EE5904/ME5404: Neural Networks Lecture 04

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Reminder: Assignments 1 & 2

Due 23:59 (SGT), Sunday, 15 February 2026.
Late submission will not be accepted unless it is well justified!

Submission instructions

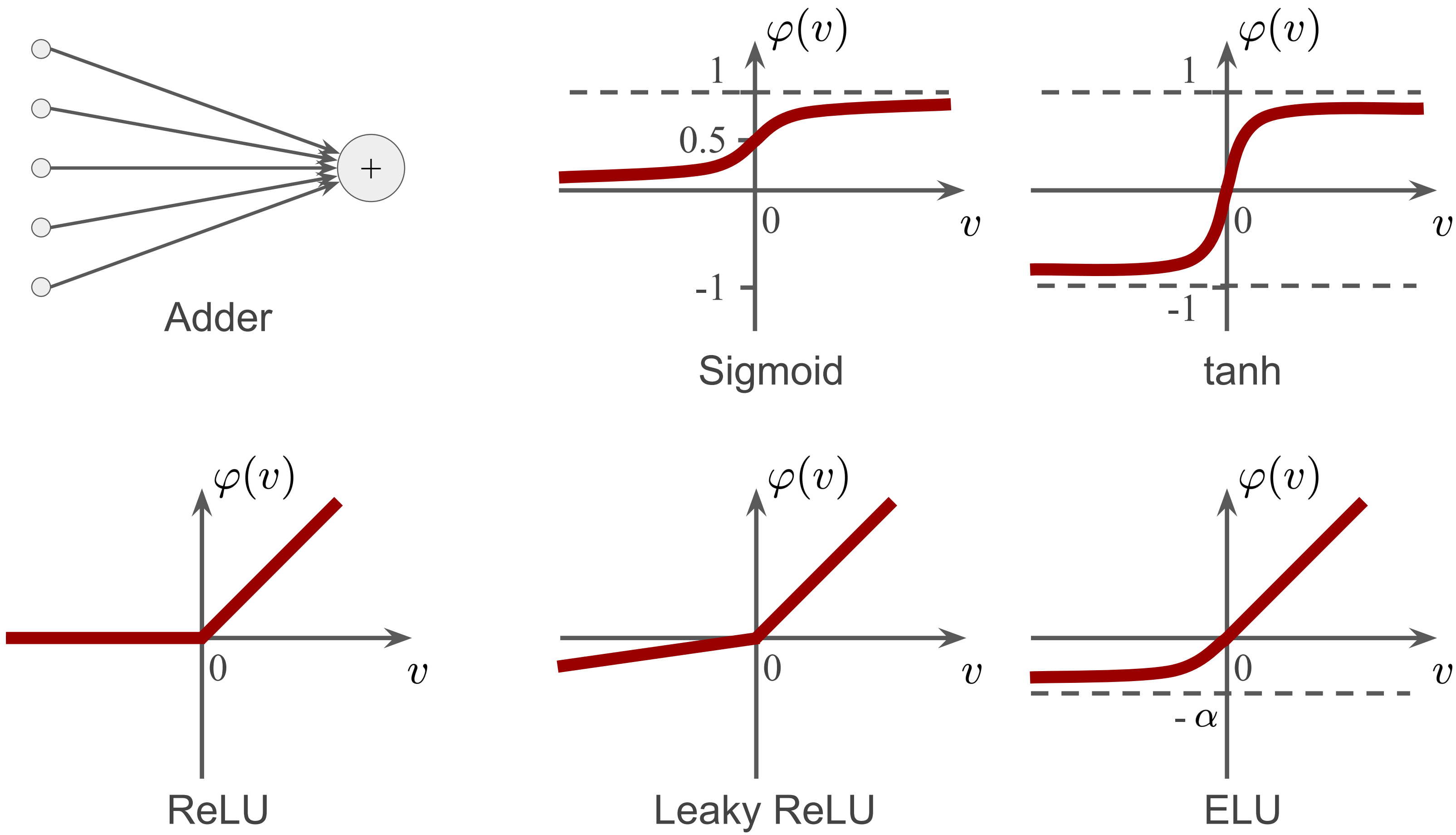
- Submit the assignment via Canvas.
- Any **Python code** and **Python code generated results** should be included as an attachment.

Handwritten submissions are encouraged!

- If all questions (except the **Python code** and **code generated results such as figures**) are handwritten, you will receive a **10% bonus** on the assignment score.
- For handwritten work, **take clear photos of the pages** and upload them to Canvas.
- Ensure that your handwriting and photos are **clear and legible**. Illegible submissions may lose marks。

Assignment 2 will be out shortly!

Recap of last lecture: activation functions

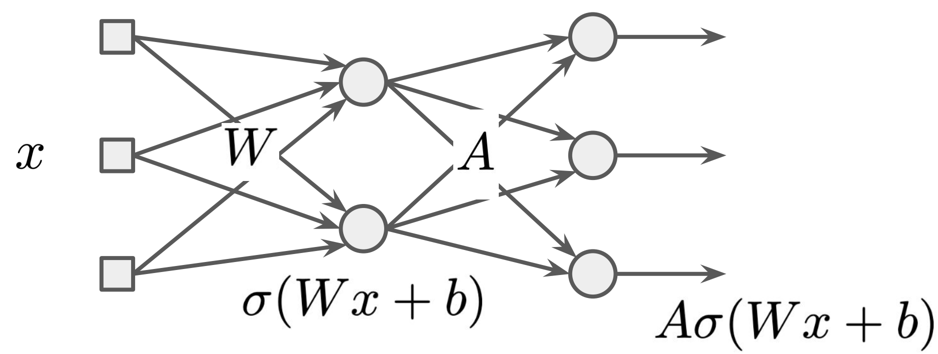


Recap of last lecture: Universal Approximation Theorem (UAT)

Theorem

For any compact set $K \subset \mathbb{R}^m$, any continuous function $f : K \to \mathbb{R}^n$ and any $\varepsilon > 0$, there exist $N, W \in \mathbb{R}^{N \times m}, b \in \mathbb{R}^N, A \in \mathbb{R}^{n \times N}$, such that

$$\sup_{x \in K} \|f(x) - A\sigma(Wx + b)\| < \varepsilon$$



It means ***a <u>two-layer</u> neural network with <u>sufficient number of hidden layer neurons</u> can approximate any continuous vector-valued function defined on a <u>bounded</u> high-dimensional region***.

Recap of last lecture: Frequently used loss functions

1. L2 loss (squared error) for regression:

$$\mathcal{L}(f_\theta(x), y) = \|f_\theta(x) - y\|_2^2$$

2. L1 loss (absolute error) for regression:

$$\mathcal{L}(f_\theta(x), y) = \|f_\theta(x) - y\|_1$$

3. Logistic loss (binary cross-entropy loss) for binary classification:

$$\mathcal{L}(f_\theta(x), y) = -y \log \sigma(f_\theta(x)) - (1 - y) \log(1 - \sigma(f_\theta(x)))$$

4. Softmax cross-entropy loss for multi-class classification:

$$\mathcal{L}(f_\theta(x), y) = -\sum_{k=1}^{K} y_k \log\left(\frac{e^{f_k(x)}}{\sum_{j=1}^{K} e^{f_j(x)}}\right)$$

where $y_k = \begin{cases} 1, & k = c \\ 0, & k \neq c \end{cases}$, and $c \in \{1, 2, \ldots, K\}$ is the true class

Training of Neural Network

Big picture: What training a neural network really is

During the training of neural networks, we want to find the neural network parameters (weights and biases) that can minimize the total loss, i.e. the sum of loss over training data.

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Today's agenda:

- **Backpropagation**: how to compute gradients efficiently
- **Batched training**: how to organize data during training
- **Optimizers**: how to use those gradients
- **Hyperparameter tuning**: how to choose the training setup

Big picture: What training a neural network really is

Neural Network computation

Suppose input is x

The result at each layer of an MLP is:

$$f_1(x) = \sigma(W_1 x + b_1)$$

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$$f_M(x) = W_M \sigma(W_{M-1} x + \sigma(W_{M-2} x + \ldots + b_1) + b_2) + \ldots) + b_{M-1}) + b_M$$

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$$

How to find $\underset{W_1, b_1, W_2, b_2, \ldots, W_M, b_M}{\arg\min} \mathbb{E}_{(x,y)\sim p_{\text{data}}} \left[\mathcal{L}(f_M(x), y)\right]$?

$$
\begin{aligned}
&= \arg\min_\theta \mathbb{E}_{(x,y)\sim p_{\text{data}}} \left[\mathcal{L}(f_M(x), y)\right] \\
&= \arg\min_\theta \mathcal{L}(\theta)
\end{aligned}
$$

Which way should I go to best vertically descent from where I am?

Follow the slope!

Gradient and gradient descent

The gradient of $\nabla_\theta L(\theta)$ is defined as

$$\nabla_\theta L(\theta) = \begin{bmatrix} \frac{\partial L}{\partial \theta_1} \\ \frac{\partial L}{\partial \theta_2} \\ \cdots \\ \frac{\partial L}{\partial \theta_m} \end{bmatrix}$$

Its direction is the **direction of steepest ascent**

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Its direction is the **direction of steepest ascent**

This is because according to the first-order Taylor expansion:

$$L(\theta + \delta\theta) = L(\theta) + \langle \nabla_\theta L(\theta), \delta\theta \rangle + o(\|\delta\theta\|)$$

The value of $L(\theta)$ is maximized if $\delta\theta$ aligns with $\nabla_\theta L(\theta)$ given a fixed norm of $\delta\theta$

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The **direction of steepest descent** will be the **negative gradient** $-\nabla_\theta L(\theta)$

Gradient and gradient descent

Though it is difficult to find the global optima directly, we can update the parameters of the neural network along the direction of negative gradient to update the parameters to at least **locally decrease the loss**

By accumulating many such local updates of parameters, we hope to obtain a globally good solution.

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This is **Gradient Descent (GD)**:

$$\theta \leftarrow \theta - \alpha \nabla_\theta \mathcal{L}(\theta)$$

where the step size coefficient α is called **learning rate**

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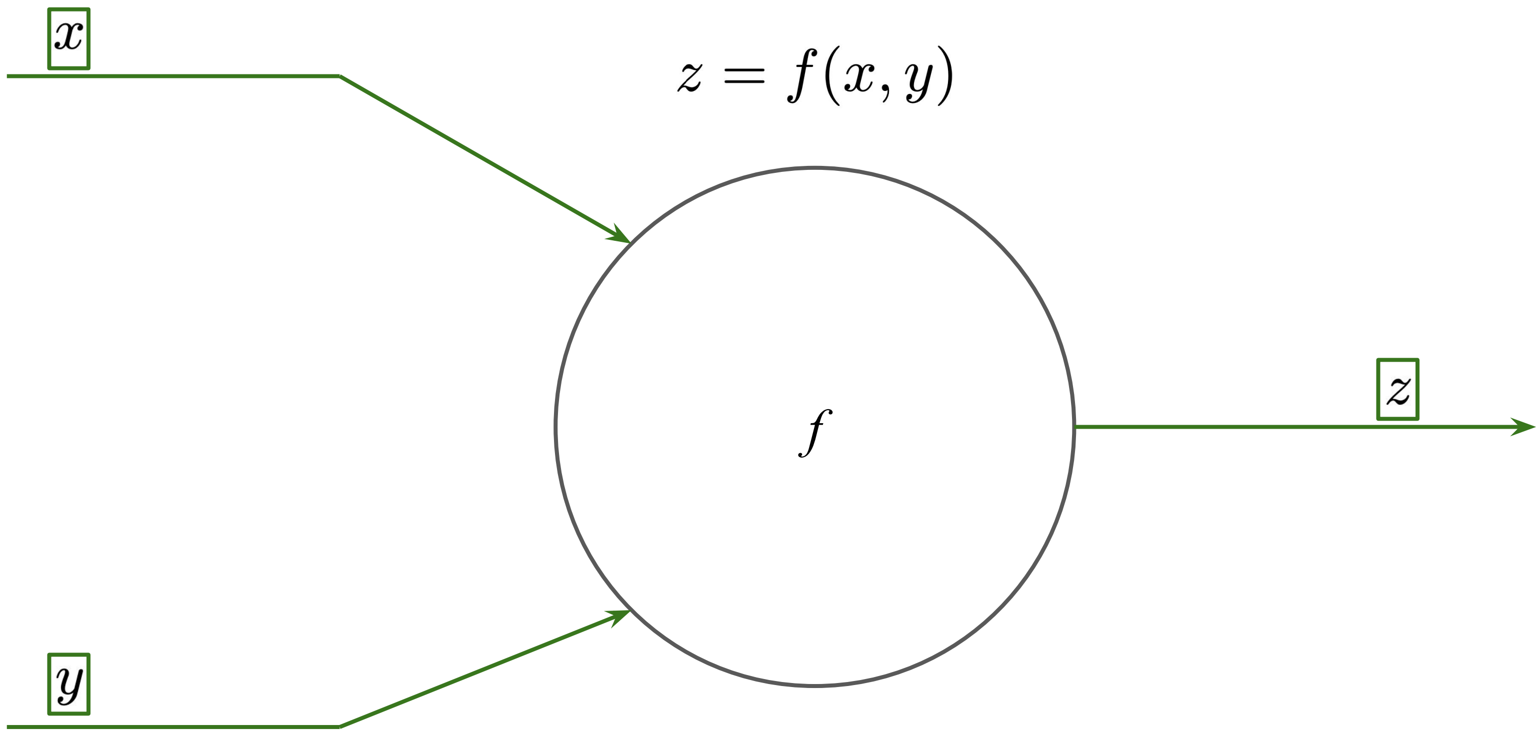
How to compute the gradient of loss w.r.t. NN parameters $\nabla_\theta L(\theta)$?

Backpropagation: scalar functions

A neural network is a parameterized computational graph.
Gradients are computed efficiently using the **chain rule**, implemented as **backpropagation** on the graph.



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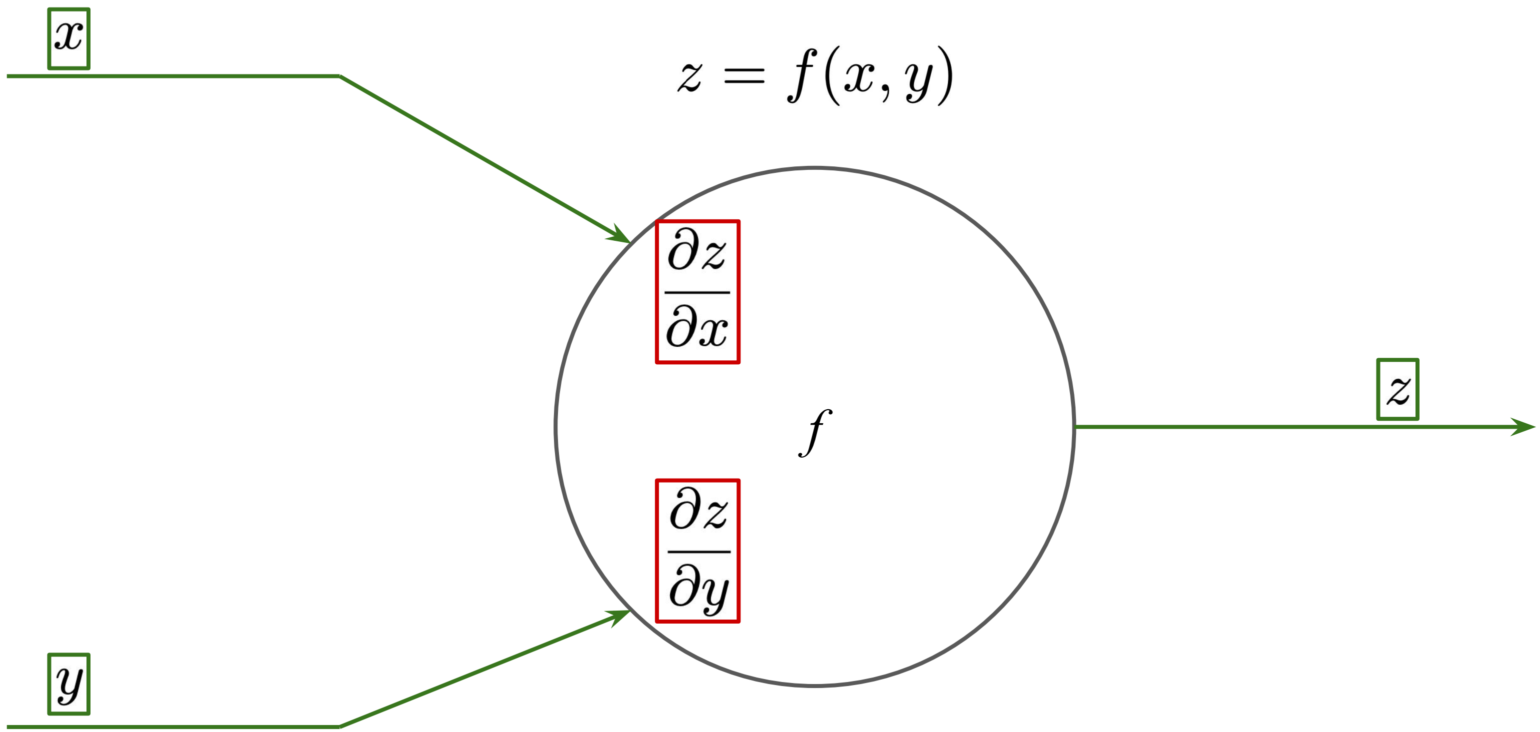

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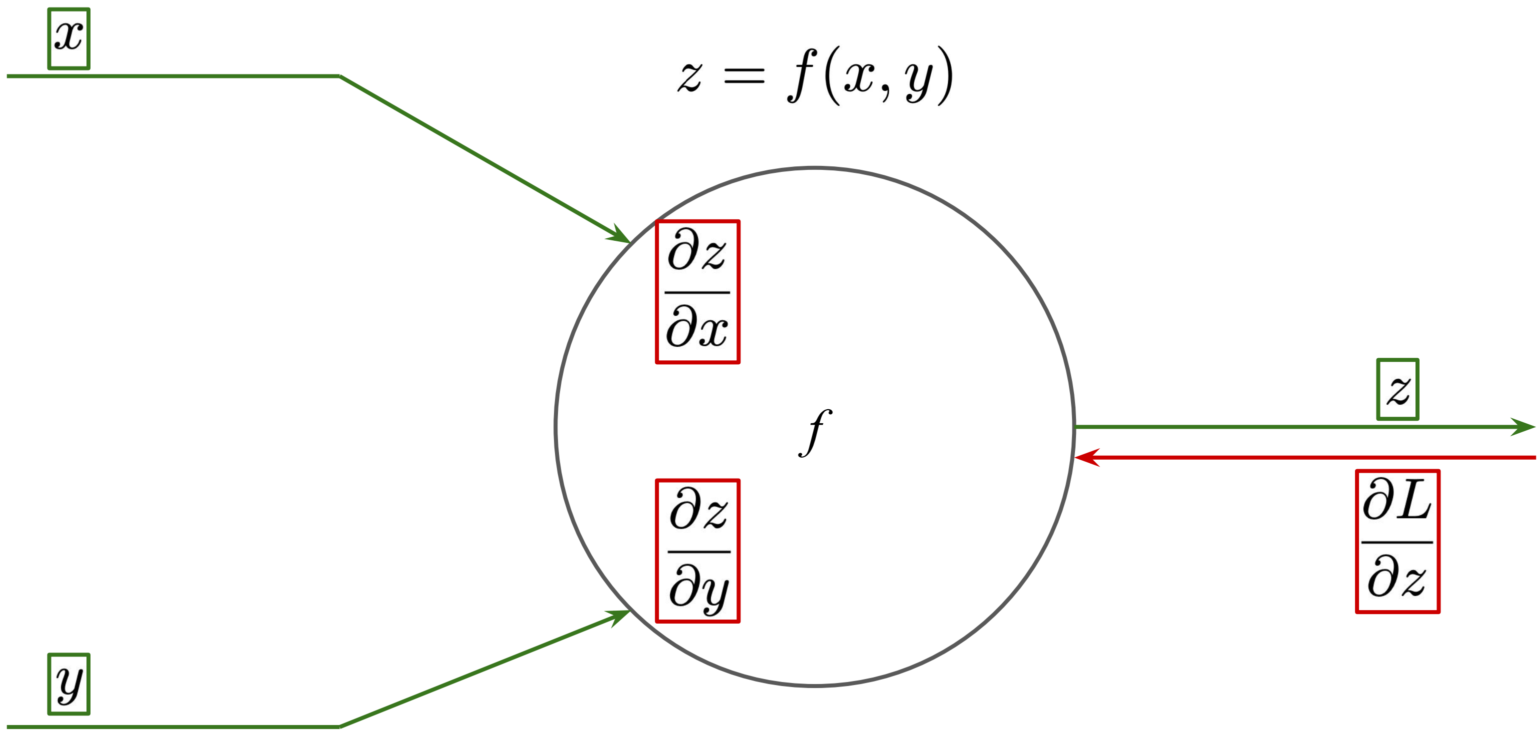

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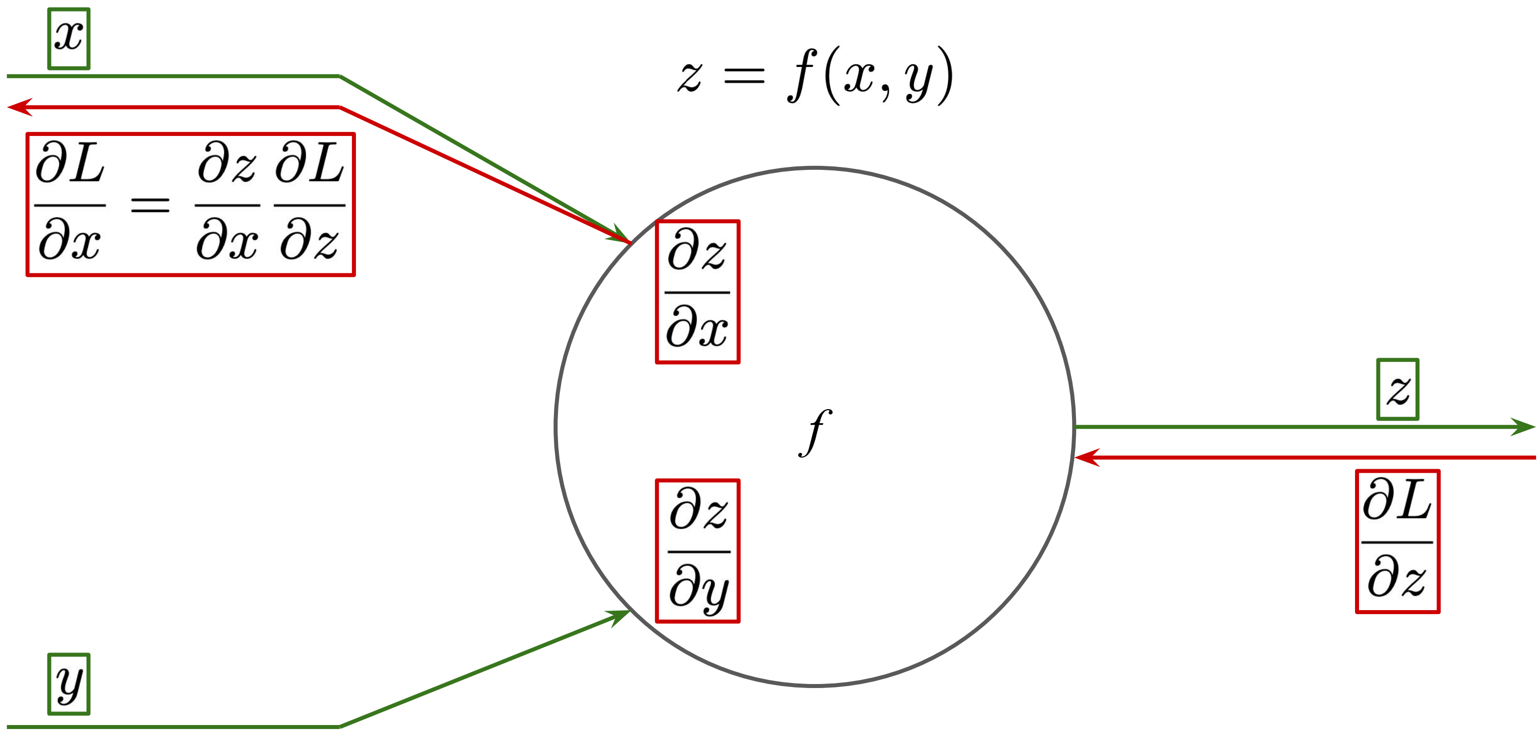

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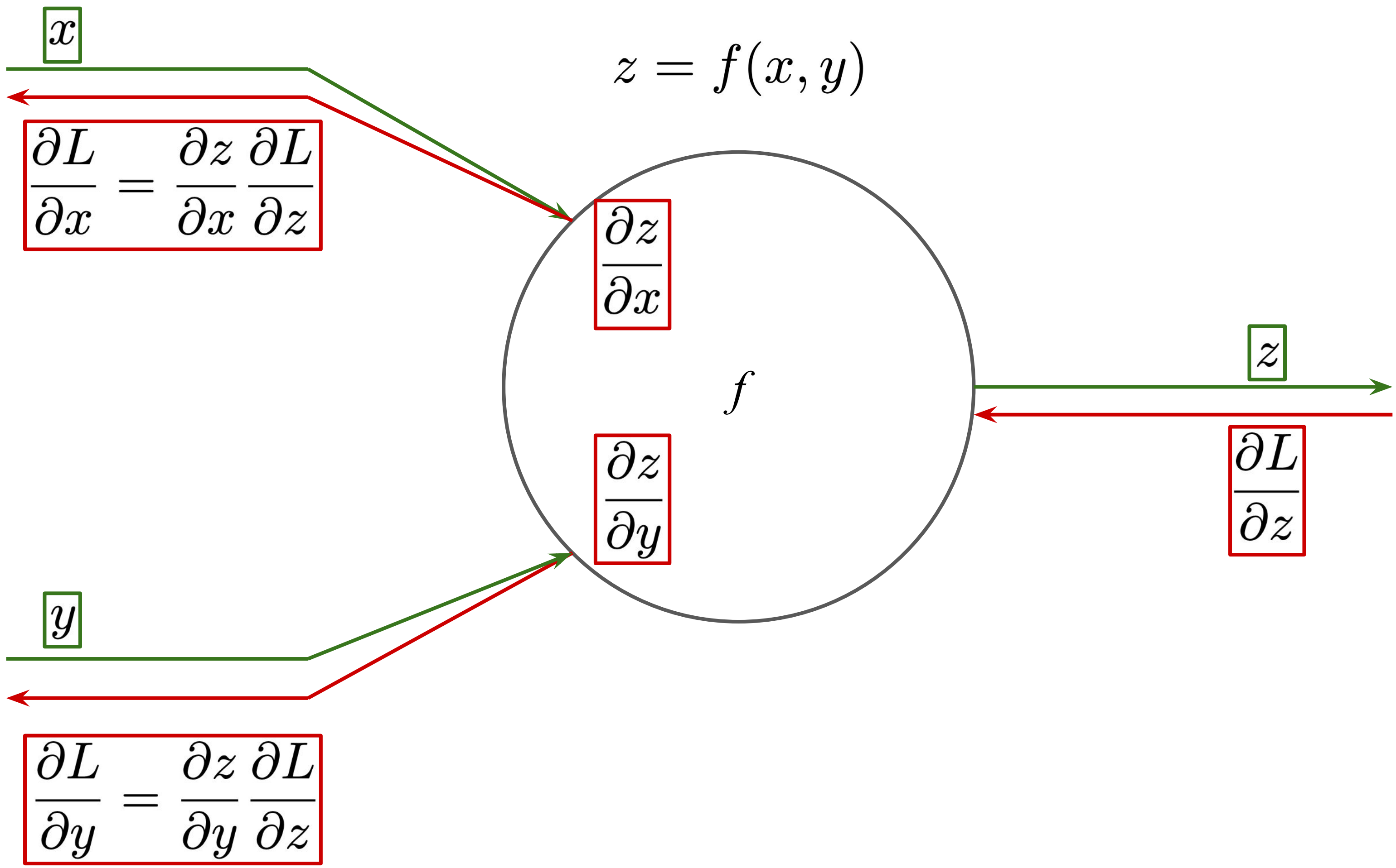

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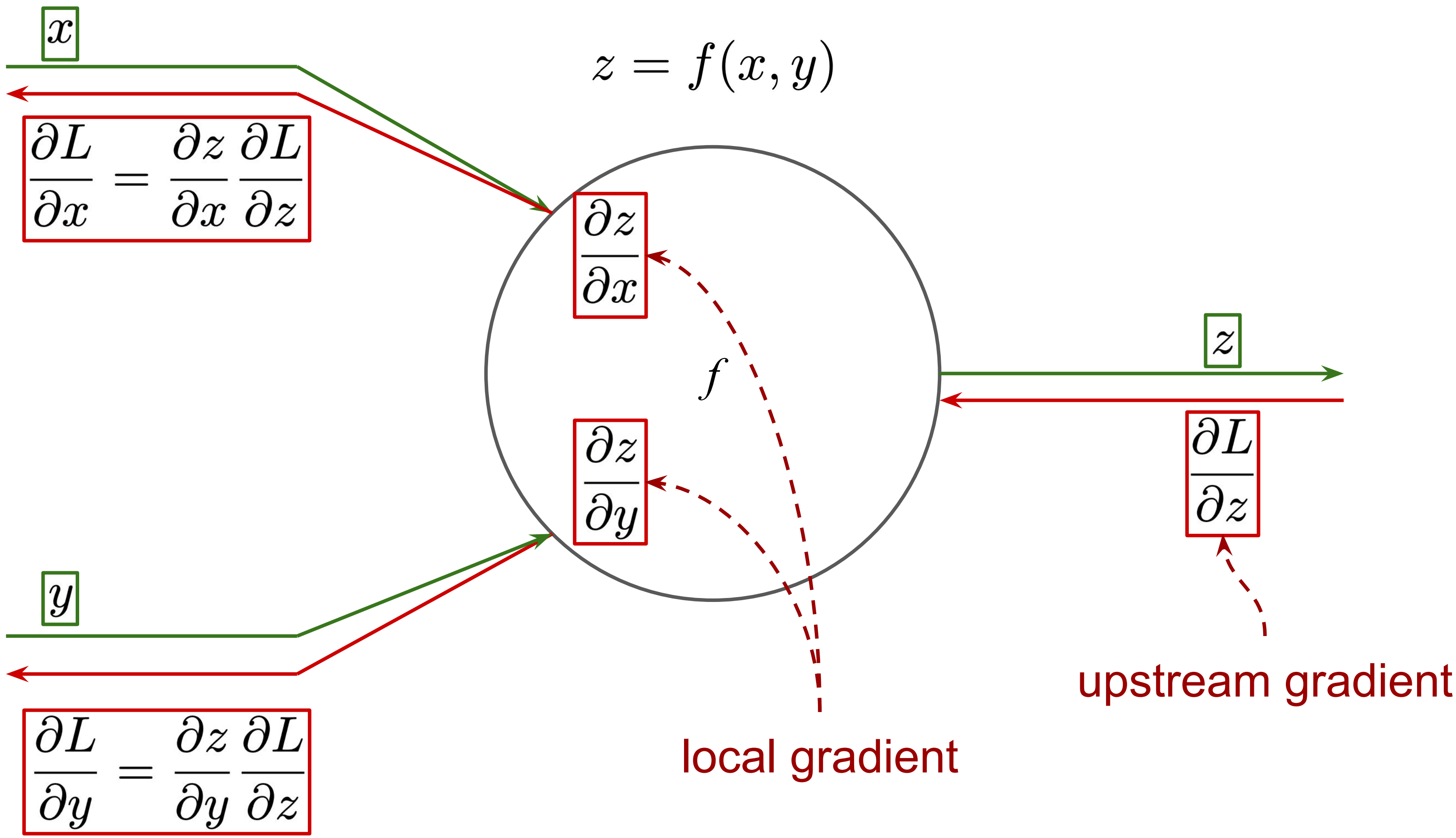
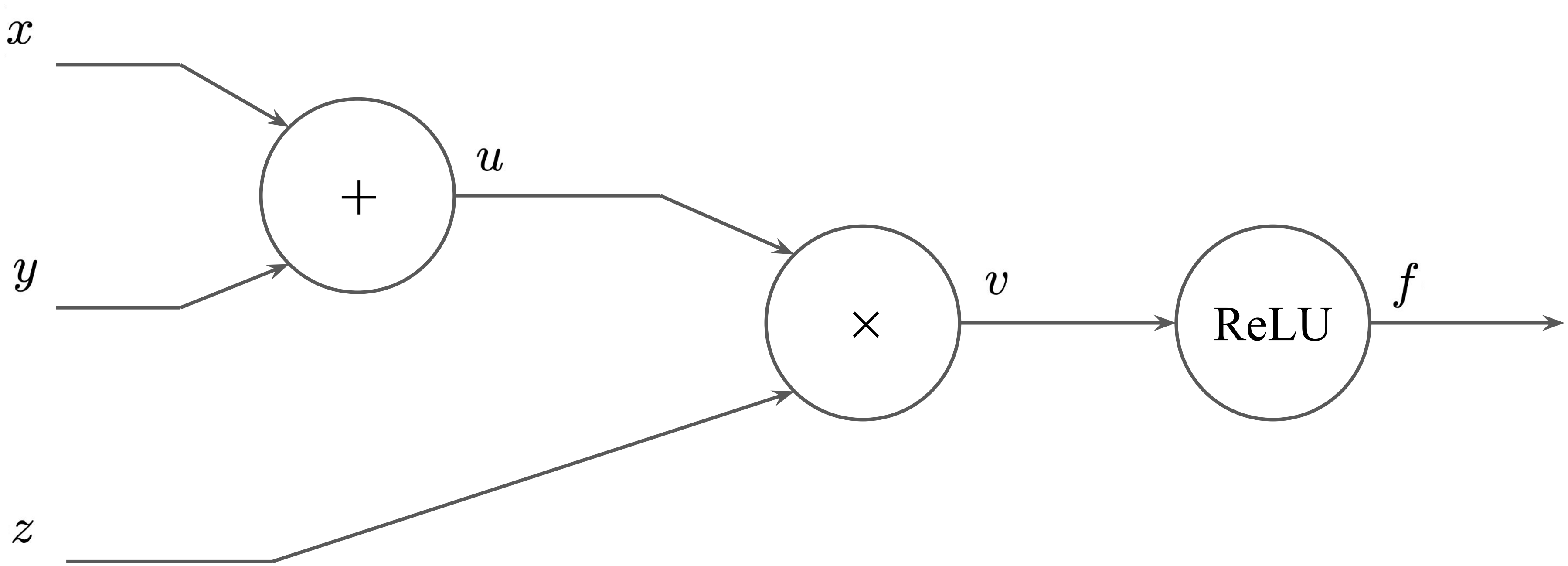


Backpropagation: scalar functions

A simple example: $f(x, y, z) = \mathrm{ReLU}((x + y)z)$
Let $u = x + y$ and $v = uz$



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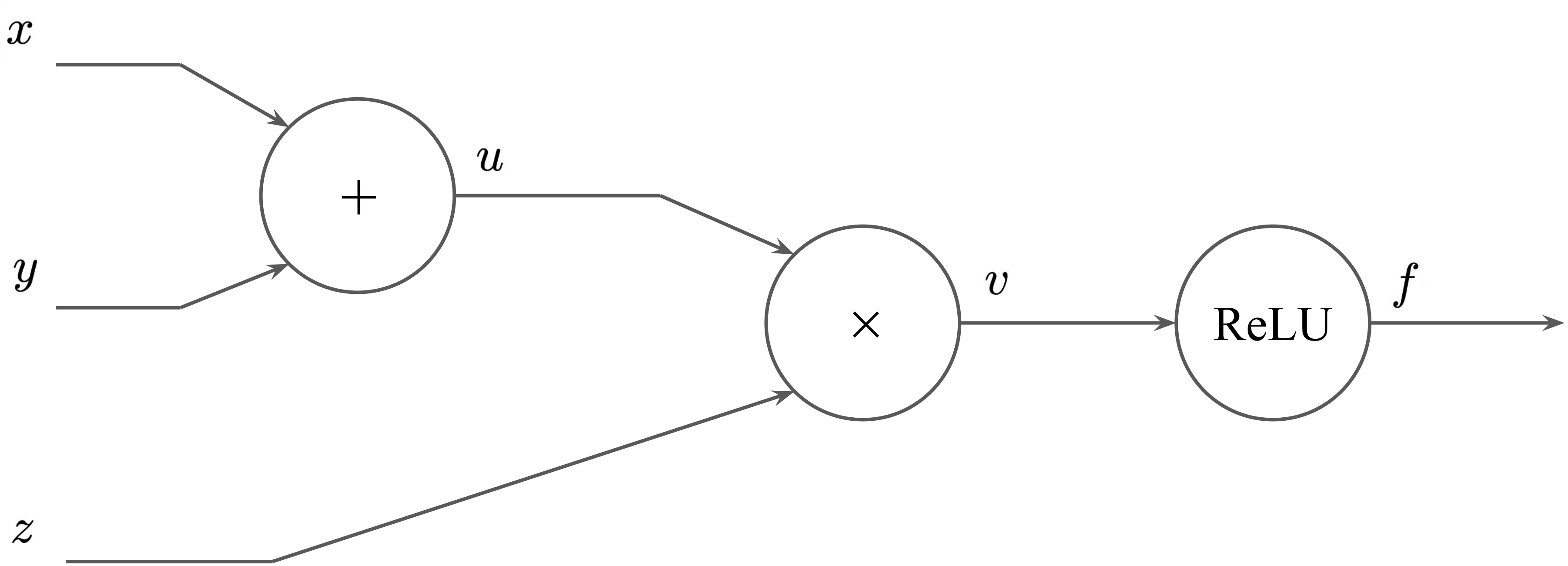

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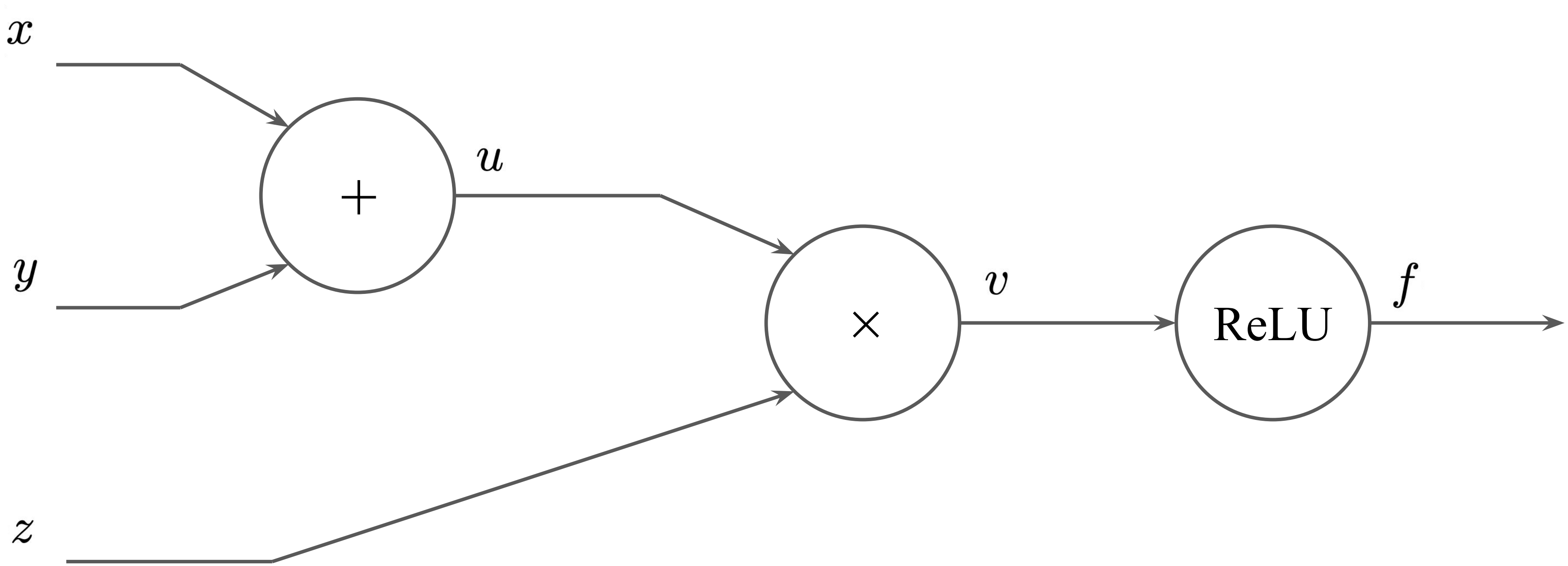

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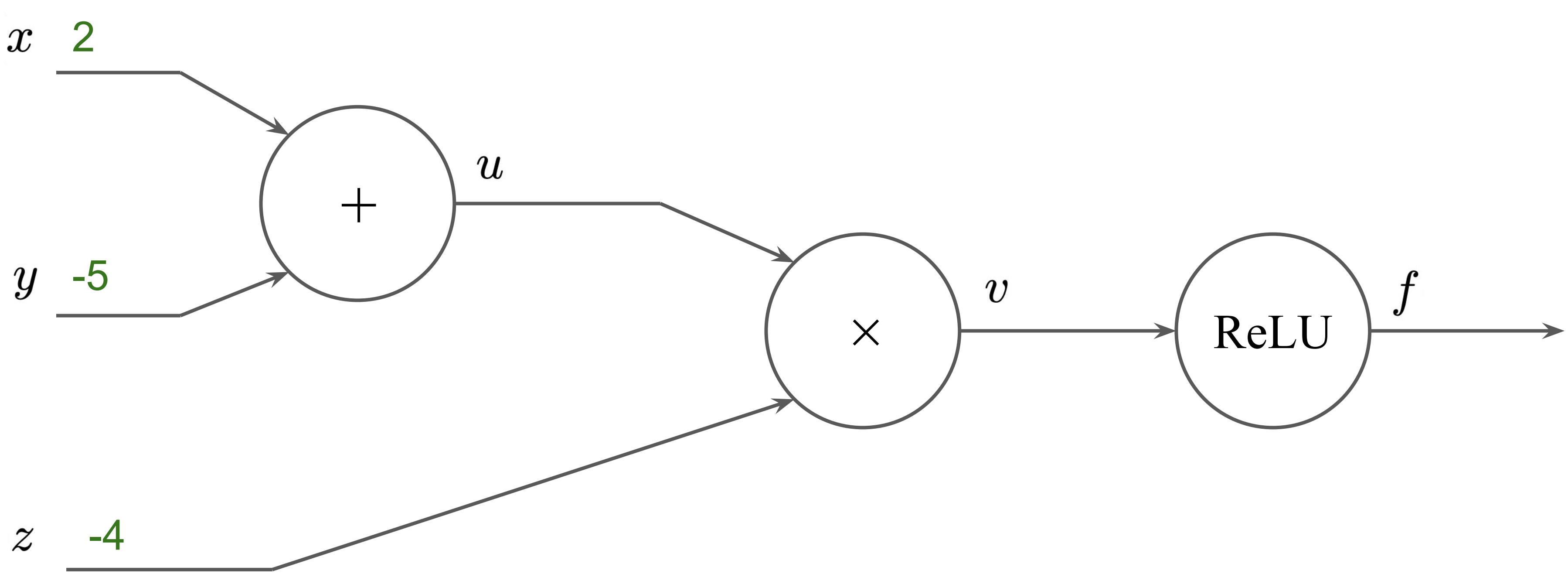

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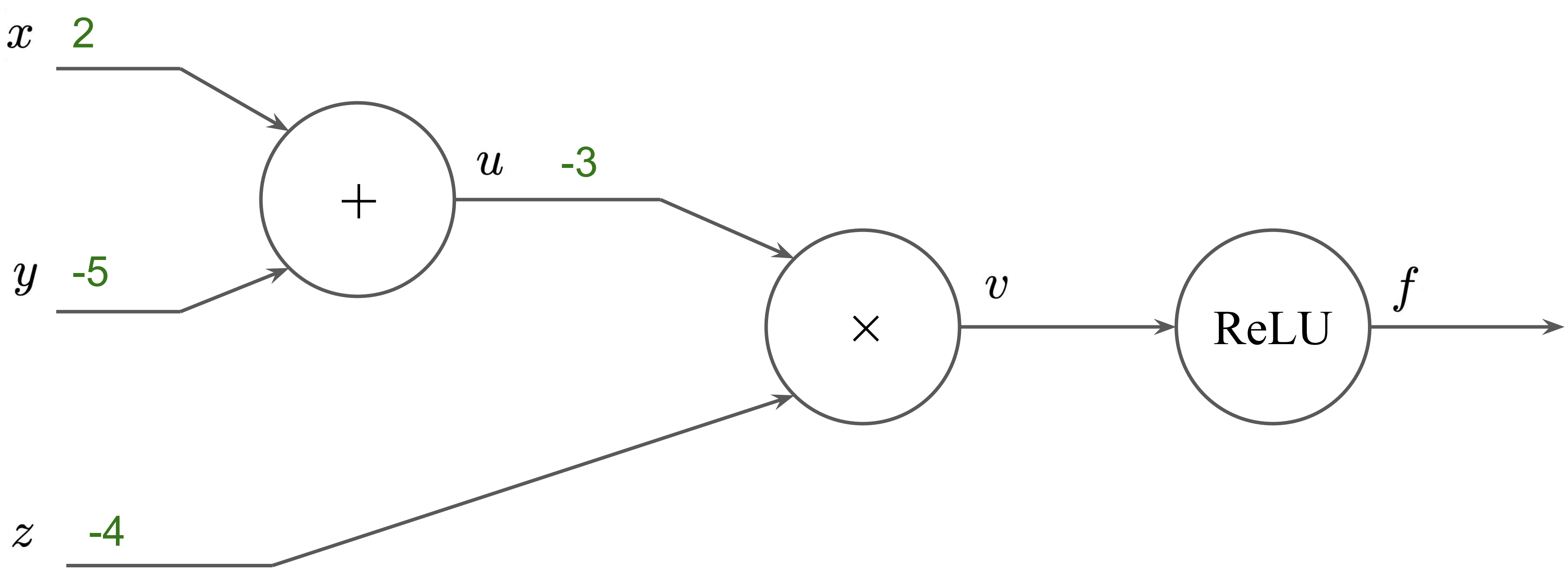

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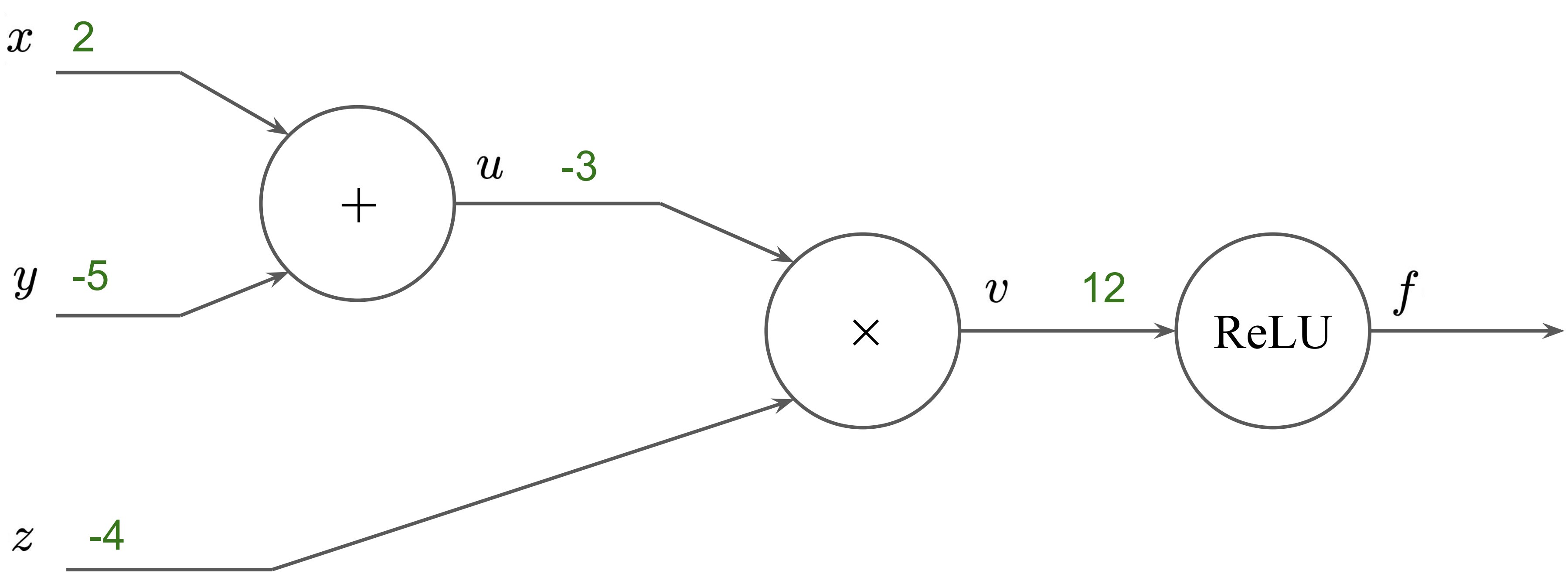

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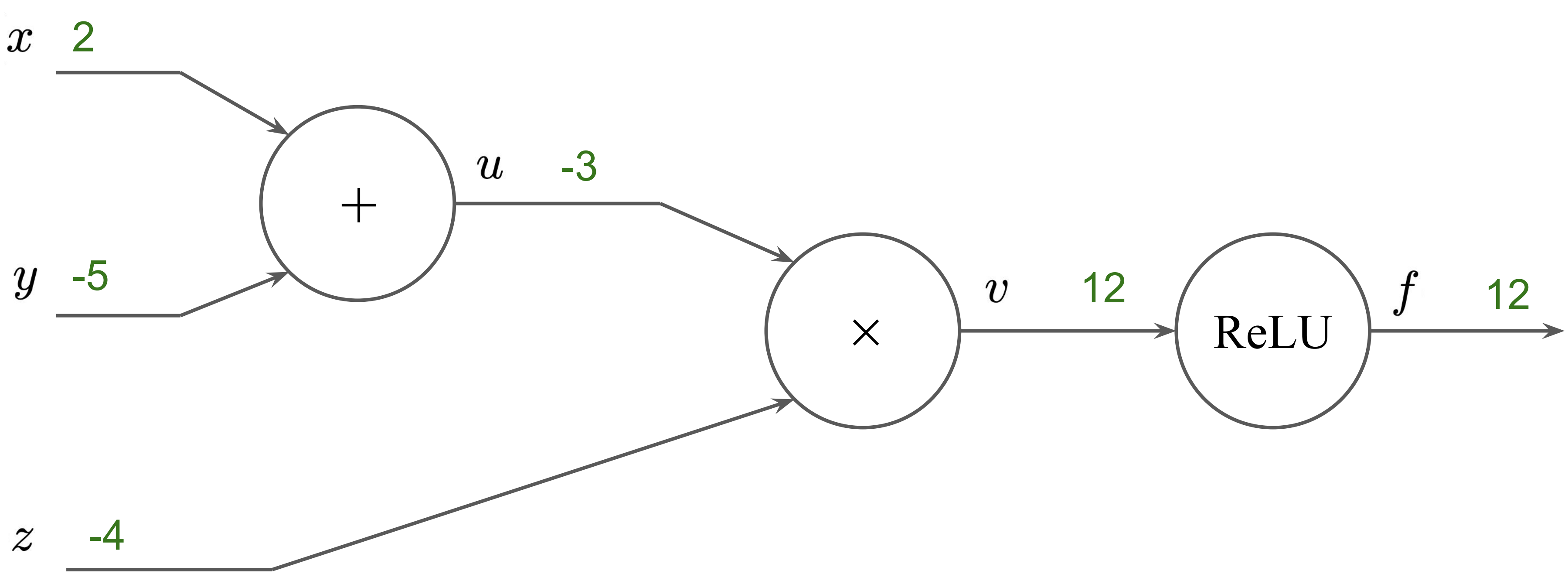

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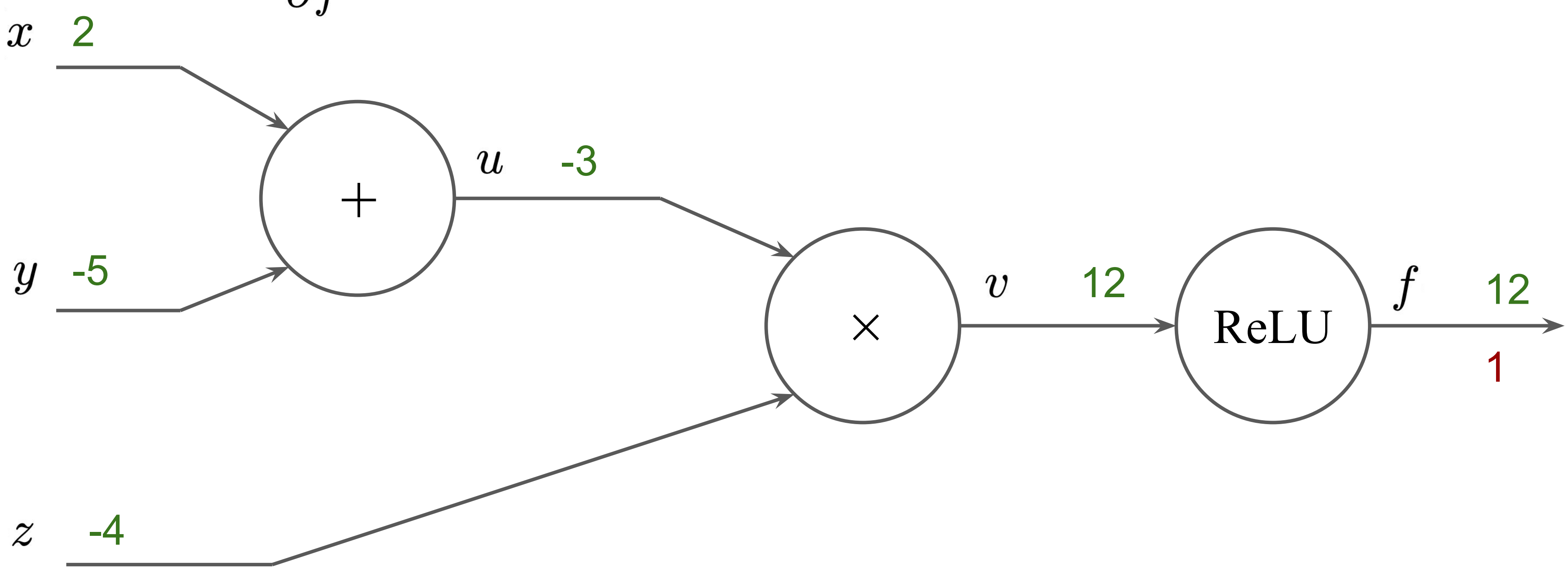
Suppose $\frac{\partial L}{\partial f} = 1$



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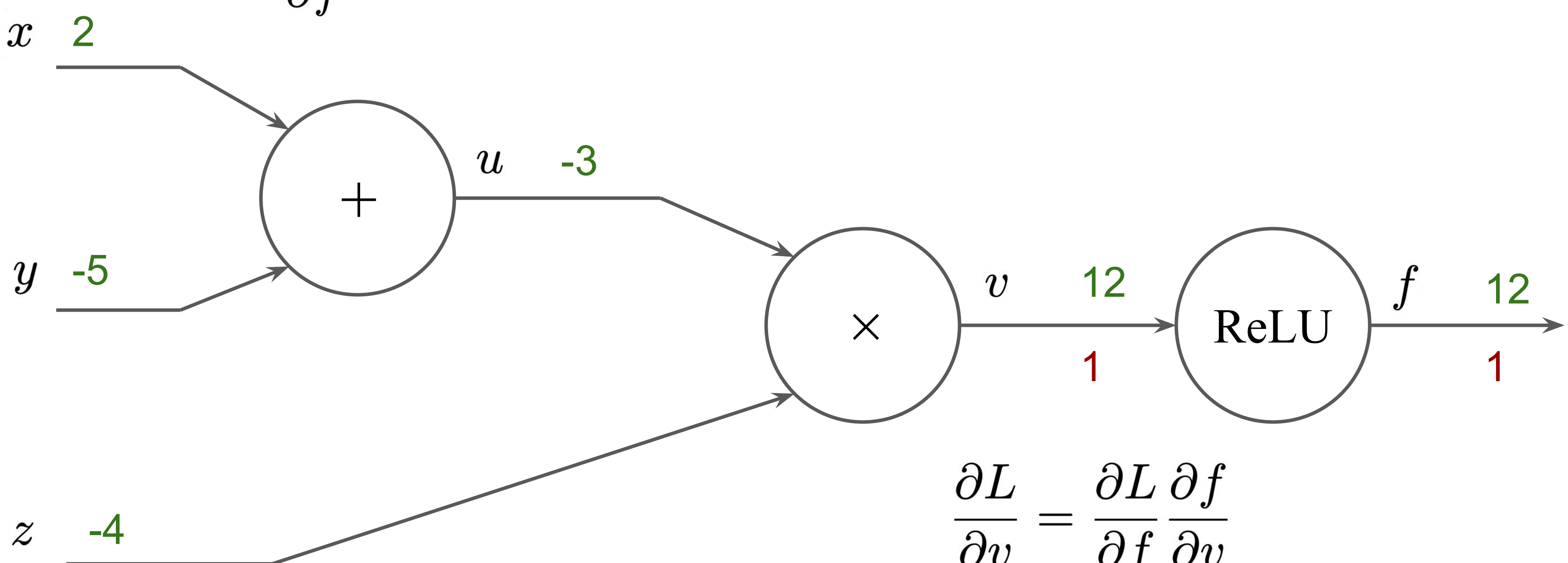

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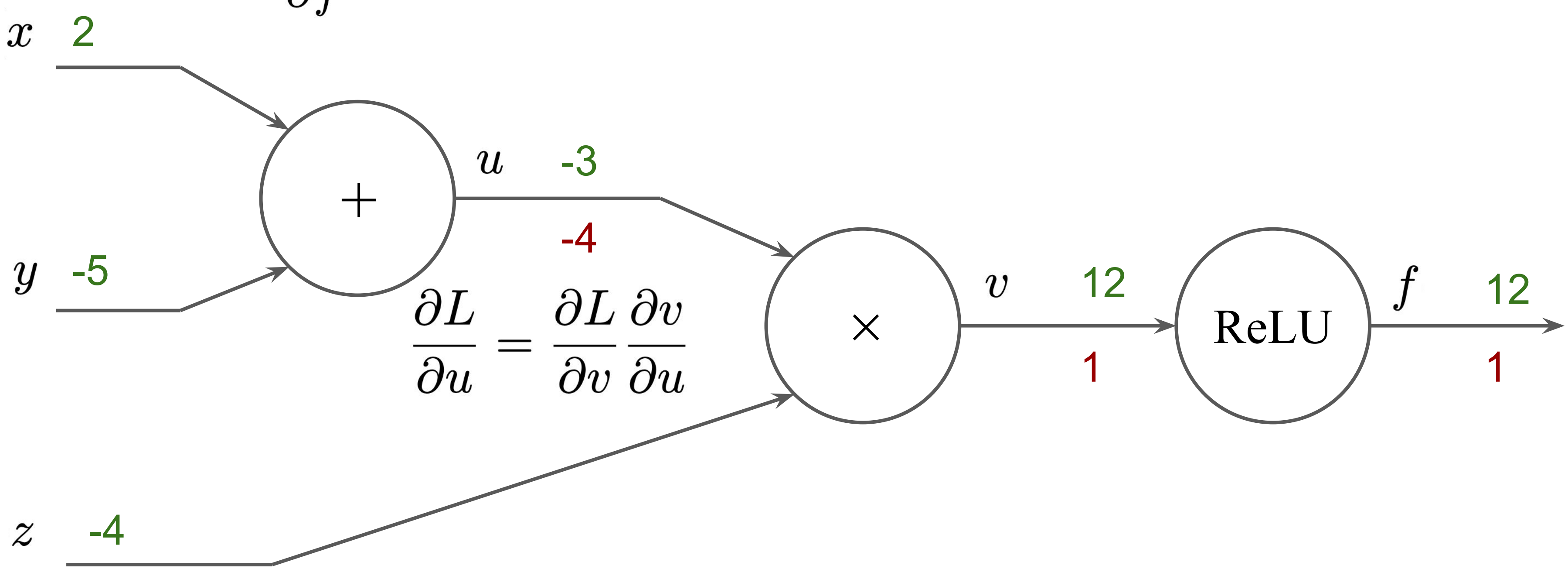

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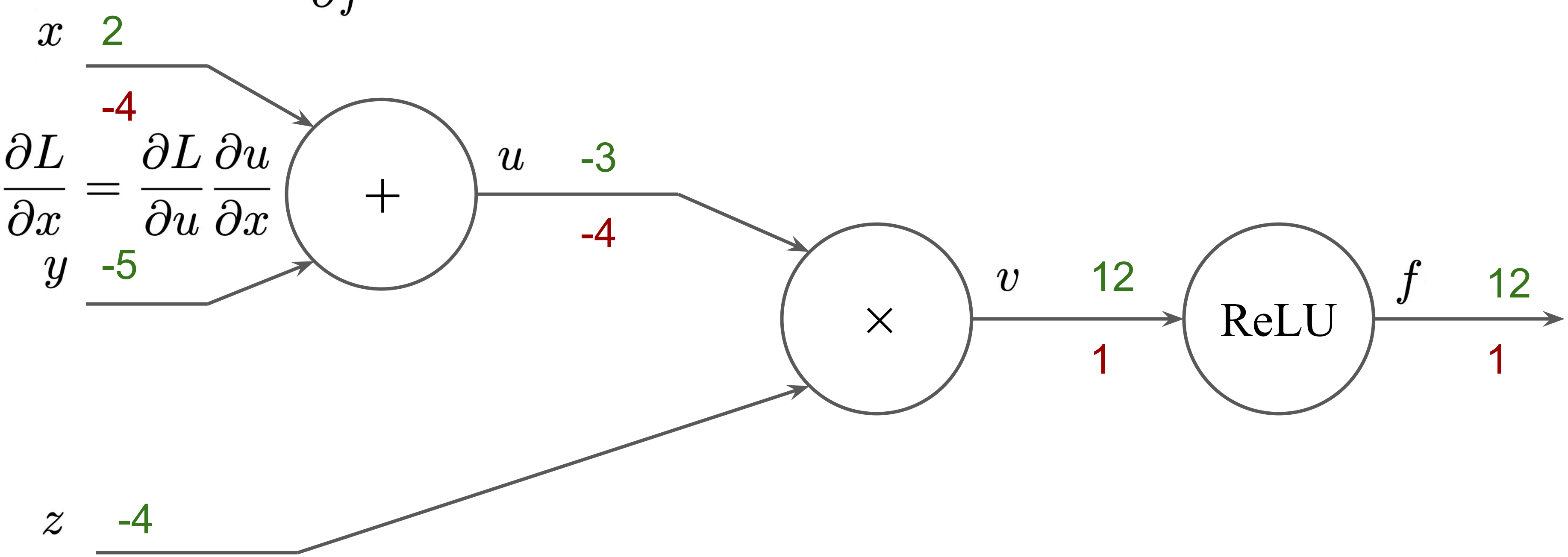

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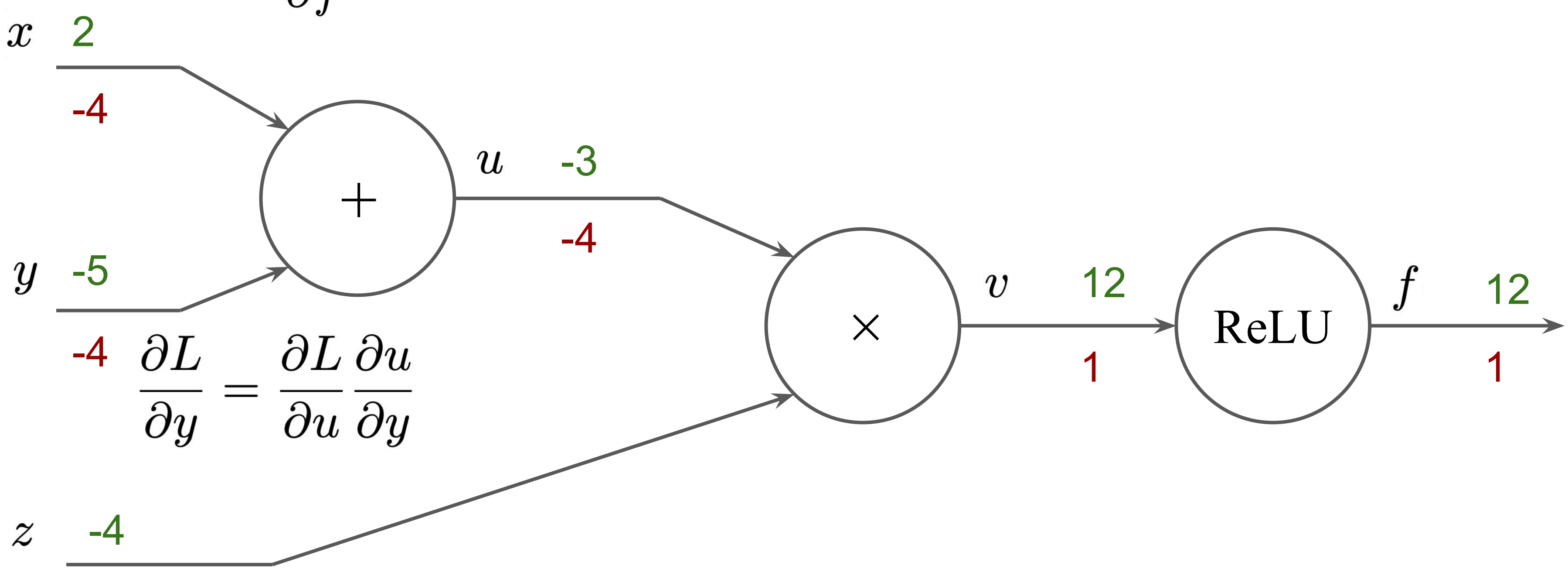

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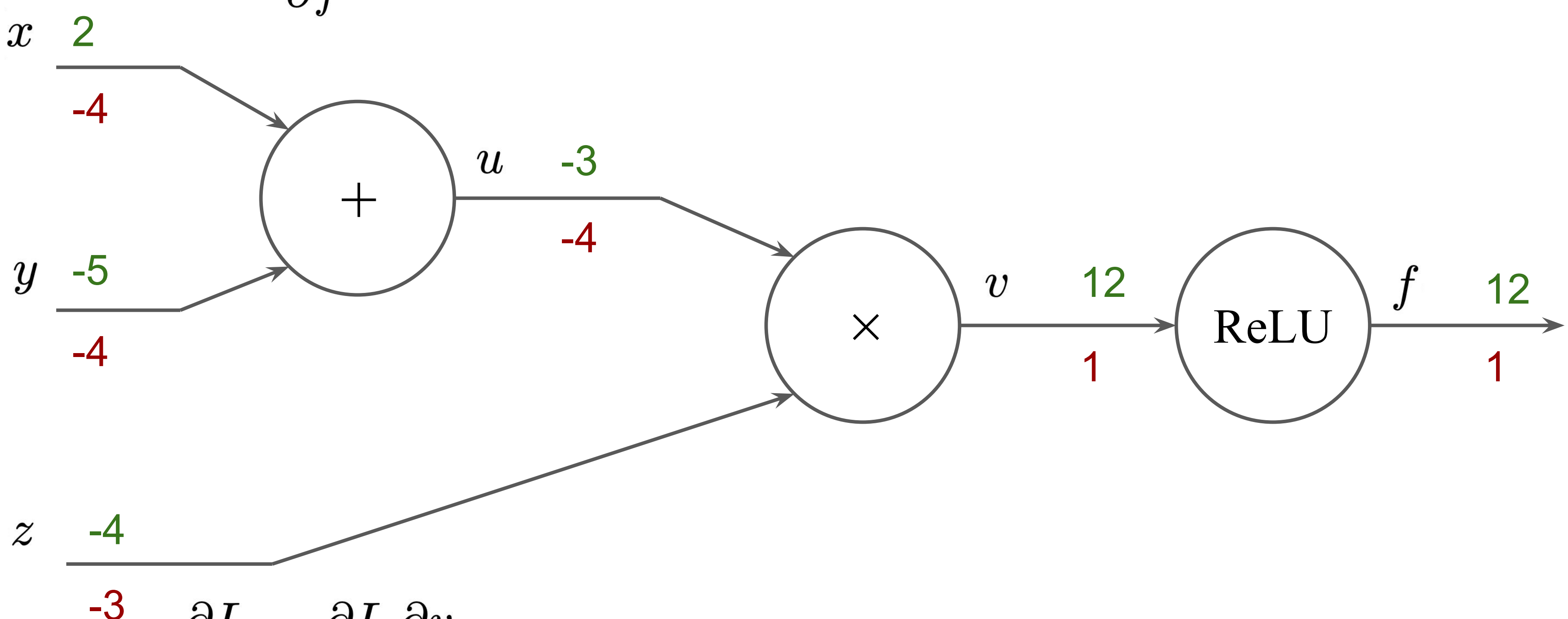

$$\frac{\partial L}{\partial z} = \frac{\partial L}{\partial v}\frac{\partial v}{\partial z}$$

Backpropagation: vector-valued functions

A more practical example of neural networks: $\boldsymbol{y} = \sigma(W\boldsymbol{x} + \boldsymbol{b})$
Let $\boldsymbol{u} = W\boldsymbol{x}$ and $\boldsymbol{v} = \boldsymbol{u} + \boldsymbol{b}$

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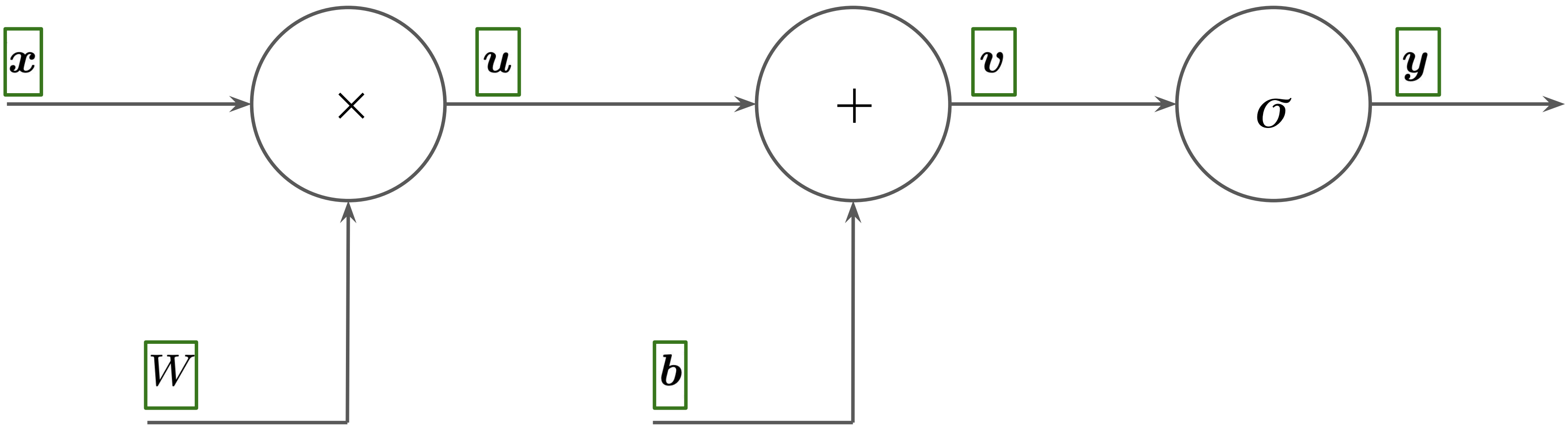

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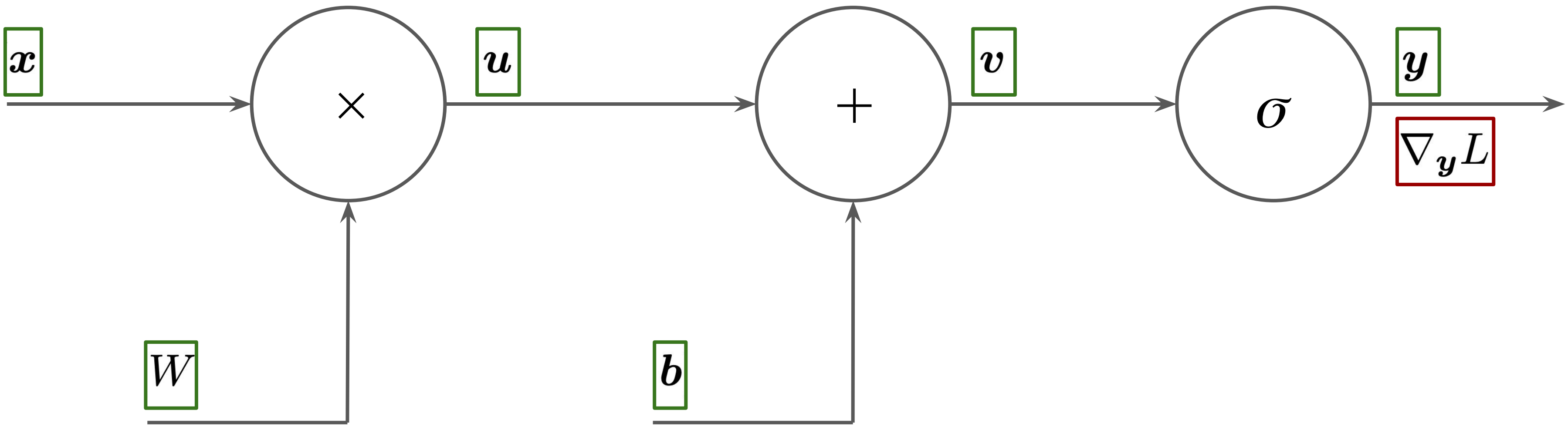

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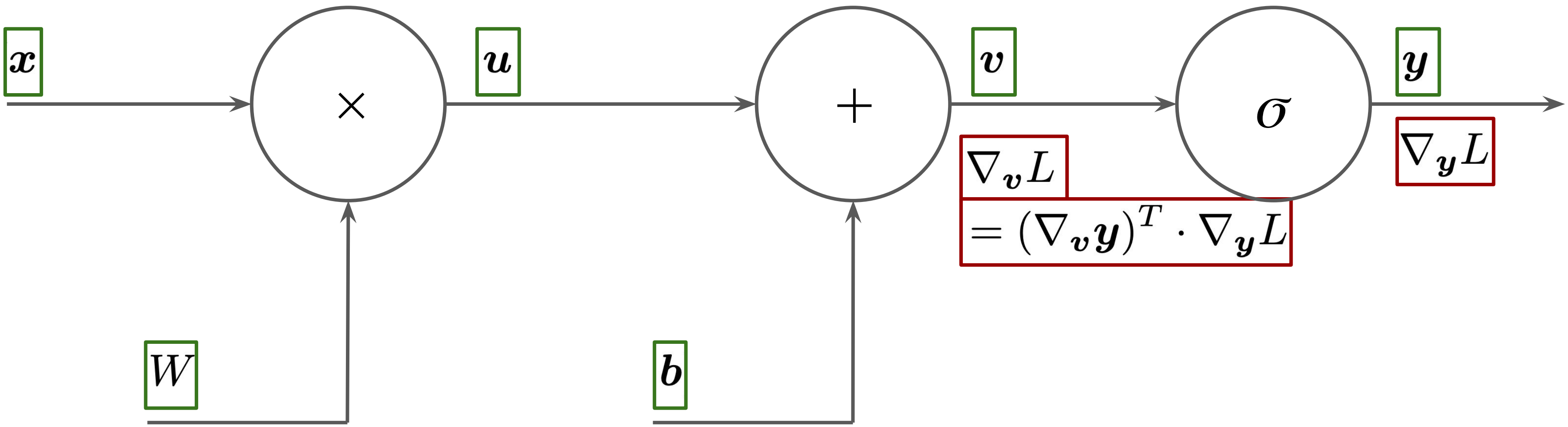

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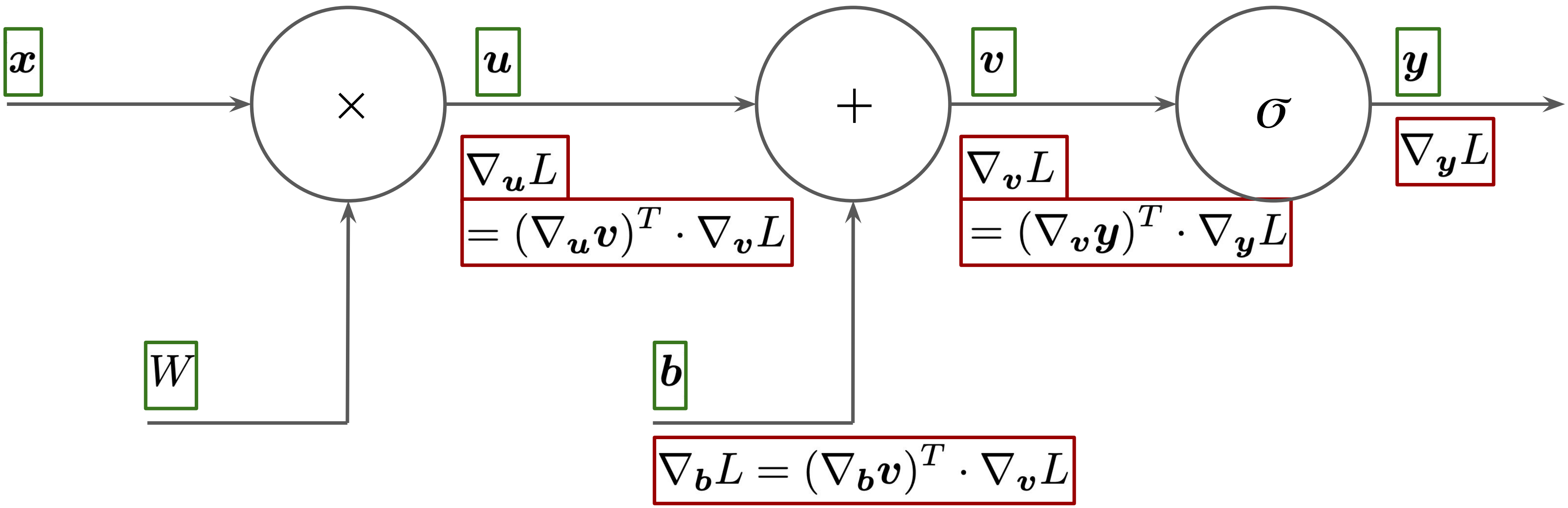

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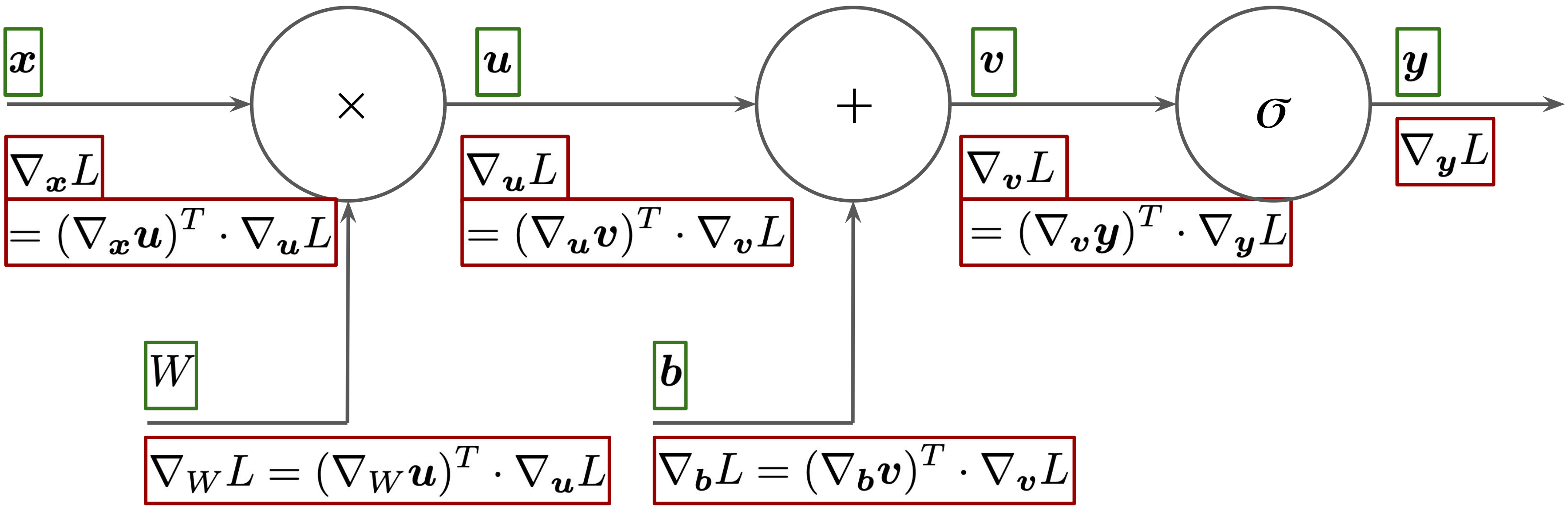
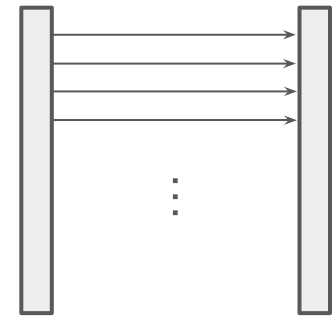


Backpropagation: vector-valued functions

Element-wise operations

Each output element depends on only one corresponding input element

Examples:



- Activation functions $\sigma()$
- Element-wise summation $\boldsymbol{x} + \boldsymbol{y}$
- Element-wise multiplication $\boldsymbol{x} \odot \boldsymbol{y}$

Gradient: also element-wise, represented by a diagonal matrix

Backpropagation: vector-valued functions

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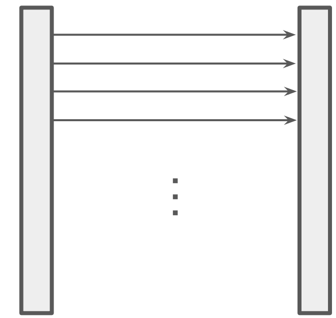
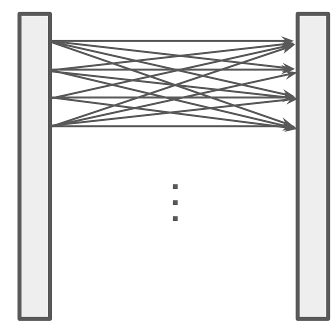


Gradient: also element-wise, represented by a diagonal matrix

More general vectorized operations
Each output element depends on many input elements



Examples:

- Matrix multiplication $\boldsymbol{y} = W\boldsymbol{x}$
- Softmax $y_i = \frac{e^{x_i}}{\sum_k e^{x_k}}$

Gradient: a dense matrix

Vanilla Gradient Descent

The loss used in vanilla version of **Gradient Descent (GD)**:

$$\theta \leftarrow \theta - \alpha \nabla_\theta \mathcal{L}(\theta)$$

is across the entire dataset

$$\begin{aligned}
\mathcal{L}(\theta) &= \mathbb{E}_{(x,y)\sim p_{\text{data}}}\left([\mathcal{L}(f_\theta(x), y)]\right) \\
&= \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(f_\theta(x_i), y_i)
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<u>Can we make faster progress?</u>

Make more frequent updates by using only a subset of data at each iteration!

Mini-batch Stochastic Gradient Descent (SGD)

At each iteration, sample a mini-batch (subset) $\mathcal{B} \subset \{1, 2, \ldots, N\}$ to compute loss

$$\mathcal{L}_{\mathcal{B}}(\theta) = \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \ell_i(\theta) = \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \mathcal{L}(f_\theta(x_i), y_i)$$

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Though the selection of mini-batch $\mathcal{B}$ is random, we want every data sample to have equal opportunity to be used in training.

This is to guarantee that the original data distribution in the dataset is unchanged!

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In practice, we randomly permute the dataset indices

$$(\pi_1, \pi_2, \ldots, \pi_N) \leftarrow \text{random\_permute}(1, 2, \ldots, N)$$

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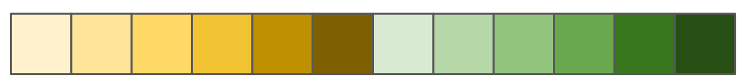

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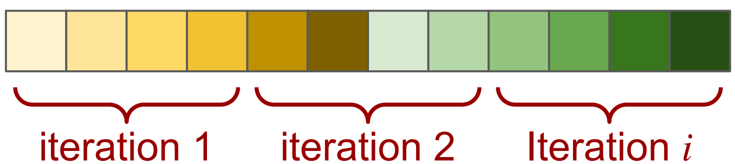

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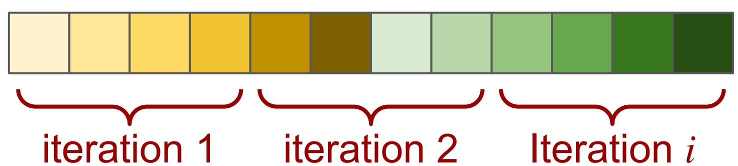
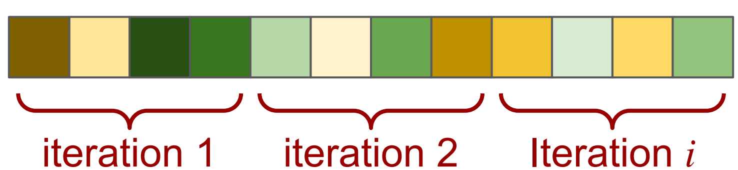


Mini-batch **stochastic** gradient descent (SGD):



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A short break

We will be back in 5 mins

Problems of Stochastic Gradient Descent (SGD):

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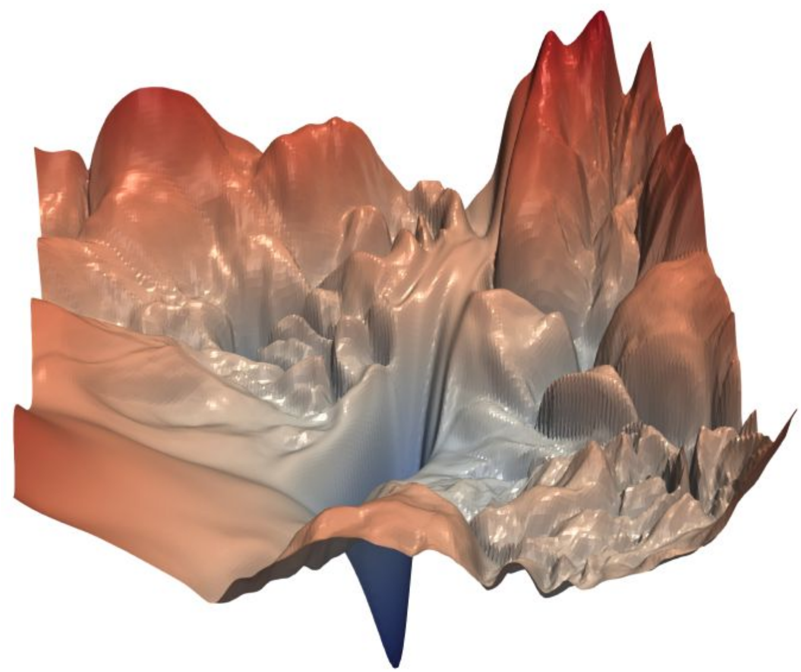

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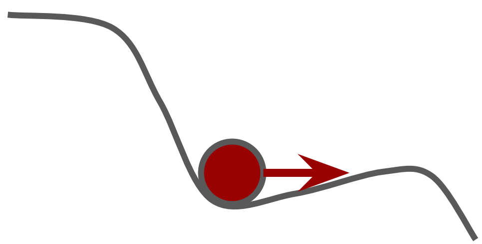
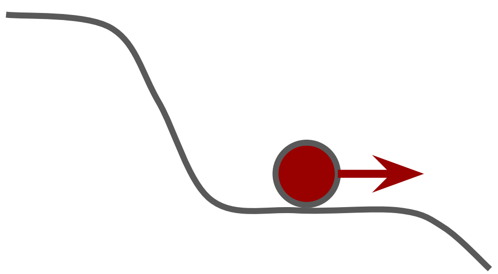


Local minima



Saddle points

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- Parameters can have different scales
    - A single learning rate may not be optimal for all parameters

Stochastic Gradient Descent (SGD) + Momentum

Solution: SGD + Momentum:

- Build up "velocity of gradients" as a **running mean** of gradients
- Dampens oscillations in the gradients
- Decay rate ρ is usually set as 0.9 or 0.99

SGD:	**SGD + Momentum**:
while True **do**	**while** True **do**
Sample batch $\mathcal{B}$	Sample batch $\mathcal{B}$
$\theta_{t+1} \leftarrow \theta_t - \alpha \nabla_\theta \mathcal{L}_\mathcal{B}(\theta_t)$	$m_{t+1} \leftarrow \rho \cdot m_t + \nabla_\theta \mathcal{L}_\mathcal{B}(\theta_t)$
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SGD + Momentum (equivalent):
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θ_t

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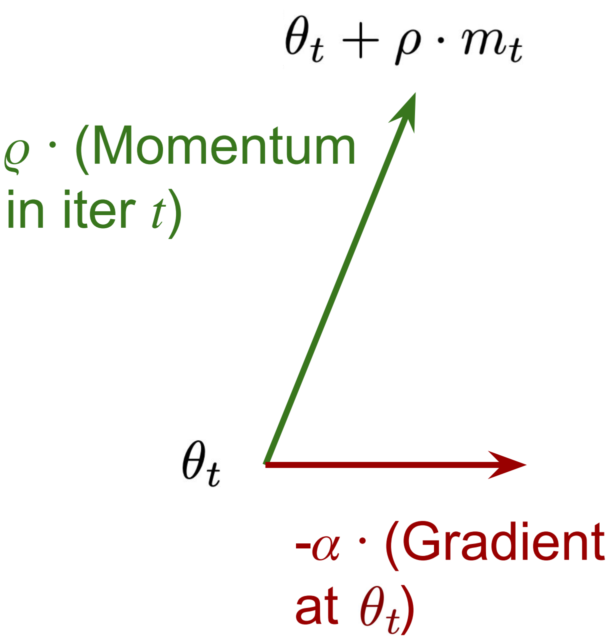

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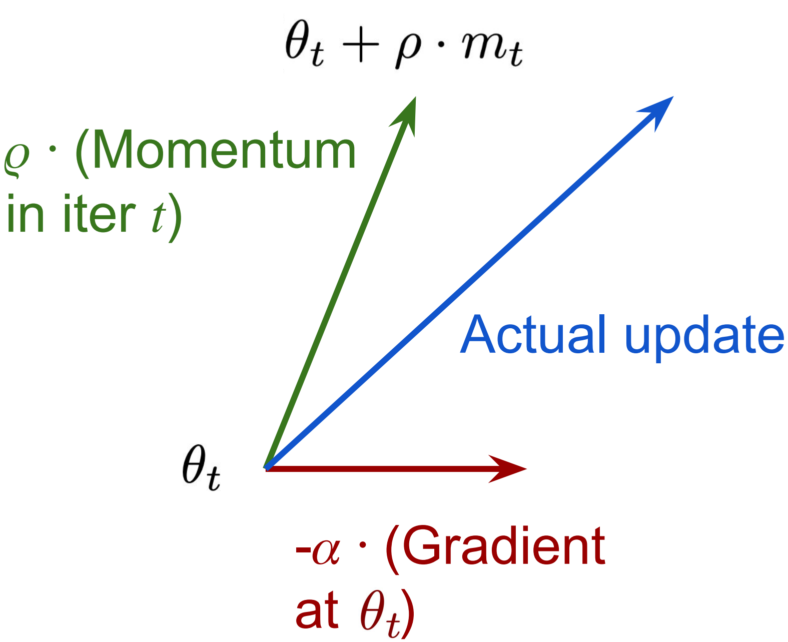

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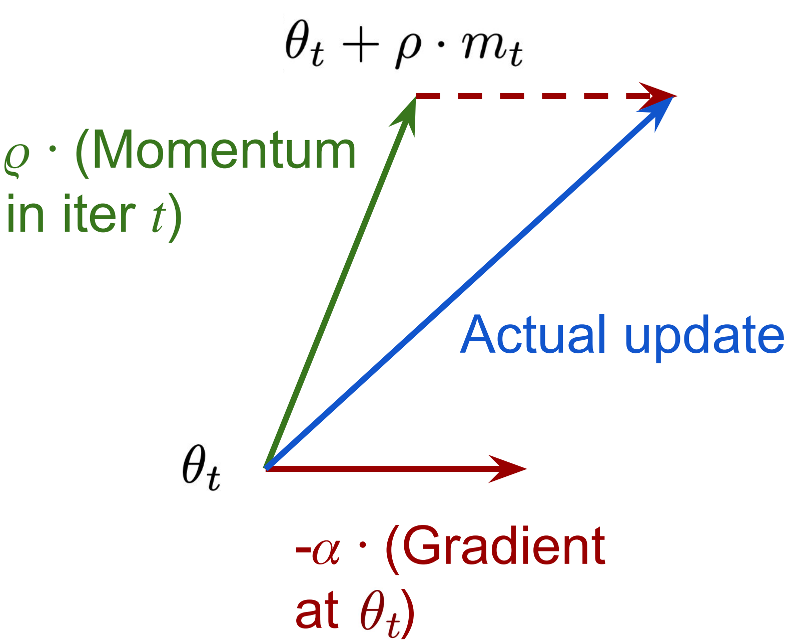

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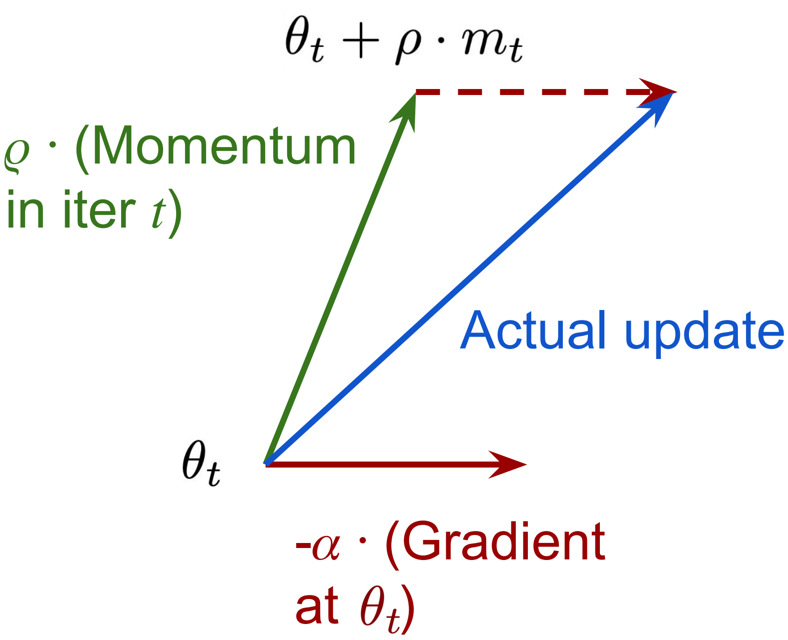

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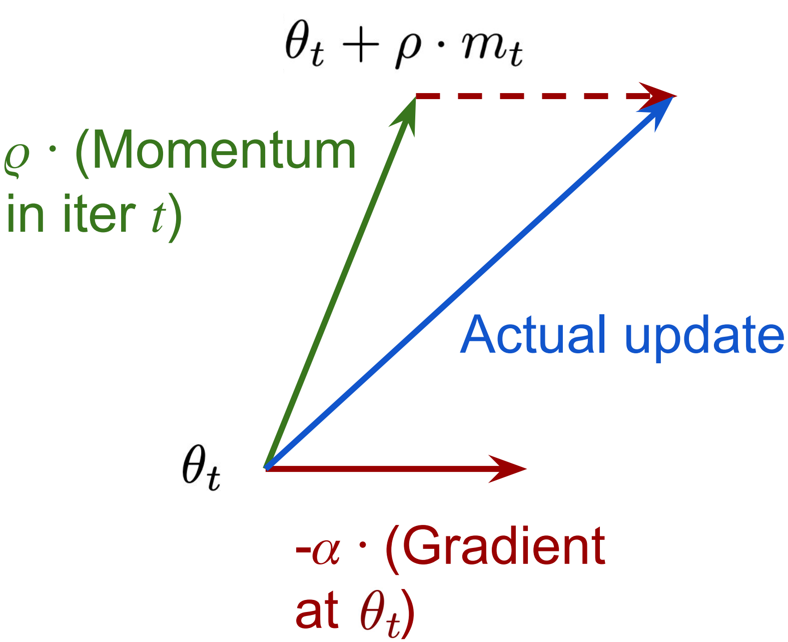

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Instead, where should the gradient be evaluated at?

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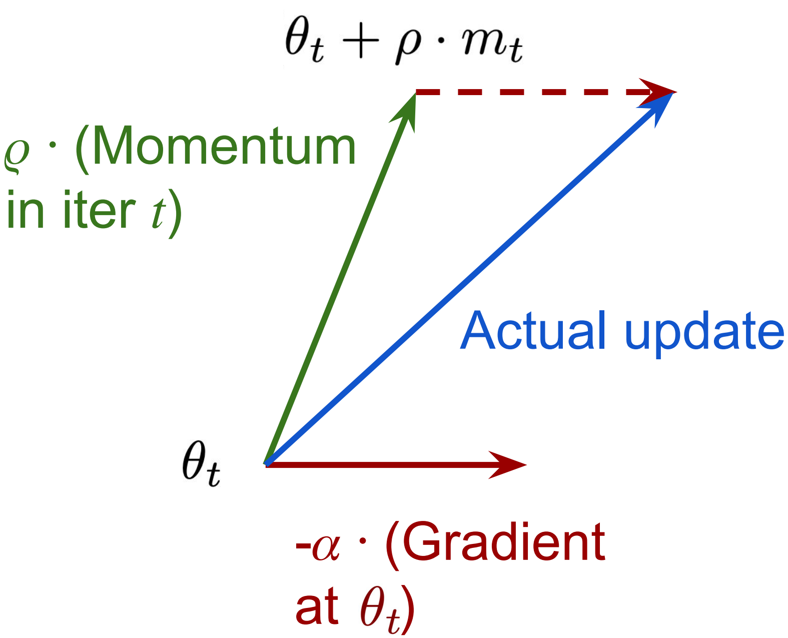

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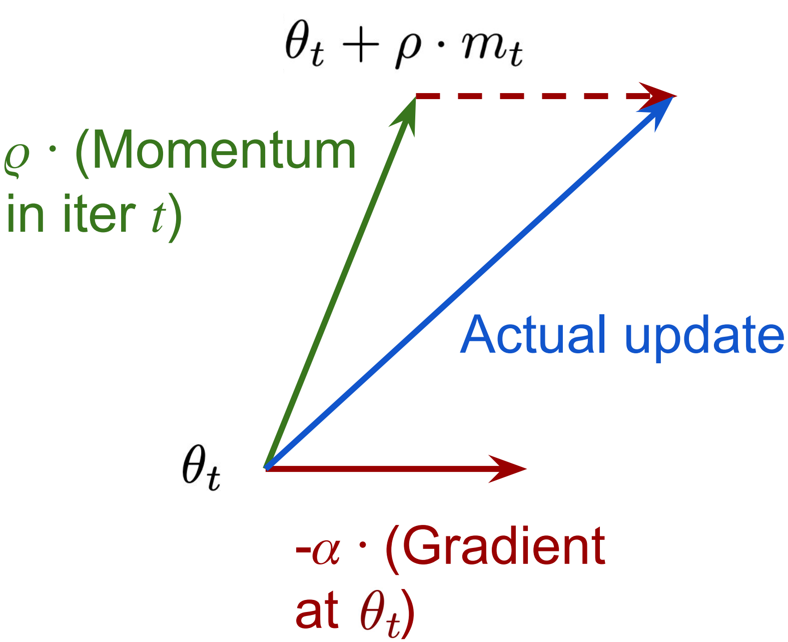

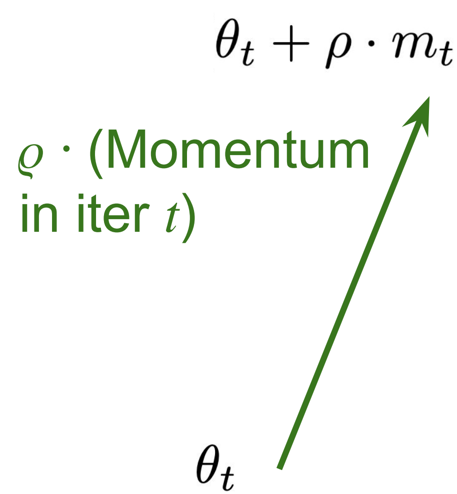

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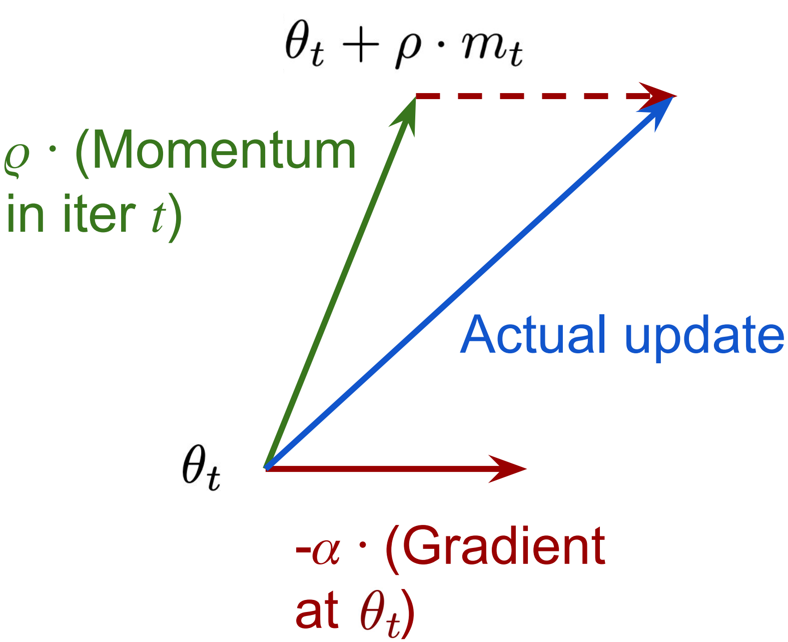

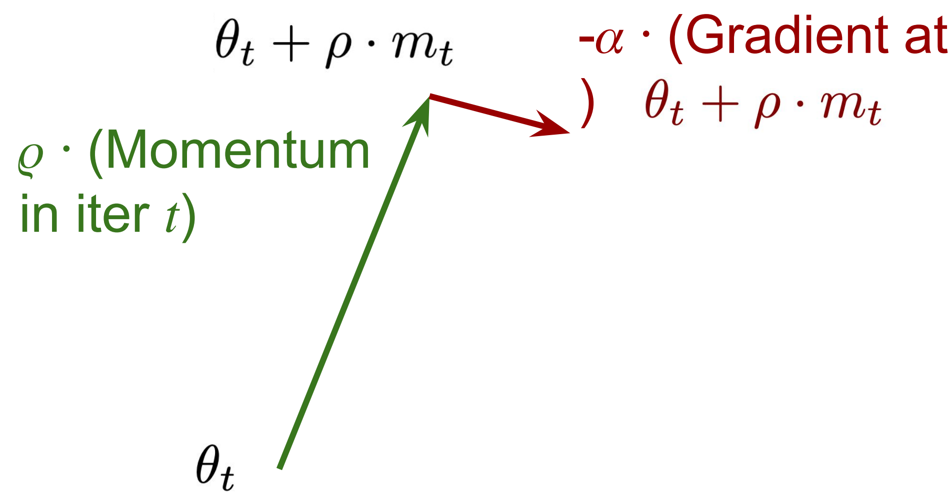

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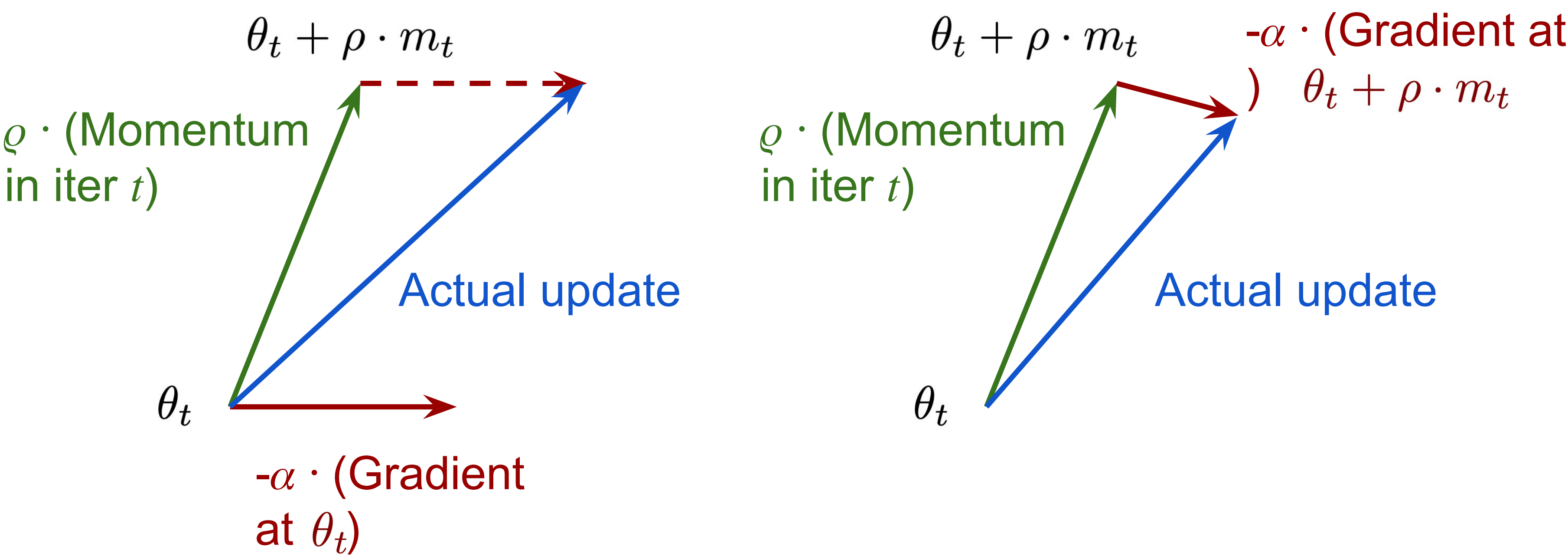

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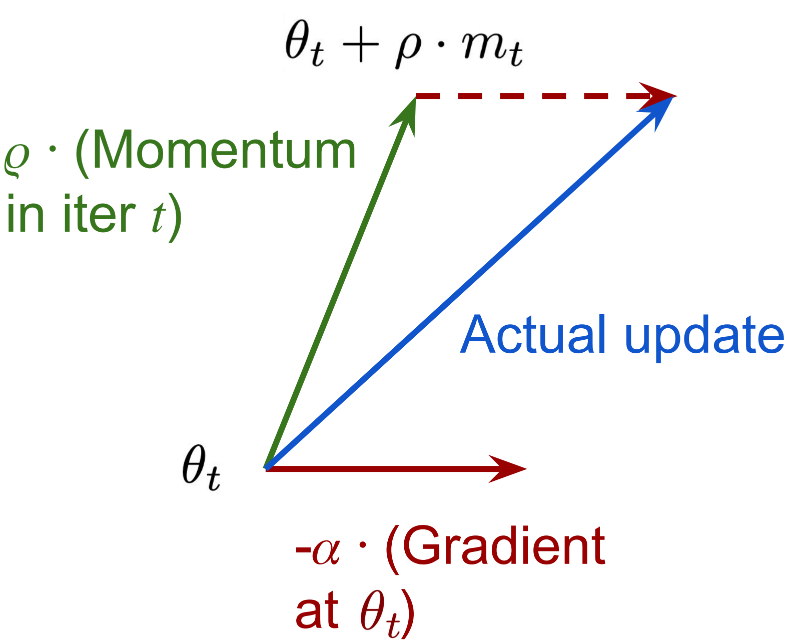

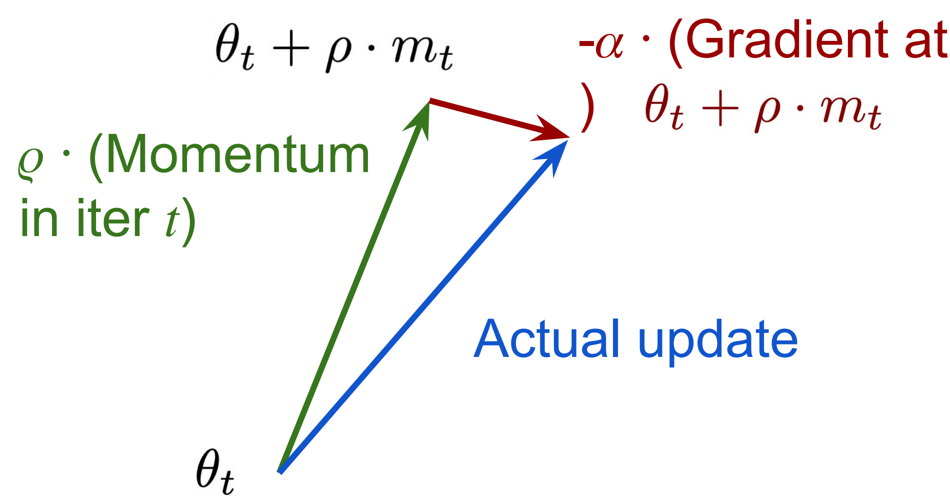

In most cases shows faster or more stable convergence than vanilla gradient

How to deal with parameters with different scales?

Adagrad

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Initialize $v \leftarrow 0$
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Duchi et al, “Adaptive subgradient methods for online learning and stochastic optimization”, JMLR 2011

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Historical element-wise sum of squares in each dimension of gradient

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However, when $t \rightarrow +\infty, v \rightarrow +\infty$, the update will decay to zero!

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

RMSProp

How to deal with parameters with different scales?

Adagrad

Initialize $v \leftarrow 0$
while True **do**
    Sample batch $\mathcal{B}$
    $v \leftarrow v + [\nabla_\theta \mathcal{L}_\mathcal{B}(\theta_t)]^2$
    $$\theta_{t+1} \leftarrow \theta_t - \alpha \cdot \frac{\nabla_\theta \mathcal{L}_\mathcal{B}(\theta_t)}{\sqrt{v} + \epsilon}$$
end

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From **accumulation** to **running mean** of element-wise square of gradient

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Can we combine the ideas of both:

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while True **do**

Sample batch $\mathcal{B}$

$$m \leftarrow \beta_1 \cdot m + (1 - \beta_1) \cdot \nabla_\theta \mathcal{L}_\mathcal{B}(\theta_t)$$

$$v \leftarrow \beta_2 \cdot v + (1 - \beta_2) \cdot [\nabla_\theta \mathcal{L}_\mathcal{B}(\theta_t)]^2$$

$$\theta_{t+1} \leftarrow \theta_t - \alpha \cdot \frac{m}{\sqrt{v} + \epsilon}$$

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Kingma and Ba, “Adam: A method for stochastic optimization”, ICLR 2015

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A good starting point: $\beta_1 = 0.9, \beta_2 = 0.999$

Kingma and Ba, “Adam: A method for stochastic optimization”, ICLR 2015

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$$m \leftarrow \frac{m}{1 - \beta_1^t}$$

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$$\boxed{\begin{aligned} m &\leftarrow \frac{m}{1 - \beta_1^t} \\ v &\leftarrow \frac{v}{1 - \beta_2^t} \end{aligned}}$$

Bias correction (<u>**why is it needed?**</u>)

$$\theta_{t+1} \leftarrow \theta_t - \alpha \cdot \frac{m}{\sqrt{v} + \epsilon}$$

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Adam (full form):

Where do the biases come from?
Both running means start at 0, and it needs time to warm up!

Suppose the gradient is roughly stationary with mean $\mathbb{E}[\nabla_\theta \mathcal{L}_\mathcal{B}(\theta)]$
We will have

$$\mathbb{E}[m_1] = \mathbb{E}[\beta_1 \cdot m_0] + \mathbb{E}[(1-\beta_1) \cdot \nabla_\theta \mathcal{L}_\mathcal{B}(\theta)]$$

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\cdots \\
\mathbb{E}[m_t] &= (1-\beta_1^t) \cdot \mathbb{E}[\nabla_\theta \mathcal{L}_\mathcal{B}(\theta)]
\end{aligned}$$

So it needs to be scaled by $1/(1-\beta_1^t)$

Another way to view it: the influence of the zero initialization decays exponentially at rates β_1^t

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Learning rate scheduling

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a **hyperparameter**.

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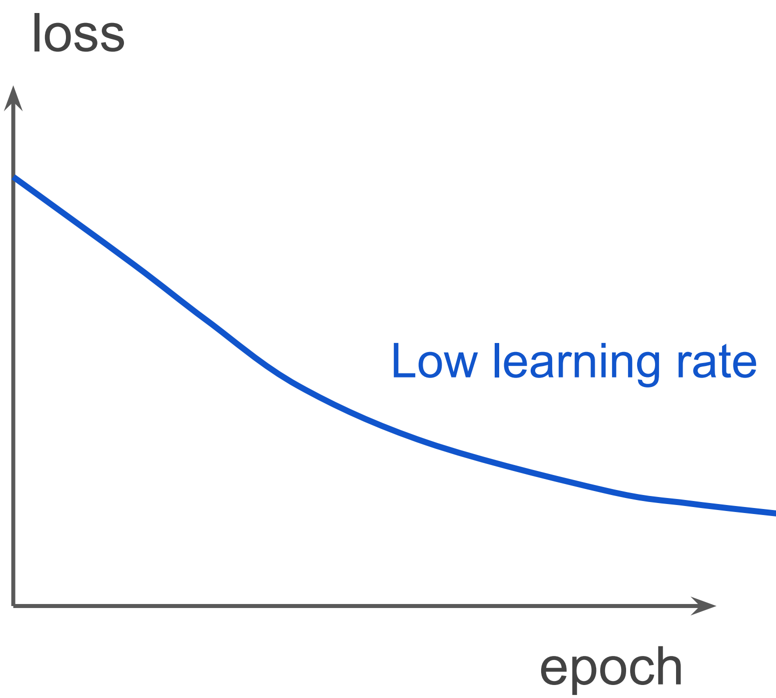

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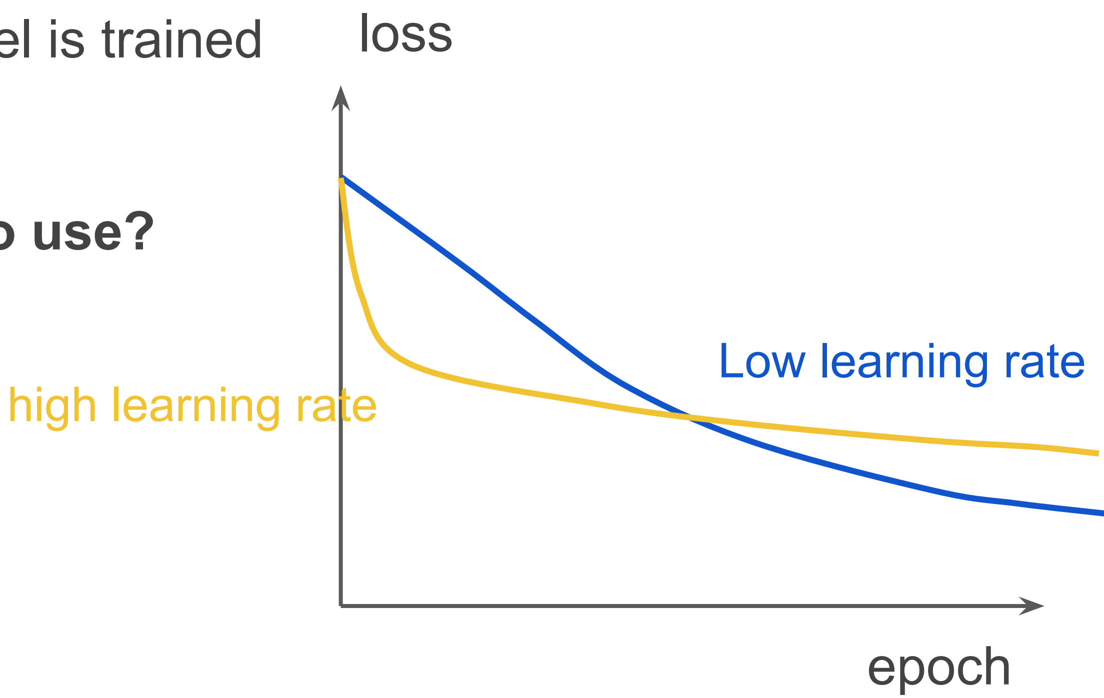

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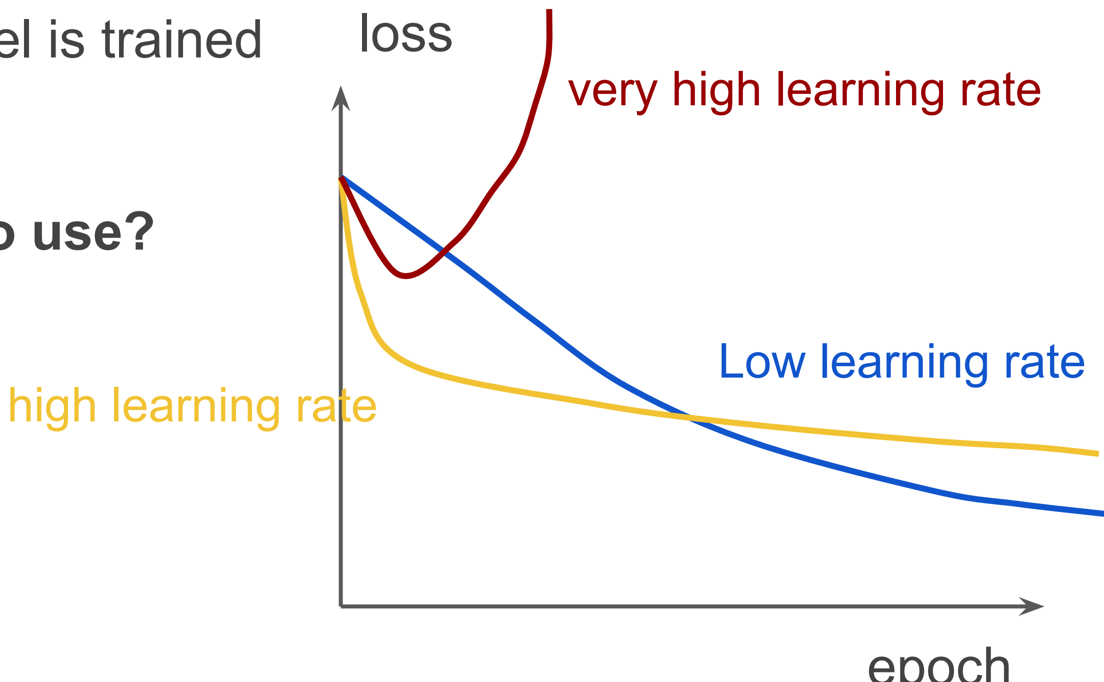

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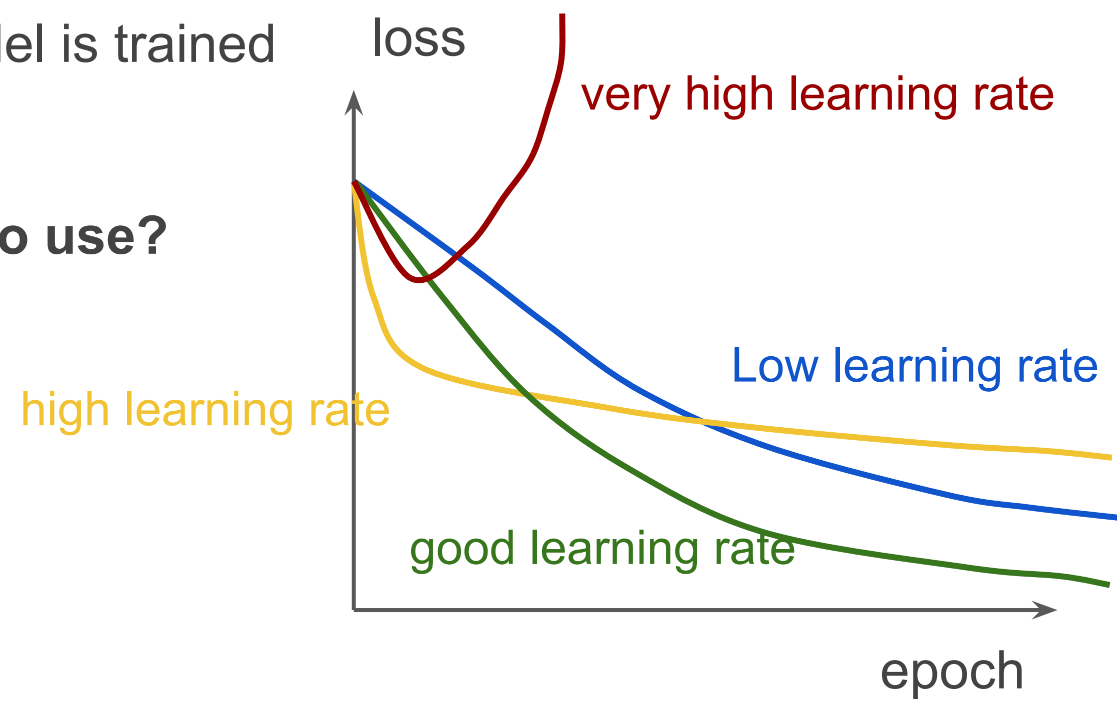

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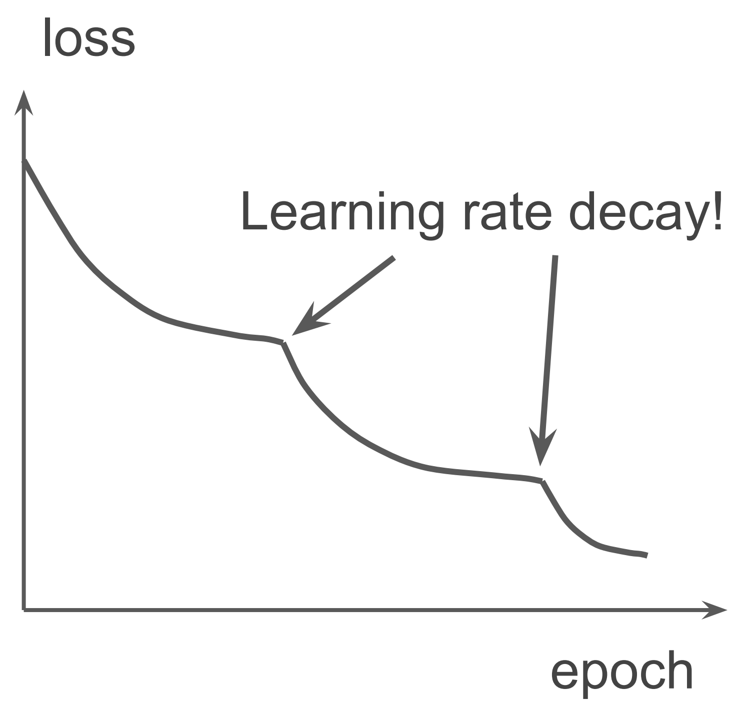

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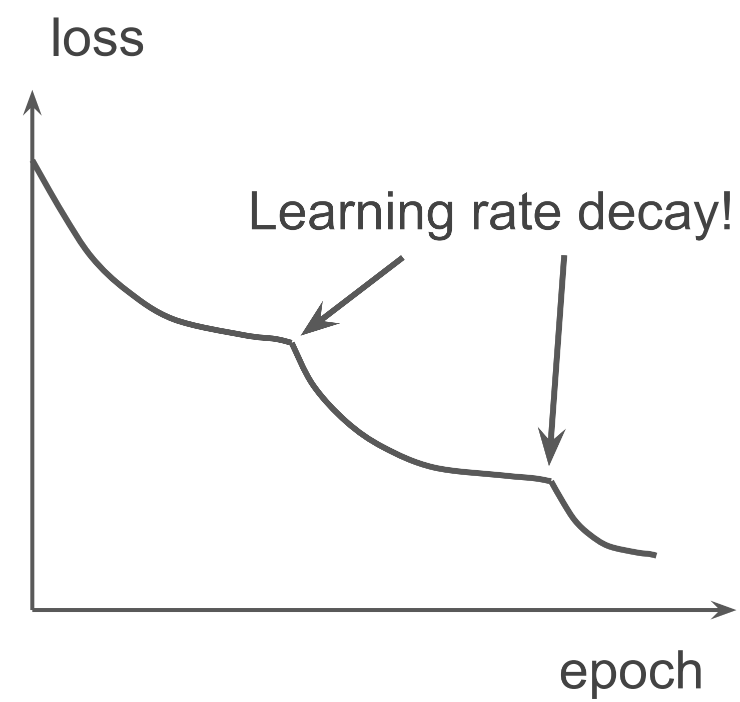

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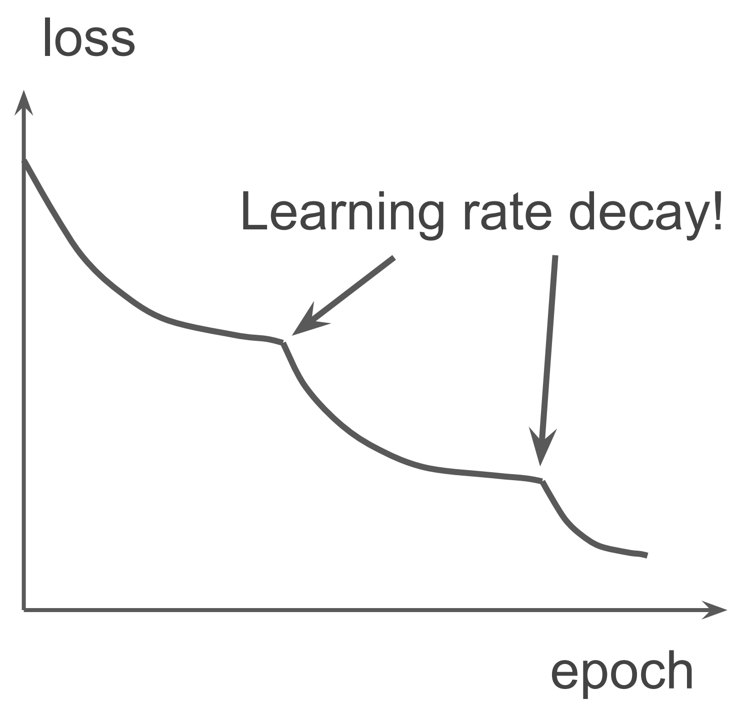

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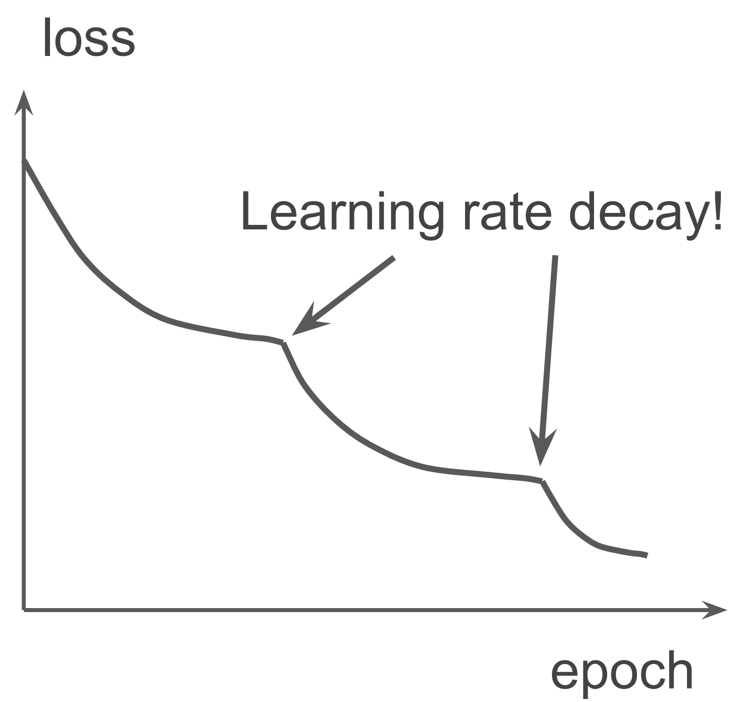
Critical for SGD+Momentum, less common with Adam



Hyperparameter selection

Neural networks have a lot of hyperparameters, for example:

- Number of layers, number of neurons in each layer
- (Initial) learning rate α_0 and learning rate scheduling parameters
- Batch size $|\mathcal{B}|$
- Number of epochs
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How do we do it given a limited amount of data?
- **Training data**: accessible during training, used to learn parameters
- **Test data**: not accessible during training, only for final evaluation

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Idea 1: train the neural network on training data, and directly evaluate it on test data

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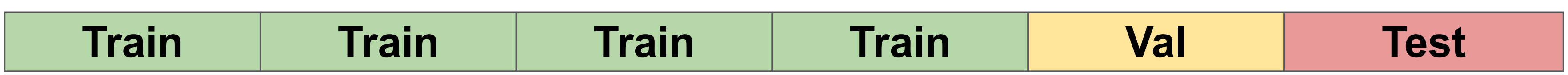
- Train neural network on both training and validation data with the best hyperparameters, and final evaluation on test data.



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Train	**Train**	**Train**	**Train**	**Val**	**Test**

<u>Can we use the given training data more efficiently?</u>

Hyperparameter selection

Idea 3 (cross-validation): Split training data into **folds**

- Try each fold as validation data (the rest as training data) and average the results, find the hyperparameters that work best
- Train neural network on both training and validation data with the best hyperparameters, and final evaluation on test data.

Train	**Train**	**Train**	**Train**	**Val**	**Test**
Train	**Train**	**Train**	**Val**	**Train**	**Test**
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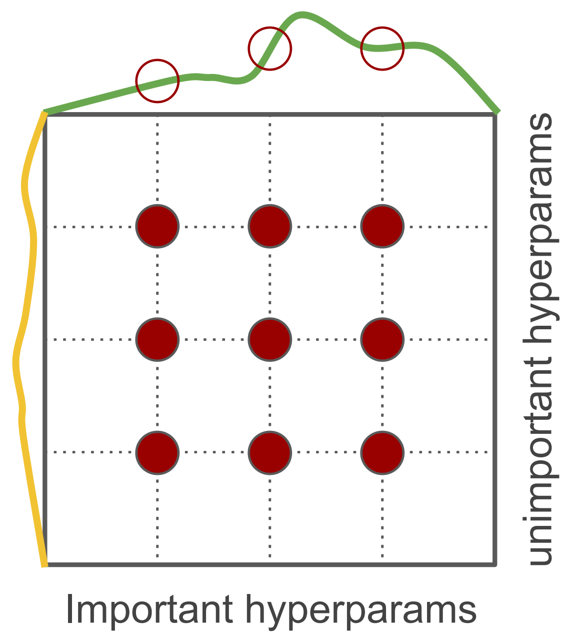
Search for *multiple* hyperparameter:

Grid search



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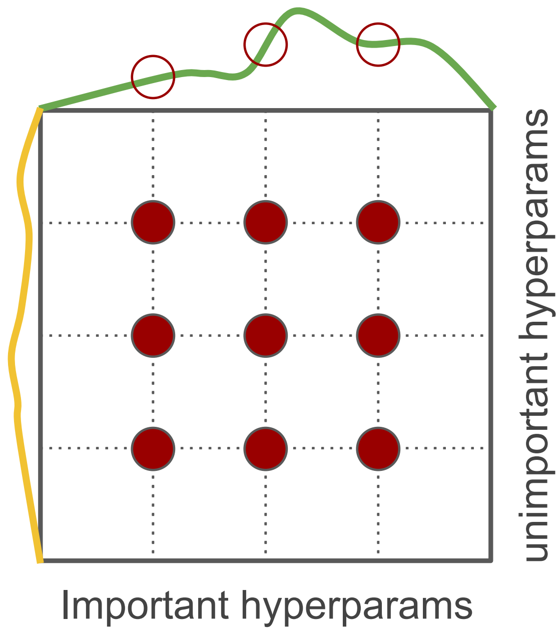

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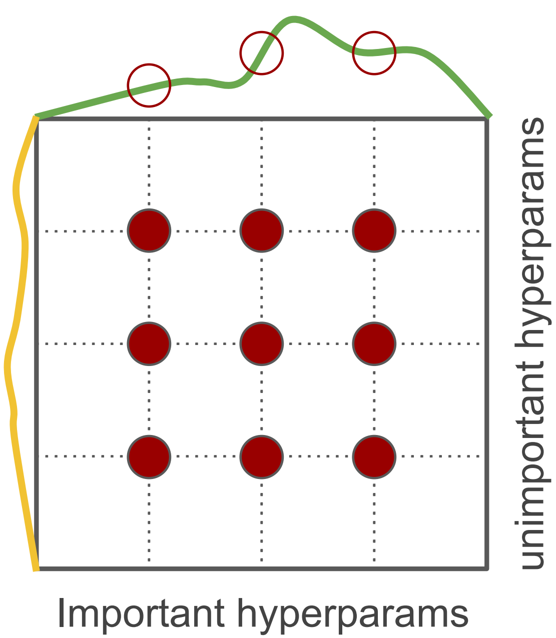
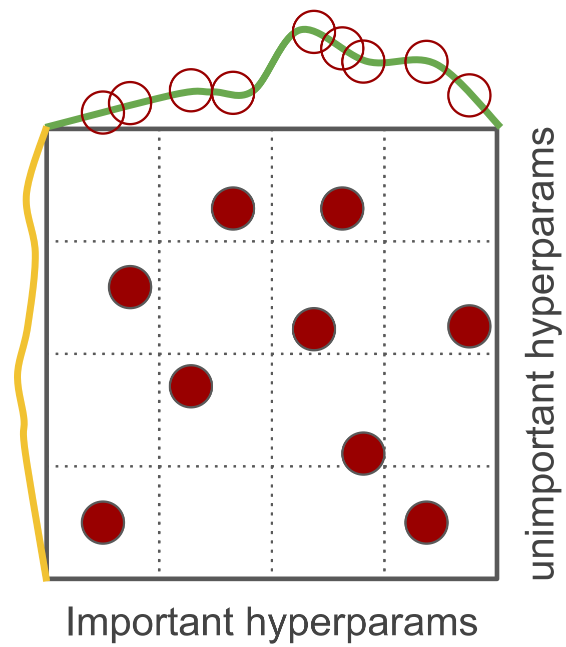


Random search



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- **Finds good values faster when only a few hyperparameters matter**

Random Search for Hyper-Parameter Optimization, Bergstra and Bengio, 2012

Thanks