Deep Learning Refresher

Week 6

Tirtharaj Dash

Limitations of MLP or CNN:

- They accept a fixed-sized vector as input (e.g. an image) and produce a fixed-sized vector as output (e.g. probabilities of different classes). [Too constrained]
- These models perform this mapping using a fixed amount of computational steps (e.g. the number of layers in the model). [Expressivity]
- Not effective data with temporal dependencies (e.g. time-series, sentences) [Problem-specific limitation]

*** We will need network structures that allow us to operate over sequences of vectors.

State and Recurrence I

- We call a hidden representation of a network as a 'state', denoted as $\mathbf{h}$.
- We will be attaching a time information (t) to this:

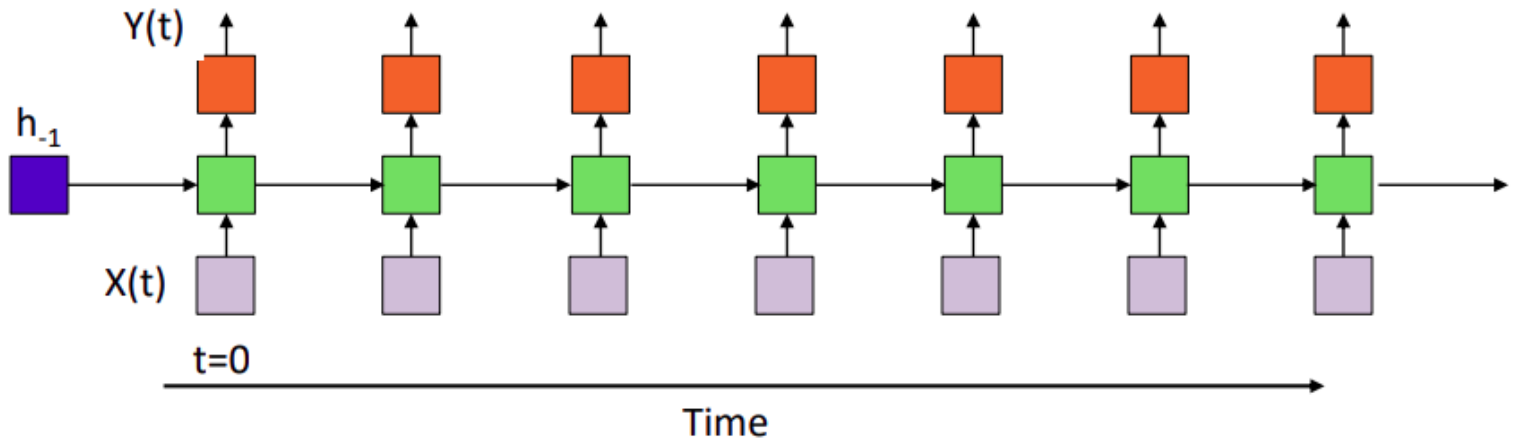
$$\mathbf{h}_t = f(\mathbf{x}_t, \mathbf{h}_{t-1})$$

and,

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

- An initial state has to be defined: $\mathbf{h}_0$ (or, sometimes, people use $\mathbf{h}_{-1}$)
- State summarises information about the entire past.
- The neural network architecture that implements the above is a fully recurrent neural network.

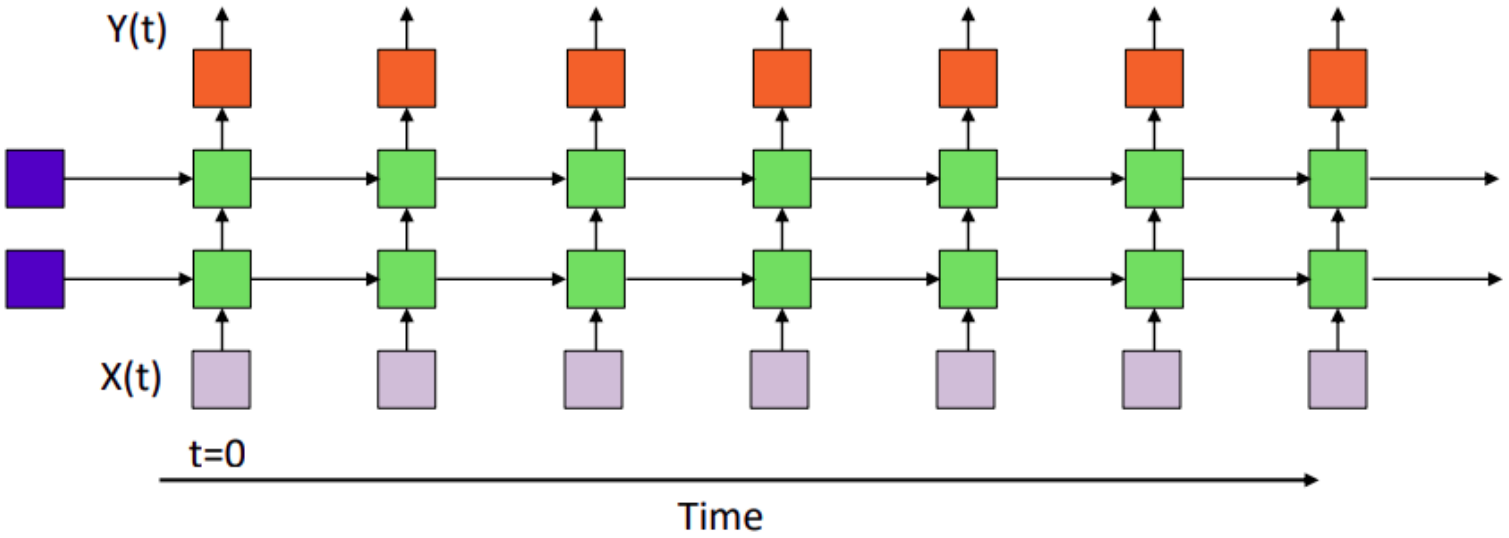
State and Recurrence II



- A state at any time is determined by the input at that time, and the previous state.
- This is a typical recurrent neural network (RNN), with one hidden layer.
- Also note that this is a generic case: where, input and output lengths are same. In other cases, we just remove some of the inputs or outputs or both.

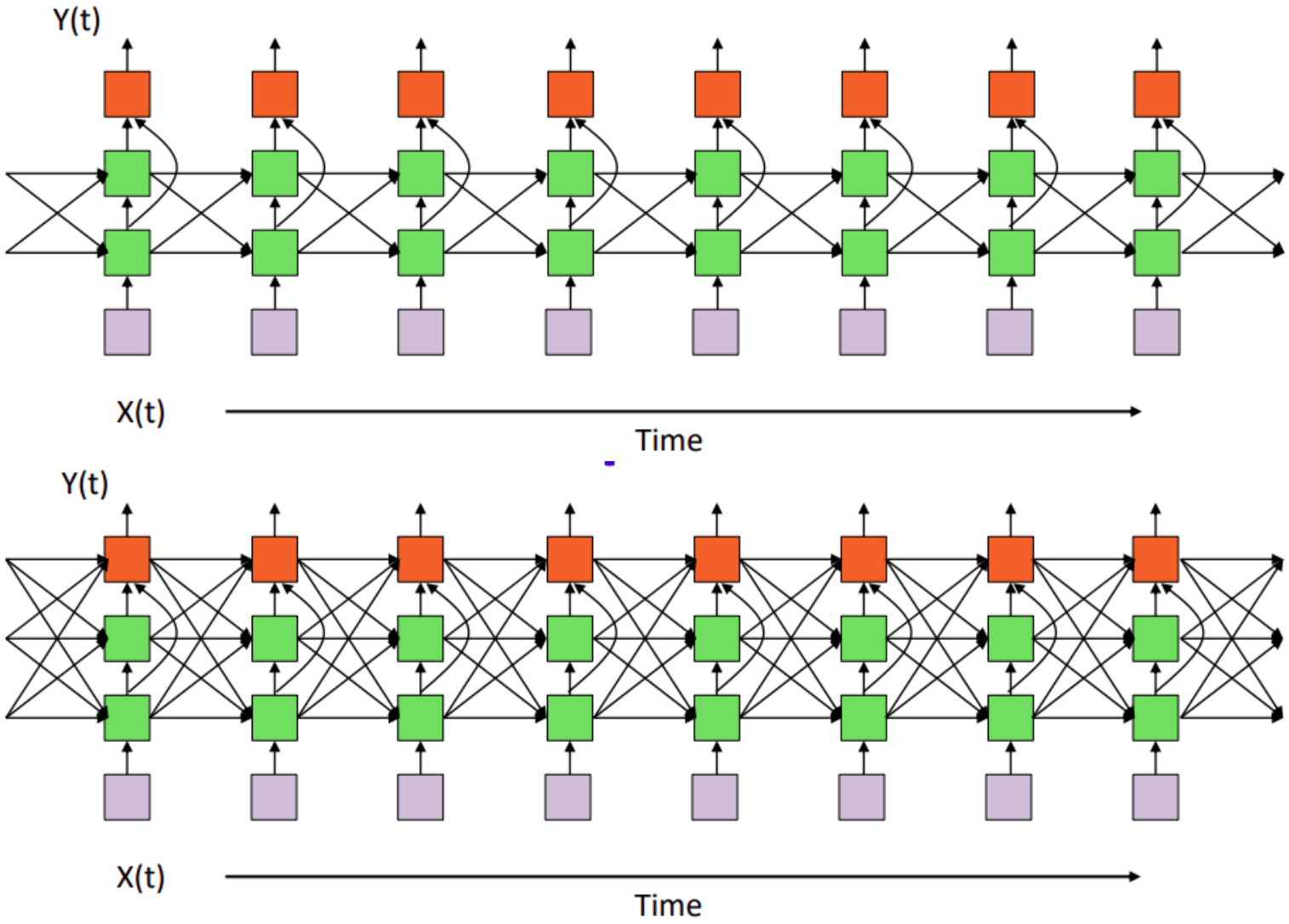
State and Recurrence III

- The state can be arbitrarily complex. Like this:



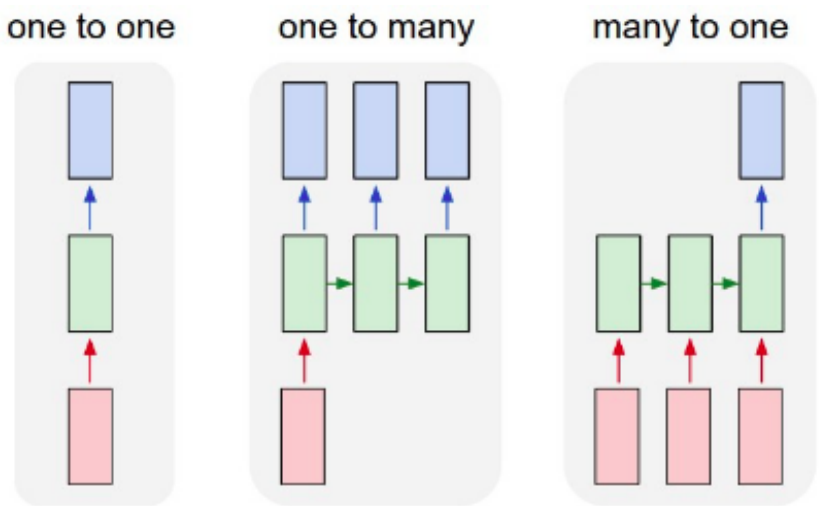
State and Recurrence IV

or, these:



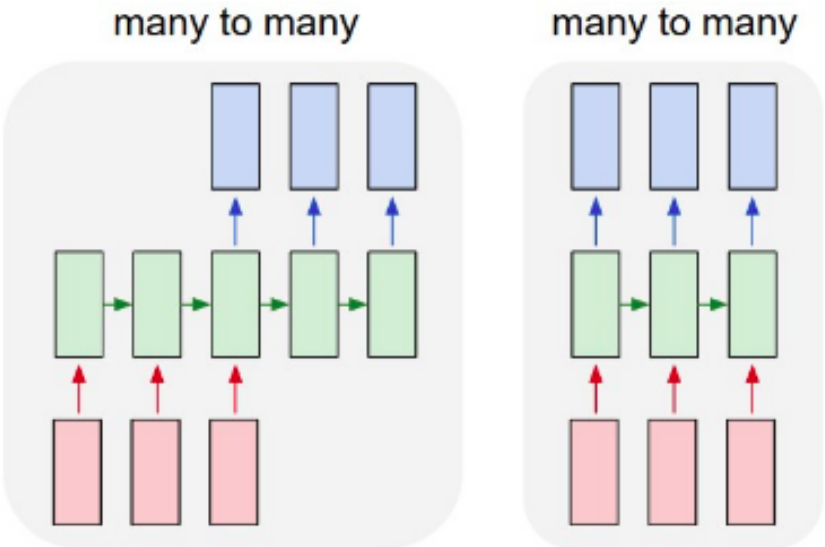
Variants of architectures I

- (1) One-to-one: Vanilla network; from fixed-sized input to fixed-sized output (e.g. image classification).
  (2) One-to-many: Sequence output (e.g. image captioning takes an image and outputs a sentence of words).
  (3) Many-to-one: Sequence input (e.g. sentiment analysis where a given sentence is classified as expressing positive or negative sentiment).



Variants of architectures II

- (4) Sequence input and sequence output (e.g. Machine Translation: an RNN reads a sentence in English and then outputs a sentence in French).
  (5) Synced sequence input and output (e.g. video classification where we wish to label each frame of the video).

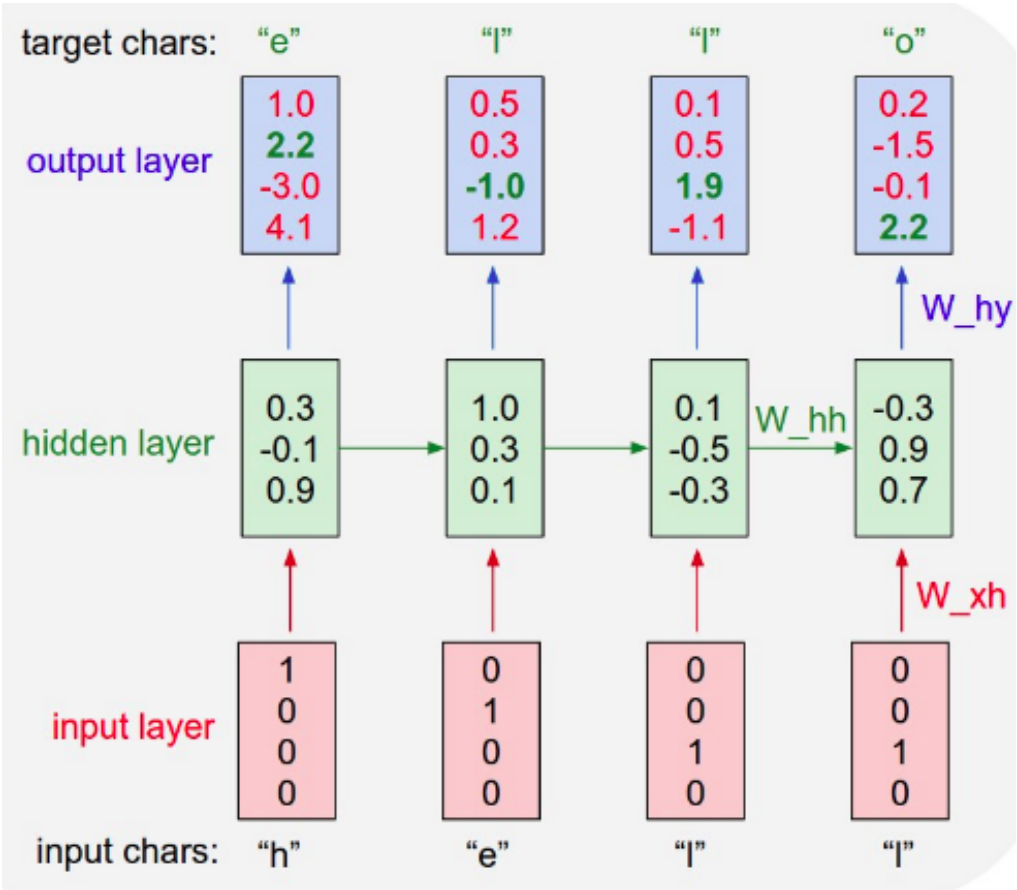


Ref: `http://karpathy.github.io/2015/05/21/rnn-effectiveness/`

A simple example I

- Character-level language model (Ref: Karpathy):
  - Input: a huge chunk of text
  - Models: probability distribution of the next character in the sequence given a sequence of previous characters.
  - Usage: It will allow us to generate new text one character at a time.
- Suppose we only had a vocabulary of 4 possible letters "helo", and wanted to train an RNN on the training sequence "hell".
  - The probability of "e" should be likely given the context of "h"
  - "l" should be likely in the context of "he"
  - "l" should also be likely given the context of "hel"
  - "o" should be likely given the context of "hell"

A simple example II



- State allows the network to understand a "context".
- It uses its recurrent connections to keep track of the context.

Gradient analysis in RNN I

- Let's consider a simplified model (general case). Making the notations also simple.
  - h_t: hidden state
  - x_t: input
  - o_t: output at time-step t
- Let's denote some weights:
  - w_{hx}: $x \rightarrow h$
  - w_{hh}: $h \rightarrow h$
  - w_o: $h \rightarrow o$
- For convenience of explanation (and, also done in practice), we concatenate h_{t-1} and x_t; and the weights are then stacked. Let's call this weight as w_h.

Gradient analysis in RNN II

- These are the forward computation of hidden layer and output at every time step t:

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

$$o_t = g(h_t, w_o)$$

where, f and g are activations at hidden and output layer respectively.

- We have now a chain of values that are dependend on each other due to recurrence:

$$\{\ldots, (x_{t-1}, h_{t-1}, o_{t-1}), (x_t, h_t, o_t), \ldots\}$$

Gradient analysis in RNN III

- Now, for finishing up with the forward computation we need to *loop* through each of the triplets at every time-step: $t = 1, \ldots, T$ and compute a total loss:

$$L(x_1, \ldots, x_T, y_1, \ldots, y_T, w_h, w_o) = \frac{1}{T} \sum_{t=1}^{T} \ell(y_t, o_t)$$

Gradient analysis in RNN IV

- Recall that we need to use backprop for learning the parameters of the network. This will require
  - Gradient of L w.r.t. w_o (easy)
  - Gradient of L w.r.t. w_h (tricky)

Gradient analysis in RNN V

- The gradient of L w.r.t. w_h:

$$\begin{aligned}\frac{\partial L}{\partial w_h} &= \frac{1}{T}\sum_{t=1}^{T}\frac{\partial \ell(y_t, o_t)}{\partial w_h} \\ &= \frac{1}{T}\sum_{t=1}^{T}\frac{\partial \ell(y_t, o_t)}{\partial o_t}\frac{\partial o_t}{\partial h_t}\frac{\partial h_t}{\partial w_h} \\ &= \frac{1}{T}\sum_{t=1}^{T}\frac{\partial \ell(y_t, o_t)}{\partial o_t}\frac{\partial g(h_t, w_h)}{\partial h_t}\frac{\partial h_t}{\partial w_h}\end{aligned}$$

  First and second term above: easy to compute

- The term $\frac{\partial h_t}{\partial w_h}$ is tricky to compute due to recurrence.

Gradient analysis in RNN VI

$\frac{\partial h_t}{\partial w_h}$:

- Recurrently compute the effect of w_h on h_t.
- h_t depends on both w_h and h_{t-1}; again h_{t-1} depends on w_h.
- Therefore,

$$\frac{\partial h_t}{\partial w_h} = \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial w_h} + \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial w_h}$$

- Do you see a chain there in the red term above?

Gradient analysis in RNN VII

Let's now assume that we have 3 sequences: $\{a_t\}$, $\{b_t\}$, and $\{c_t\}$.

- Let these sequences satisfy: $a_0 = 0$ and $a_t = b_t + c_t a_{t-1}$ for $t = 1, 2, \ldots$
- For any $t \geq 1$, we can show that:

$$a_t = b_t + \sum_{i=1}^{t-1} \left(\prod_{j=i+1}^{t} c_j \right) b_i$$

(Taken from `d2l.ai`)

Gradient analysis in RNN VIII

This is what we had:

$$a_t = b_t + \sum_{i=1}^{t-1} \left(\prod_{j=i+1}^{t} c_j \right) b_i$$

Okay!!! Let's now substitute:

$$a_t = \frac{\partial h_t}{\partial w_h}$$

$$b_t = \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial w_h}$$

$$c_t = \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial h_{t-1}}$$

Gradient analysis in RNN IX

Therefore,

$$\frac{\partial h_t}{\partial w_h} = \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial w_h} + \sum_{i=1}^{t-1} \left(\prod_{j=i+1}^{t} \frac{\partial f(x_j, h_{j-1}, w_h)}{\partial h_{j-1}} \right) \frac{\partial f(x_i, h_{i-1}, w_h)}{\partial w_h}$$

We are doing backprop through time (BPTT).

Do you see some potential problems:

- Q What will happen if t is large?
- Q What will happen if the bracketted term is < 0 or large?

Gradient analysis in RNN X

Strategies to deal with some problems in computing (note that full computation of the equation is not desirable in practice):

$$\sum_{i=1}^{t-1}\left(\prod_{j=i+1}^{t}\frac{\partial f(x_j, h_{j-1}, w_h)}{\partial h_{j-1}}\right)\frac{\partial f(x_i, h_{i-1}, w_h)}{\partial w_h}$$

Trucating time-steps (Jaeger, 2002):

- Truncate the sum after τ steps: $\frac{\partial h_{t-\tau}}{\partial w_h}$ (leads to an approximation of the true gradient)
- In practice, this works quite well. It is referred to as truncated backpropgation through time.
- The model focuses primarily on short-term influence rather than long-term consequences.
- Outcome is a simple and stable model.

Gradient analysis in RNN XI

Read:

- Randomized Truncation (Tallec & Ollivier, 2017) that uses a random variable to replace $\frac{\partial h_t}{\partial w_h}$.
- Gradient clipping: limits the magnitude of the gradient. (Goodfellow et al., DL book)

RNNs are good for handling short-term dependencies. To deal with long-term dependencies, the structure of the RNN needs change. (e.g. LSTM, GRU cells)

Gradient analysis in RNN XII

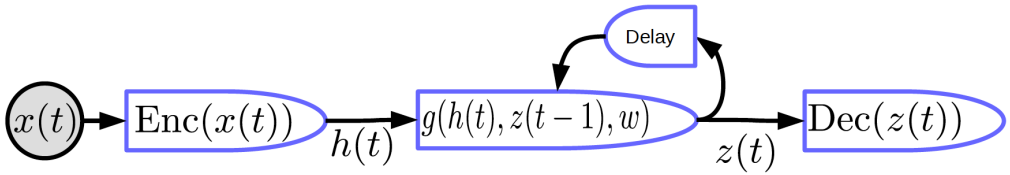
While explaining this, in the lecture you will see the following example:

```
The input is the characters from a C program.  The
system will tell whether it is a syntactically
correct program.  A syntactically correct program
should have a valid number of braces and
parentheses....
```

This is a bad example. You DO NOT need machine learning for the above problem. A simple regex program could do the job. Just because you are doing machine learning, don't just use it where you don't need it.

From lecture I

- Rolled structure of RNN:



$$h(t) = \text{Enc}(x(t))$$

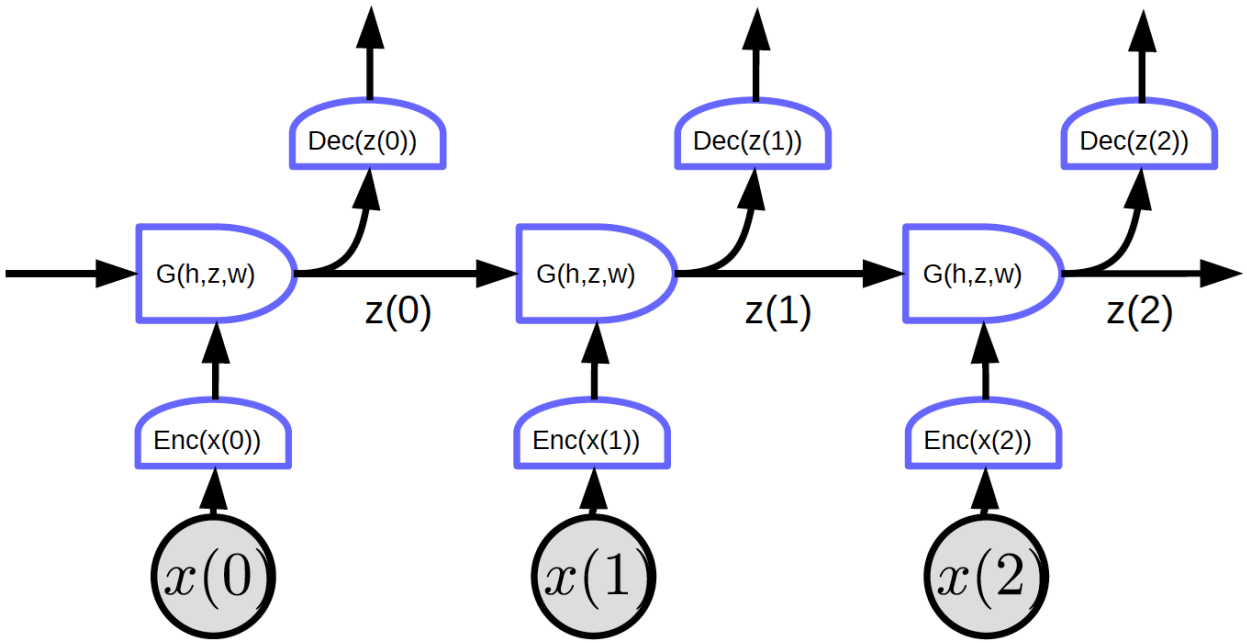
$$z(t) = g(h(t), z(t-1), w)$$

$$y(t) = \text{Dec}(z(t))$$

- Notations:
  - $x(t)$: input that varies across time
  - $Enc(x(t))$: encoder that generates a representation of input
  - $h(t)$: a representation of the input
  - $z(t-1)$: previous hidden state
  - $z(t)$: current hidden state
  - g: a neural network
  - $Dec(z(t))$: decoder that generates the output

From lecture II

- Unrolled version:



Multiplicative Modules

- In multiplicative modules rather than only computing a weighted sum of inputs, we compute products of inputs and then compute weighted sum of that.
- Suppose: $x \in \mathbb{R}^{n \times 1}$, $W \in \mathbb{R}^{m \times n}$, $U \in \mathbb{R}^{m \times n \times d}$, and $z \in \mathbb{R}^{d \times 1}$

$$w_{ij} = u_{ij}^\top z = \begin{pmatrix} u_{ij1} & u_{ij2} & \cdots & u_{ijd} \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_d \end{pmatrix} = \sum_k u_{ijk} z_k$$

$$s = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_m \end{pmatrix} = Wx = \begin{pmatrix} w_{11} & w_{12} & \cdots & w_{1n} \\ w_{21} & w_{22} & \cdots & w_{2n} \\ \vdots & & & \\ w_{m1} & w_{m2} & \cdots & w_{mn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

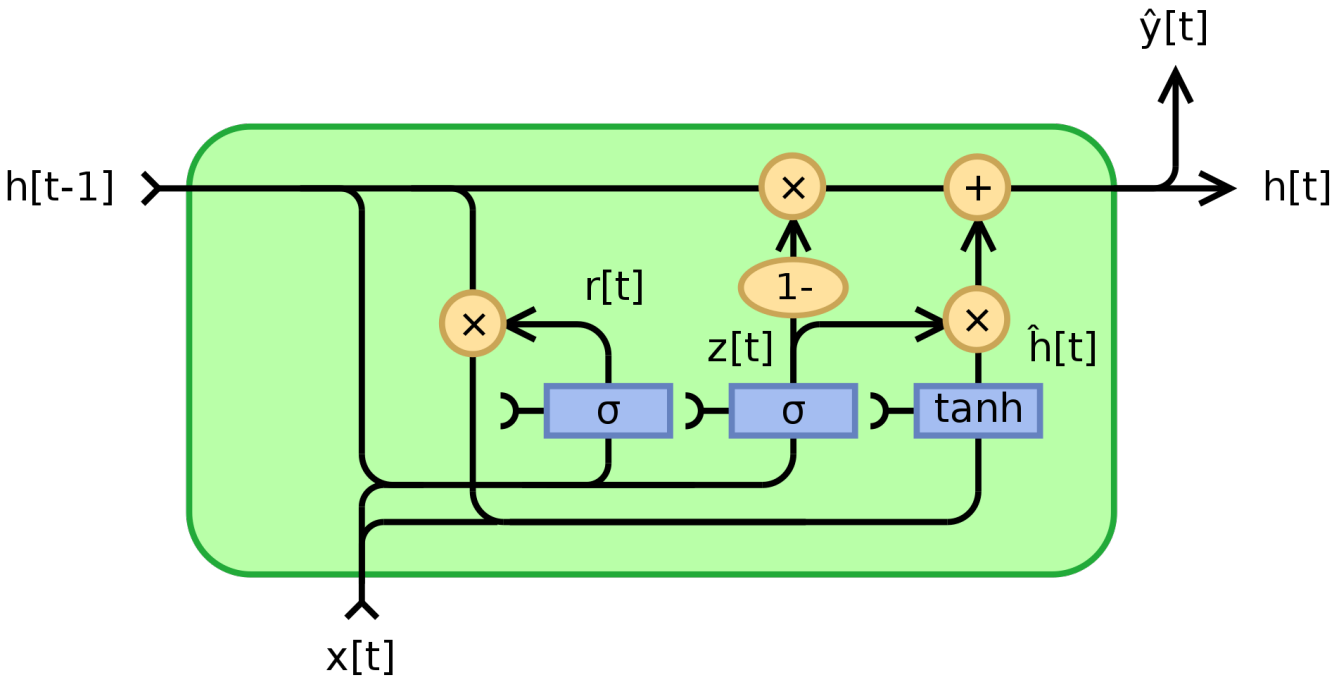
where $s_i = w_i^\top x = \sum_j w_{ij} x_j$.

Attention

- Let x_1 and x_2 are vectors (e.g. different words in a sentence); and w_1 and w_2 are scalars after softmax where $w_1 + w_2 = 1$ (probabilities).
- By appropriately choosing w_1 and w_2, we can vary the output of $w_1x_1 + w_2x_2$ to either x_1, x_2 or a linear combination of both.
- Usually, this is done by the systeml; i.e. the system will find out ws that find an appropriate combination of inputs xs.
- An attention mechanism allows the neural network to focus its attention on particular input(s) and ignore the others.
- Attention is increasingly important in NLP systems that use transformer architectures or other types of attention.

Gated Recurrent Unit (GRU) I

- RNN suffers from vanishing or exploding gradients and can't remember states for very long.
- GRU (Cho, 2014) is an application of multiplicative modules that attempts to solve these problems with the help of a memory.



Gated Recurrent Unit (GRU) II

- Equations:

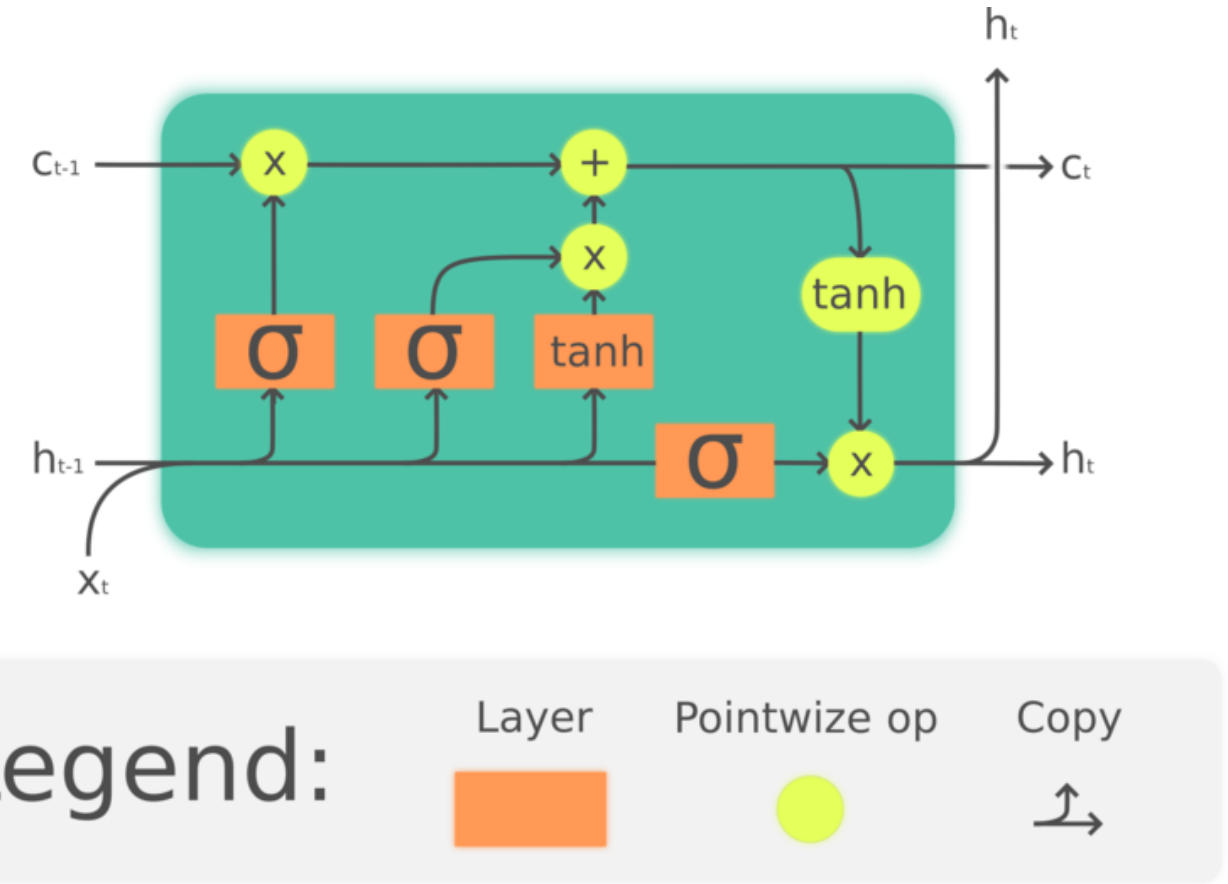
$$
\begin{aligned}
z_t &= \sigma_g(W_z x_t + U_z h_{t-1} + b_z) \\
r_t &= \sigma_g(W_r x_t + U_r h_{t-1} + b_r) \\
h_t &= z_t \odot h_{t-1} + (1 - z_t) \odot \phi_h(W_h x_t + U_h(r_t \odot h_{t-1}) + b_h)
\end{aligned}
$$

  where $\odot$ is Hadamard product (element-wise multiplication).

- x_t: input vector; h_t: output vector; z_t: update gate vector; r_t: reset gate vector.
- z_t: It is a gating vector that determines how much of the past information should be passed along to the future. (behaves like a key)
- r_t: It is used to decide how much of the past information to forget.
- If $r_t = 0$ and $z_t = 0$: then the system is completely reset.

Long Short-Term Memory (LSTM) I

- Solves long-term dependency problem by using memory cell (Hochreiter, Schmidhuber, 1997)



Long Short-Term Memory (LSTM) II

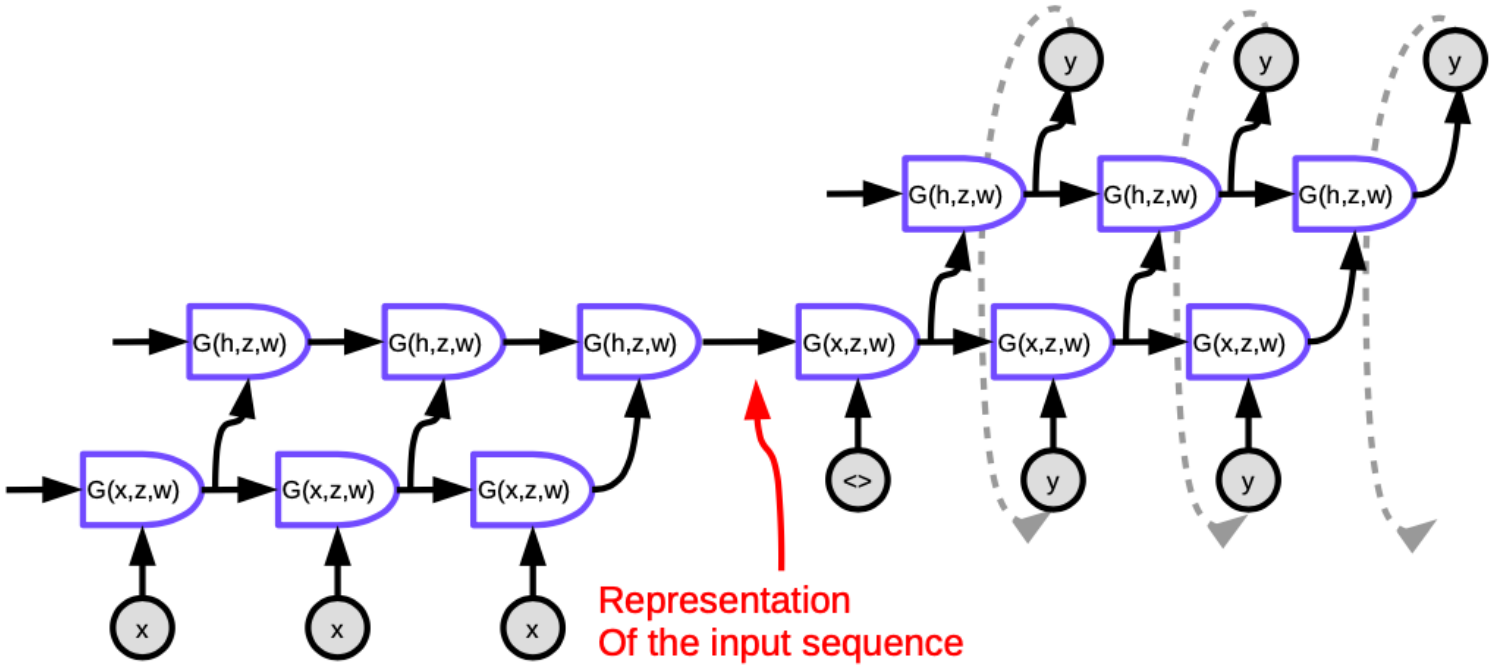
- Equations:

$$
\begin{aligned}
f_t &= \sigma_g(W_f x_t + U_f h_{t-1} + b_f) \\
i_t &= \sigma_g(W_i x_t + U_i h_{t-1} + b_i) \\
o_t &= \sigma_o(W_o x_t + U_o h_{t-1} + b_o) \\
c_t &= f_t \odot c_{t-1} + i_t \odot \tanh(W_c x_t + U_c h_{t-1} + b_c) \\
h_t &= o_t \odot \tanh(c_t)
\end{aligned}
$$

- Cell state c_t: conveys the information through the unit. It regulates how information is preserved or removed from the cell state through structures called gates.
- Forget gate f_t: decides how much information we want to keep from the previous cell state c_{t-1}.

Sequence to Sequence Model I

- Machine-translation system (Sutskever, 2014) using multi-layered LSTM-based encoder-decoder structure.



- Each G cell in the figure is an LSTM.
- For the encoder (the part on the left), the number of time steps equals the length of the sentence to be translated.

Sequence to Sequence Model II

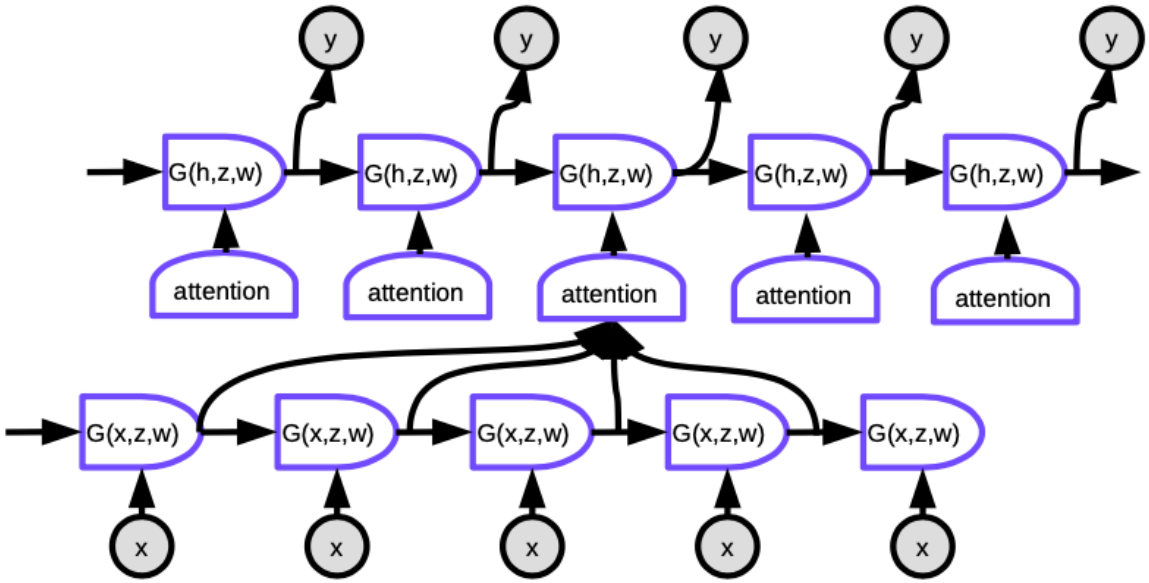
- The encoder constructs a representation (meaning) of the whole input sequence.
- Issues:
  - Entire meaning of the sentence has to be squeezed into the hidden state between the encoder and decoder.
  - It assumes that a word is only dependent on the previous words. However, that maynot always be the case. E.g.

    Last year's christmas songs were beautiful.

    Last year's christmas cakes were tasty.
- To deal with these problems: Use a bi-directional RNN (e.g. Bi-LSTM), which runs two LSTMs in opposite directions.
- In a Bi-LSTM the meaning is encoded in two vectors, one generated by running LSTM from left to right, and another from right to left. This allows doubling the length of the sentence without losing too much information.

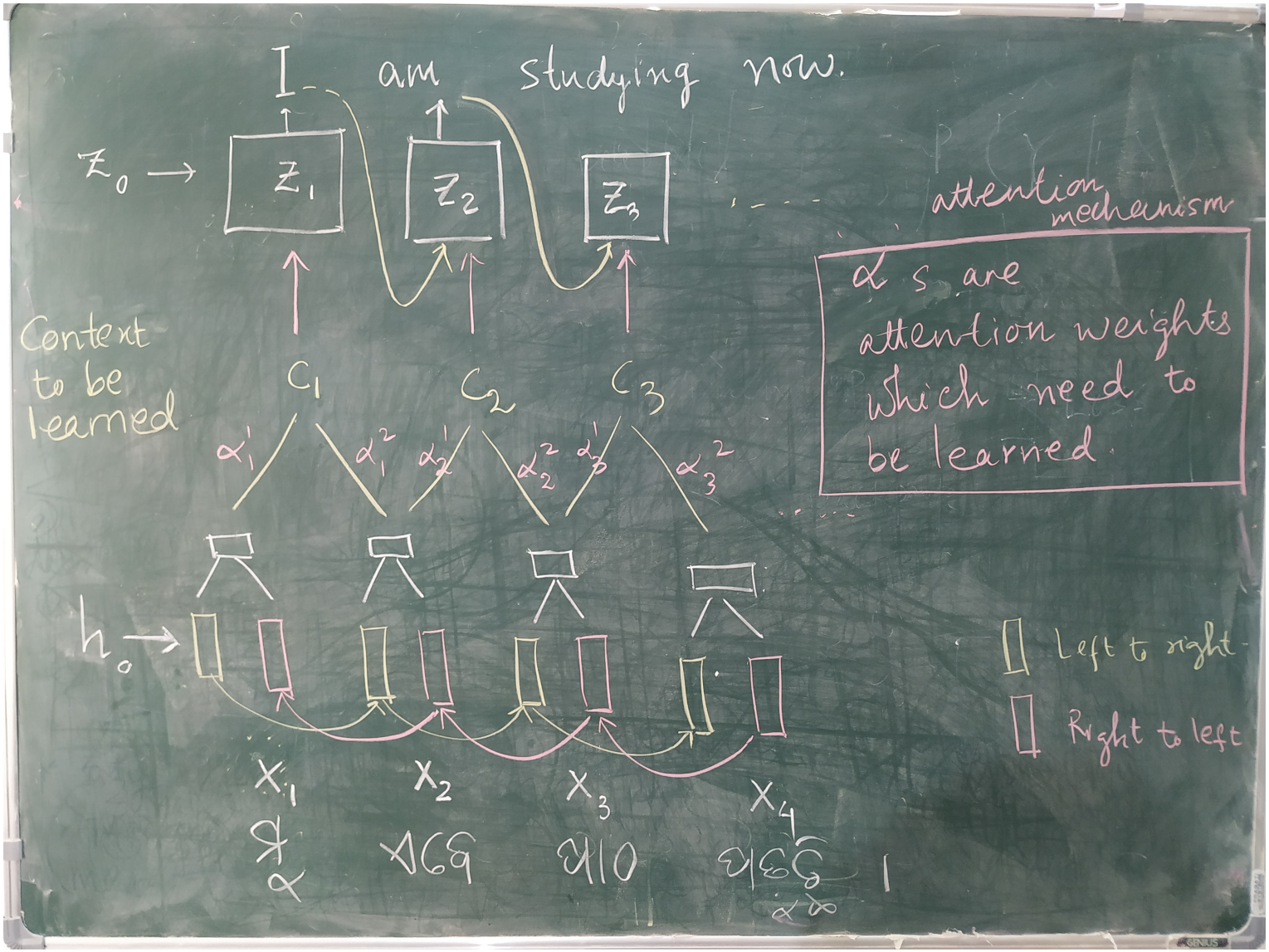
Sequence to Sequence Model with attention I

- Instead of constructing a single representation for the whole sentence, focus the (model's) attention on the relevant locations in the original input.



- In Attention, to produce the current word at each time step, we first need to decide which hidden representations of words in the input sentence to focus on.

Sequence to Sequence Model with attention II



Sequence to Sequence Model with attention III

- A network will learn to score how well each encoded input matches the current output of the decoder.
- A way to think 'attention' is thinking about 'probabilities' (or, probability distribution). Whenever there is a probability involved there is `softmax`.

Sequence to Sequence Model with attention IV

- Some little steps (without maths):
  1. Look at the set of encoder hidden states it received – each encoder hidden states is most. associated with a certain word in the input sentence
  2. Give each hidden states a score (let's ignore how the scoring is done for now).
  3. Multiply each hidden states by its softmaxed score, thus amplifying hidden states with high scores, and drowning out hidden states with low scores.

An excellent visualisation of machine translation with attention:
`https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2se`