Natural Language Processing

AI51701/CSE71001

Lecture 6

09/19/2023

Instructor: Taehwan Kim

Announcements

- Reminder: Assignment 1
  - Due: Sep. 24 at 11:59:00pm

- No class on Sep 21 due to *2023 UNIST AI Technology Open Workshop*
  - You are encouraged to attend

- Due to attending a conference, we will have **no class on Oct. 5** and instead **a substitute class on Oct. 12 at 5:20pm**
  - If you cannot make it, please let me know ASAP

Announcements

- We will have final project proposal presentation on Oct. 12
  - Written proposal submission due: Oct. 11 at 11:59pm (BlackBoard)

word2vec (Mikolov et al., 2013a)

Efficient Estimation of Word Representations in Vector Space

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word2vec (Mikolov et al., 2013b)

Distributed Representations of Words and Phrases and their Compositionality

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Neural Network for Sentiment Classification

$$\mathbf{z}^{(1)} = g\left(\mathbf{U}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

$$\mathbf{s} = \mathbf{U}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

vector of label scores

Neural Network for Sentiment Classification

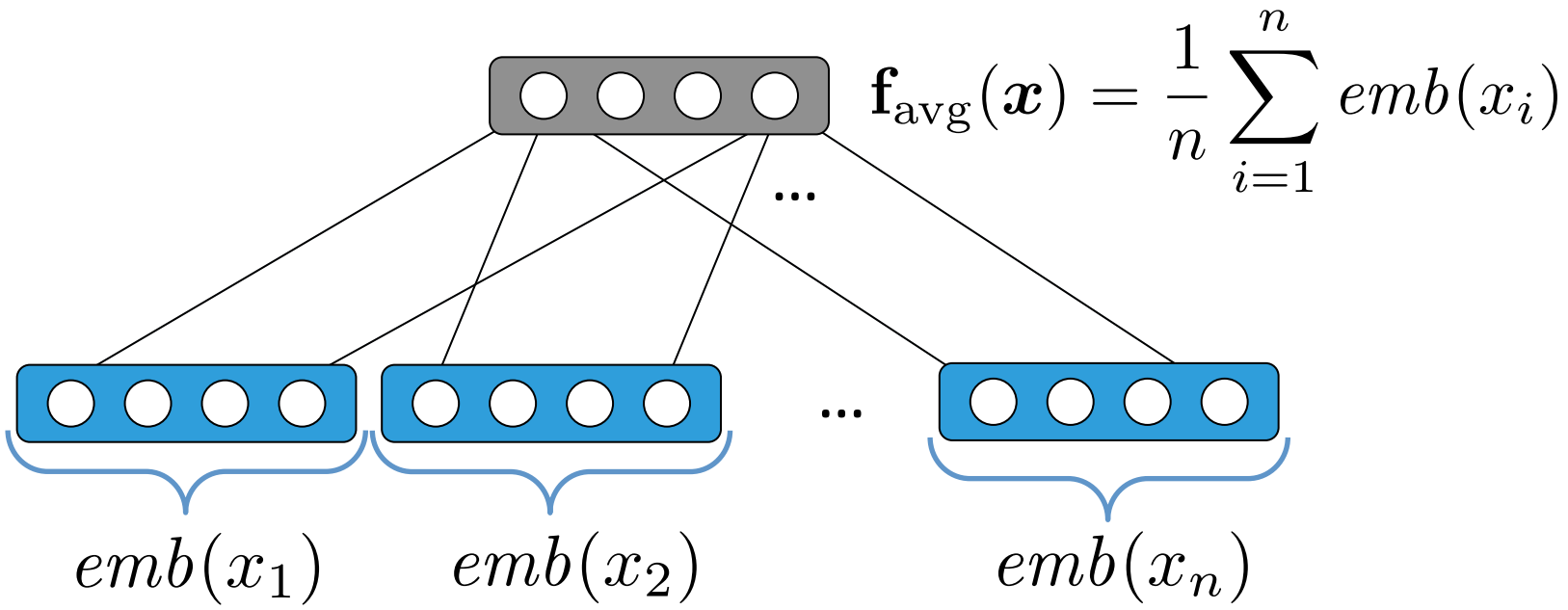
$$\mathbf{z}^{(1)} = g\left(\mathbf{U}^{(0)}\mathbf{x} + \mathbf{b}^{(0)}\right)$$

$$\mathbf{s} = \mathbf{U}^{(1)}\mathbf{z}^{(1)} + \mathbf{b}^{(1)}$$

$$\mathbf{s} = \begin{bmatrix} \text{score}(\boldsymbol{x}, \text{positive}, \boldsymbol{w}) \\ \text{score}(\boldsymbol{x}, \text{negative}, \boldsymbol{w}) \end{bmatrix}$$

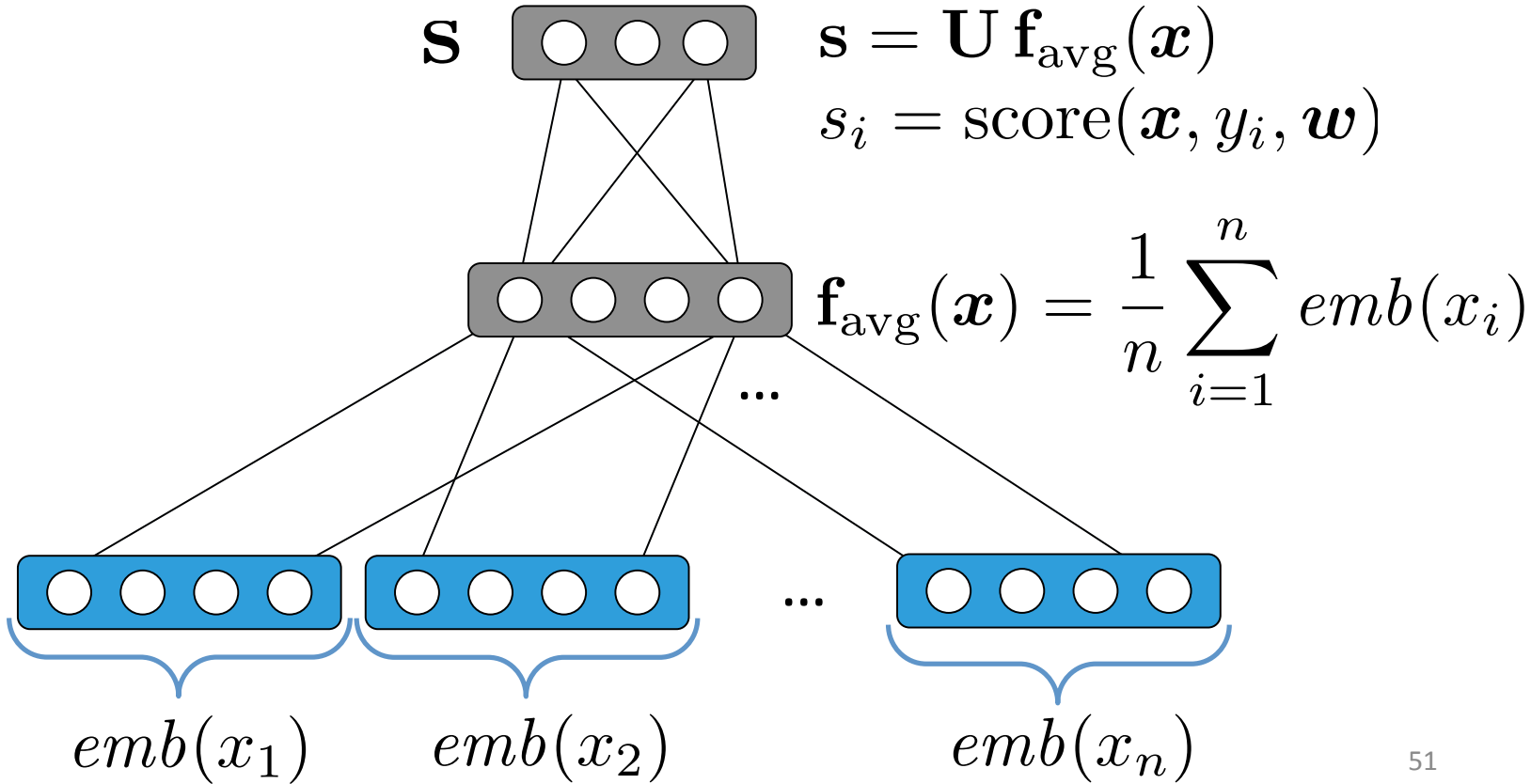
A Simple Neural Text Classification Model

- Given a word sequence ***x***, predict its label
- Represent ***x*** by averaging its word embeddings:



A Simple Neural Text Classification Model

- Represent x by averaging its word embeddings
- Output is a score vector over all possible labels:



Averaging Word Embeddings

- Effective encoder for text classification and many other tasks
- Sometimes called a neural bag of words (NBOW) model (Kalchbrenner et al., 2014)
- Or a deep averaging network (DAN), especially if hidden layers are used (Iyyer et al., 2015)

Encoders

- Encoder: a function to represent a word sequence as a vector
- Simplest: average word embeddings:

$$\mathbf{f}_{\text{avg}}(\boldsymbol{x}) = \frac{1}{n}\sum_{i=1}^{n} emb(x_i)$$

- Many other functions possible!
- Lots of recent work on developing better ways to encode word sequences

Deep Learning Classification Task: Named Entity Recognition (NER)

- The task: **find** and **classify** names in text, for example:

  Last night , Paris Hilton wowed in a sequin gown .

  PER PER

  Samuel Quinn was arrested in the Hilton Hotel in Paris in April 1989 .

  PER PER LOC LOC LOC DATE DATE

- Possible uses:
  - Tracking mentions of particular entities in documents
  - For question answering, answers are usually named entities
  - Relating sentiment analysis to the entity under discussion
- Often followed by Entity Linking/Canonicalization into a Knowledge Base such as Wikidata

Simple NER: Window classification using binary logistic classifier

- **Idea**: **classify each word in its context window** of neighboring words
- Train logistic classifier on hand-labeled data to classify center word {yes/no} for each class based on a **concatenation of word vectors** in a window
  - Really, we usually use multi-class softmax, but we're trying to keep it simple
- **Example:** Classify "Paris" as +/– location in context of sentence with window length 2:

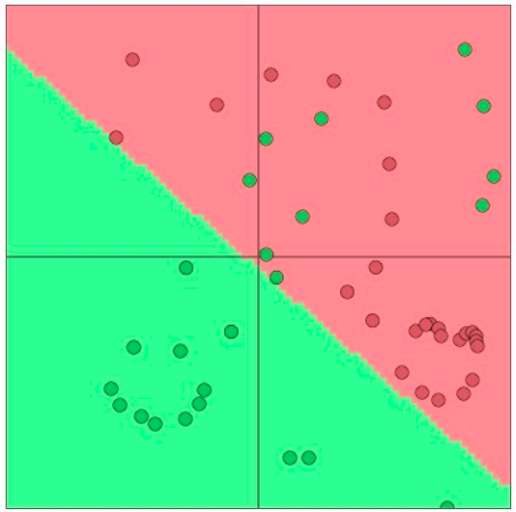
the museums in Paris are amazing to see .

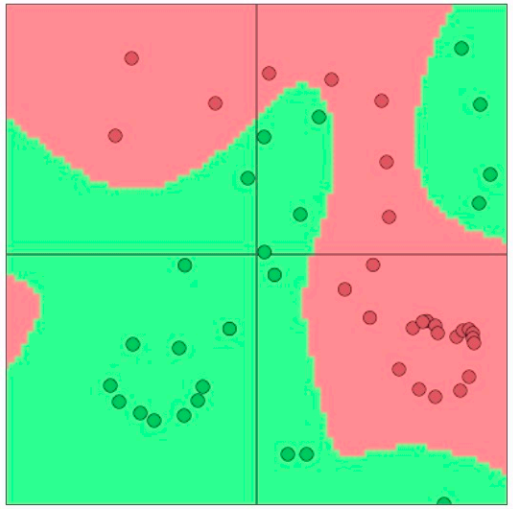
$$X_{window} = [\ x_{museums} \quad x_{in} \quad x_{Paris} \quad x_{are} \quad x_{amazing}\ ]^T \qquad x \in R^{5d}$$

- To classify all words: run classifier for each class on the vector centered on each word in the sentence

Neural Network Classifiers

- Typical ML/stats softmax classifier: $$p(y|x) = \frac{\exp(W_y.x)}{\sum_{c=1}^{C} \exp(W_c.x)}$$
  - Learned parameters θ are just elements of W (not input representation x, which has sparse symbolic features)
  - Classifier gives linear decision boundary, which can be limiting
- Neural networks can learn much more complex functions with nonlinear decision boundaries!





From Stanford CS224n course

Neural Network Classifiers

- A neural network classifier differs in that:
  - We learn **both** *W* **and (distributed!)** representations for words
  - The word vectors *x* re-represent one-hot vectors, moving them around in an intermediate layer vector space, for easy classification with a (linear) softmax classifier
    - Conceptually, we have an embedding layer: $x=Le$
  - We use deep networks—more layers—that let us re-represent and compose our data multiple times, giving a non-linear classifier

Training with “cross entropy loss”

- Until now, our objective was stated as to **maximize the probability of the correct class** y or equivalently we can **minimize the negative log probability of that class**
- Now restated in terms of **cross entropy**, a concept from information theory
- Let the true probability distribution be *p*; let our computed model probability be *q*
- The cross entropy is:

$$H(p,q) = -\sum_{c=1}^{C} p(c) \log q(c)$$

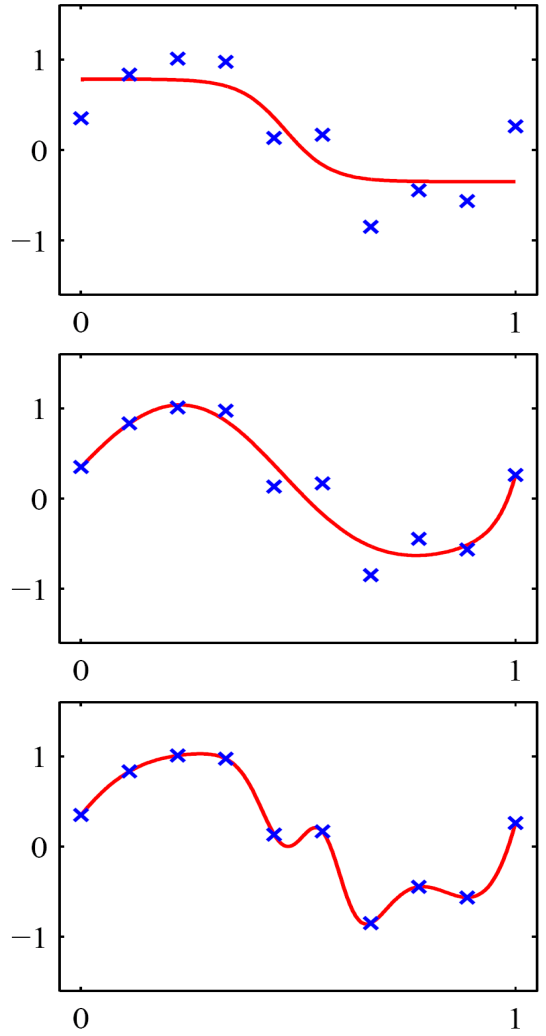
Training with “cross entropy loss”

- Let the true probability distribution be *p*; let our computed model probability be *q*
- The cross entropy is: $$H(p,q) = -\sum_{c=1}^{C} p(c) \log q(c)$$

- Assuming a ground truth (or true or gold or target) probability distribution that is 1 at the right class and 0 everywhere else, *p* = [0, ..., 0, 1, 0, ..., 0], then:
- **Because of one-hot *p*, the only term left is the negative log probability of the true class y_i:** $-\log p(y_i|x_i)$

Why nonlinearities?

- Neural networks do function approximation, e.g., regression or classification
  - Without non-linearities, deep neural networks can't do anything more than a linear transform
  - Extra layers could just be compiled down into a single linear transform: $W_1 W_2 x = Wx$
  - But, with more layers that include non-linearities, they can approximate more complex functions!

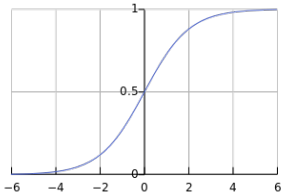


NER: Binary classification for center word being location

- We do supervised training and want high score if it's a location

$$J_t(\theta) = \sigma(s) = \frac{1}{1 + e^{-s}}$$

predicted model probability of class



$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad \text{(input)}$$

f = Some element-wise non-linear function, e.g., logistic, tanh, ReLU

From Stanford CS224n course

Stochastic Gradient Descent

- Update equation: $\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$

  α = *step size* or *learning rate*

  - I.e., for each parameter: $\theta_j^{new} = \theta_j^{old} - \alpha \frac{\partial J(\theta)}{\partial \theta_j^{old}}$
  - In deep learning, θ includes the data representation (e.g., word vectors) too!
- How can we compute $\nabla_\theta J(\theta)$?
  - By hand
  - Algorithmically: the backpropagation algorithm

Gradients

- Given a function with 1 output and 1 input

$$f(x) = x^3$$

- It's gradient (slope) is its derivative

$$\frac{df}{dx} = 3x^2$$

  - "How much will the output change if we change the input a bit?"
    - At *x* = 1 it changes about 3 times as much: 1.013 = 1.03
    - At x = 4 it changes about 48 times as much: 4.013 = 64.48

Gradients

- Given a function with 1 output and n inputs

$$f(\boldsymbol{x}) = f(x_1, x_2, ..., x_n)$$

- Its gradient is a vector of partial derivatives with respect to each input

$$\frac{\partial f}{\partial \boldsymbol{x}} = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_n}\right]$$

Jacobian Matrix: Generalization of the Gradient

- Given a function with ***m* outputs** and *n* inputs

$$f(\boldsymbol{x}) = f(x_1, x_2, ..., x_n)$$

- It's Jacobian is an ***m* x *n* matrix** of partial derivatives

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

$$\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)_{ij} = \frac{\partial f_i}{\partial x_j}$$

Jacobian Matrix: Generalization of the Gradient

- For composition of one-variable functions: **multiply derivatives**

$$z = 3y$$

$$y = x^2$$

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx} = (3)(2x) = 6x$$

- For multiple variables at once: **multiply Jacobians**

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} = \dots$$

Example Jacobian: Elementwise activation Function

$$\boldsymbol{h} = f(\boldsymbol{z}), \text{what is } \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}? \qquad \boldsymbol{h}, \boldsymbol{z} \in \mathbb{R}^n$$

$$h_i = f(z_i)$$

- Function has n outputs and n inputs → *n* by *n* Jacobian

Example Jacobian: Elementwise activation Function

$$\boldsymbol{h} = f(\boldsymbol{z}), \text{what is } \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}? \qquad \boldsymbol{h}, \boldsymbol{z} \in \mathbb{R}^n$$

$$h_i = f(z_i)$$

$$\left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\right)_{ij} = \frac{\partial h_i}{\partial z_j} = \frac{\partial}{\partial z_j} f(z_i) \qquad \text{definition of Jacobian}$$

$$= \begin{cases} f'(z_i) & \text{if } i = j \\ 0 & \text{if otherwise} \end{cases} \qquad \text{regular 1-variable derivative}$$

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} = \begin{pmatrix} f'(z_1) & & 0 \\ & \ddots & \\ 0 & & f'(z_n) \end{pmatrix} = \text{diag}(\boldsymbol{f}'(\boldsymbol{z}))$$

Other Jacobians

$$\frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{W}\boldsymbol{x}+\boldsymbol{b}) = \boldsymbol{W}$$

$$\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{W}\boldsymbol{x}+\boldsymbol{b}) = \boldsymbol{I} \ \ (\text{Identity matrix})$$

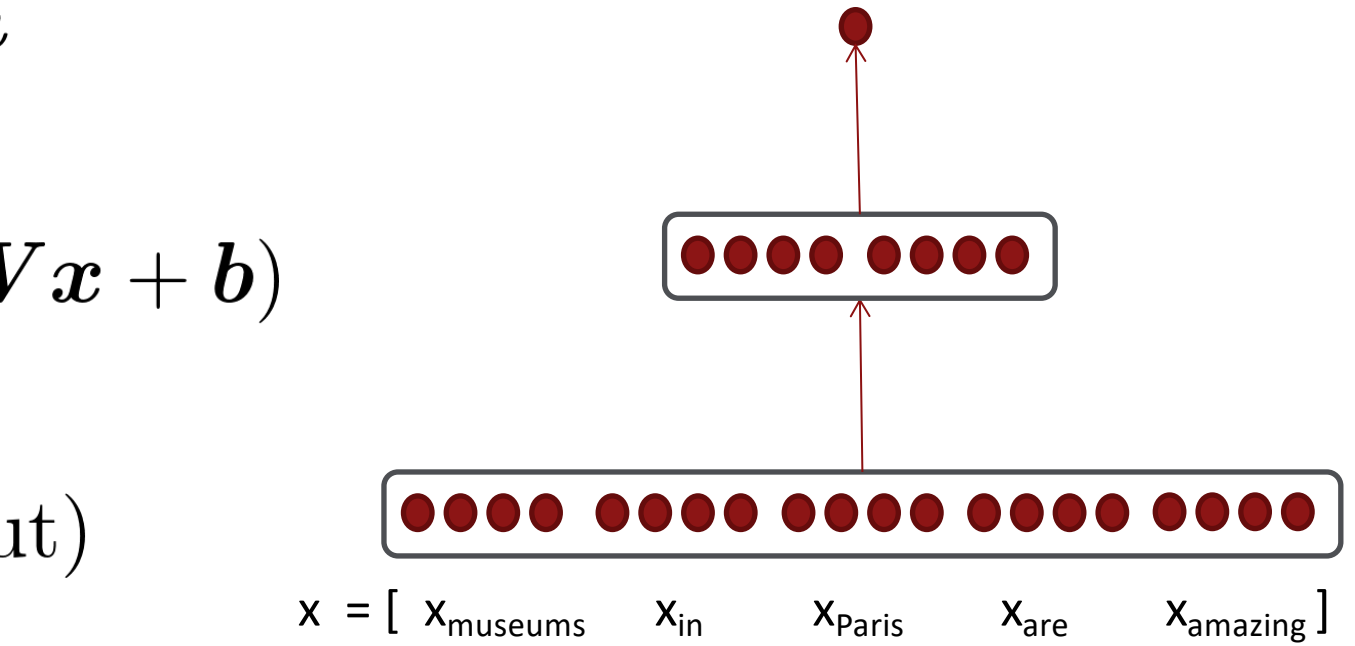
$$\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{u}^T\boldsymbol{h}) = \boldsymbol{h}^{\boldsymbol{T}}$$

Back to our Neural Net!

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad (\text{input})$$



Back to our Neural Net!

- Let's find $\frac{\partial s}{\partial \boldsymbol{b}}$
- Really, we care about the gradient of the loss J_t but we will compute the gradient of the score for simplicity

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

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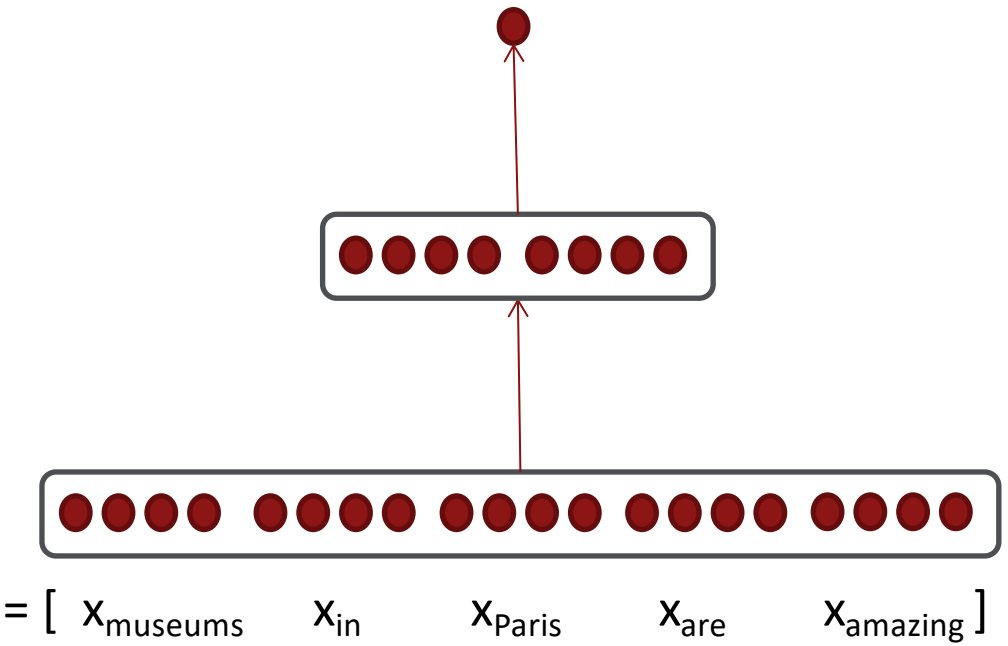

1. Break up equations into simple pieces

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad \text{(input)}$$

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad \text{(input)}$$

- Carefully define your variables and keep track of their dimensionality!

2. Apply the chain rule

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad (\text{input})$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

2. Apply the chain rule

$$\boxed{s = \boldsymbol{u}^T \boldsymbol{h}}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad (\text{input})$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \boxed{\frac{\partial s}{\partial \boldsymbol{h}}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

3. Write out the Jacobians

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad (\text{input})$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

Useful Jacobians from previous slide

$$\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{u}^T \boldsymbol{h}) = \boldsymbol{h}^T$$

$$\frac{\partial}{\partial \boldsymbol{z}}(f(\boldsymbol{z})) = \text{diag}(f'(\boldsymbol{z}))$$

$$\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{I}$$

3. Write out the Jacobians

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad (\text{input})$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

$$\downarrow$$

$$\boldsymbol{u}^T$$

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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

$$\boldsymbol{u}^T \operatorname{diag}(f'(\boldsymbol{z}))$$

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$$\boldsymbol{x} \quad (\text{input})$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

$$= \boldsymbol{u}^T \operatorname{diag}(f'(\boldsymbol{z}))\boldsymbol{I}$$

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3. Write out the Jacobians

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$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad (\text{input})$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

$$= \boldsymbol{u}^T \operatorname{diag}(f'(\boldsymbol{z}))\boldsymbol{I}$$

$$= \boldsymbol{u}^T \odot f'(\boldsymbol{z})$$

Useful Jacobians from previous slide

$$\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{u}^T \boldsymbol{h}) = \boldsymbol{h}^T$$

$$\frac{\partial}{\partial \boldsymbol{z}}(f(\boldsymbol{z})) = \operatorname{diag}(f'(\boldsymbol{z}))$$

$$\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{I}$$

$\odot$ = Hadamard product = element-wise multiplication of 2 vectors to give vector

Re-using Computation

- Suppose we now want to compute $\frac{\partial s}{\partial \boldsymbol{W}}$
  - Using the chain rule again:

$$\frac{\partial s}{\partial \boldsymbol{W}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$$

Re-using Computation

- Suppose we now want to compute $\frac{\partial s}{\partial \boldsymbol{W}}$
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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

The same! Let's avoid duplicated computation ...

Re-using Computation

- Suppose we now want to compute $\frac{\partial s}{\partial \boldsymbol{W}}$
  - Using the chain rule again:

$$\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \boldsymbol{\delta} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}} = \boldsymbol{\delta}$$

$$\boldsymbol{\delta} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} = \boldsymbol{h}^T \circ f'(\boldsymbol{z})$$

δ is the local error signal

Derivative with respect to Matrix

- What does $\frac{\partial s}{\partial \boldsymbol{W}}$ look like? $\boldsymbol{W} \in \mathbb{R}^{n \times m}$
- 1 output, *nm* inputs: 1 by *nm* Jacobian?
  - Inconvenient to then do $\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$

- Instead, we leave pure math and use the shape convention: the shape of the gradient is the shape of the parameters!

  - So $\frac{\partial s}{\partial \boldsymbol{W}}$ is *n* by *m*:

$$\begin{bmatrix} \frac{\partial s}{\partial W_{11}} & \cdots & \frac{\partial s}{\partial W_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial s}{\partial W_{n1}} & \cdots & \frac{\partial s}{\partial W_{nm}} \end{bmatrix}$$

Derivative with respect to Matrix

- What is $\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$
  - The other term should be $\boldsymbol{x}$ because $\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$

- Answer is: $\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta}^T \boldsymbol{x}^T$

δ is local error signal at z; x is local input signal

Deriving local input gradient in backprop

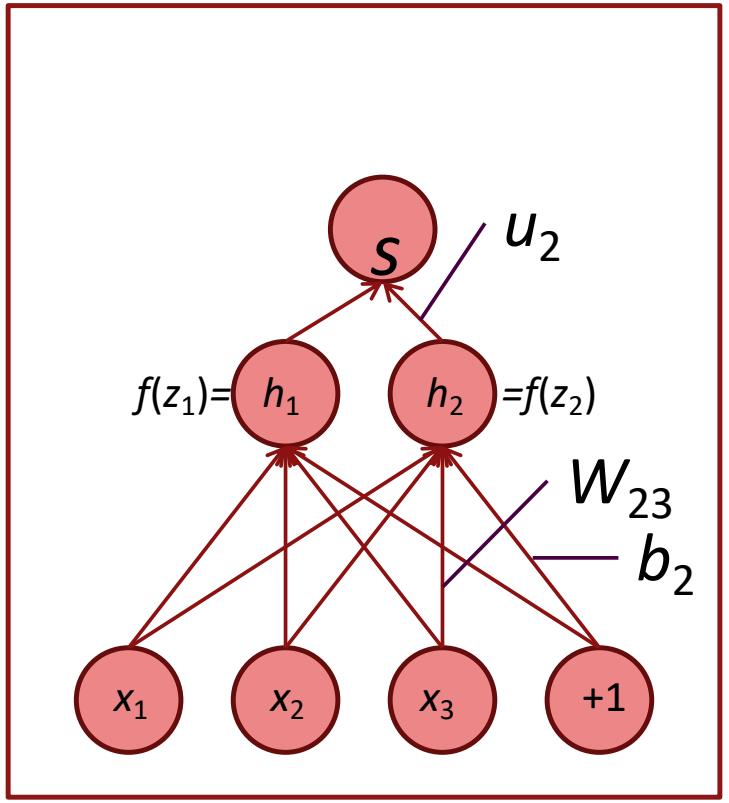
- For $\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}$ in our equation:

$$\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta}\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}} = \boldsymbol{\delta}\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

- Let's consider the derivative of a single weight W_{ij}
- W_{ij} only contributes to z_i
- For example: W_{23} is only used to compute z_2 not z_1

$$\frac{\partial z_i}{\partial W_{ij}} = \frac{\partial}{\partial W_{ij}}\boldsymbol{W}_{i.}\boldsymbol{x} + b_i$$

$$= \frac{\partial}{\partial W_{ij}}\sum_{k=1}^{d} W_{ik}x_k = x_j$$



Why the Transposes?

$$\frac{\partial s}{\partial \boldsymbol{W}} = \boldsymbol{\delta}^T \quad \boldsymbol{x}^T$$

$$[n \times m] \quad [n \times 1][1 \times m]$$

$$= \begin{bmatrix} \delta_1 \\ \vdots \\ \delta_n \end{bmatrix} [x_1, ..., x_m] = \begin{bmatrix} \delta_1 x_1 & \dots & \delta_1 x_m \\ \vdots & \ddots & \vdots \\ \delta_n x_1 & \dots & \delta_n x_m \end{bmatrix}$$

- Hacky answer: this makes the dimensions work out!
  - Useful trick for checking your work!
  - Each input goes to each output – you want to get outer product

3. Backpropagation

- We've almost shown you backpropagation
  - It's taking derivatives and using the (generalized, multivariate, or matrix) chain rule
- Other trick:
  - We **re-use** derivatives computed for higher layers in computing derivatives for lower layers to minimize computation

Computation Graphs and Backpropagation

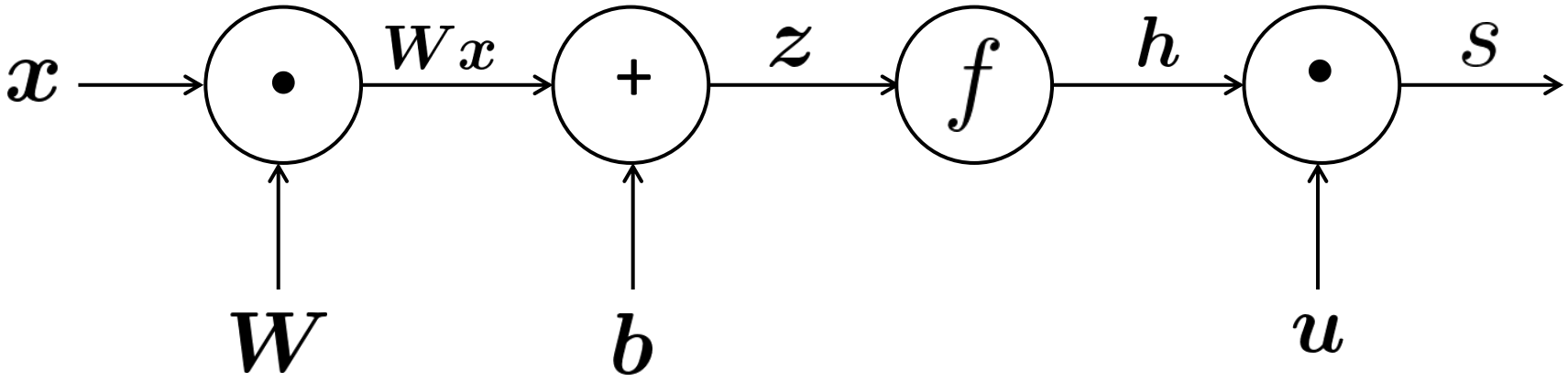
- Software represents our neural net equations as a graph
  - Source nodes: inputs
  - Interior nodes: operations
  - Edges pass along result of the operation

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad (\text{input})$$

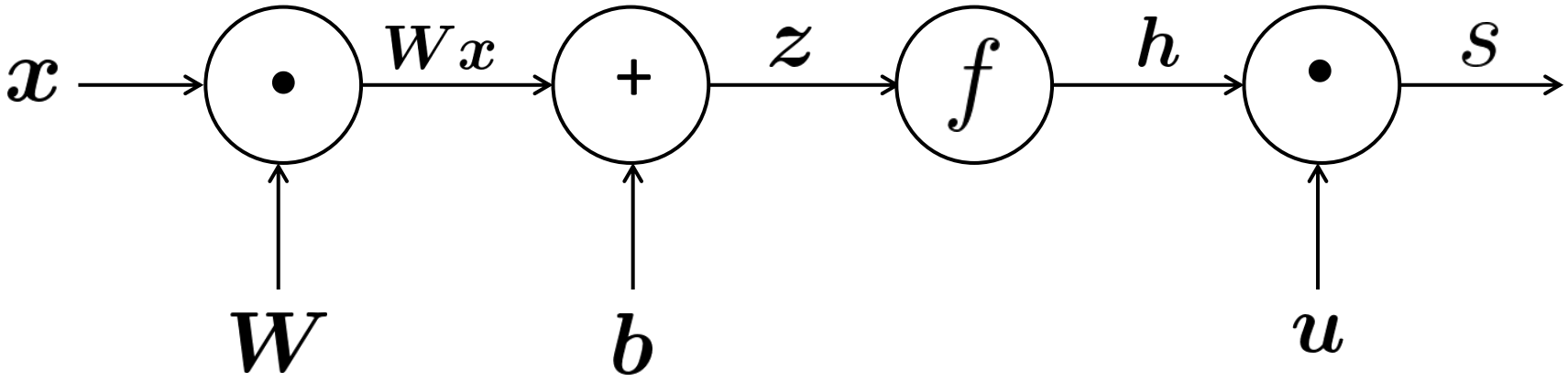


Computation Graphs and Backpropagation

- Software represents our neural net equations as a graph
  - Source nodes: inputs
  - Interior r
  - Edges pa

"Forward Propagation"

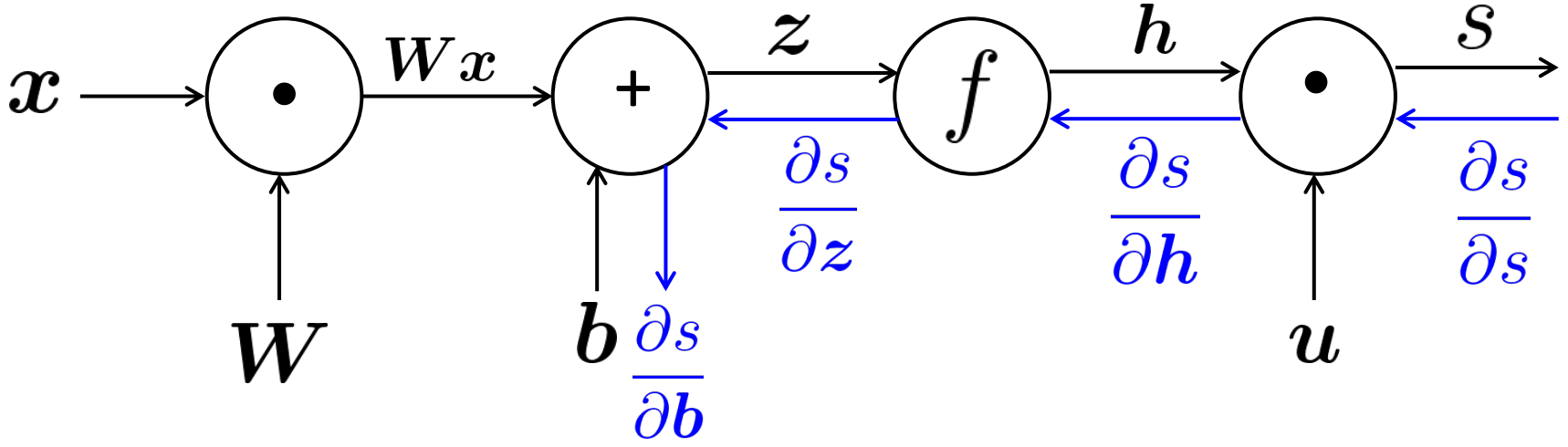
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



Computation Graphs and Backpropagation

- Then go backwards along edges
  - Pass along **gradients**

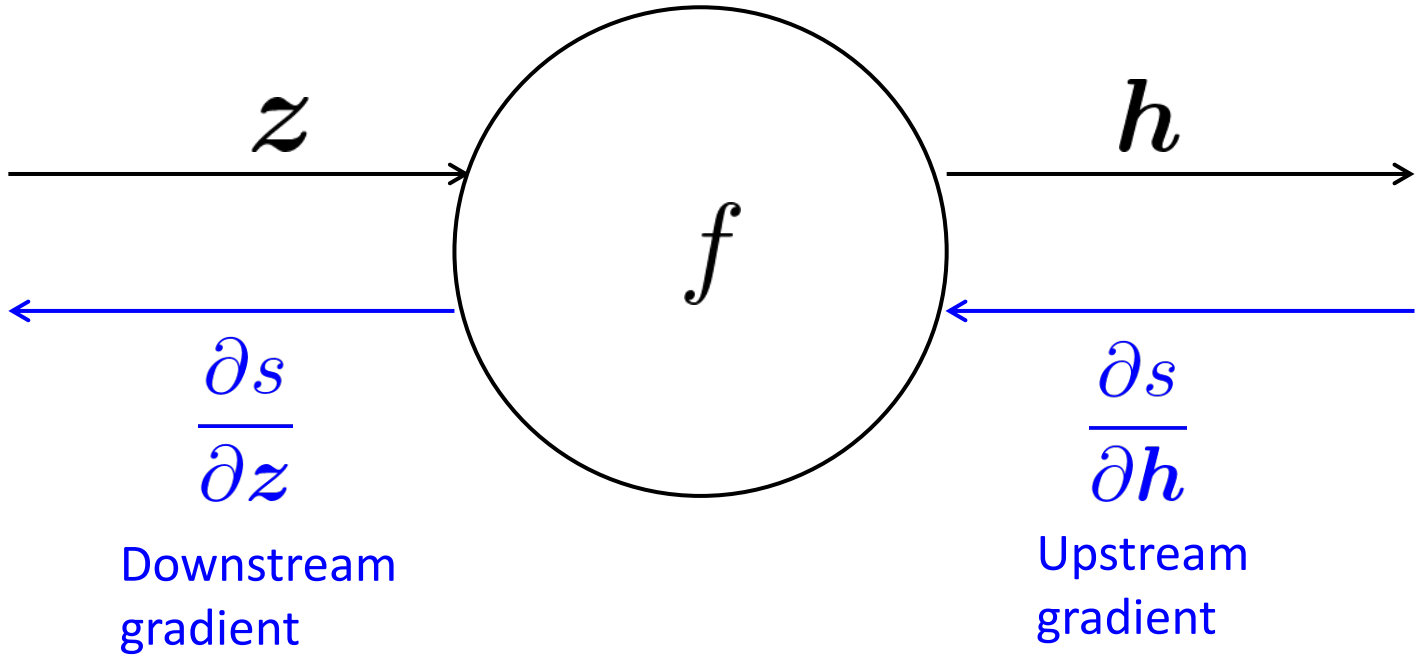
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



Backpropagation: Single Node

- Node receives an “upstream gradient”
- Goal is to pass on the correct “downstream gradient”

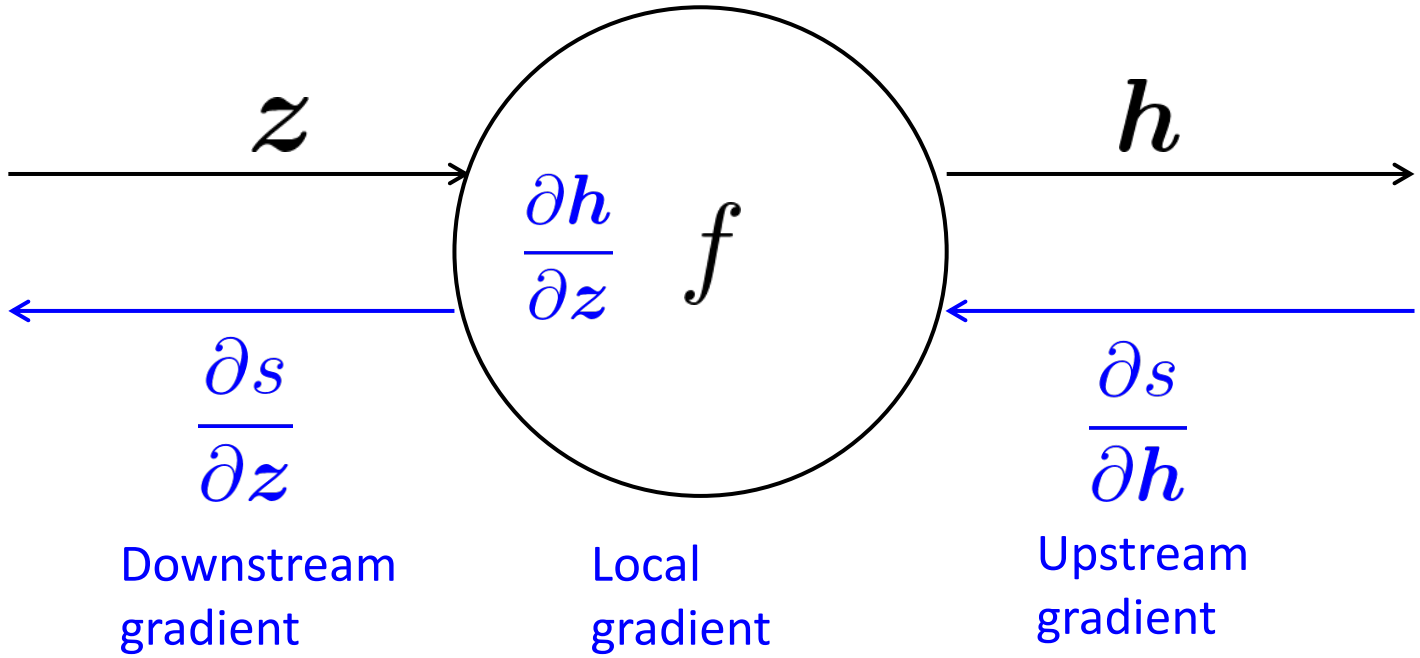
$$\boldsymbol{h} = f(\boldsymbol{z})$$



Backpropagation: Single Node

- Each node has a local gradient
  - The gradient of its output with respect to its input

$$\boldsymbol{h} = f(\boldsymbol{z})$$



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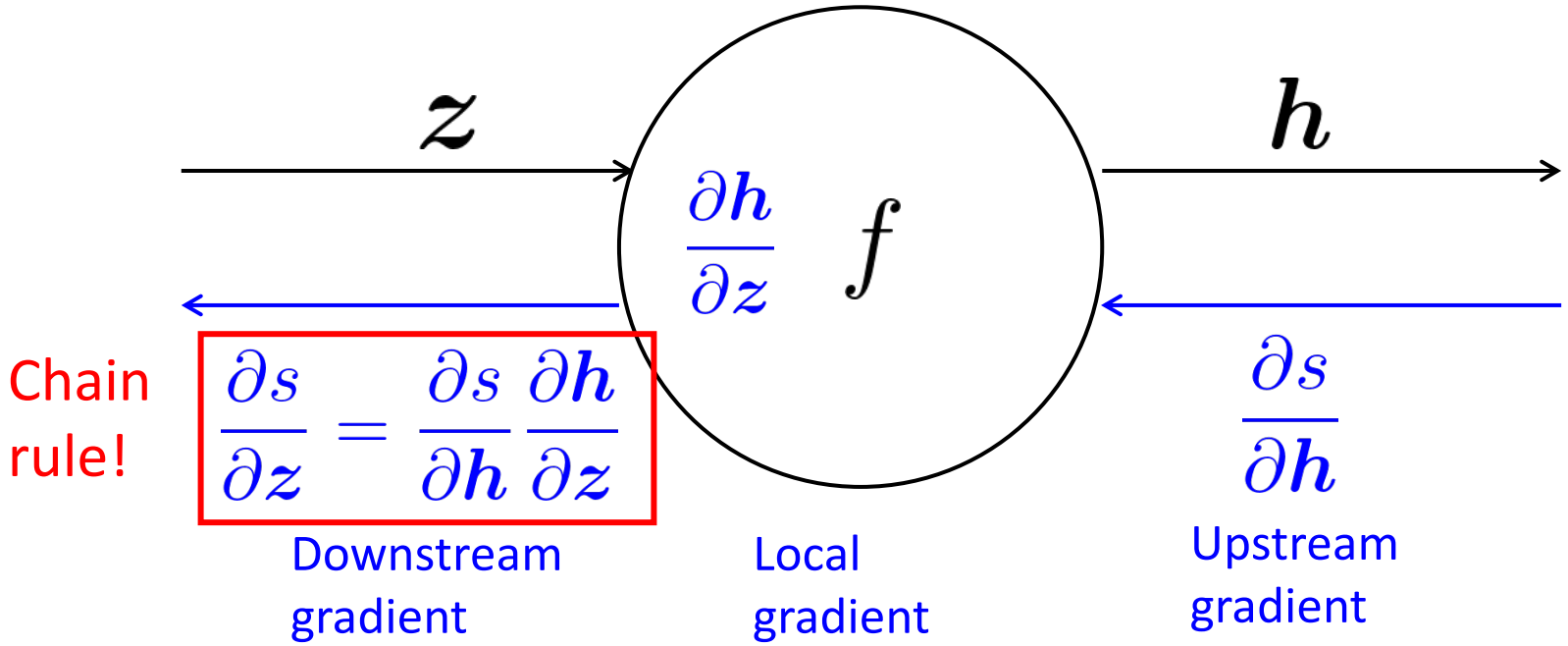
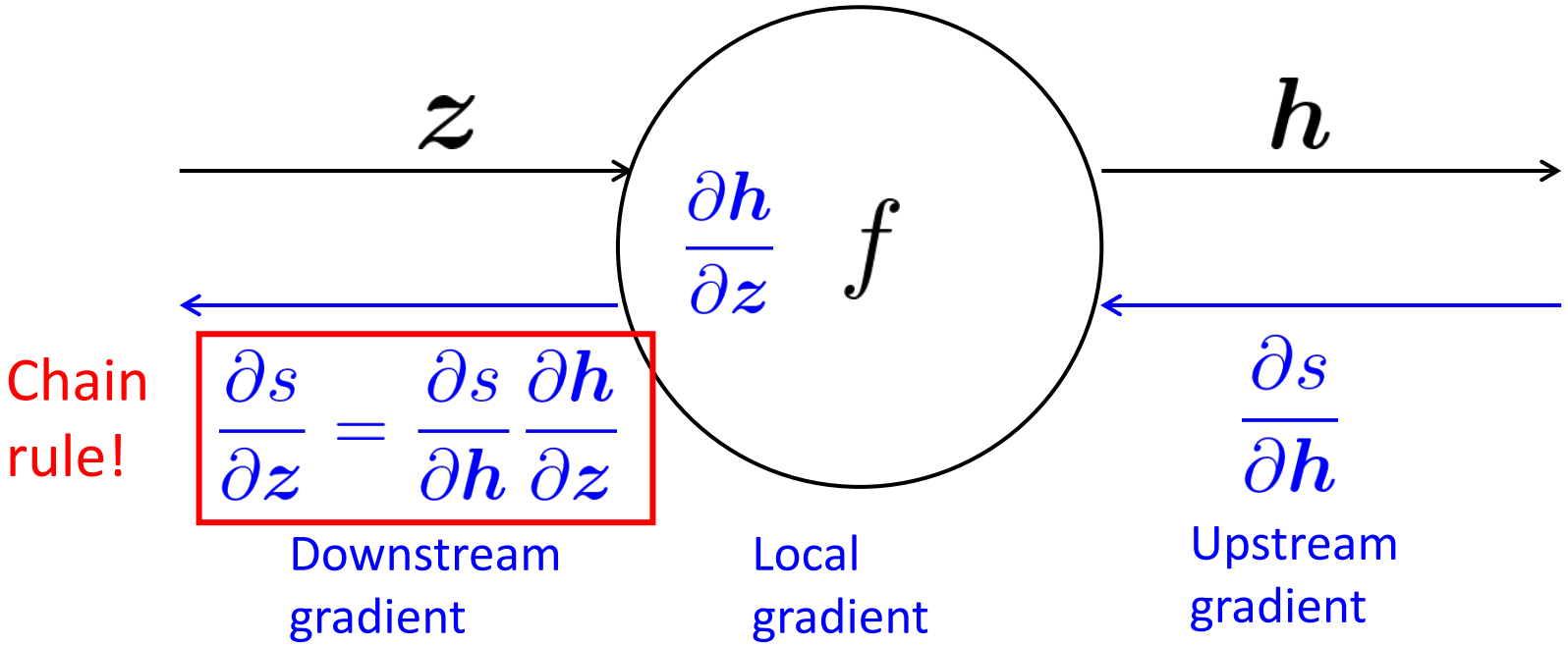


Backpropagation: Single Node

- Each node has a local gradient
  - The gradient of its output with respect to its input

$$\boldsymbol{h} = f(\boldsymbol{z})$$

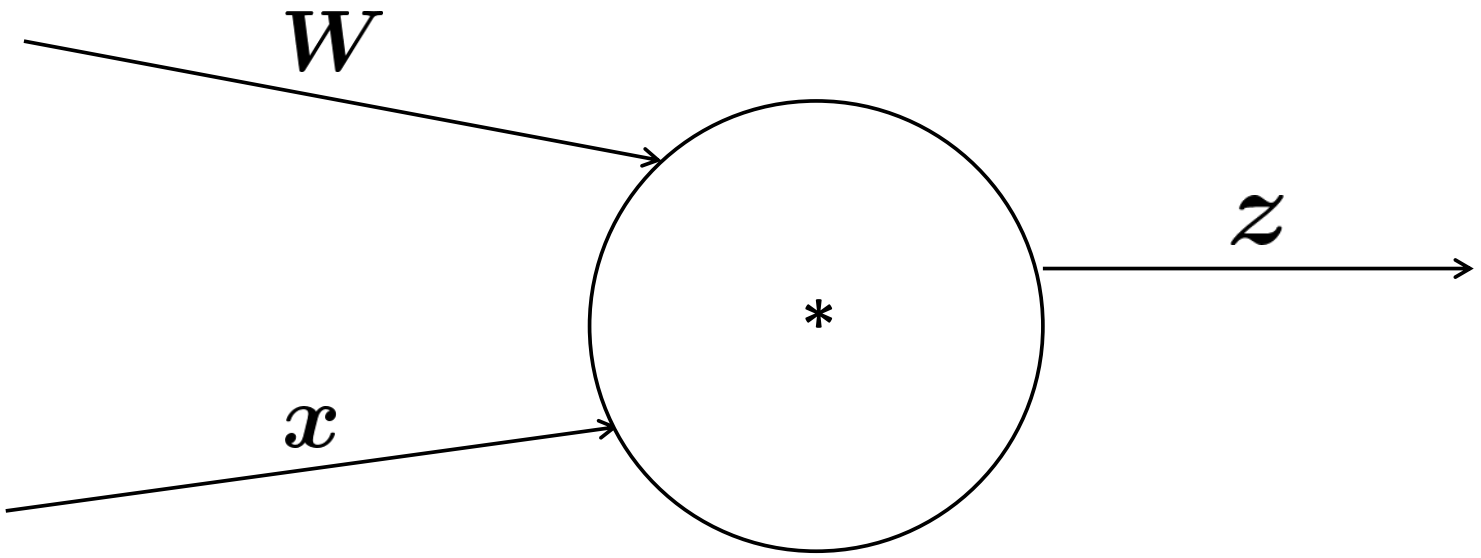
- [downstream gradient] = [upstream gradient] x [local gradient]



Backpropagation: Single Node

- What about nodes with multiple inputs?

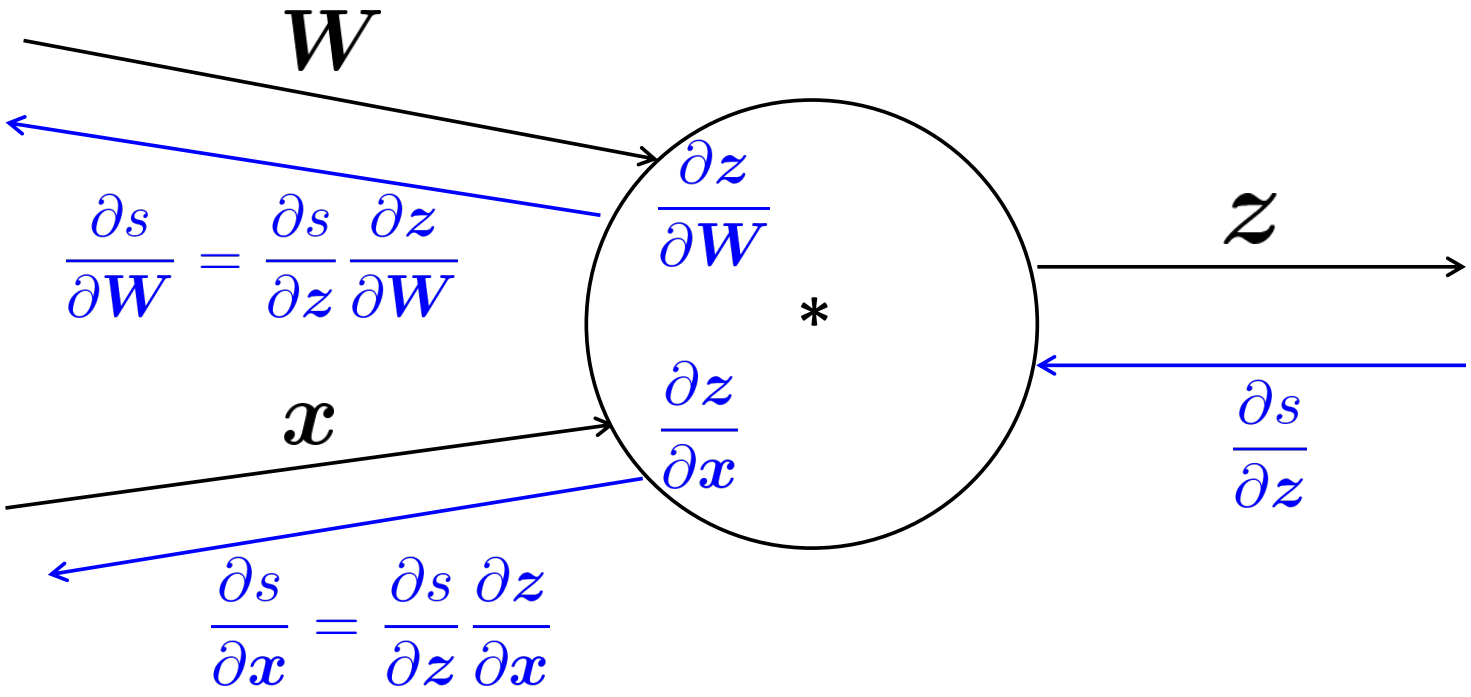
$$z = Wx$$



Backpropagation: Single Node

- Multiple inputs → multiple local gradients

$$z = Wx$$



Downstream gradients

Local gradients

Upstream gradient

An Example

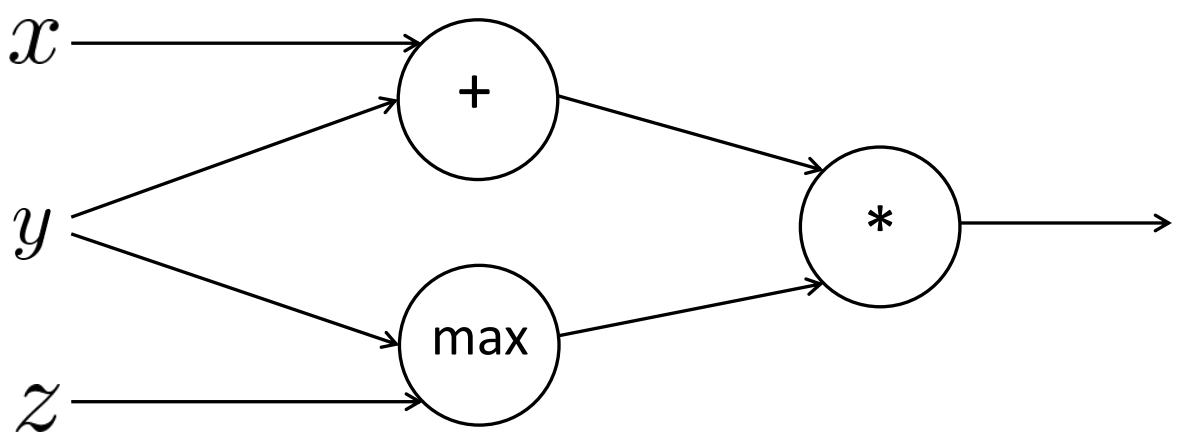
$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$

$$b = \max(y, z)$$

$$f = ab$$



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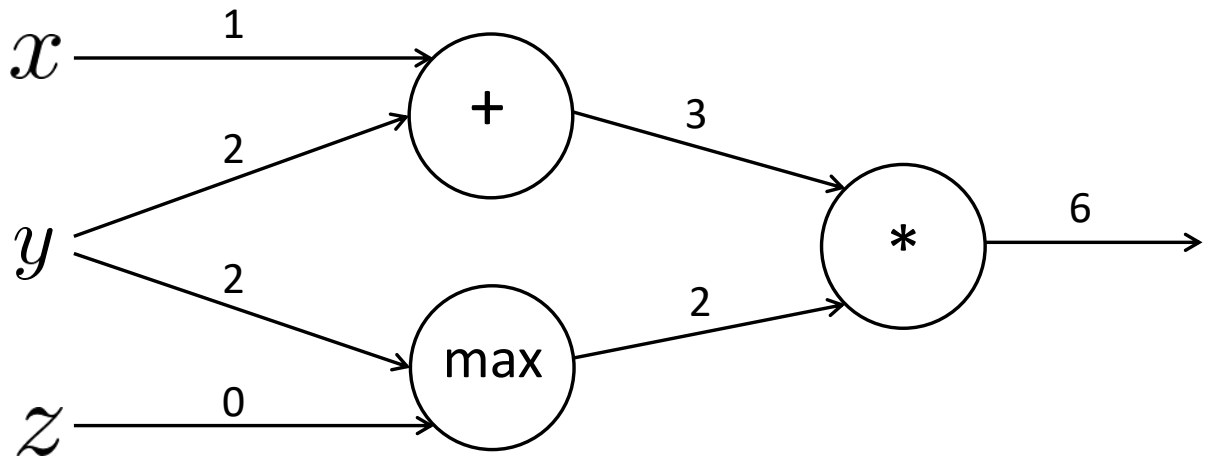

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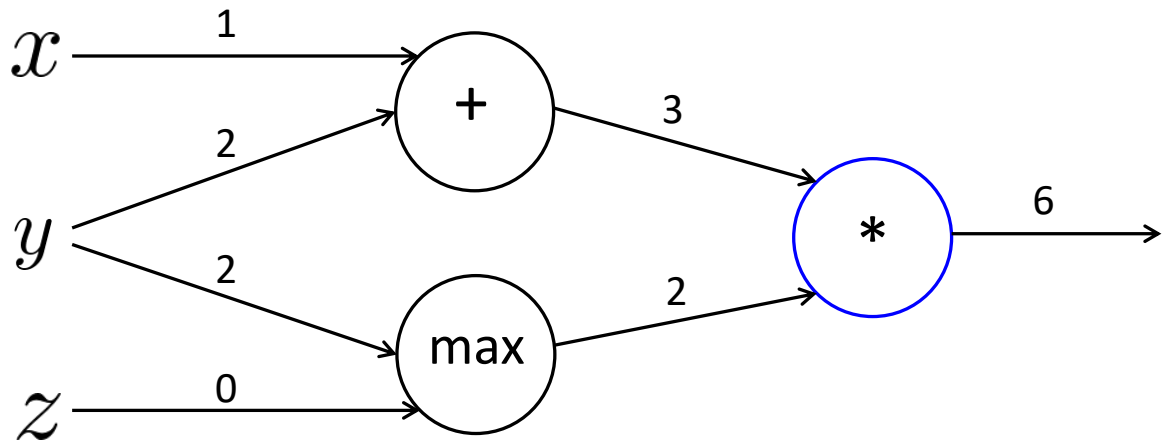
Local gradients

$$\frac{\partial a}{\partial x} = 1 \quad \frac{\partial a}{\partial y} = 1$$
$$\frac{\partial b}{\partial y} = \mathbf{1}(y > z) = 1 \quad \frac{\partial b}{\partial z} = \mathbf{1}(z > y) = 0$$
$$\frac{\partial f}{\partial a} = b = 2 \quad \frac{\partial f}{\partial b} = a = 3$$



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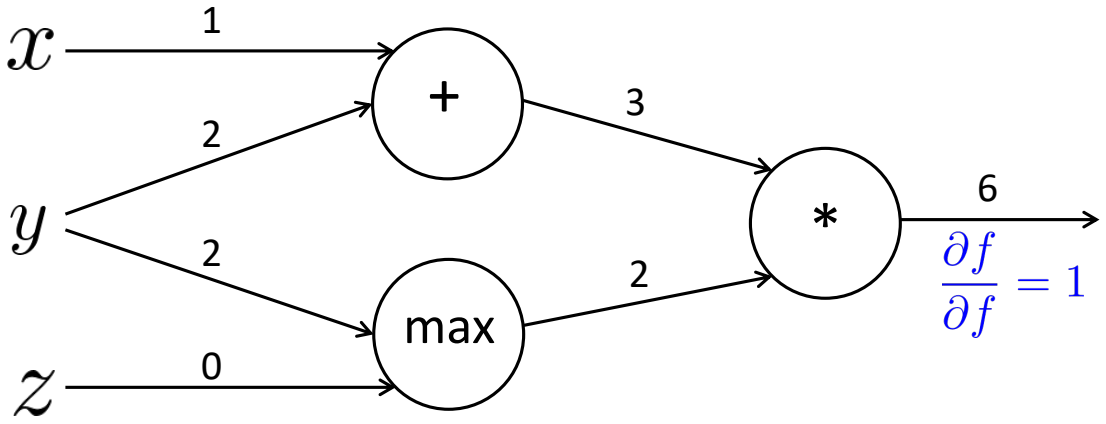

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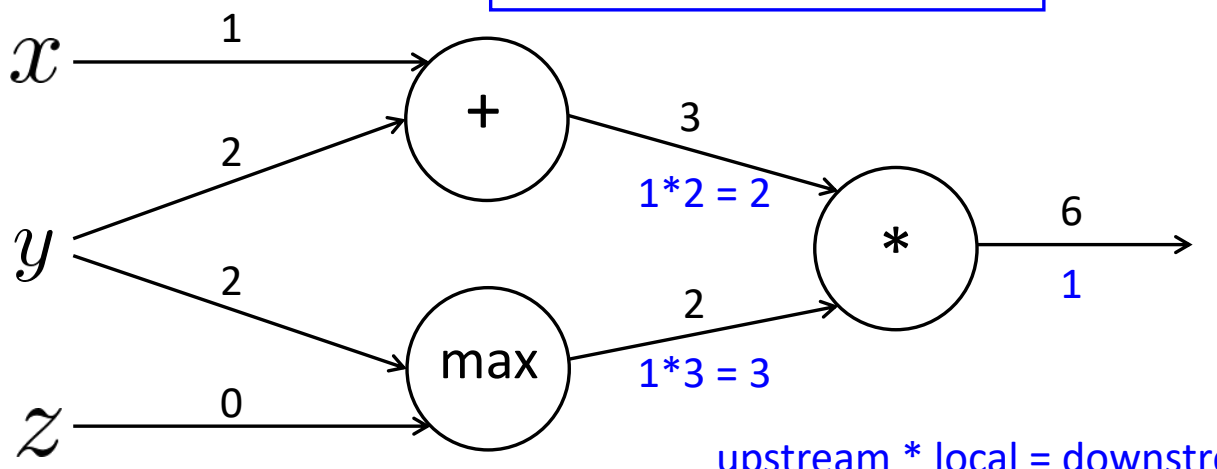

upstream * local = downstream

An Example

$$f(x, y, z) = (x + y)\max(y, z)$$
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Forward prop steps

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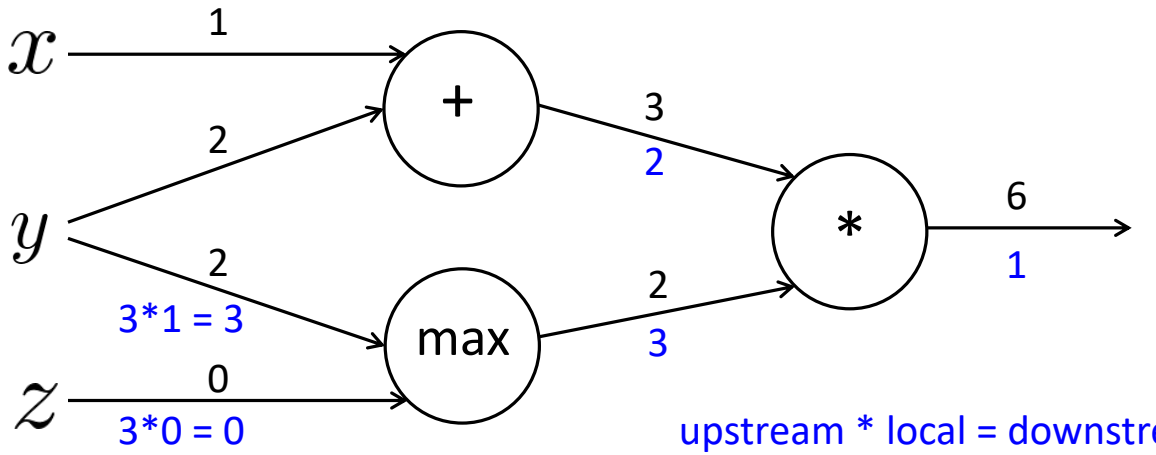

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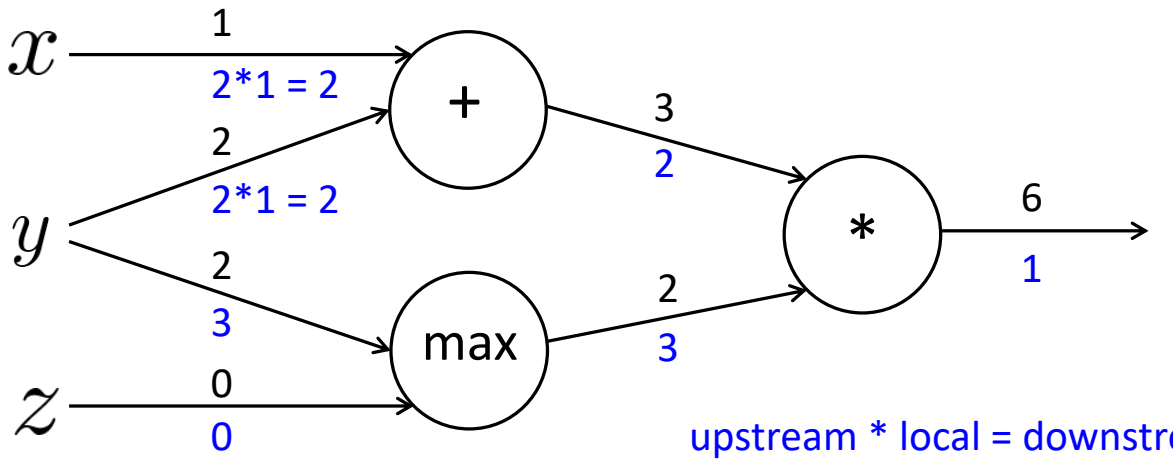

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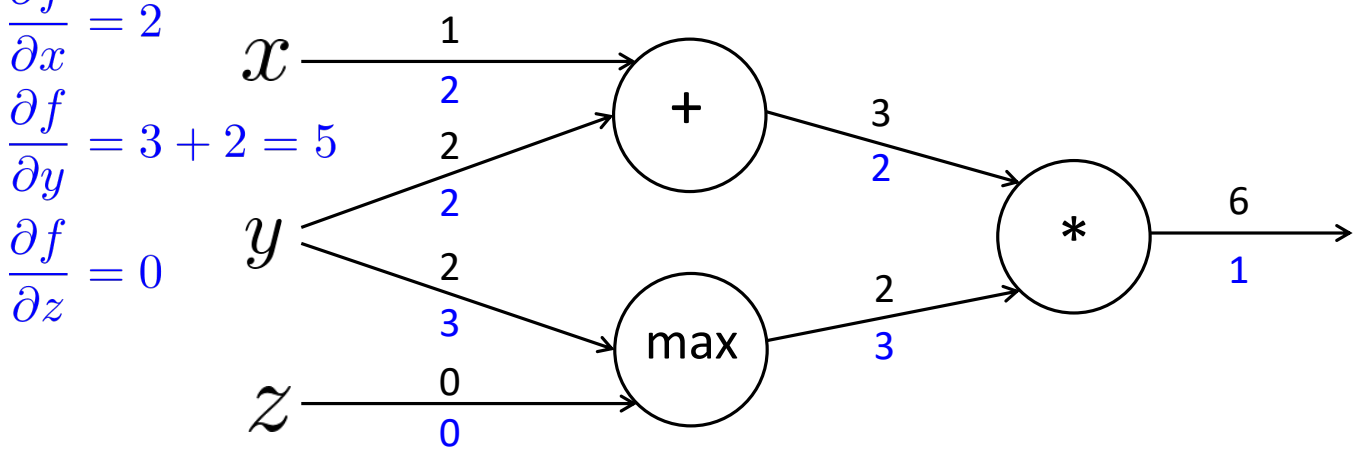
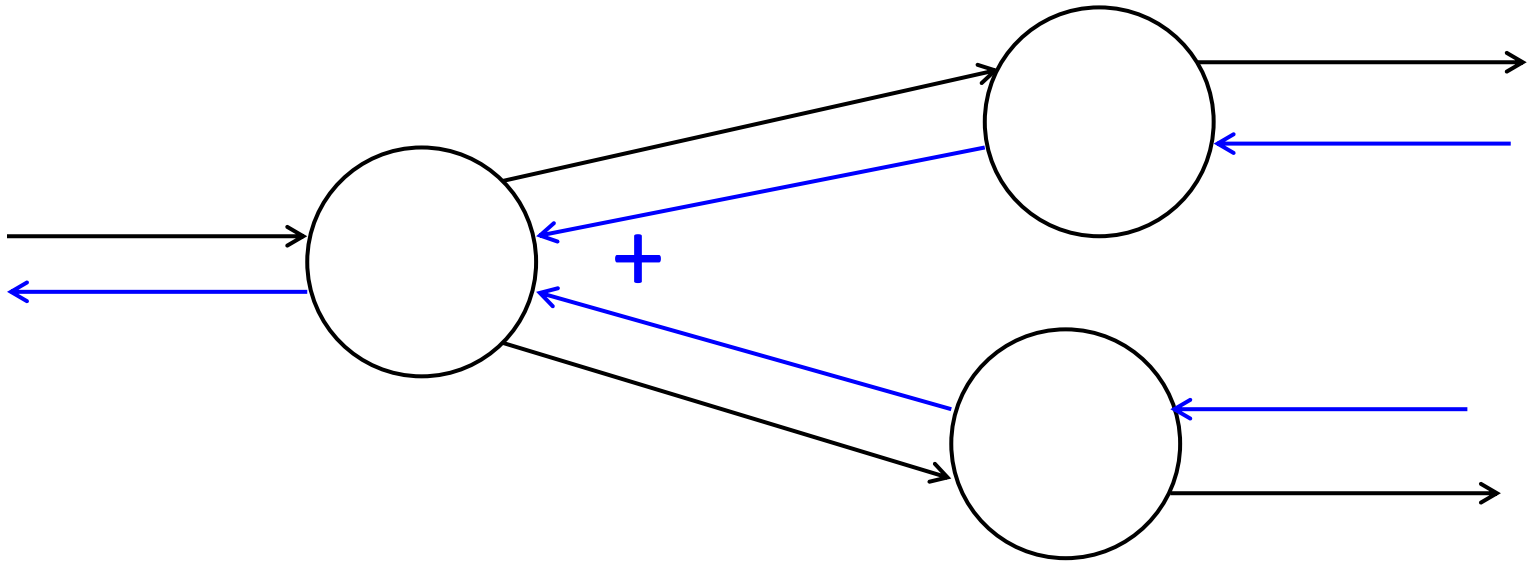


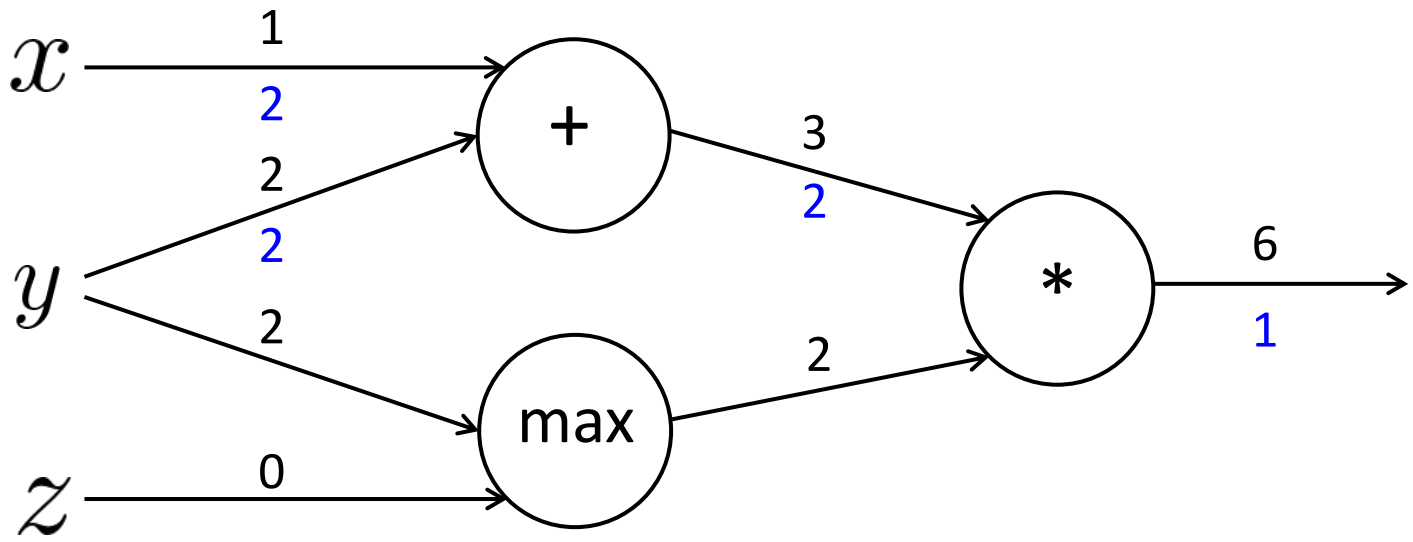
Gradients sum at outward branches



Node Intuitions

$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

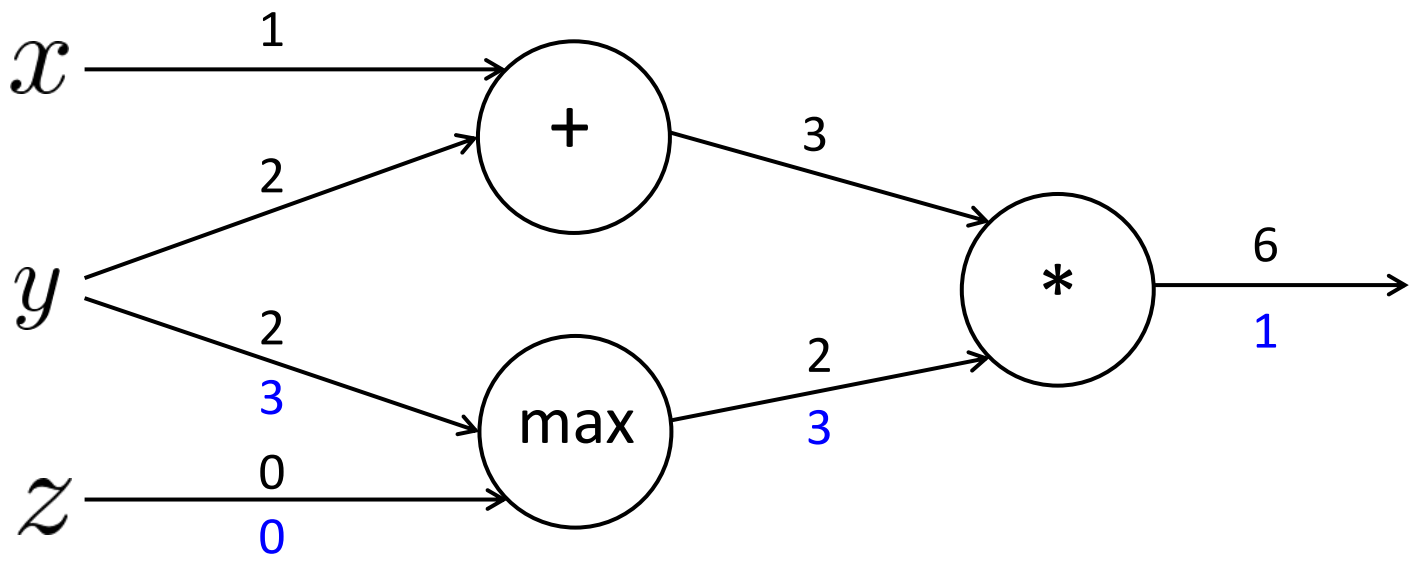
- + "distributes" the upstream gradient to each summand



Node Intuitions

$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

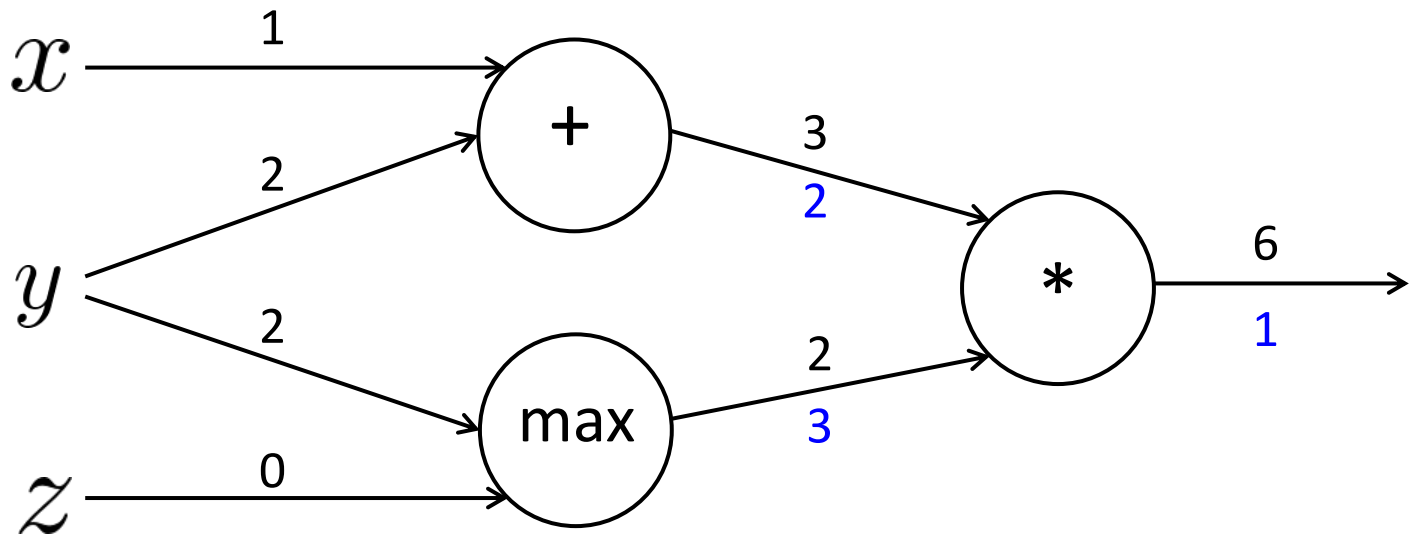
- + "distributes" the upstream gradient to each summand
- max "routes" the upstream gradient



Node Intuitions

$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

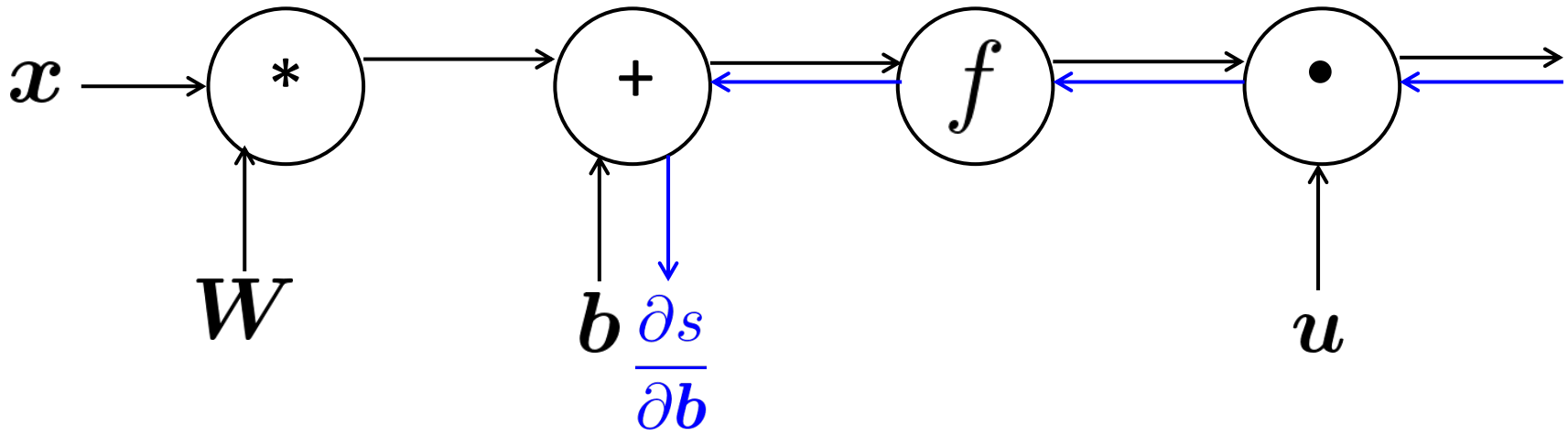
- + “distributes” the upstream gradient to each summand
- max “routes” the upstream gradient
- * “switches” the upstream gradient



Efficiency: compute all gradients at once

- Incorrect way of doing backprop:
  - First compute $\frac{\partial s}{\partial \boldsymbol{b}}$

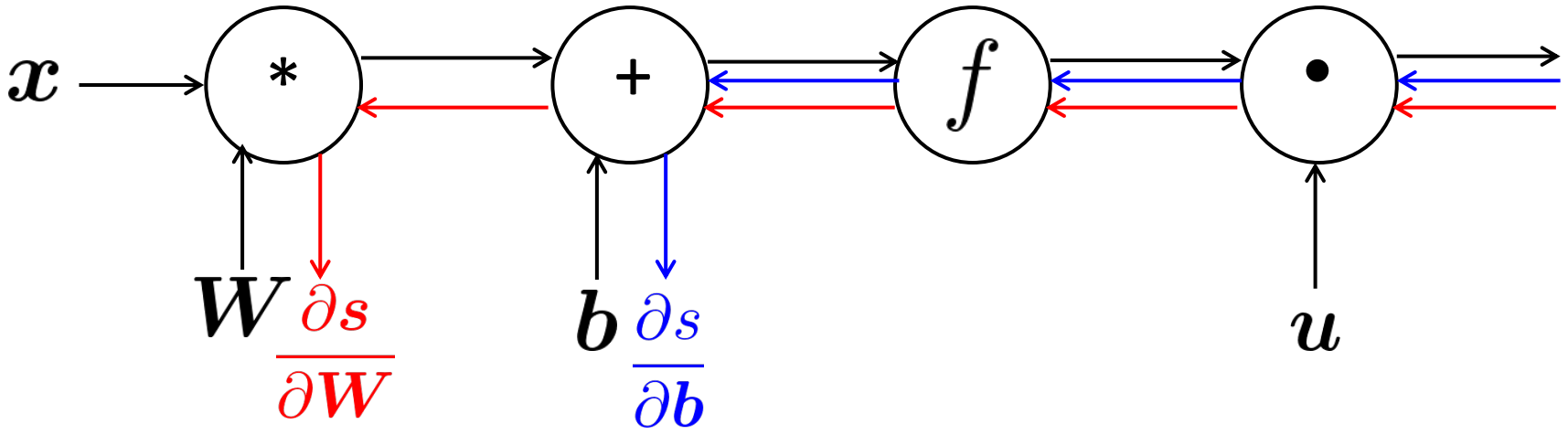
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



Efficiency: compute all gradients at once

- Incorrect way of doing backprop:
  - First compute $\frac{\partial s}{\partial \boldsymbol{b}}$
  - Then independently compute $\frac{\partial \boldsymbol{s}}{\partial \boldsymbol{W}}$
  - Duplicated computation!

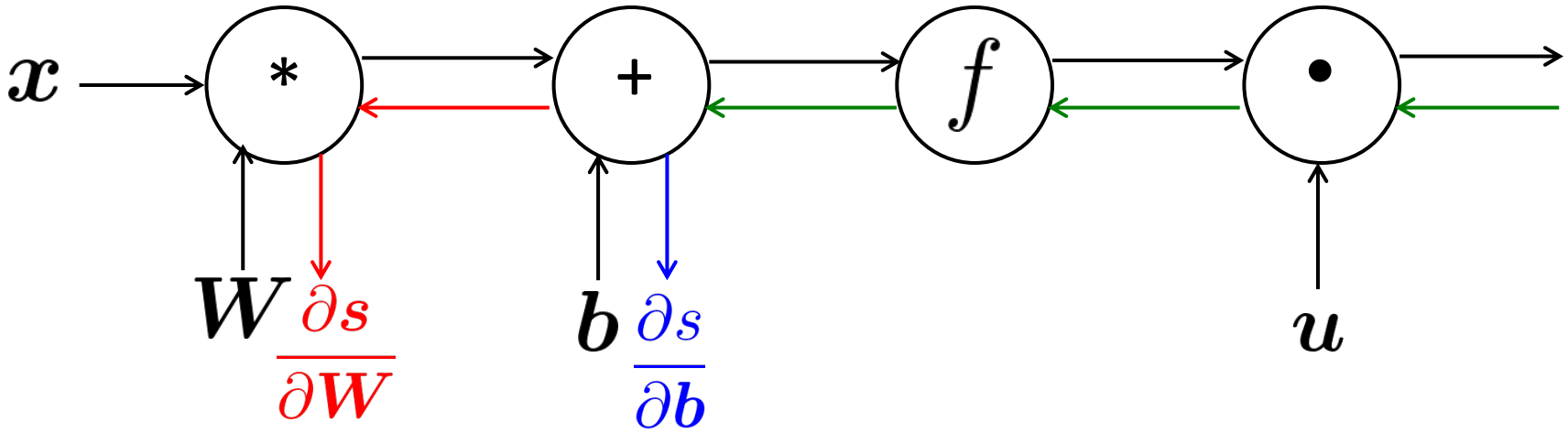
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



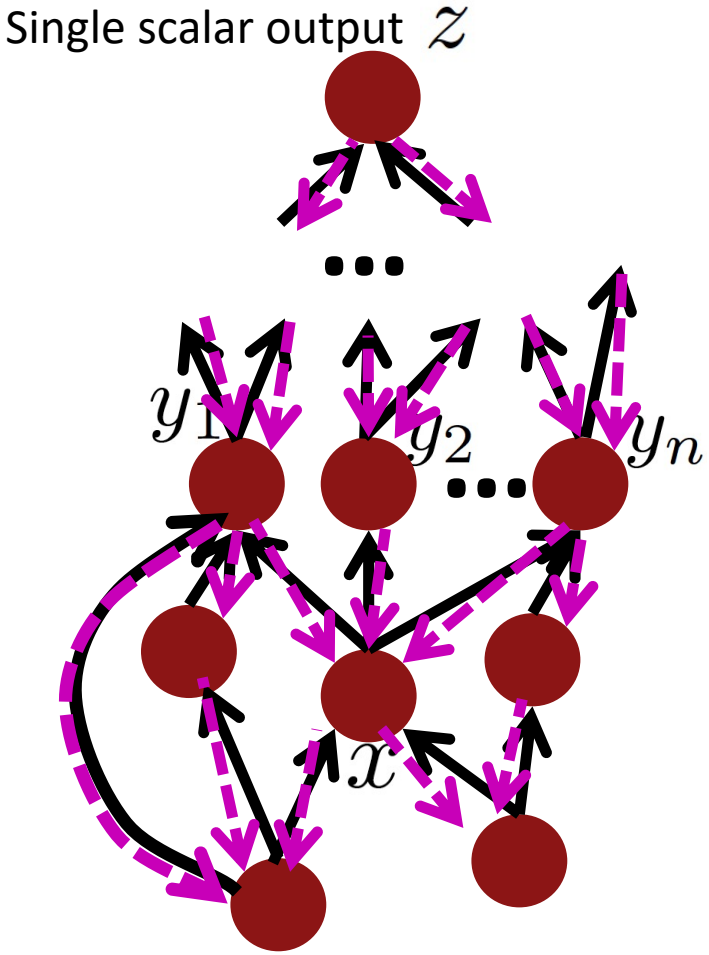
Efficiency: compute all gradients at once

- Correct way:
  - Compute all the gradients at once
  - Analogous to using $\boldsymbol{\delta}$ when we computed gradients by hand

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$



Back-Prop in General Computation Graph



1. Fprop: visit nodes in topological sort order
   - Compute value of node given predecessors
2. Bprop:
   - initialize output gradient = 1
   - visit nodes in reverse order:
   Compute gradient wrt each node using gradient wrt successors

$\{y_1, y_2, \ldots y_n\}$ = successors of x

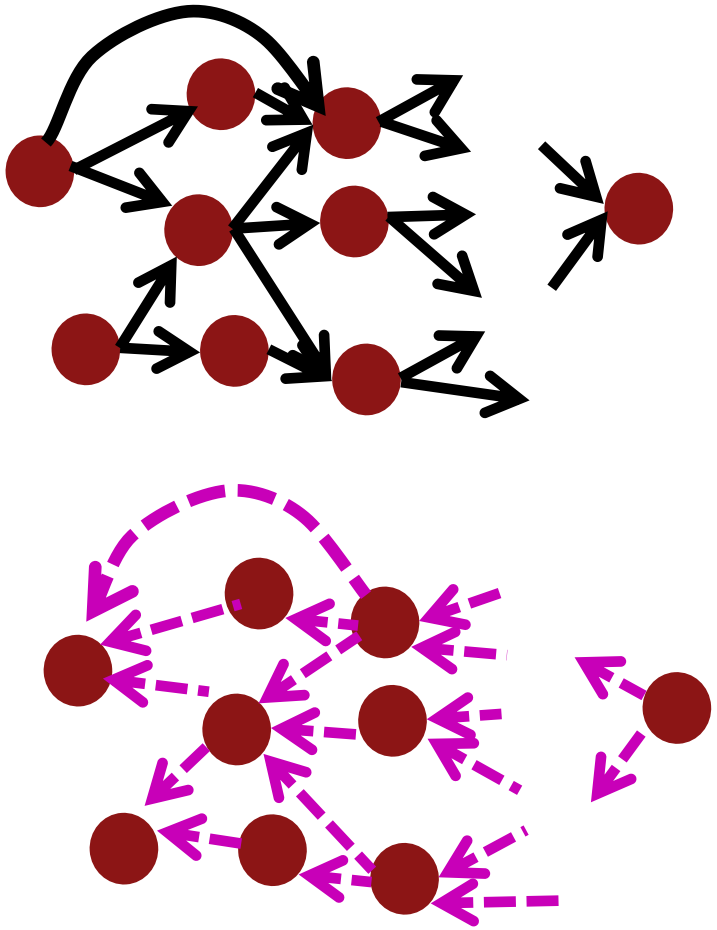
$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Done correctly, big O() complexity of fprop and bprop is **the same**

In general, our nets have regular layer-structure and so we can use matrices and Jacobians…

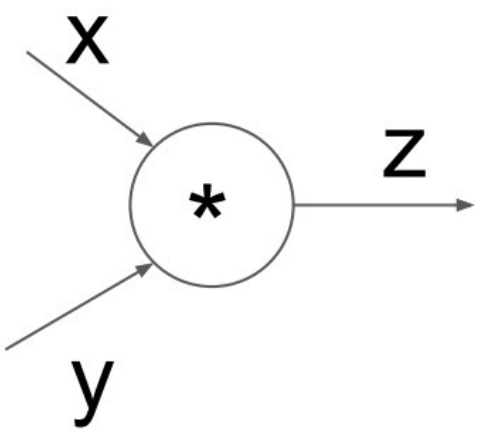
From Stanford CS224n course

Automatic Differentiation



- The gradient computation can be automatically inferred from the symbolic expression of the fprop
- Each node type needs to know how to compute its output and how to compute the gradient w.r.t. its inputs given the gradient w.r.t. its output
- Modern DL frameworks (PyTorch, Tensorflow, etc.) do backpropagation for you but mainly leave layer/node writer to hand-calculate the local derivative

Implementation: forward/backward API



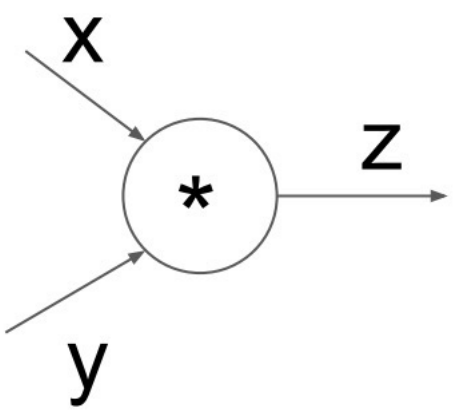
(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

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

$\frac{\partial L}{\partial x}$

Implementation: forward/backward API



(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

Manual Gradient checking: Numeric Gradient

- For small h (≈ 1e-4),

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

- Easy to implement correctly
- But approximate and **very** slow:
  - You have to recompute *f* for **every parameter** of our model
- Useful for checking your implementation
  - In the old days, we hand-wrote everything, doing this everywhere was the key test
  - Now much less needed; you can use it to check layers are correctly implemented

Summary

- Backpropagation: recursively (and hence efficiently) apply the chain rule along computation graph
  - [downstream gradient] = [upstream gradient] x [local gradient]

- Forward pass: compute results of operations and save intermediate values
- Backward pass: apply chain rule to compute gradients

Why learn all these details about gradients?

- Modern deep learning frameworks compute gradients for you!
  - There will a lecture for PyTorch soon

- But why take a class on compilers or systems when they are implemented for you?
  - Understanding what is going on under the hood is useful!

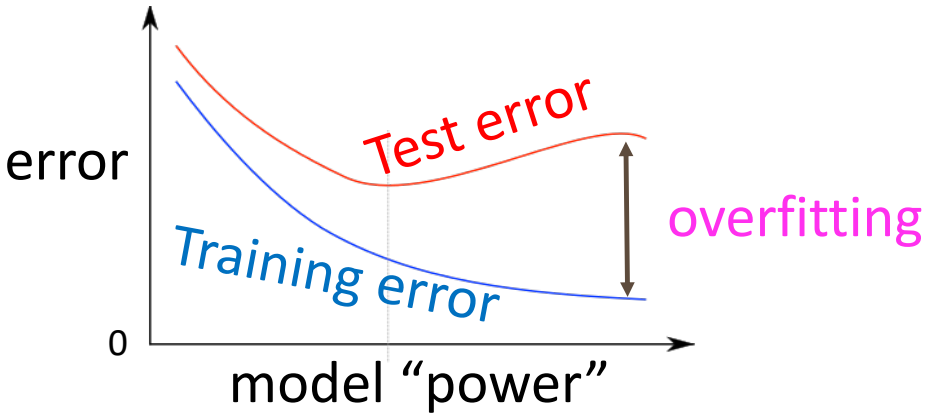
- Backpropagation doesn't always work perfectly out of the box
  - Understanding why is crucial for debugging and improving models
  - See Karpathy article: https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b
  - Example in future lecture: exploding and vanishing gradients

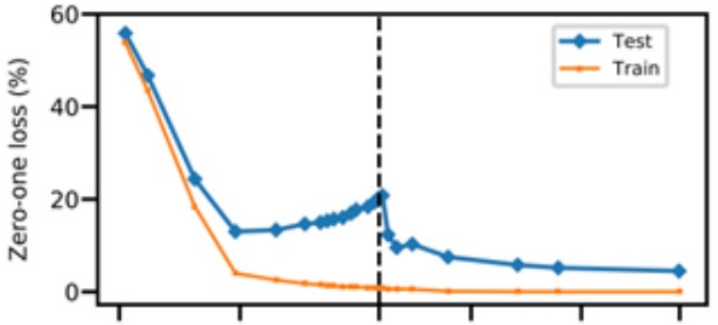
We have models with many parameters! Regularization!

- A full loss function includes **regularization** over all parameters θ, e.g., L2 regularizati

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} -\log\left(\frac{e^{f_{y_i}}}{\sum_{c=1}^{C} e^{f_c}}\right) + \lambda \sum_k \theta_k^2$$

- Classic view: Regularization works to prevent **overfitting** when we have a lot of features (or later a very powerful/deep model, etc.)
- Now: Regularization **produces models that generalize well** when we have a "big" model
  - We do not care that our models overfit on the training data, even though they are **hugely** overfit!





Dropout (Srivastava, Hinton, Krizhevsky, Sutskever, & Salakhutdinov 2012/JMLR 2014)

- Preventing Feature Co-adaptation = Good Regularization Method! Use it widely!
  - Training time: at each instance of evaluation (in online SGD-training), randomly set 50% of the inputs to each neuron to 0
  - Test time: halve the model weights (now twice as many)
  - (Except usually only drop first layer inputs a little (~15%) or not at all)
  - This prevents feature co-adaptation: A feature cannot only be useful in the presence of particular other features
  - In a single layer: A kind of middle-ground between Naïve Bayes (where all feature weights are set independently) and logistic regression models (where weights are set in the context of all others)
  - Can be thought of as a form of model bagging (i.e., like an ensemble model)
  - Nowadays usually thought of as strong, feature-dependent regularizer [Wager, Wang, & Liang 2013]

“Vectorization”

- E.g., looping over word vectors versus concatenating them all into one large matrix and then multiplying the softmax weights with that matrix:

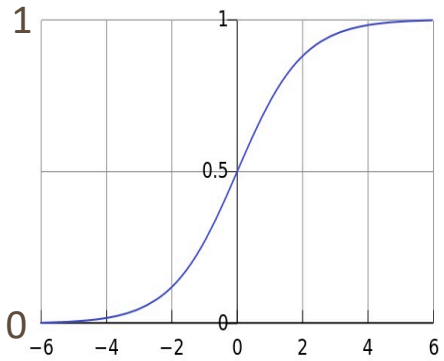
```
from numpy import random
N = 500 # number of windows to classify
d = 300 # dimensionality of each window
C = 5 # number of classes
W = random.rand(C,d)
wordvectors_list = [random.rand(d,1) for i in range(N)]
wordvectors_one_matrix = random.rand(d,N)

%timeit [W.dot(wordvectors_list[i]) for i in range(N)]
%timeit W.dot(wordvectors_one_matrix)
```

- 1000 loops, best of 3: 639 µs per loop
  10000 loops, best of 3: 53.8 µs per loop <- Now using a single a C x N matrix
- Matrices are awesome!!! Always try to use vectors and matrices rather than for loops!
- The speed gain goes from 1 to 2 orders of magnitude with GPUs!

Non-linearities, old and new

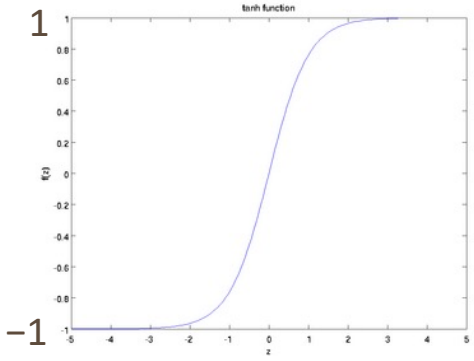
logistic ("sigmoid")

$$f(z) = \frac{1}{1 + \exp(-z)}.$$



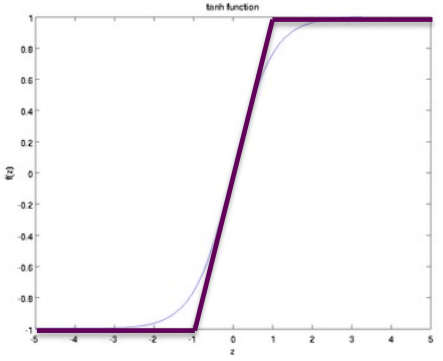
tanh

$$f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}},$$



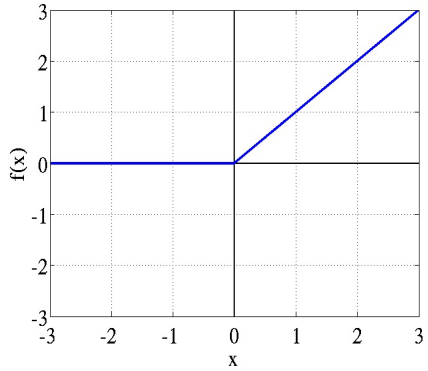
hard tanh

$$\text{HardTanh}(x) = \begin{cases} -1 & \text{if } x < -1 \\ x & \text{if } -1 <= x <= 1 \\ 1 & \text{if } x > 1 \end{cases}$$



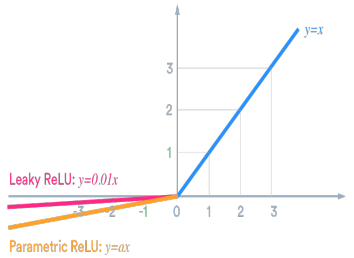
ReLU (Rectified Linear Unit)

$$\text{ReLU}(z) = \max(z, 0)$$

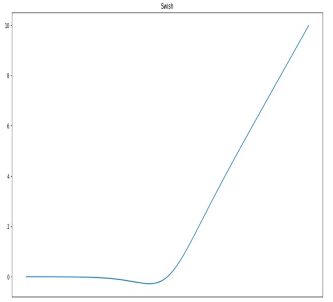


- Both logistic and tanh are still used in various places (e.g., to get a probability), but are no longer the defaults for making deep networks
- For building a deep network, the first thing you should try is ReLU — it trains quickly and performs well due to good gradient backflow

Leaky ReLU / Parametric ReLU



Swish [Ramachandran, Zoph & Le 2017]



Parameter Initialization

- You normally must initialize weights to small random values (i.e., not zero matrices!)
  - To avoid symmetries that prevent learning/specialization
- Initialize hidden layer biases to 0 and output (or reconstruction) biases to optimal value if weights were 0 (e.g., mean target or inverse sigmoid of mean target)
- Initialize **all other weights** ~ Uniform(*–r, r*), with r chosen so numbers get neither too big or too small (later the need for this is removed with use of layer normalization)
- Xavier initialization has variance inversely proportional to fan-in nin (previous layer size) and fan-out n_{out} (next layer size):

$$\mathrm{Var}(W_i) = \frac{2}{n_{\mathrm{in}} + n_{\mathrm{out}}}$$

Optimizers

- Usually, plain SGD will work just fine!
  - However, getting good results will often require hand-tuning the learning rate
    - E.g., start it higher and halve it every *k* epochs (passes through full data, **shuffled** or sampled)
- For more complex nets and situations, or just to avoid worry, you often do better with one of a family of more sophisticated "adaptive" optimizers that scale the adjustment to individual parameters by an accumulated gradient.
  - These models give differential per-parameter learning rates
    - Adagrad
    - RMSprop
    - Adam <- A fairly good, safe place to begin in many cases
    - AdamW
    - SparseAdam
    - ...
  - Can just start them with an initial learning rate, around 0.001

Language Modeling + RNNs

Language Modeling

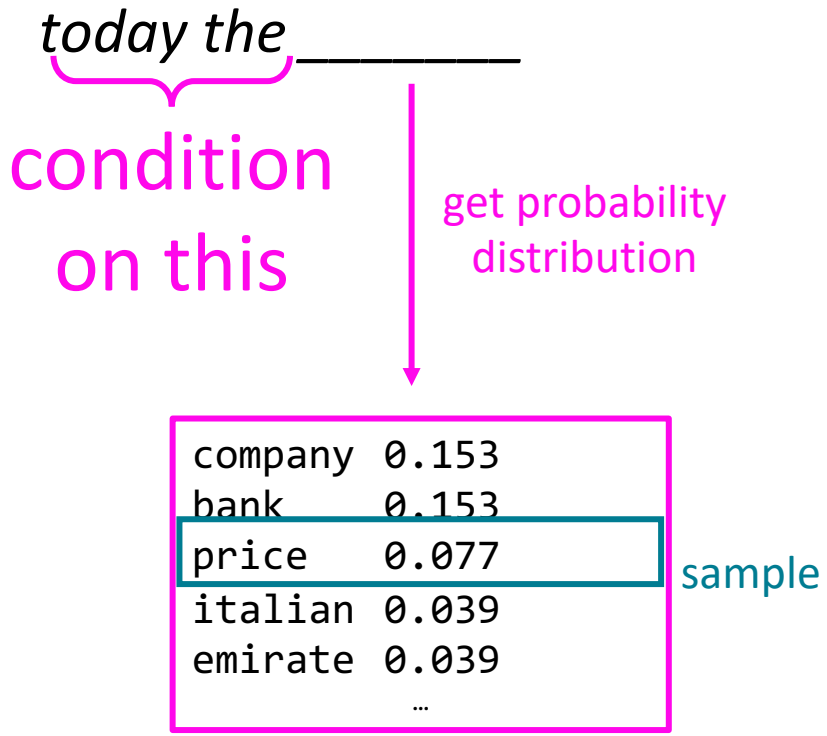
- **Language Modeling** is the task of predicting what word comes next

$$P(w_k \mid w_1, w_2, \ldots, w_{k-1})$$

- A system that compute the probability distribution of the next word is called a **Language Model**

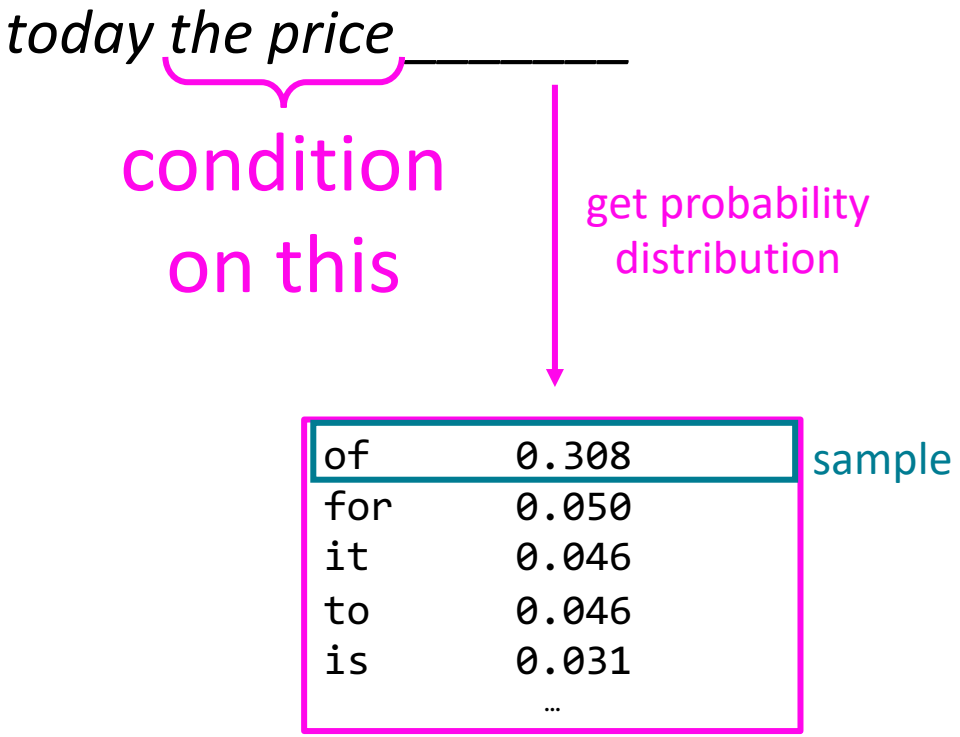
Generating text with a n-gram Language Model

- You can use a Language Model to generate text



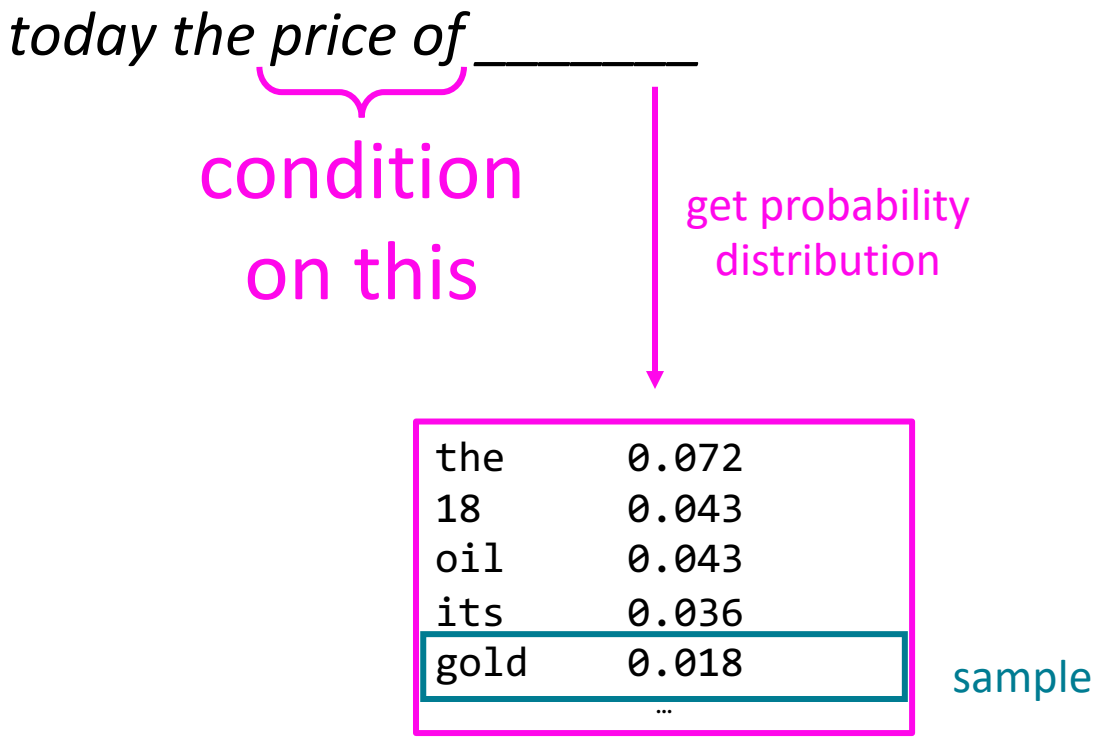
Generating text with a n-gram Language Model

- You can use a Language Model to generate text



Generating text with a n-gram Language Model

- You can use a Language Model to generate text



A fixed-window neural Language Model

~~as the proctor started the clock~~ the students opened their _____

discard

fixed window

A fixed-window neural Language Model

output distribution

$$\hat{\boldsymbol{y}} = \text{softmax}(\boldsymbol{U}\boldsymbol{h} + \boldsymbol{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

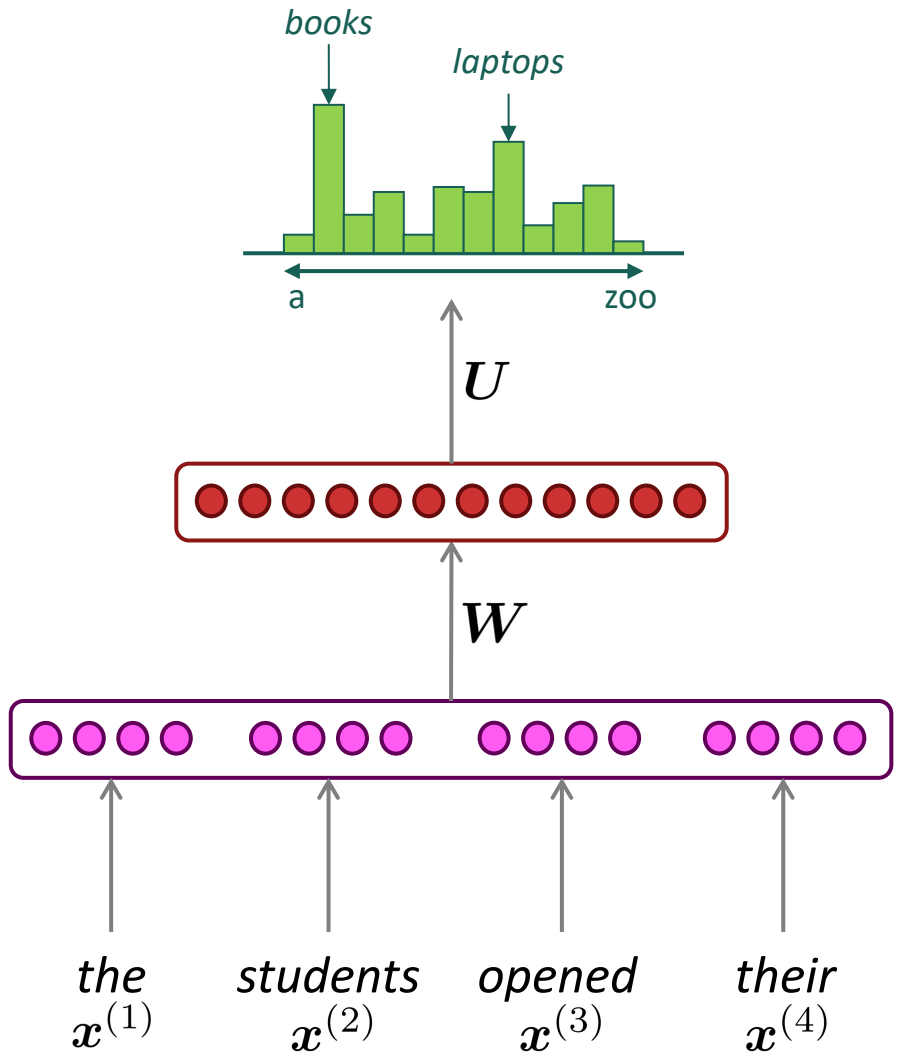
$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{e} + \boldsymbol{b}_1)$$

concatenated word embeddings

$$\boldsymbol{e} = [\boldsymbol{e}^{(1)}; \boldsymbol{e}^{(2)}; \boldsymbol{e}^{(3)}; \boldsymbol{e}^{(4)}]$$

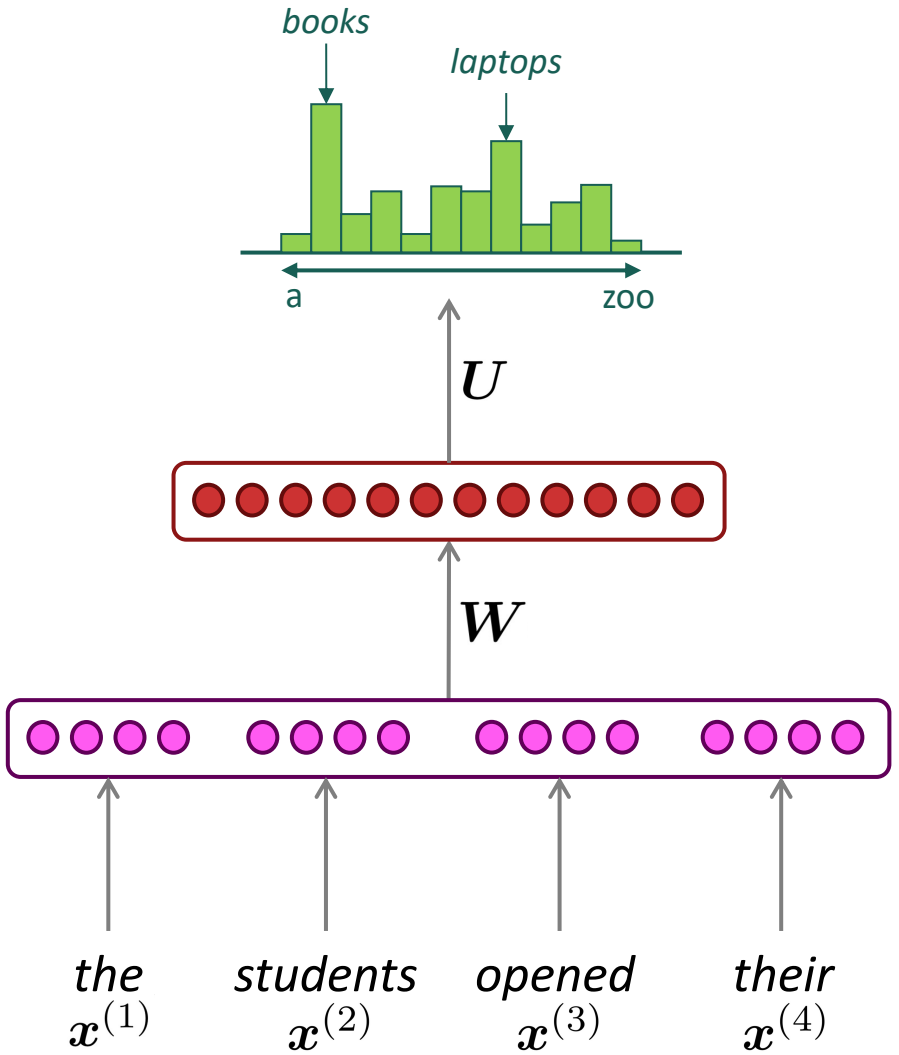
words / one-hot vectors

$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}, \boldsymbol{x}^{(4)}$$



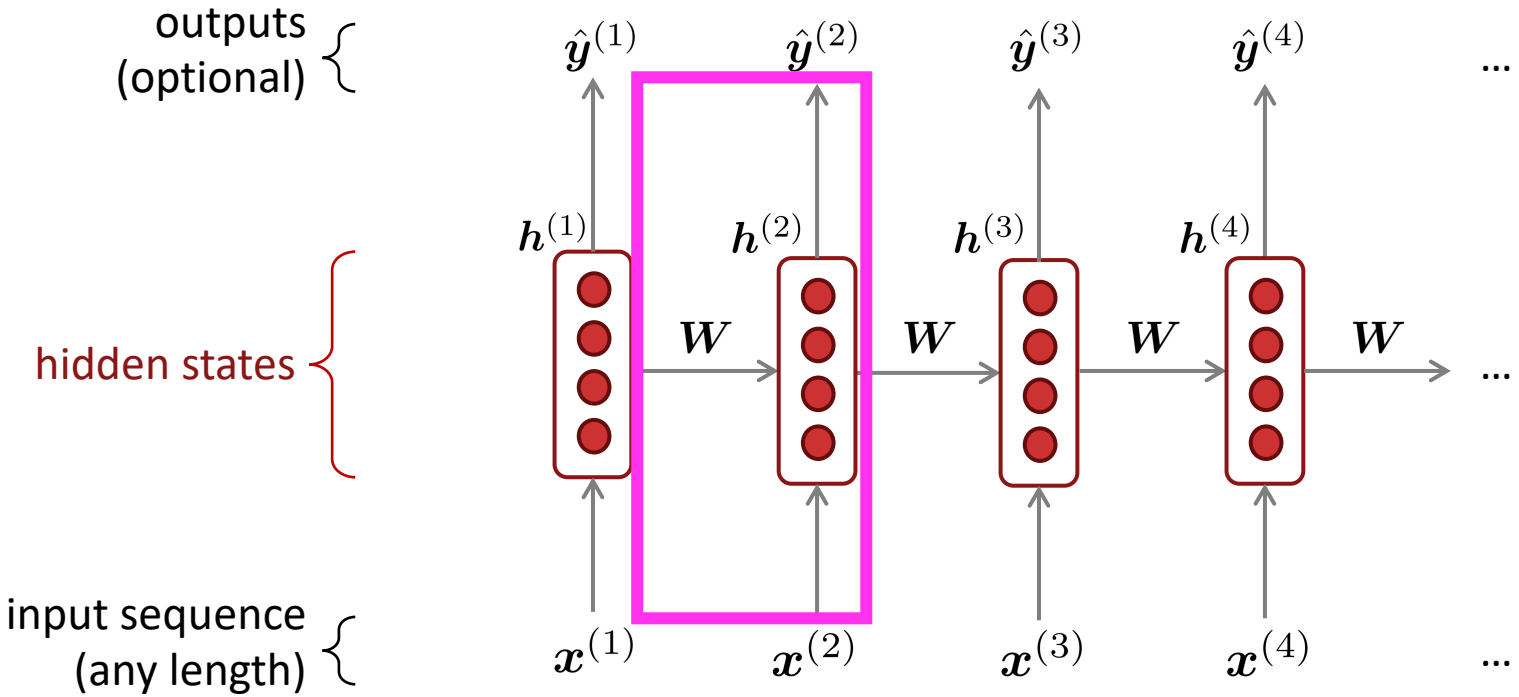
A fixed-window neural Language Model

- Improvements over n-gram LM:
  - No sparsity problem
  - Don't need to store all observed n-grams
- Remaining problems:
  - Fixed window is too small
  - Enlarging window enlarges W
  - Window can never be large enough!
  - $x(0)$ and $x(1)$ are multiplied by completely different weights in W. No symmetry in how the inputs are processed.
  - We need a neural architecture that can process **any length input**!



Recurrent Neural Networks (RNN)

- A family of neural architectures
- Core idea: Apply the same weights W repeatedly



A Simple RNN Language Model

output distribution

$$\hat{\boldsymbol{y}}^{(t)} = \text{softmax}\left(\boldsymbol{U}\boldsymbol{h}^{(t)} + \boldsymbol{b}_2\right) \in \mathbb{R}^{|V|}$$

hidden states

$$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_e\boldsymbol{e}^{(t)} + \boldsymbol{b}_1\right)$$

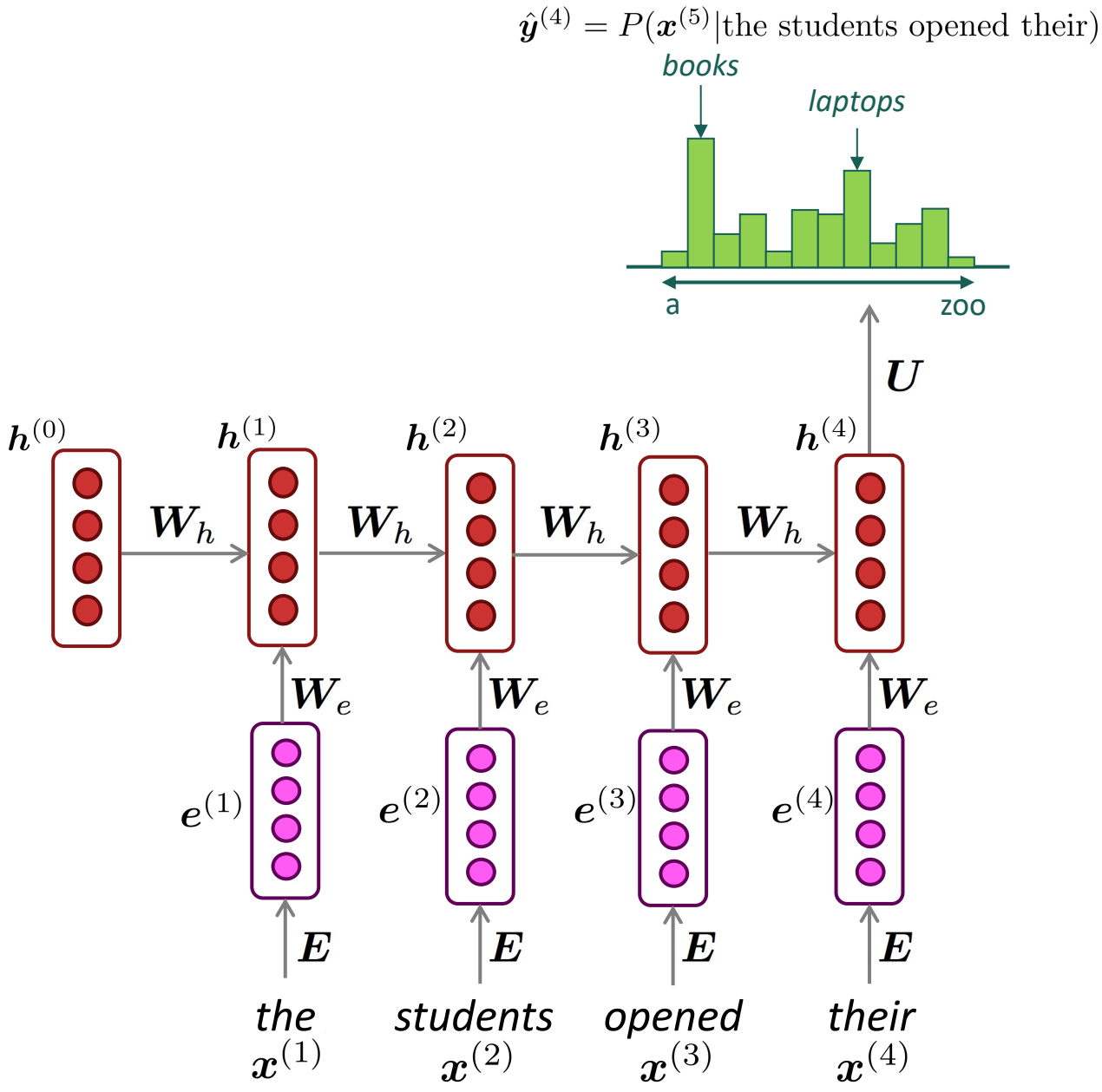
$\boldsymbol{h}^{(0)}$ is the initial hidden state

word embeddings

$$\boldsymbol{e}^{(t)} = \boldsymbol{E}\boldsymbol{x}^{(t)}$$

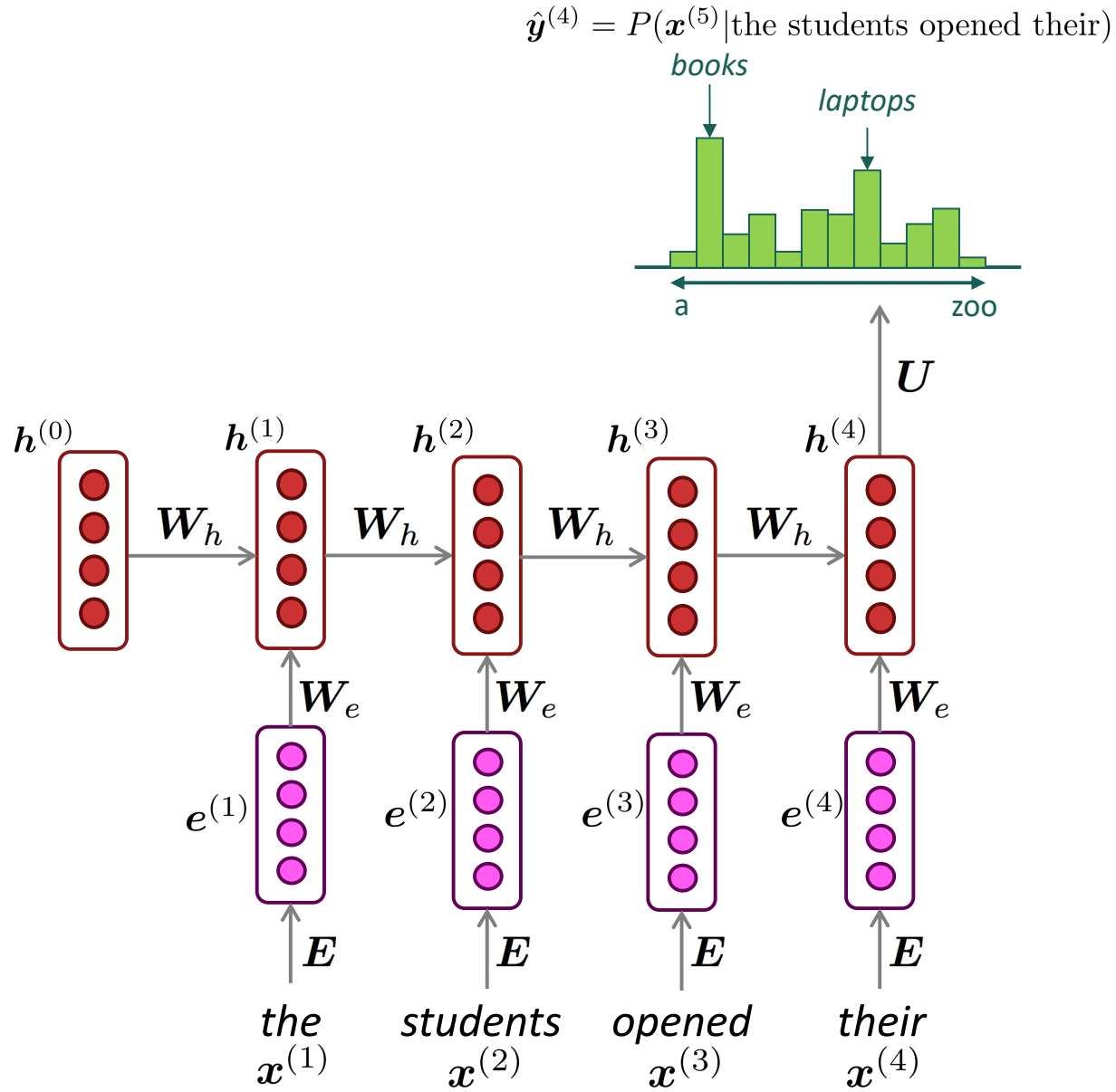
words / one-hot vectors

$$\boldsymbol{x}^{(t)} \in \mathbb{R}^{|V|}$$



RNN Language Models

- RNN **Advantages**:
  - Can process any length input
  - Computation for step t can (in theory) use information from many steps back
  - Model size doesn't increase for longer input context
  - Same weights applied on every timestep, so there is symmetry in how inputs are processed.
- RNN **Disadvantages**:
  - Recurrent computation is slow
  - In practice, difficult to access information from many steps back



Training an RNN Language Model

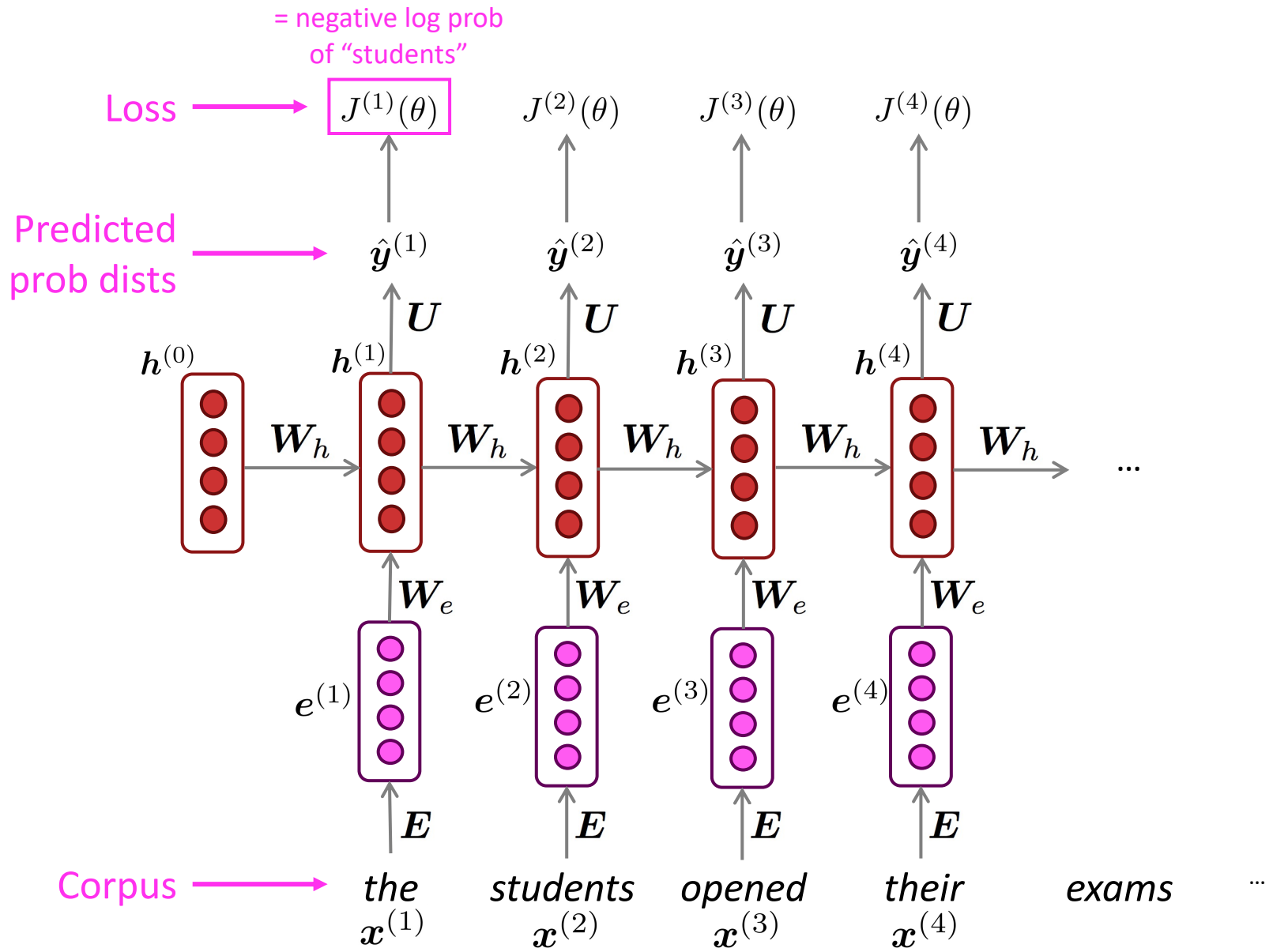
- Get a **big corpus of text** which is a sequence of words $x^{(1)}, \ldots, x^{(T)}$
- Feed into RNN-LM; compute output distribution $\hat{y}^{(t)}$ *for every step t*
  - i.e. predict probability distribution of *every word*, given words so far
- **Loss function** on step t is **cross-entropy** between predicted probability distribution $\hat{y}^{(t)}$, and the true next word $y^{(t)}$ (one-hot for $x^{(t+1)}$):

$$J^{(t)}(\theta) = CE(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)}) = -\sum_{w \in V} \boldsymbol{y}_w^{(t)} \log \hat{\boldsymbol{y}}_w^{(t)} = -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

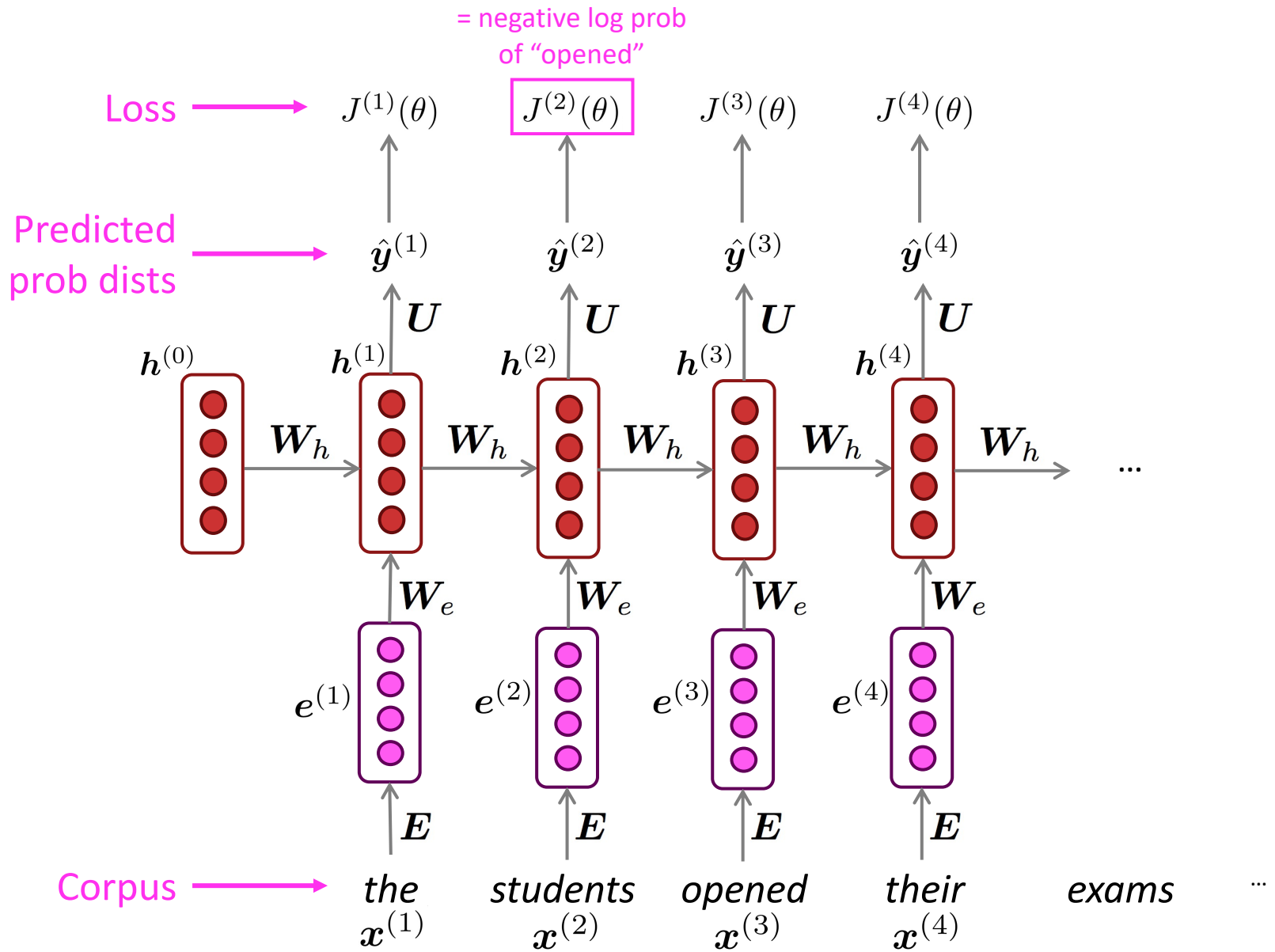
- Average this to get **overall loss** for entire training set:

$$J(\theta) = \frac{1}{T} \sum_{t=1}^{T} J^{(t)}(\theta) = \frac{1}{T} \sum_{t=1}^{T} -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

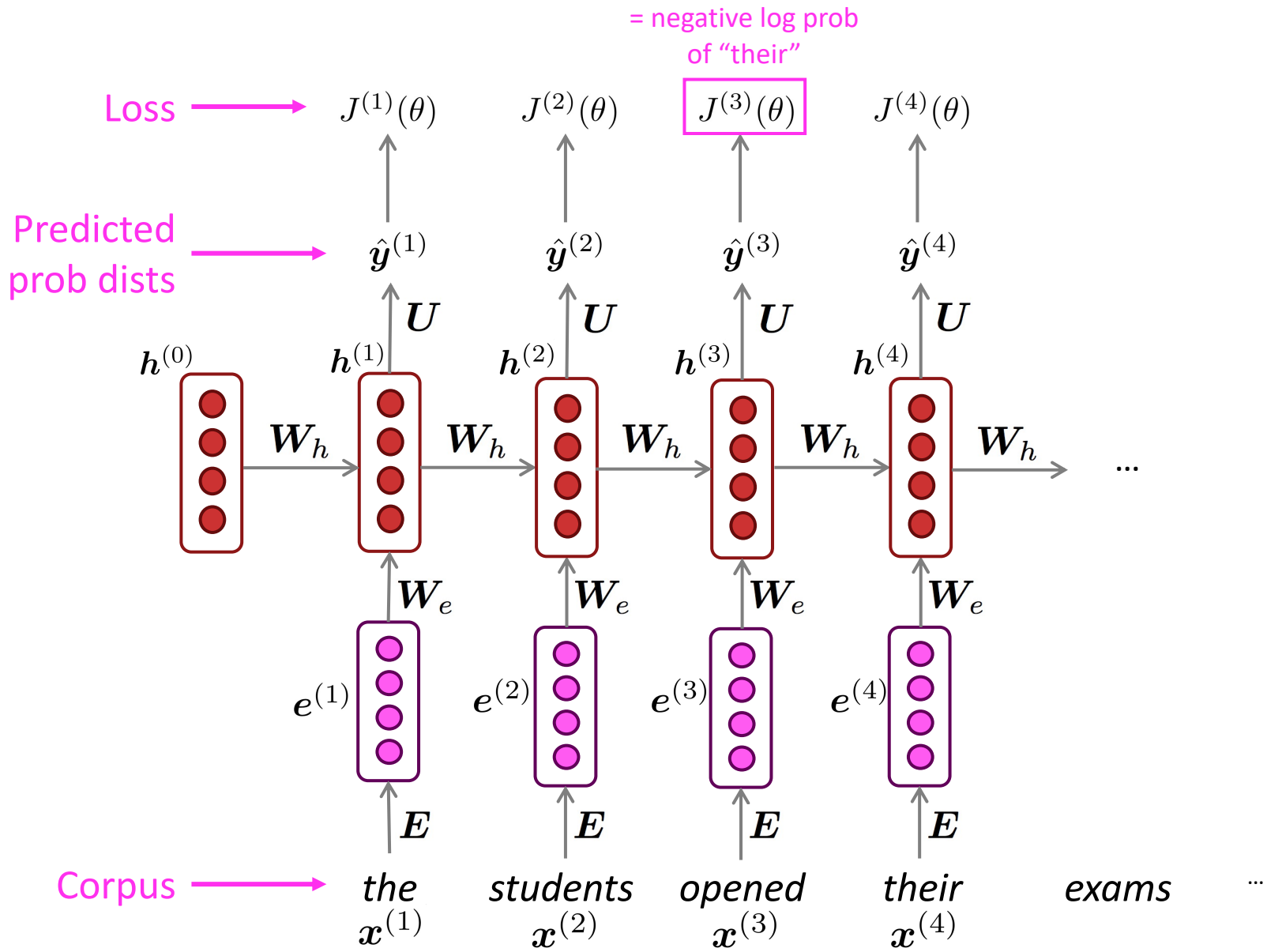
Training an RNN Language Model



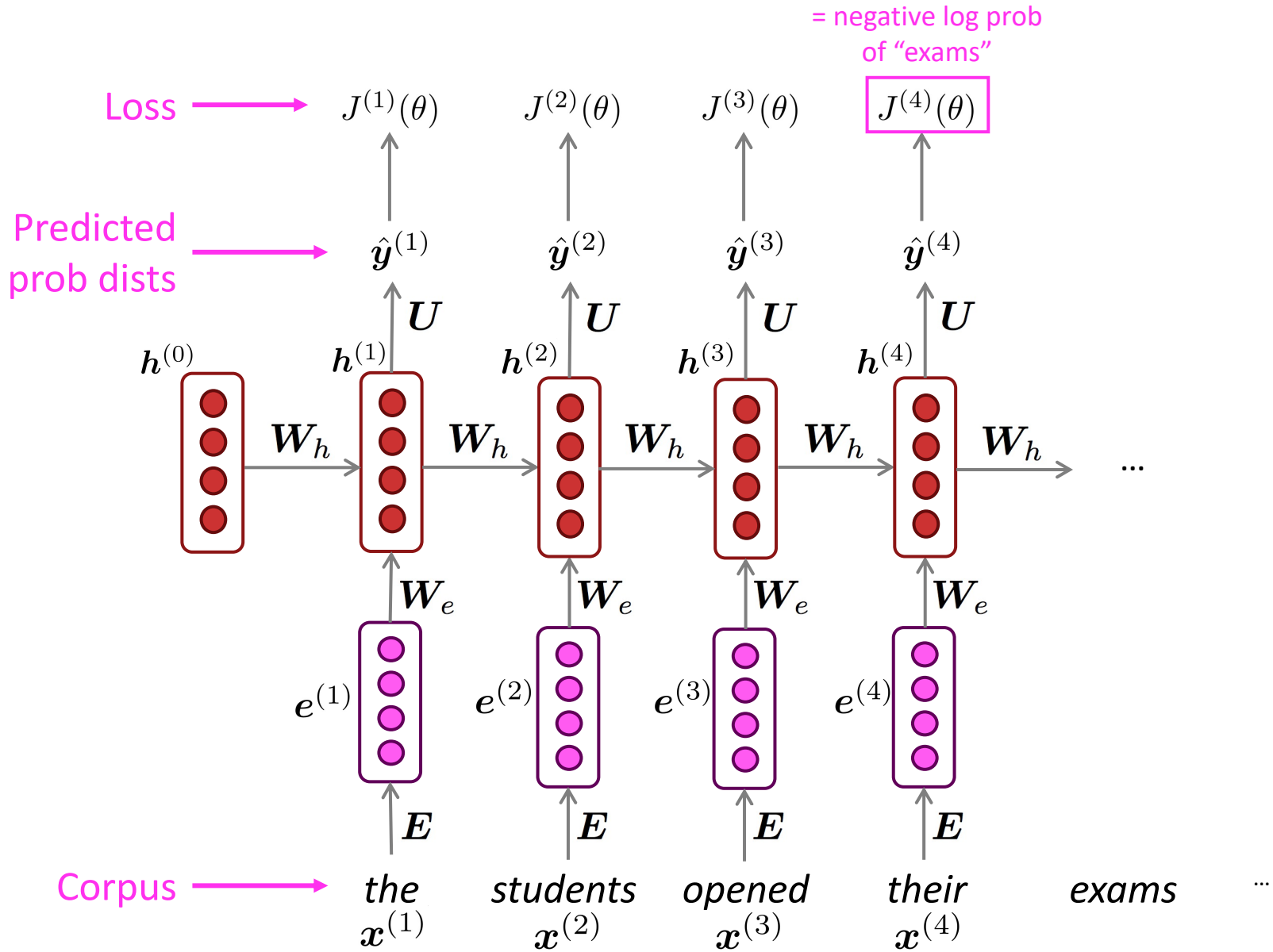
Training an RNN Language Model



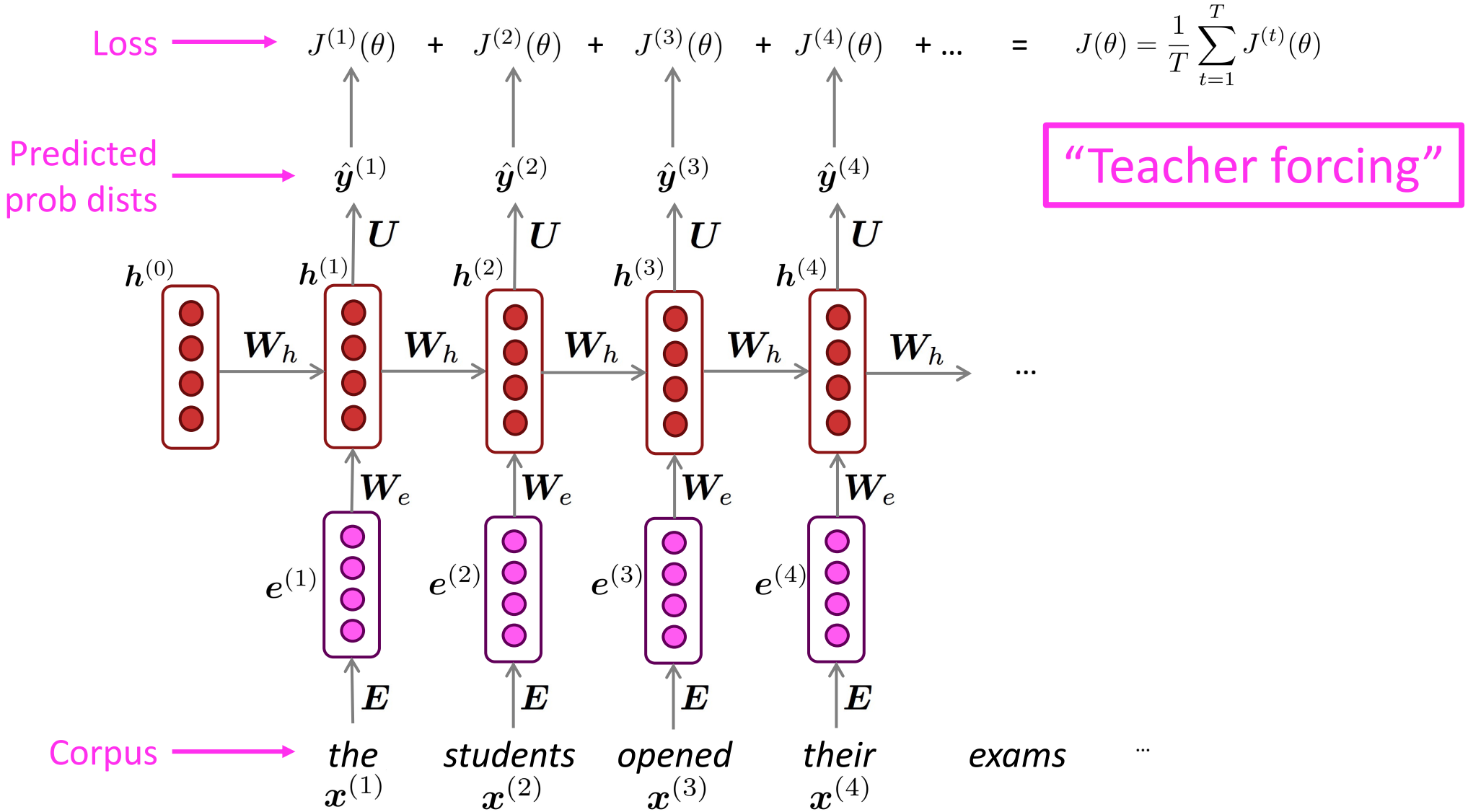
Training an RNN Language Model



Training an RNN Language Model



Training an RNN Language Model



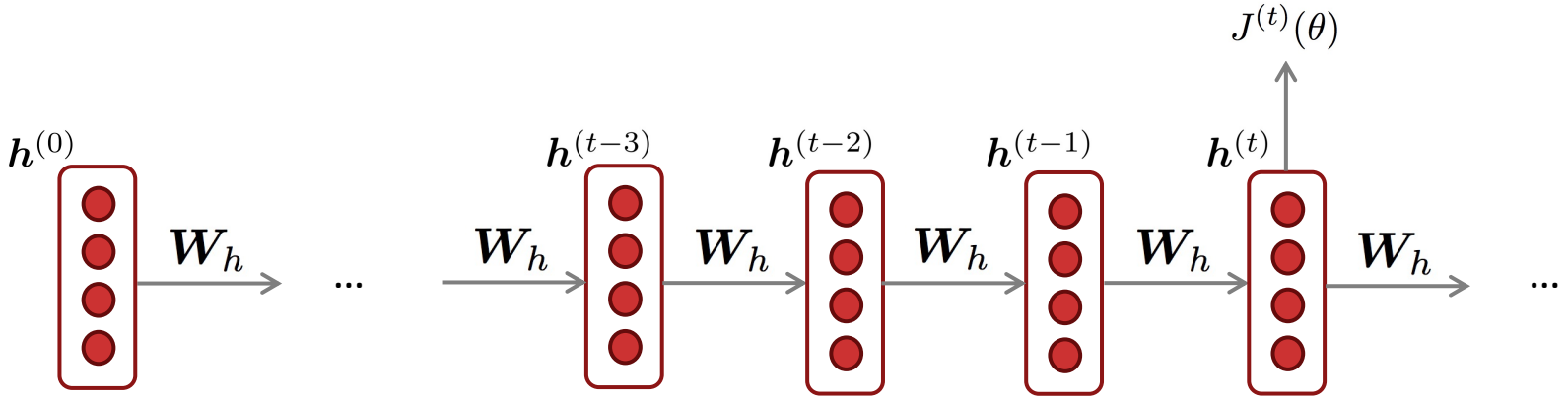
Training an RNN Language Model

- However: Computing loss and gradients across **entire corpus** $x^{(1)}, \ldots, x^{(T)}$ is too expensive!

$$J(\theta) = \frac{1}{T} \sum_{t=1}^{T} J^{(t)}(\theta)$$

- In practice, consider $x^{(1)}, \ldots, x^{(T)}$ as a **sentence** (or a **document**)
- Recall: **Stochastic Gradient Descent** allows us to compute loss and gradients for small
- Compute loss $J(\theta)$ for a sentence (actually, a batch of sentences), compute gradients and update weights. Repeat.

Backpropagation for RNNs



- **Question**: What's the derivative of $J^{(t)}(\theta)$ w.r.t. the repeated weight matrix $\boldsymbol{W_h}$?

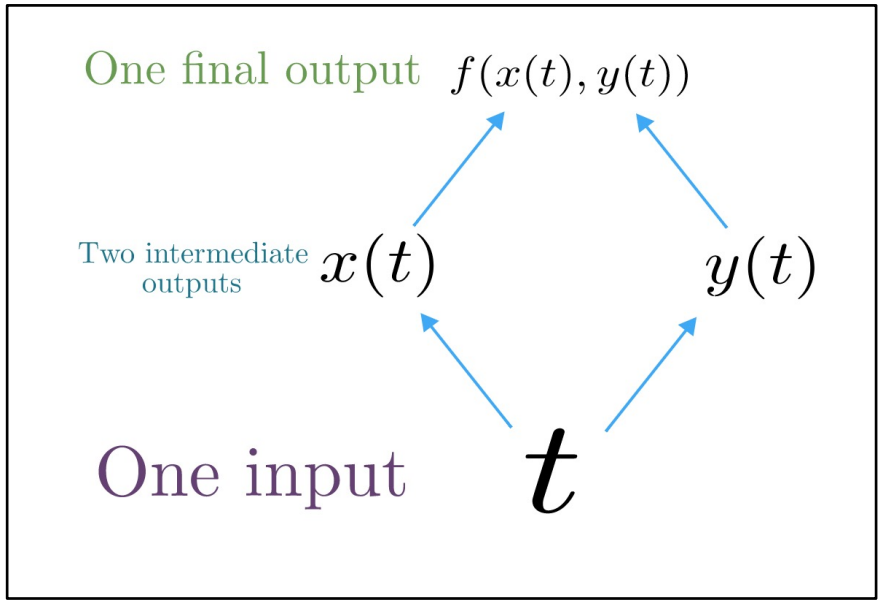
- **Answer:** $$\frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} = \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}}\bigg|_{(i)}$$

- "The gradient w.r.t. a repeated weight is the sum of the gradient w.r.t. each time it appears"

Multivariable Chain Rule

- Given a multivariable function $f(x,y)$, and two single variable functions $x(t)$ and $y(t)$, here's what the multivariable chain rule says:

$$\underbrace{\frac{d}{dt} f(x(t), y(t))}_{\text{Derivative of composition function}} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt}$$



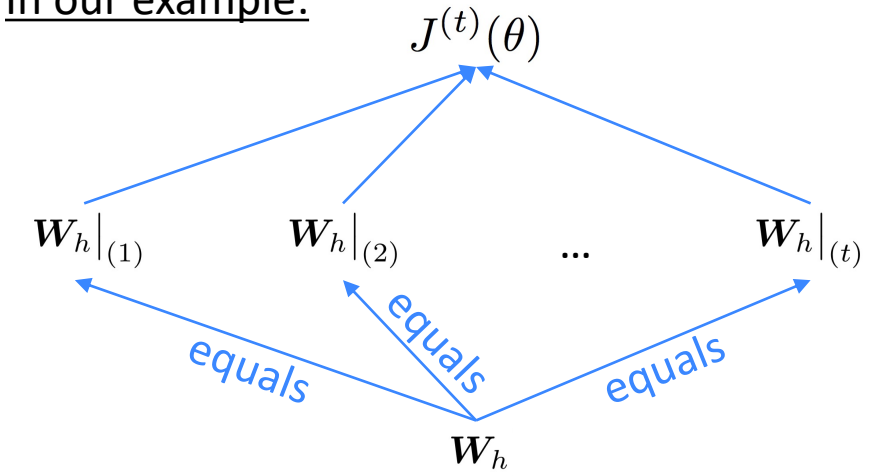
Source: https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives/differentiating-vector-valued-functions/a/multivariable-chain-rule-simple-version

Backpropagation for RNNs: Proof sketch

- Given a multivariable function $f(x,y)$, and two single variable functions $x(t)$ and $y(t)$, here's what the multivariable chain rule says:

$$\underbrace{\frac{d}{dt} f(x(t), y(t))}_{\text{Derivative of composition function}} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt}$$

In our example:



Apply the multivariable chain rule:

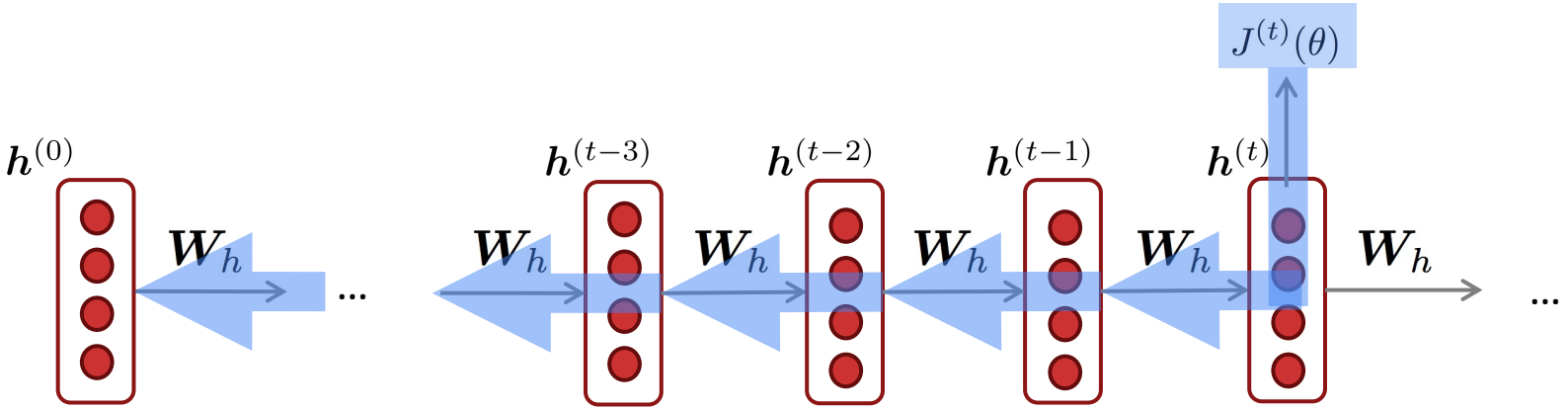
= 1

$$\frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h} = \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h}\bigg|_{(i)} \frac{\partial \boldsymbol{W}_h|_{(i)}}{\partial \boldsymbol{W}_h}$$

$$= \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h}\bigg|_{(i)}$$

Source: https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives/differentiating-vector-valued-functions/a/multivariable-chain-rule-simple-version

Backpropagation for RNNs



$$\frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} = \sum_{i=1}^{t} \left. \frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} \right|_{(i)}$$

Question: How do we calculate this?

Answer: Backpropagate over timesteps *i=t,…,0*, summing gradients as you go. This algorithm is called **"backpropagation through time"** [Werbos, P.G., 1988, *Neural Networks* **1**, and others]

In practice, often "truncated" after ~20 timesteps for training efficiency reasons

From Stanford CS224n course

Generating text with a RNN Language Model

- Just like a n-gram Language Model, you can use a RNN Language Model to **generate text** by **repeated sampling**. Sampled output becomes next step's input.