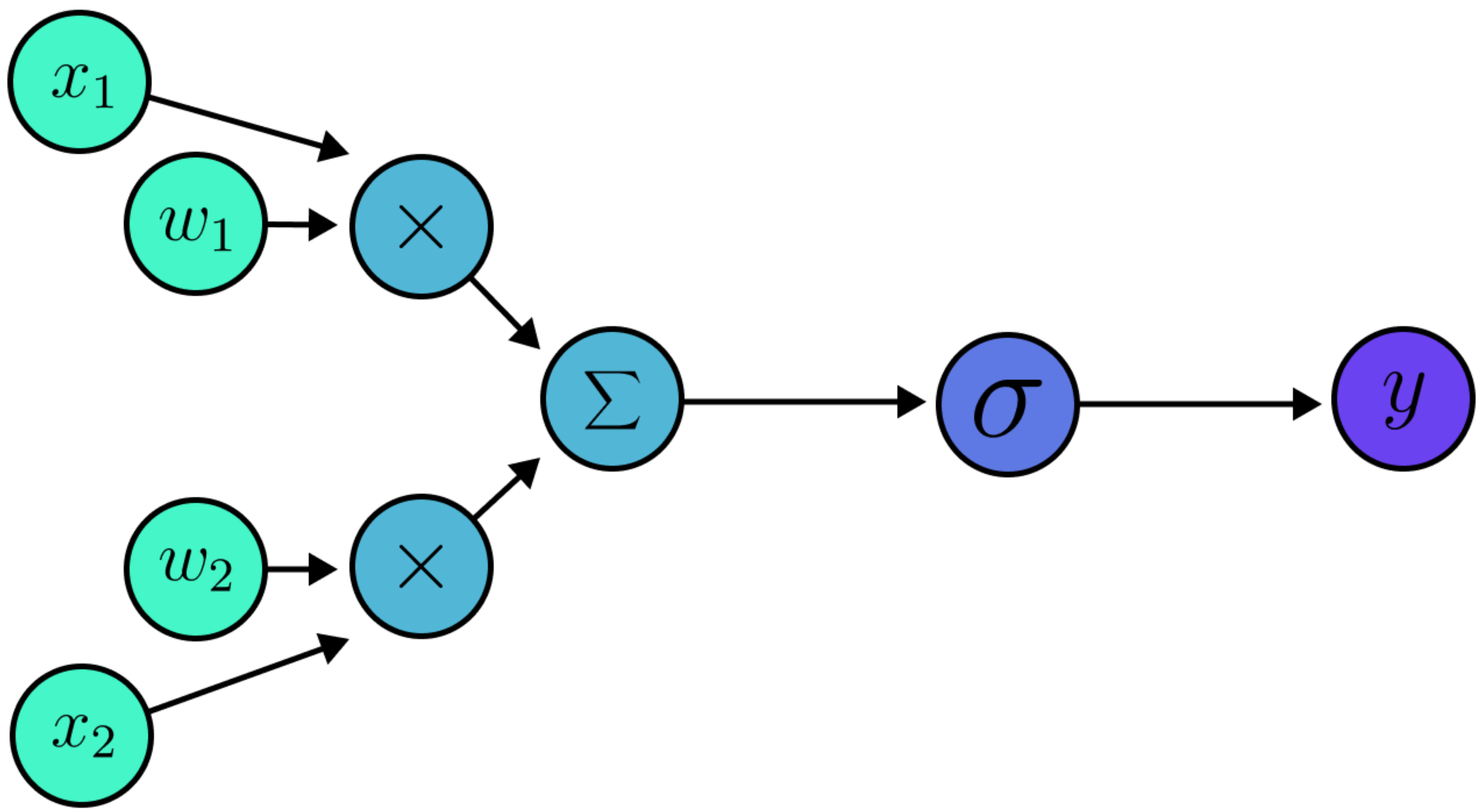
Computational graph



a) $\boldsymbol{x} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} 0.5 \\ 1.3 \end{bmatrix}$

b) $\boldsymbol{x} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} 0.5 \\ -1.3 \end{bmatrix}$

c) $\boldsymbol{x} = \begin{bmatrix} 0.4 \\ 0.9 \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} -1.5 \\ 0.8 \end{bmatrix}$

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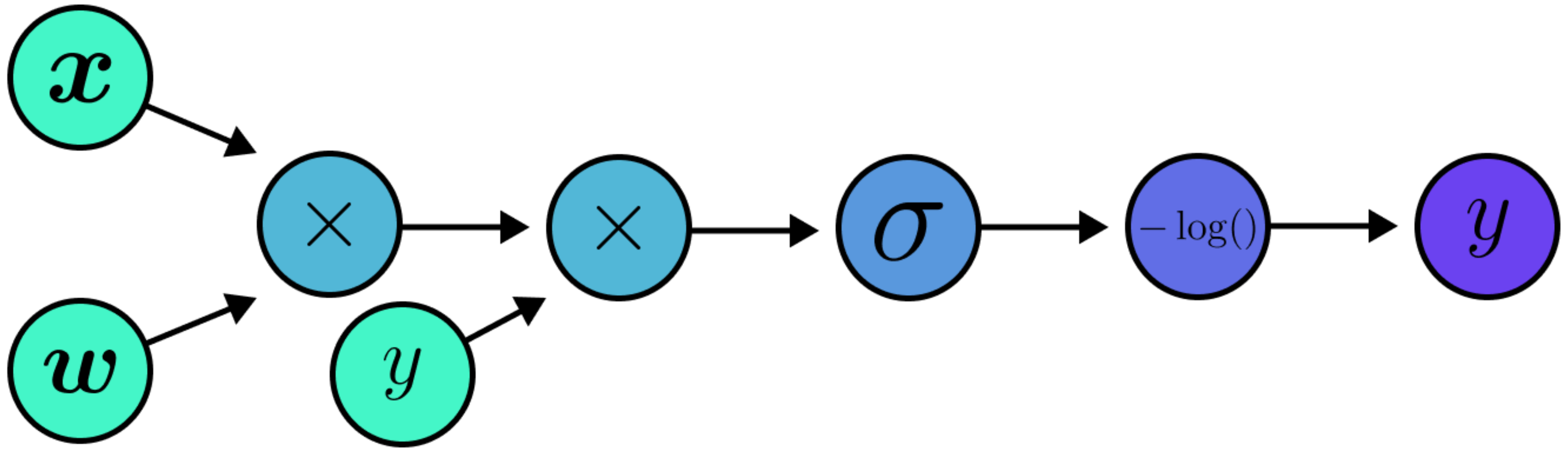
Training weights



$$\boldsymbol{x} = \begin{bmatrix} 0.7 \\ 0.4 \\ 1.2 \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} 0.3 \\ 0.3 \\ 0.3 \end{bmatrix}, y = 1$$

Individual task

You are given the following equation

$$y = \sin\left(\boldsymbol{w}^\top \boldsymbol{x}\right) - b$$

with

$$\boldsymbol{x} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} \frac{\pi}{2} \\ \pi \end{bmatrix}, b = 0, \hat{y} = 2$$

a) Draw a computational graph

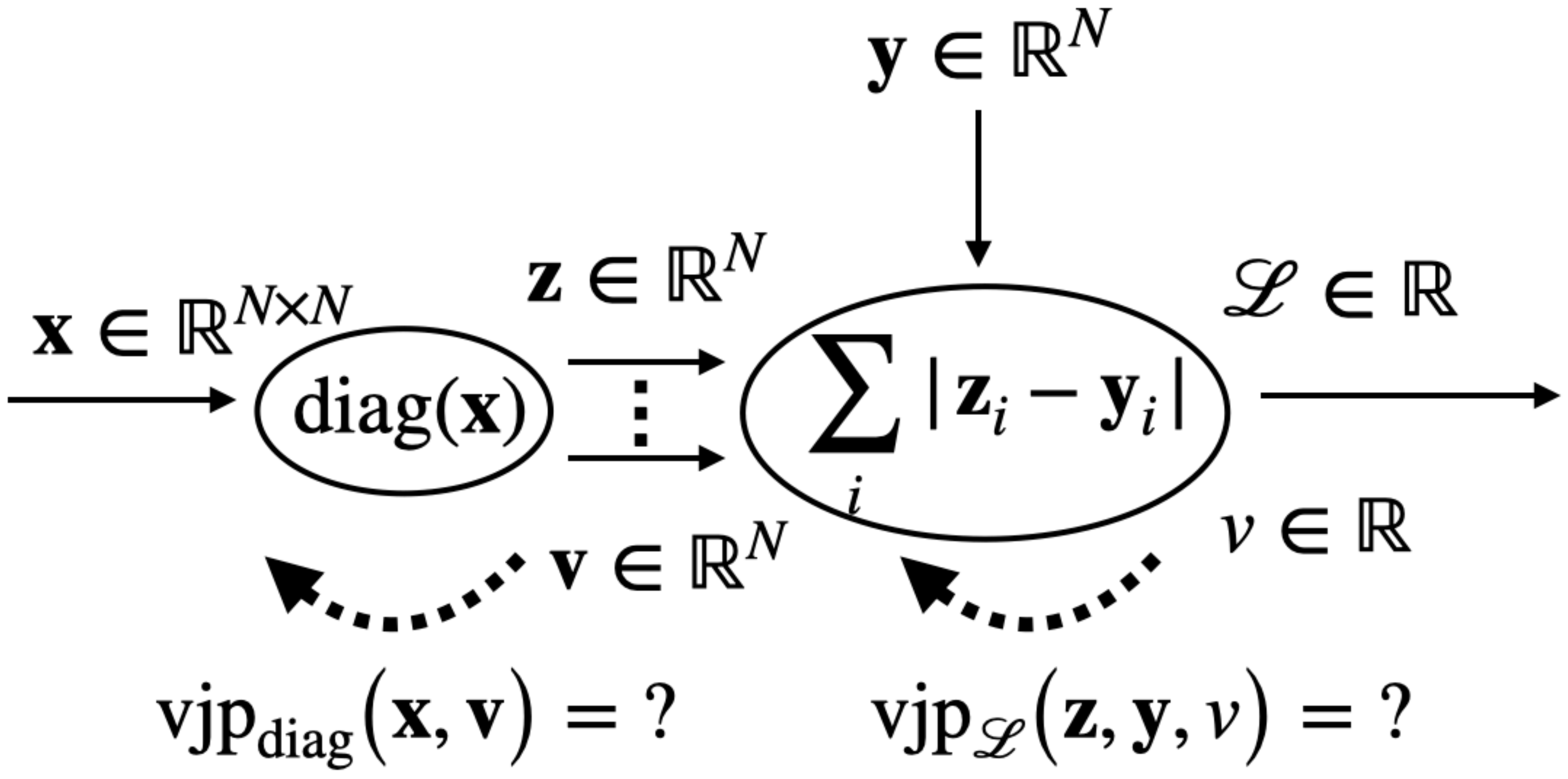
b) Compute feedforward pass

c) Calculate gradient $\frac{\partial y}{\partial \boldsymbol{w}}$

d) Calculate MSE loss, add to graph

e) Update weights with $\alpha = 0.5$

Vector-Jacobian product



a) Implementation of $\mathrm{vjp}_{\mathrm{diag}}(\boldsymbol{v}, \boldsymbol{x})$, where $\boldsymbol{v}$ is the upstream gradient

b) Derive the $\dfrac{\partial \mathscr{L}}{\partial \boldsymbol{x}}$

Backpropagation in code

Under the hood of autograd library

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Activation functions

Sigmoid

$$f(x) = \frac{1}{1 + e^{-x}}$$

$$\frac{\partial f(x)}{\partial x} = \frac{e^{-x}}{(e^{-x} + 1)^2}$$

ReLU

$$f(x) = \max(0,\ x)$$

$$\frac{\partial f(x)}{\partial x} = 1,\ x \geq 0 \\ = 0,\ x < 0$$

Tanh

$$f(x) = \frac{1 - e^{-2x}}{1 + e^{-2x}}$$

$$\frac{\partial f(x)}{\partial x} = \frac{4e^{2x}}{\left(e^{2x} + 1\right)^2}$$

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Logistic loss

$$f(x, y) = \log\left(1 + e^{-xy}\right)$$

$$\frac{\partial f(x, y)}{\partial x} = -\frac{y}{1 + e^{xy}}$$

HW2 Autograd

Creating your own library

For next week

Matrix multiplication

Mathematical derivatives

$$\begin{bmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & & \vdots \\ x_{m1} & \cdots & x_{mn} \end{bmatrix} \times \begin{bmatrix} y_{11} & \cdots & y_{1m} \\ \vdots & & \vdots \\ y_{n1} & \cdots & y_{nm} \end{bmatrix} = \begin{bmatrix} x_{11} \cdot y_{11} + \cdots + x_{1n} \cdot y_n 1 & \cdots & x_{11} \cdot y_{1m} + \cdots + x_{1n} \cdot y_{nm} \\ \vdots & & \vdots \\ x_{m1} \cdot y_{11} + \cdots + x_{mn} \cdot y_{n1} & \cdots & x_{m1} \cdot y_{1m} + \cdots + x_{mn} \cdot y_{nm} \end{bmatrix}$$

$$\frac{\partial f}{\partial \boldsymbol{Y}} = \boldsymbol{X}^\top \quad \frac{\partial f}{\partial \boldsymbol{X}} = \boldsymbol{Y}^\top$$

Backward pass in code (using vjp)

$$\mathrm{vjp}_f(\boldsymbol{v}, \boldsymbol{X}) = \boldsymbol{v} \times \frac{\partial f}{\partial \boldsymbol{X}} = \boldsymbol{v} \times \boldsymbol{Y}^\top$$

$$\mathrm{vjp}_f(\boldsymbol{v}, \boldsymbol{Y}) = \frac{\partial f}{\partial \boldsymbol{Y}} \times \boldsymbol{v} = \boldsymbol{X}^\top \times \boldsymbol{v}$$

https://math.stackexchange.com/questions/1846339/why-does-the-gradient-of-matrix-product-ab-w-r-t-a-equal-bt

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Regularization loss

$$f(\boldsymbol{x}, y) = y \cdot \sum_{i=1}^{n} x_i^2$$

$$\boldsymbol{x} \in \mathbb{R}^n,\ y \in \mathbb{R}$$

$$\frac{\partial f(\boldsymbol{x}, y)}{\partial x_i} = 2 \cdot y \cdot x_i$$

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Cross-entropy loss

$$f(\boldsymbol{x}, \boldsymbol{y}) = -\frac{1}{n}\sum_{i=1}^{n} [\![y_i = c_i]\!] \log(x_i)$$

$$\frac{\partial f(\boldsymbol{x}, \boldsymbol{y})}{\partial \boldsymbol{x}} = -\frac{1}{n}\sum_{i=1}^{n} [\![y_i = c_i]\!] \frac{1}{x_i}$$

$\boldsymbol{x} \in \mathbb{R}^n$ is a vector with class **probabilities** for input

$\boldsymbol{y} \in \mathbb{R}^n$ is a vector of correct class predictions for input

$\boldsymbol{c} \in \mathbb{R}^n$ is a vector of all possible classes

$[\![\cdot]\!]$ is an Iverson Bracket

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Cross-entropy loss with softmax

With proof, do not learn the proof just the result is enough

$$f(\boldsymbol{x},\boldsymbol{y}) = -\sum_i y_i \log\left(a_i\right), \quad a_i = h\left(x_i\right) = \frac{e^{x_i}}{\sum_j e^{x_j}}$$

$$\frac{\partial f}{\partial a_i} = \frac{\partial\left(-\sum_j y_j \cdot \log\left(a_j\right)\right)}{\partial a_i} = \frac{\partial\left(-y_i \cdot \log\left(a_i\right)\right)}{\partial a_i} = -\frac{y_i}{a_i}$$

$$\frac{\partial f}{\partial x_i} = \sum_j \frac{\partial f}{\partial a_j} \cdot \frac{\partial a_j}{\partial x_i}$$

$$\frac{\partial a_i}{\partial x_i} = \frac{\partial\left(\frac{e^{x_i}}{\sum_j e^{x_j}}\right)}{\partial x_i} = \frac{e^{x_i}}{\sum_j e^{x_j}}\left(\frac{e^{x_j}}{e^{x_j}} - \frac{e^{x_i}}{\sum_j e^{x_j}}\right) = a_i\left(1 - a_i\right)$$

$$\frac{\partial f}{\partial x_i} = \sum_{j \neq i} \frac{\partial f}{\partial a_j} \cdot \frac{\partial a_j}{\partial x_i} + \frac{\partial f}{\partial a_i} \cdot \frac{\partial a_i}{\partial x_i}$$

$$\frac{\partial f}{\partial a_j} = \frac{\partial\left(-\sum_k y_k \cdot \log(a_k)\right)}{\partial a_j} = -\frac{y_j}{a_j}$$

$$\frac{\partial f}{\partial x_i} = \sum_{j \neq i} y_j \cdot a_i - y_i\left(1 - a_i\right) = \sum_{j \neq i} y_j \cdot a_i + y_i \cdot a_i - y_i$$

$$\frac{\partial a_j}{\partial x_i} = \frac{\partial\left(\frac{e^{x_j}}{\sum_k e^{x_k}}\right)}{\partial x_i} = \frac{e^{x_j}}{\sum_k e^{x_k}}\left(\frac{\frac{\partial e^{x_j}}{\partial x_i}}{e^{x_j}} - \frac{\frac{\partial \sum_k e^{x_k}}{\partial x_i}}{\sum_k e^{x_k}}\right) = \frac{e^{x_j}}{\sum_k e^{x_k}}\left(0 - \frac{e^{x_i}}{\sum_k e^{x_k}}\right) = -a_j \cdot a_i$$

$$\frac{\partial f}{\partial x_i} = \sum_j y_j \cdot a_i - y_i = a_i \sum_j y_j - y_i$$

$$\boxed{\frac{\partial f}{\partial x_i} = a_i - y_i}$$

https://towardsdatascience.com/deriving-backpropagation-with-cross-entropy-loss-d24811edeaf9