NLU: Lecture 14
LLMs as Formal Machines

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(based on slides from Butoi et al.)

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School of informatics

Why formal study of LLMs?

- Opening the black box of LLMs: what are the underlying computations they do?
- We can better understand the limitations of LLMs
- Find connections to previous models may help deriving new methodology for LLMs

What are language models?

- Let $y = y_1 \cdots y_n$
- An autoregressive language model defines $p(y)$

$$p(y) = p(\text{EOS} \mid y) \prod_{t=1}^{n} p(y_t \mid y_{<t})$$

Nothing new! Any distribution over strings can be written that way

Food for thought: Why is that the case?

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Food for thought: Why is that the case? The chain rule

Representation-based language model

Remember the conditional probability model over words given a representation, which is roughly:

$$p(y_t \mid y_1 \cdots y_{t-1}) = \text{softmax}(Eh(y_1 \cdots y_{t-1}))_{y_t}$$

Recurrent Neural Networks

We are given a sequence of $x_1, \ldots x_n$.

The hidden state:

$$h_{t+1} = f(h_t, x_t)$$

f is a function that maps the current state and symbol into a new state, so $f : \mathbb{R}^d \times \Sigma \rightarrow \mathbb{R}^d$

Elman RNNs

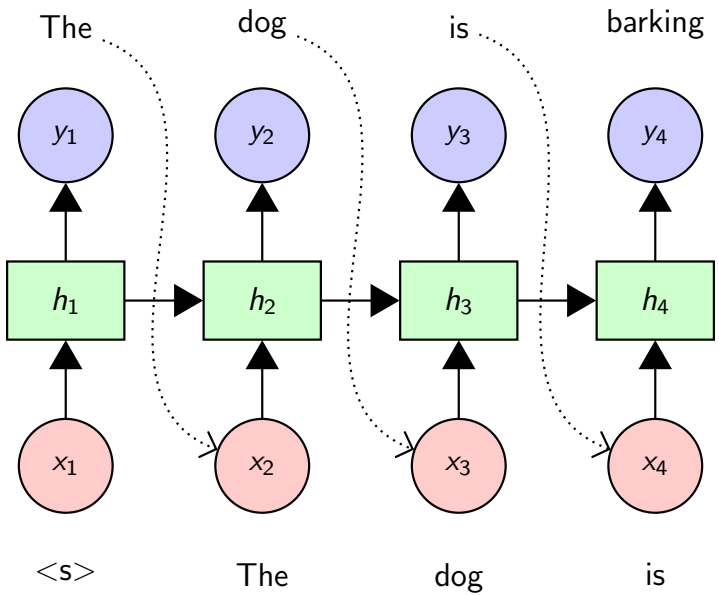
We will focus on so-called Elman RNNs, an older model that has been studied:

$$h_{t+1} = f(h_t, x_t) = \sigma(Uh_t + Vr(x_t) + b)$$

where r is an embedding function, U and V are matrices and b is a vector

RNNs as language models

If we want to turn an RNN into a language model, we add another layer that takes as input h_t and returns a probability distribution over the vocabulary



Every y_t is fed as an x_{t+1} in the next step

RNNs as language models

Food for thought: What is the connection to n-grams?

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Both approaches provide a probability distribution over sentences

> *We multiply the probability of the n-grams together,*
> *OR*
> *We multiply the probability of the words emitted by the RNN,*

to get the probability over the string $p(y_1 \cdots y_n)$.

Food for thought: Why is it important that the mapping f is deterministic?

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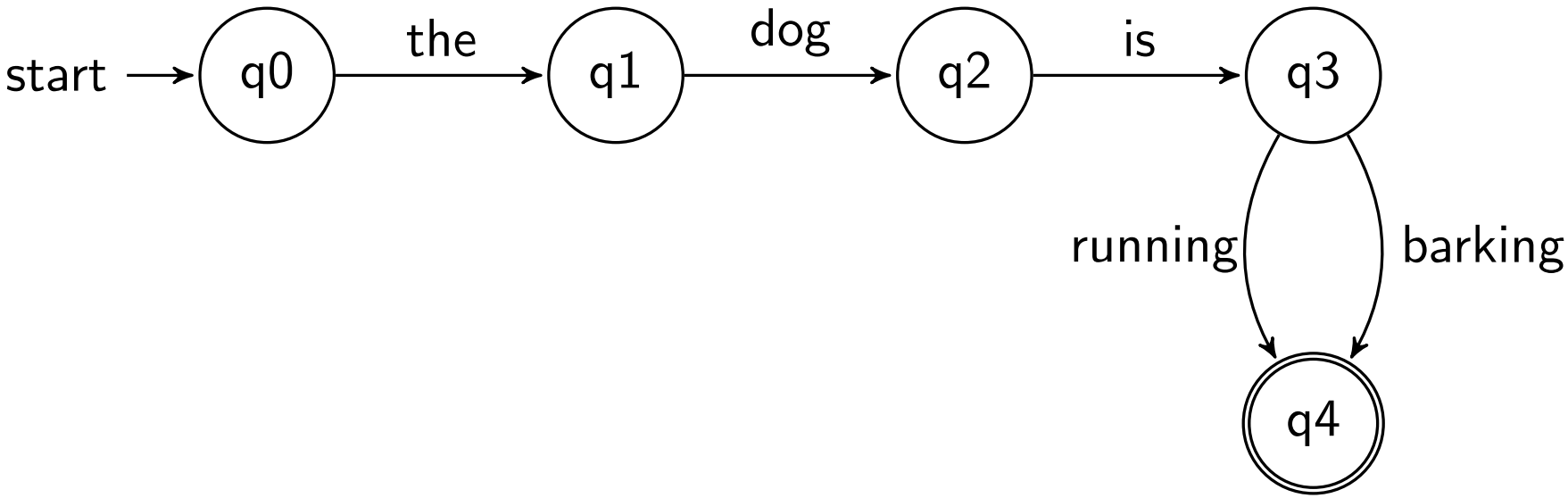
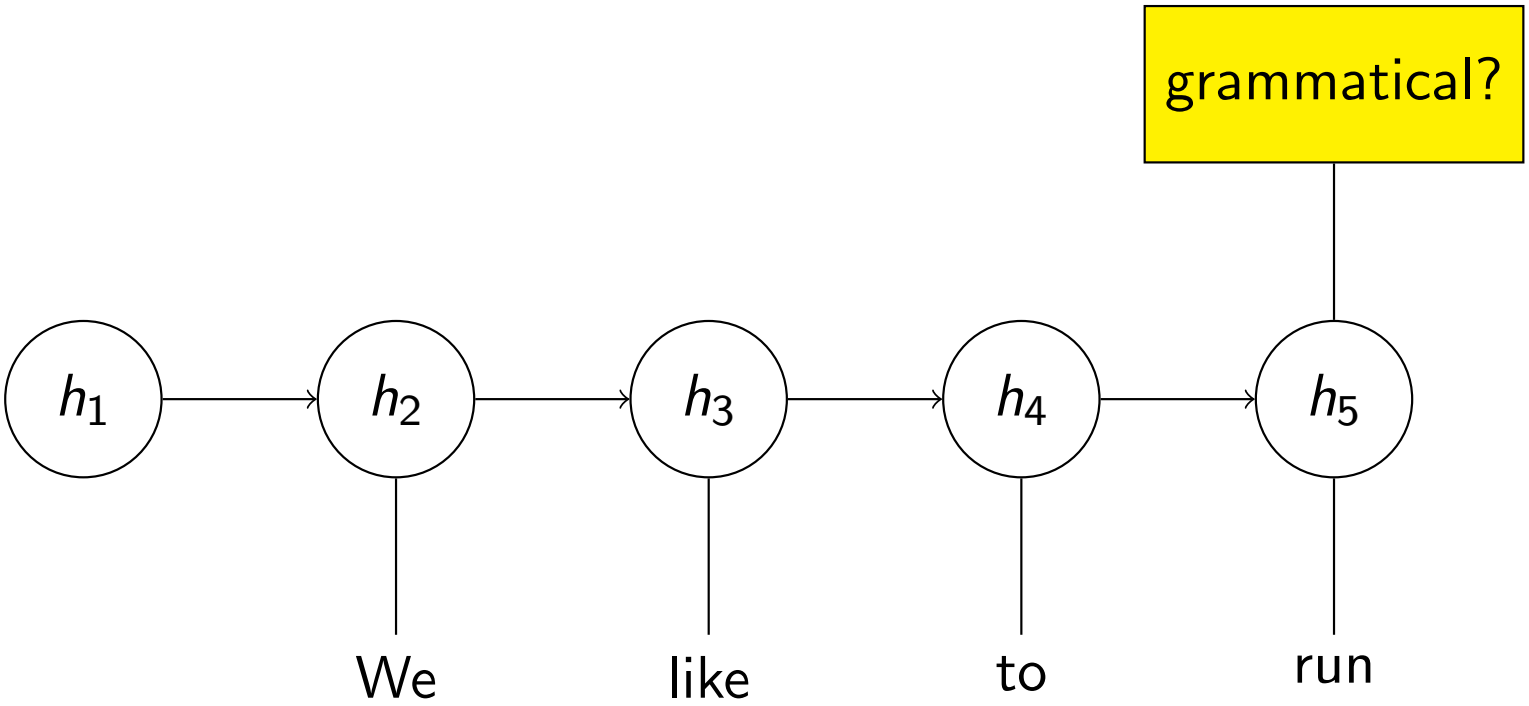
Food for thought: Why is it important that the mapping f is deterministic? We do not need to "sum out" h!

Reminder: Finite State Machines



A set of states Q with q_0 the initial state, an alphabet Σ, a transition function $\delta(q, y) = q'$ and a set of final states $F \subseteq Q$.

RNNs as Recognisers



- Apply a softmax or some other activation unit to binarise the state after encoding into *grammatical* or *not grammatical*
- Given an RNN, its language is defined as the set of all strings it classifies as "grammatical"

RNNs Have States Like Automata

- RNNs have many similarities to automata
- At each step, consume an input symbol, and calculate a new state
- Rather than using a look-up table like transition, use a mathematical formula to calculate a state *vector*

Food for thought: Does that change anything?

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Food for thought: Does that change anything?

Answer: It depends!

Characterising a formalism through its languages

Let $\mathcal{F}$ be a "formalism", whether all RNNs as acceptors or FSMs

Each specific instance in $A \in \mathcal{F}$ is a single RNN or an FSM

It defines a language $L(A)$. We can characterise the formalism by the set $L(\mathcal{F}) = \{L(A) \mid A \in \mathcal{F}\}$.

Two formalisms $\mathcal{F}, \mathcal{F}'$ are equivalent if $L(\mathcal{F}) = L(\mathcal{F}')$.

Do you remember? Which languages do FSMs accept?

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Do you remember? Which languages do FSMs accept?
Regular languages
Indeed, the regular languages fully characterise FSMs.
$L(\text{FSM}) = \textit{regular languages}$

State Space in RNNs

- In principle, the state space for RNNs is infinite, not only infinite, but continuous

- Can we use this fact somehow to simulate really complex algorithms?

We will test RNNs in two cases: the case of unbounded precision and computation and the case of bounded computation and finite precision

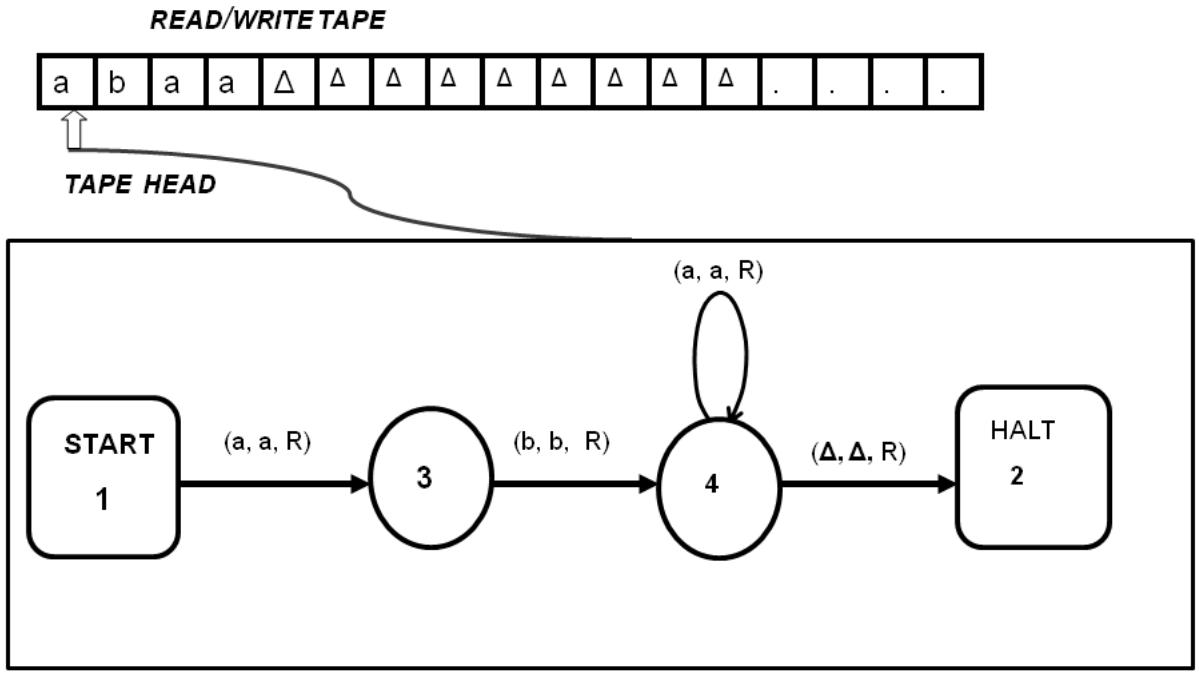
Food for thought: What do you think the outcome will be?

RNNs Power

Depending on the amount of power we provide to the latent states of RNNs, they can either:

- Implement any computable function
- Be significantly limited to finite state languages

Turing Machines



A Turing Machine for aba*

Church-Turing thesis: any reasonably computable function can be implemented using a Turing machine!

Two-stack Pushdown Automaton

An equivalent formalism to Turing machines

Rather than having an infinite tape, we have two stacks. A two-stack PD automaton has:

- Q - a finite set of states
- Σ - a finite alphabet
- Γ - a finite stack alphabet (for both stacks)
- δ - a transition function in $Q \times (\Sigma \cup \{\epsilon\}) \times \Gamma \times \Gamma \rightarrow Q \times \Gamma^* \times \Gamma^*$.
  The transition outputs a new state and strings to replace the top of the two stacks based on the current input symbol and the top symbols of the two stacks
- $q_0 \in Q$ - an initial state
- $q_A \in Q$ - an accepting state
- $q_R \in Q$ - a reject state

RNNs Power

Depending on the amount of power we provide to the latent states of RNNs, they can either:

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  We will start here and show how a 2-PDA can be **simulated** using an RNN. This means we need to bridge the continuous approach of RNNs with the discrete manner PDAs work

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Class exercise: Spend a few minutes to try and construct this simulation

Encoding a Stack

- We will assume that our alphabet is $\Gamma = \{0, 1\}$ in the stack $y_1 \cdots y_n$. (This is enough, why?)

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- We will assume that our alphabet is $\Gamma = \{0, 1\}$ in the stack $y_1 \cdots y_n$. (This is enough, why?)
- A stack can be represented as a number: $0.\gamma_N \gamma_{N-1} \ldots \gamma_1$ where $\gamma_i = \begin{cases} 1 & \text{if } y_i = 0, \\ 3 & \text{otherwise.} \end{cases}$
- We need operations on the stack: mostly pushing and popping

Food for thought: How do we simulate pushing and popping on a number?

Performing Stack Operations

Stack operations can be performed by manipulating a real number that represents the whole stack:

- Popping $y_N = 0 : 10 \times 0.\gamma_N\gamma_{N-1}\ldots\gamma_1 - 1$
- Popping $y_N = 1 : 10 \times 0.\gamma_N\gamma_{N-1}\ldots\gamma_1 - 3$
- Pushing $y = 0 : \frac{1}{10} \times 0.\gamma_N\gamma_{N-1}\ldots\gamma_1 + \frac{1}{10}$
- Pushing $y = 1 : \frac{1}{10} \times 0.\gamma_N\gamma_{N-1}\ldots\gamma_1 + \frac{3}{10}$

Note: Automata transition between configurations

A configuration is a "state of the world" for the two-stack automaton

It includes:

- The current state of the two stacks
- The current state the machine is in

The two-stack automaton can be thought of as transitioning between configurations based on the input!

Configurations

Given a 2-stack PDA, and an input x, there is a sequence of configurations $c_1, \ldots, c_n$ that we transition to

$$c_1 \rightarrow c_2 \rightarrow \cdots \rightarrow c_n$$

If we know how to move between configurations, we can simulate any machine

We will show how RNNs can move between configurations, represented by their latent state

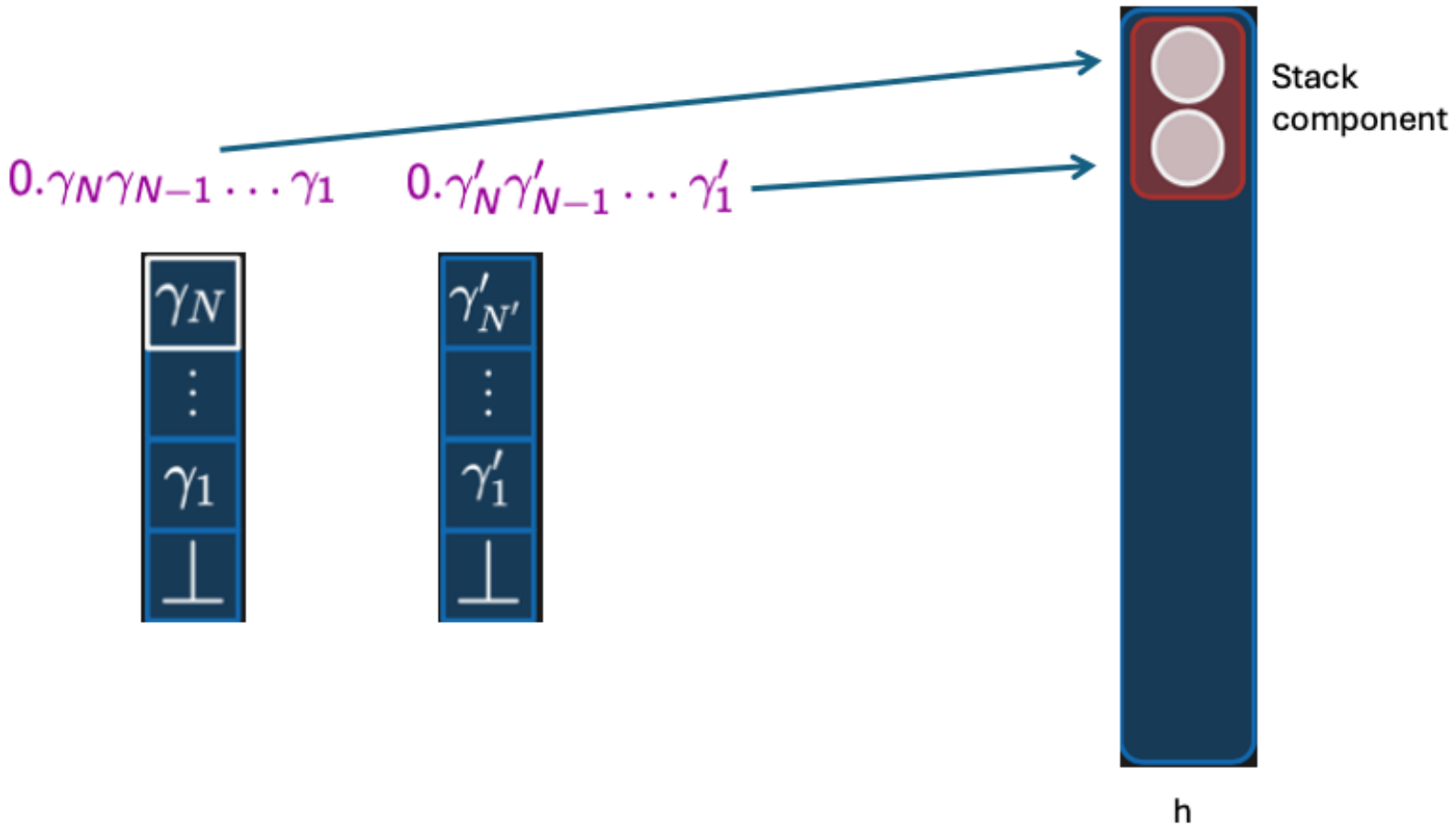
How to encode a "configuration" of a 2-stack PDA machine?

- A vector in the RNN will be in $\mathbb{R}^d$ where $d = 2 + 3 + 3 + N$ where N is the number of states in the Turing machine

- How to encode a configuration of a Turing machine using a vector in the RNN h?
  - h_1 is the first stack encoded as before
  - h_2 is the second stack encoded as before
  - h_3, h_4 and h_5 encode the top element of the first stack (remember the alphabet is $\{0, 1\}$ and we need one more slot for denoting an empty stack!)
  - h_6, h_7 and h_8 encode the top element of the second stack
  - The rest of the vector (positions 9 to $8 + N$) indicate which state the Turing machine is currently in

The Construction (adapted from Butoi et al.)

- Encode the contents of the two stacks



The Construction (adapted from Butoi et al.)

- Encode the contents of the two stacks
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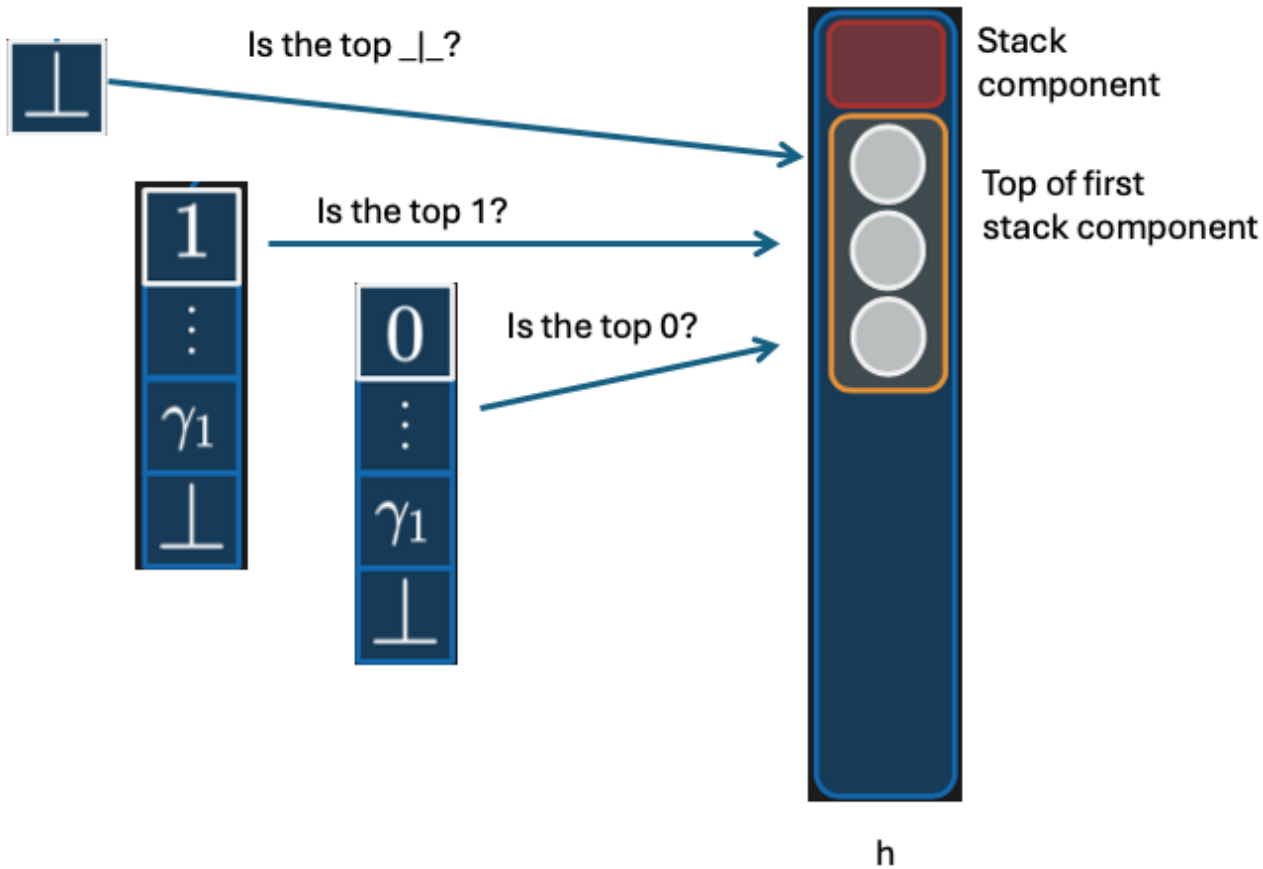
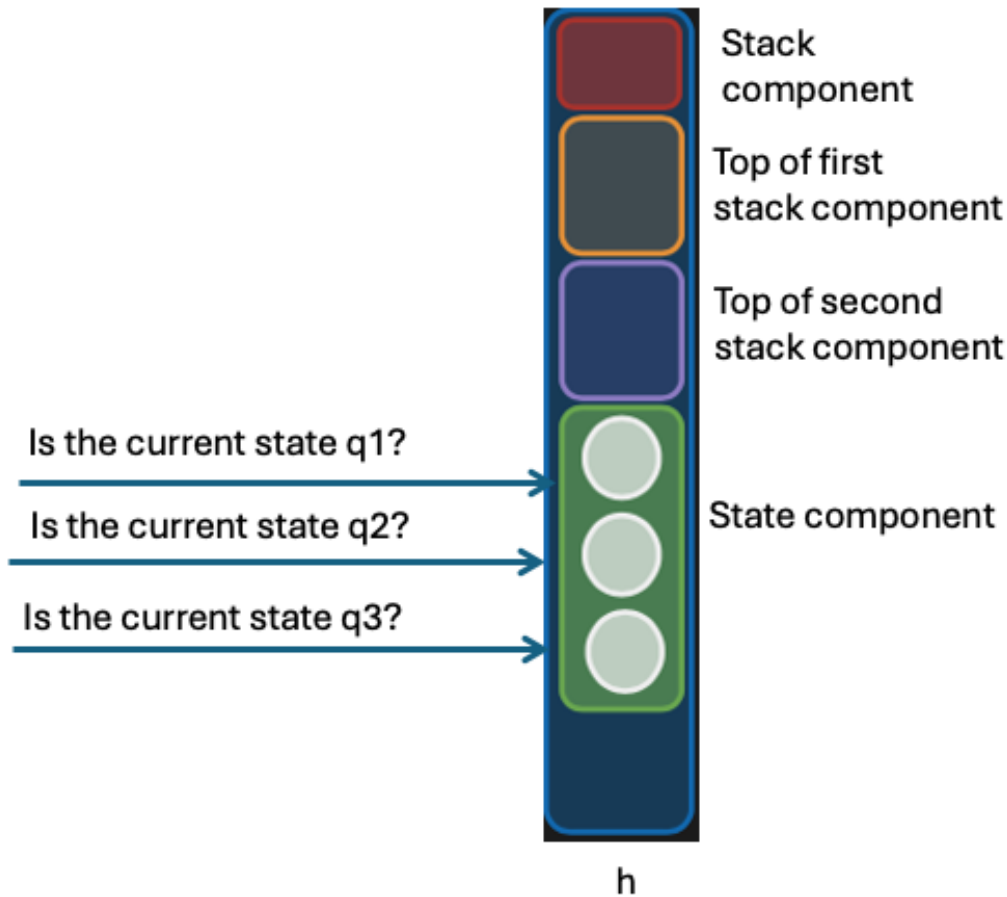


The Construction (adapted from Butoi et al.)

- Encode the contents of the two stacks
- Encode the top of the two stacks
- Encode the current state



How to simulate a 2-stack PDA?

We can set the parameters of the RNN U, V, b such that it will transition between configurations of the Turing machine according to its transition rules

For more details, see Siegelmann and Songtag (1992)

Note that we are not doing **any** training here! We figure out the parameters in a constructive manner, not learning from data

Summary: Turing Machines and RNNs

- Turing machines can be simulated using two-stack automata
- Two-stack automata can be simulated using RNNs with unbounded precision and computation
- The state in the RNN encodes the two stacks and the state in the two-stack automaton (a "configuration")
- Therefore: **RNNs with unbounded precision and computation are as powerful as Turing machines!**

Back to RNNs Power

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  If RNNs are bounded in precision and computation, they are equivalent to FSMs!

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Bounded precision and computation

- An RNN with the update rule

$$h_{t+1} = H(Uh_t + Vr(y_t) + b)$$

can simulate any deterministic automaton (where $H(x) = 0$ if $x \leq 0$ and 1 otherwise; The Heaviside function)

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- An RNN with bounded precision is no more expressive than a finite state automaton

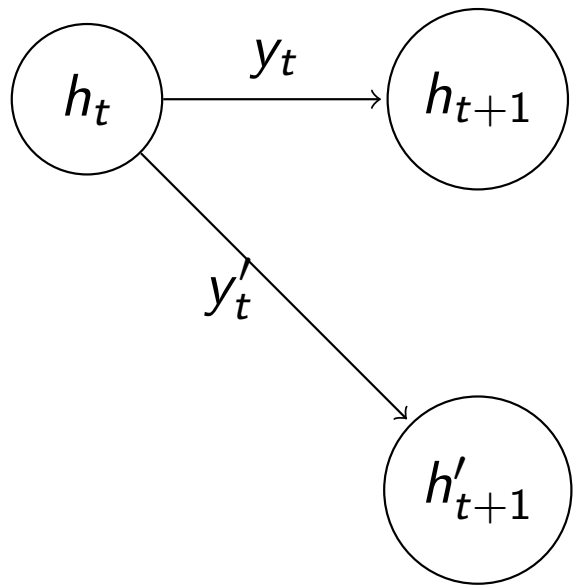
  Class exercise: Try to construct the latter argument

Any RNN can be an FSM

(Note we assume that the activation leads to binary states!)

$$h_{t+1} = f(h_t, y_t)$$

$$h'_{t+1} = f(h_t, y'_t)$$



RNNs can simulate FSMs

- The construction takes any **deterministic** FSM and transforms it into an RNN
  Food for thought: What about non-deterministic FSMs?

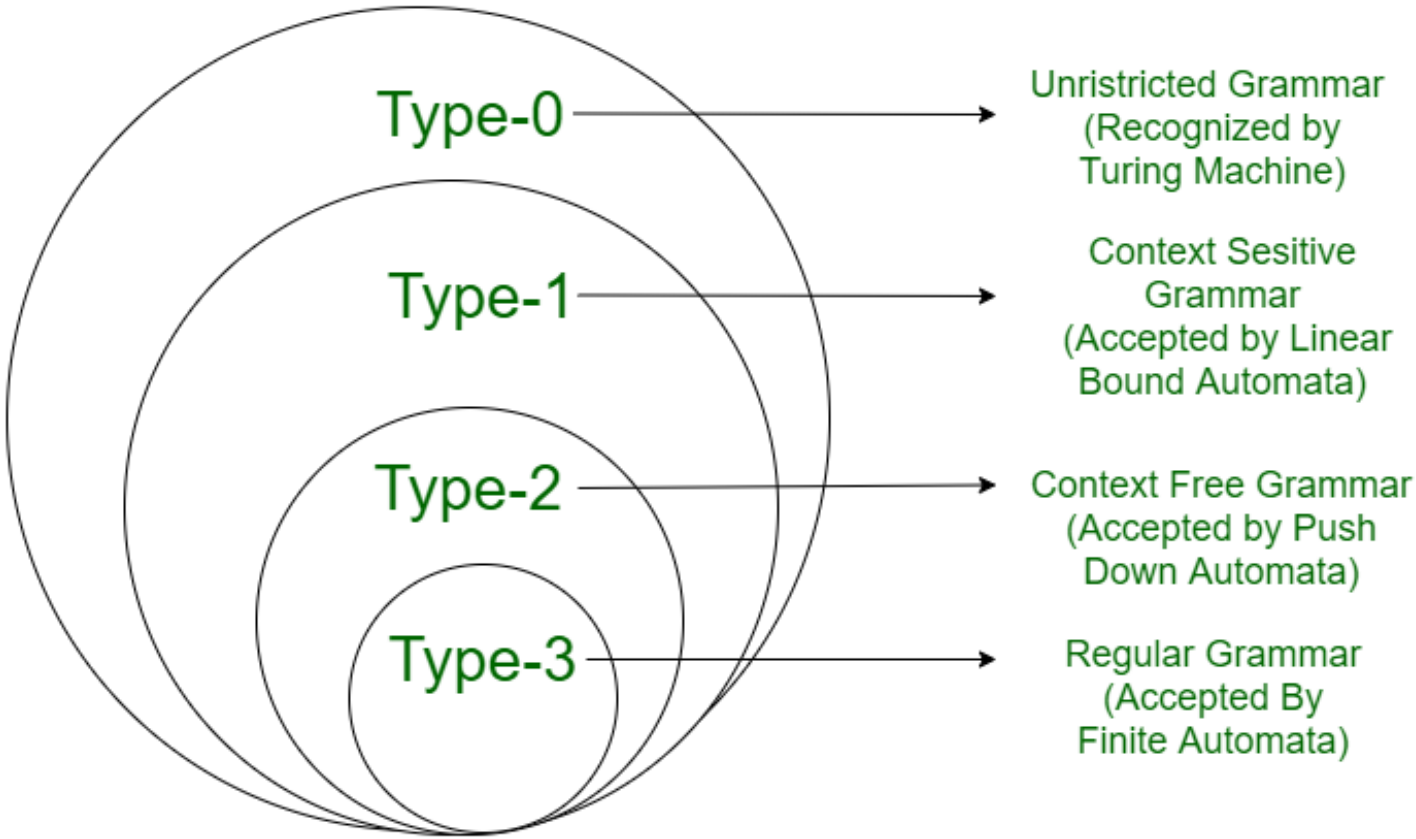
RNNs can simulate FSMs

- The construction takes any **deterministic** FSM and transforms it into an RNN
  Food for thought: What about non-deterministic FSMs? Any non-deterministic FSM can be determinised
- The latent state h_t will be indexed by a pair of state and symbol. The state provides the current state in the simulated machine, and the symbol provides the symbol we are being fed
- $h_{t+1} = H(Uh_t + Vr(y_t) + b)$. We will set U to give 0.5 for all elements in the vector (q, a) ranging over a such that transition from q in h_t provides q'; We will set V to add another 0.5 to all elements in the vector that correspond to y_t
- The H function now will zero out all those that are just 0.5 and keep only one element that is 1.0. We get from that h_{t+1}.

The devil is in the details

- To make the construction work we need more attention to details, but that's the construction at a high level

A stark difference in the Chomsky hierarchy



RNNs with finite precision and bounded computation are reduced from Type-0 to Type-3.

Summary

- Studying LLMs in formal terms is a fertile ground to understand them better

References

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H. T. Siegelman and E. D. Sontag. Neural networks with real weights: analog computational complexity. COLT 1992.