Autograd

Computational graphs, backpropagation and the automatic gradient computation.

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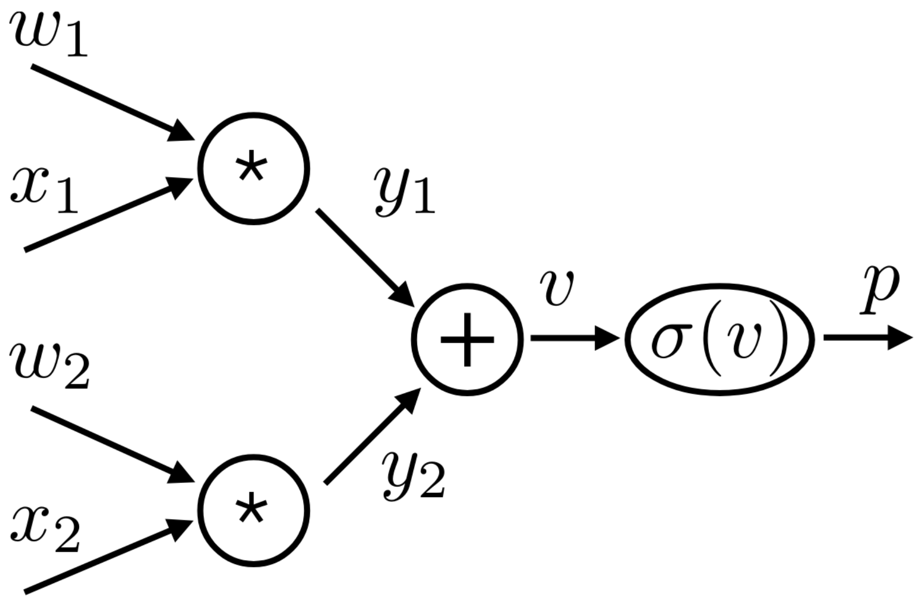
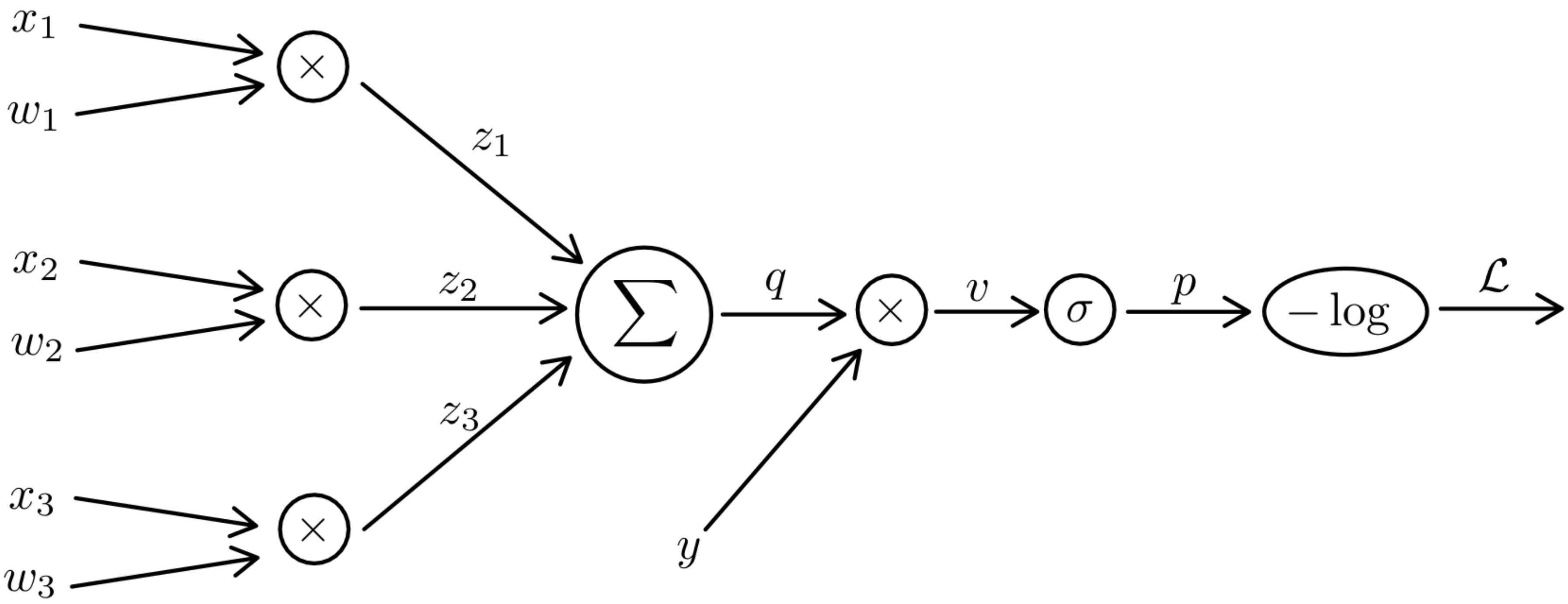
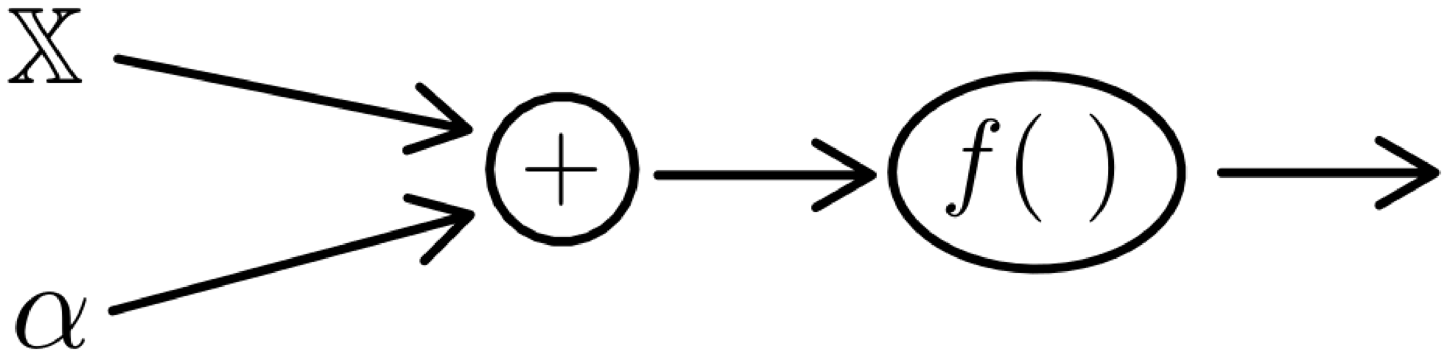
Computational graph



Training weights



Gradient in broadcasting



Backpropagation in code

Under the hood of autograd library

Activation functions

Sigmoid

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

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

ReLU

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

$$\frac{\partial f}{\partial x} = \begin{matrix} 1, x \geq 0 \\ 0, x < 0 \end{matrix}$$

Tanh

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

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

Logistic loss

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

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

HW1 Autograd

Creating your own library

Matrix multiplication

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

$$\frac{\partial f}{\partial Y} = X^T \qquad \frac{\partial f}{\partial X} = Y^T$$

Backward pass in code

$$vjp_f(v, X) = v \times \frac{\partial f}{\partial X} = v \times Y^T \qquad vjp_f(v, Y) = \frac{\partial f}{\partial Y} \times v = X^T \times v$$

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

Reqularization loss

$$f(x, y) = y \cdot \sum_i x_i^2$$

$$y \in R$$

$$\frac{\partial f}{\partial x_i} = 2 \cdot y \cdot x_i$$

Cross-entropy loss

$$f(x, y) = -\sum_{c \in Y} [\![y = c]\!] \log(x) \qquad \frac{\partial f}{\partial x} = -\sum_{c \in Y} [\![y = c]\!] \frac{1}{x}$$

x is a matrix with class probabilities for inputs
y is a vector of correct class predictions for inputs
Y is a matrix of all possible classes

Cross-entropy loss

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

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

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

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

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

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

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

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

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

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

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

Direct kinematic task

Use of backpropagation