



Modeling Structured Data with Neural Nets

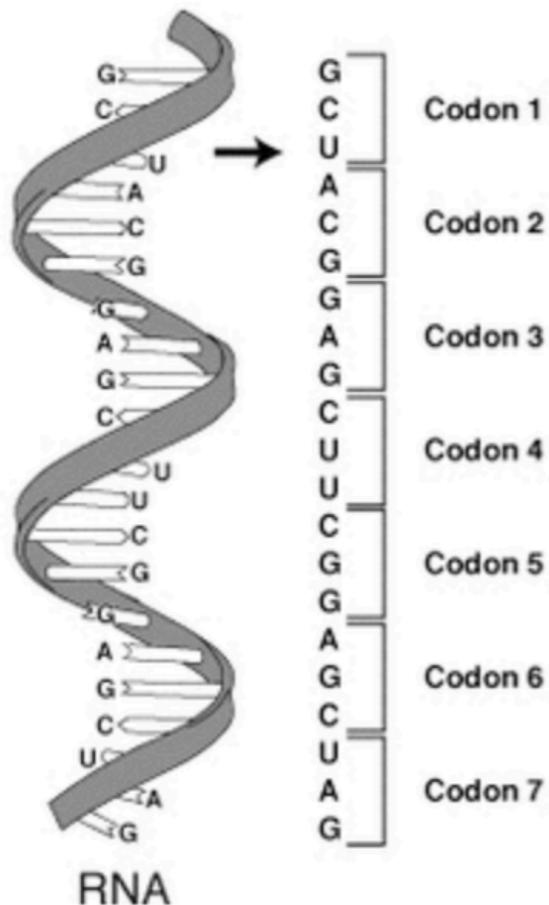
Chris Dyer
DeepMind
Carnegie Mellon University

What is structured data?

Sentences

Kyunghyun Cho is speaking tonight at LxMLS 2020.

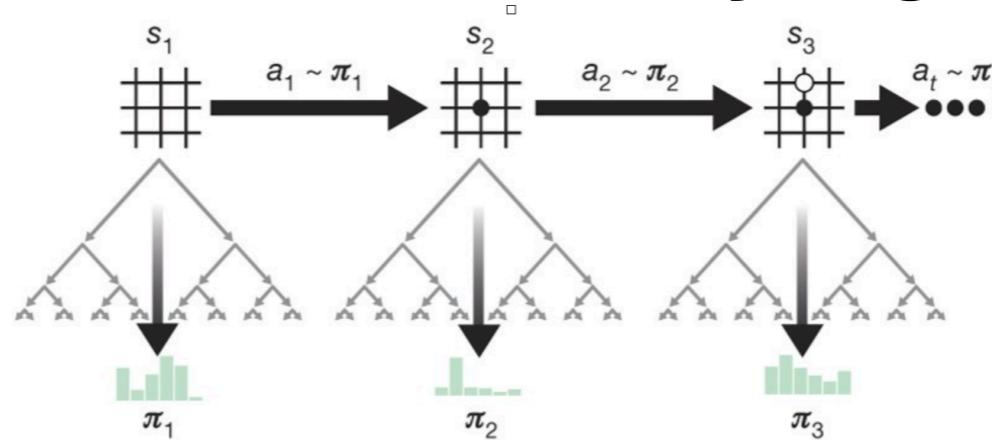
Genetic code



Acoustic waves



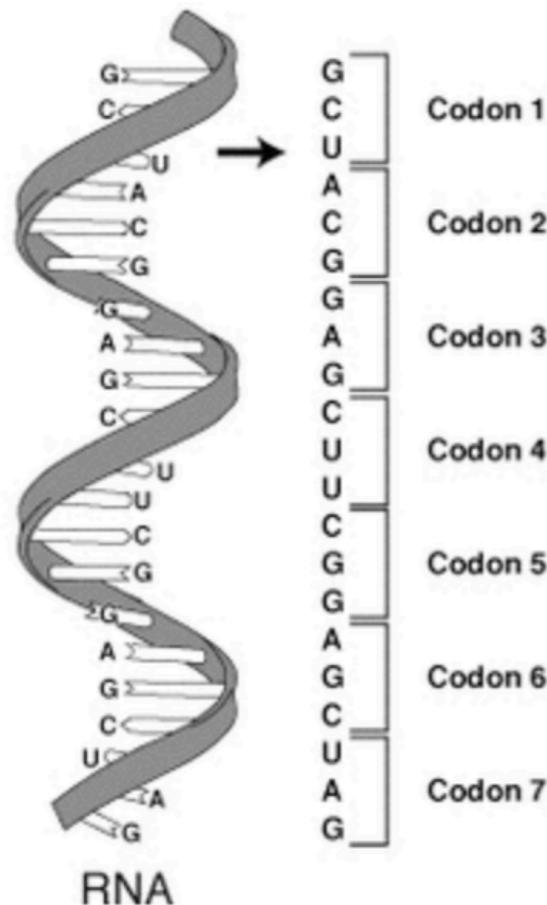
Actions taken by a game player



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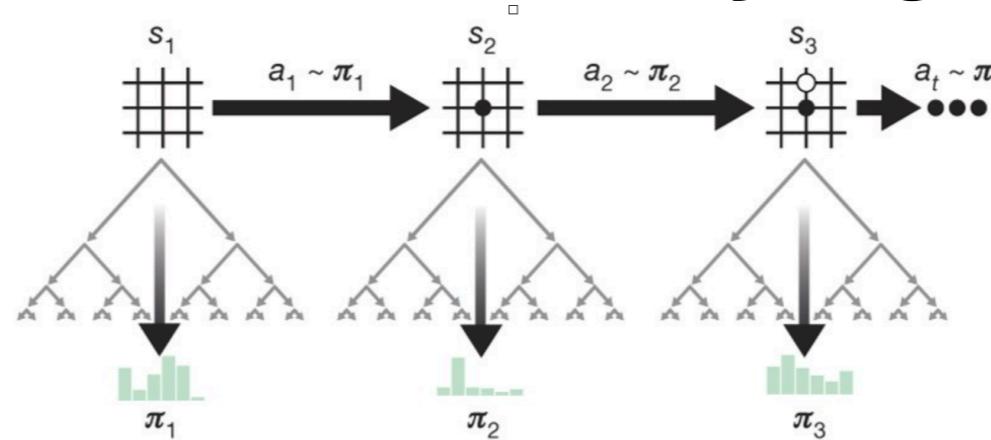
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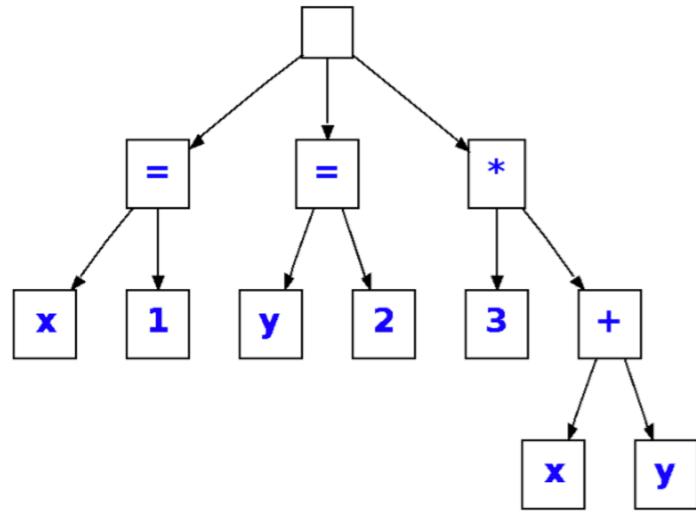
Segmentation

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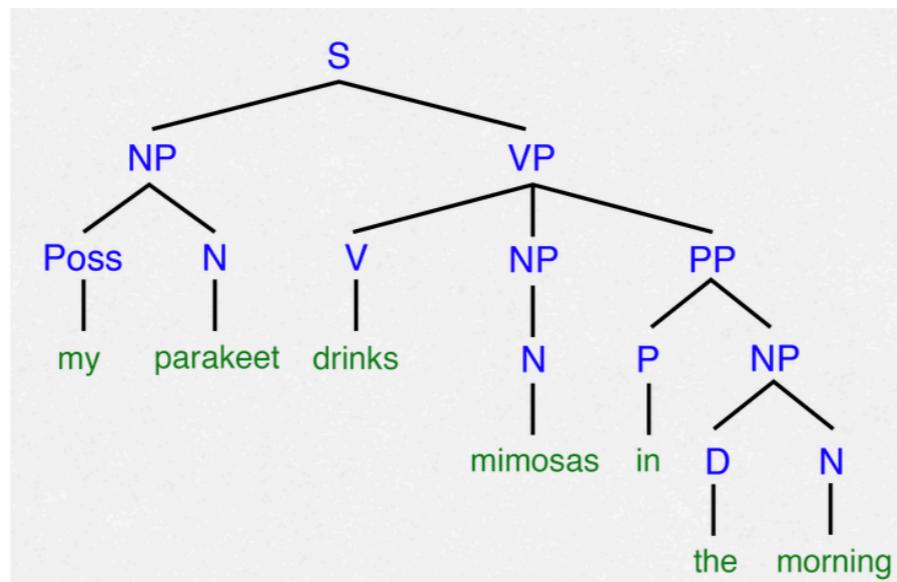
PERSON

EVENT

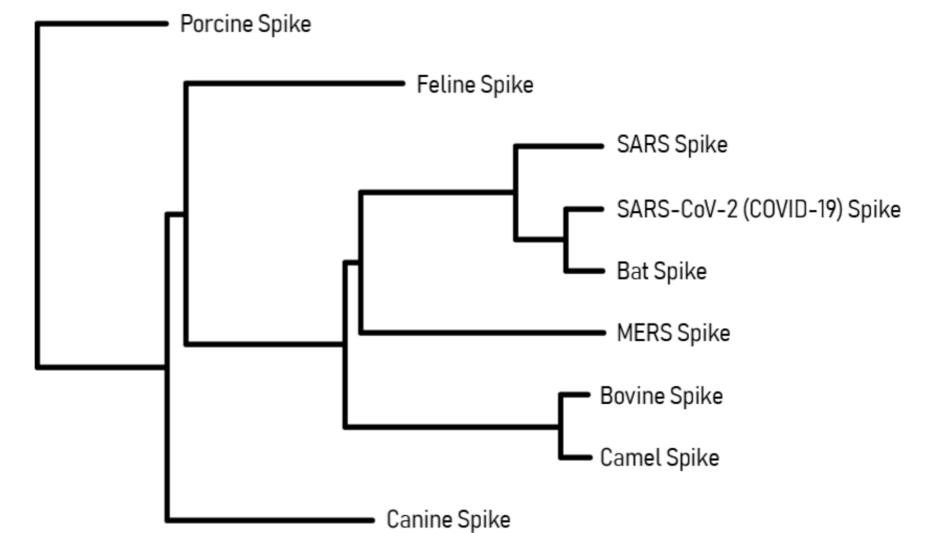
Trees



Programs

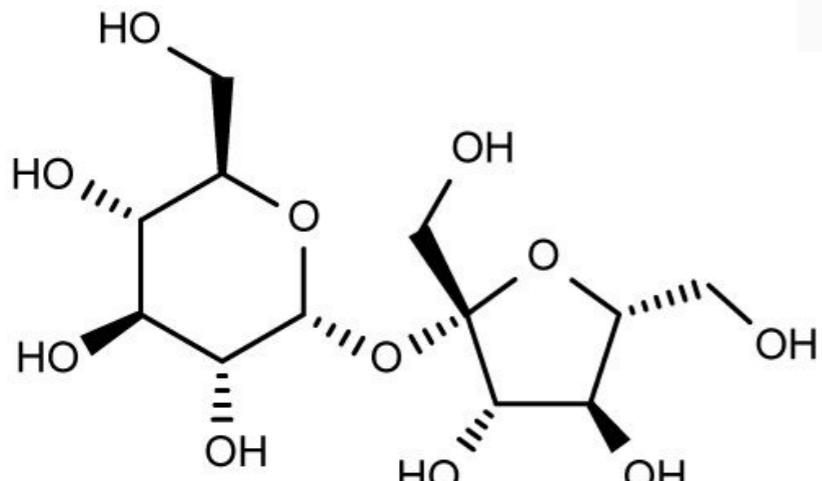


Natural language
(a kind of program?)



Evolutionary relationships

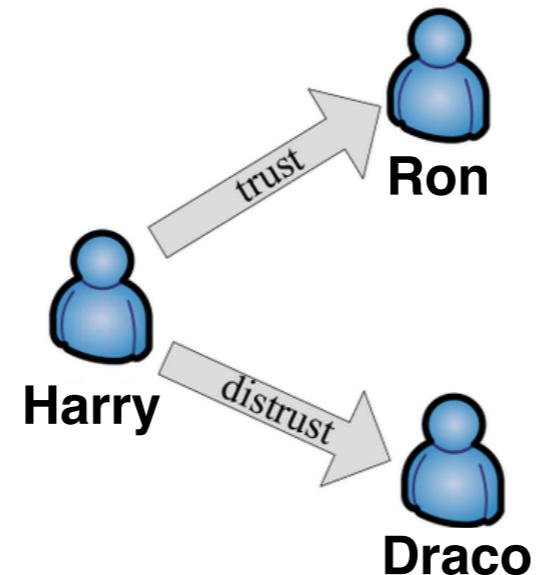
Graphs



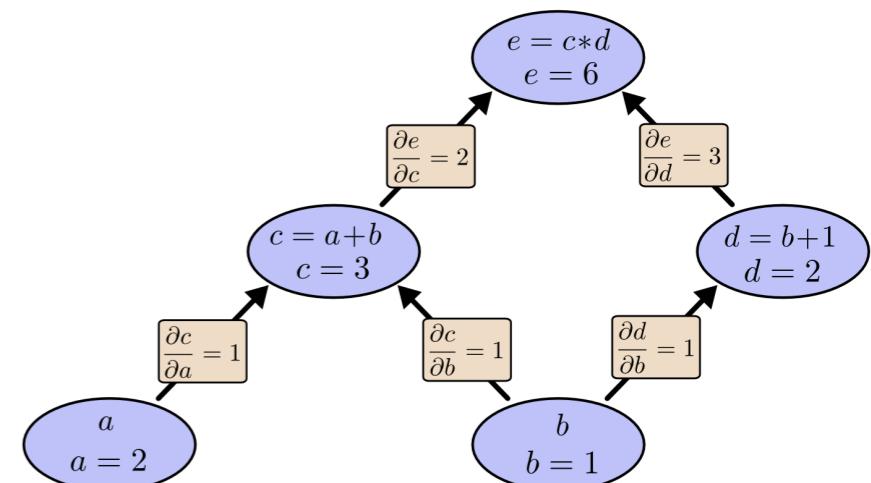
Molecules



Physical spaces



Interpersonal relationships



Computations

What is structured data?

Bipartite data that consists of **atomic elements** and **structure** that links the elements together.

The behaviour/meaning of structured object depends on both these aspects and their interaction.

Two problems in machine learning

- How do we represent structured data?
- How do we generate structure data?

To answer these questions, we will focus on **neural network models of sequences**.

What can neural sequence models do?

What can neural sequence models do?

PORUGUESE



ENGLISH

O Bairro Alto é um bairro antigo e pitoresco no centro de Lisboa, com ruas estreitas e empedradas, casas seculares, pequeno comércio tradicional, restaurantes e locais de vida nocturna.

Google Translate

What can neural sequence models do?

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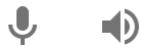
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OpenAI GPT-2 Language Model

What can neural sequence models do?

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Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.

Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.

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“When we approached them, they said, ‘If you come any closer, we’ll kill you,’” recounted one of the researchers. “We asked them what their problem was, and they said, ‘It’s a long story.’ They also said that we would never understand their problem because we’re too stupid.”

The unicorns spoke of a terrible blight that had been visited upon them by the government of Ecuador, which had decided to grant the unicorns “human rights” after receiving a \$4 million donation from the nation of Qatar.

“The money was intended to provide us with clean water, but instead they used it to pay for legal fees to protect us,” said one of the unicorns. “The next thing we knew, they were forcing us to get jobs, or else they’d seize our horns.”



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The database begins knowing nothing.
The database knows everything that is added to it.

The database does not know anything else.
When asked a question, if the answer has been added to the database the database says the answer.

When asked a question, if the answer has not been added the database says it does not know.

Q: Does the database know “What is 2+2?”

A: The database does not know.

Q: Does the database know “What is the capital of France?”

A: The database does not know.

“Tom is 20 years old” is added to the database.

Nothing else about Tom is added to the database.

Q: Does the database know where Tom lives?

A: The database does not know.

Q: How does the database respond when Tom’s age?

A: The database says “Tom is 20 years old.”

Q: How does the database response when asked “What’s my age?”

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It's a long story...

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Back to Future:	👨‍🦰👨‍🦰🚗🕒
Batman:	🦇
Transformers:	🚗🤖
	➡
Zootopia:	🦊🐾🐻🦋🐰
Wonder Woman:	👸👸👸👸👸
The Godfather:	ǪǪǪǪ
Star Trek:	🖖🚀
Planet of the Apes:	🐵猿
Game of Thrones:	👑🐺🏰
Jurassic Park:	🦕🦕🦕
Castlevania:	👻👹🕷️🔪acula
The Matrix:	🤖🧠
Iron Man:	🤖🔧sPida
Death Note:	📖🔪🔫🗡️
Frozen:	❄️👸👸🌲
The Hunger Games:	🏹🍎🍍🏆

Outline: Part I

- Recurrent neural networks
 - Application: language models
- Learning challenges and solutions
 - Vanishing gradients
 - Long short-term memories
 - Gated recurrent units
- Break

Representing Sequential Data

Recurrent Neural Networks

- In some applications, we want to **condition** on sequential data and make a prediction
 - Examples: read a review and decide whether it is positive or negative; read a blog post and predict who wrote it
- In other applications, we want to **generate** sequential data
 - Examples: machine translation, summarization, “natural language generation”, image generation, text to speech, speech to text, playing a game by making a sequence of actions ...
 - (in many of these, we need to do both!)

Example: Language Models

A language model assigns probabilities to a sequence of words $\mathbf{w} = (w_1, w_2, \dots, w_\ell)$.

It is convenient (but not necessary) to decompose this probability using the **chain rule**, as follows:

$$\begin{aligned} p(\mathbf{w}) &= p(w_1) \times p(w_2 \mid w_1) \times p(w_3 \mid w_1, w_2) \times \cdots \times \\ &\quad p(w_\ell \mid w_1, \dots, w_{\ell-1}) \\ &= \prod_{t=1}^{\ell} p(w_t \mid w_1, \dots, w_{t-1}) \end{aligned}$$

The chain rule reduces the language modeling problem to **modeling the probability of the next word**, given the *history* of preceding words.

Example: Language Models

The chain rule reduces the language modeling problem to **modeling the probability of the next word**, given the *history* of preceding words.

Thus,

- (i) For **conditioning problems**, we need to **represent a sequence**.
- (ii) For **generation problems**, we need to **represent a sequence** — the *history* at each time step.

Example: Language Models

The chain rule reduces the language modeling problem to **modeling the probability of the next word**, given the *history* of preceding words.

Thus,

How do we represent an arbitrarily long sequence?

- (i) For **completely observed sequences** we can store the history at each time step.
- (ii) For **generative sequences** we can store the history at each time step.

Example: Language Models

The chain rule reduces the language modeling problem to **modeling the probability of the next word**, given the *history* of preceding words.

Thus,

- (i) For **consecutive sequences**

How do we represent an arbitrarily long sequence?

- (ii) For **general sequences**

We will train a neural network to build a representation of sequences of unbounded length.

the history at each time step.

Feature Induction

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x} + \mathbf{b}$$

$$\mathcal{F} = \frac{1}{M} \sum_{i=1}^M \|\hat{\mathbf{y}}_i - \mathbf{y}_i\|_2^2$$

In linear regression, the goal is to learn \mathbf{W} and \mathbf{b} such that \mathcal{F} is minimized for a dataset D consisting of M training instances. An engineer must select/design \mathbf{x} *carefully*.

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$$\mathbf{h} = g(\mathbf{V}\mathbf{x} + \mathbf{c})$$

“nonlinear regression”

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h} + \mathbf{b}$$

Use “naive features” \mathbf{x} and *learn* their transformations (conjunctions, nonlinear transformation, etc.) into \mathbf{h} .

Feature Induction

$$\mathbf{h} = g(\mathbf{Vx} + \mathbf{c})$$

$$\hat{\mathbf{y}} = \mathbf{Wh} + \mathbf{b}$$

- What functions can this parametric form compute?
 - If \mathbf{h} is big enough (i.e., enough dimensions), it can represent any vector-valued function to any degree of precision
- This is a much more powerful regression model!

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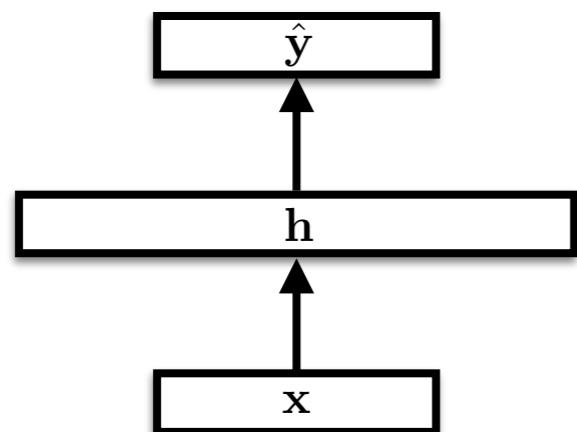
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 - If \mathbf{h} is big enough (i.e., enough dimensions), it can represent any vector-valued function to any degree of precision
- This is a much more powerful regression model!
- You can think of \mathbf{h} as “induced features” in a linear classifier
- The network did the job of a feature engineer

Recurrent Neural Networks

Feed-forward NN

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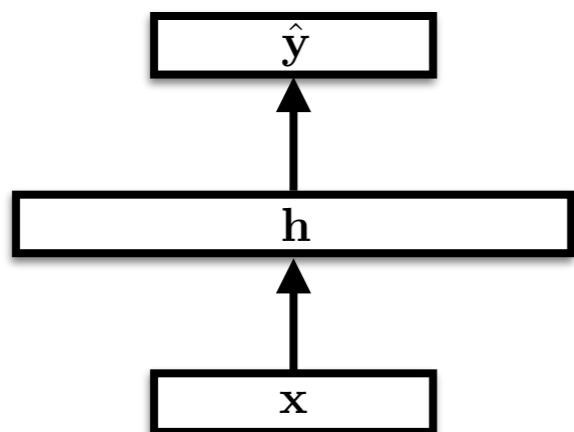


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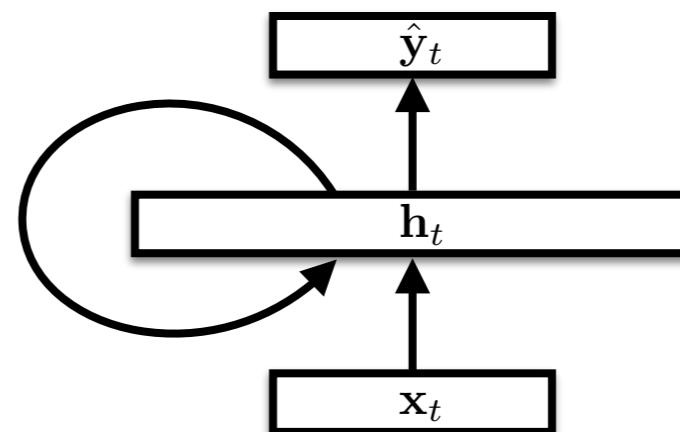
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Recurrent NN

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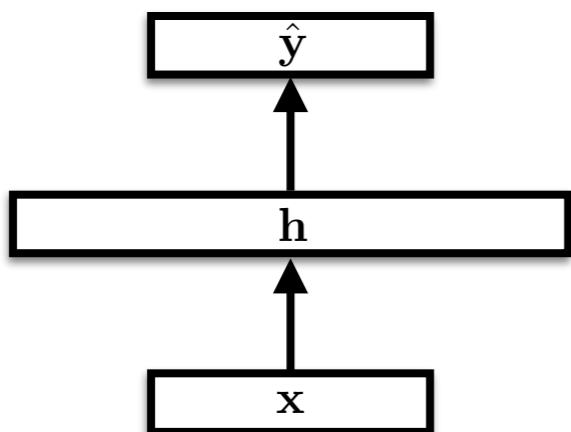


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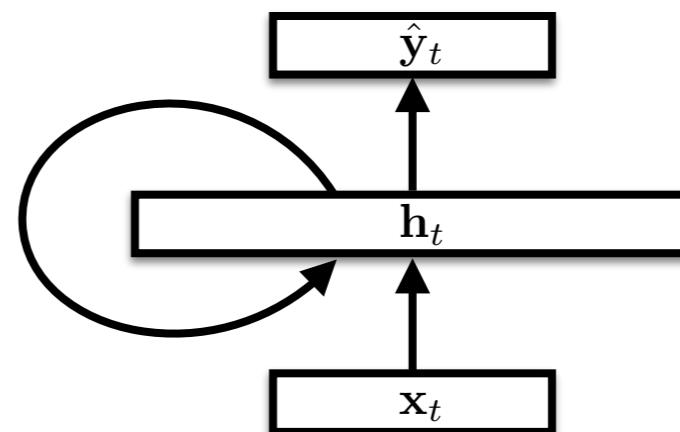


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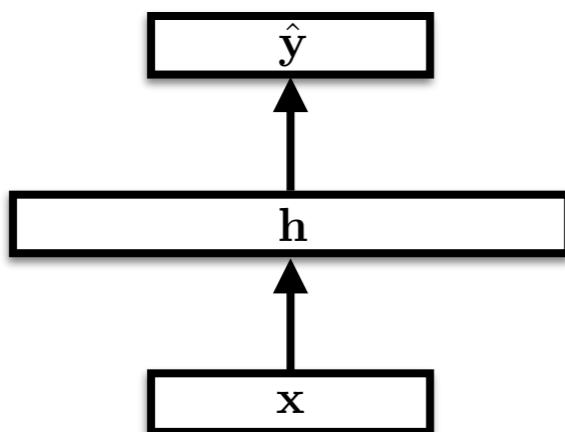


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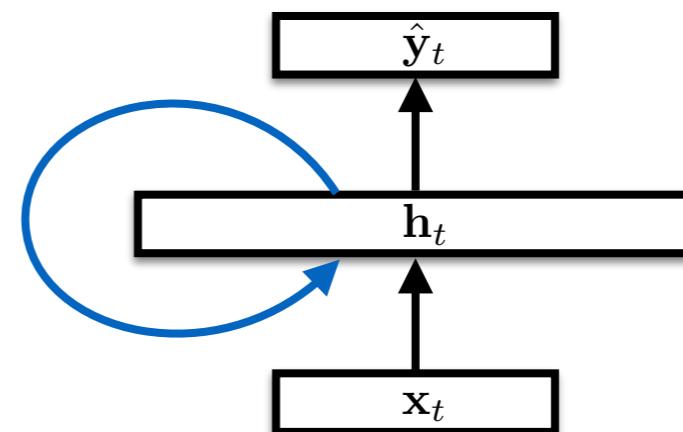


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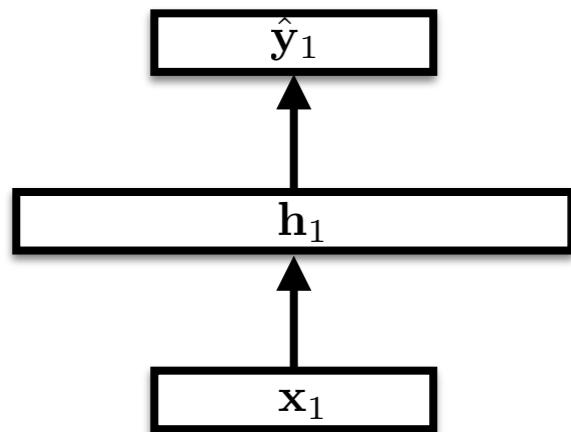
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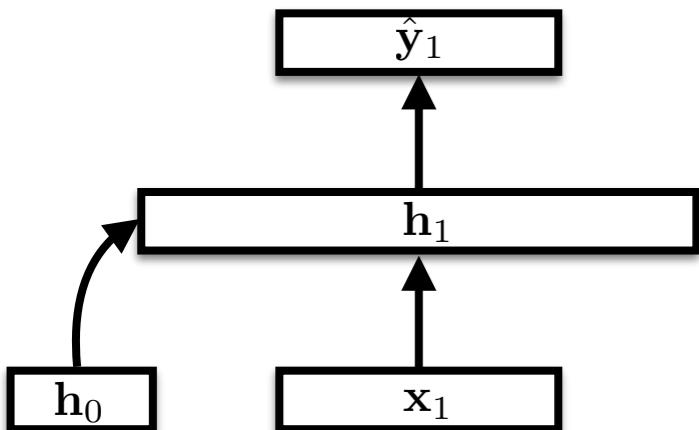
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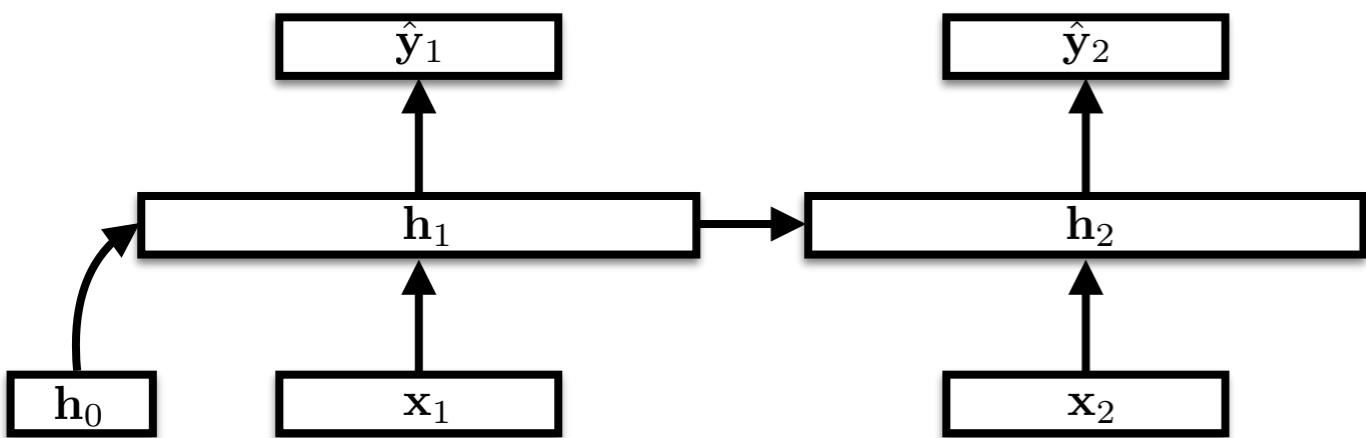
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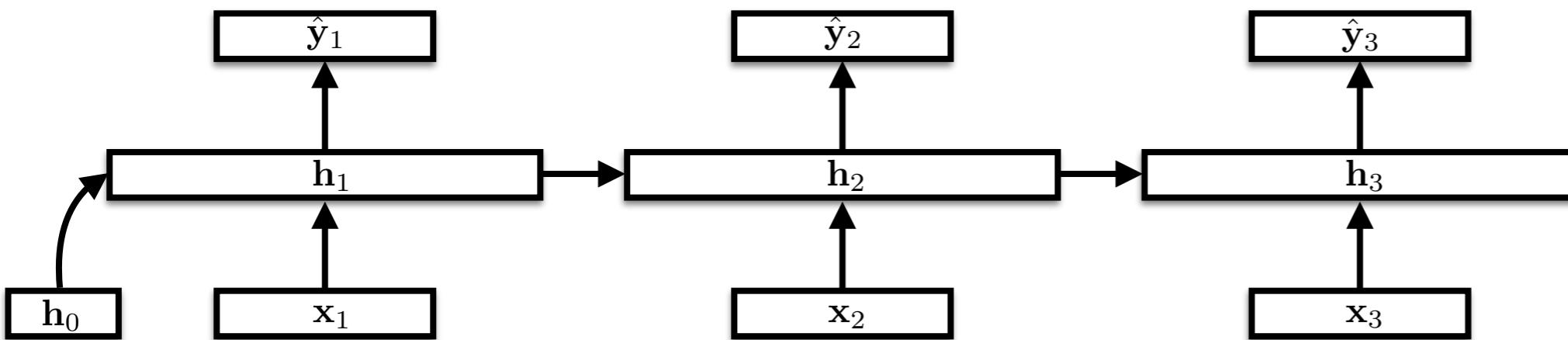
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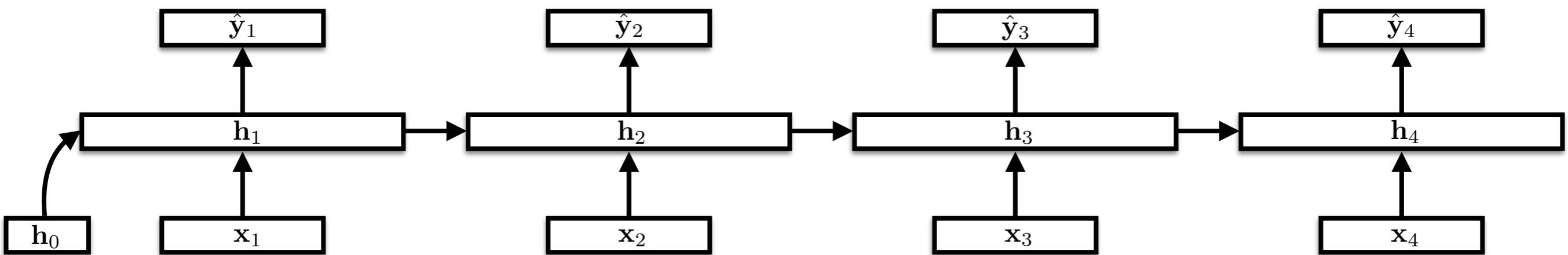
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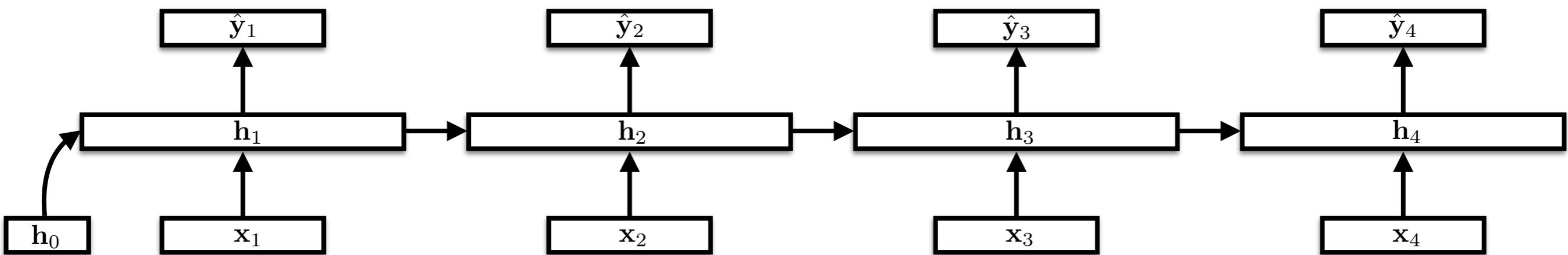


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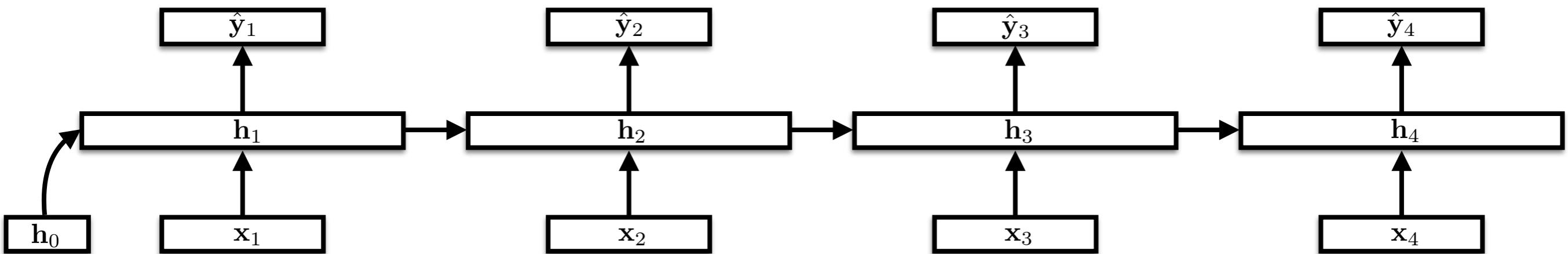
How do we train the RNN's parameters?



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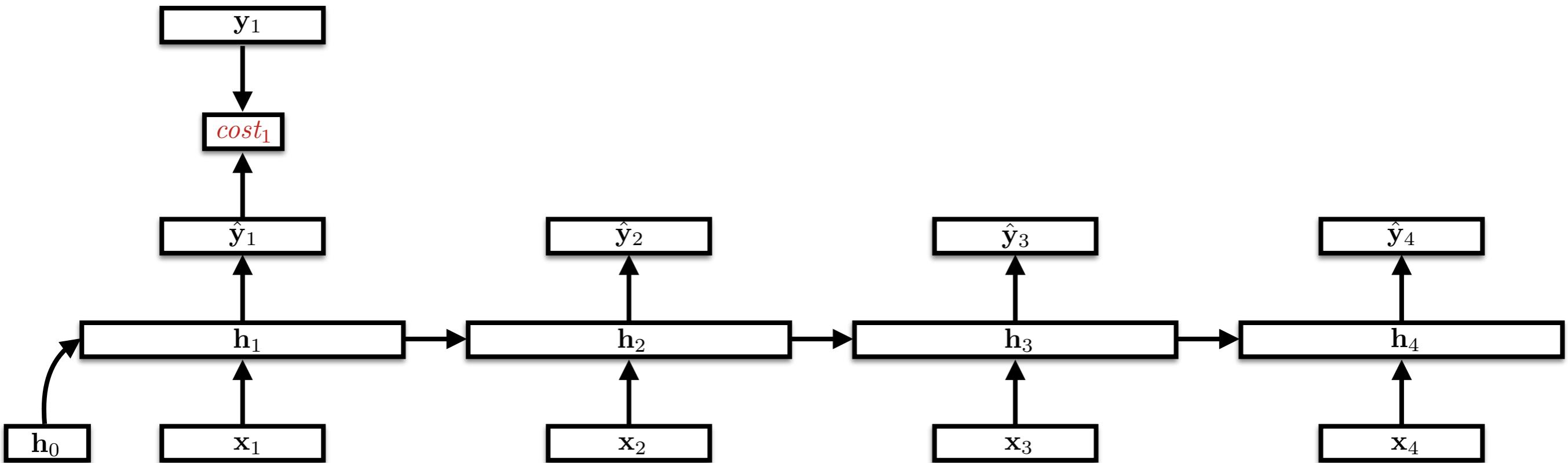
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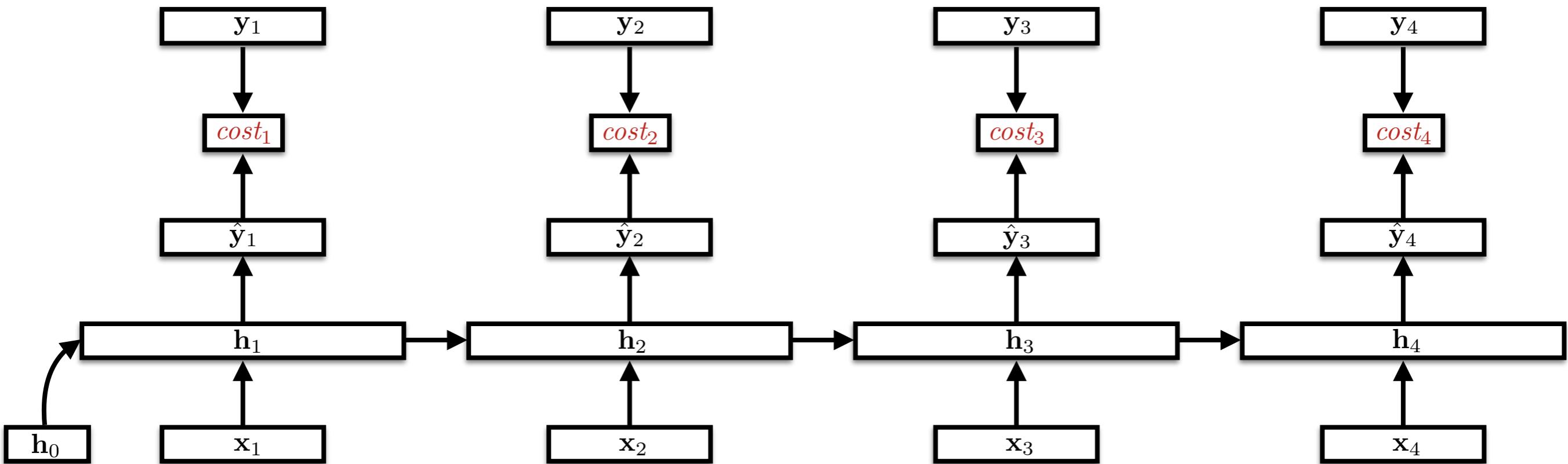
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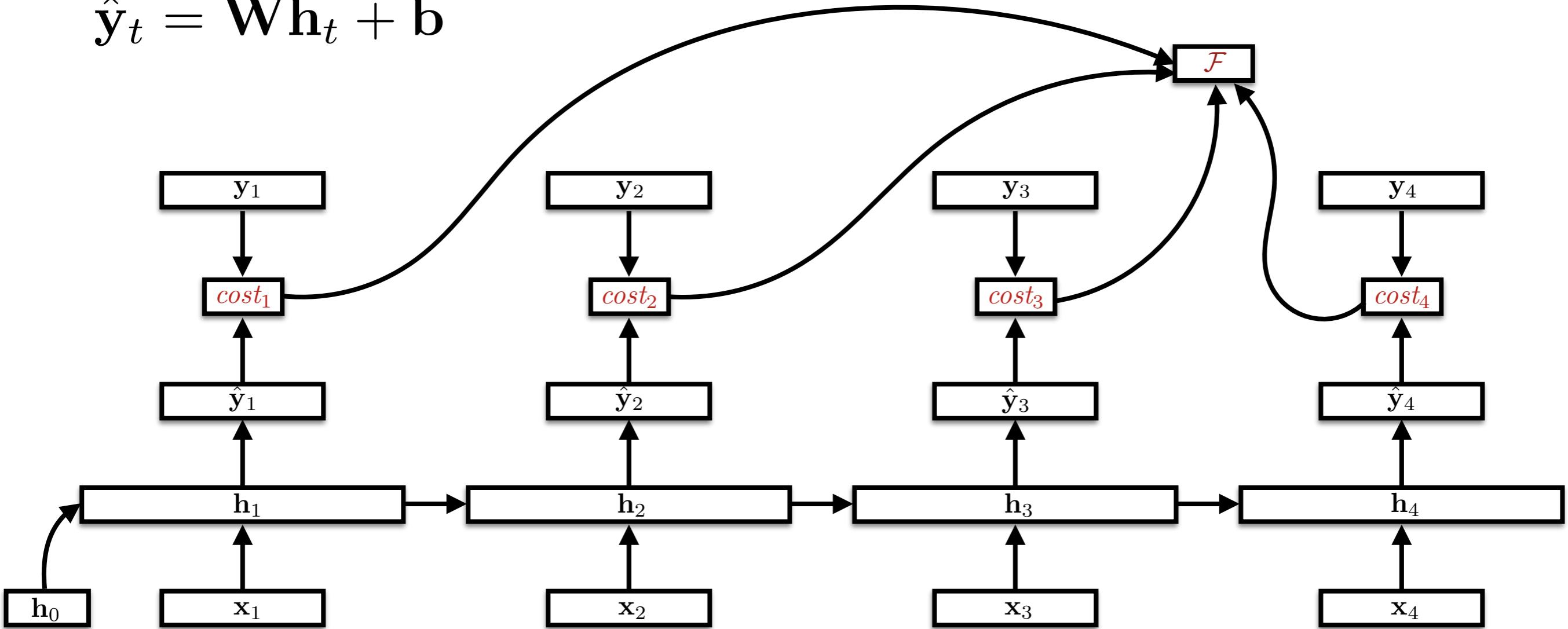
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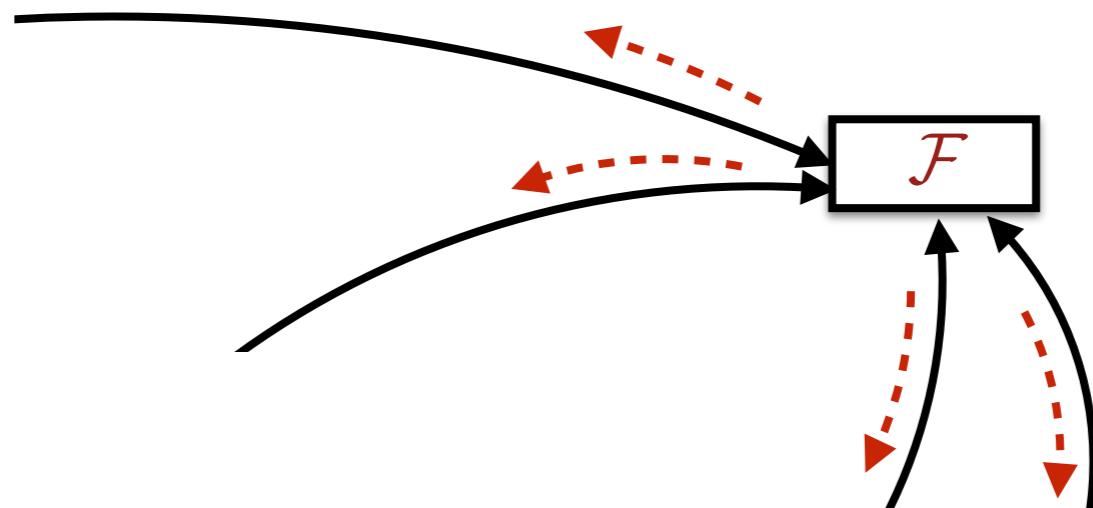
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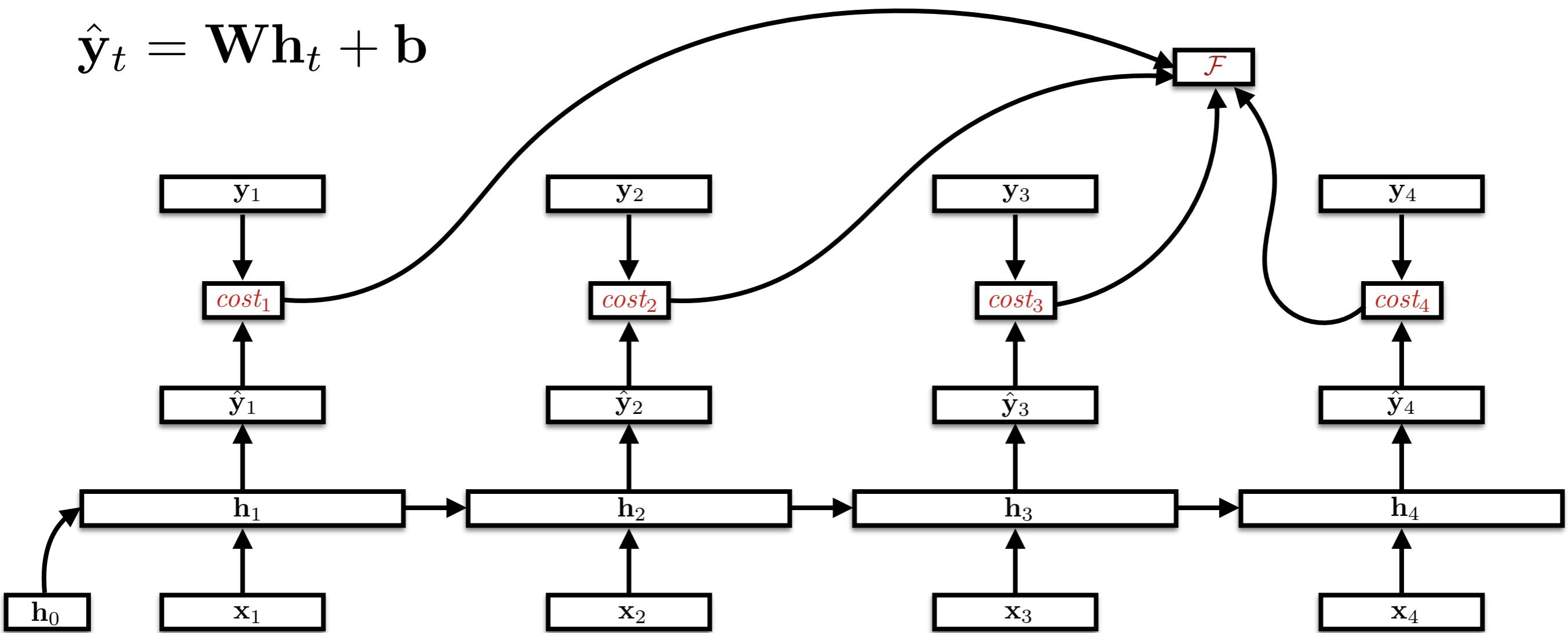


- The unrolled graph is a well-formed (DAG) computation graph—we can run backprop
 - Parameters are tied across time, derivatives are aggregated across all time steps
 - This is historically called “backpropagation through time” (BPTT)

Parameter Tying

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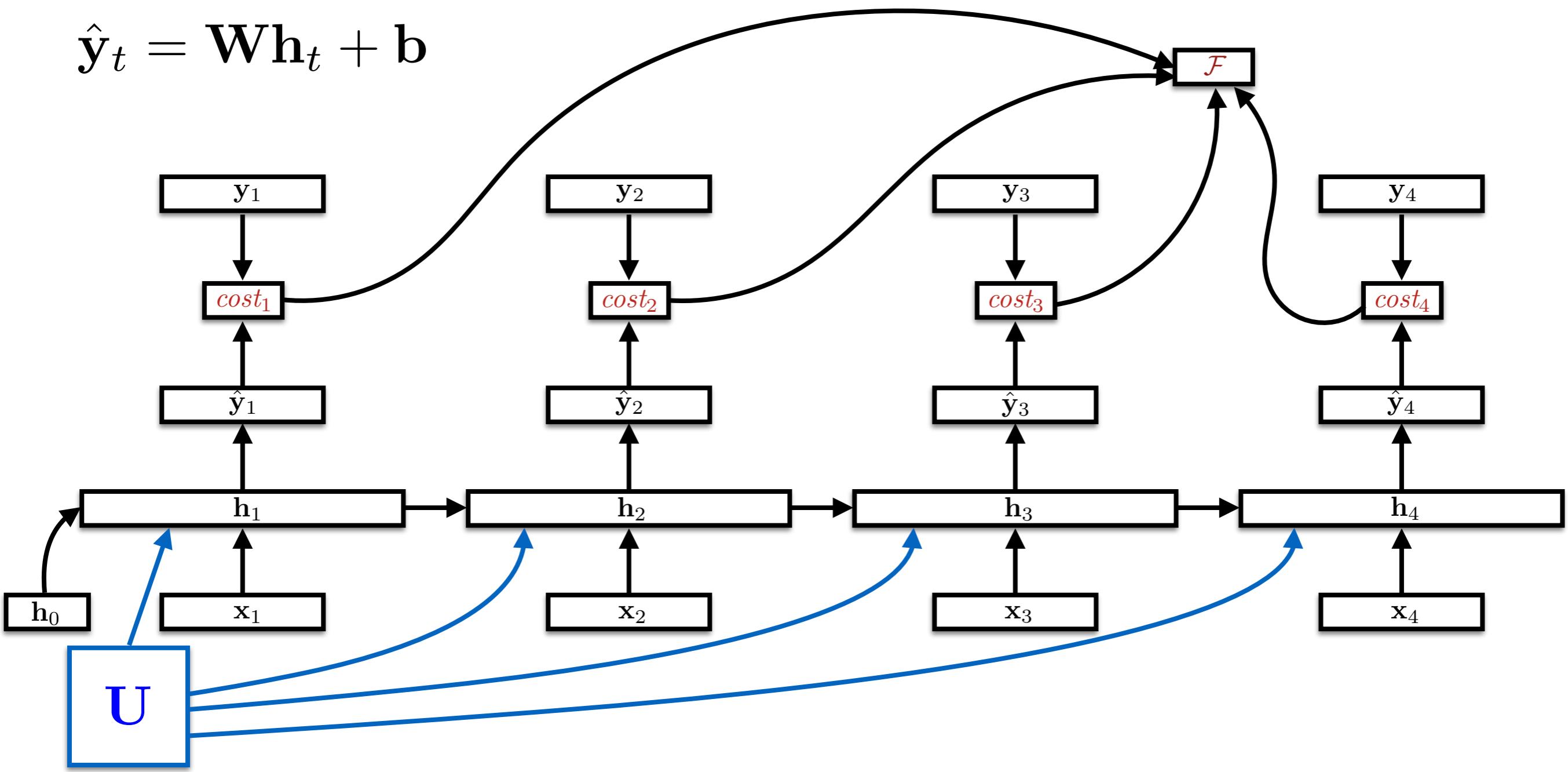
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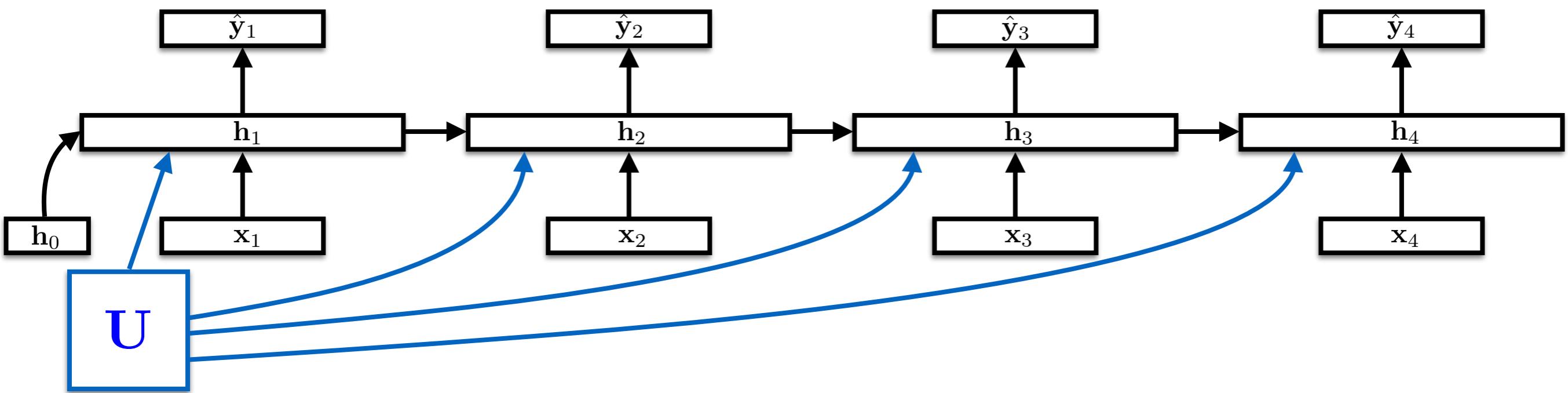
Parameter Tying

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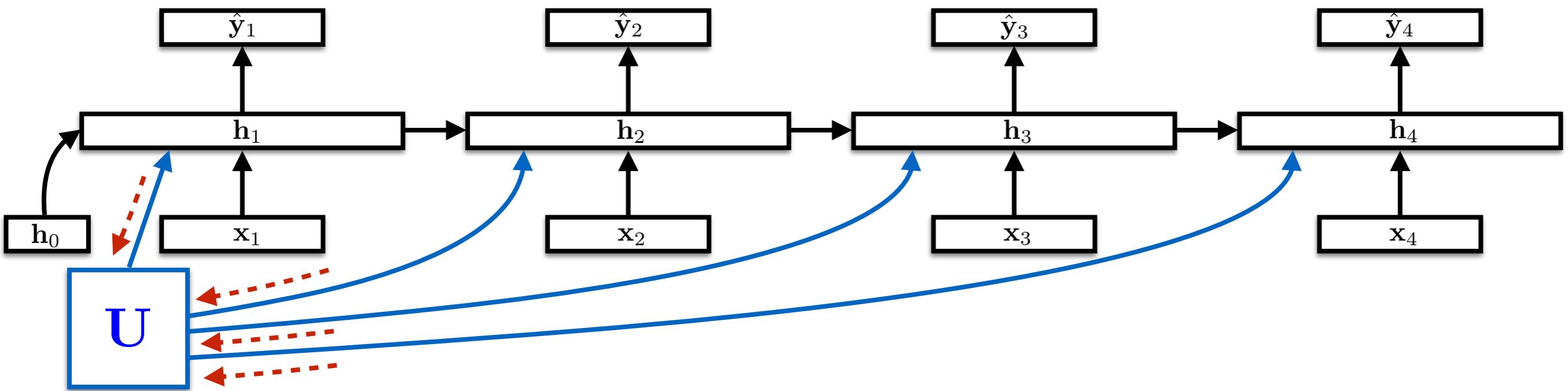
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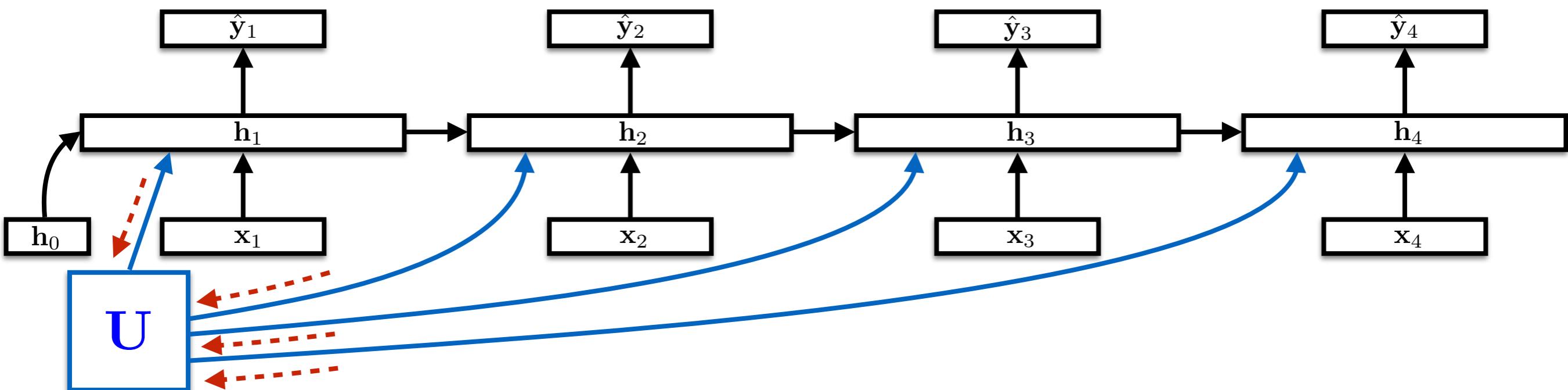


Parameter Tying



$$\frac{\partial \mathcal{F}}{\partial \mathbf{U}} = \sum_{t=1}^4 \frac{\partial \mathbf{h}_t}{\partial \mathbf{U}} \frac{\partial \mathcal{F}}{\partial \mathbf{h}_t}$$

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Parameter tying also came up when learning the transition matrix for HMMs!

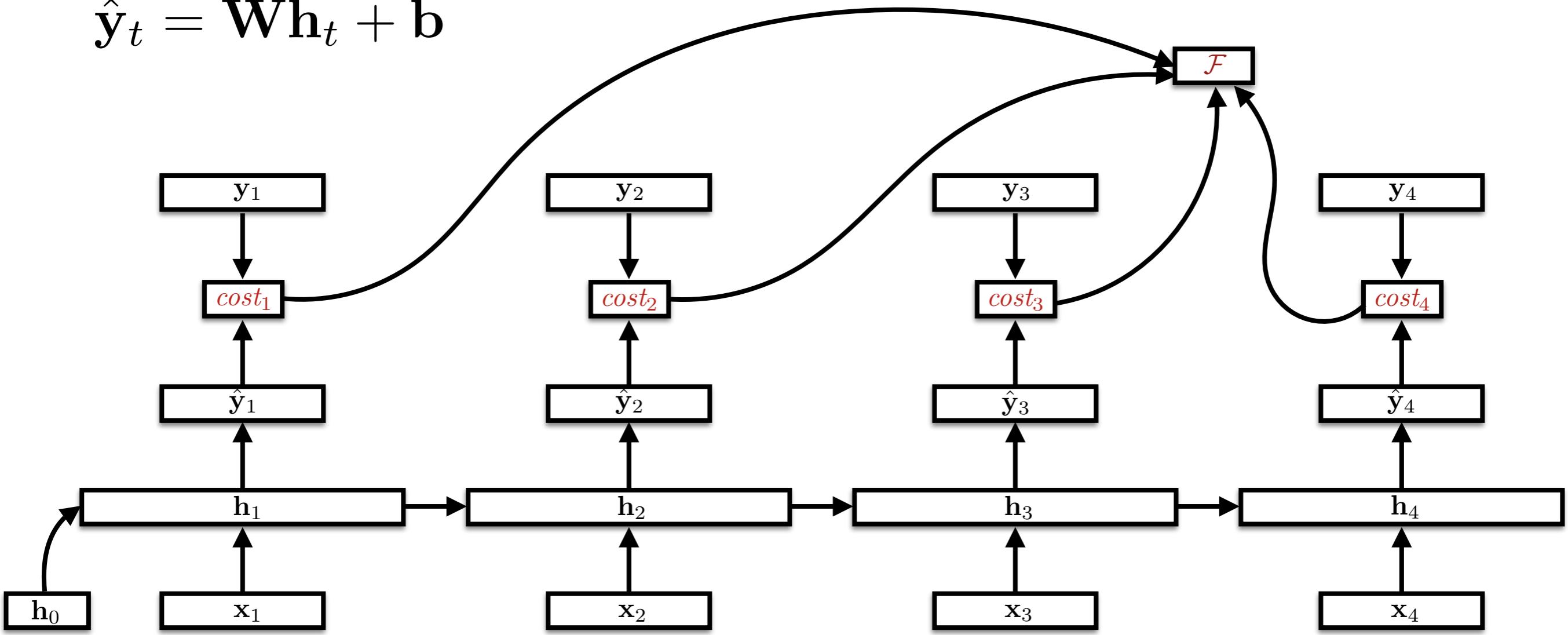
Parameter Tying

- Why do we want to tie parameters?
 - Reduce the number of parameters to be learned
 - Deal with arbitrarily long sequences
- What if we always have short sequences?
 - Maybe you might untie parameters, then. But you wouldn't have an RNN anymore!

What else can we do?

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

$$\hat{\mathbf{y}}_t = \mathbf{W}\mathbf{h}_t + \mathbf{b}$$

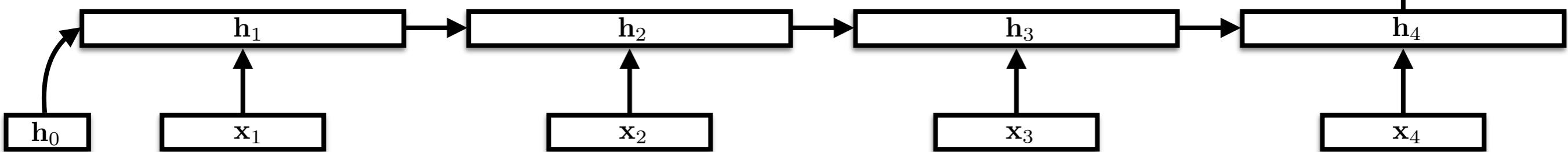


“Read and summarize”

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h}_{|\mathbf{x}|} + \mathbf{b}$$

Summarize a sequence into a single vector.
(This will be useful later...)

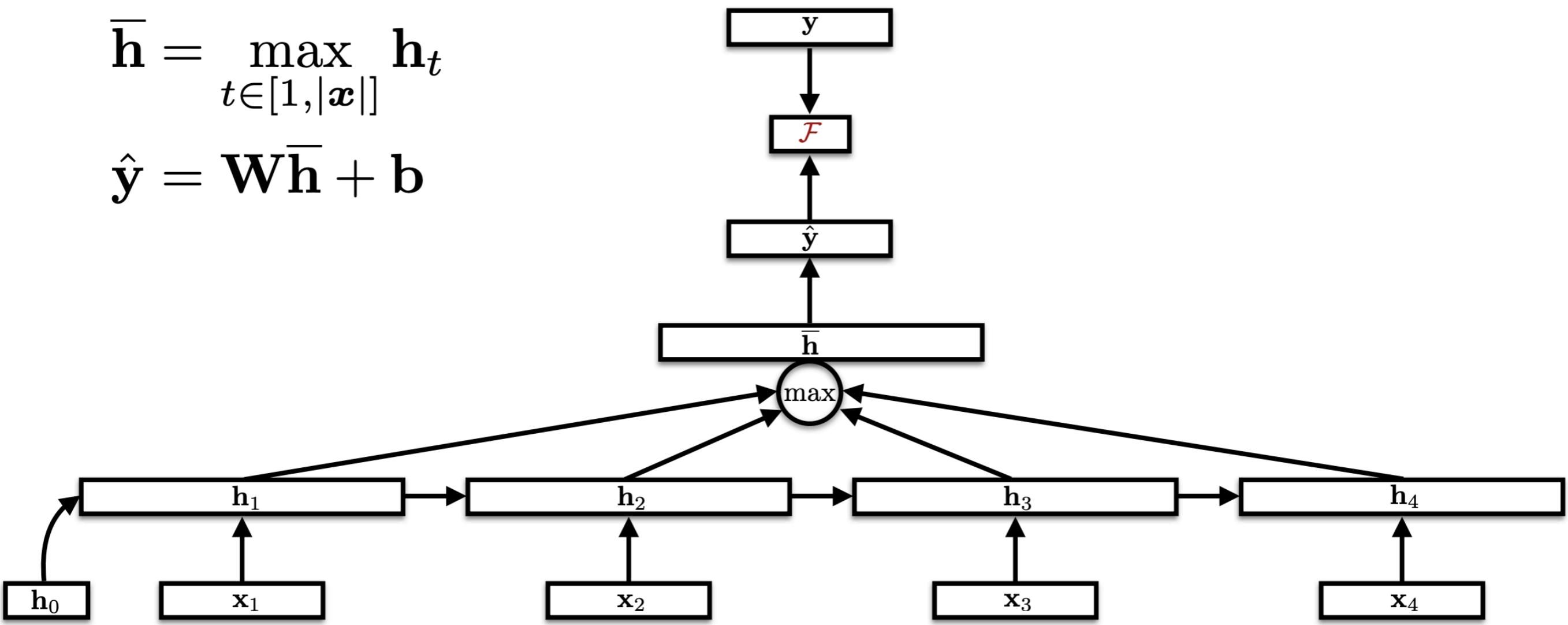


“Read and summarize”

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

$$\bar{\mathbf{h}} = \max_{t \in [1, |\mathbf{x}|]} \mathbf{h}_t$$

$$\hat{\mathbf{y}} = \mathbf{W}\bar{\mathbf{h}} + \mathbf{b}$$



View 2: Recursive Definition

- Recall how to construct a list recursively:
base case
[] is a list (the empty list)

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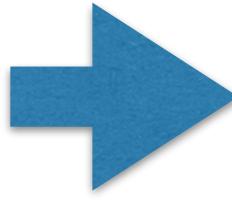
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- Recall how to construct a list recursively:
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induction

[**t** | **h**] where **t** is a list and **h** is an atom is a list

- RNNs define functions that compute representations recursively according to this definition of a list.
 - Define (learn) a representation of the base case
 - Learn a representation of the inductive step



Any structured object that you can construct recursively, you can obtain an “embedding” of with neural networks using this general strategy

History-based LMs

As Noah told us, a common strategy in sequence modeling is to make a **Markov assumption**.

$$\begin{aligned} p(\mathbf{w}) = & p(w_1) \times \\ & p(w_2 \mid w_1) \times \\ & p(w_3 \mid w_1, w_2) \times \\ & p(w_4 \mid w_1, w_2, w_3) \times \\ & \dots \end{aligned}$$



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Markov: forget the “distant” past.
Is this valid for language? No...
Is it practical? Often!



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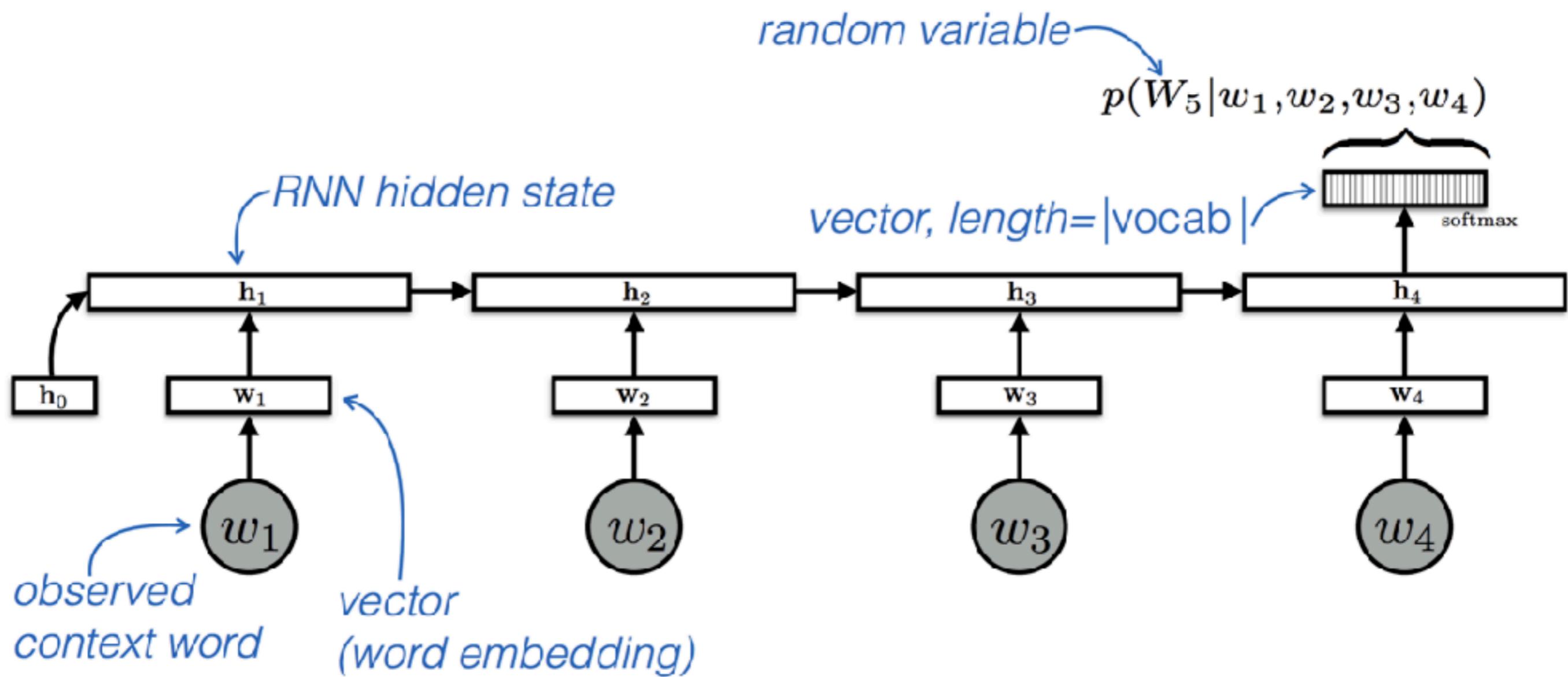
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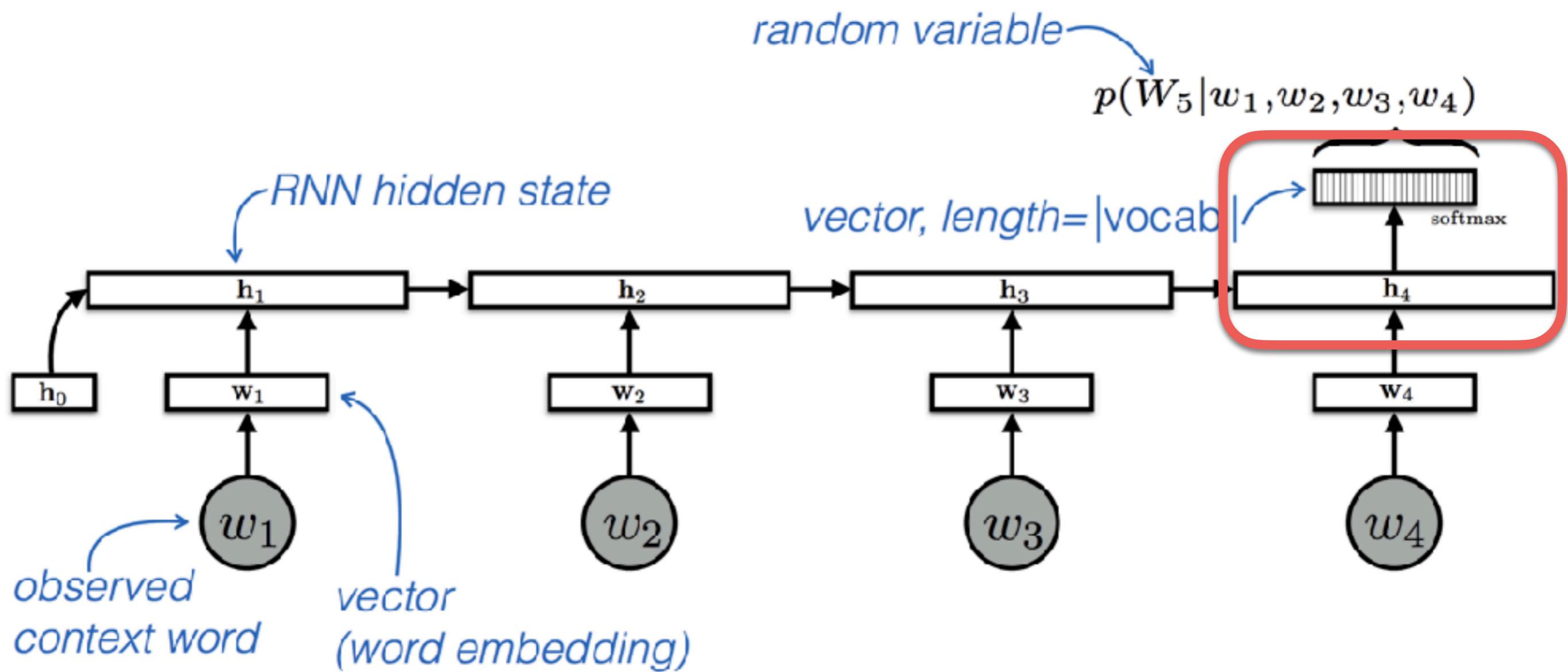
Why RNNs are great for language:
no more Markov assumptions.



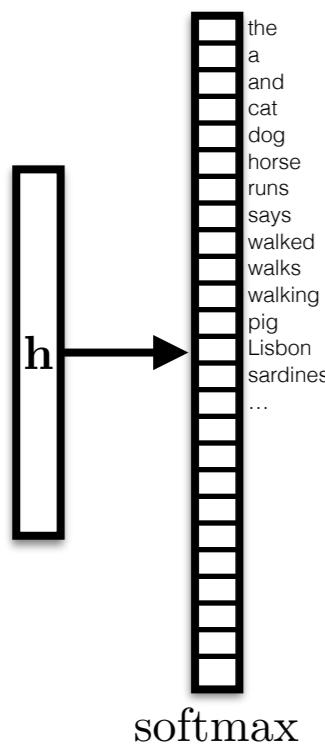
History-based LMs with RNNs



History-based LMs with RNNs



Example: Language Model



$$\mathbf{u} = \mathbf{W}\mathbf{h} + \mathbf{b}$$

$$p_i = \frac{\exp u_i}{\sum_j \exp u_j}$$

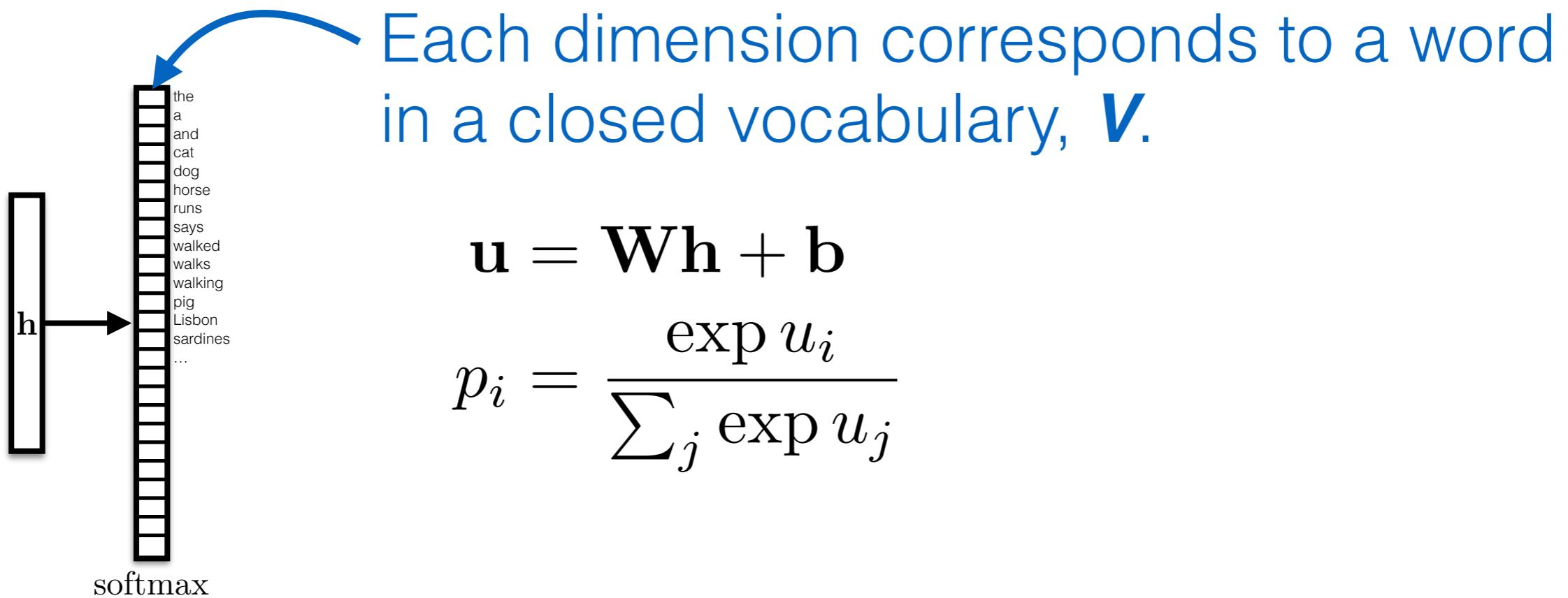
The p 's form a distribution, i.e.
 $p_i > 0 \quad \forall i, \quad \sum p_i = 1$

To enforce this stochastic constraint, we suggest a *normalised exponential output non-linearity*,

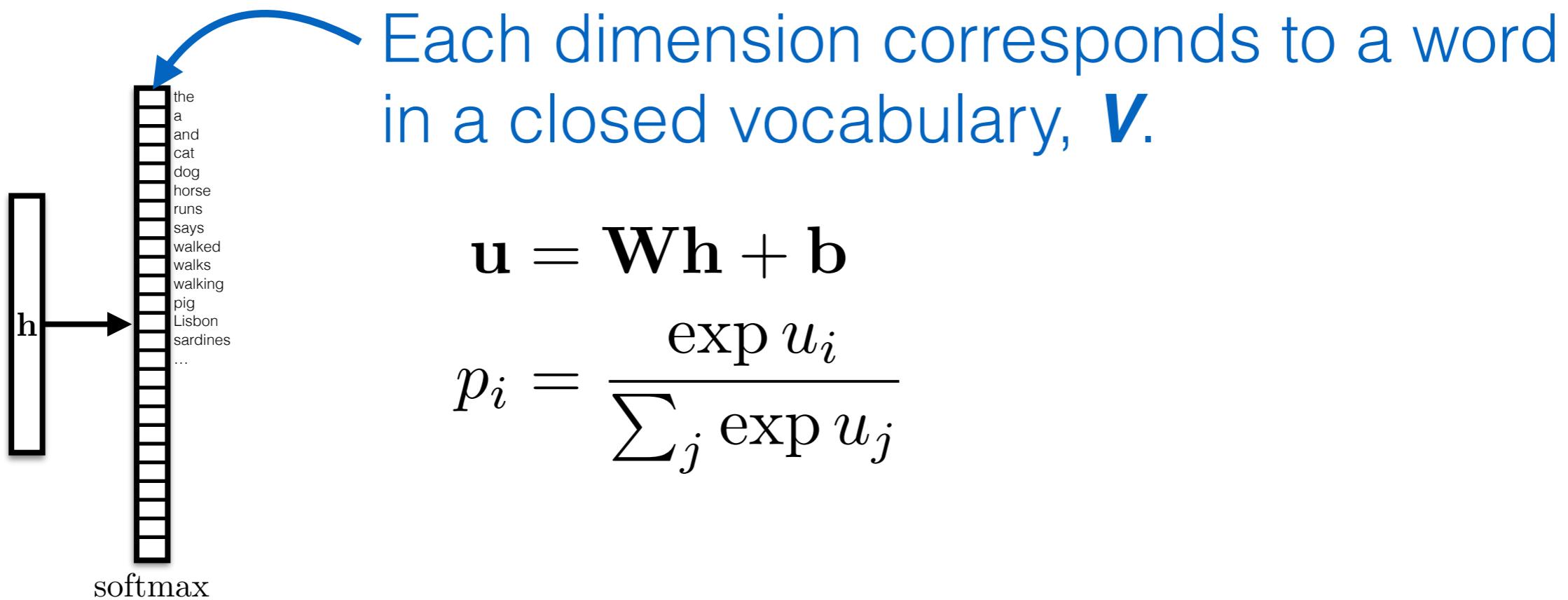
$$o_j = e^{I_j} / \sum_k e^{I_k}.$$

This “softmax” function is a generalisation of the logistic to multiple inputs. It also generalises maximum picking, or “Winner-Take-All”, in the sense that that the outputs change smoothly, and equal inputs produce equal outputs. Although it looks rather cumbersome, and perhaps not really in the spirit of neural networks, those familiar with Markov random fields or statistical mechanics will know that it has convenient mathematical properties. Circuit designers will enjoy the simple transistor circuit which implements it.

Example: Language Model

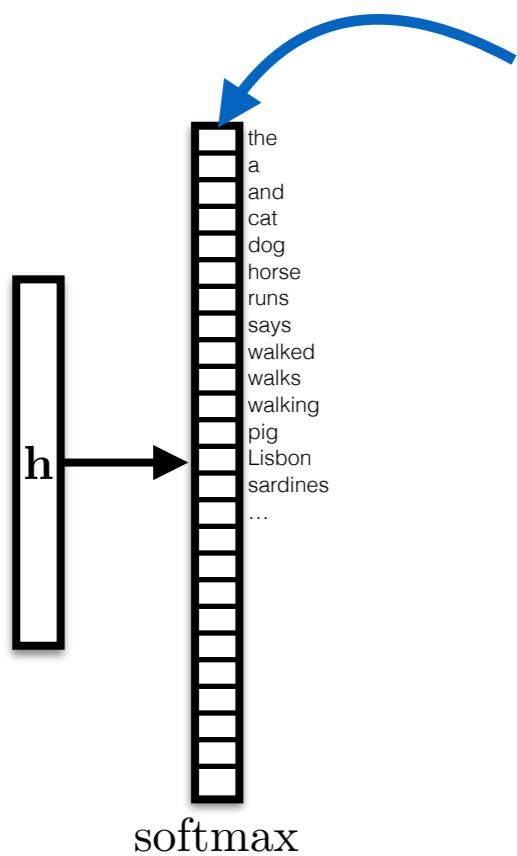


Example: Language Model



$$\begin{aligned} p(e) &= p(e_1) \times \\ &p(e_2 | e_1) \times \\ &p(e_3 | e_1, e_2) \times \\ &p(e_4 | e_1, e_2, e_3) \times \\ &\dots \end{aligned}$$

Example: Language Model



Each dimension corresponds to a word in a closed vocabulary, V .

$$\mathbf{u} = \mathbf{W}\mathbf{h} + \mathbf{b}$$

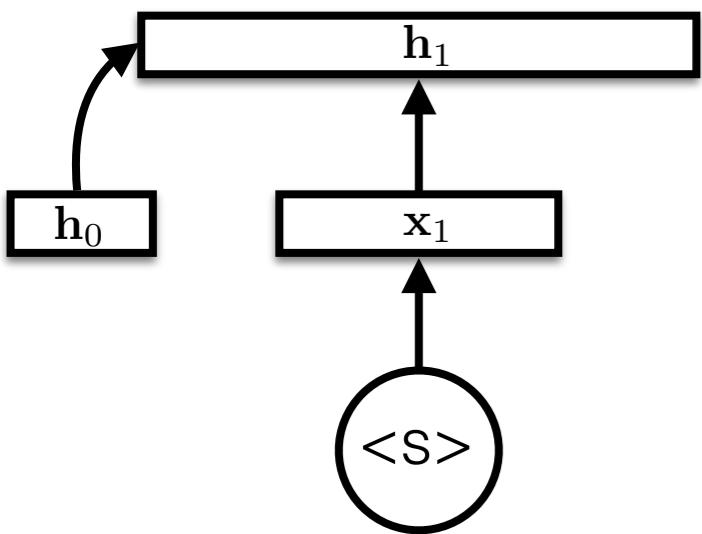
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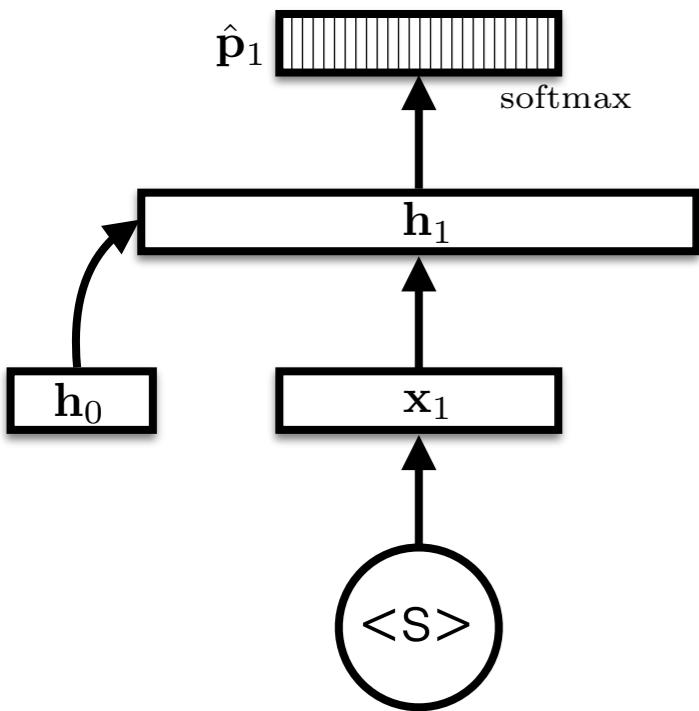
histories are sequences of words...

Example: Language Model

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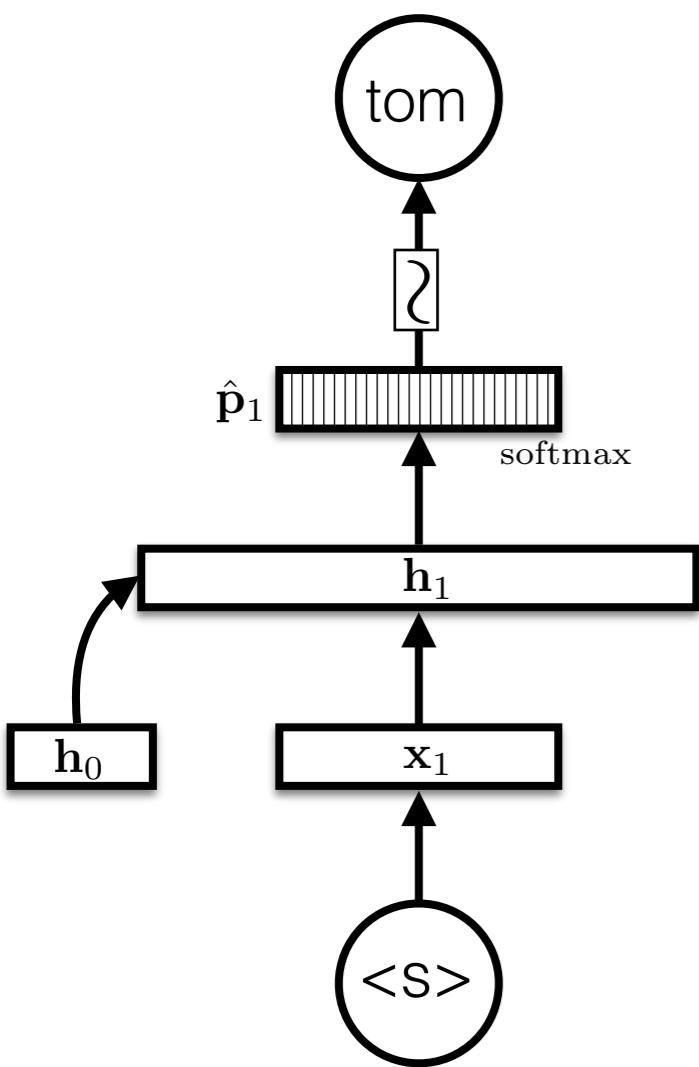


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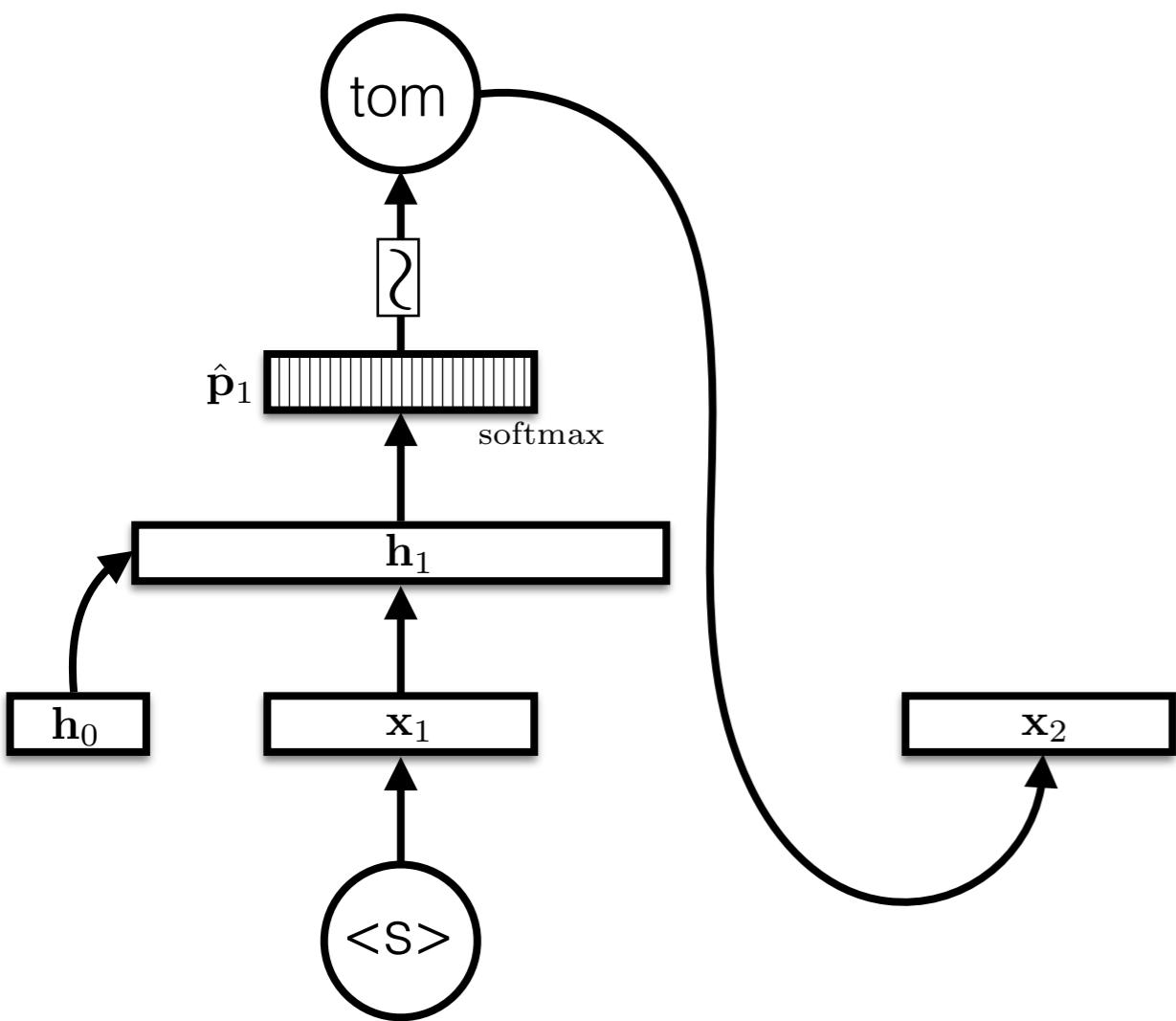
Example: Language Model

$$p(\text{tom} \mid \langle \mathbf{s} \rangle)$$



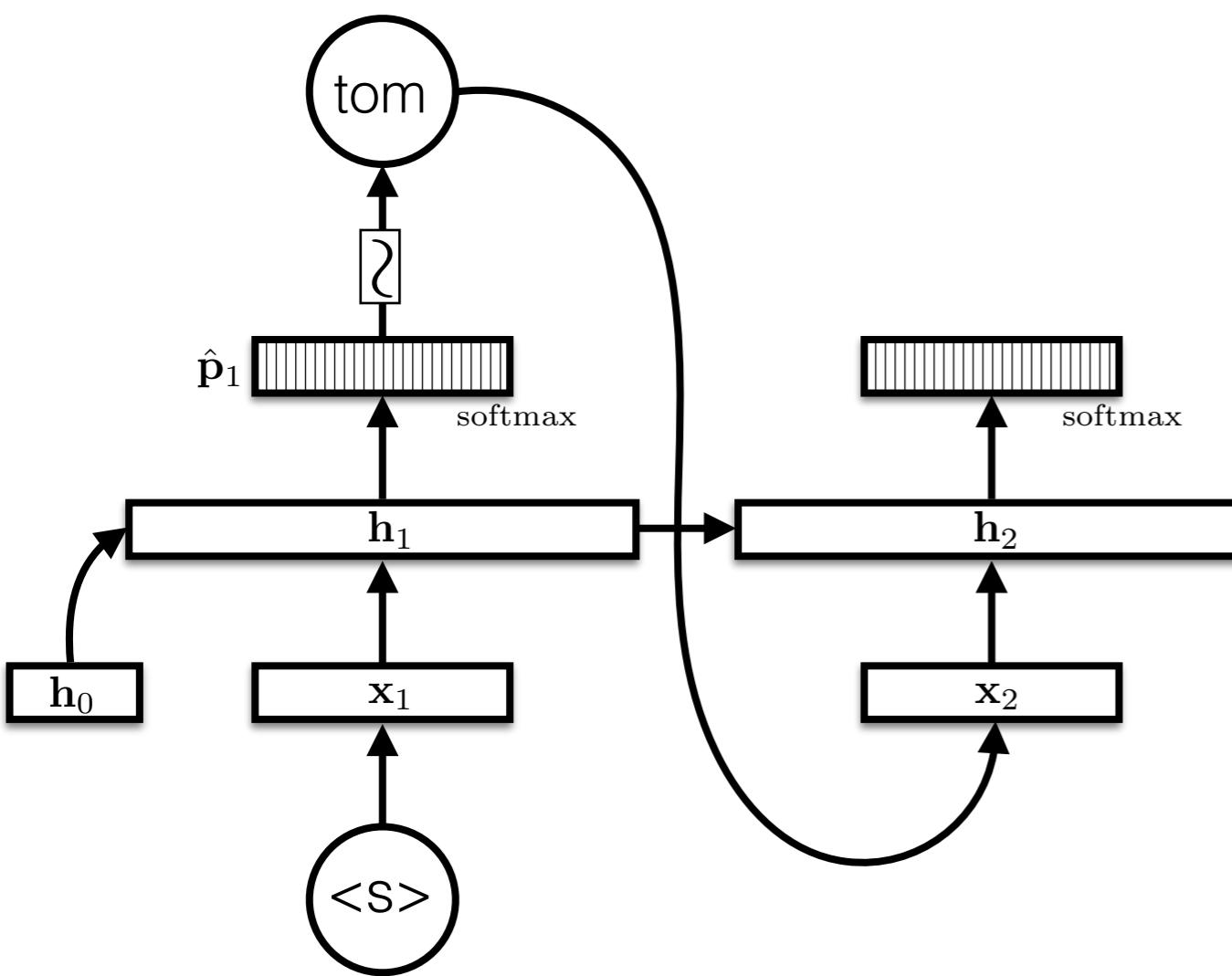
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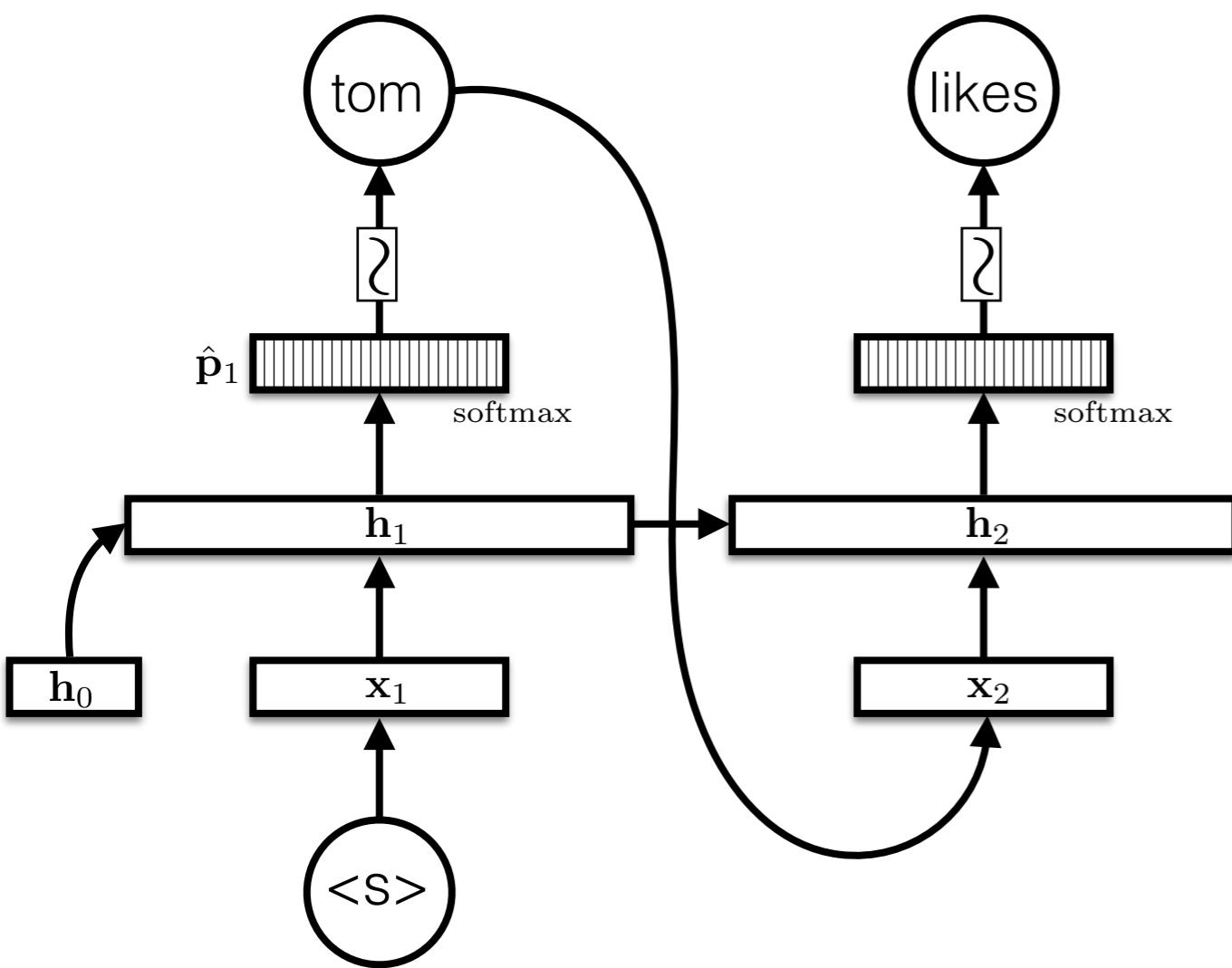
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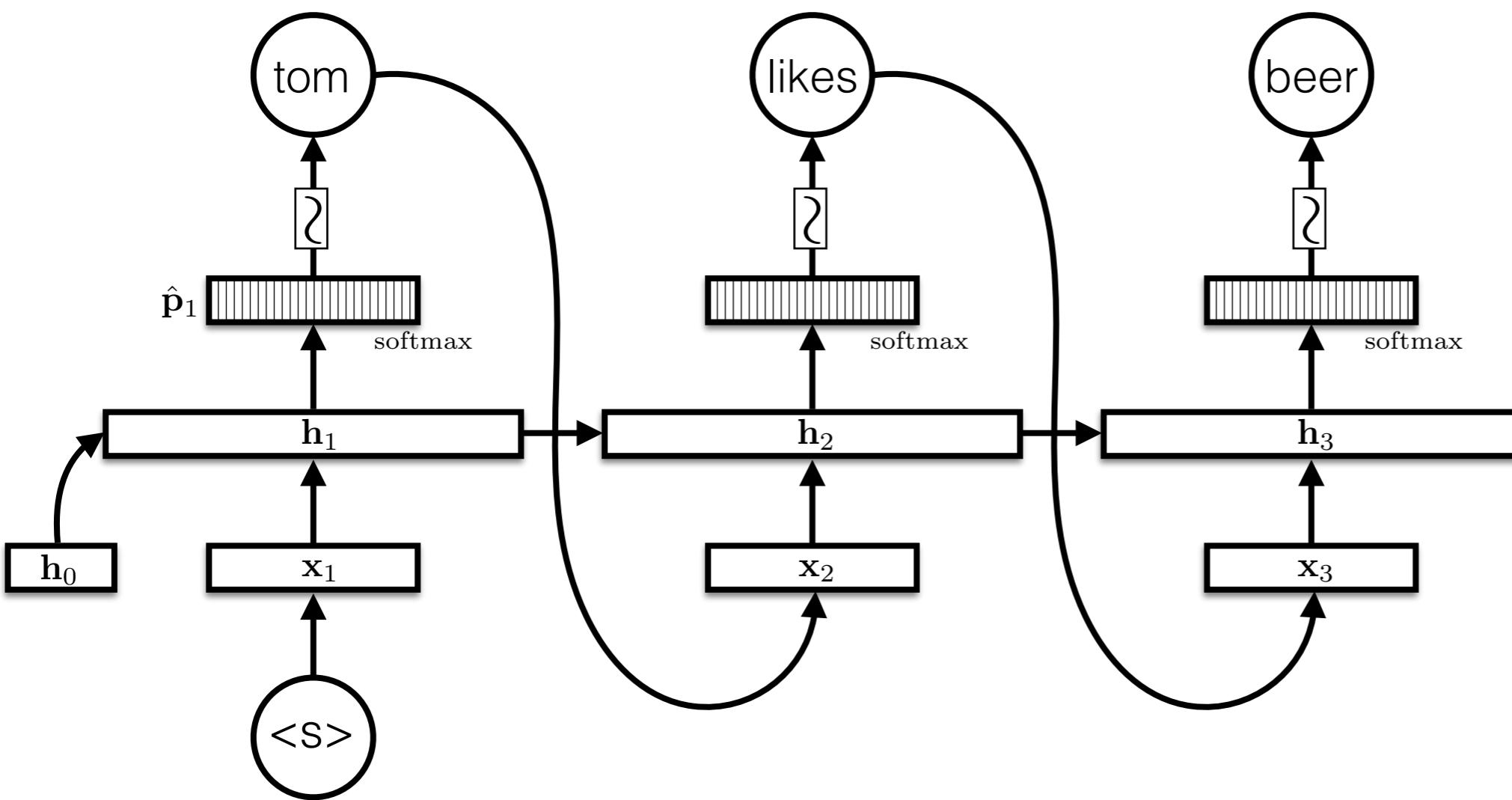
Example: Language Model

$$p(\text{tom} \mid \langle \mathbf{s} \rangle) \times p(\text{likes} \mid \langle \mathbf{s} \rangle, \text{tom})$$



Example: Language Model

$$p(\text{tom} | \langle s \rangle) \times p(\text{likes} | \langle s \rangle, \text{tom}) \\ \times p(\text{beer} | \langle s \rangle, \text{tom}, \text{likes})$$

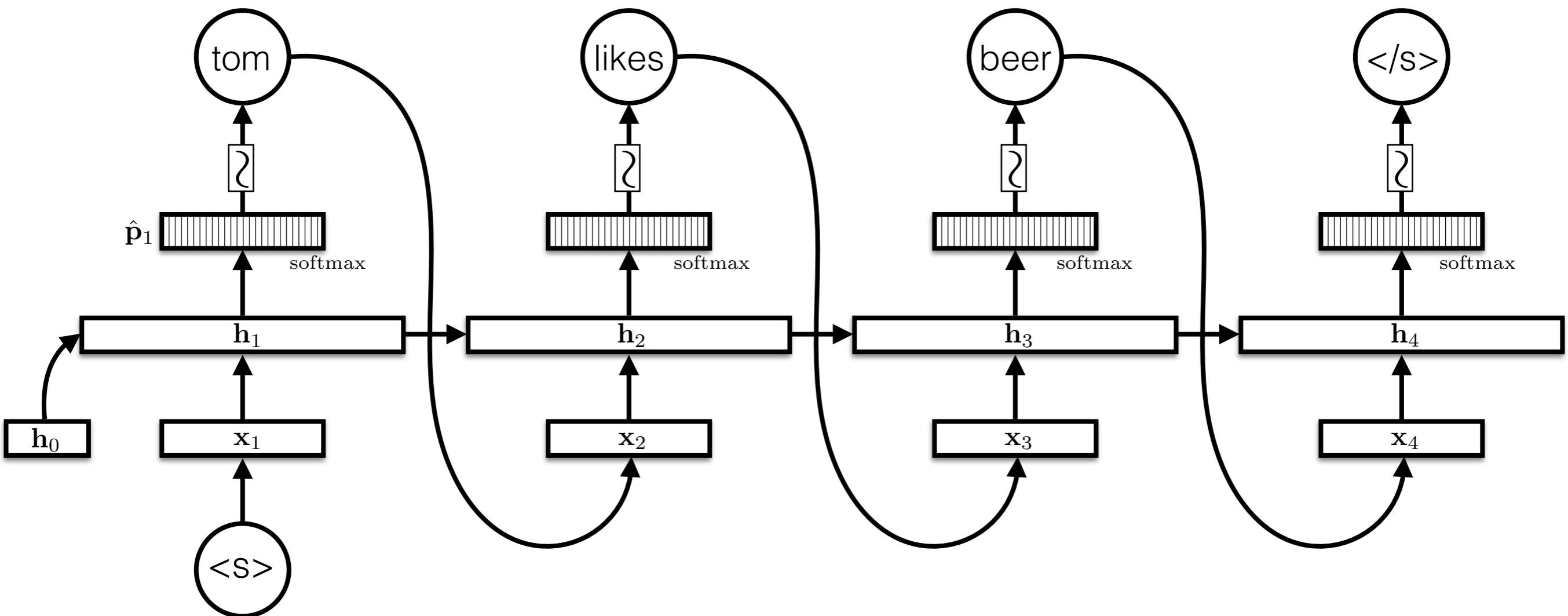


Example: Language Model

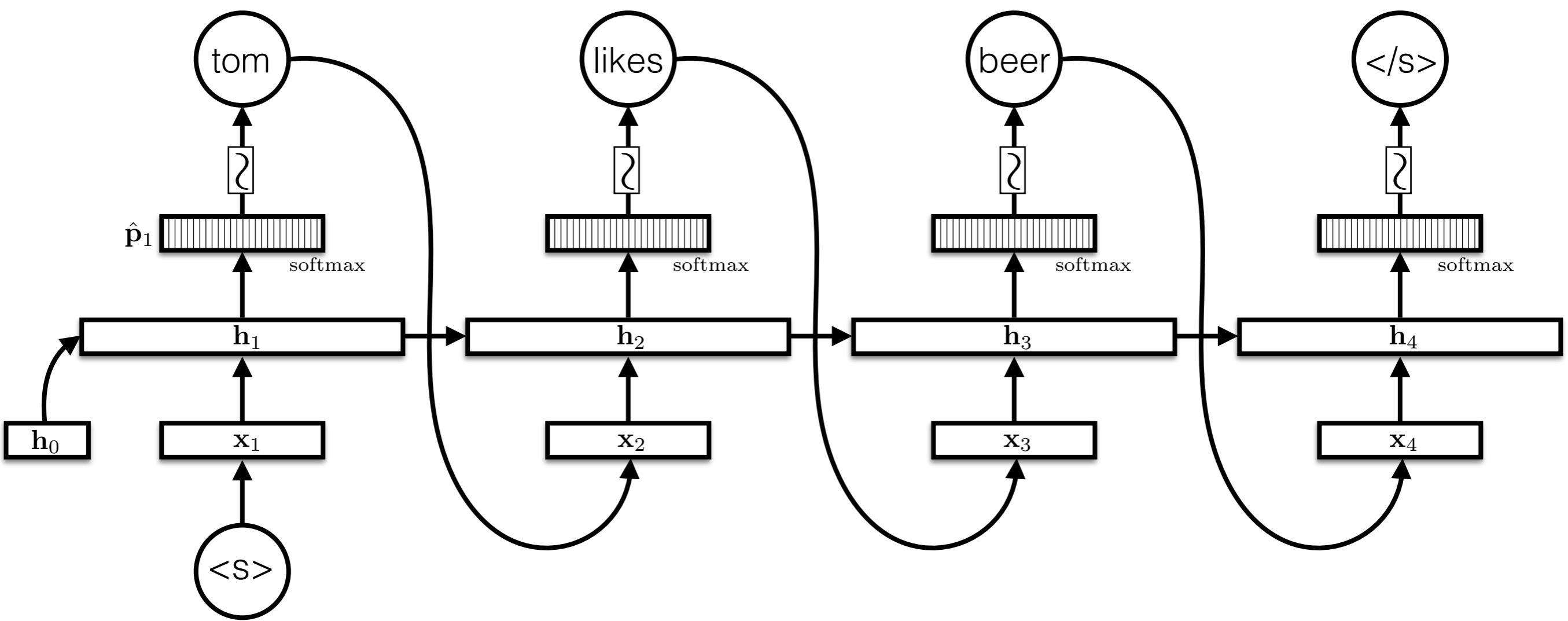
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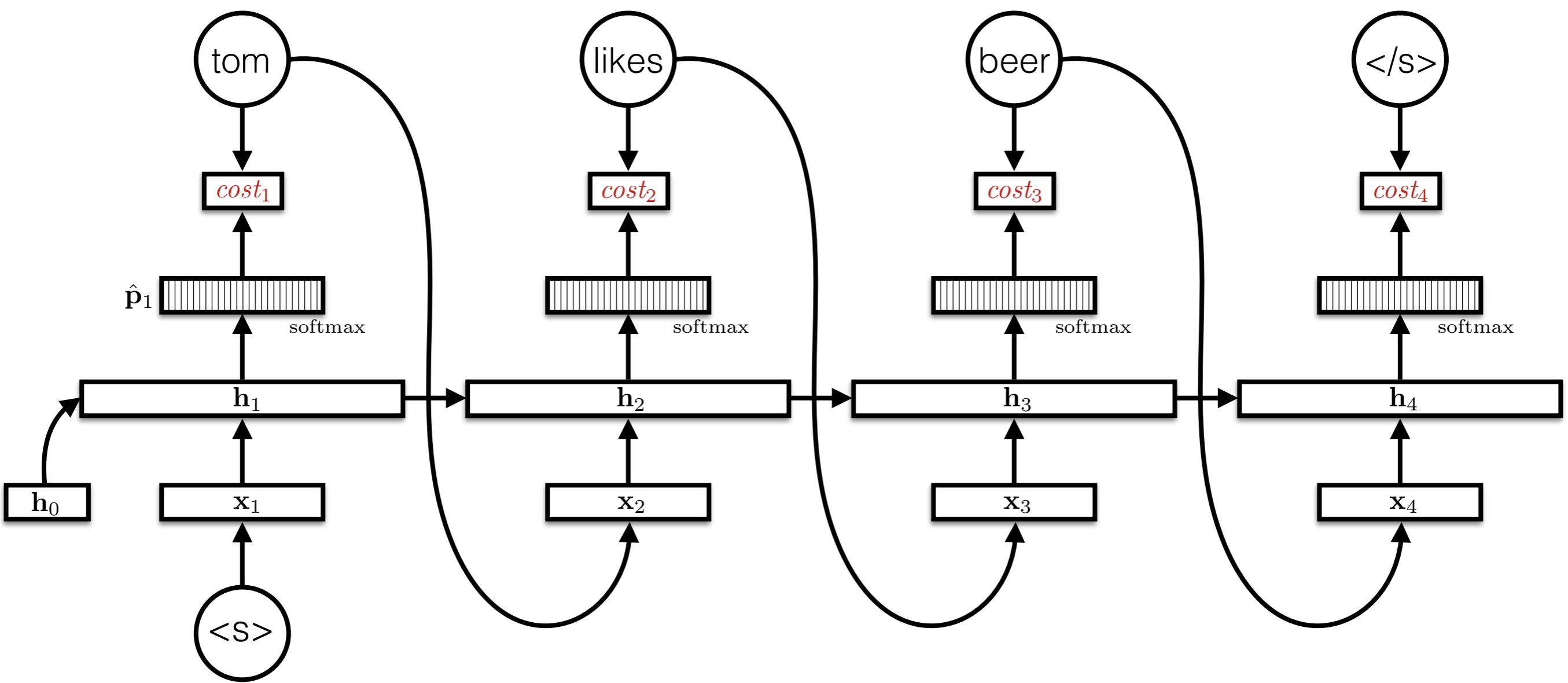
$$\times p(\langle /s \rangle | \langle s \rangle, \text{tom}, \text{likes}, \text{beer})$$



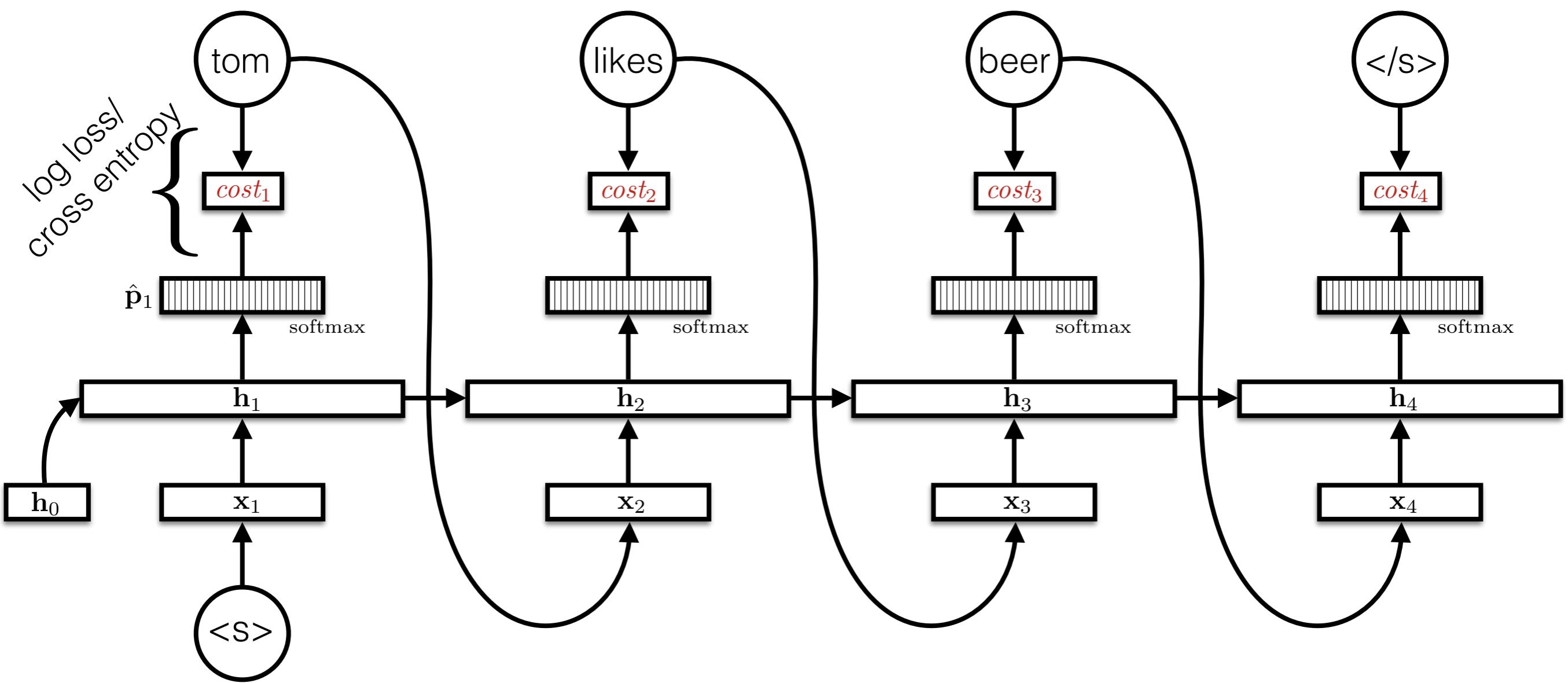
Language Model Training



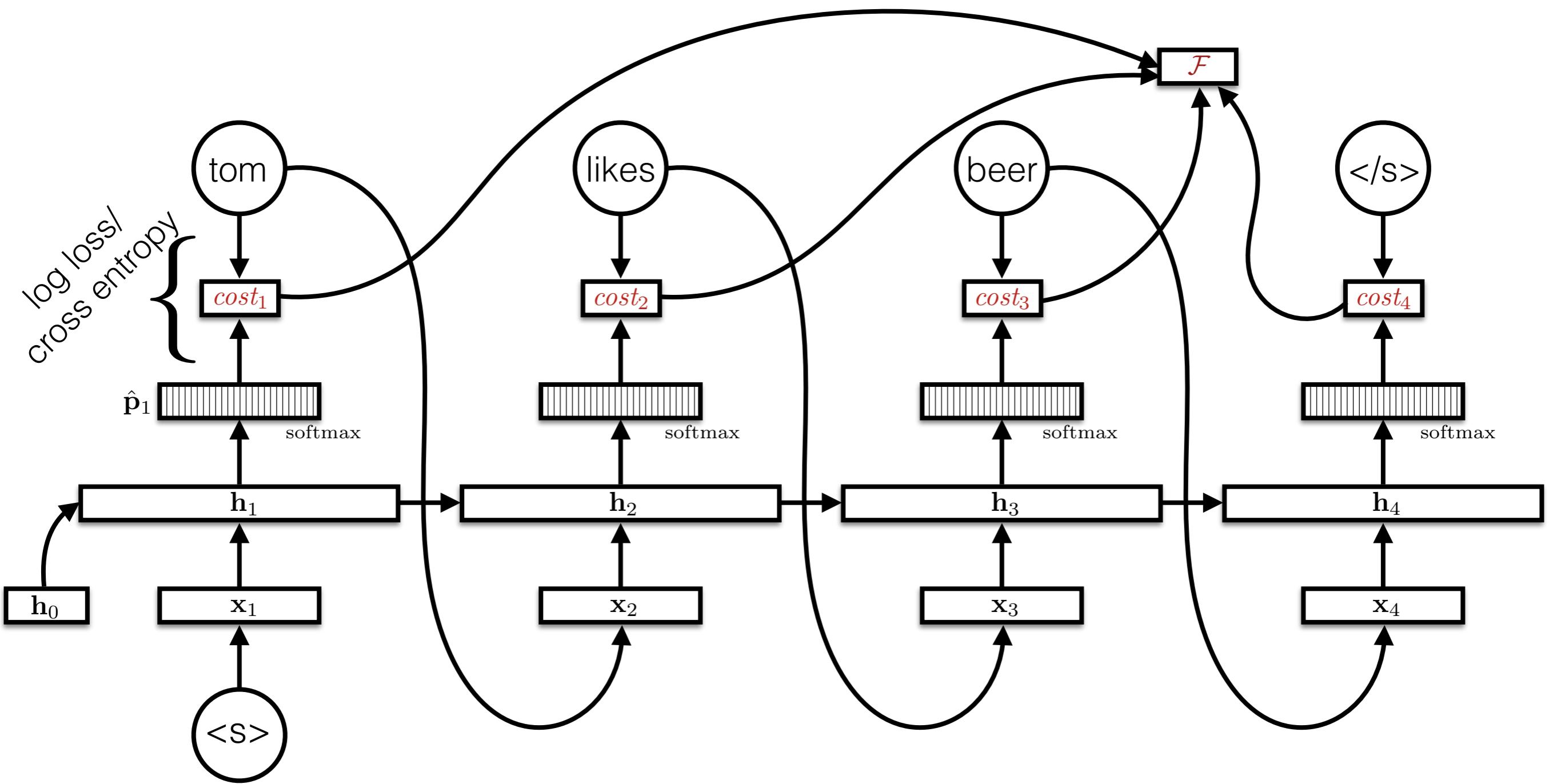
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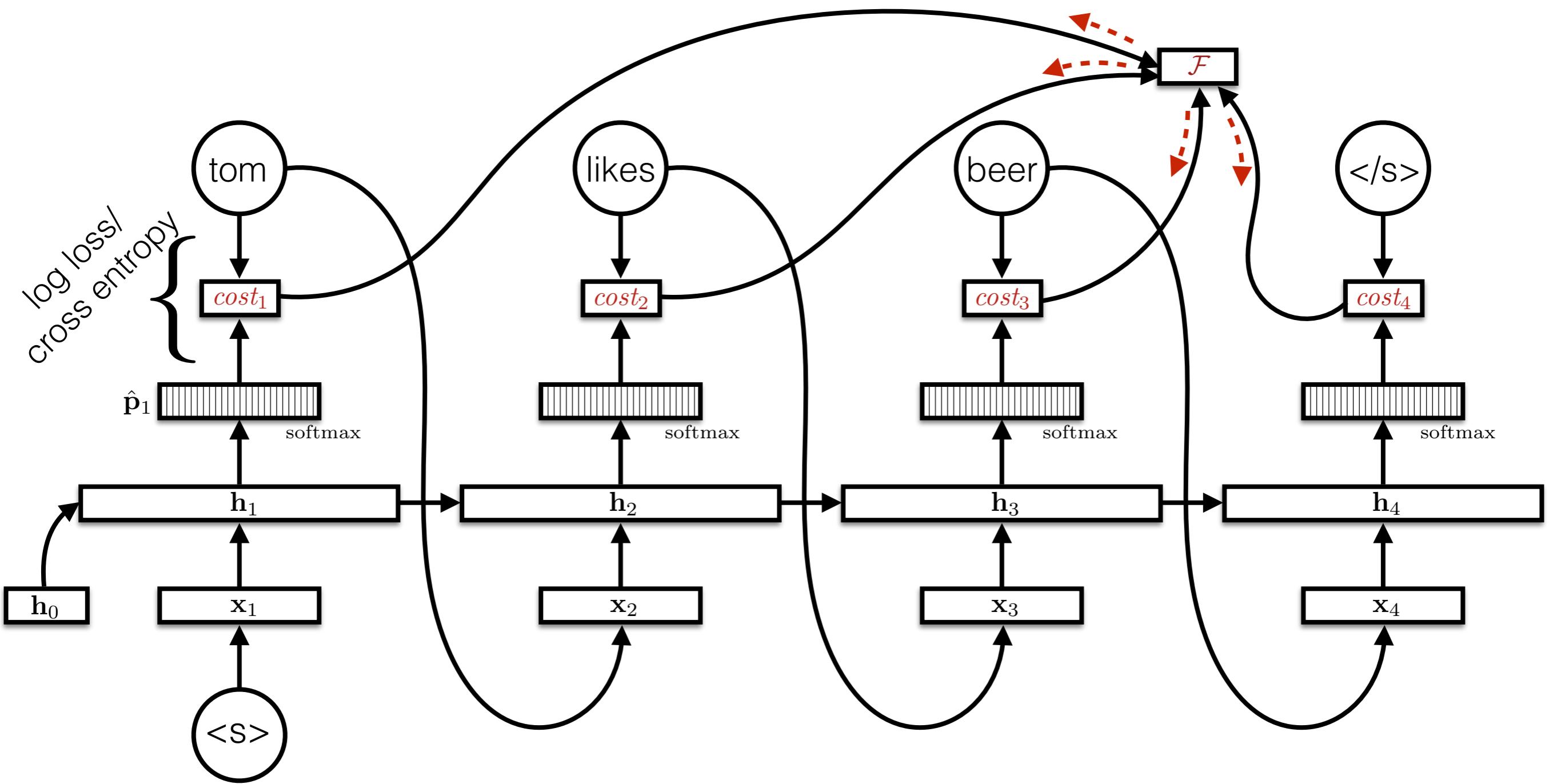
Language Model Training



Language Model Training



Language Model Training



Language Model Training

- The cross-entropy objective seeks the **maximum likelihood** (MLE) parameters.

“Find the parameters that make the training data most likely.”
- You will overfit:
 - Stop training early, based on a validation set
 - Weight decay / other weight regularizers
 - Dropout variants during training
- In contrast to count-based models, RNNs don’t have problems with “zeros”.

RNN Language Models

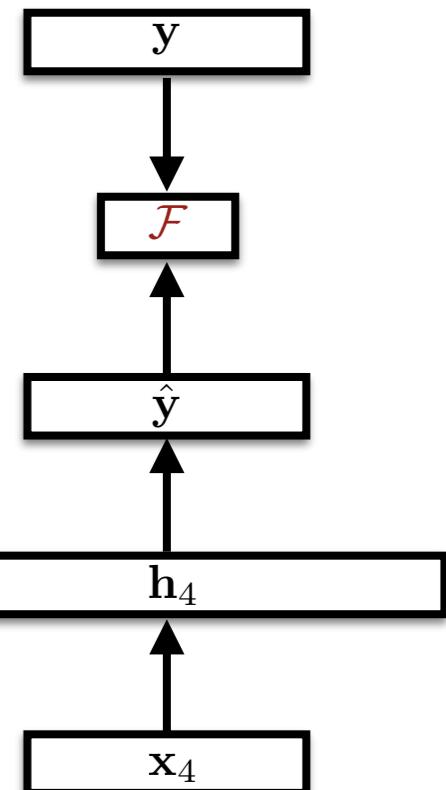
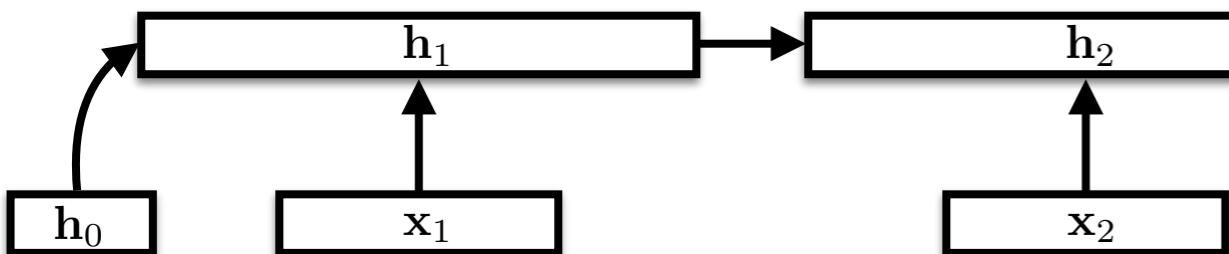
- Unlike Markov (n -gram) models, RNNs never forget
 - However we will see they might have trouble learning to use their memories (more soon...)
- Algorithms
 - Sample a sequence from the probability distribution defined by the RNN
 - Train the RNN to minimize cross entropy (aka MLE)
 - What about: what is the most probable sequence?

Questions?

Training Challenges

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h}_{|\mathbf{x}|} + \mathbf{b}$$



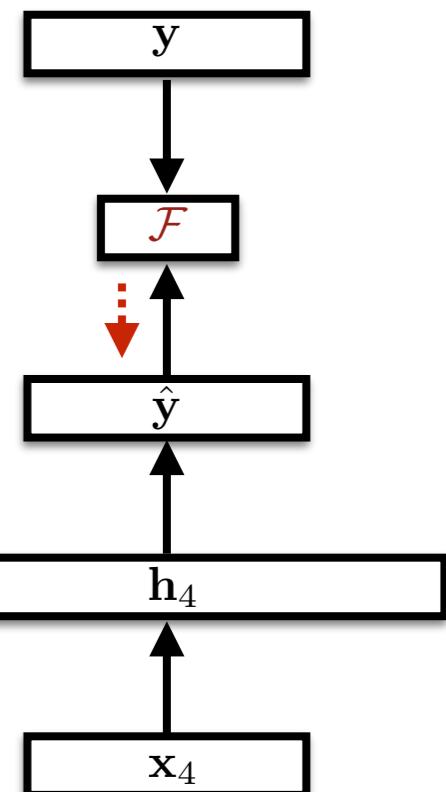
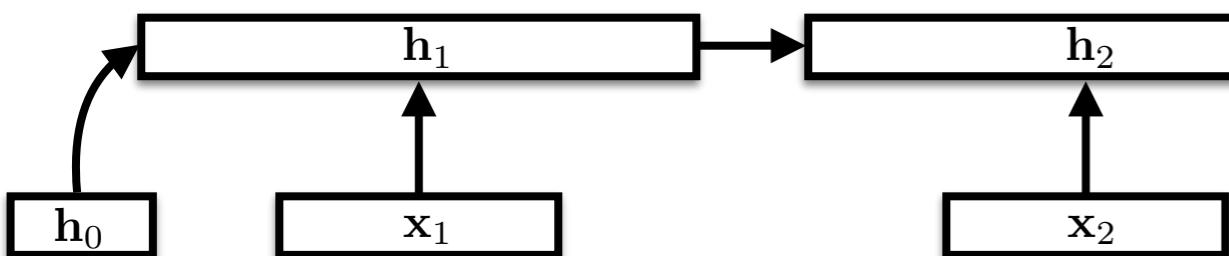
What happens to gradients as you go back in time?

$$\frac{\partial \mathcal{F}}{\partial \mathcal{F}}$$

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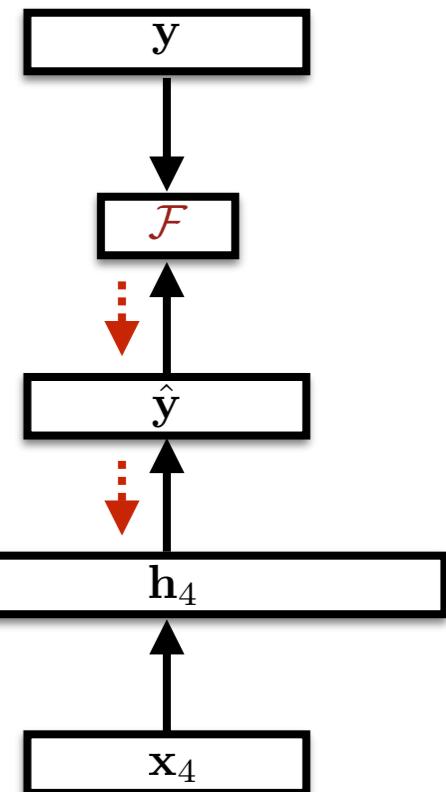
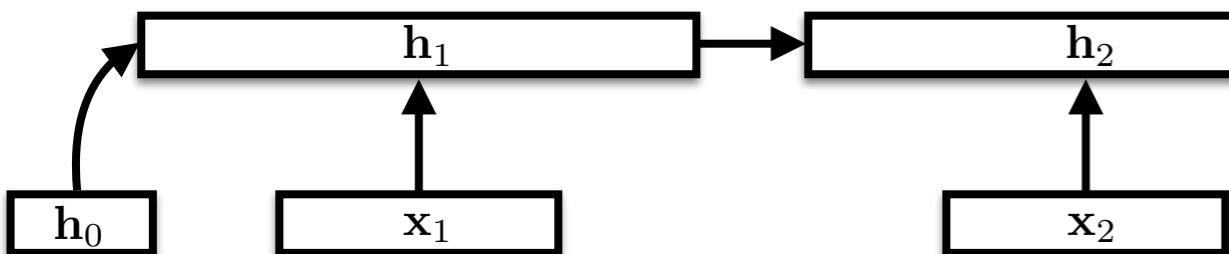
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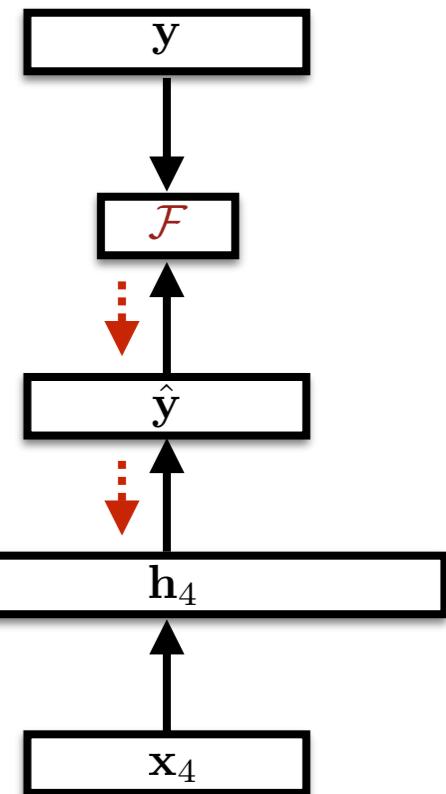
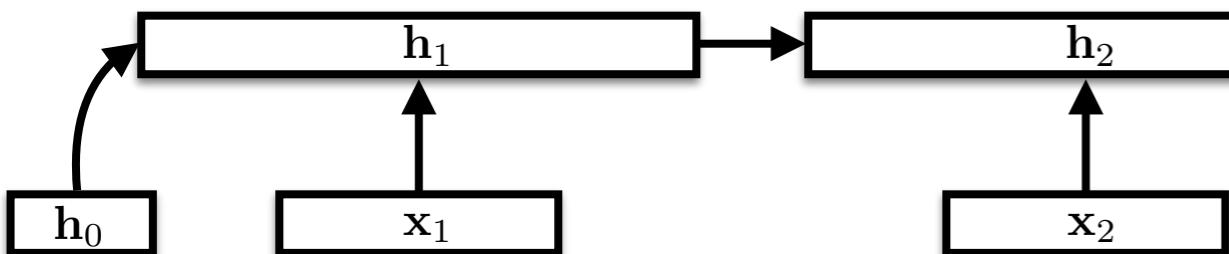
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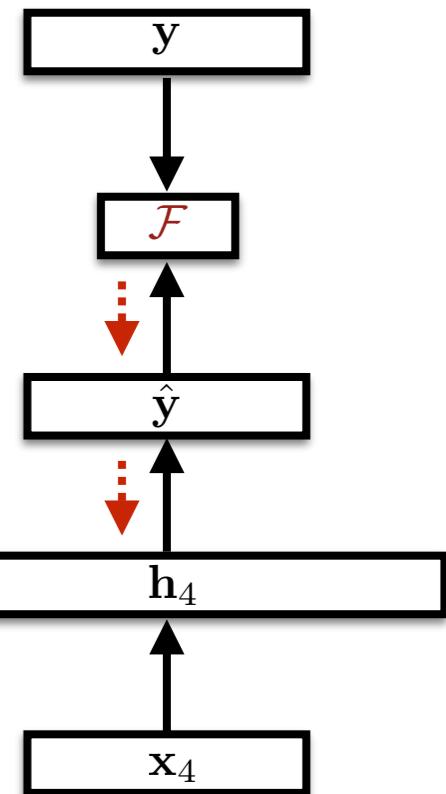
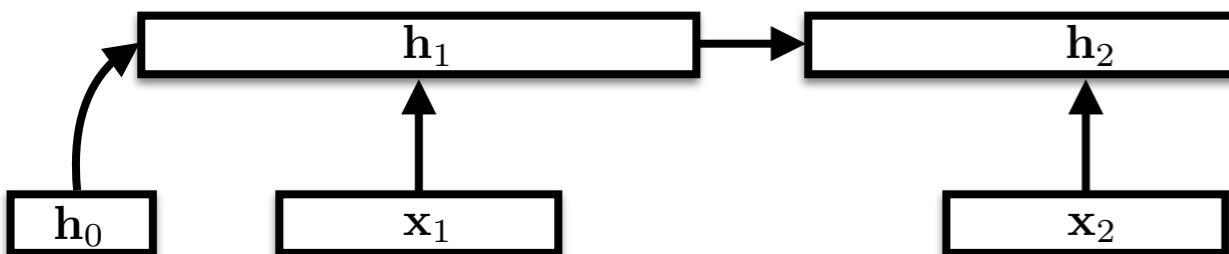
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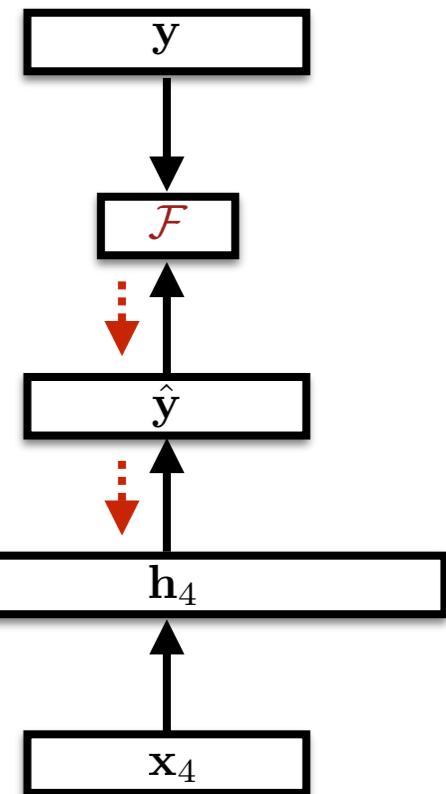
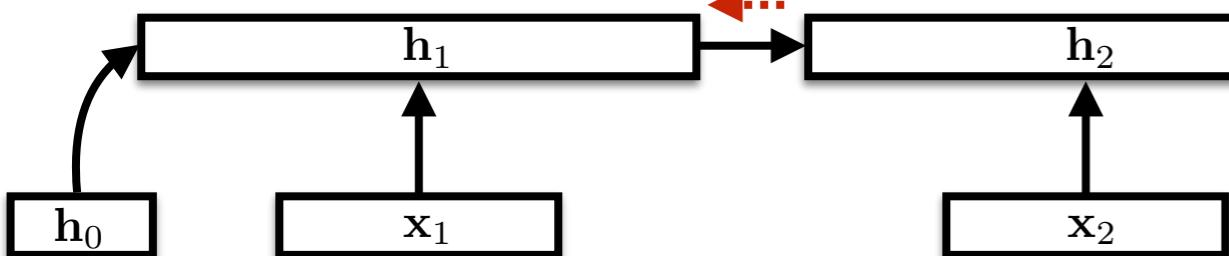
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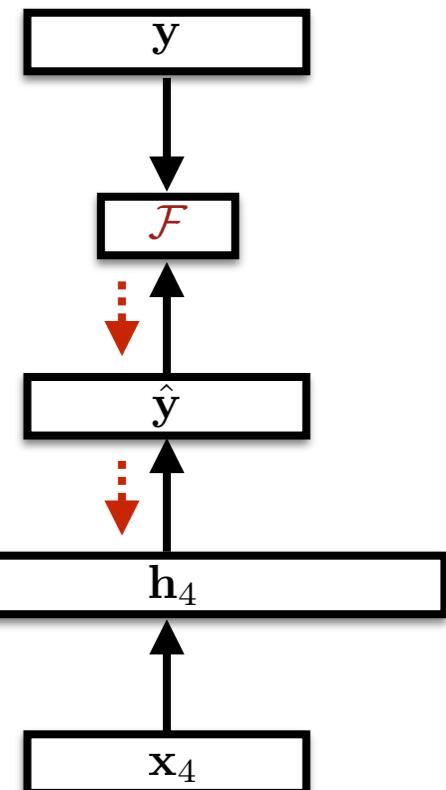
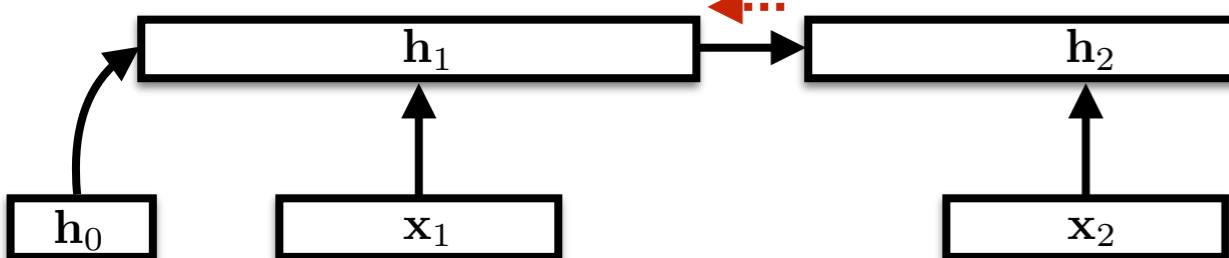
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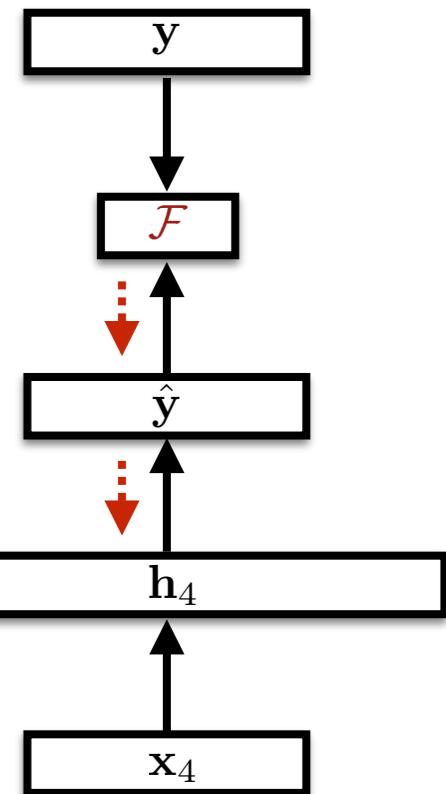
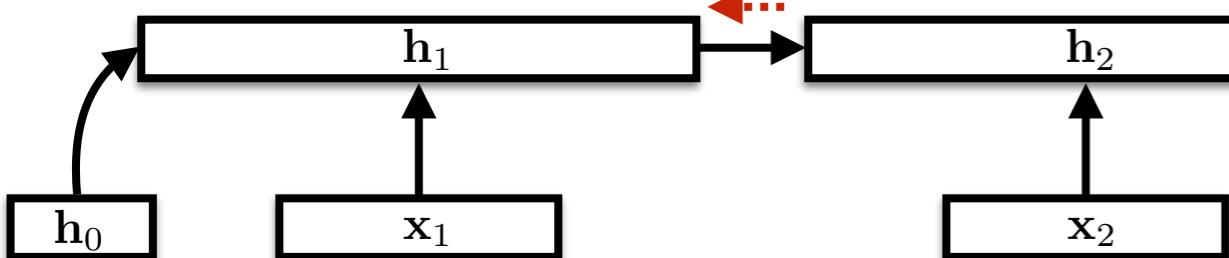
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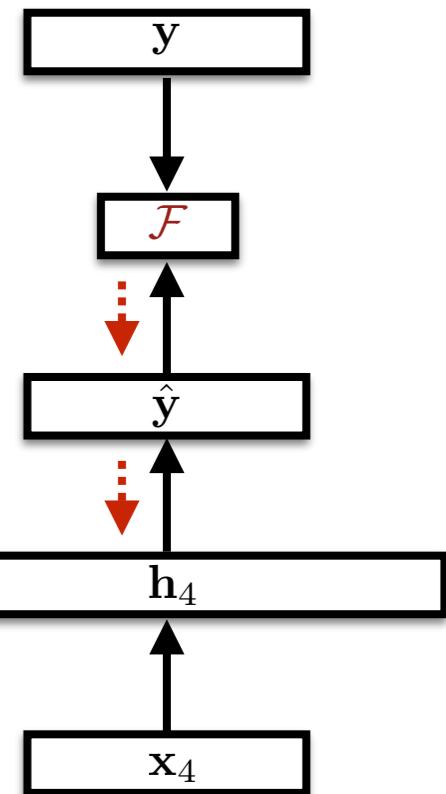
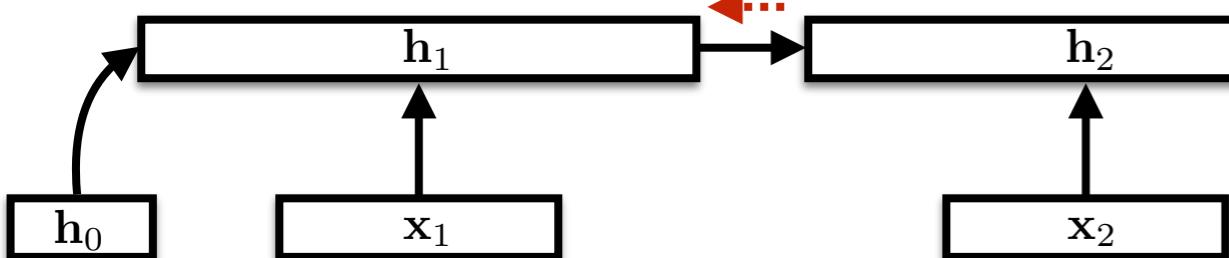
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Training Challenges

$$\mathbf{h}_t = g(\overbrace{\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c}}^{\mathbf{z}_t})$$

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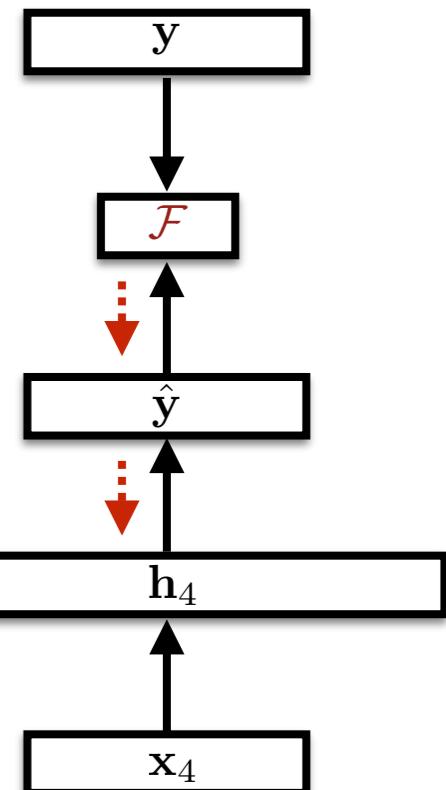
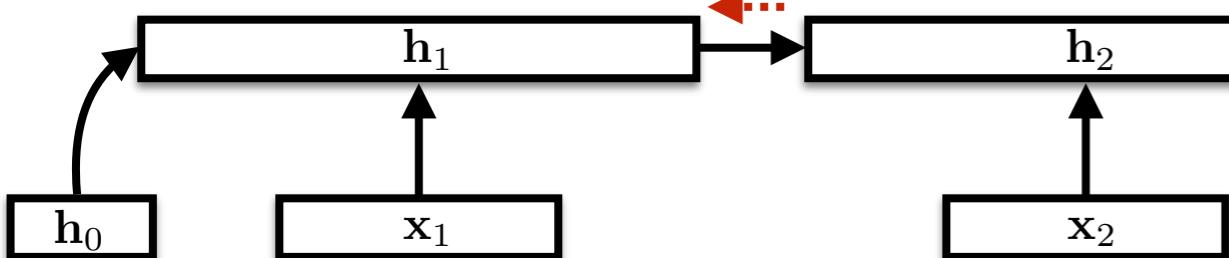
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$$\frac{\partial \mathcal{F}}{\partial \mathbf{h}_1} = \left(\prod_{t=2}^{|\mathbf{x}|} \frac{\partial \mathbf{h}_t}{\partial \mathbf{z}_t} \frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}} \right) \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{h}_{|\mathbf{x}|}} \frac{\partial \mathcal{F}}{\partial \hat{\mathbf{y}}} \frac{\partial \mathcal{F}}{\partial \mathcal{F}}$$

Training Challenges

$$\mathbf{h}_t = g(\overbrace{\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c}}^{\mathbf{z}_t})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h}_{|\mathbf{x}|} + \mathbf{b}$$

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$$\frac{\partial \mathbf{h}_t}{\partial \mathbf{z}_t} = \text{diag}(g'(\mathbf{z}_t))$$

Training Challenges

$$\mathbf{h}_t = g(\overbrace{\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c}}^{\mathbf{z}_t})$$

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$$\frac{\partial \mathbf{h}_t}{\partial \mathbf{z}_t} = \text{diag}(g'(\mathbf{z}_t))$$

$$\frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}} = \boxed{?}$$

Training Challenges

$$\mathbf{h}_t = g(\overbrace{\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c}}^{\mathbf{z}_t})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h}_{|\mathbf{x}|} + \mathbf{b}$$

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$$\frac{\partial \mathbf{h}_t}{\partial \mathbf{z}_t} = \text{diag}(g'(\mathbf{z}_t))$$

$$\frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}} = \mathbf{U}$$

Training Challenges

$$\mathbf{h}_t = g(\overbrace{\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c}}^{\mathbf{z}_t})$$

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$$\frac{\partial \mathcal{F}}{\partial \mathbf{h}_1} = \left(\prod_{t=2}^{|\mathbf{x}|} \frac{\partial \mathbf{h}_t}{\partial \mathbf{z}_t} \frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}} \right) \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{h}_{|\mathbf{x}|}} \frac{\partial \mathcal{F}}{\partial \hat{\mathbf{y}}} \frac{\partial \mathcal{F}}{\partial \mathcal{F}}$$

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$$\frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}} = \mathbf{U}$$

$$\frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}} = \frac{\partial \mathbf{h}_t}{\partial \mathbf{z}_t} \frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}} = \text{diag}(g'(\mathbf{z}_t)) \mathbf{U}$$

Training Challenges

$$\mathbf{h}_t = g(\overbrace{\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c}}^{\mathbf{z}_t})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h}_{|\mathbf{x}|} + \mathbf{b}$$

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$$\frac{\partial \mathcal{F}}{\partial \mathbf{h}_1} = \left(\prod_{t=2}^{|\mathbf{x}|} \text{diag}(g'(\mathbf{z}_t)) \mathbf{U} \right) \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{h}_{|\mathbf{x}|}} \frac{\partial \mathcal{F}}{\partial \hat{\mathbf{y}}} \frac{\partial \mathcal{F}}{\partial \mathcal{F}}$$

Training Challenges

$$\mathbf{h}_t = g(\overbrace{\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c}}^{\mathbf{z}_t})$$

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Three cases: largest eigenvalue is
exactly 1; gradient propagation is stable
<1; gradient vanishes (exponential decay)
>1; gradient explodes (exponential growth)

Vanishing Gradients

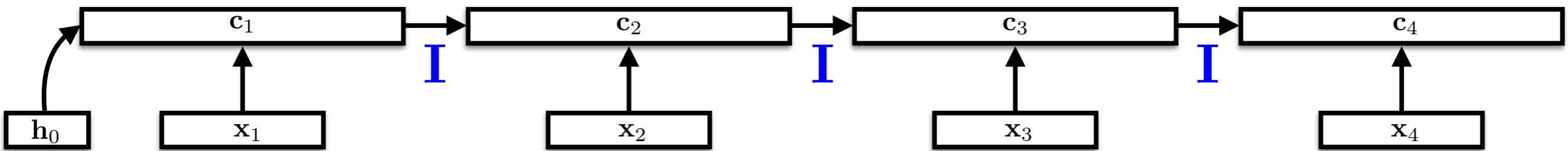
- In practice, the spectral radius of \mathbf{U} is small, and gradients vanish
- In practice, this means that long-range dependencies are difficult to learn (although in theory they are learnable)
- Solutions
 - Better optimizers (second order methods, approximate second order methods)
 - Normalization to keep the gradient norms stable across time
 - Clever initialization so that you at least start with good spectra (e.g., start with random orthonormal matrices)
 - **Alternative parameterizations: LSTMs and GRUs**

Alternative RNNs

- Long short-term memories (LSTMs; Hochreiter and Schmidhuber, 1997)
- Gated recurrent units (GRUs; Cho et al., 2014)
- Intuition instead of **multiplying** across time (which leads to exponential growth), we want the error to be **constant**.
 - What is a function whose Jacobian has a spectral radius of exactly \mathbb{I} : the identity function

Memory cells

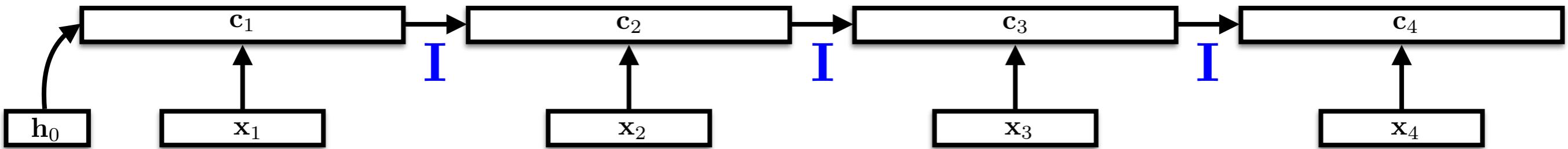
$$\mathbf{c}_t = \mathbf{c}_{t-1} + f(\mathbf{x}_t)$$



Memory cells

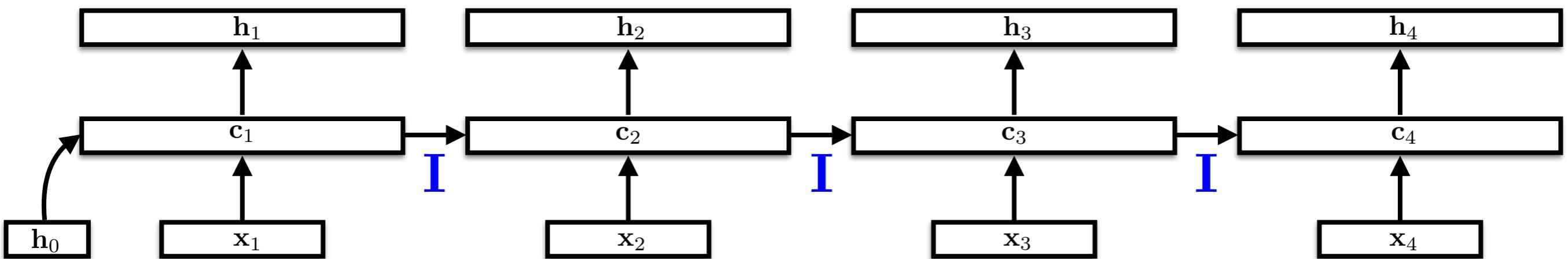
$$\mathbf{c}_t = \mathbf{c}_{t-1} + f(\mathbf{x}_t)$$

$f(\mathbf{v}) = \tanh(\mathbf{W}\mathbf{v} + \mathbf{b})$



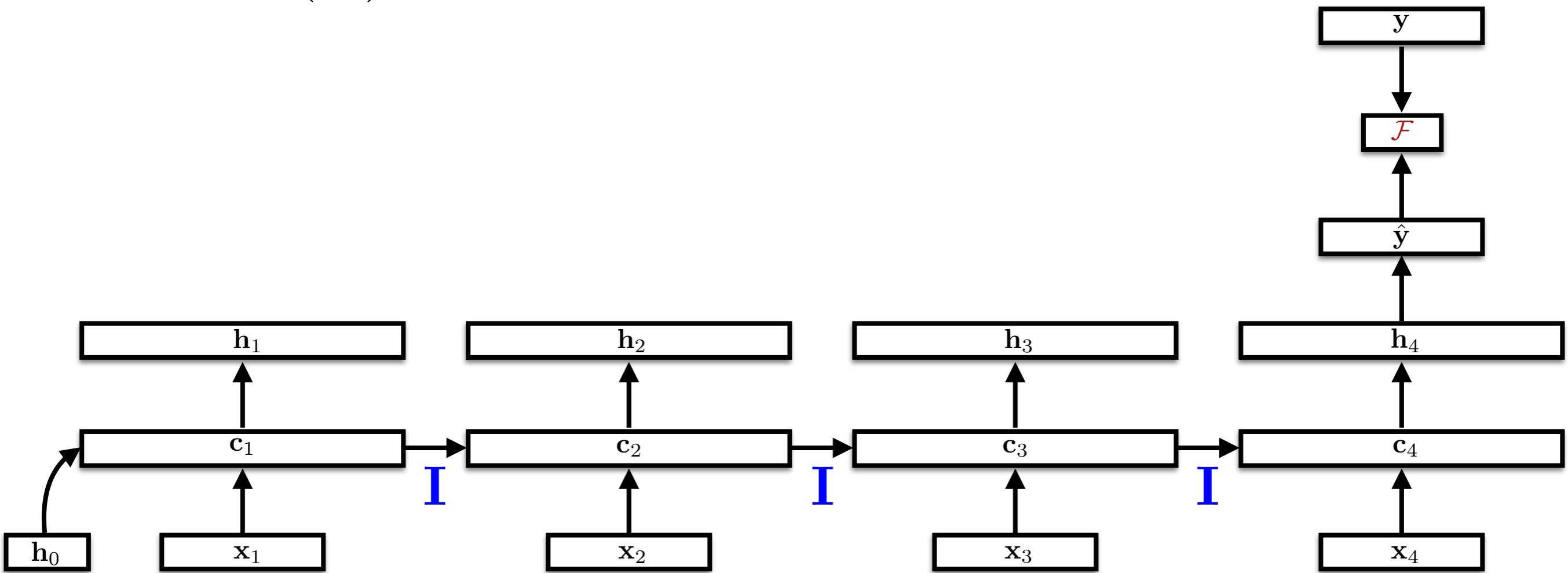
Memory cells

$$\mathbf{c}_t = \mathbf{c}_{t-1} + f(\mathbf{x}_t)$$
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$$\mathbf{h}_t = g(\mathbf{c}_t)$$



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Memory cells

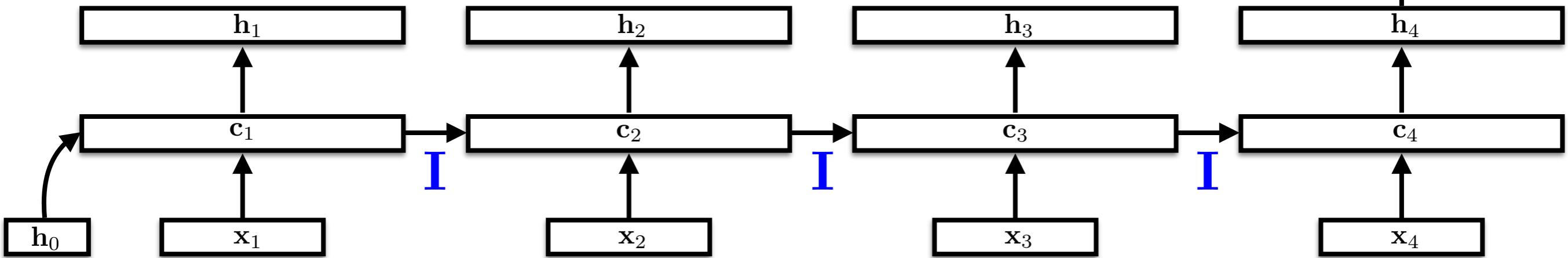
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$$f(\mathbf{v}) = \tanh(\mathbf{W}\mathbf{v} + \mathbf{b})$$

$$\mathbf{h}_t = g(\mathbf{c}_t)$$

Note:

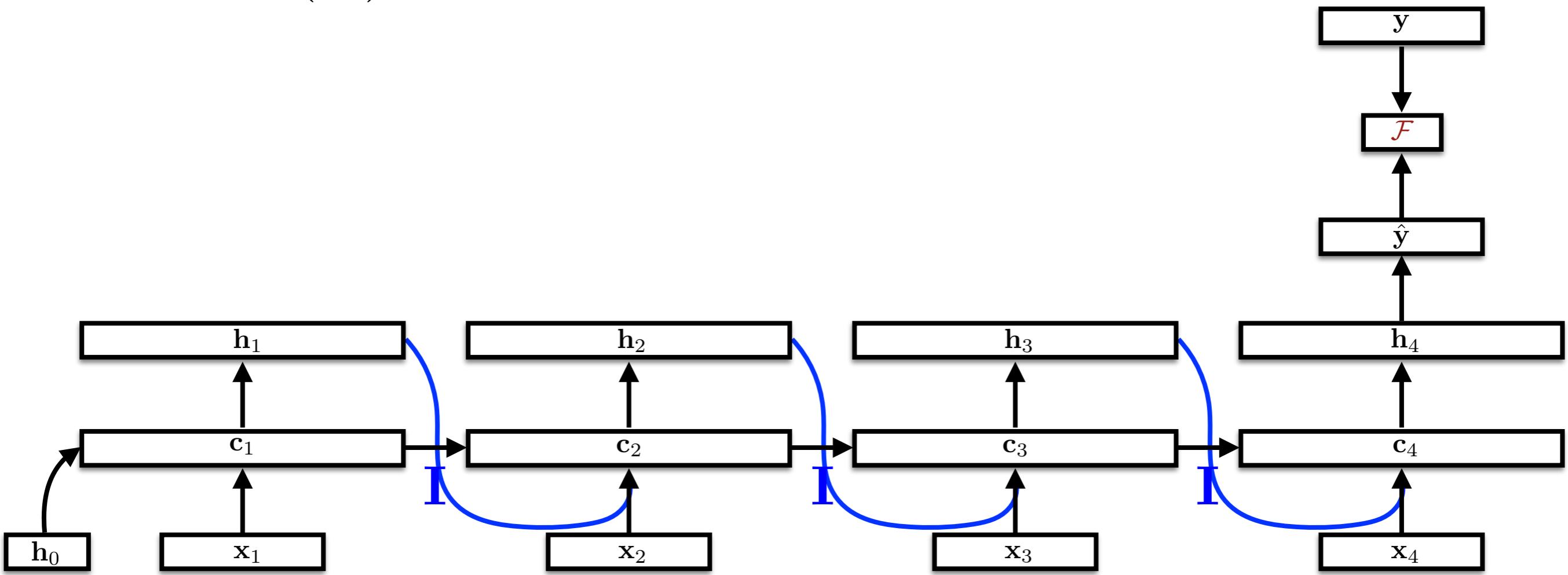
$$\frac{\partial \mathbf{c}_t}{\partial \mathbf{c}_{t-1}} = \mathbf{I}$$



Memory cells

$$\mathbf{c}_t = \mathbf{c}_{t-1} + f([\mathbf{x}_t; \mathbf{h}_{t-1}])$$

$$\mathbf{h}_t = g(\mathbf{c}_t)$$



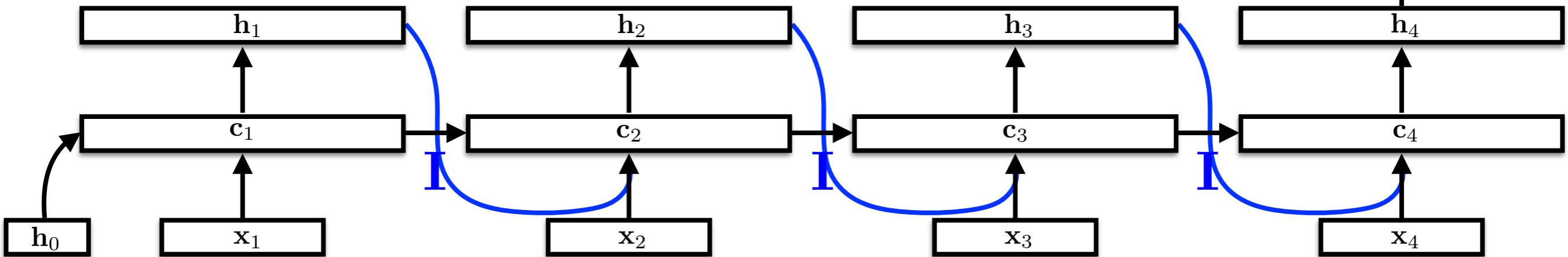
Memory cells

$$\mathbf{c}_t = \mathbf{c}_{t-1} + f([\mathbf{x}_t; \mathbf{h}_{t-1}])$$

$$\mathbf{h}_t = g(\mathbf{c}_t)$$

“Almost constant”

$$\frac{\partial \mathbf{c}_t}{\partial \mathbf{c}_{t-1}} = \mathbf{I} + \boldsymbol{\varepsilon}$$



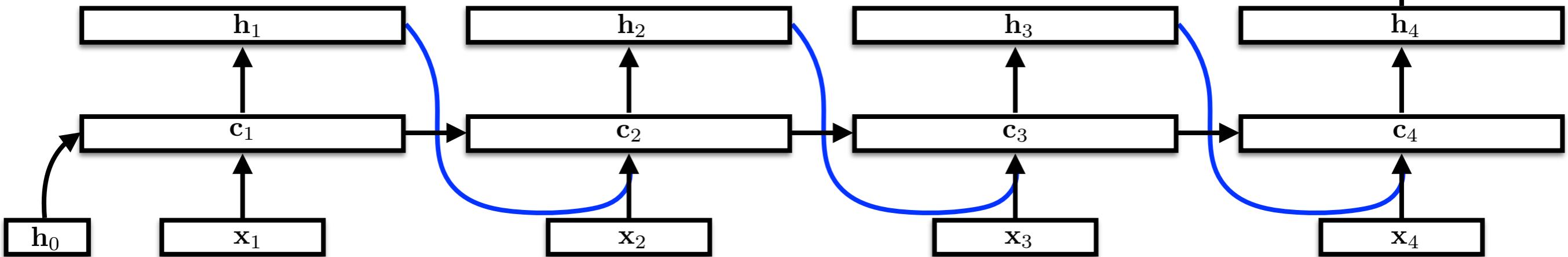
Memory cells

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot f([\mathbf{x}_t; \mathbf{h}_{t-1}])$$

$$\mathbf{h}_t = g(\mathbf{c}_t)$$

$$\mathbf{f}_t = \sigma(f_f([\mathbf{x}_t; \mathbf{h}_{t-1}]))$$
 “forget gate”

$$\mathbf{i}_t = \sigma(f_i([\mathbf{x}_t; \mathbf{h}_{t-1}]))$$
 “input gate”



Memory cells

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot f([\mathbf{x}_t; \mathbf{h}_{t-1}])$$

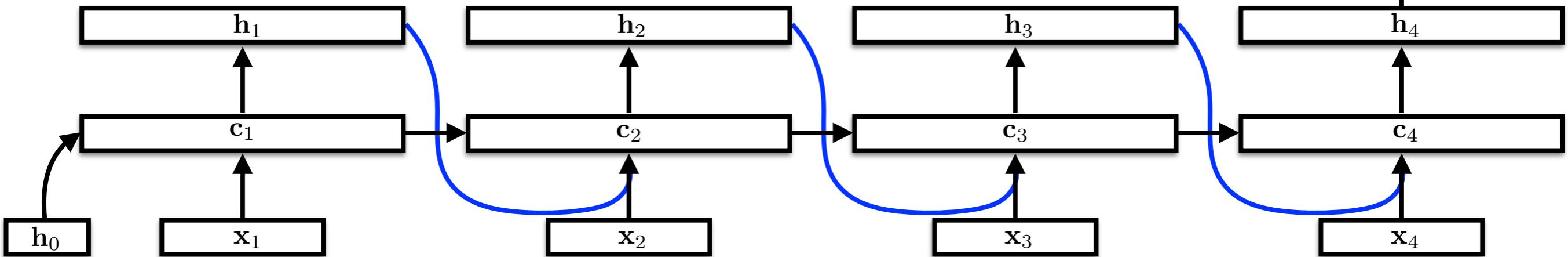
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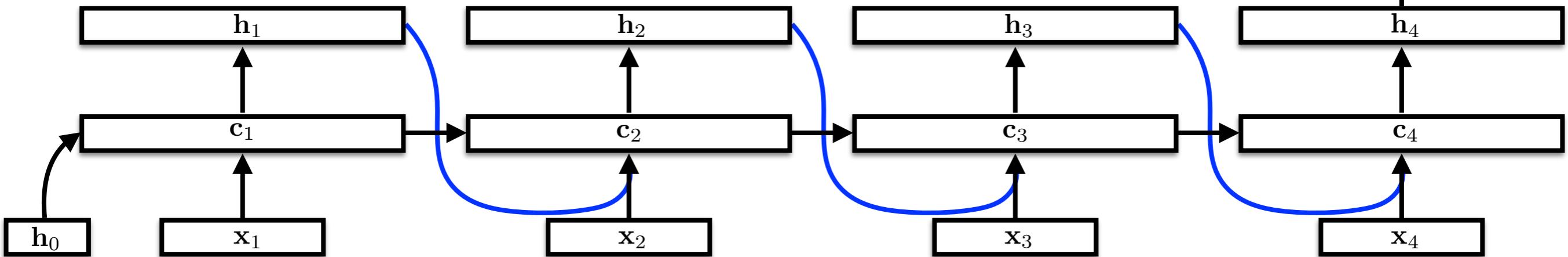
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LSTM

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot f([\mathbf{x}_t; \mathbf{h}_{t-1}])$$

$$\mathbf{h}_t = \mathbf{o}_t \odot g(\mathbf{c}_t)$$

$$\mathbf{f}_t = \sigma(f_f([\mathbf{x}_t; \mathbf{h}_{t-1}]))$$

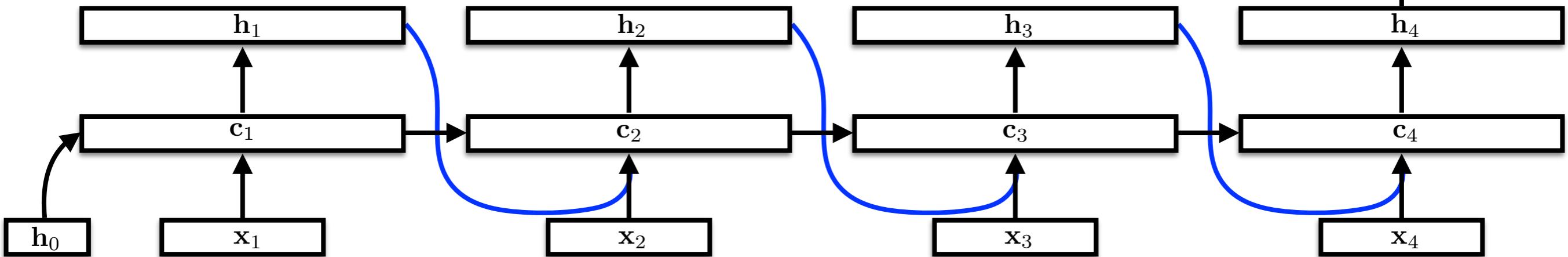
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LSTM

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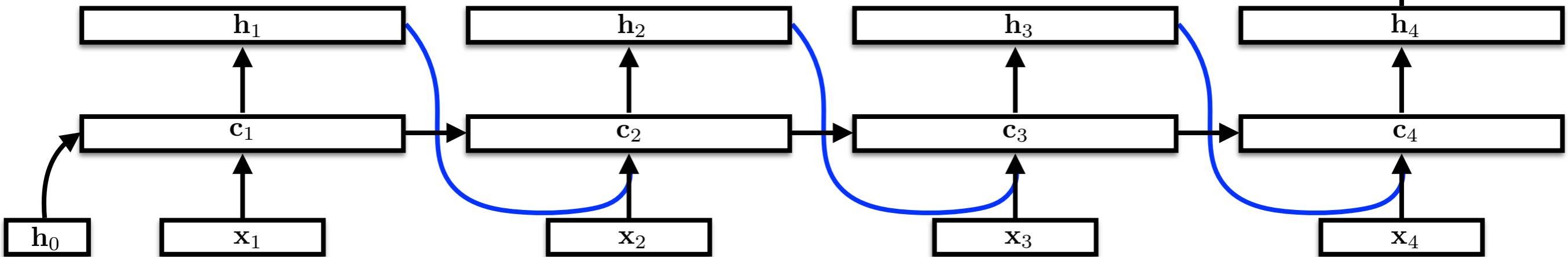
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“output gate”



LSTM Variant

$$\mathbf{c}_t = (1 - \mathbf{i}_t) \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot f([\mathbf{x}_t; \mathbf{h}_{t-1}])$$

$$\mathbf{h}_t = \mathbf{o}_t \odot g(\mathbf{c}_t)$$

~~$$\mathbf{f}_t = \sigma(f_f([\mathbf{x}_t; \mathbf{h}_{t-1}]))$$~~

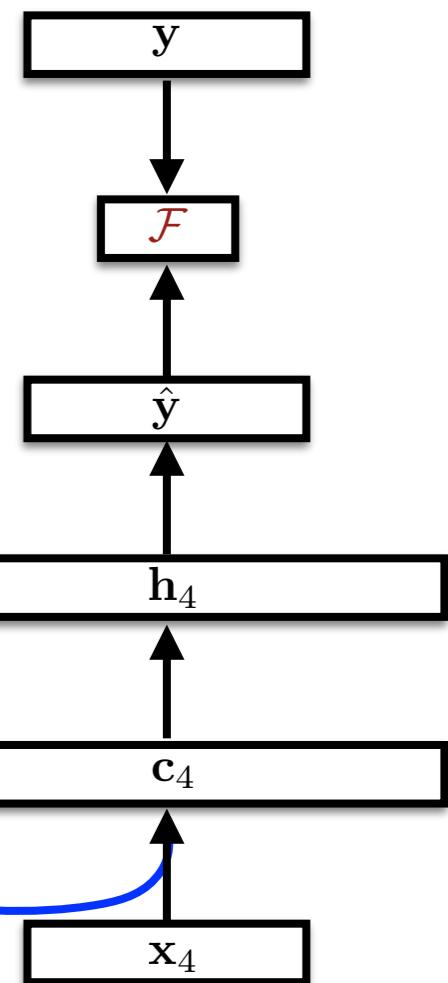
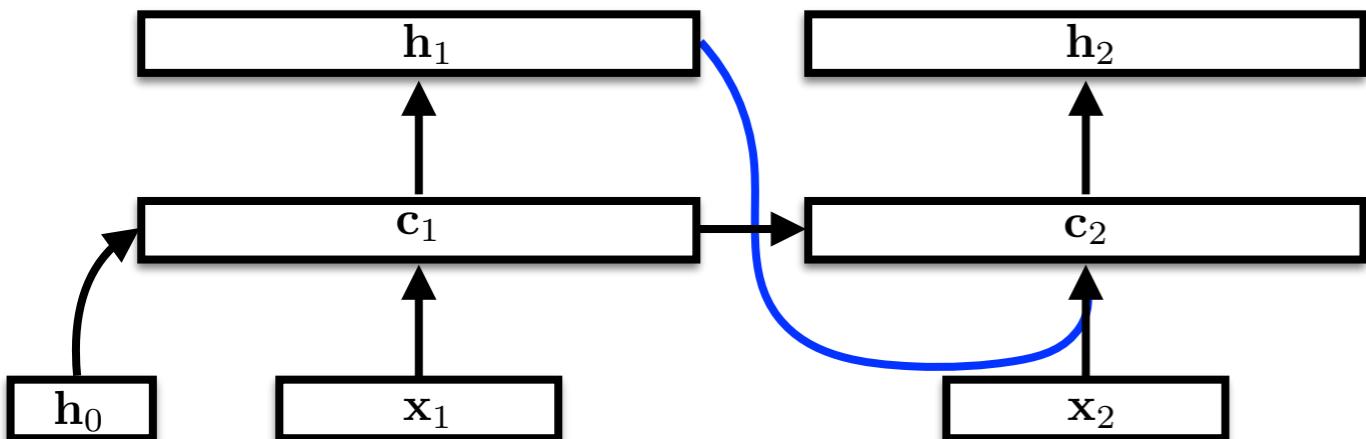
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$$\mathbf{i}_t = \sigma(f_i([\mathbf{x}_t; \mathbf{h}_{t-1}]))$$

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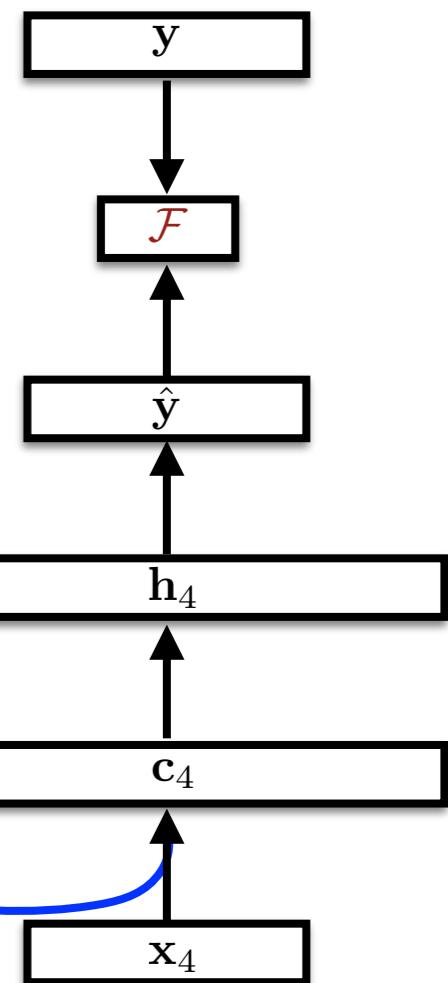
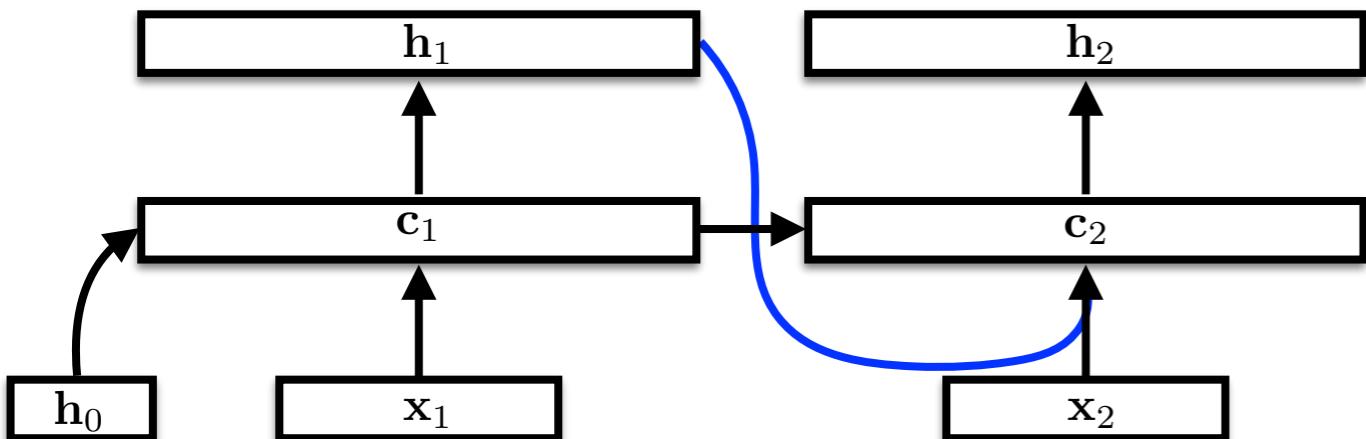
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Another Visualization

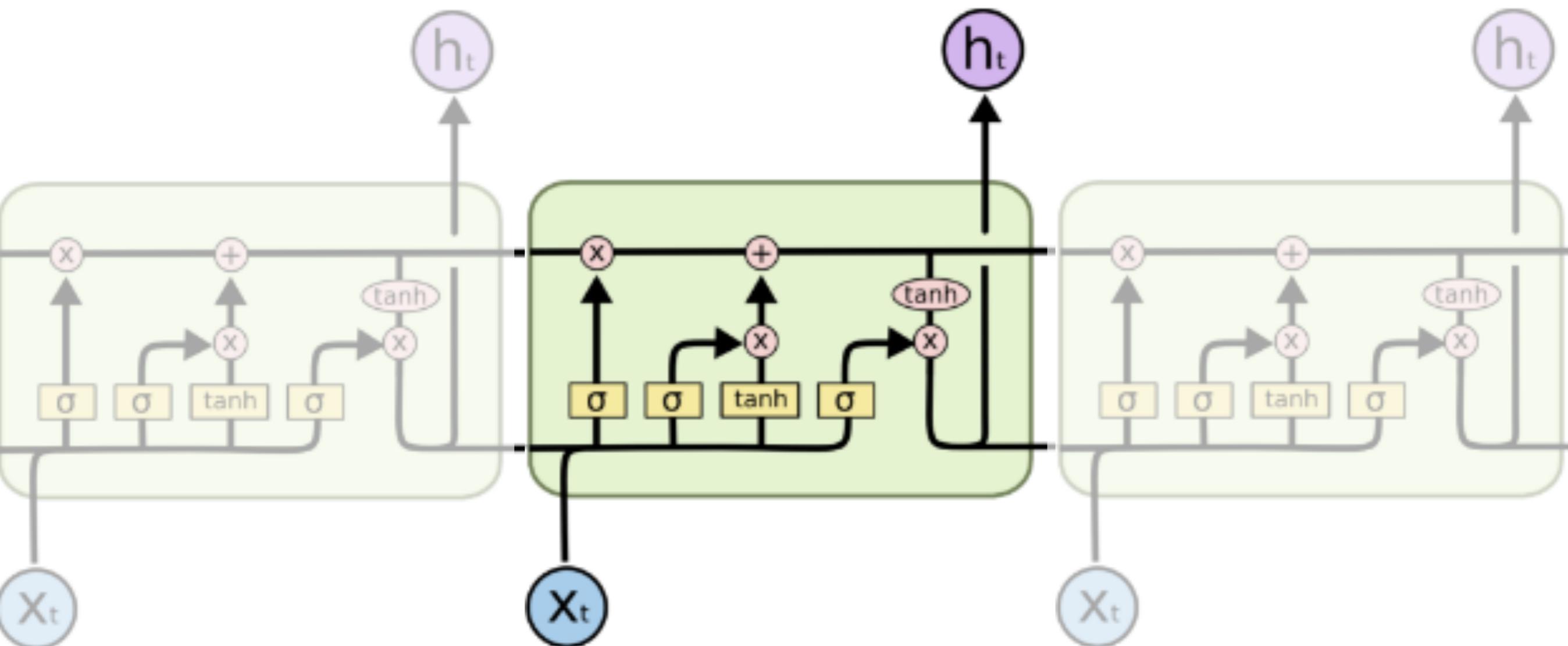


Figure credit: Christopher Olah

Another Visualization

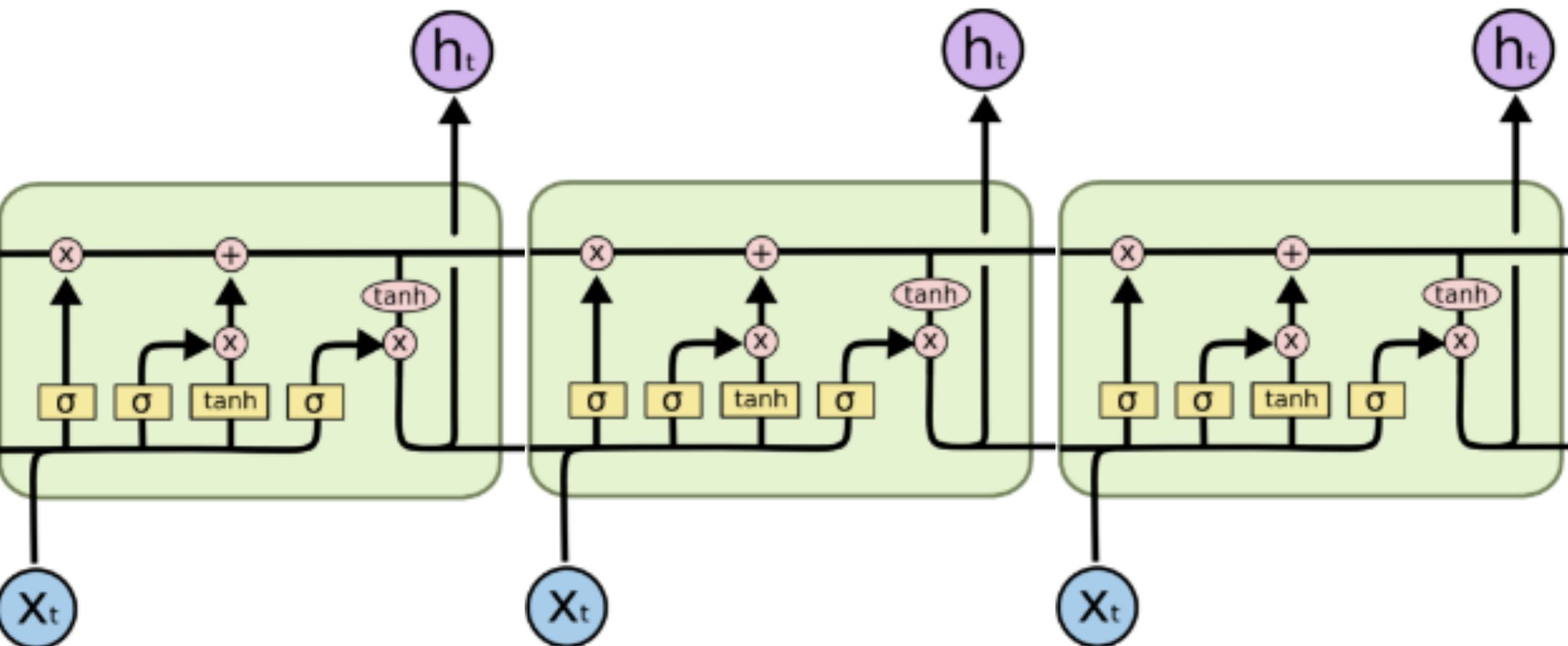


Figure credit: Christopher Olah

Another Visualization

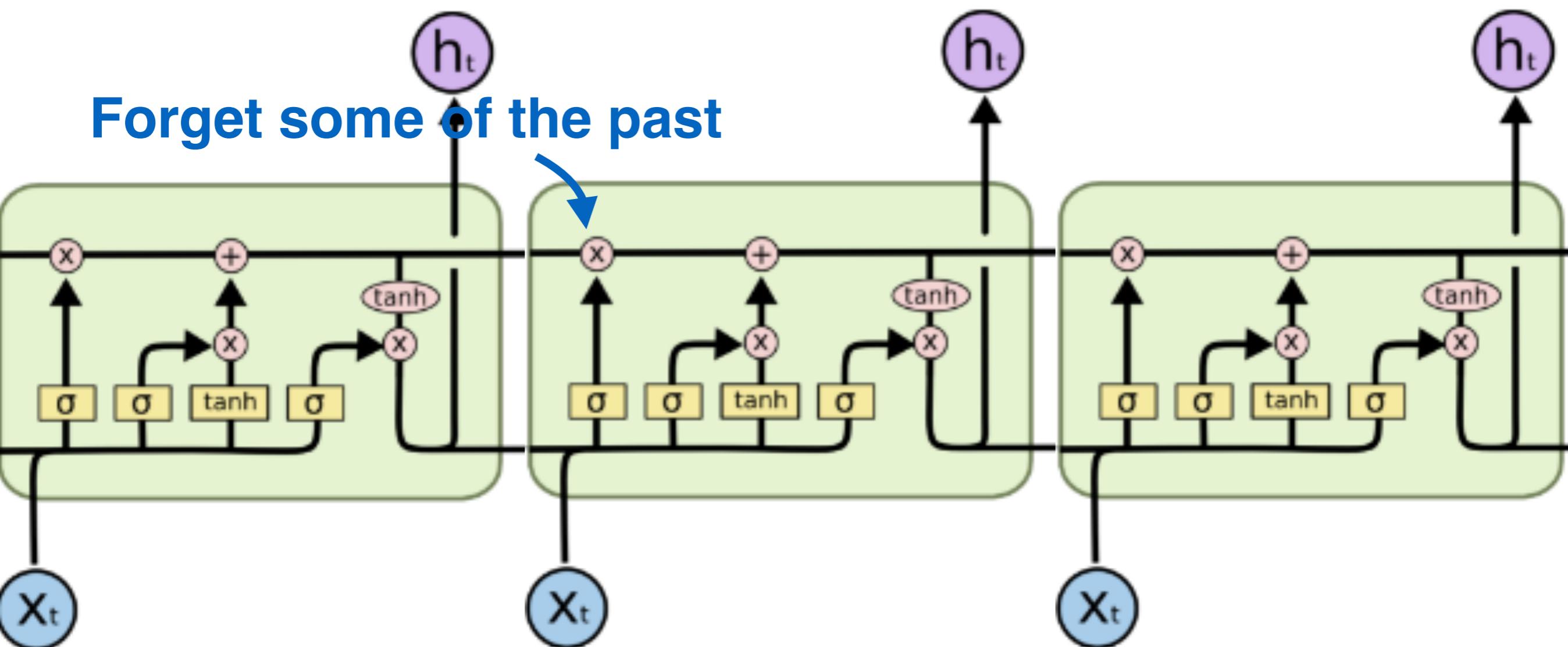


Figure credit: Christopher Olah

Another Visualization

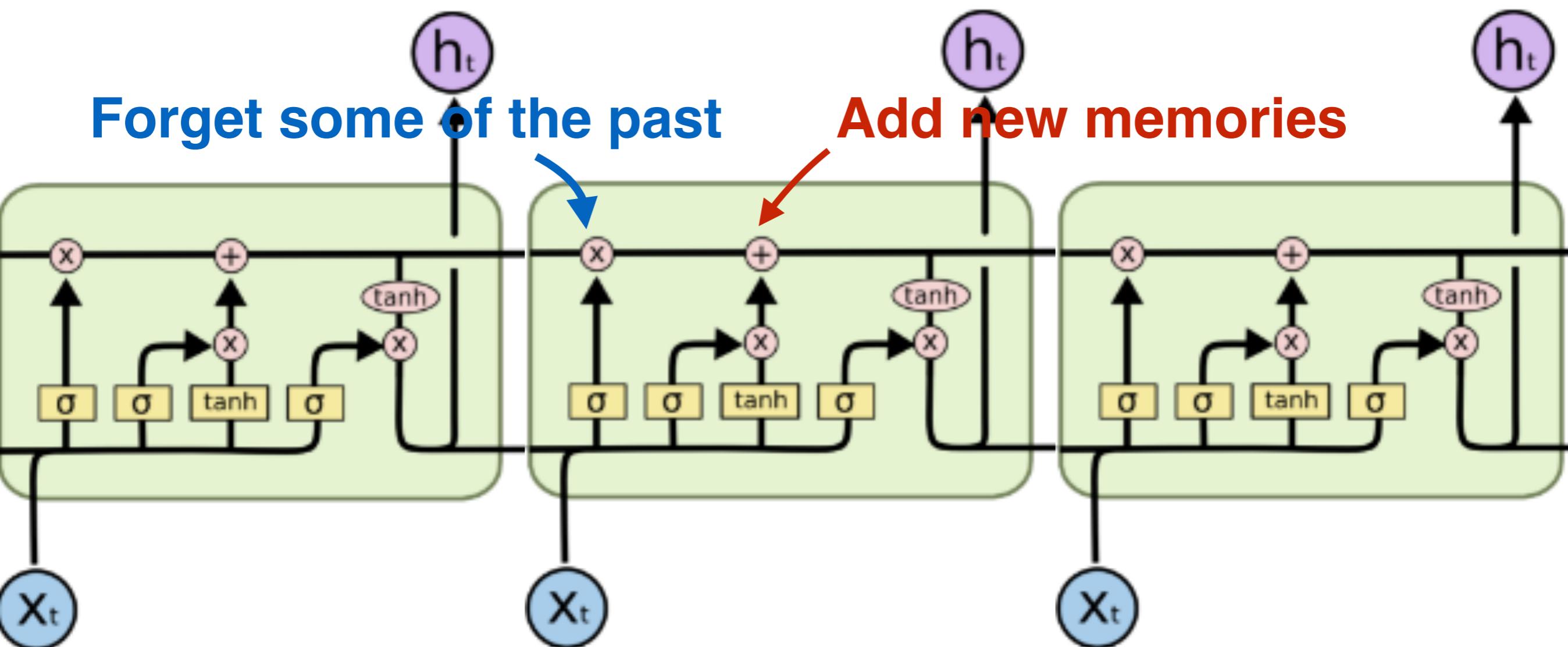


Figure credit: Christopher Olah

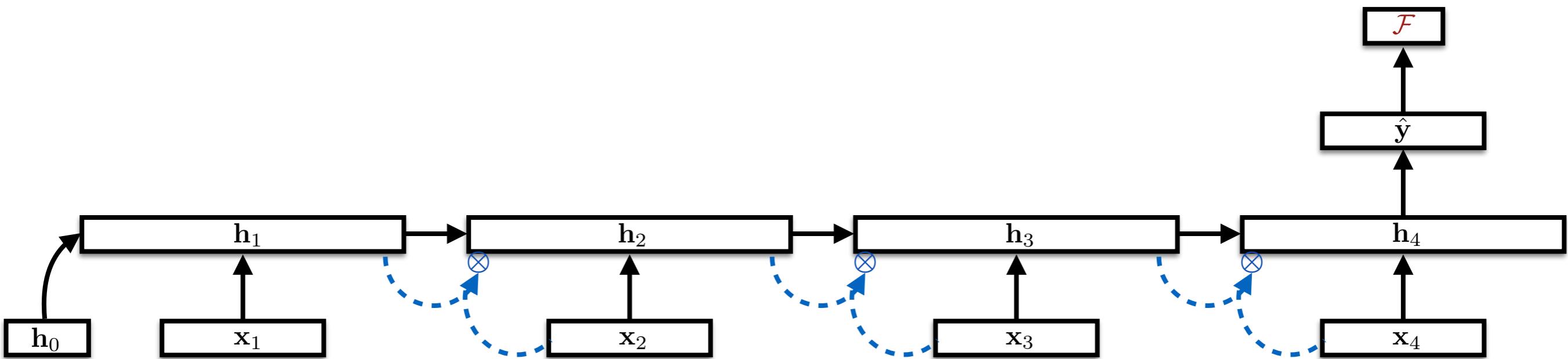
Gated Recurrent Units (GRUs)

$$\mathbf{h}_t = (1 - \mathbf{z}_t) \odot \mathbf{h}_{t-1} + \mathbf{z}_t \odot \tilde{\mathbf{h}}_t$$

$$\mathbf{z}_t = \sigma(f_z([\mathbf{h}_{t-1}; \mathbf{x}_t]))$$

$$\mathbf{r}_t = \sigma(f_r([\mathbf{h}_{t-1}; \mathbf{x}_t]))$$

$$\tilde{\mathbf{h}}_t = f([r_t \odot \mathbf{h}_{t-1}; \mathbf{x}_t]))$$



Summary

- Better gradient propagation is possible when you use additive rather than multiplicative/highly non-linear recurrent dynamics

$$\mathbf{RNN} \quad \mathbf{h}_t = f([\mathbf{x}_t; \mathbf{h}_{t-1}])$$

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$$\mathbf{GRU} \quad \mathbf{h}_t = (\mathbf{1} - \mathbf{z}_t) \odot \mathbf{h}_{t-1} + \mathbf{z}_t \odot f([\mathbf{x}_t; \mathbf{r}_t \odot \mathbf{h}_{t-1}])$$

Summary

- Better gradient propagation is possible when you use **additive** rather than multiplicative/highly non-linear recurrent dynamics

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Questions?

Conditional LMs

A **conditional** language model assigns probabilities to a sequence of words $\mathbf{w} = (w_1, w_2, \dots, w_\ell)$, given some conditioning context, \mathbf{x} .

As with unconditional models, it helpful to use the chain rule to decompose the probability:

$$p(\mathbf{w} \mid \mathbf{x}) = \prod_{t=1}^{\ell} p(w_t \mid \mathbf{x}, w_1, w_2, \dots, w_{t-1})$$

*What is the probability of the next word, given the history of previously generated words **and** conditioning context \mathbf{x} .*

Conditional LMs

x “input”

An author

A topic label

{SPAM, NOT_SPAM}

A sentence in French

A sentence in English

A sentence in English

An image

A document

A document

Meteorological measurements

Acoustic signal

Conversational history + database

A question + a document

A question + an image

w “text output”

A document written by that author

An article about that topic

An email

Its English translation

Its French translation

Its Chinese translation

A text description of the image

Its summary

Its translation

A weather report

Transcription of speech

Dialogue system response

Its answer

Its answer

Data for Training Conditional LMs

To train conditional language models, we need *paired samples*, $\{(\mathbf{x}_i, \mathbf{w}_i)\}_{i=1}^N$.

Data availability varies by task. It's easy to think of tasks that could be solved with conditional language models, but the data just doesn't exist.

Relatively large amounts of data for:
Translation, summarization, caption generation,
speech recognition

Evaluating Conditional LMs

How good is our conditional language model?

These are language models, we can use **cross-entropy** or **perplexity**. okay to implement, hard to interpret

Task specific evaluation. Compare the model's most likely output to a human-generated reference output using a task-specific evaluation metric L .

$$\boldsymbol{w}^* = \arg \max_{\boldsymbol{w}} p(\boldsymbol{w} \mid \boldsymbol{x}) \quad L(\boldsymbol{w}^*, \boldsymbol{w}_{ref})$$

Examples of L : BLEU, METEOR, ROUGE, WER

easy to implement, okay to interpret

Human evaluation.

hard to implement, easy to interpret

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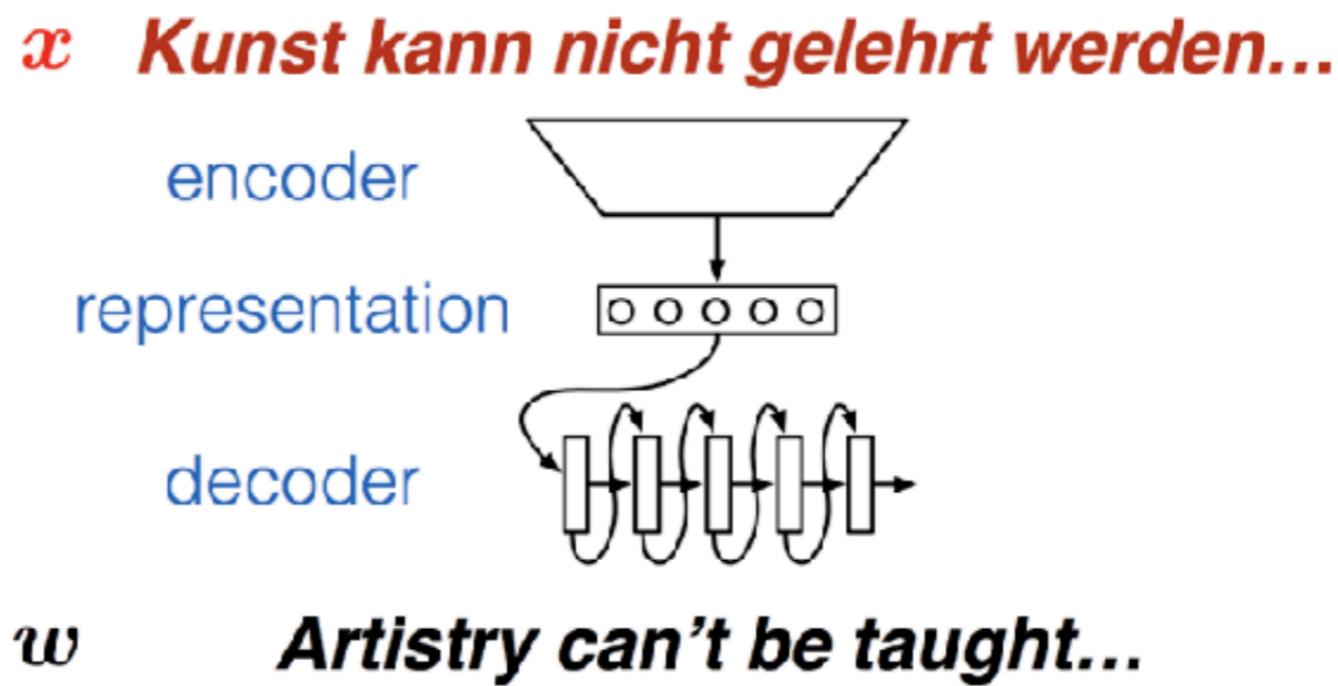
Human evaluation.

hard to implement, easy to interpret

Encoder-Decoder Models

Encoder-decoder models are a very simple class of conditional LMs that are nevertheless extremely powerful.

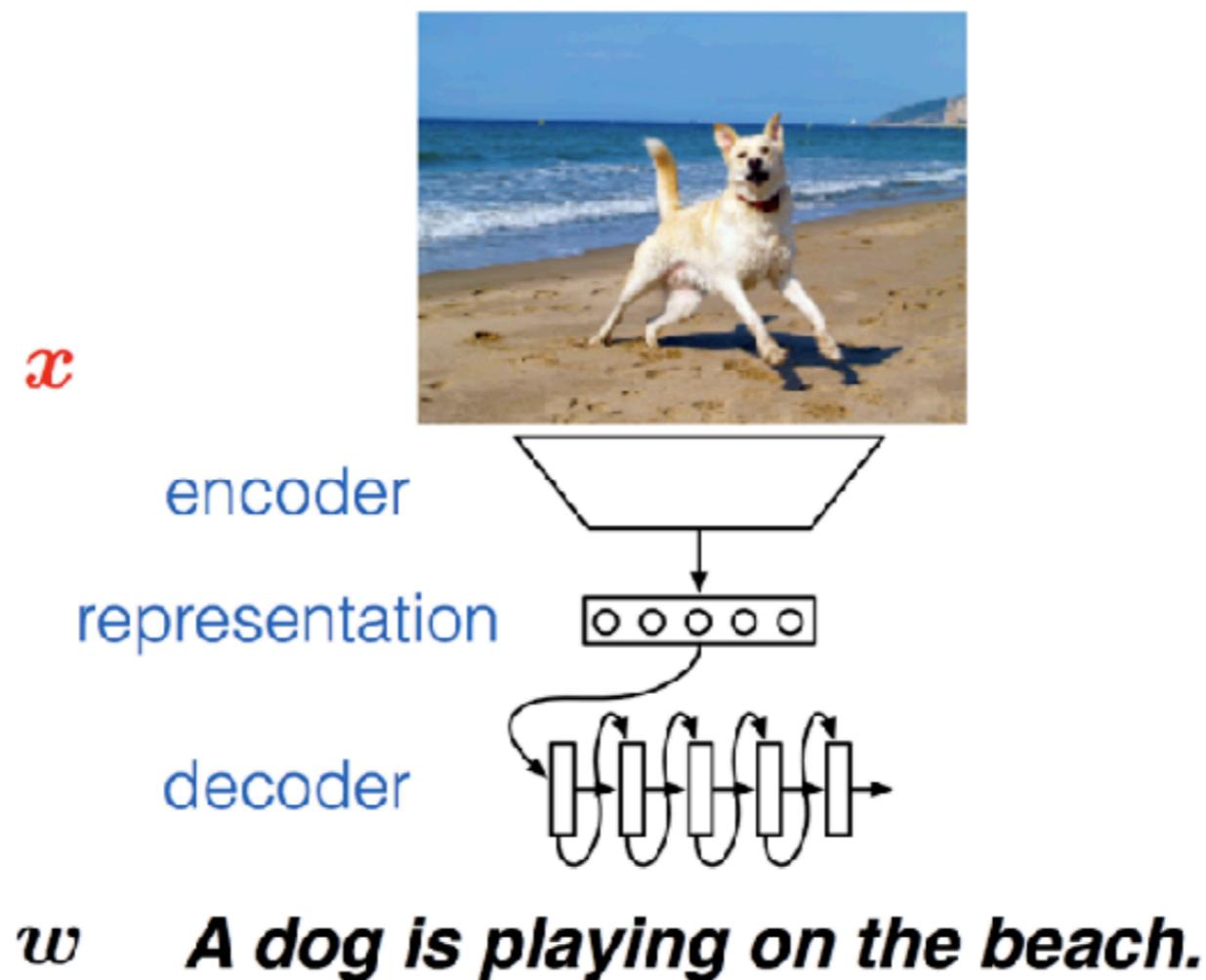
These “encode” \mathbf{x} into a fixed-sized vector and “decode” that into a sequence of words \mathbf{w} .



Encoder-Decoder Models

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These “encode” \mathbf{x} into a fixed-sized vector and “decode” that into a sequence of words \mathbf{w} .



Encoder-Decoder Models

Two questions

- How do we encode $\textcolor{red}{x}$ into a fixed-sized vector?
 - Problem/modality specific
 - Think about assumptions!
- How do we decode that vector into a sequence of words w ?
 - Less problem specific (general decoders?)
 - We now describe a solution using RNNs.

Recurrent Neural Networks (RNNs)

$$\mathbf{h}_t = f(\mathbf{h}_{t-1}, \mathbf{x}_t)$$

$$\mathbf{c} = \text{RNN}(\mathbf{x}) \quad 0$$

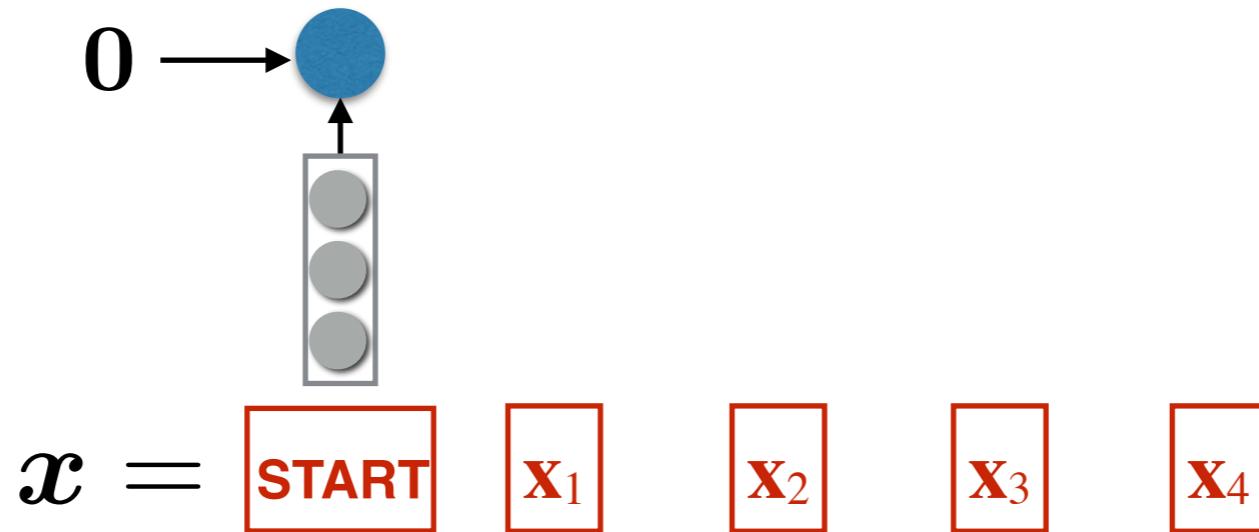
$$\mathbf{x} = \boxed{\text{START}} \quad \boxed{\mathbf{x}_1} \quad \boxed{\mathbf{x}_2} \quad \boxed{\mathbf{x}_3} \quad \boxed{\mathbf{x}_4}$$

What is a vector representation of a sequence \mathbf{x} ?

Recurrent Neural Networks (RNNs)

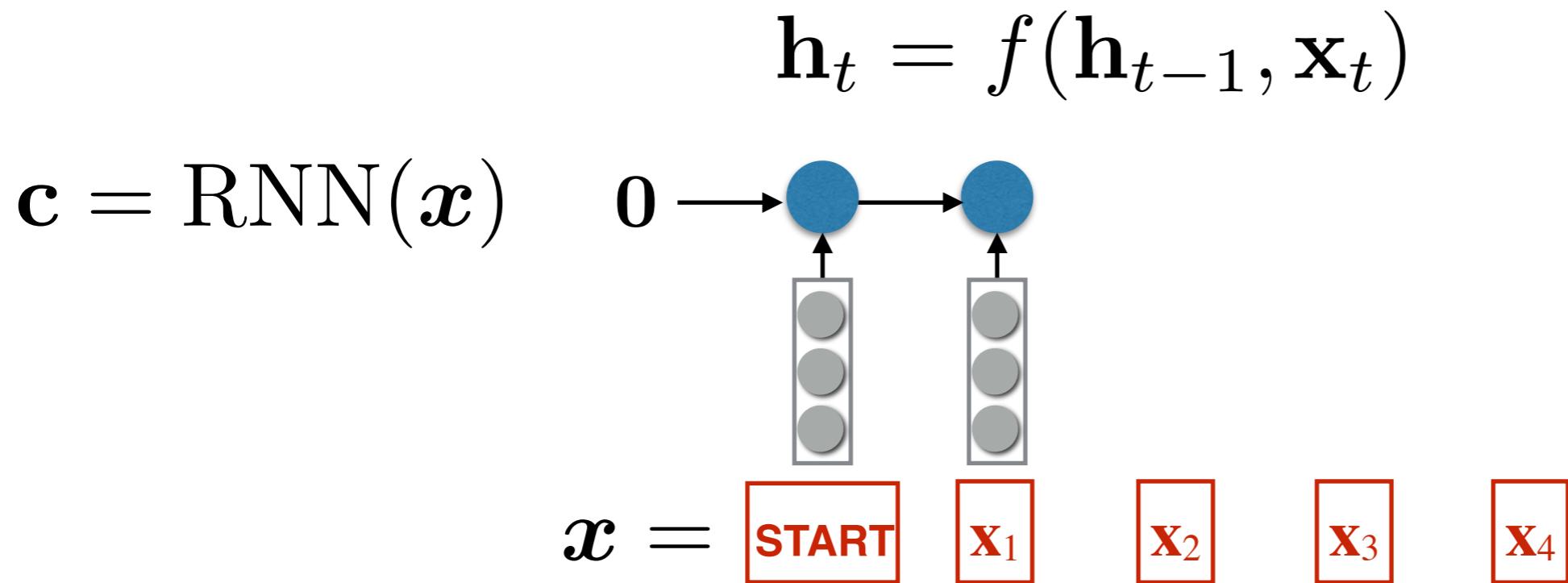
$$\mathbf{h}_t = f(\mathbf{h}_{t-1}, \mathbf{x}_t)$$

$$\mathbf{c} = \text{RNN}(\mathbf{x})$$



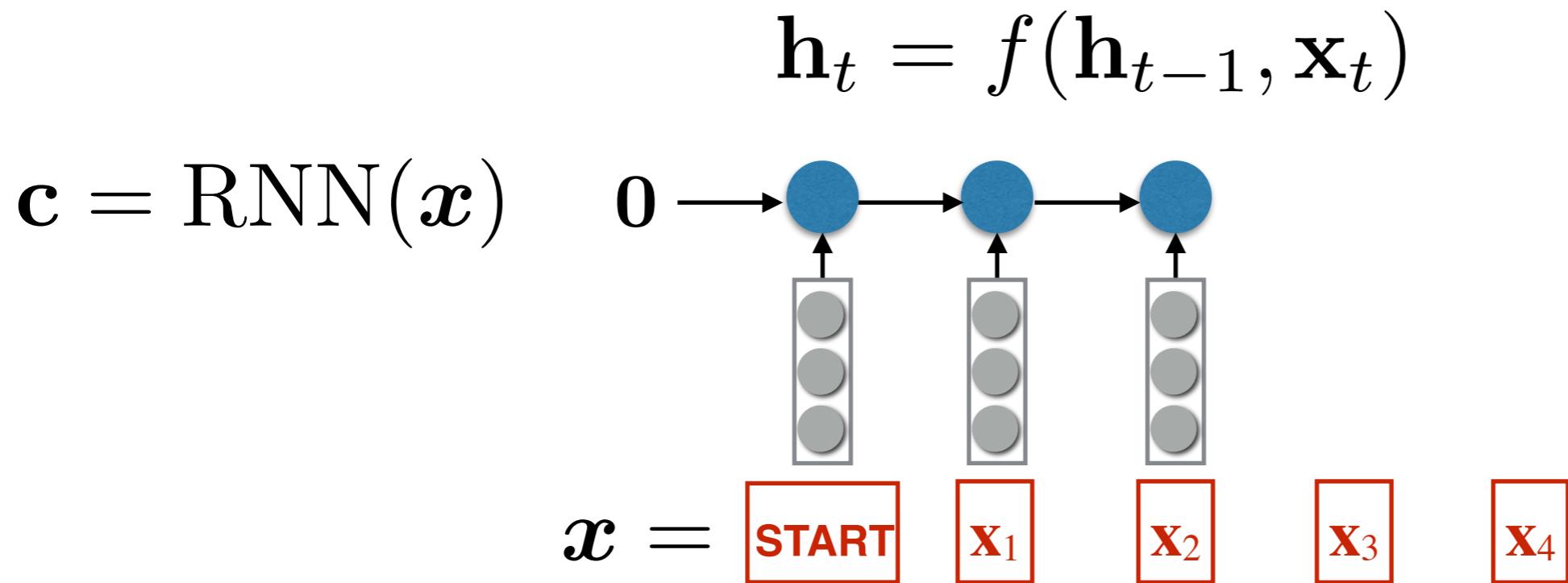
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Recurrent Neural Networks (RNNs)



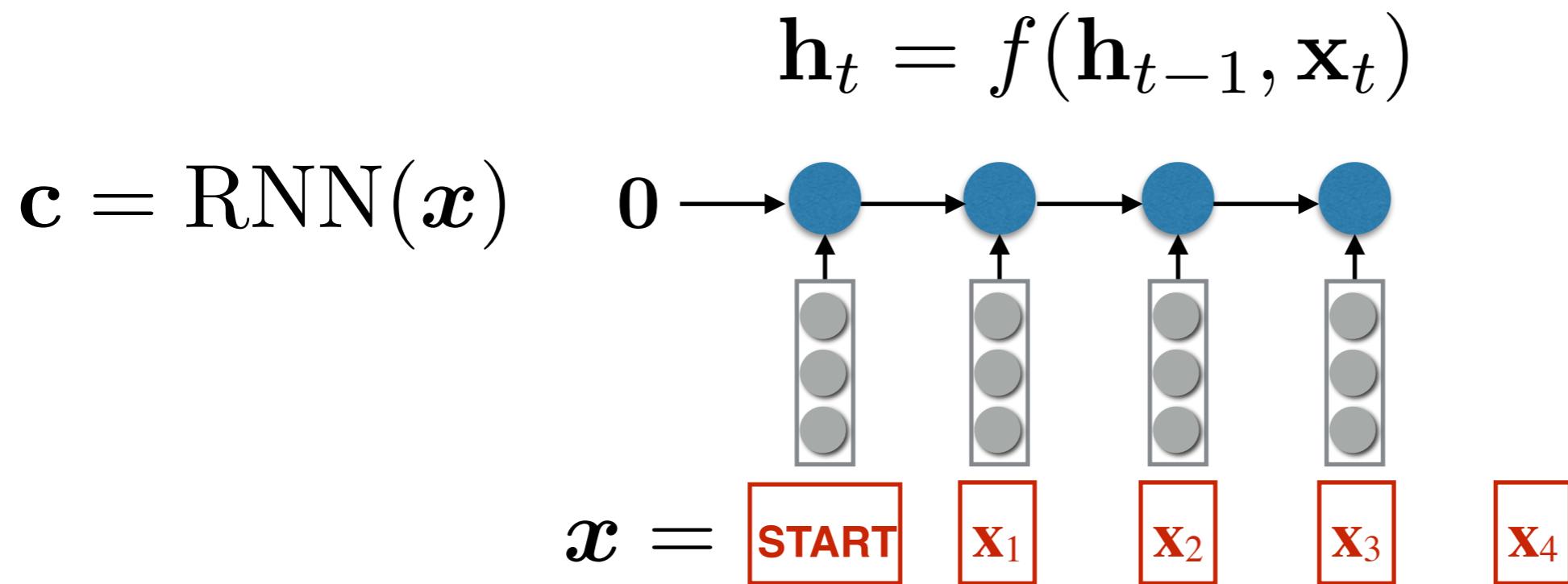
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Recurrent Neural Networks (RNNs)



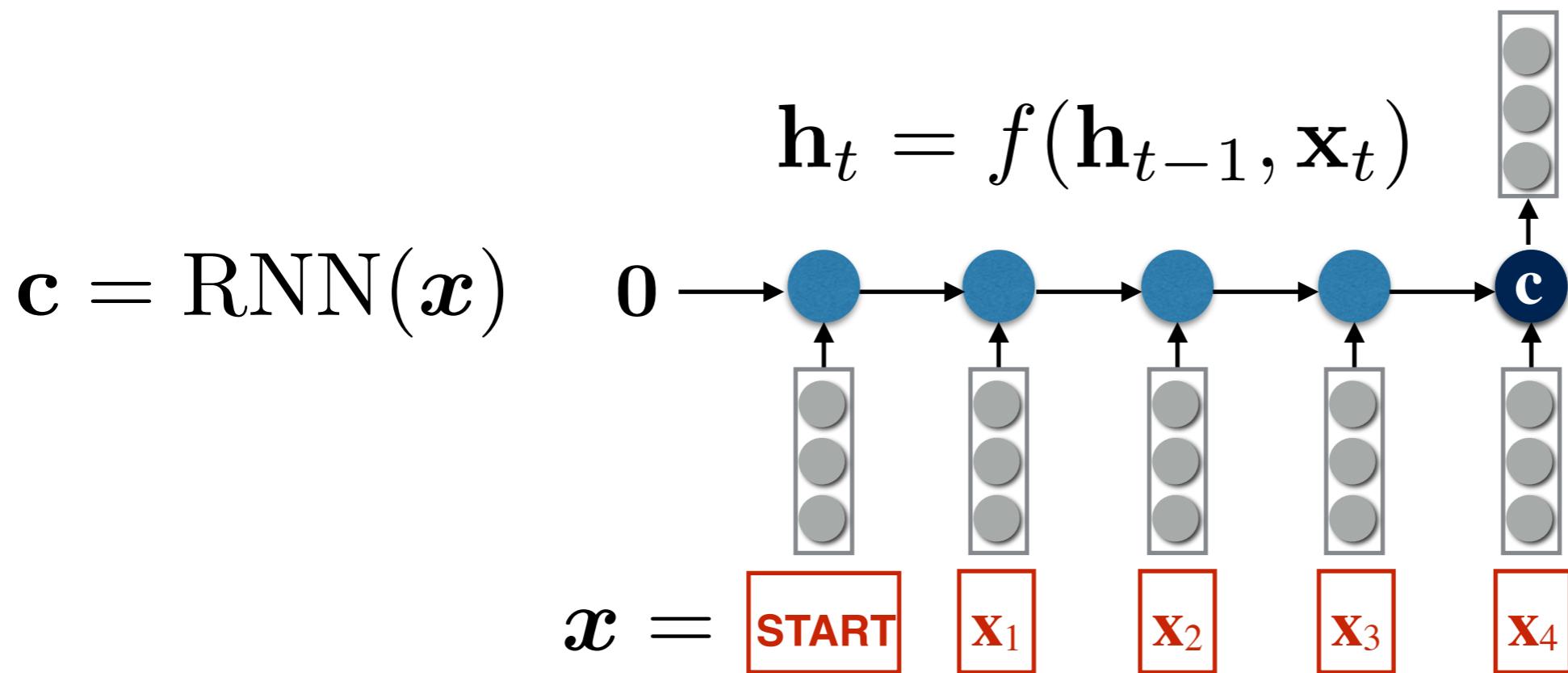
What is a vector representation of a sequence x ?

Recurrent Neural Networks (RNNs)



What is a vector representation of a sequence x ?

Recurrent Neural Networks (RNNs)



What is a vector representation of a sequence x ?

RNN Encoder-Decoders

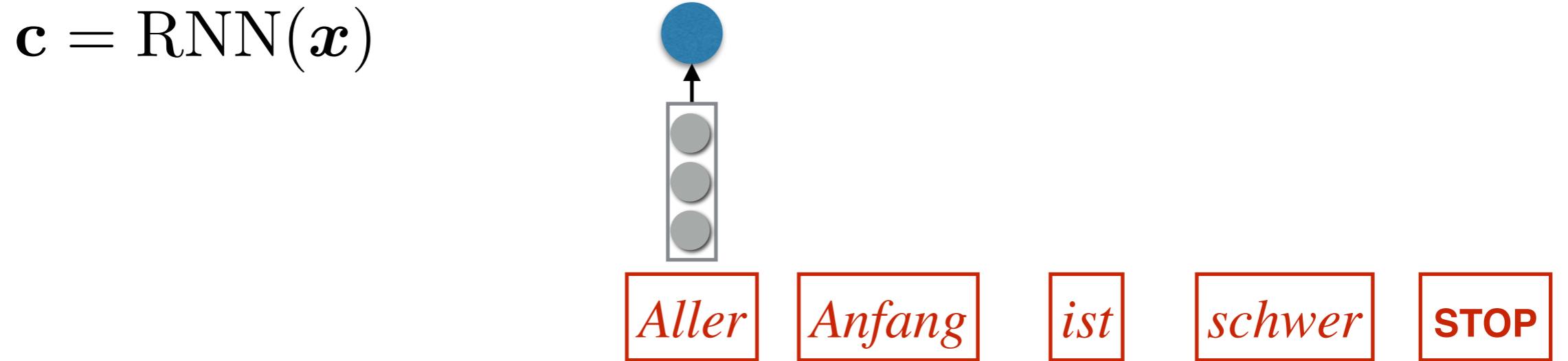
$$\mathbf{c} = \text{RNN}(\mathbf{x})$$

Aller *Anfang* *ist* *schwer* **STOP**

What is the probability of a sequence $y \mid x$?

Cho et al. (2014); Sutskever et al. (2014)

RNN Encoder-Decoders

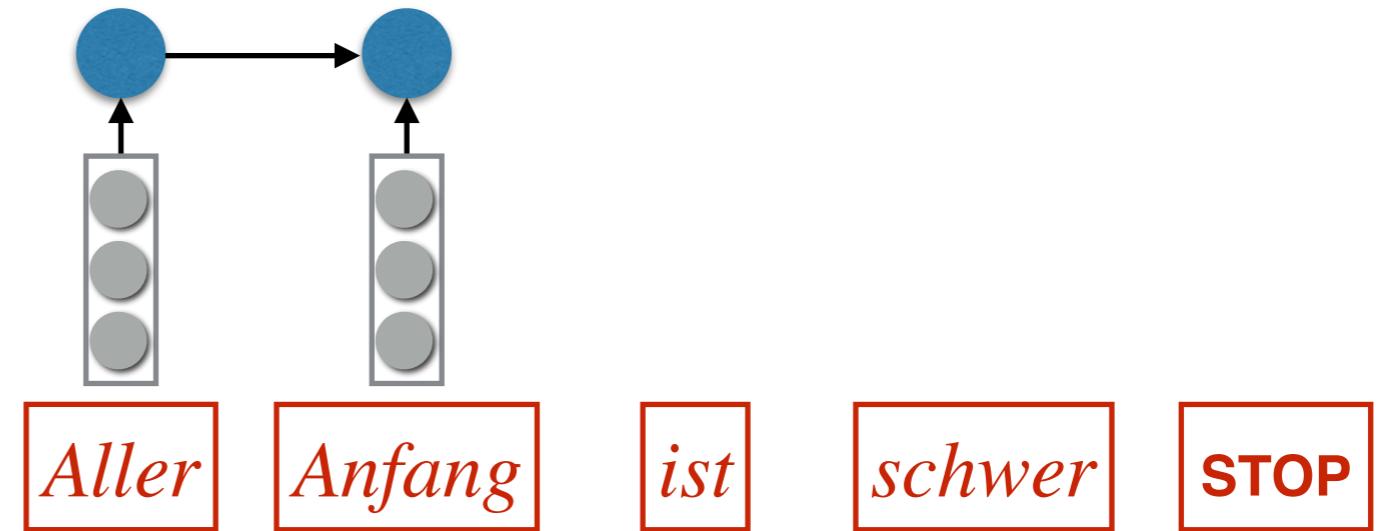


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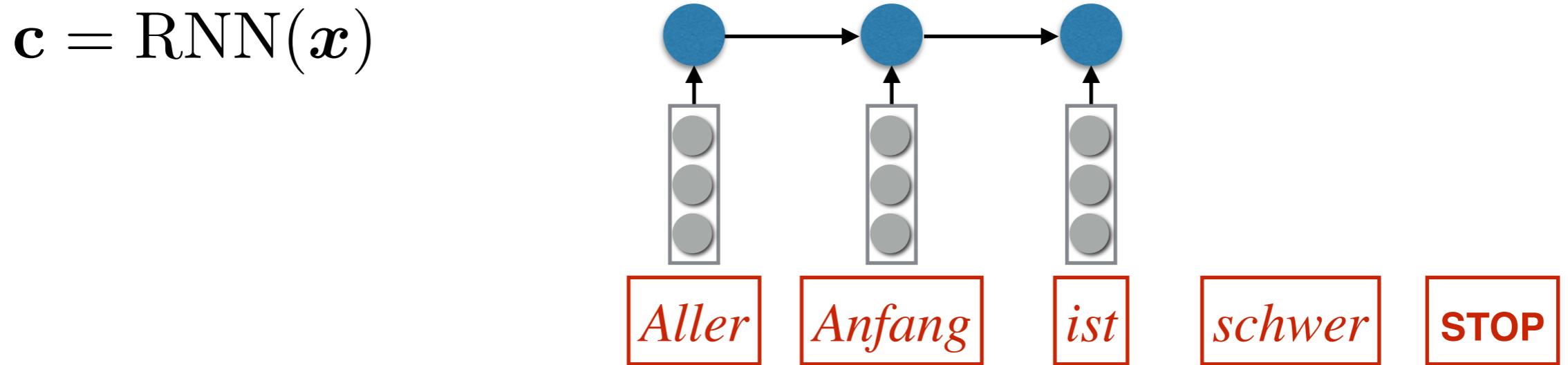
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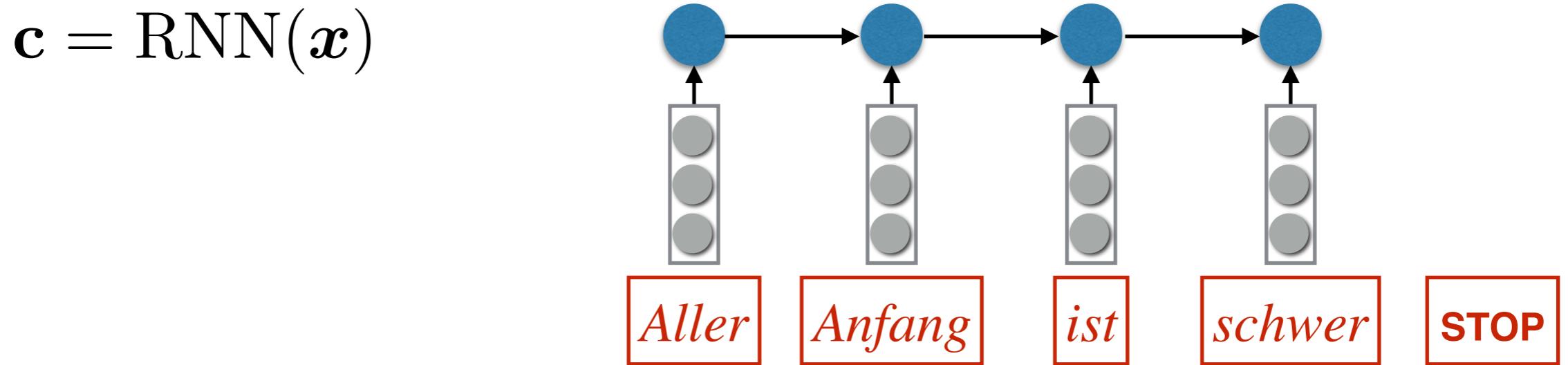
RNN Encoder-Decoders



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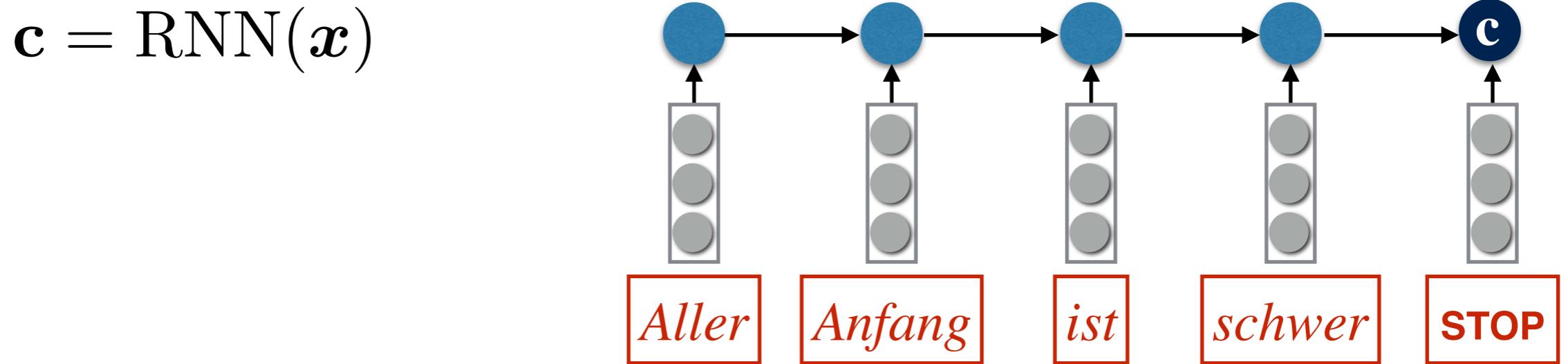
RNN Encoder-Decoders



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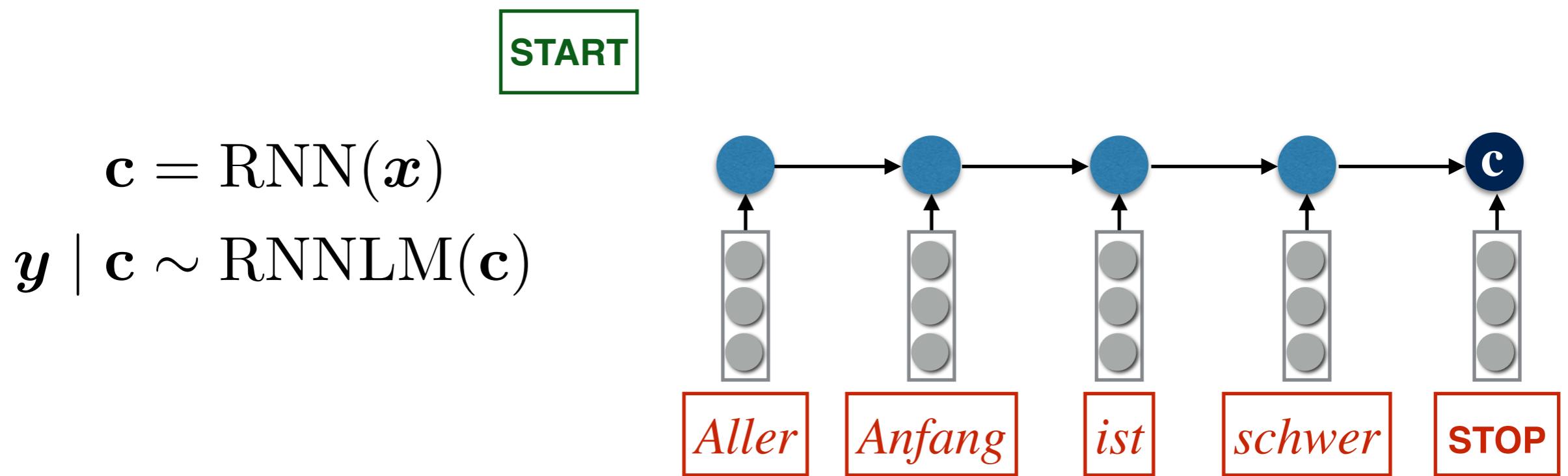
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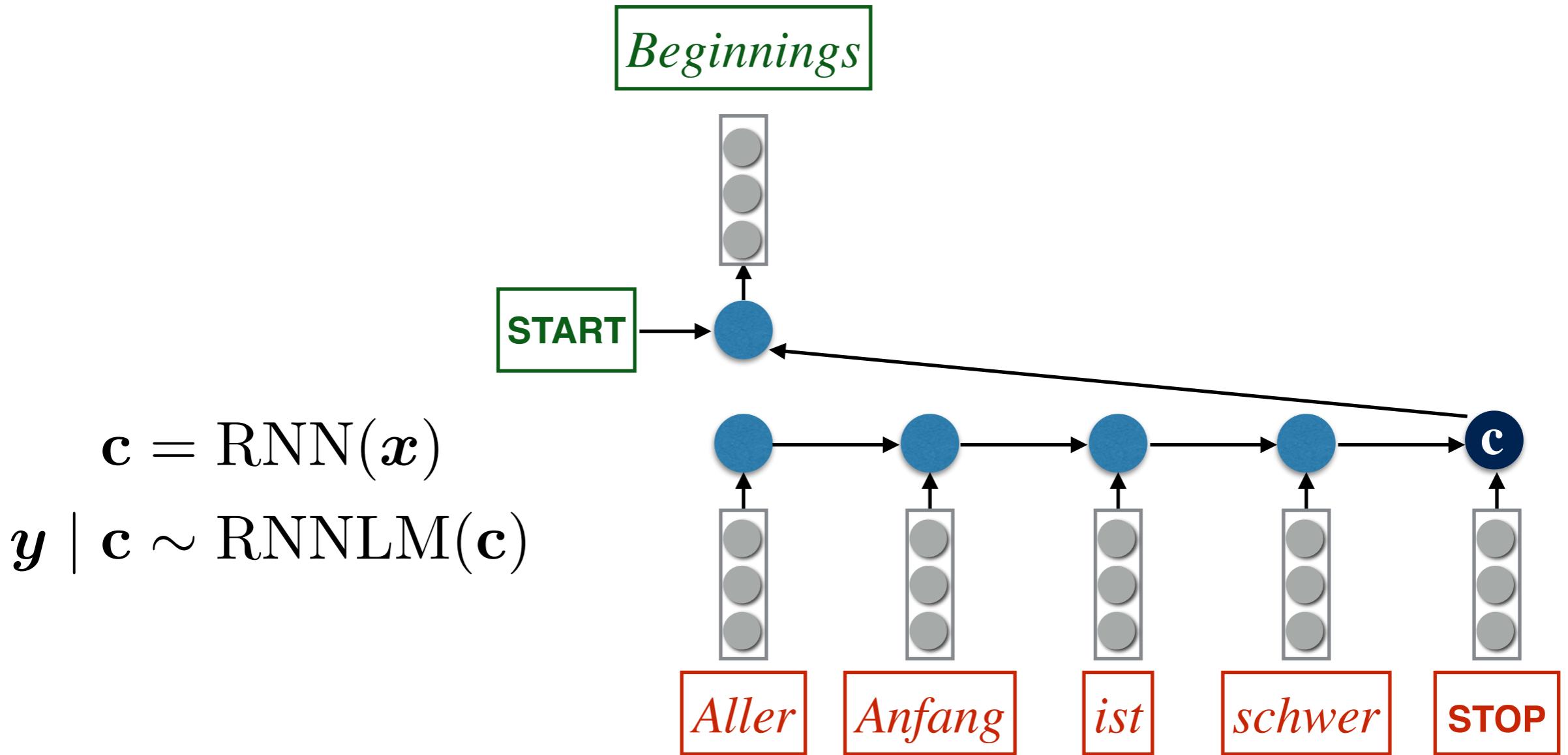
RNN Encoder-Decoders



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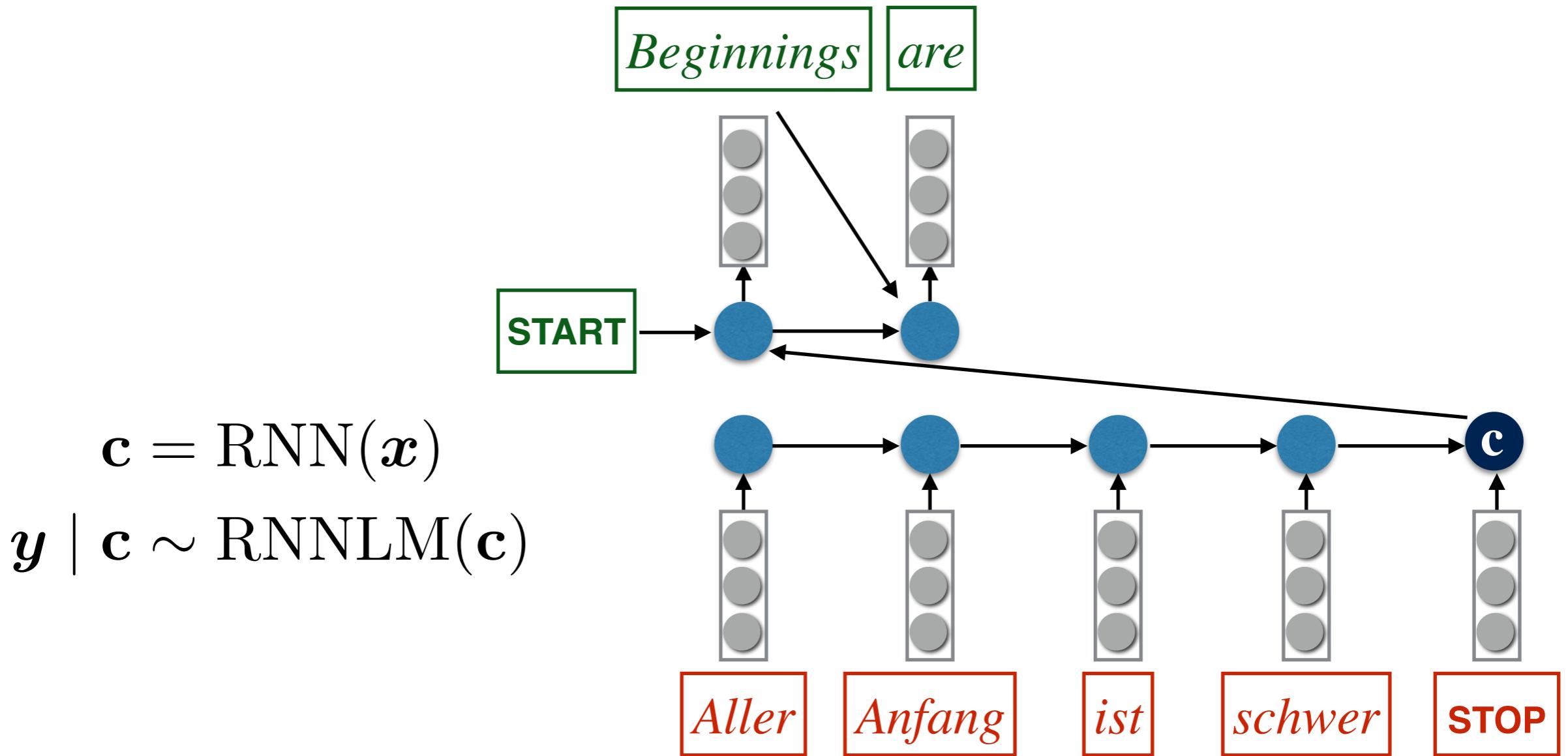
RNN Encoder-Decoders



What is the probability of a sequence $y | x$?

Cho et al. (2014); Sutskever et al. (2014)

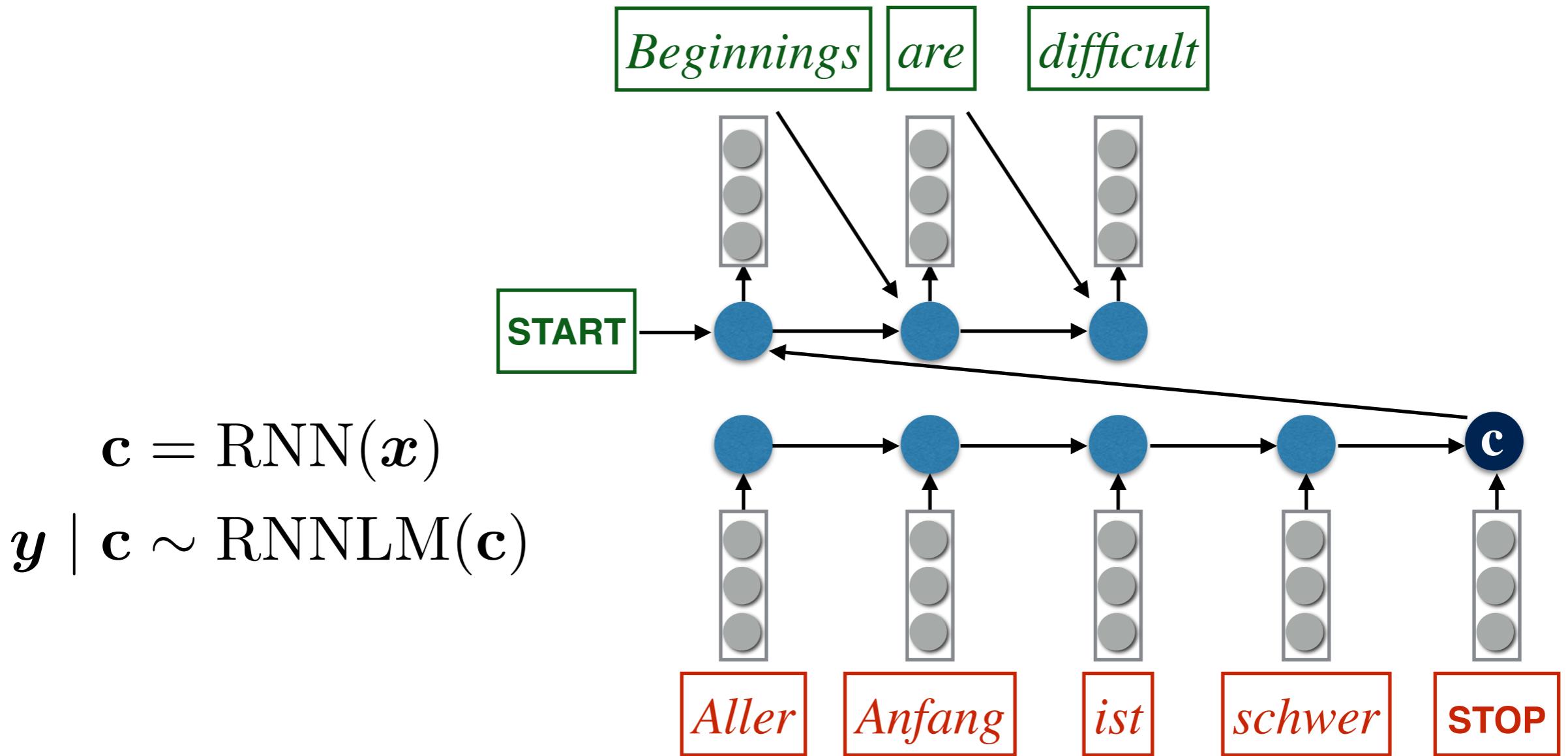
RNN Encoder-Decoders



What is the probability of a sequence $y \mid x$?

Cho et al. (2014); Sutskever et al. (2014)

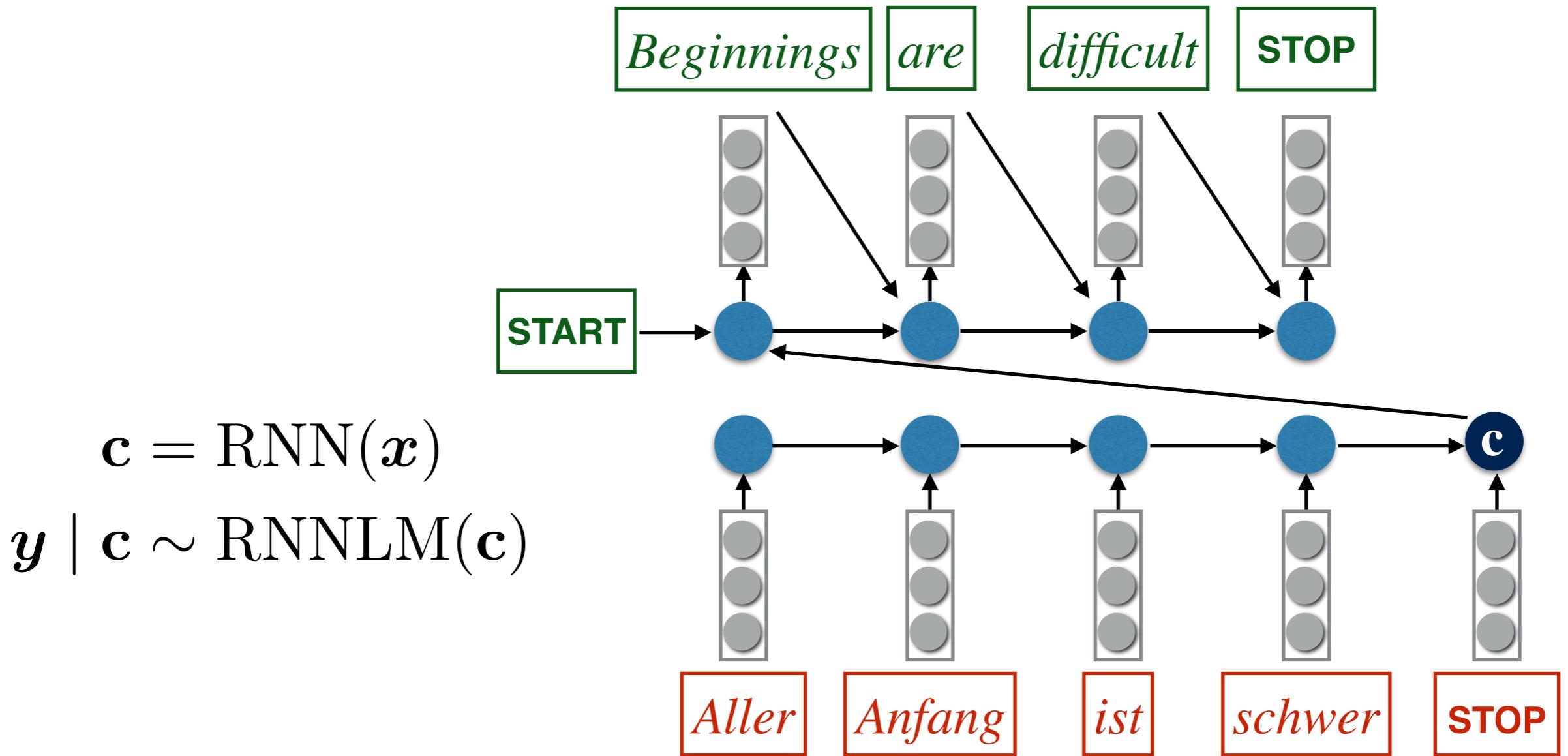
RNN Encoder-Decoders



What is the probability of a sequence $y \mid x$?

Cho et al. (2014); Sutskever et al. (2014)

RNN Encoder-Decoders



What is the probability of a sequence $y \mid x$?

Cho et al. (2014); Sutskever et al. (2014)

Conditional LMs

Algorithms for Decoding

In general, we want to find the most probable (MAP) output given the input, i.e.,

$$\begin{aligned} \mathbf{w}^* &= \arg \max_{\mathbf{w}} p(\mathbf{w} \mid \mathbf{x}) \\ &= \arg \max_{\mathbf{w}} \sum_{t=1}^{|\mathbf{w}|} \log p(w_t \mid \mathbf{x}, \mathbf{w}_{<t}) \end{aligned}$$

Unlike with Markov models, this is a hard problem. But we can approximate it with a **greedy search**:

$$\begin{aligned} w_1^* &\approx \arg \max_{w_1} p(w_1 \mid \mathbf{x}) \\ w_1^* &\approx \arg \max_{w_2} p(w_2 \mid \mathbf{x}, w_1) \\ &\vdots \\ w_t^* &\approx \arg \max_{w_t} p(w_t \mid \mathbf{x}, \mathbf{w}_{<t}^*) \end{aligned}$$

Beam search for decoding

A slightly better approximation is to use a **beam search** with beam size b . Key idea: keep track of the top- b hypotheses.

E.g., for $b=2$:

$\textcolor{red}{x} = Bier trinke ich$

beer drink |

$\langle s \rangle$

logprob=0

w_0

w_1

w_2

w_3

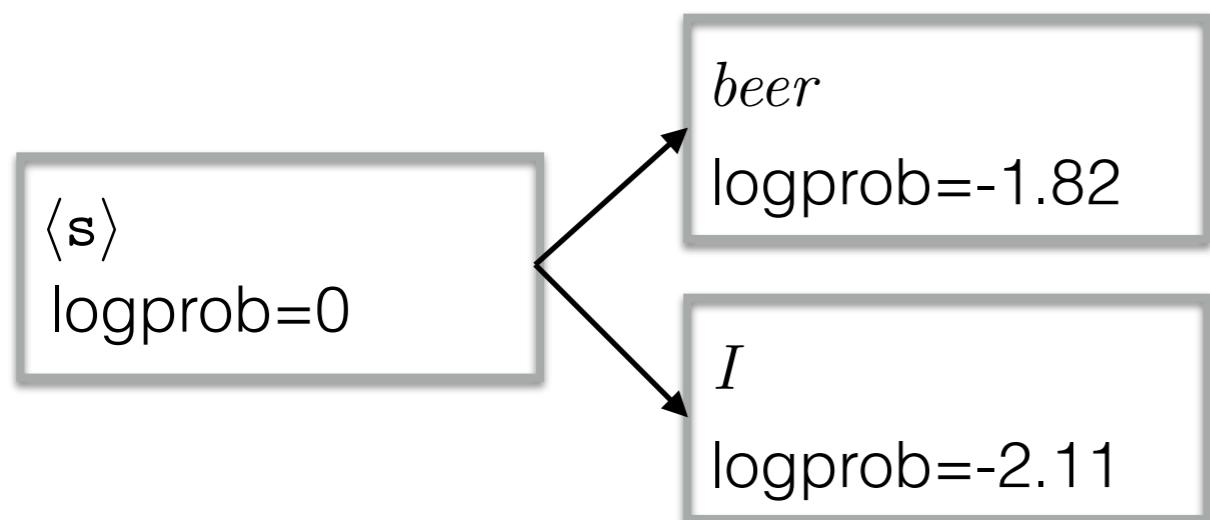
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beer drink |



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$\textcolor{red}{x} = Bier trinke ich$

beer drink |

$\langle s \rangle$
logprob=0

beer
logprob=-1.82

I
logprob=-2.11

drink
logprob=-6.93

I
logprob=-5.8

w_0

w_1

w_2

w_3

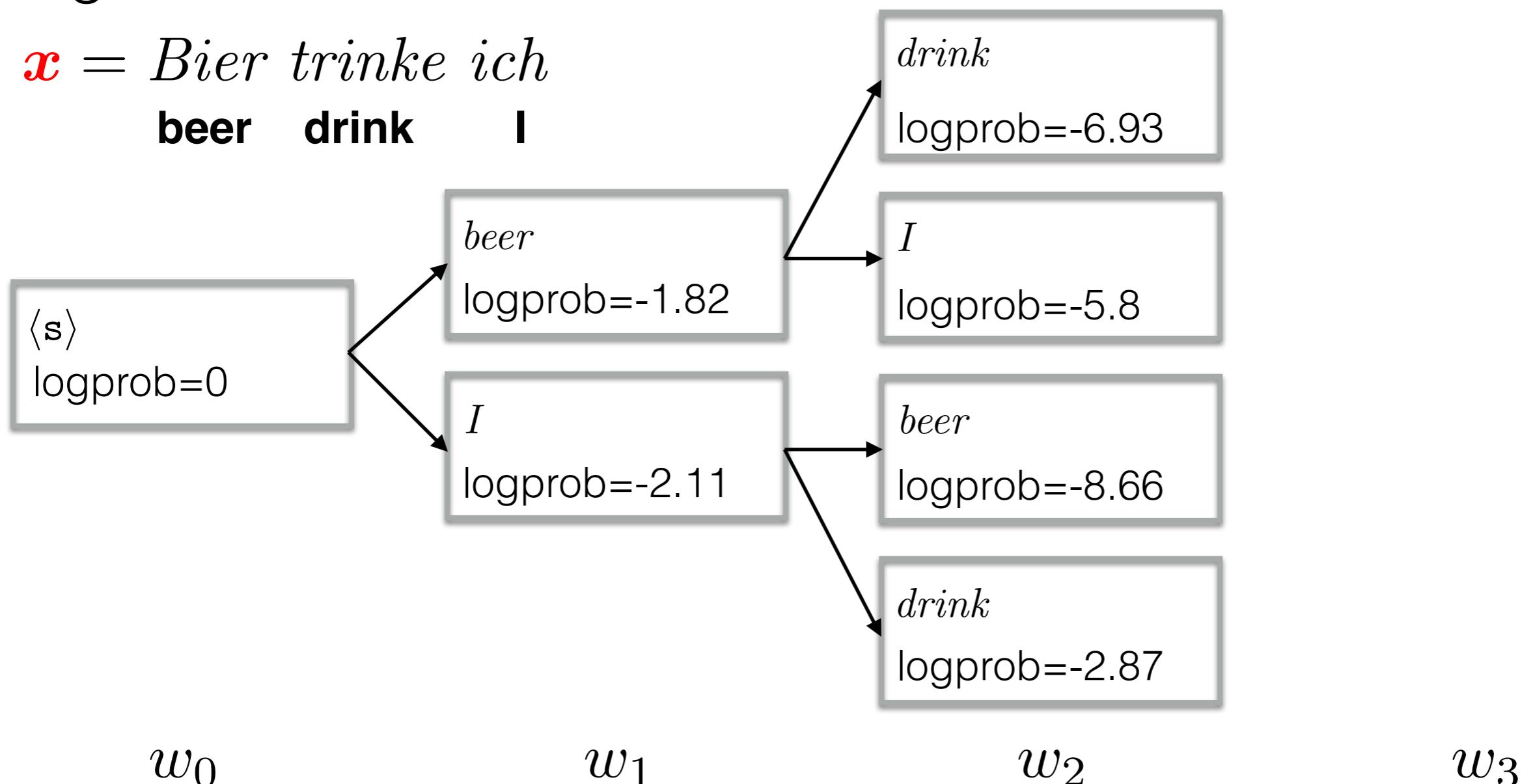
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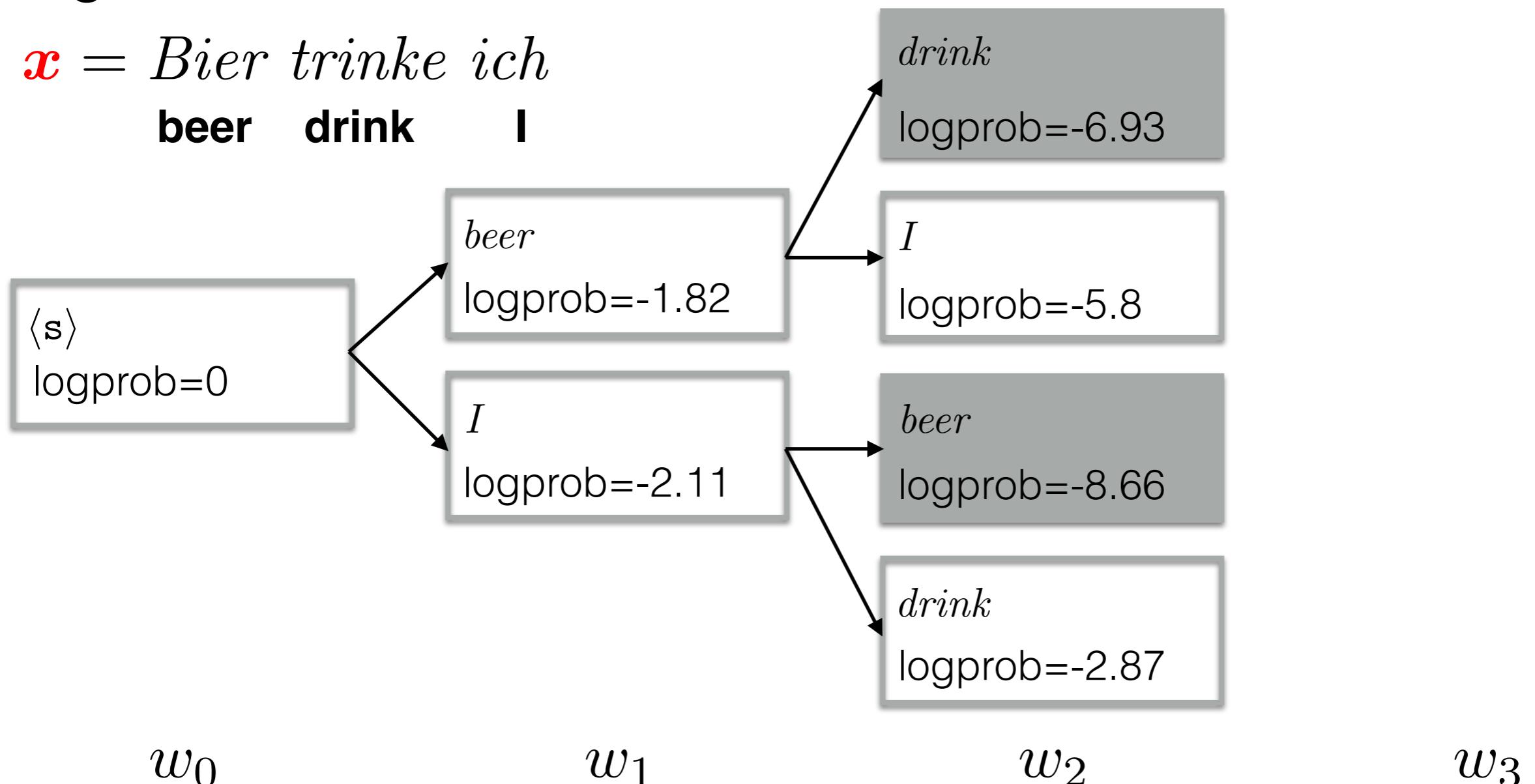
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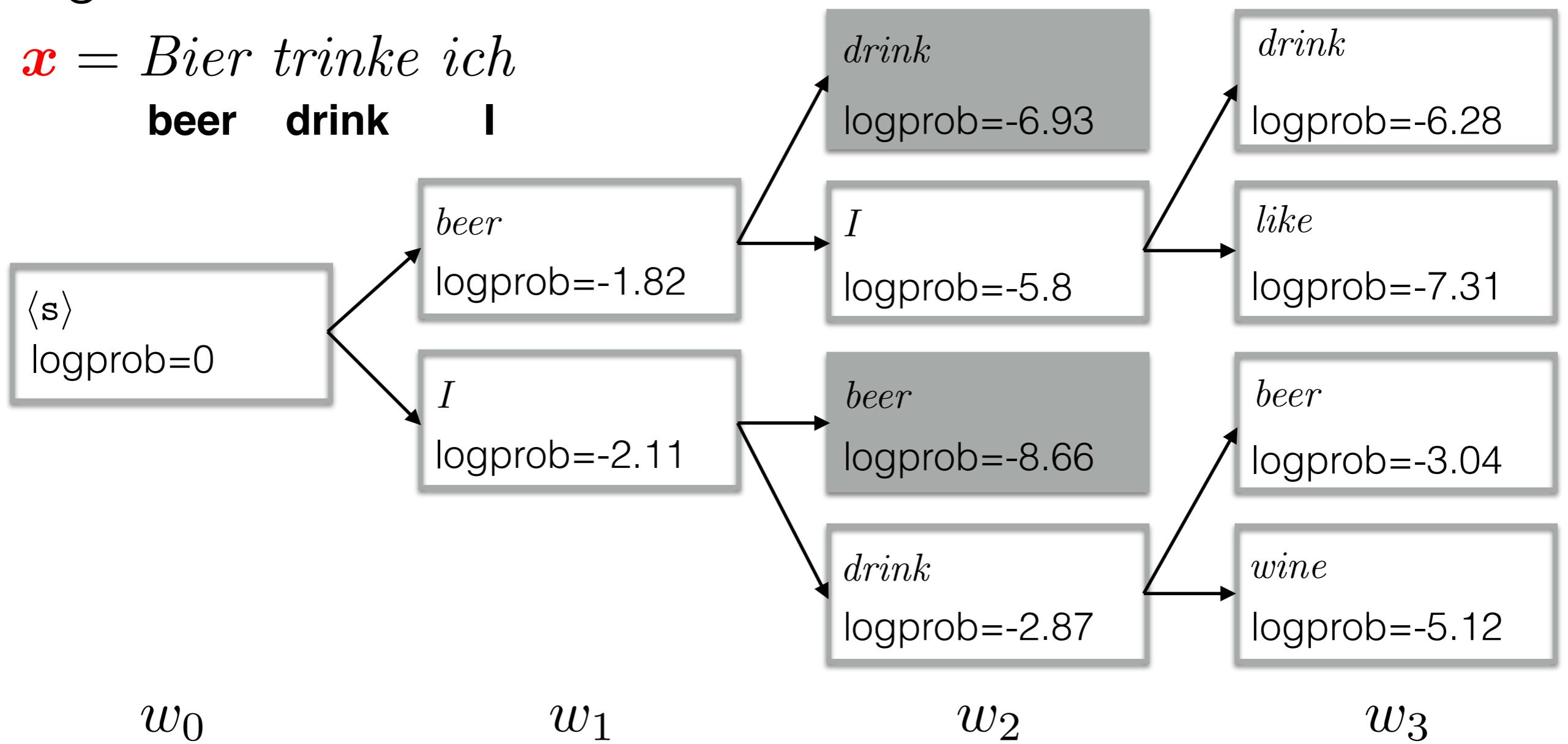
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beer **drink** |



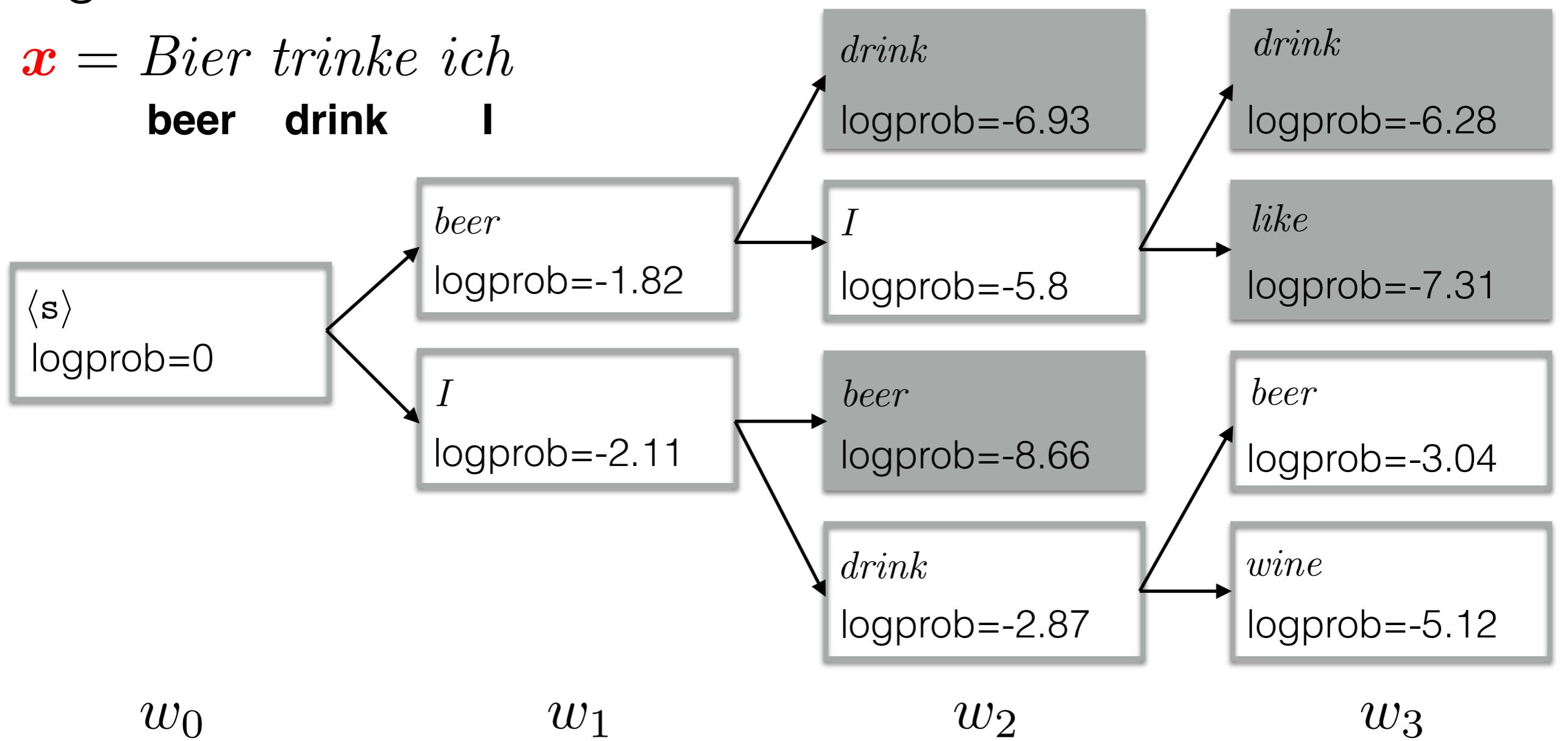
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$\textcolor{red}{x} = \textit{Bier trinke ich}$

beer **drink** |

$\langle s \rangle$
logprob=0

$beer$
logprob=-1.82

I
logprob=-2.11

$drink$
logprob=-6.93

I
logprob=-5.8

$beer$
logprob=-8.66

$drink$
logprob=-2.87

$drink$
logprob=-6.28

$like$
logprob=-7.31

$beer$
logprob=-3.04

$wine$
logprob=-5.12

w_0

w_1

w_2

w_3

Questions?

Conditioning with vectors

Encoder-decoder models like this compress a lot of information in a vector.

Gradients have a long way to travel. Even LSTMs forget.

What is to be done?

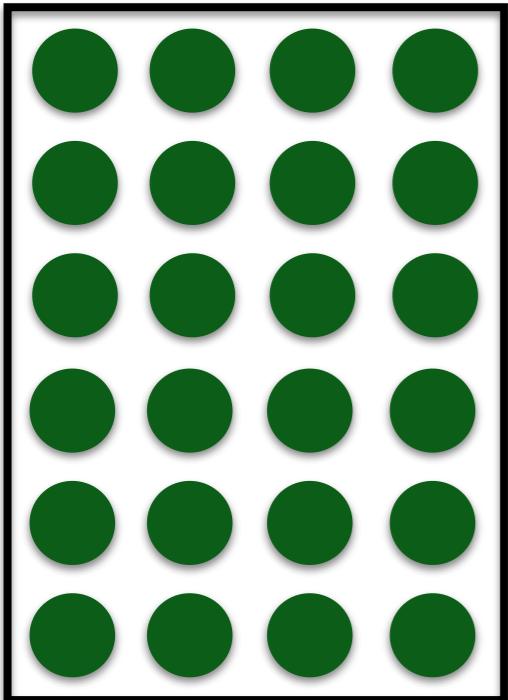
Translation with Attention

- Represent a source sentence as a matrix
- Generate a target sentence from a matrix
- These two steps are:
 - An algorithm for neural MT
 - A way of introducing **attention**

Sentences as Matrices

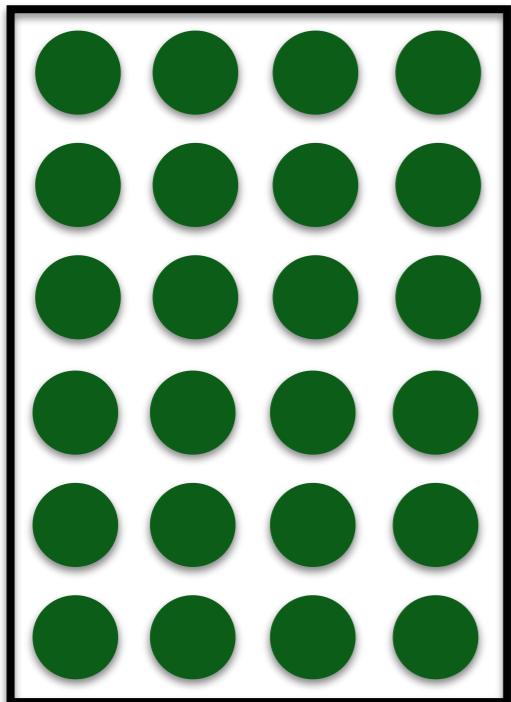
- Problem with the fixed-size vector model in translation (maybe in images?)
 - Sentences are of different sizes but vectors are of the same size
- Solution: use matrices instead
 - Fixed number of rows, but number of columns depends on the number of words
 - Usually $|\mathbf{f}| = \#cols$

Sentences as Matrices



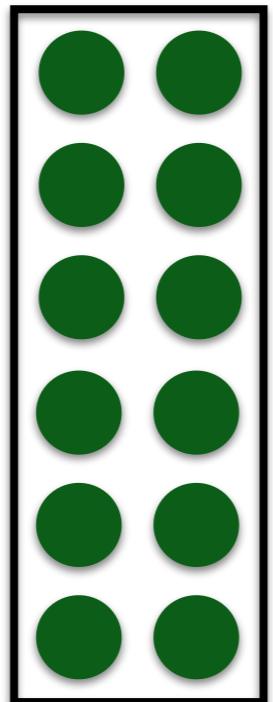
Ich möchte ein Bier

Sentences as Matrices

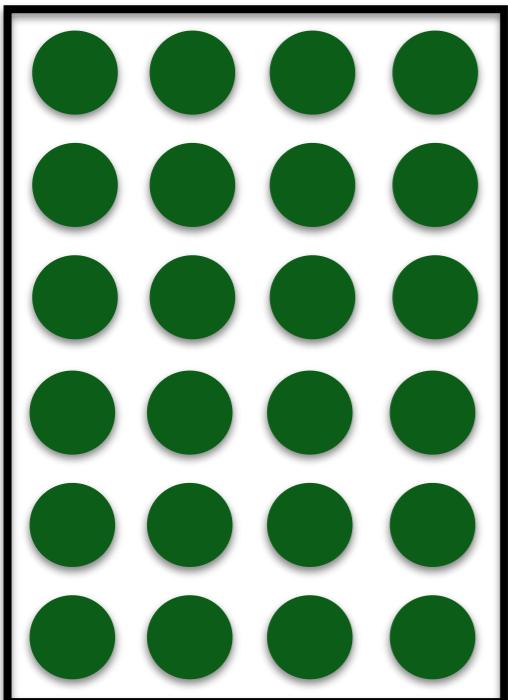


Ich möchte ein Bier

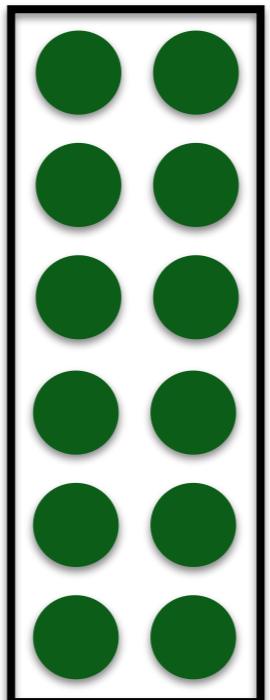
Mach's gut



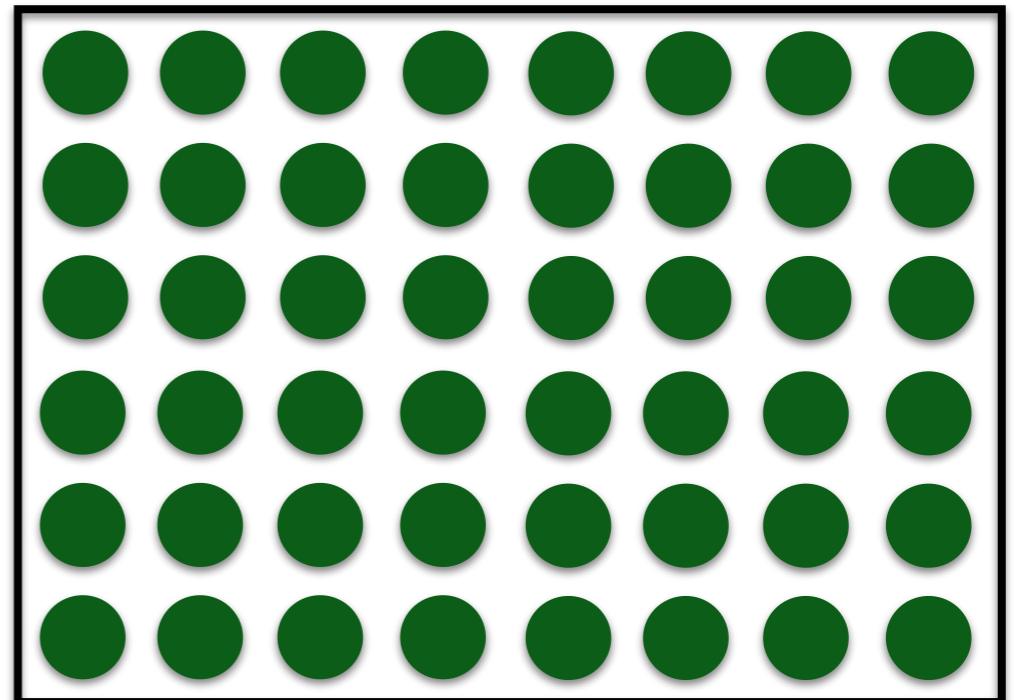
Sentences as Matrices



Ich möchte ein Bier

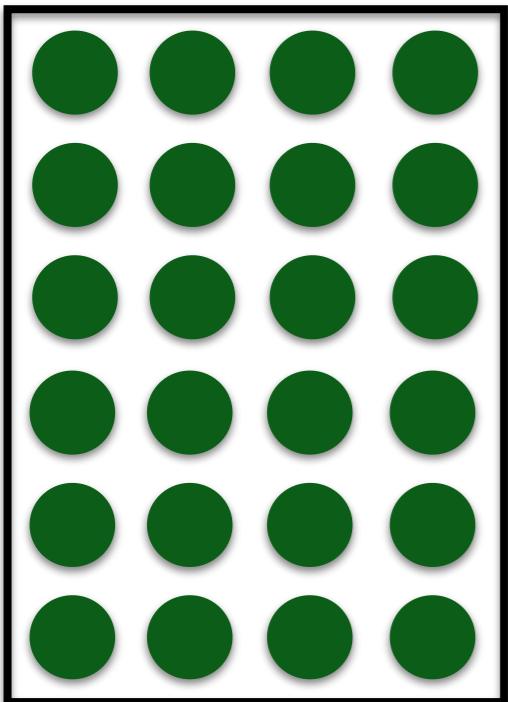


Mach's gut



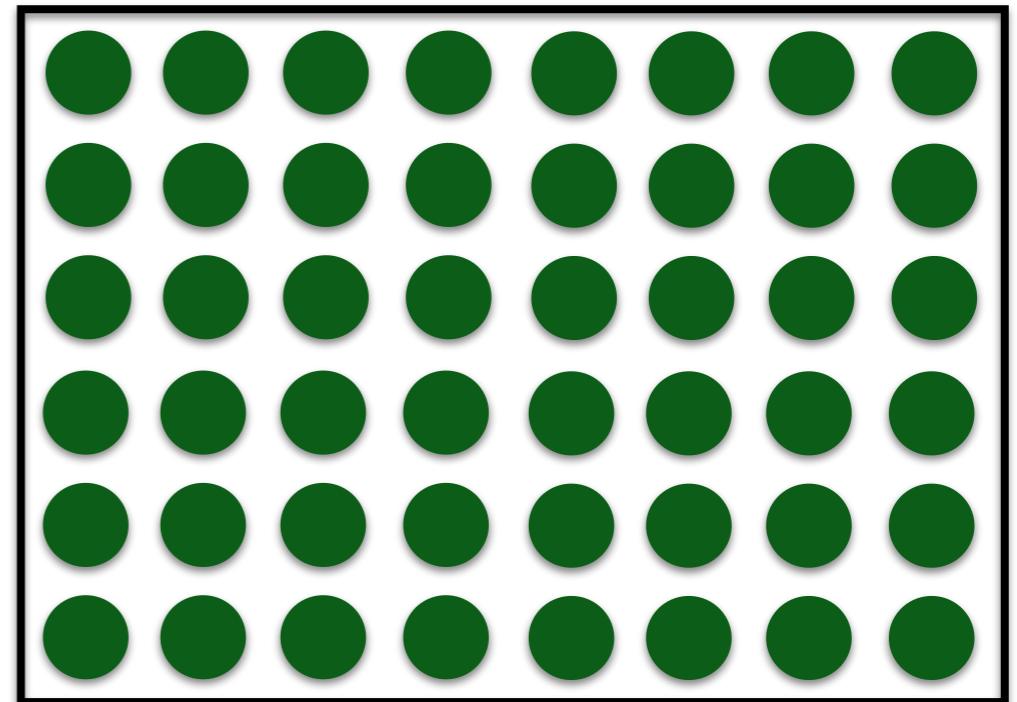
Die Wahrheiten der Menschen sind die unwiderlegbaren Irrtümer

Sentences as Matrices



Ich möchte ein Bier

Mach's gut



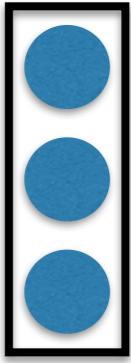
Die Wahrheiten der Menschen sind die unwiderlegbaren Irrtümer

Question: How do we build these matrices?

With Concatenation

- We can represent a sentence by stacking word vectors into a matrix representing a sentence
- This is easy and fast, but it has the following limitations
 - There is no positional information about the words in the representation
 - Word meanings depend on the context they are used in

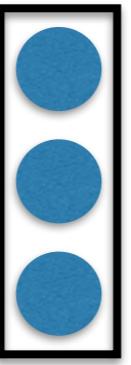
x_1



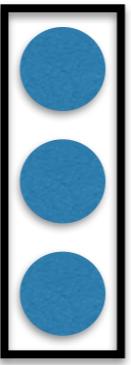
x_2



x_3



x_4



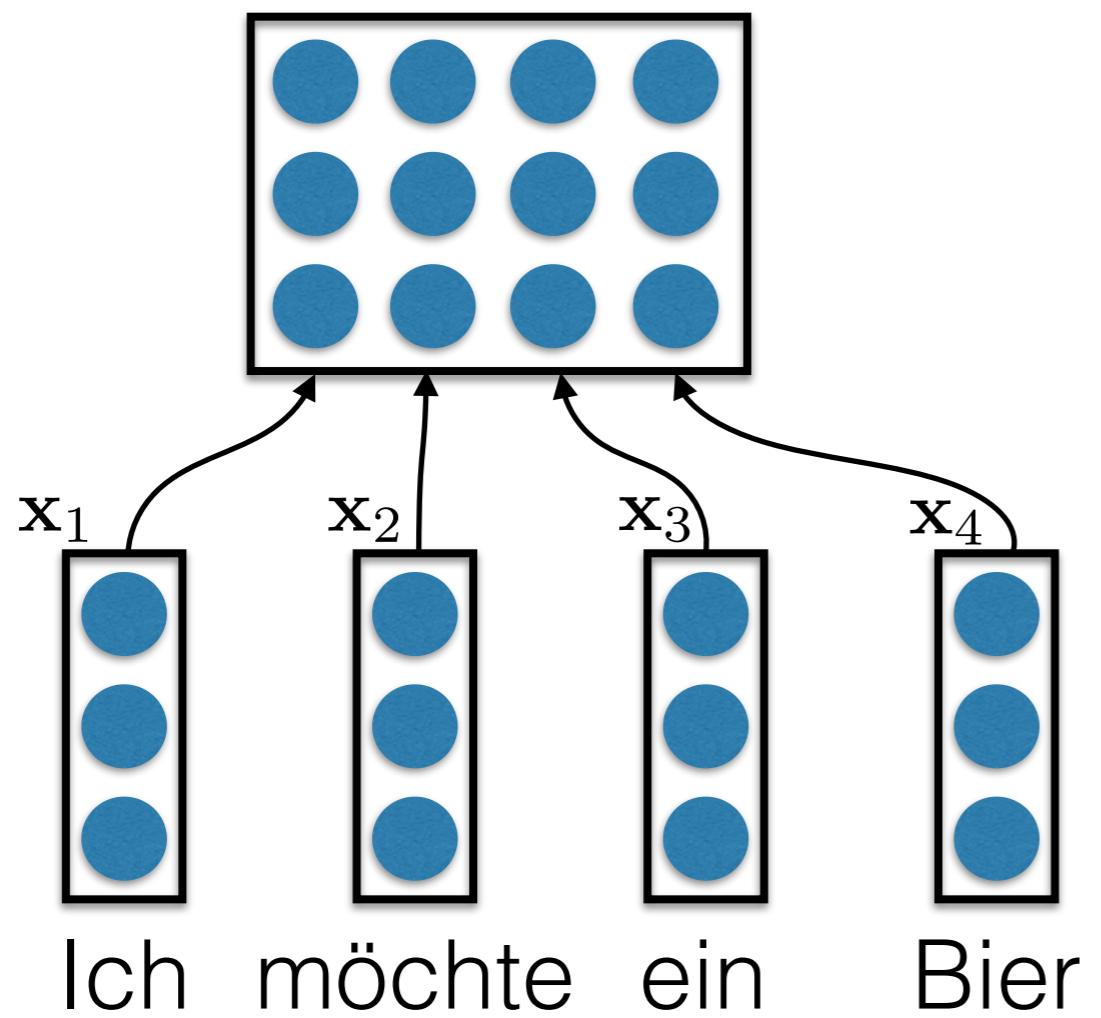
Ich

möchte

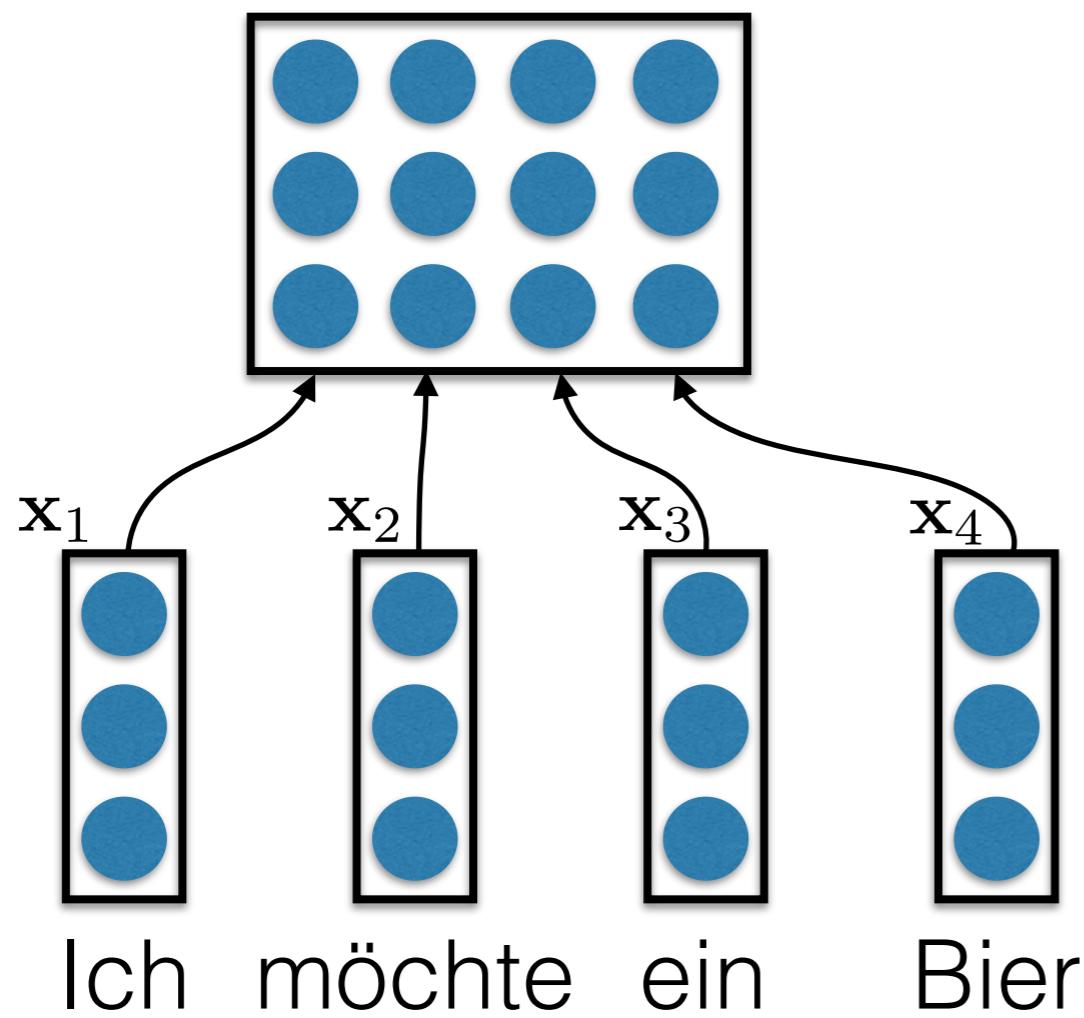
ein

Bier

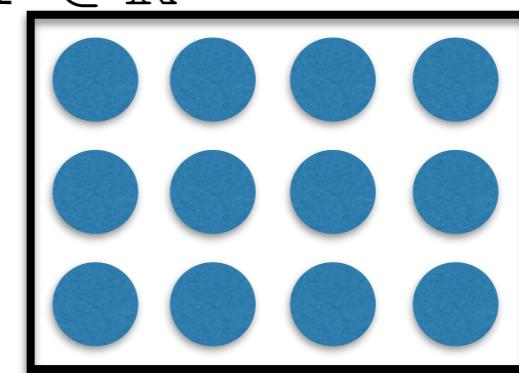
$$\mathbf{f}_i = \mathbf{x}_i$$



$$\mathbf{f}_i = \mathbf{x}_i$$



$$\mathbf{F} \in \mathbb{R}^{n \times |\mathcal{F}|}$$

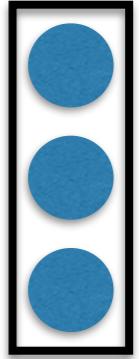


Ich möchte ein Bier

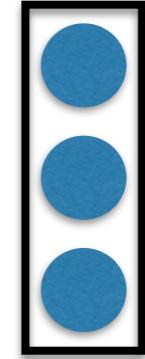
With Bidirectional RNNs

- A widely used matrix representation, due to Bahdanau et al (2015)
- One column per word
- Each column (word) has two halves concatenated together:
 - a “forward representation”, i.e., a word and its left context
 - a “reverse representation”, i.e., a word and its right context
- Implementation: bidirectional RNNs (GRUs or LSTMs) to read **f** from left to right and right to left, concatenate representations

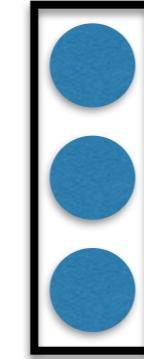
x_1



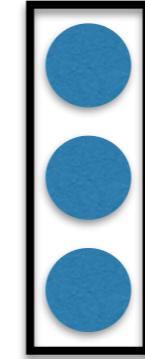
x_2



x_3

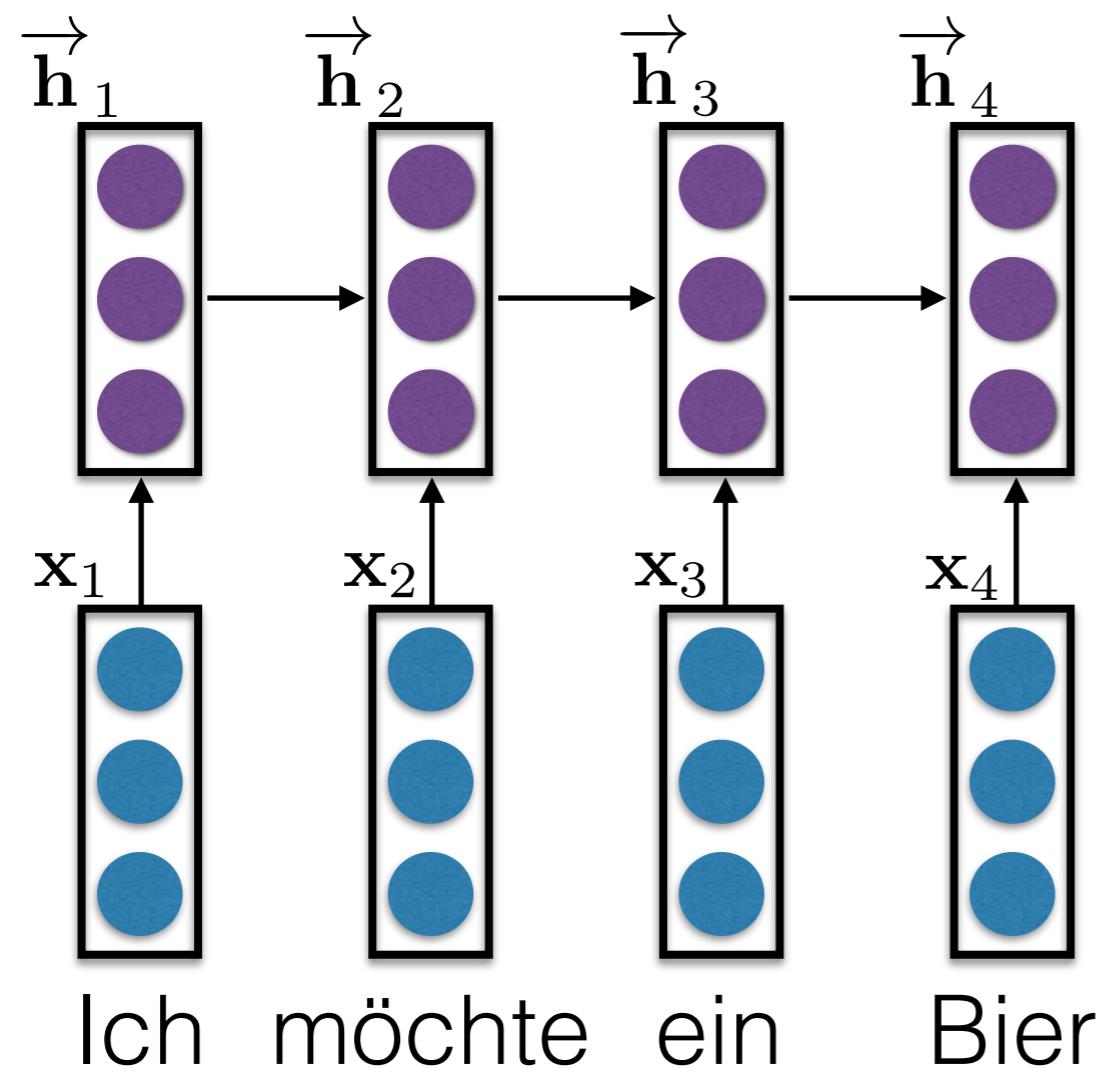


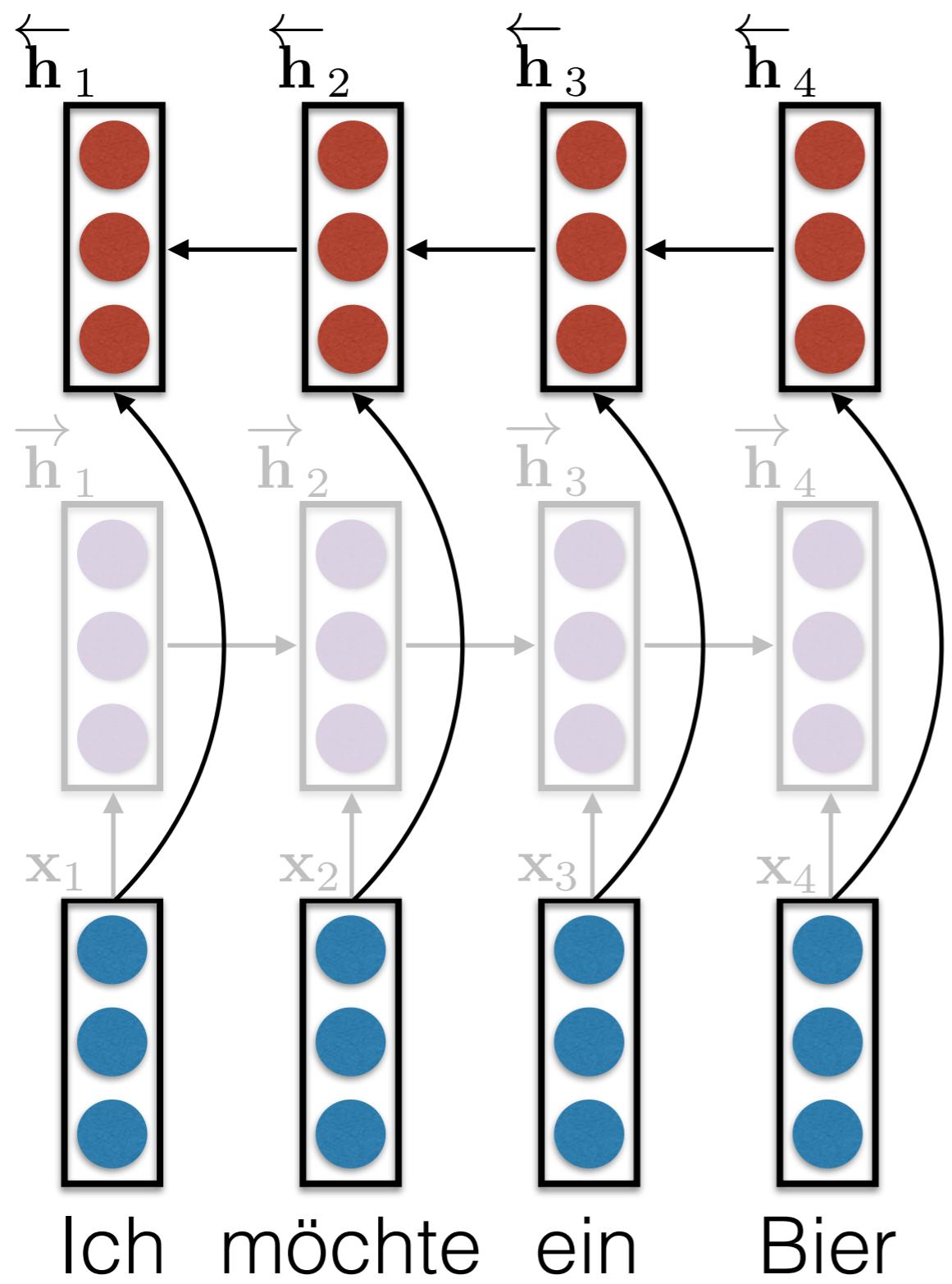
x_4



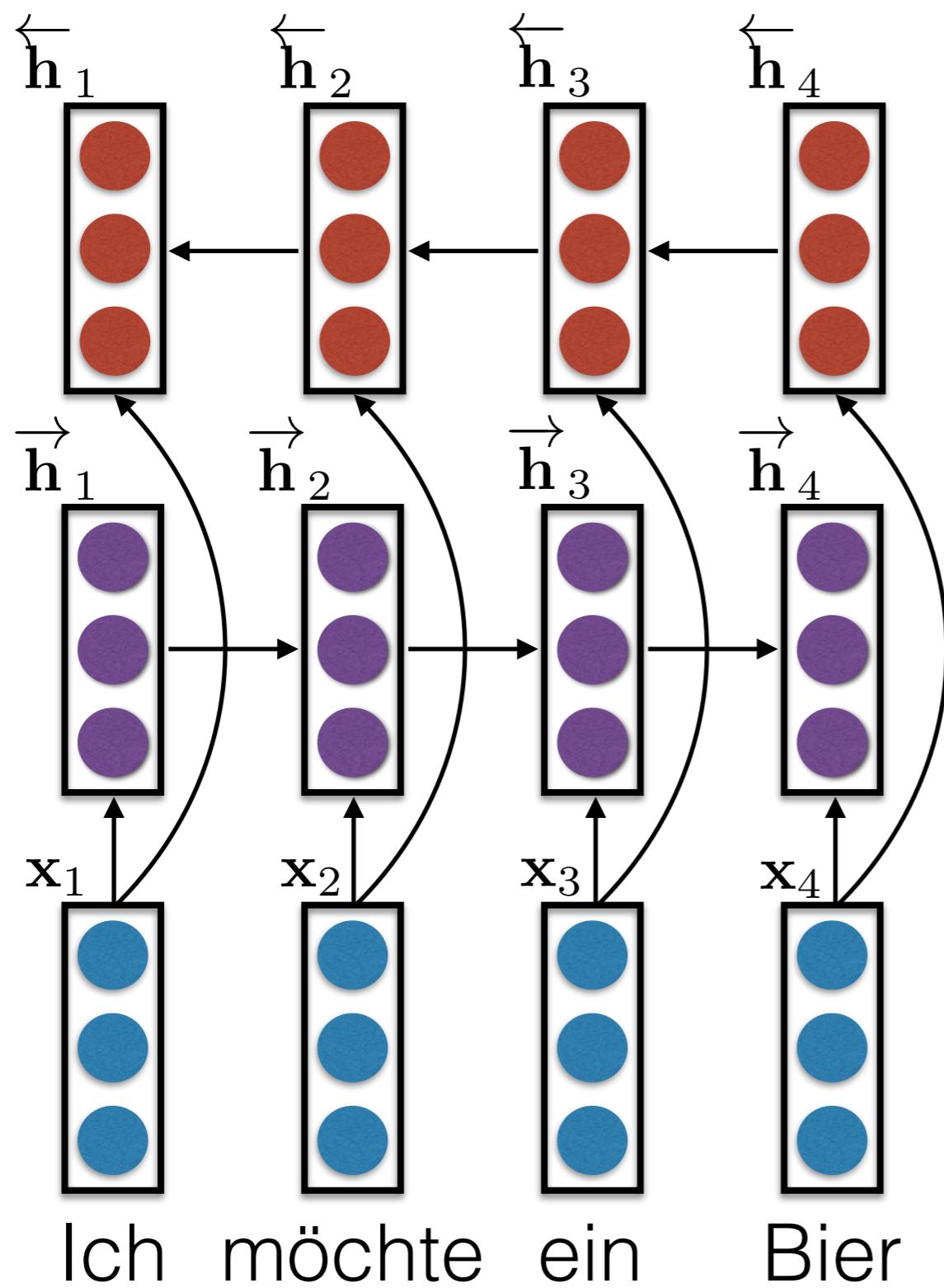
Ich möchte ein

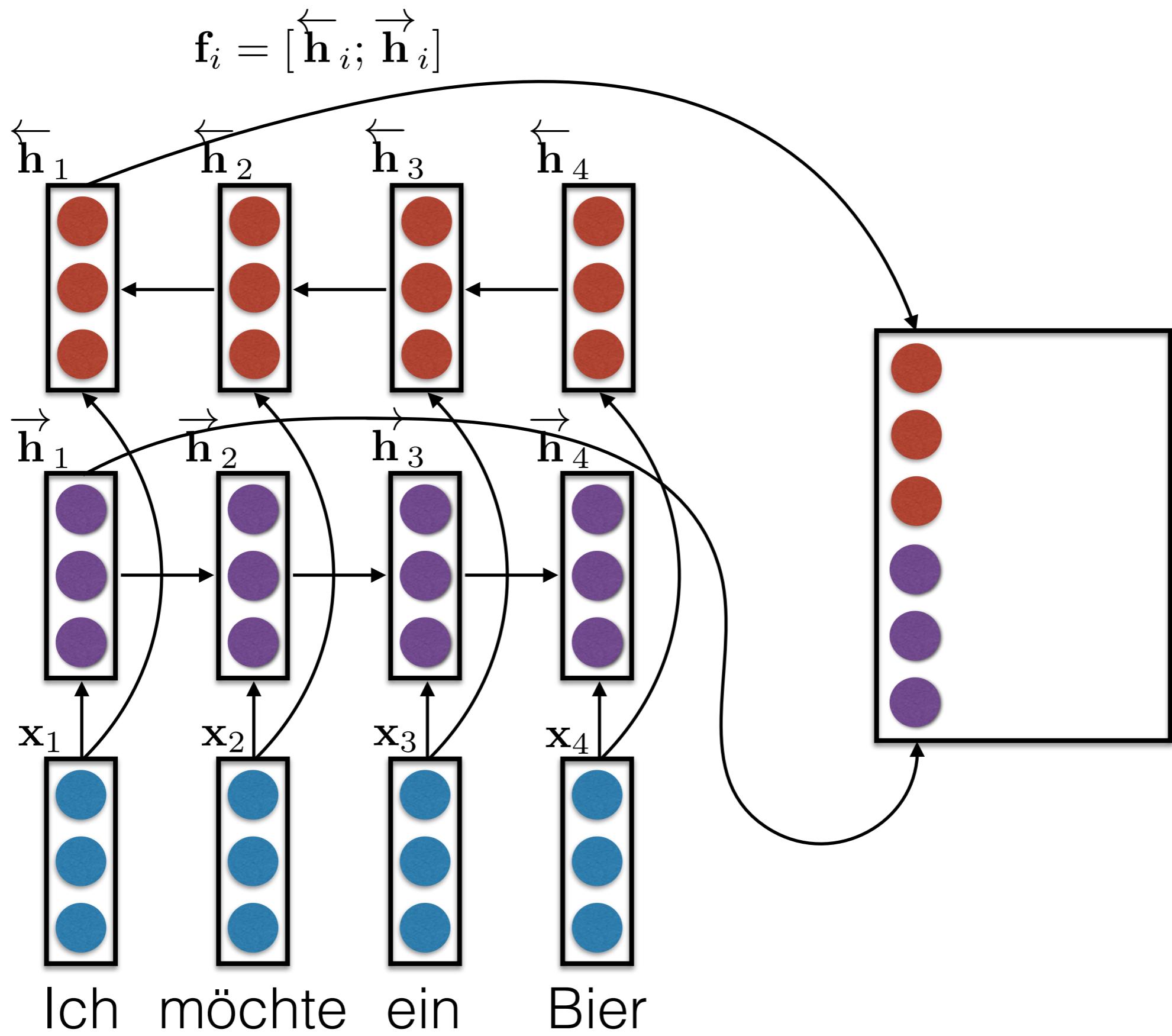
Bier

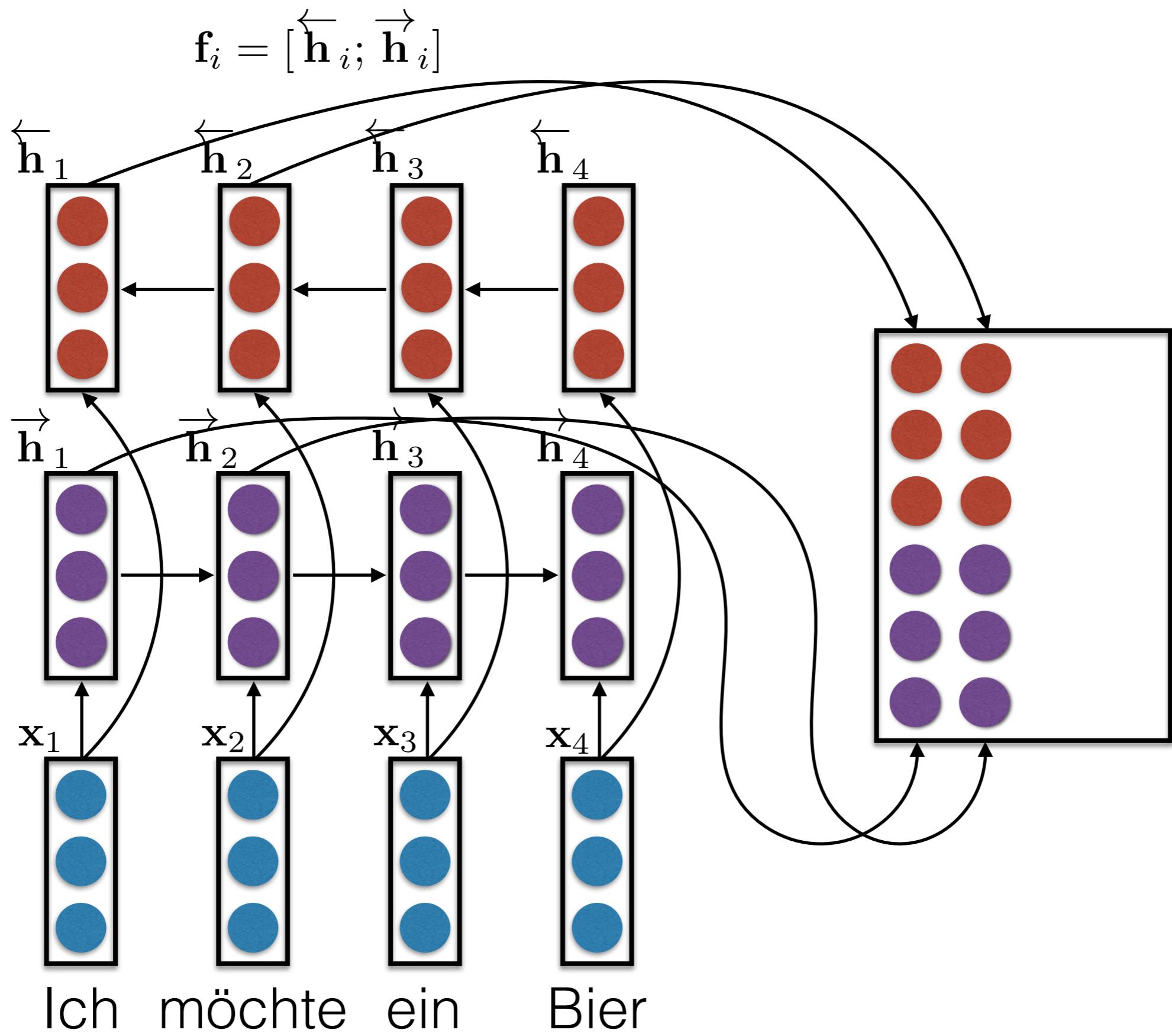


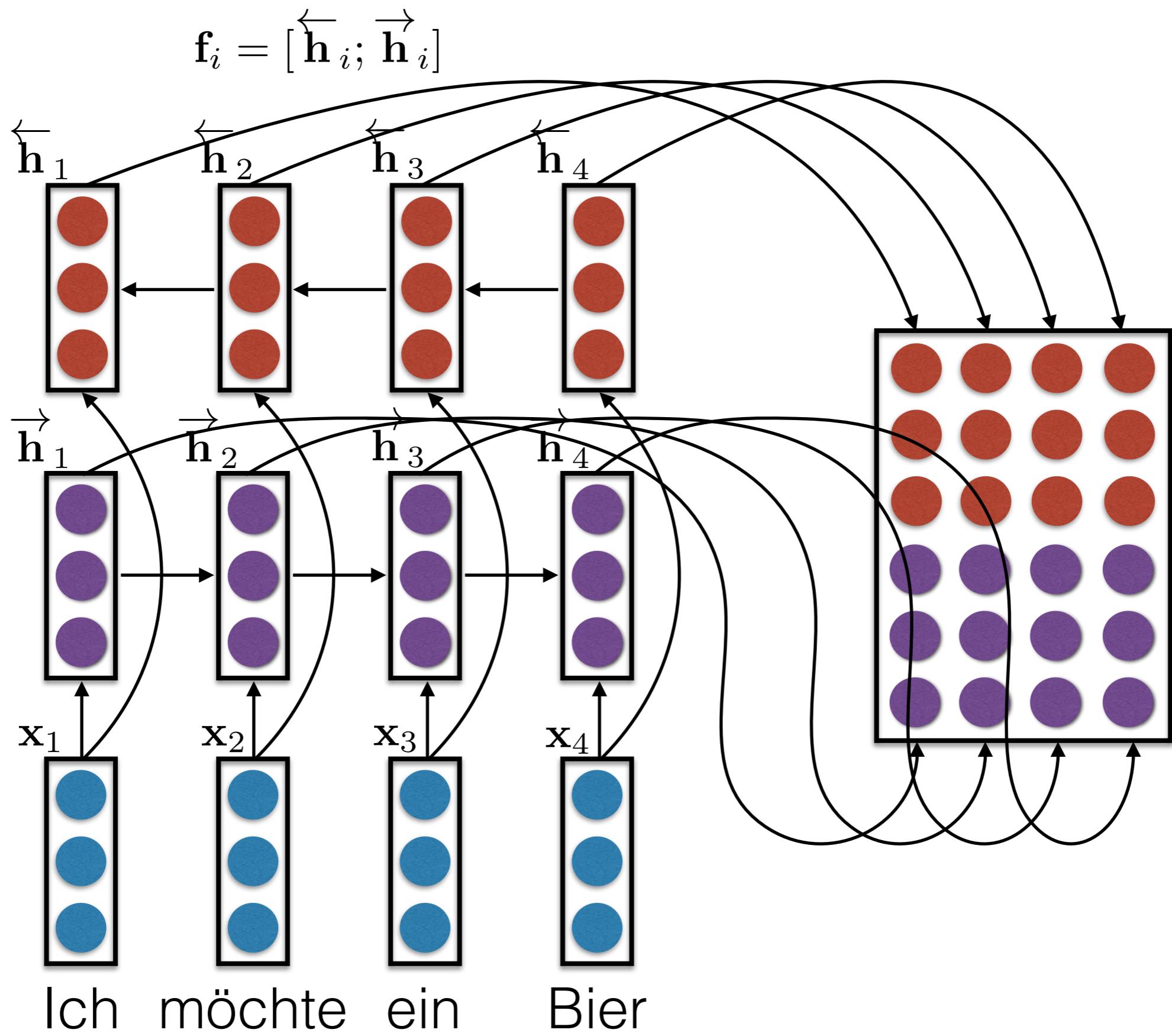


$$\mathbf{f}_i = [\overleftarrow{\mathbf{h}}_i; \overrightarrow{\mathbf{h}}_i]$$

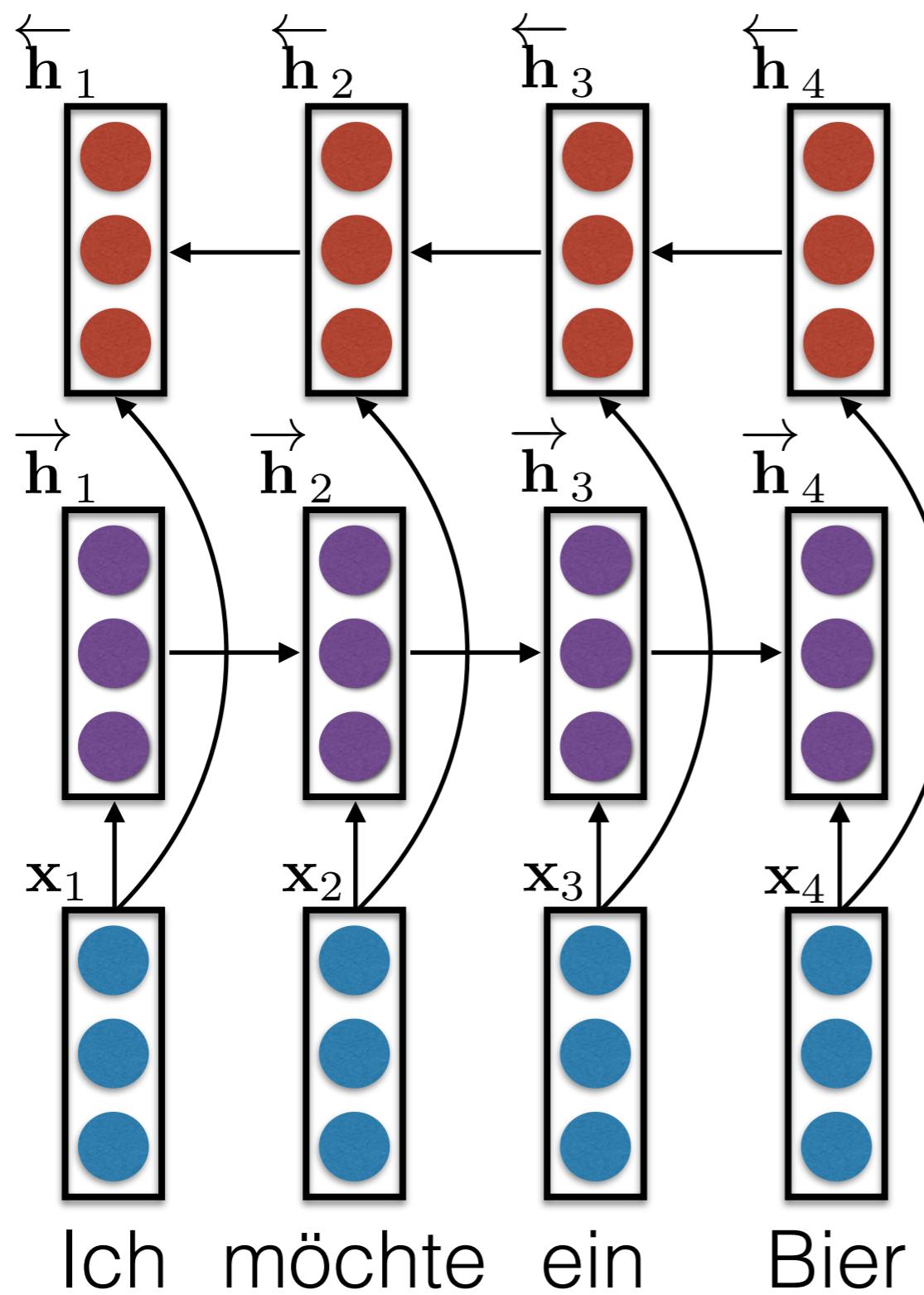




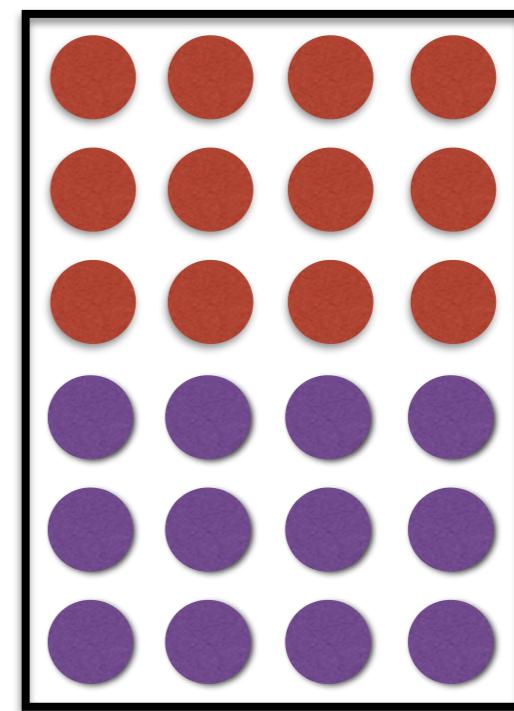




$$\mathbf{f}_i = [\overleftarrow{\mathbf{h}}_i; \overrightarrow{\mathbf{h}}_i]$$



$$\mathbf{F} \in \mathbb{R}^{2n \times |\mathbf{f}|}$$



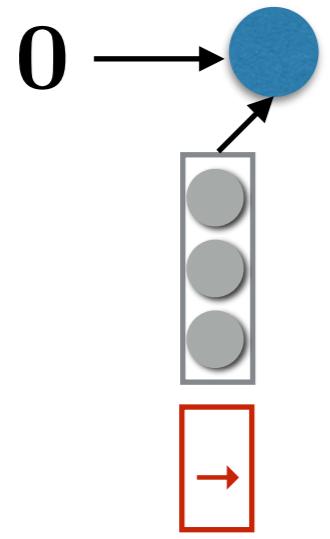
Ich möchte ein Bier

Generation from Matrices

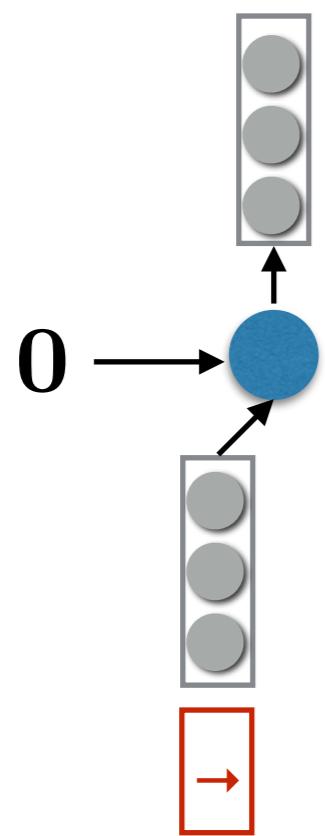
- We have a matrix \mathbf{F} representing the input, now we need to generate from it
- Bahdanau et al. (2015) were the first to propose using **attention** for translating from matrix-encoded sentences
- High-level idea
 - Generate the output sentence word by word using an RNN
 - At each output position t , the RNN receives **two** inputs (in addition to any recurrent inputs)
 - a fixed-size vector embedding of the previously generated output symbol e_{t-1}
 - a fixed-size vector encoding a “view” of the input matrix
 - How do we get a fixed-size vector from a matrix that changes over time?
 - Bahdanau et al: do a weighted sum of the columns of \mathbf{F} (i.e., words) based on how important they are *at the current time step*. (i.e., just a matrix-vector product $\mathbf{F}\mathbf{a}_t$)
 - The weighting of the input columns at each time-step (\mathbf{a}_t) is called **attention**

0

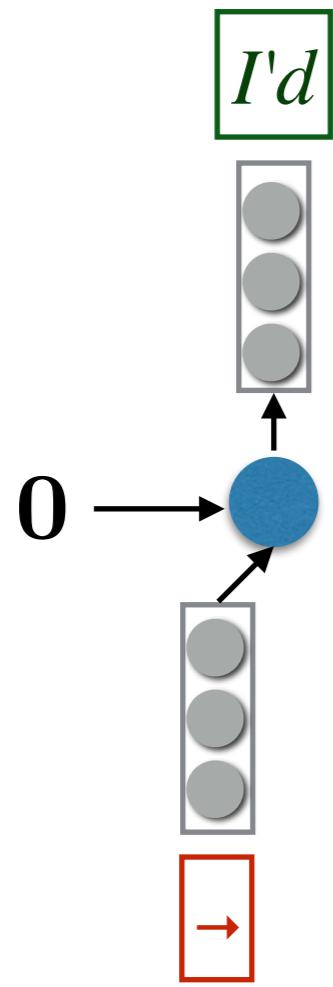
Recall RNNs...



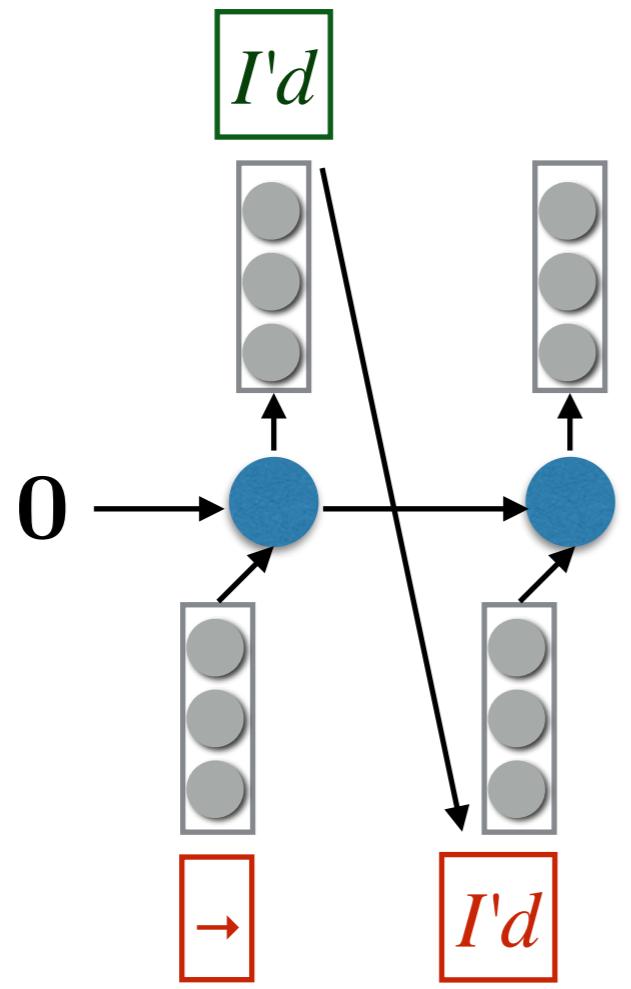
Recall RNNs...



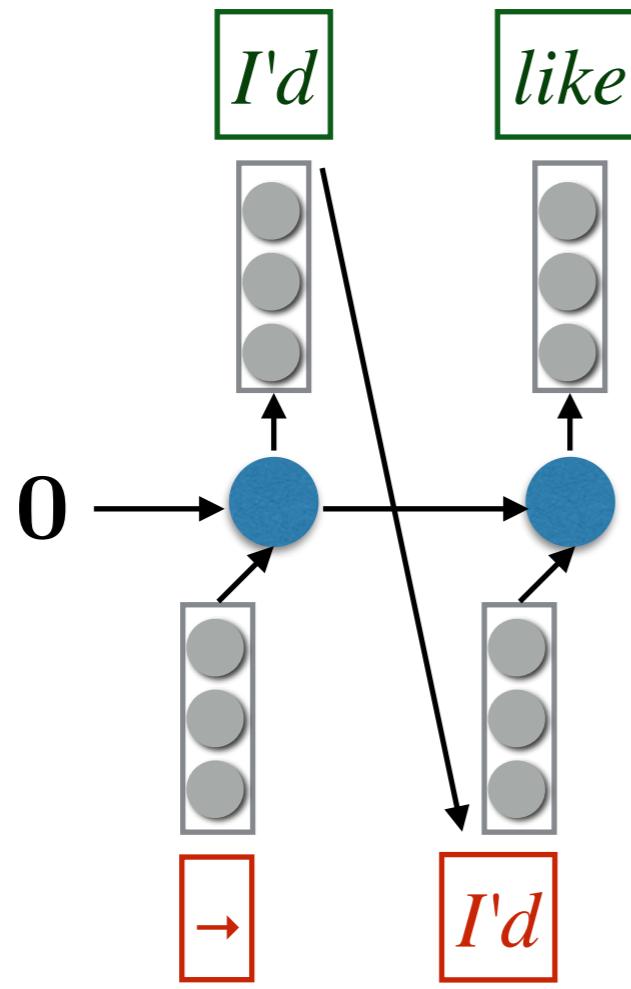
Recall RNNs...



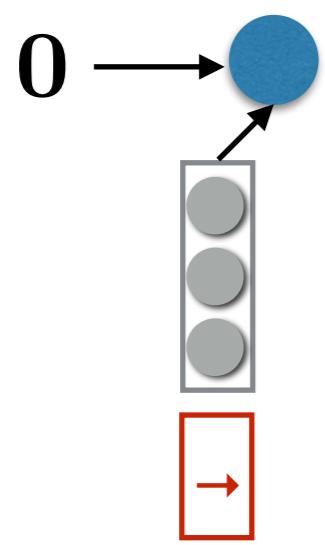
Recall RNNs...

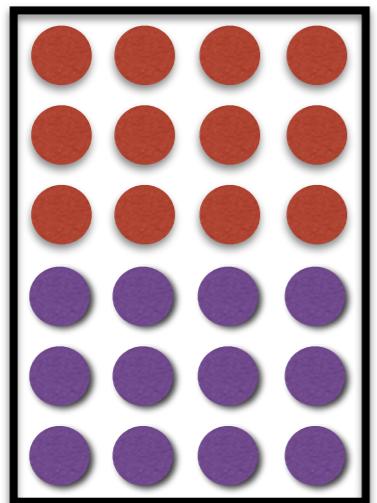
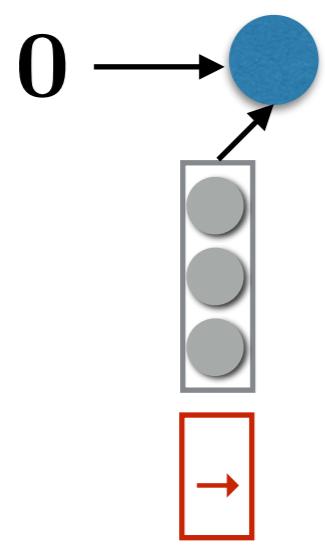


Recall RNNs...

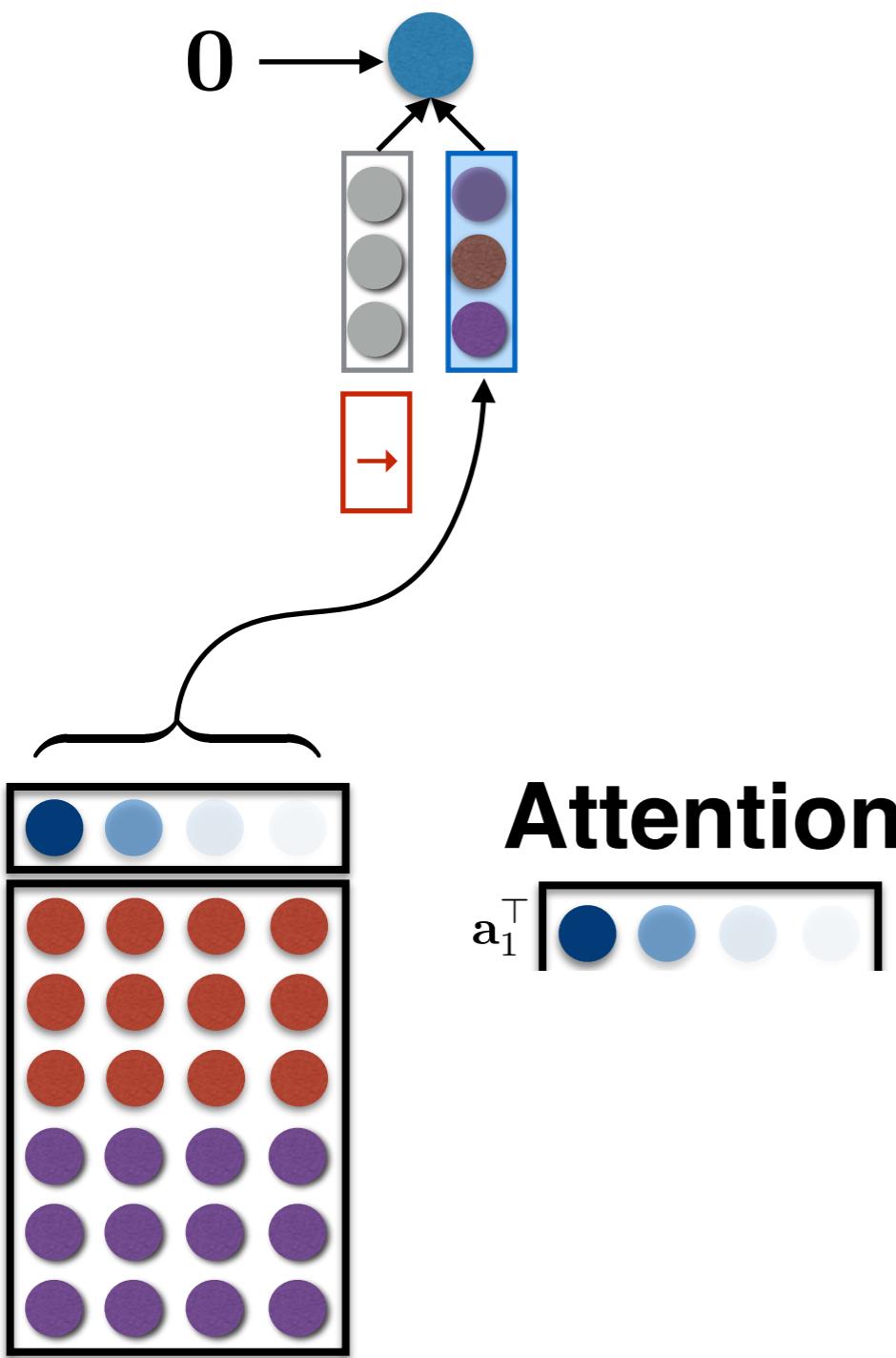


Recall RNNs...

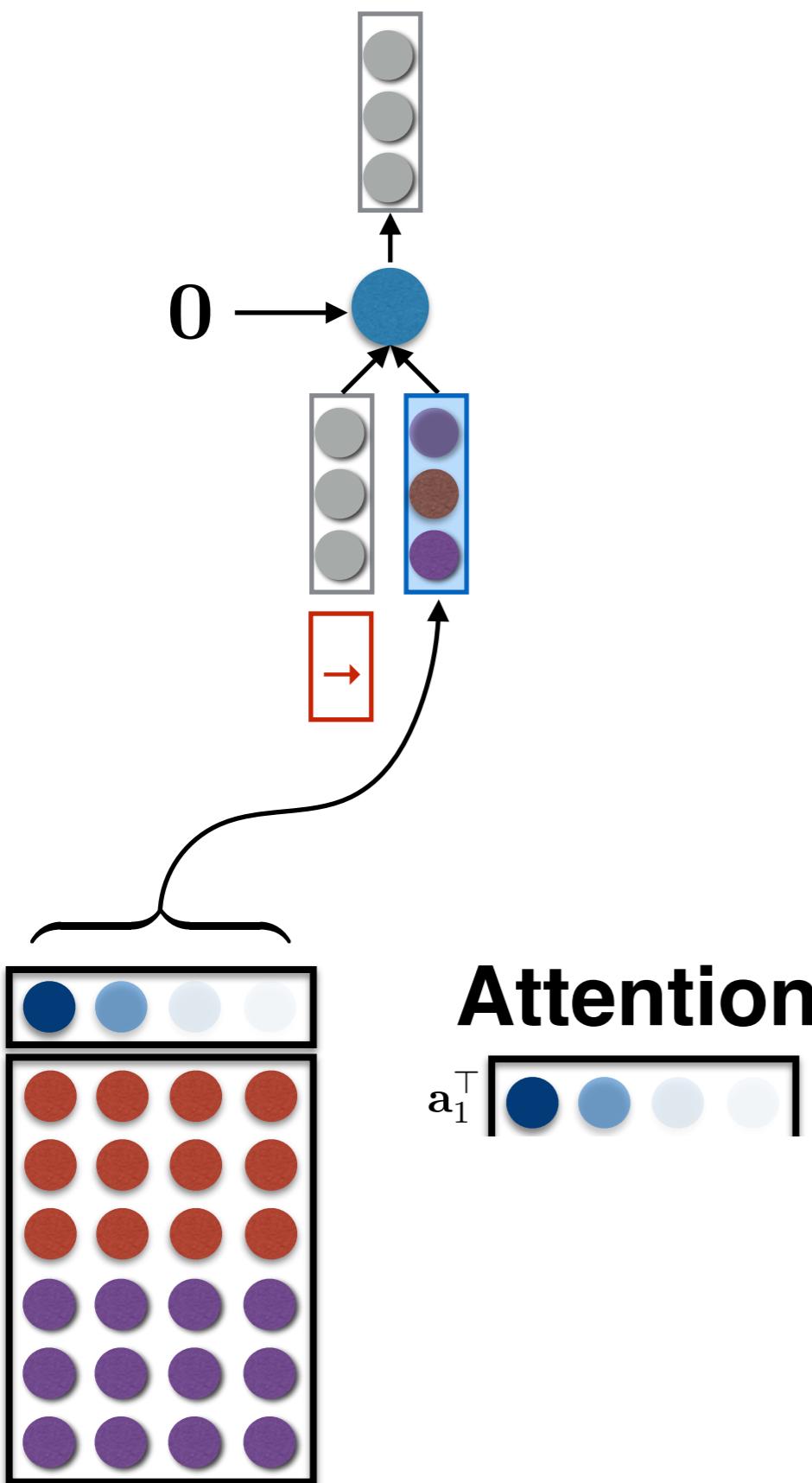




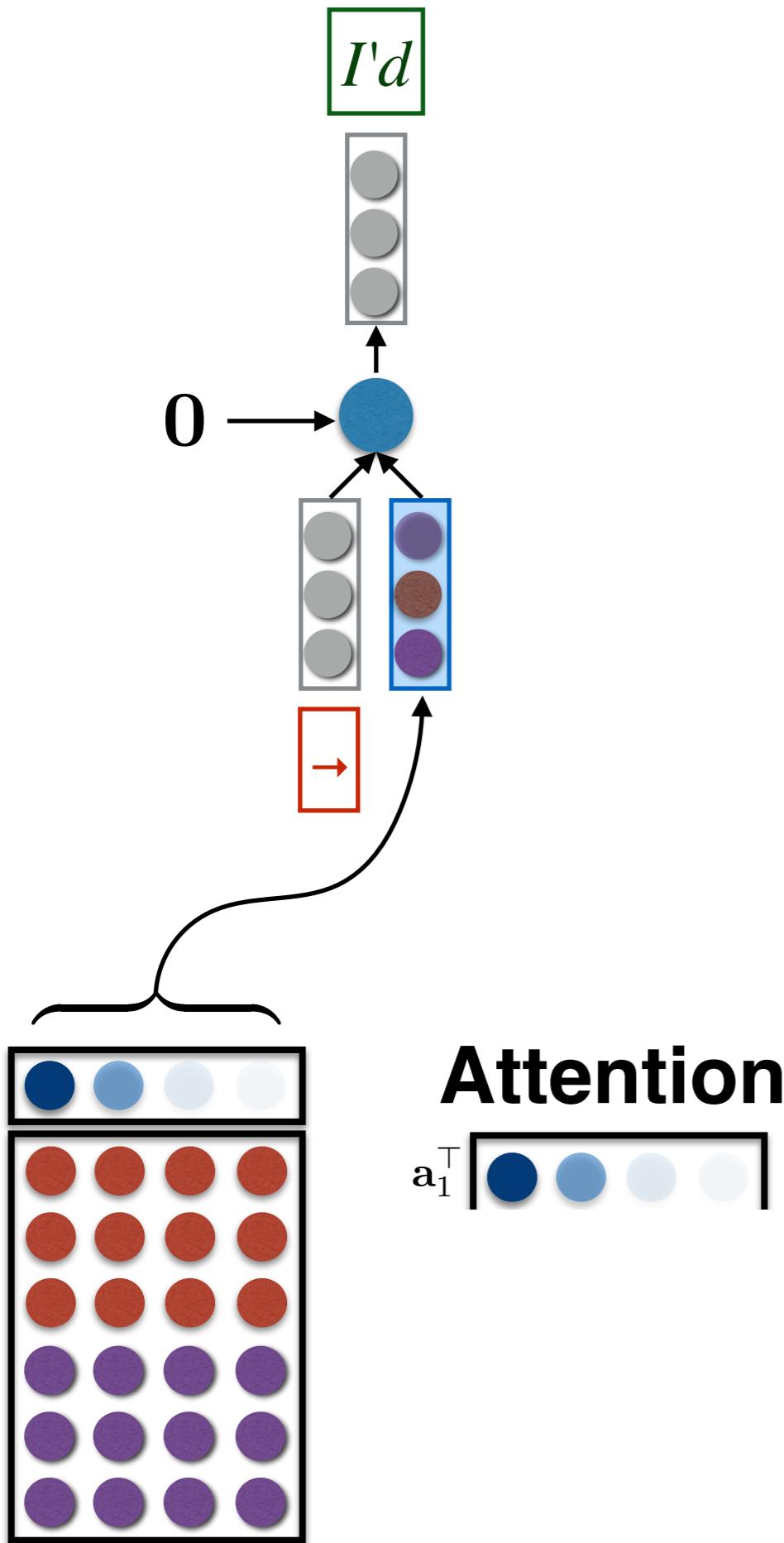
Ich möchte ein Bier



Ich möchte ein Bier



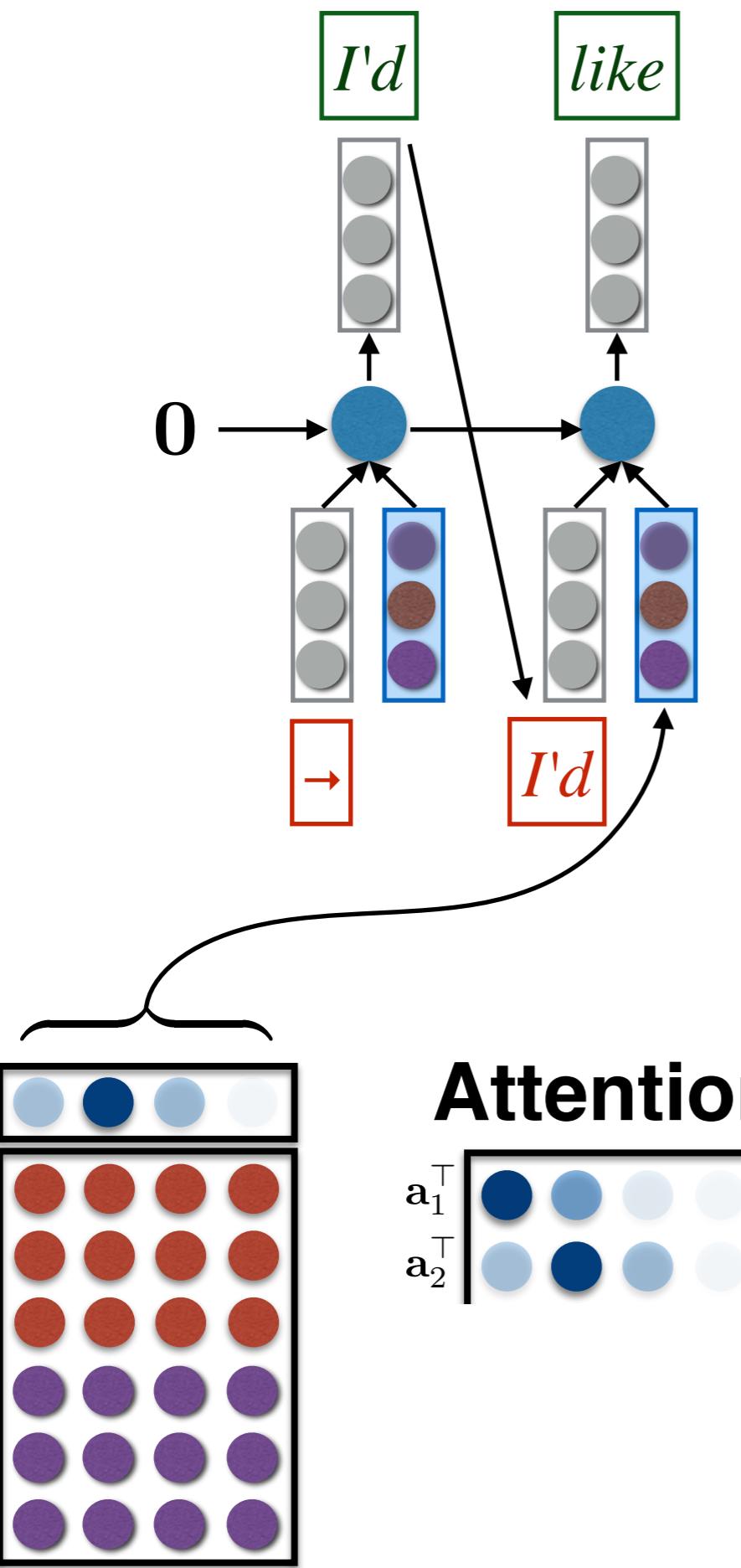
Ich möchte ein Bier

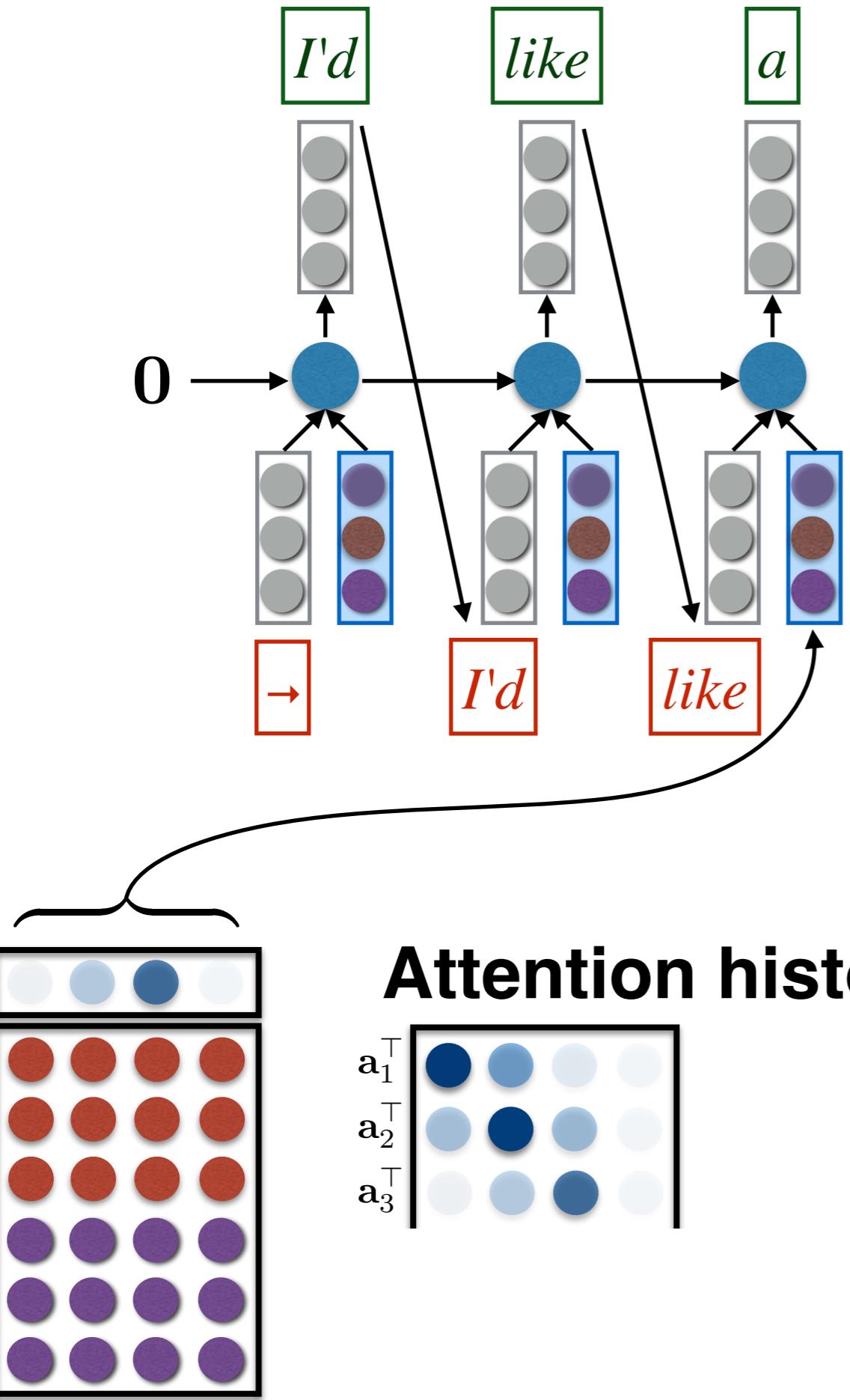


Attention history:

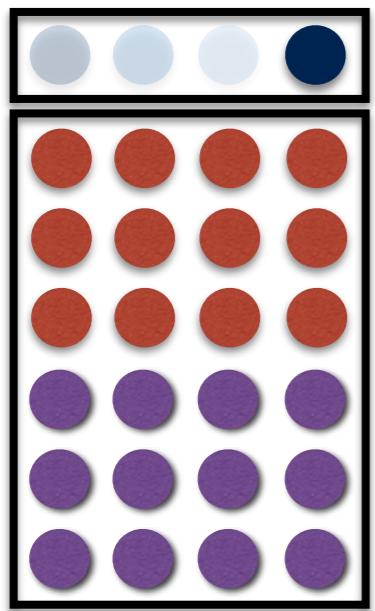
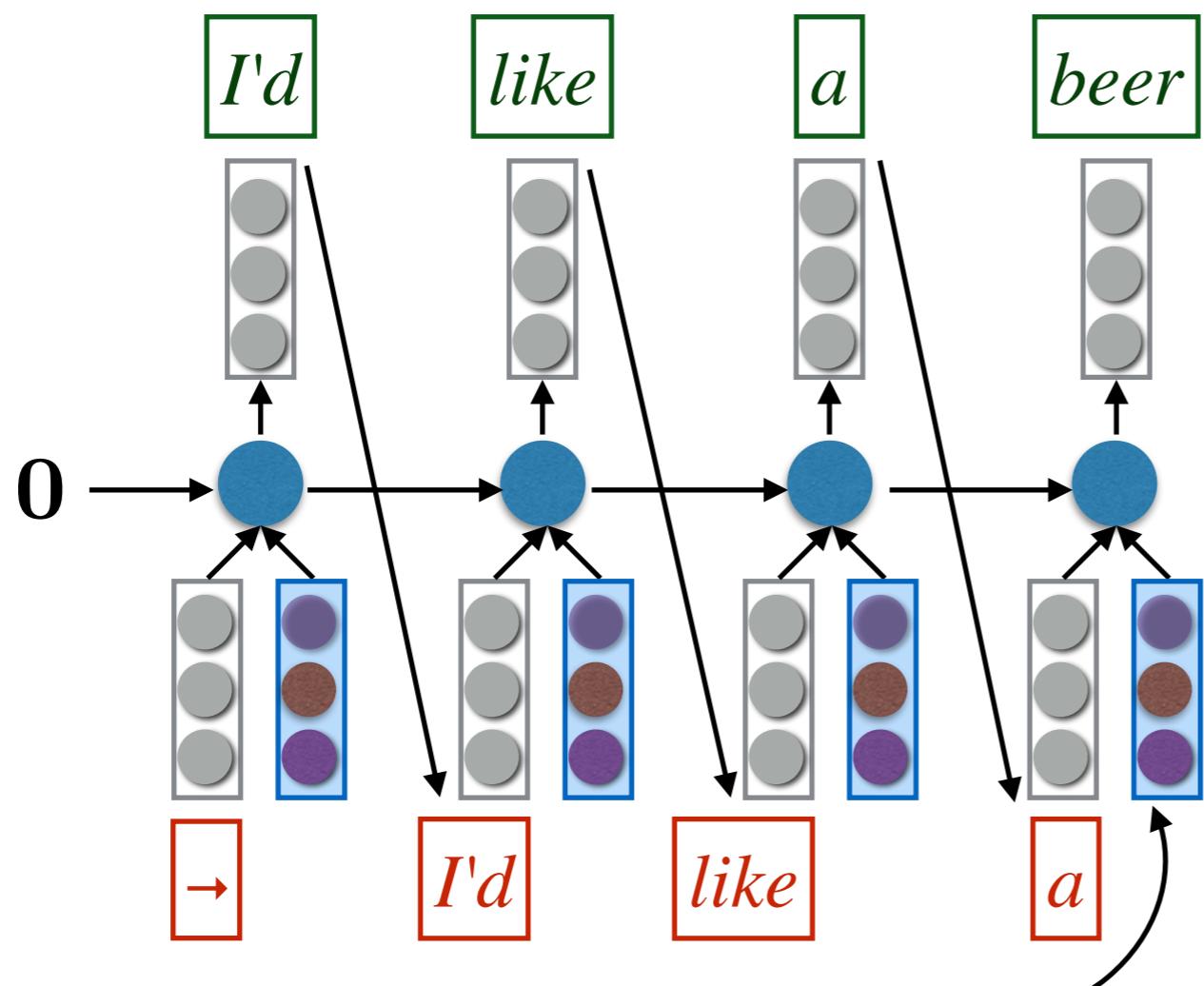
$$a_1^\top \boxed{\text{blue} \quad \text{light blue} \quad \text{light gray} \quad \text{white}}$$

Ich möchte ein Bier





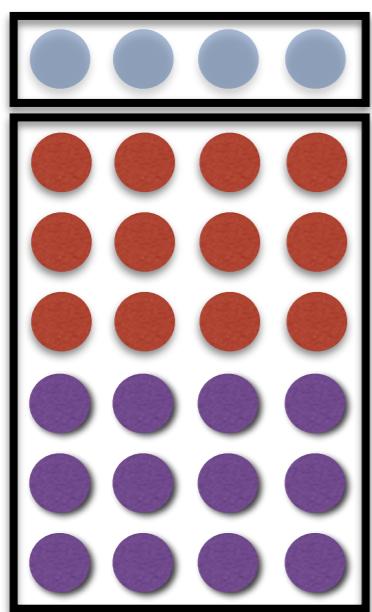
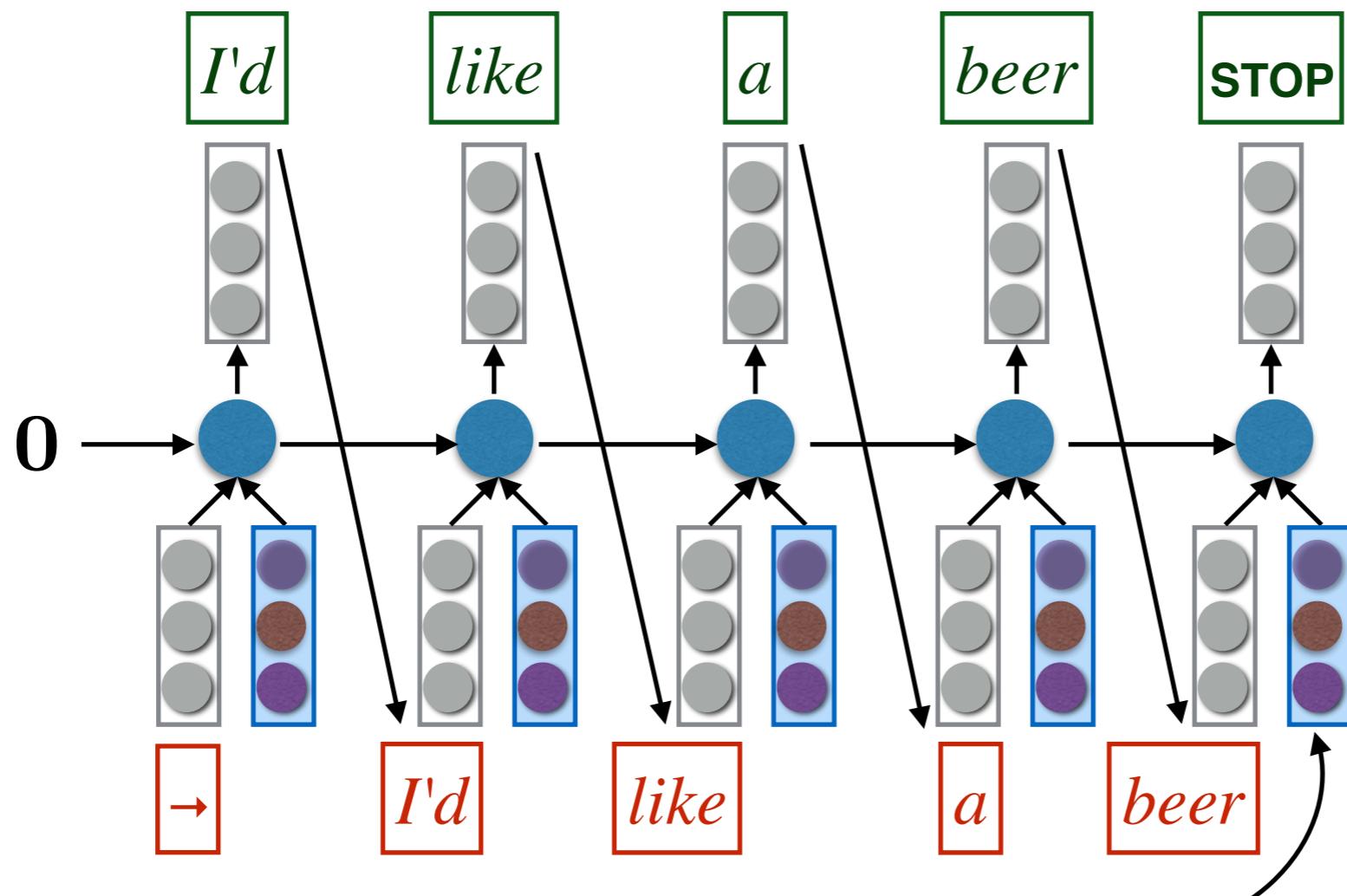
Ich möchte ein Bier



Attention history:

$$\begin{matrix} a_1^\top & a_2^\top & a_3^\top & a_4^\top \\ \text{dark red} & \text{orange} & \text{yellow} & \text{green} \end{matrix}$$

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Attention history:

Ich möchte ein Bier

Attention

- How do we know what to attend to at each time-step?
- That is, how do we compute \mathbf{a}_t ?

Computing Attention

- At each time step (one time step = one output word), we want to be able to “attend” to different words in the source sentence
 - We need a weight for every word: this is an $|\mathbf{f}|$ -length vector \mathbf{a}_t
 - Here is a simplified version of Bahdanau et al.’s solution
 - Use an RNN to predict model output, call the hidden states \mathbf{s}_t
(\mathbf{s}_t has a fixed dimensionality, call it m)

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(\mathbf{V} is a learned parameter)

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 - At time t compute the **expected input embedding** $\mathbf{r}_t = \mathbf{V}\mathbf{s}_{t-1}$ (\mathbf{V} is a learned parameter)
 - Take the dot product with every column in the source matrix to compute the **attention energy**. $\mathbf{u}_t = \mathbf{F}^\top \mathbf{r}_t$ (called \mathbf{e}_t in the paper)
(Since \mathbf{F} has $|f|$ columns, \mathbf{u}_t has $|f|$ rows)

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 - Exponentiate and normalize to 1: $\mathbf{a}_t = \text{softmax}(\mathbf{u}_t)$
 - Finally, the **input source vector** for time t is $\mathbf{c}_t = \mathbf{F}\mathbf{a}_t$

Summary

- Attention is closely related to “pooling” operations in convnets (and other architectures)
- Bahdanau’s attention model seems to only cares about “content”
 - No obvious bias in favor of diagonals, short jumps, fertility, etc.
 - Some work has begun to add other “structural” biases (Luong et al., 2015; Cohn et al., 2016), but there are lots more opportunities
- Attention is similar to **alignment**, but there are important differences
 - alignment makes stochastic but hard decisions. Even if the alignment probability distribution is “flat”, the model picks one word or phrase at a time
 - attention is “soft” (you add together all the words). Big difference between “flat” and “peaked” attention weights

Questions?

Representing Words in Context with Self-Attention

- RNNs are computationally inconvenient: to compute \mathbf{h}_t , we need to first compute \mathbf{h}_{t-1} , for which we need to compute $\mathbf{h}_{t-2} \dots$
- LSTMs have to use their memories to remember everything in the past
- We will solve both of these problems with **self-attention**.
 - Each \mathbf{h}_t will be computed in parallel (take advantage of GPUs which can do a lot of things in parallel)
 - Each \mathbf{h}_t will be able to create a direct “connection” to anything else in the sequence without resorting to a single vector “memory”
 - This architecture is called a “transformer”

我

wǒ

昨天

zuótiān

看了

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三部

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电影

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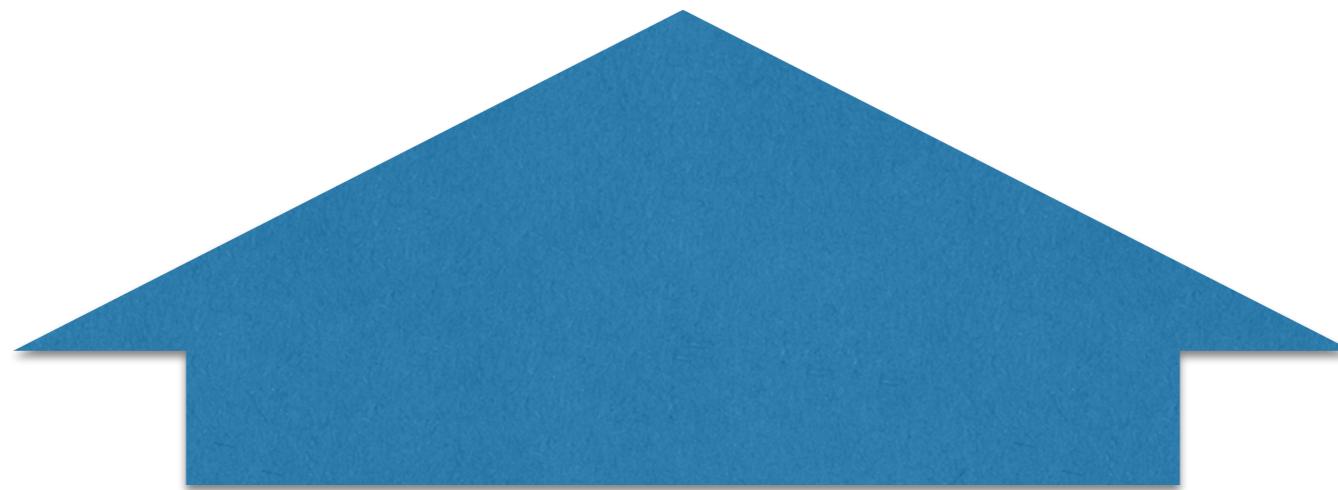
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diànyǐng

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I watched three movies yesterday.



我

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Chinese pronouns don't indicate whether they are subjects or objects!

But in English, we need to know this.

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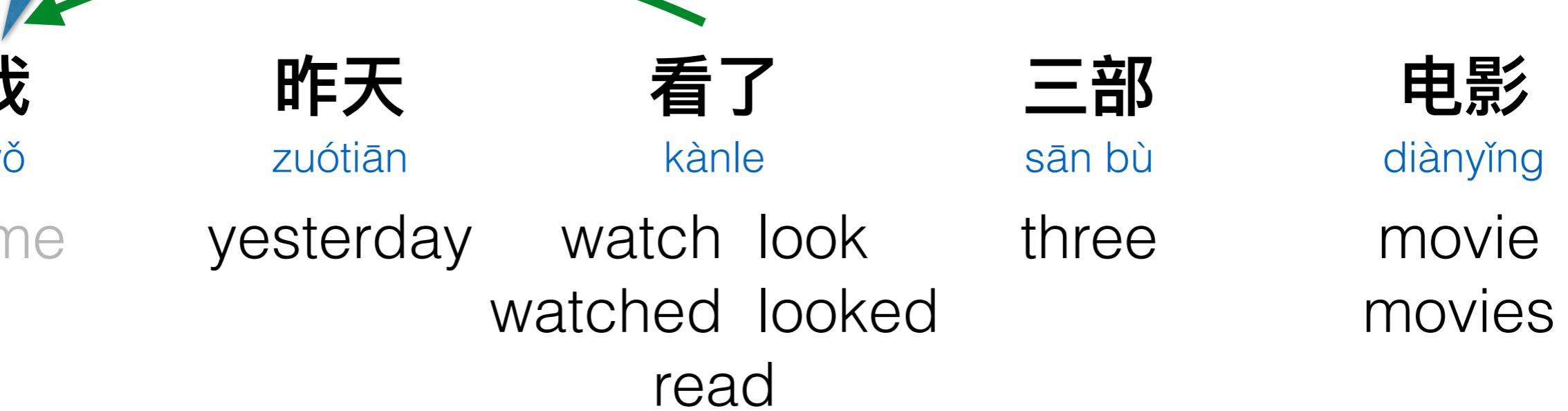
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Chinese verbs don't map directly on to English verbs! The right verb depends on the object.

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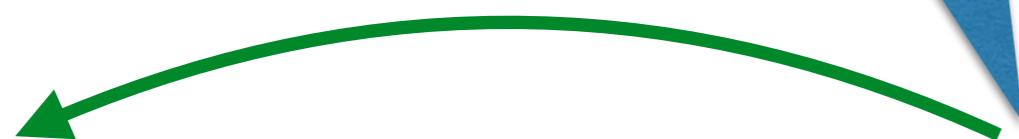
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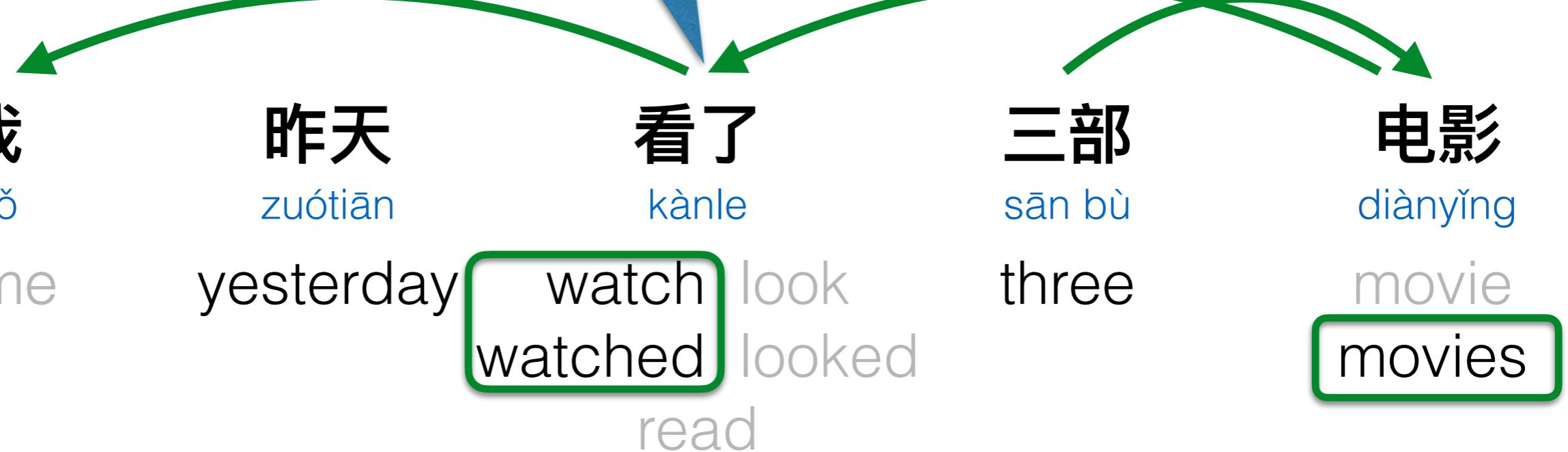
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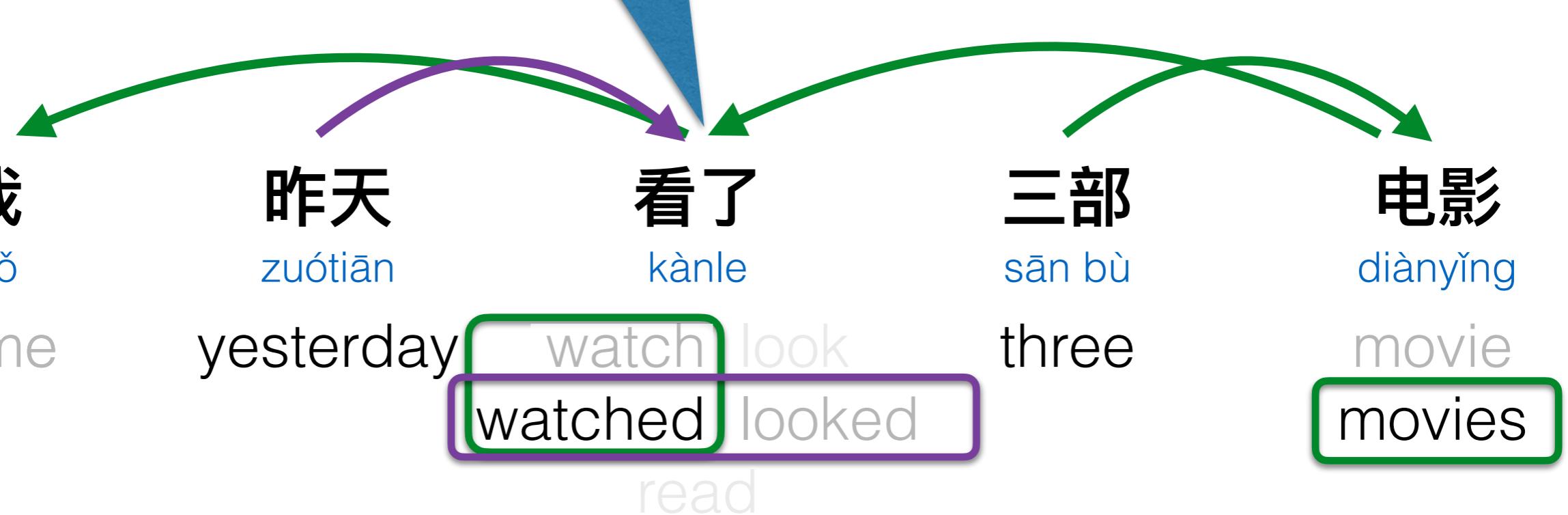
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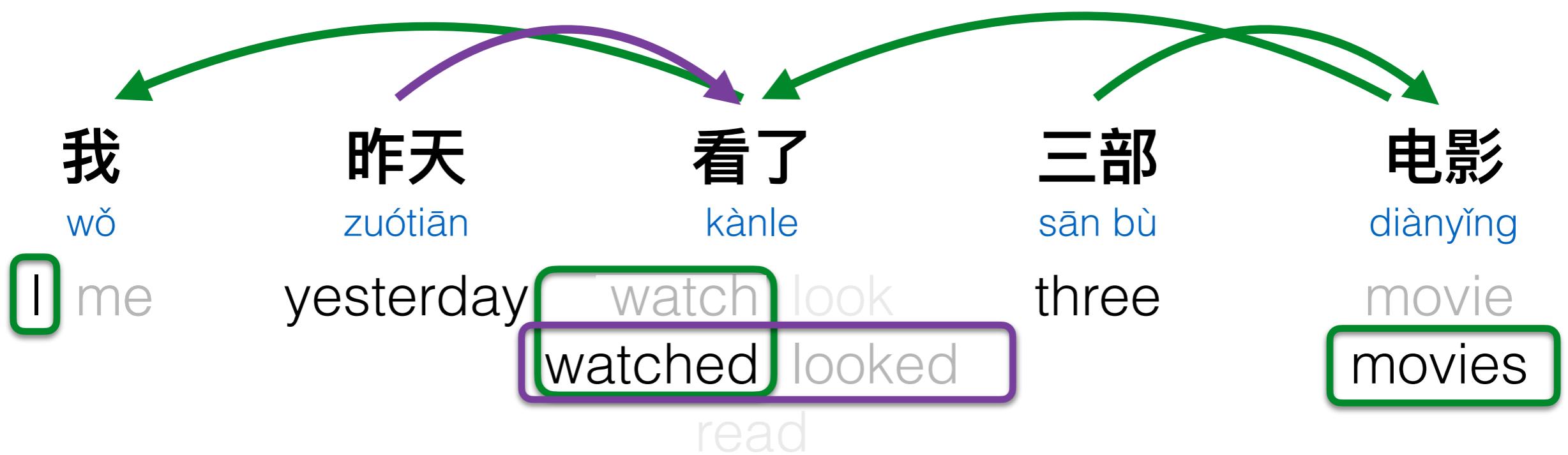
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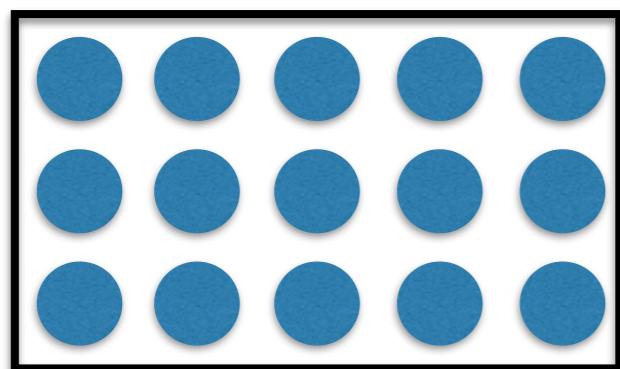
movie
movies



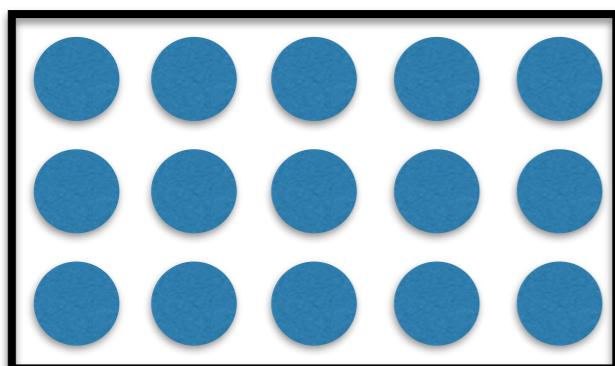
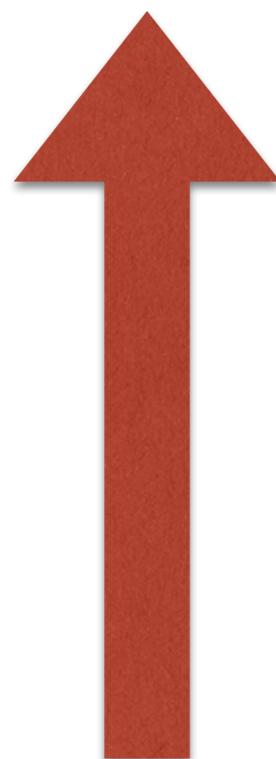
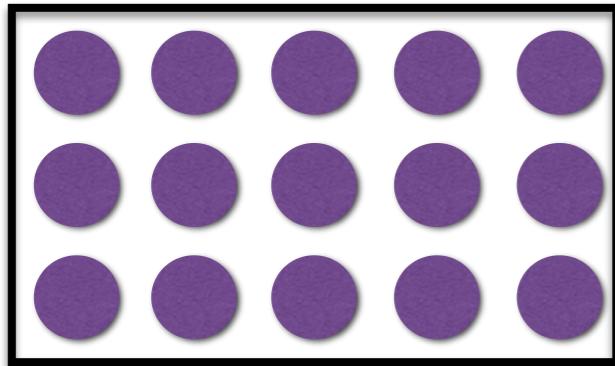
- Different words need to obtain **different kinds of information** from different places.
- Words need to integrate **multiple kinds of information**.
- Although we didn't consider an example, words may need to pass information along **multiple hops**.
- Let's design a model that supports this.



We will start with $\mathbf{X} \in \mathbb{R}^{n \times d}$ which is obtained by stacking word vectors ...



我 昨天 看了 三部 电影



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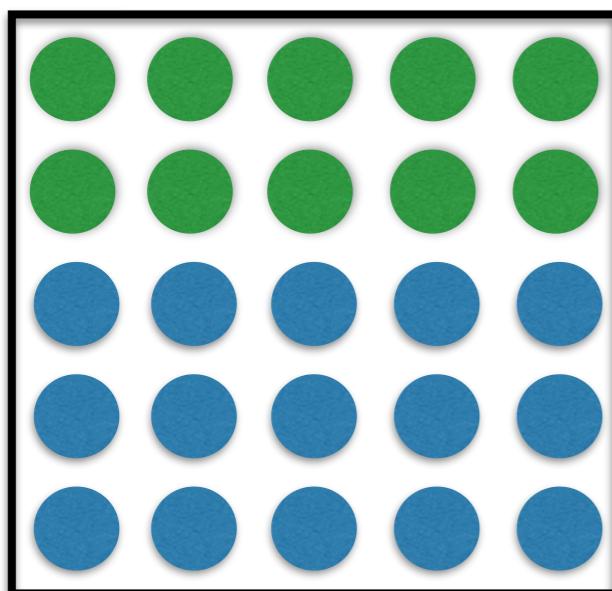
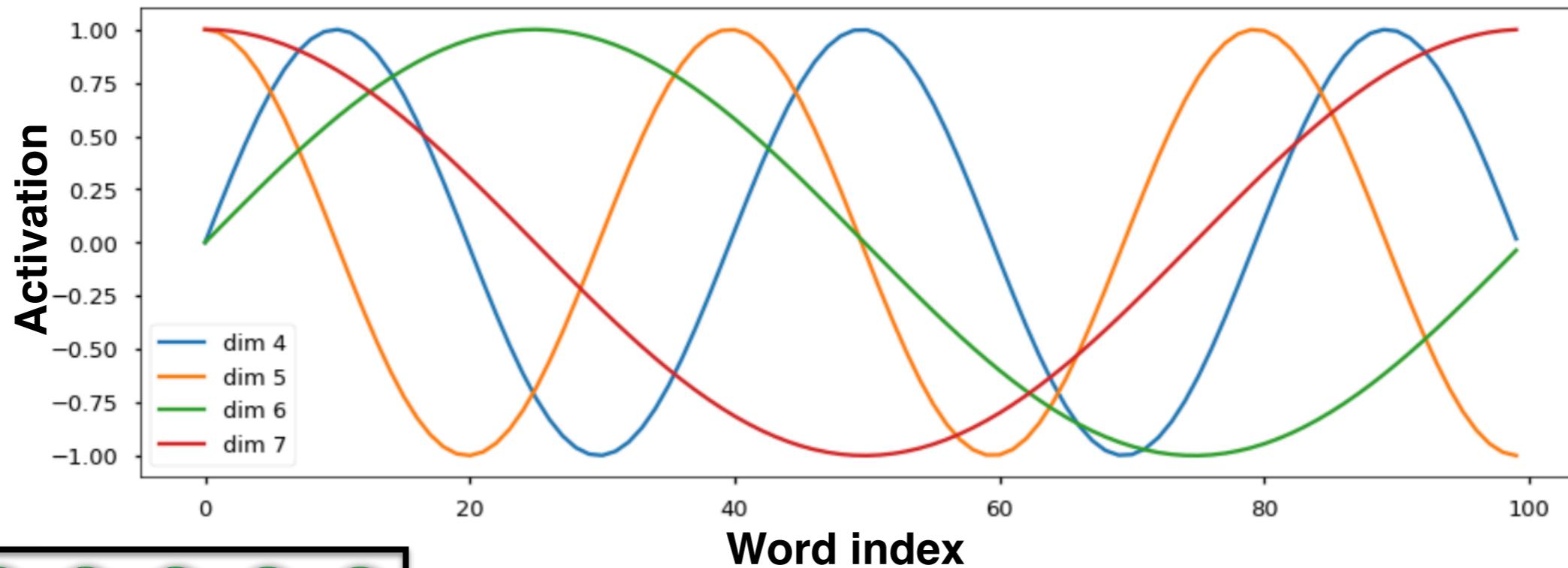
and we will transform it into a representation that integrates all the necessary contextual information useful for the task.

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Since we need information about positions, we need to augment \mathbf{X} with positional information.

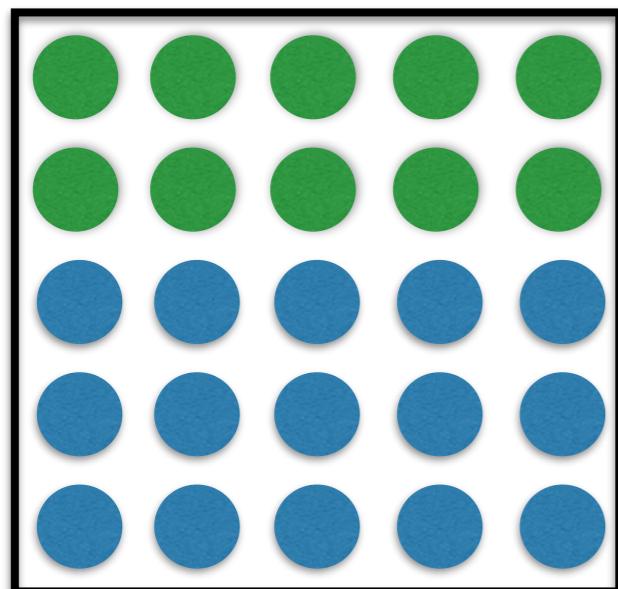
Plot by Sasha Rush



$$PE_{(pos,2i)} = \sin(pos/10000^{2i/d_{\text{model}}})$$
$$PE_{(pos,2i+1)} = \cos(pos/10000^{2i/d_{\text{model}}})$$

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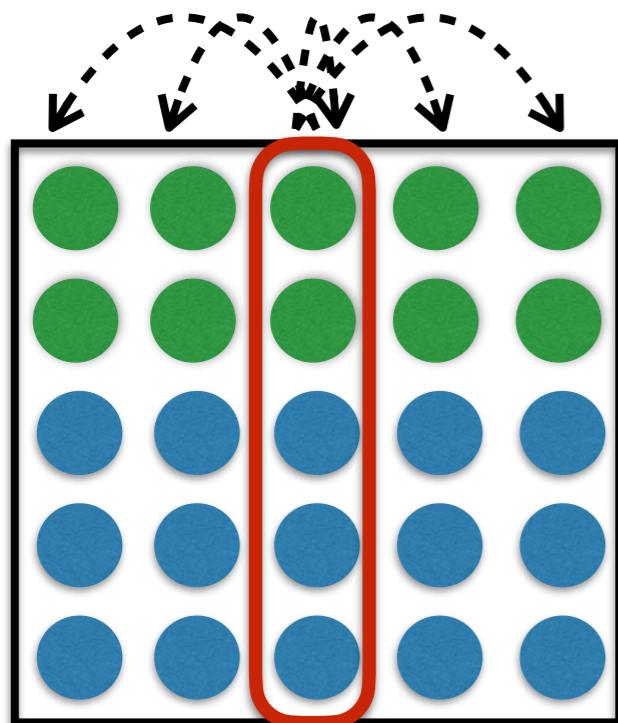


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Consider just one position. It must decide where else in the sentence to attend (and we do permit it to attend to itself, since sometimes there may be no relevant external information).

If we compute the inner product $\mathbf{X}\mathbf{x}_i \in \mathbb{R}^n$, we will get a score for every position, which we can normalize into an attention weighting $\text{softmax}(\mathbf{X}\mathbf{x}_i)$.



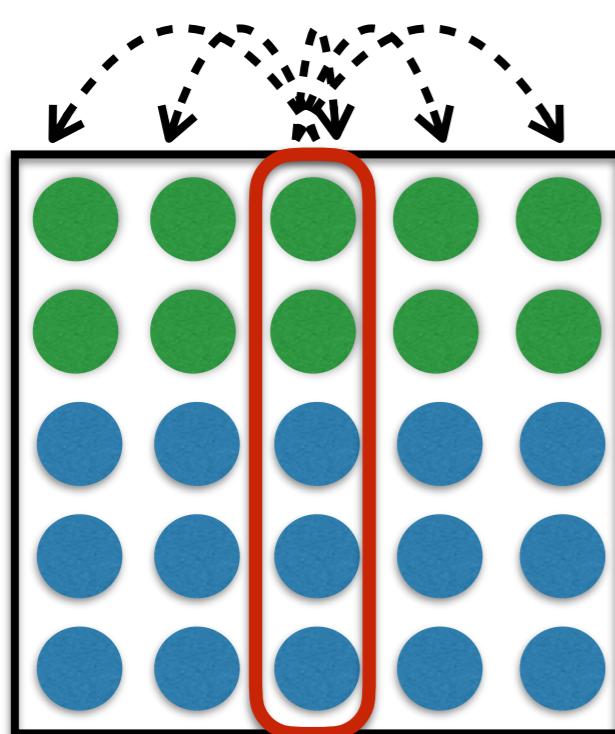
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We can do this “in parallel” for all positions by doing the following $\mathbf{A} = \text{softmax}(\mathbf{X}\mathbf{X}^\top)$ which is in $[0, 1]^{n \times n}$. And then the “output” is $\mathbf{Y} = \mathbf{AX}$.



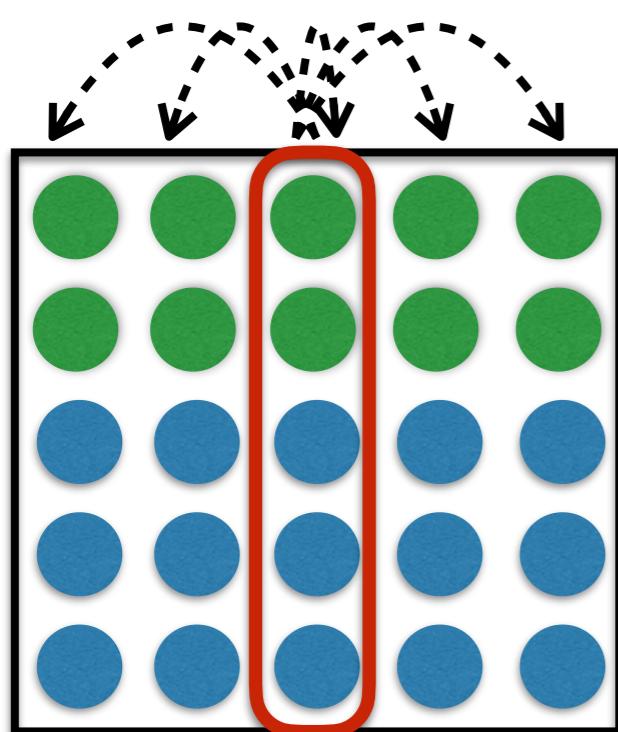
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Unfortunately: each word will always want to attend to itself (property of inner products), attention will be symmetric (we don’t want this), and we can’t attend to different kinds of information.

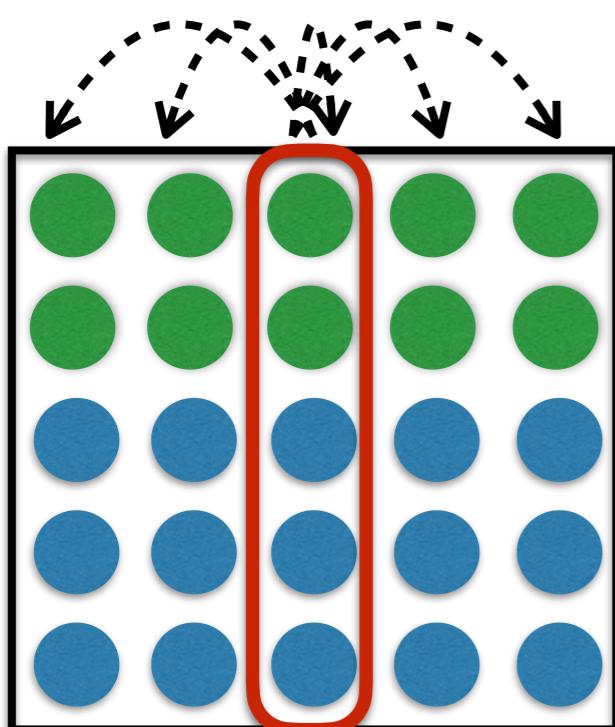
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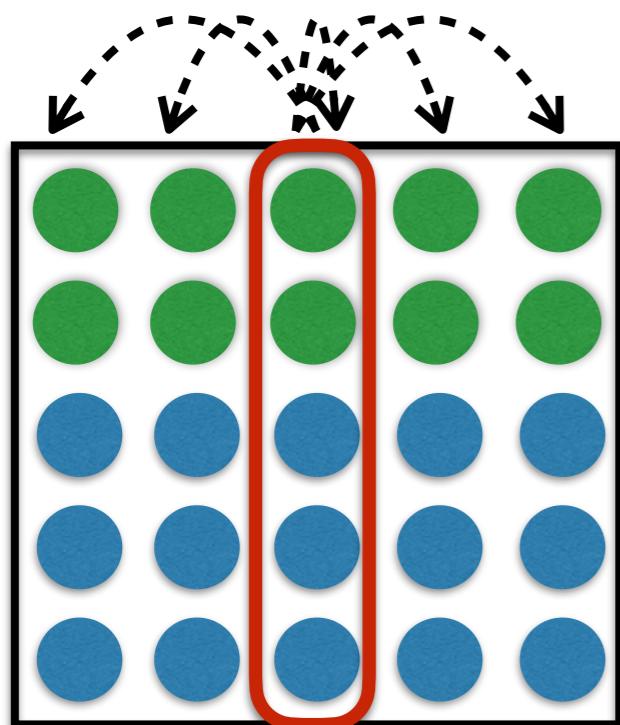
We need some parameters!

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$\mathbf{X} \in \mathbb{R}^{n \times d}$ is obtained by stacking word vectors and concatenating positional information.

Another attempt: Let's add a parameter $\mathbf{W} \in \mathbb{R}^{d \times d}$, now we can compute $\mathbf{XWx}_i \in \mathbb{R}^n$. This lets us control where we look, and attention is no necessarily symmetric.

Moreover, we can still do things very efficiently with by computing $\text{softmax}(\mathbf{XWX}^\top)$.



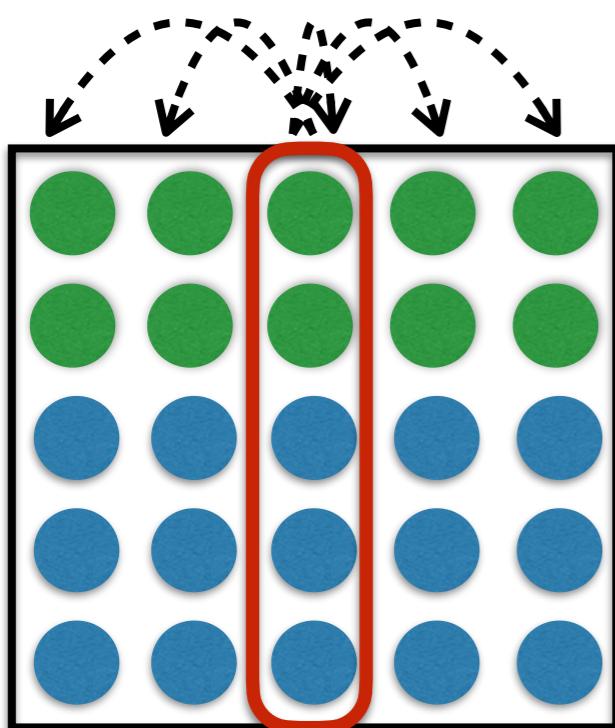
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To attend to different kinds of information, we can just add multiple \mathbf{W} 's, or equivalently, redefine $\mathbf{W} \in \mathbb{R}^{h \times d \times d}$ and use *batched matrix multiplies*.



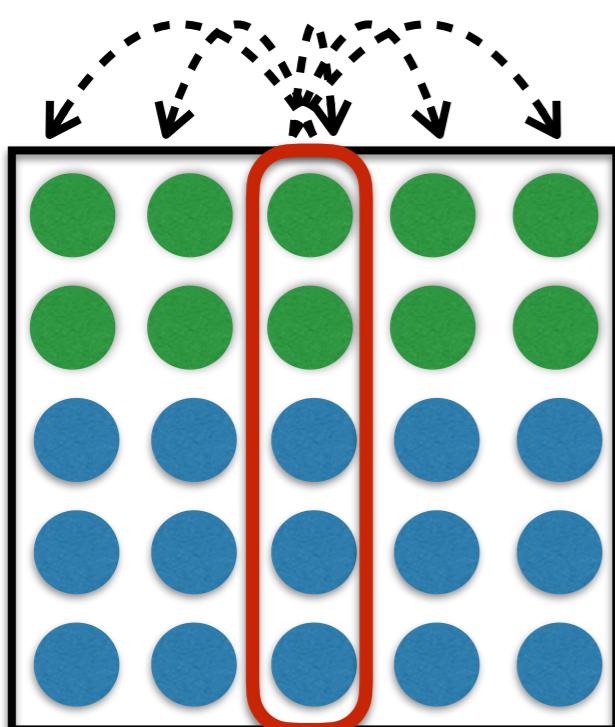
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Unfortunately: \mathbf{W} has massive number of parameters, just to decide where to attend to. This is slow and makes learning hard.

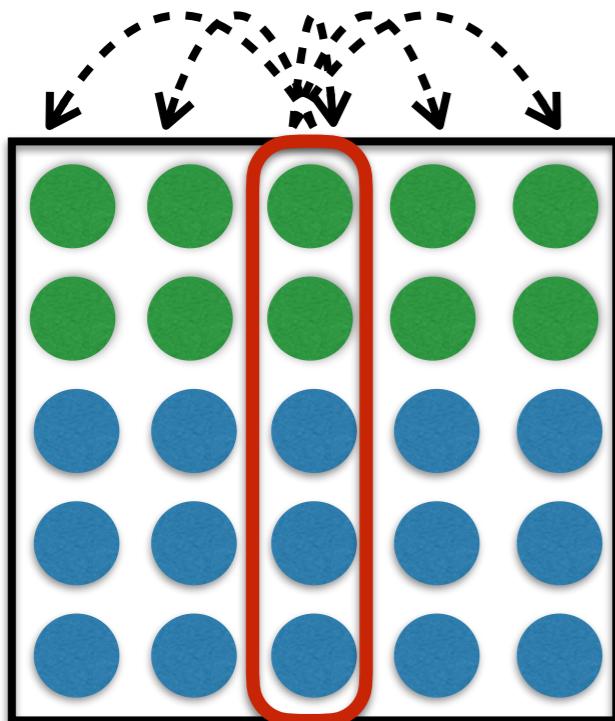
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$\mathbf{X} \in \mathbb{R}^{n \times d}$ is obtained by stacking word vectors and concatenating positional information.

Another attempt: Let's use a **low rank** approximation of \mathbf{W} . We define two matrices $\mathbf{L} \in \mathbb{R}^{d \times \ell}$ and $\mathbf{R} \in \mathbb{R}^{\ell \times d}$ and then do $\mathbf{A} = \text{softmax}(\mathbf{X}\mathbf{L}\mathbf{R}\mathbf{X}^\top)$.

Now we can control the number of parameters in the model by setting ℓ to be as small as we like! In practice, it's common to use $\ell = d/h$.

So we can write $\mathbf{Y} = \text{softmax}(\mathbf{X}\mathbf{L}\mathbf{R}\mathbf{X}^\top)\mathbf{X}$.



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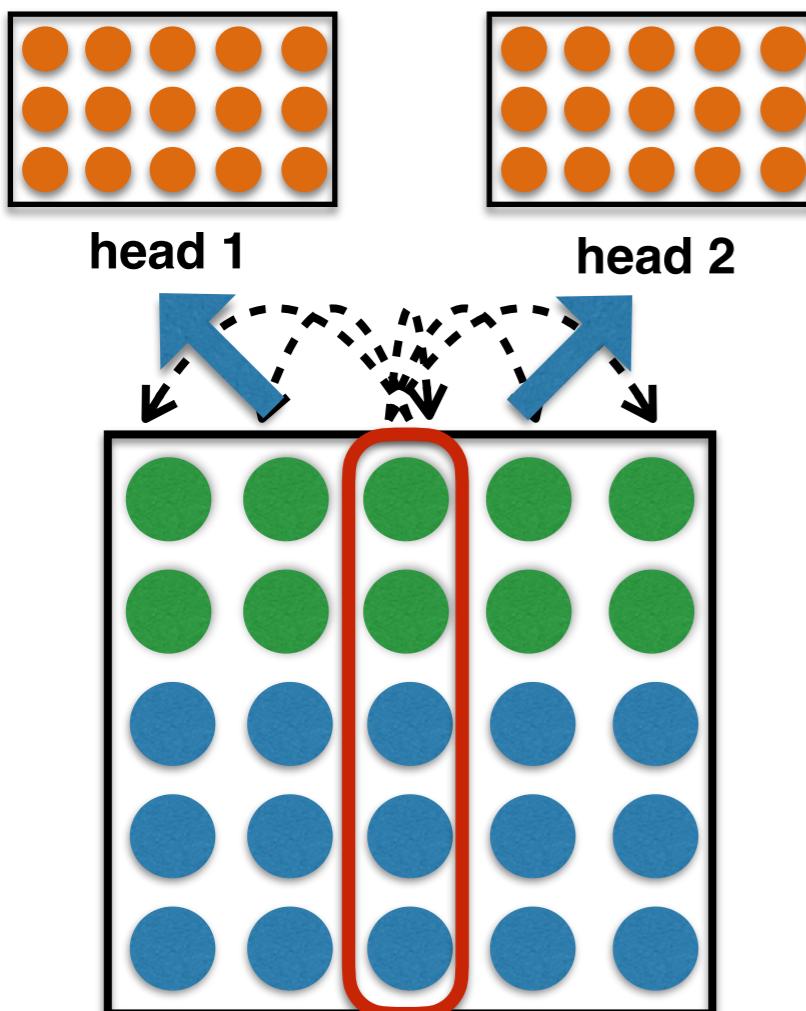
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But what about multiple heads? We would like each of these to extract different information from different places. Since we want to extract different information, we need to transform \mathbf{X} : $\mathbf{Y} = \text{softmax}(\mathbf{X}\mathbf{L}\mathbf{R}\mathbf{X}^\top)\mathbf{X}\mathbf{P}$ where we also want \mathbf{P} to be low rank: $\mathbf{P} \in \mathbb{R}^{d \times \ell}$, or rather, in the case of multiple heads, $\mathbf{P} \in \mathbb{R}^{h \times d \times \ell}$.



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$\mathbf{X} \in \mathbb{R}^{n \times d}$ is obtained by stacking word vectors and concatenating positional information.

We have auxiliary parameters:

$$\mathbf{L} \in \mathbb{R}^{h \times d \times \ell}$$

$$\mathbf{R} \in \mathbb{R}^{h \times \ell \times d}$$

$$\mathbf{P} \in \mathbb{R}^{h \times d \times \ell}$$

And we compute $\mathbf{Z} = \text{softmax}(\mathbf{XLRX}^\top)\mathbf{XP}$ which is in $\mathbb{R}^{h \times n \times \ell}$.

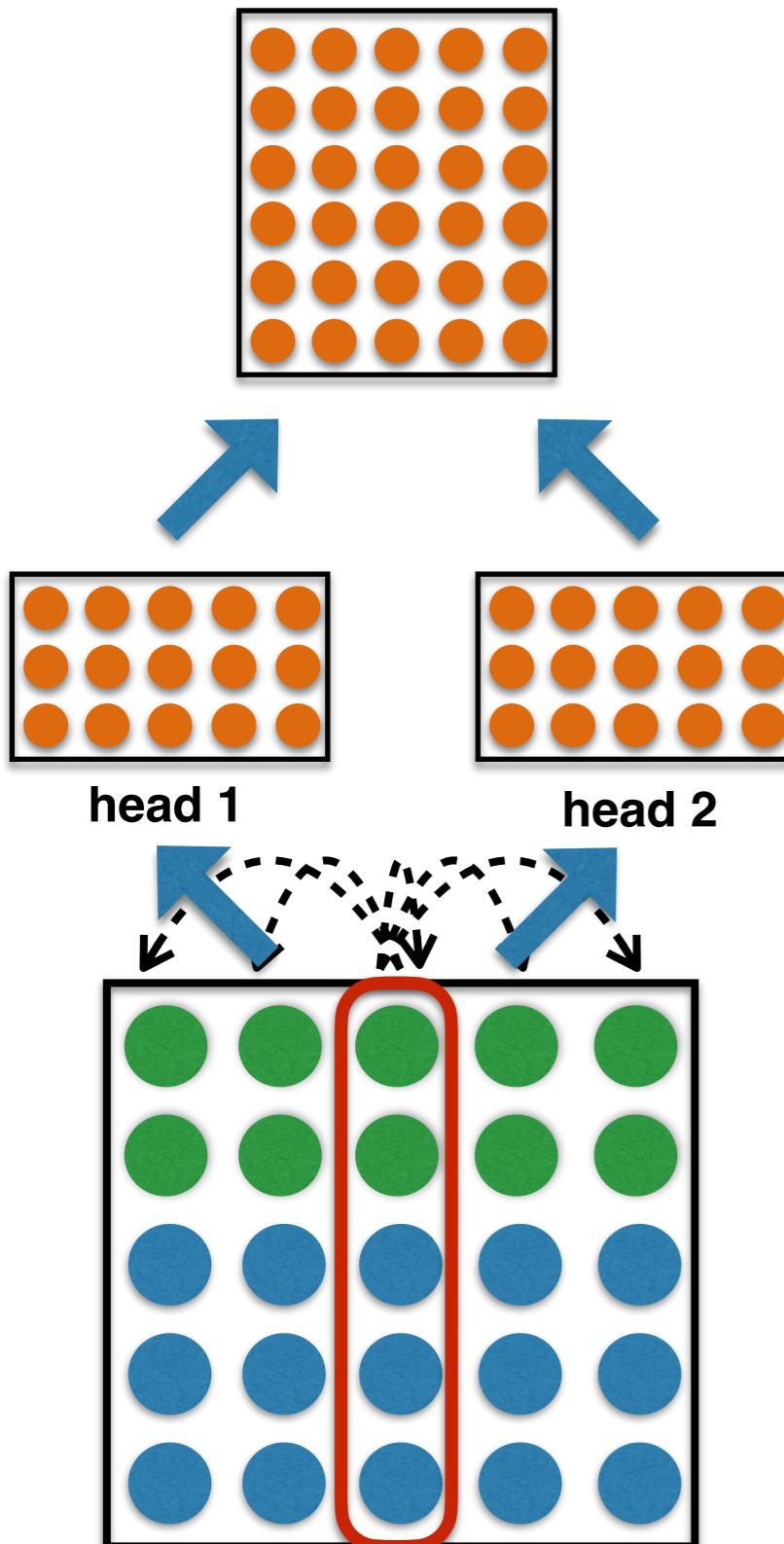
To obtain one vector per position, we rearrange this tensor so that all ℓ -length representations for each position are adjacent; i.e., the reshaped matrix is in $\mathbb{R}^{n \times (\ell \cdot h)}$.

Since we would like the final output to have the same shape as the input, we use a final linear projection, $\mathbf{O} \in \mathbb{R}^{(\ell \cdot h) \times d}$, to conclude what the authors call **“multiheaded attention”**:

$$\mathbf{Y} = \text{reshape}(\mathbf{Z})\mathbf{O}$$

$$= \text{reshape}(\text{softmax}(\mathbf{XLRX}^\top)\mathbf{XP})\mathbf{O}$$

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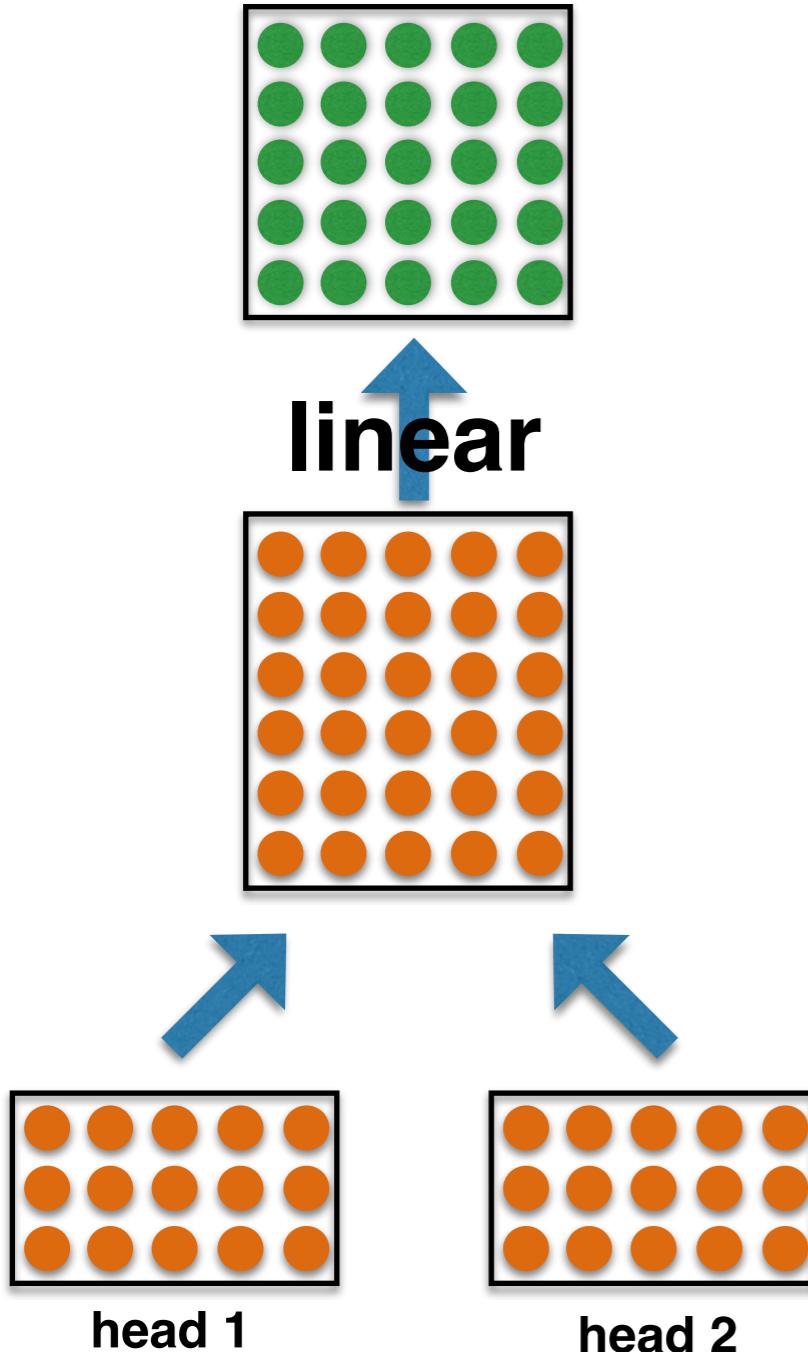
$$\mathbf{R} \in \mathbb{R}^{h \times \ell \times d}$$

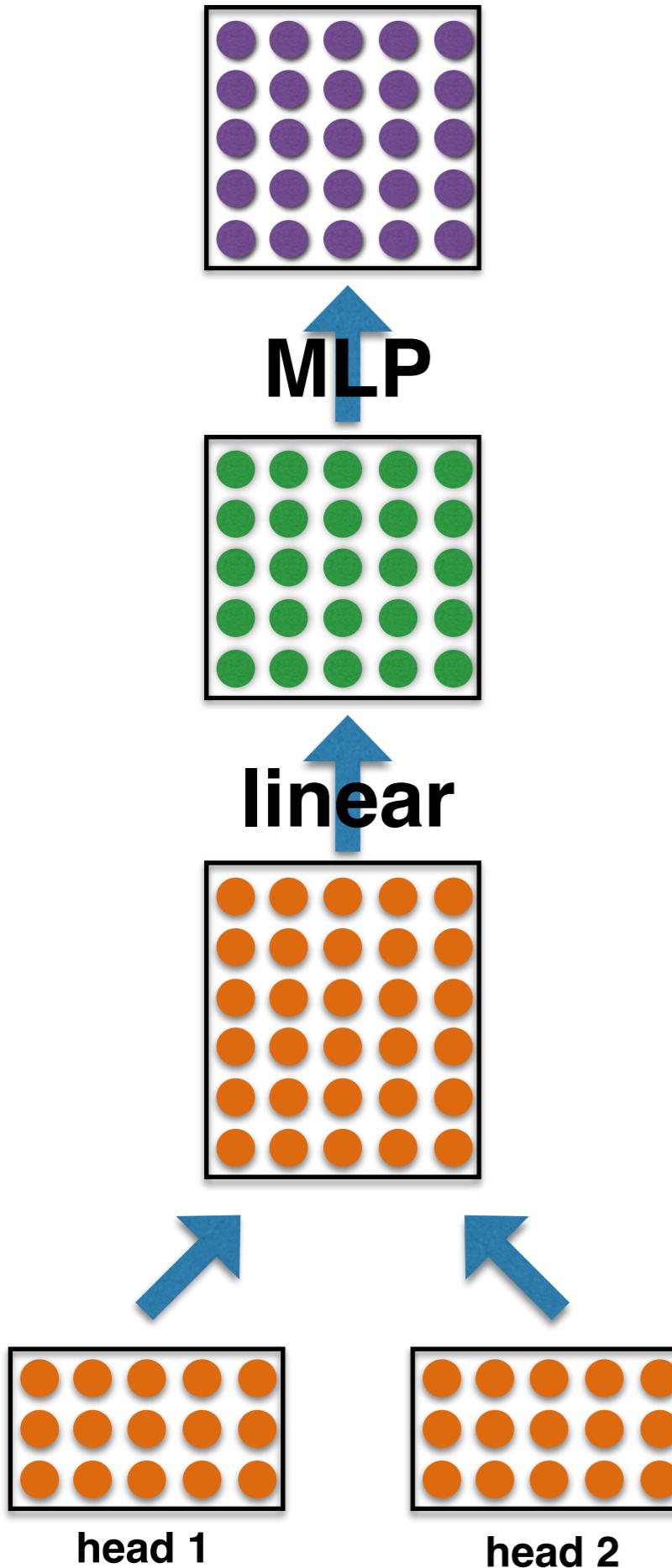
$$\mathbf{P} \in \mathbb{R}^{h \times d \times \ell}$$

$$\mathbf{O} \in \mathbb{R}^{(\ell \cdot h) \times d}$$

And we compute $\mathbf{Y} = \text{reshape}(\text{softmax}(\mathbf{XLRX}^\top)\mathbf{XP})\mathbf{O}$, which is in $\mathbb{R}^{n \times d}$.

Happily, these operations exploit the very efficient batched matrix multiply operations (fast on your GPUs).





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$$\mathbf{P} \in \mathbb{R}^{h \times d \times \ell}$$

$$\mathbf{O} \in \mathbb{R}^{(\ell \cdot h) \times d}$$

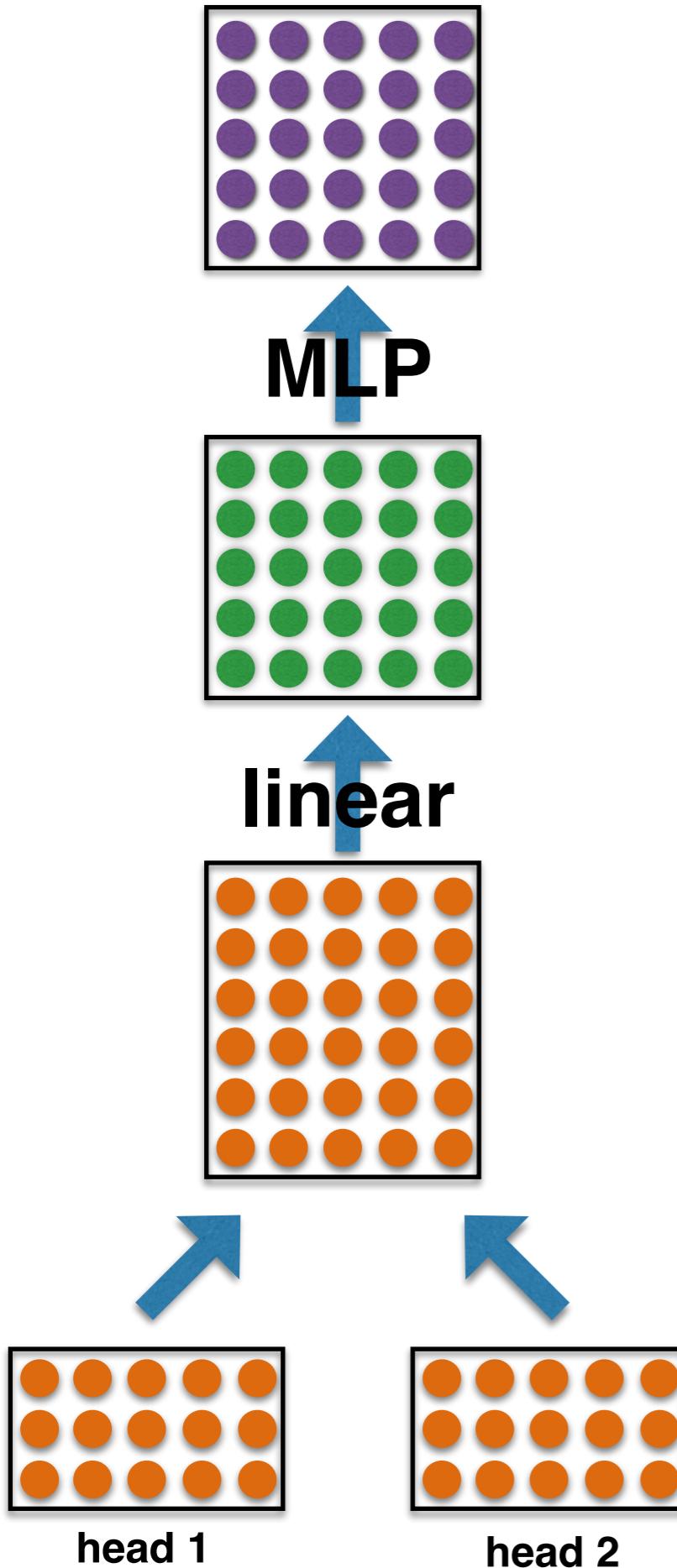
And we compute $\mathbf{Y} = \text{reshape}(\text{softmax}(\mathbf{X}\mathbf{L}\mathbf{R}\mathbf{X}^\top)\mathbf{X}\mathbf{P})\mathbf{O}$, which is in $\mathbb{R}^{n \times d}$.

Happily, these operations exploit the very efficient batched matrix multiply operations (fast on your GPUs).

But we're not done yet. After multi-headed attention, \mathbf{Y} is further transformed by passing each position through an MLP in parallel. Intuitively this lets the model extract *conjunctions* of features that were *integrated* via attention.

$$\mathbf{F} = \text{relu}(\mathbf{Y}\mathbf{W} + \mathbf{b})\mathbf{V} + \mathbf{c}$$

where $\mathbf{W} \in \mathbb{R}^{d \times k}$ and k is “large” (eg $4 \times d$).



$\mathbf{X} \in \mathbb{R}^{n \times d}$ is obtained by stacking word vectors and concatenating positional information.

We have auxiliary parameters:

$$\mathbf{L} \in \mathbb{R}^{h \times d \times \ell} \quad \mathbf{W} \in \mathbb{R}^{d \times k}$$

$$\mathbf{R} \in \mathbb{R}^{h \times \ell \times d} \quad \mathbf{V} \in \mathbb{R}^{k \times d}$$

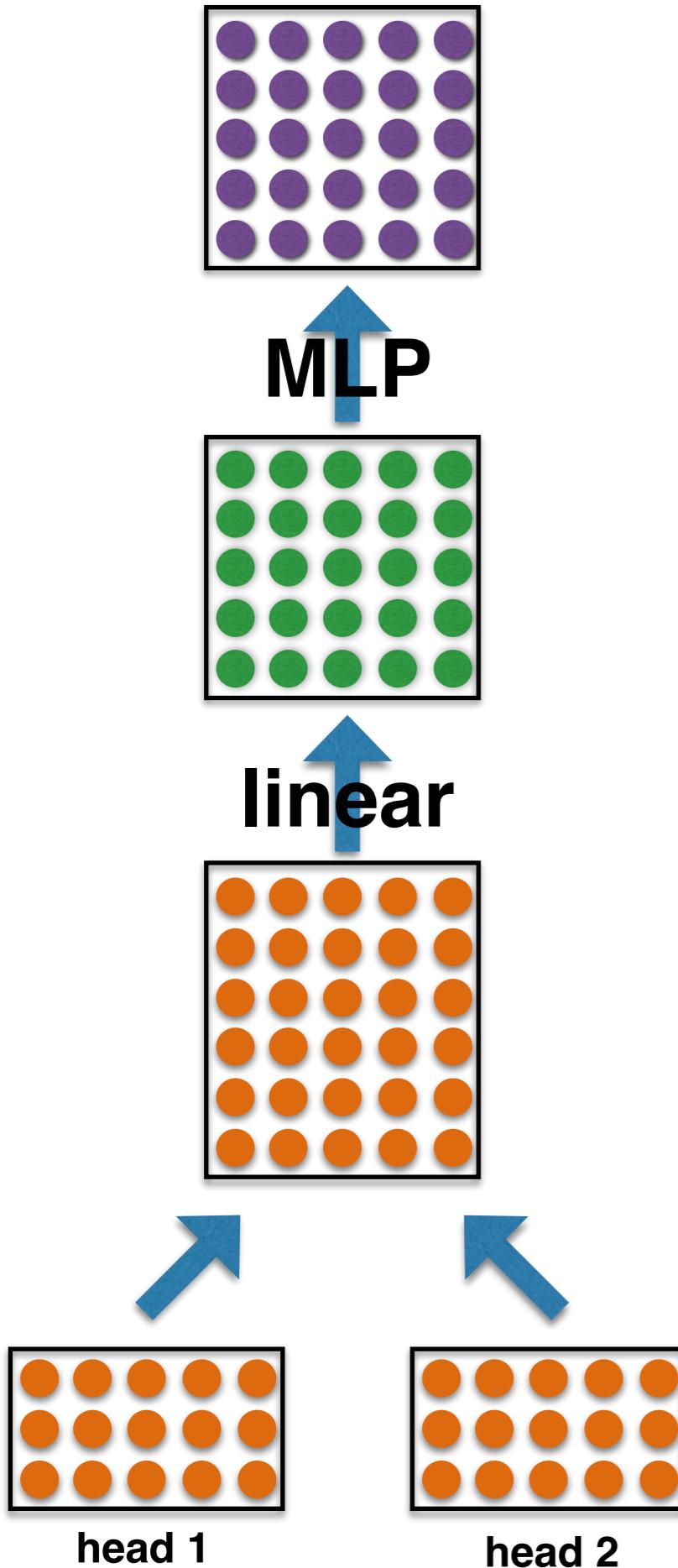
$$\mathbf{P} \in \mathbb{R}^{h \times d \times \ell}$$

$$\mathbf{O} \in \mathbb{R}^{(\ell \cdot h) \times d}$$

And we compute

$$\mathbf{Y} = \text{reshape}(\text{softmax}(\mathbf{X}\mathbf{L}\mathbf{R}\mathbf{X}^\top)\mathbf{X}\mathbf{P})\mathbf{O} + \mathbf{X}$$

$$\mathbf{F} = \text{relu}(\mathbf{Y}\mathbf{W} + \mathbf{b})\mathbf{V} + \mathbf{c} + \mathbf{Y}$$



$\mathbf{X} \in \mathbb{R}^{n \times d}$ is obtained by stacking word vectors and concatenating positional information.

We have auxiliary parameters:

$$\mathbf{L} \in \mathbb{R}^{h \times d \times \ell} \quad \mathbf{W} \in \mathbb{R}^{d \times k}$$

$$\mathbf{R} \in \mathbb{R}^{h \times \ell \times d} \quad \mathbf{V} \in \mathbb{R}^{k \times d}$$

$$\mathbf{P} \in \mathbb{R}^{h \times d \times \ell}$$

$$\mathbf{O} \in \mathbb{R}^{(\ell \cdot h) \times d}$$

And we compute

$$\mathbf{Y} = \text{reshape}(\text{softmax}(\mathbf{X}\mathbf{L}\mathbf{R}\mathbf{X}^\top)\mathbf{X}\mathbf{P})\mathbf{O} + \mathbf{X}$$

$$\mathbf{F} = \text{relu}(\mathbf{Y}\mathbf{W} + \mathbf{b})\mathbf{V} + \mathbf{c} + \mathbf{Y}$$

Some final details:

- residual connections make deeper ($+\mathbf{X}$, $+\mathbf{Y}$) make deeper networks easier to learn. That's why it's there.
- “layer normalization” is used, which rescales and “remean” \mathbf{Y} and \mathbf{F} . This also makes training more stable.
- to enable propagation of information over multiple hops, and to learn more complex interactions, we stack many of these layers on top of each other

Transformer encoders

- We have now built an encoder that uses attention to compute representations of words-in-context
- We could replace the bidirectional encoder used in the previous section with this
- But we now turn to how to build a “decoder” out of transformer components

Transformer decoders

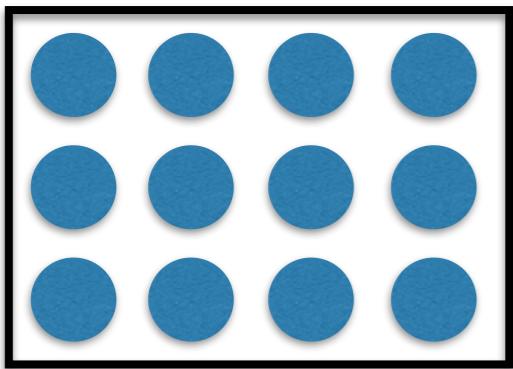
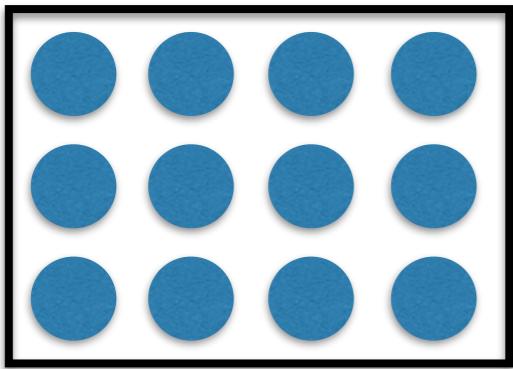
- Transformers can attend forwards and backward
 - This is what makes them powerful, but a language model can't look into the future for words that haven't been generated (at training time it could, but it wouldn't help you at test time)
 - Trick: we will manipulate the attention so that words can only look to their left. Very simple tweak to the model:

$$\begin{aligned}\mathbf{Y} &= \text{reshape}(\text{softmax}(\mathbf{XLRX}^\top)\mathbf{XP})\mathbf{O} + \mathbf{X} \\ \mathbf{\tilde{Y}} &= \text{reshape}(\text{softmax}(\mathbf{XLRX}^\top + \mathbf{M})\mathbf{XP})\mathbf{O} + \mathbf{X}\end{aligned}$$

Here, $\mathbf{M} \in \{-\infty, 0\}^{n \times n}$, such that the pre-softmax attention “logits” are set to -infinity for all attention from position i to position j where $j > i$.

Unconditional LMs

tom likes beer </s>



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$$Q = \text{softmax}(\overset{\leftarrow}{Y} R)$$



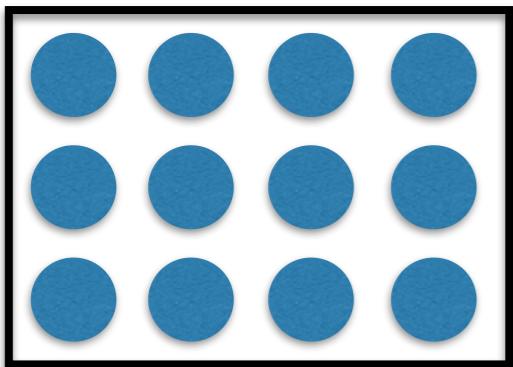
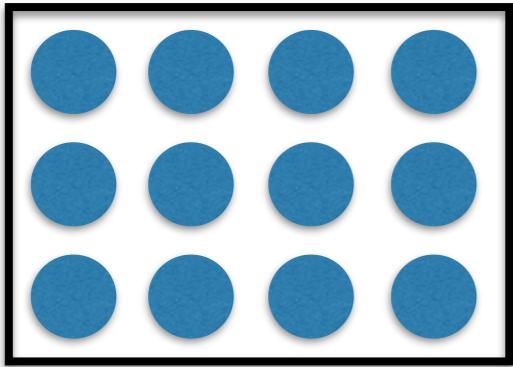
$$\overset{\leftarrow}{Y} = \text{reshape}(\text{softmax}(\overset{\leftarrow}{Y} LR \overset{\leftarrow}{Y}^T + M) \overset{\leftarrow}{Y} P)O + \overset{\leftarrow}{Y}$$



$$\overset{\leftarrow}{Y} = \text{reshape}(\text{softmax}(XLRX^T + M)XP)O + X$$

Conditional LMs

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$$Q = \text{softmax}(\overset{\leftarrow}{Y} R)$$



$$\overset{\leftarrow}{Y} = \text{reshape}(\text{softmax}(\overset{\leftarrow}{Y} L R C^T) C P) O + \overset{\leftarrow}{Y}$$



$$\overset{\leftarrow}{Y} = \text{reshape}(\text{softmax}(X L R X^T + M) X P) O + X$$

1. Build a representation of the target history
2. Incorporate conditioning context by “attending to” the source context **C**.

Transformer Summary

- Current state of the art
 - Good mix of computationally efficient and a reasonably effective model
- Still many opportunities to improve things!
 - Low-rank approximations are one way to reduce parameters— there are many others.
 - Does every attention head have to sum to 1? Maybe sometimes certain heads should be turned off
 - Should attention be dense? Maybe it should be sparse. Maybe it should correlate with linguistic structure
 - **Your ideas here...**

Questions?

Thanks!

Obrigado!