11-695: AI Engineering
Recurrent Neural Networks

Spring 2019

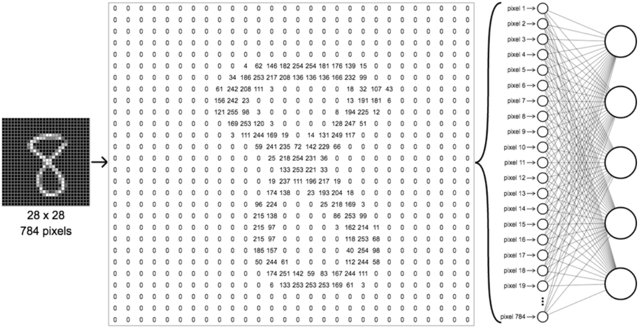
Outline

How to "model" each type of data?

- Spatial: images
- Sequential: text
- Mixed: videos
- Other structured and unstructured data

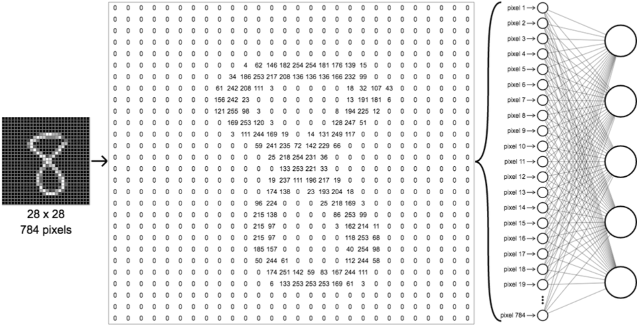
Image credit: BYU Art

MLP a one-size-fits-all approximator?



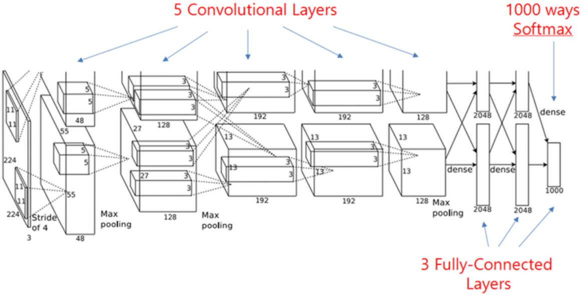
- A general solution to general data

MLP a one-size-fits-all approximator?



- A general solution to general data
- It has disadvantages: params, relations, ...

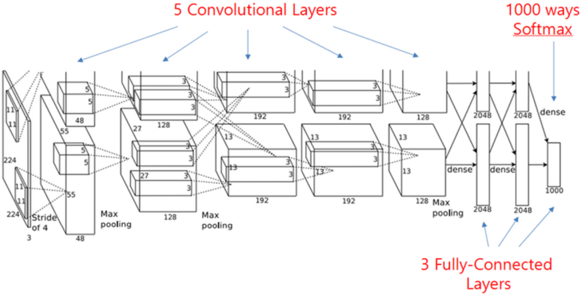
How about CNN in modelling data?



- It has a huge advantage in vision and related data

Image credit: Krizhevsky et. al 2012

How about CNN in modelling data?



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- But also requires fixed size of input

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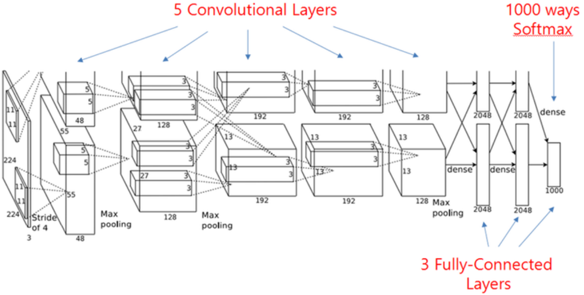

- It has a huge advantage in vision and related data
- But also requires fixed size of input
- With MLP, they are feed-foward type without "memory"

Image credit: Krizhevsky et. al 2012

Say no to over-parameterizing models

- We can either ignore any dependency in the data, just throw a deep NN as an approximator

Image credit: StyleSage

Say no to over-parameterizing models

- We can either ignore any dependency in the data, just throw a deep NN as an approximator
- Or we exploit dependencies by designing a more intepretable, and powerful models.

Image credit: StyleSage

Model sequential data

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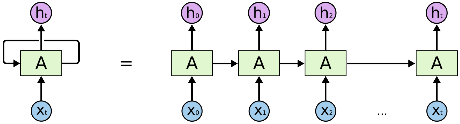

- Texts, video, trading, ...
- Treating samples indepdendently is losing information
- We need a special model for time-series data
- Markov, Graphical Model, and

Image credit: Chris Olah

Model sequential data

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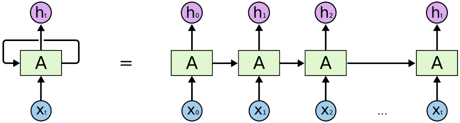

- Texts, video, trading, ...
- Treating samples indepdendently is losing information
- We need a special model for time-series data
- Markov, Graphical Model, and
- Recurrent NN

Image credit: Chris Olah

Outline

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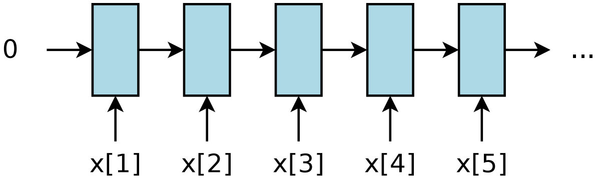
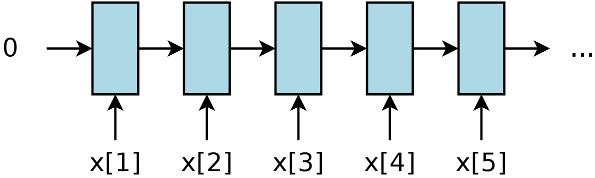
Recurrent Neural Networks



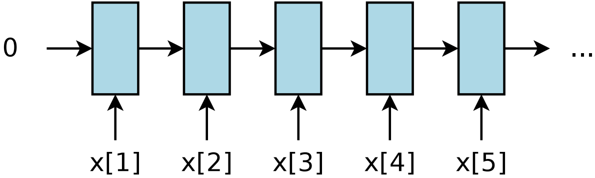
- Processes a sequence of signals
  - $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_T \in \mathbb{R}^D$
- ... in a sequential order
  - $\mathbf{h}_0 = \mathbf{0}_H$
  - $\mathbf{h}_t = \mathbf{f}(\mathbf{x}_t, \mathbf{h}_{t-1})$
- Designing an RNN means designing $\mathbf{f} : \mathbb{R}^D \times \mathbb{R}^H \to \mathbb{R}^H$.

Example 1: A Dummy RNN



- With the function $\mathbf{f}(\mathbf{x}, \mathbf{h}) = \mathbf{x} + \mathbf{h}$
  - $\mathbf{h}_0 = \mathbf{0}_H$
  - $\mathbf{h}_t = \mathbf{h}_{t-1} + \mathbf{x}_t$
- This network requires $D = H$, and is really dumb...

Example 2: Vanilla RNN



- With the function $\mathbf{f}(\mathbf{x}, \mathbf{h}) = g(\mathbf{x} \cdot \mathbf{W}_x + \mathbf{h} \cdot \mathbf{W}_h)$
  - g is an activation function, e.g. tanh, ReLU, etc.
  - $\mathbf{W}_x \in \mathbb{R}^{D \times H}$, $\mathbf{W}_h \in \mathbb{R}^{H \times H}$ are the *shared* parameters.
- Much less dumb. Invented in 1990. Drove people crazy in 2011...

Example 3: Long Short-Term Memory (LSTM)

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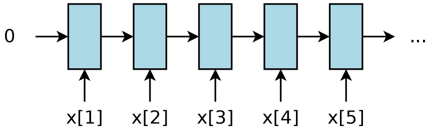


- The function $\mathbf{f}$ goes wild

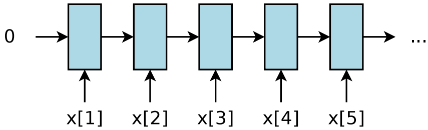
$$\begin{bmatrix} \mathbf{i} \\ \mathbf{f} \\ \mathbf{o} \\ \mathbf{g} \end{bmatrix}^\top = \begin{bmatrix} \text{sigmoid} \\ \tanh \\ \text{sigmoid} \\ \text{sigmoid} \end{bmatrix} \mathbf{W}_{H \times (D+H)} \cdot \begin{bmatrix} \mathbf{x}_t^\top \\ \mathbf{h}_t^\top \end{bmatrix} \tag{1}$$

$$\mathbf{c}_t = \mathbf{i} \otimes \mathbf{g} + \mathbf{f} \cdot \mathbf{c}_{t-1}$$

$$\mathbf{h}_t = \mathbf{o} \otimes \tanh \mathbf{c}_{t-1}$$

- Finally looks smart. Invented in 1997. Drove people crazy in 2014...

Example 4: Gated Recurrent Units (GRU)

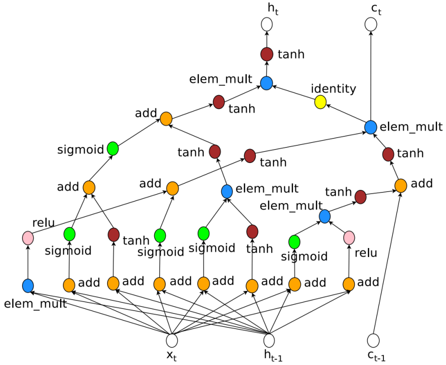


- Someone doesn't like LSTM and wants to be creative with $\mathbf{f}$

$$
\begin{aligned}
\mathbf{z} &= \text{sigmoid}(\mathbf{x}_t \cdot \mathbf{W}_{xz} + \mathbf{h}_{t-1} \cdot \mathbf{W}_{hz}) \\
\mathbf{r} &= \text{sigmoid}(\mathbf{x}_t \cdot \mathbf{W}_{xr} + \mathbf{h}_{t-1} \cdot \mathbf{W}_{hr}) \\
\tilde{\mathbf{h}} &= \text{sigmoid}(\mathbf{x}_t \cdot \tilde{\mathbf{W}}_x + (\mathbf{r} \cdot \mathbf{h}_{t-1}) \cdot \tilde{\mathbf{W}}_h) \\
\mathbf{h}_t &= (1 - \mathbf{z}) \otimes \mathbf{h}_{t-1} + \mathbf{z} \otimes \tilde{\mathbf{h}}
\end{aligned} \tag{2}
$$

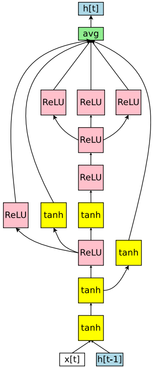
- Sure. We're so tired with different formulas for $\mathbf{f}$

Example 5: Neural Architecture Search



- You can also use a computer to generate good formulas for $\mathbf{f}$

Example 6: Efficient Neural Architecture Search



- Yet another one, also generated by a computer

Outline

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Back to the big picture

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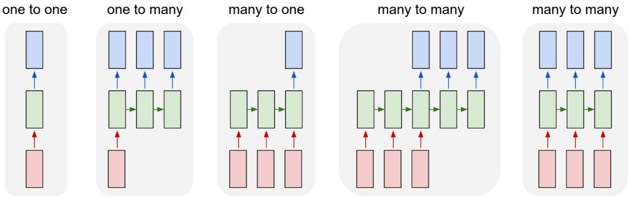
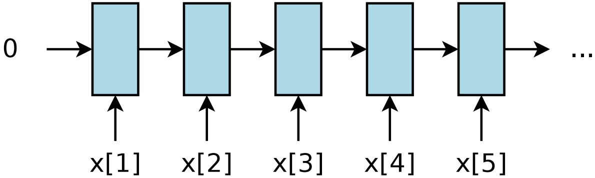


- You can be model many layouts of input and outputs

Image credit: Andrej Karpathy

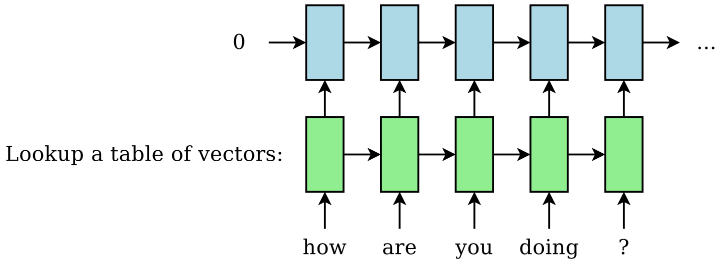
Back to the big picture



- You can be *very* creative about RNNs:
  - How to choose the input sequence $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_T$
  - What to do with the "hidden" sequence $\mathbf{h}_1, \mathbf{h}_2, ..., \mathbf{h}_T$

Outline

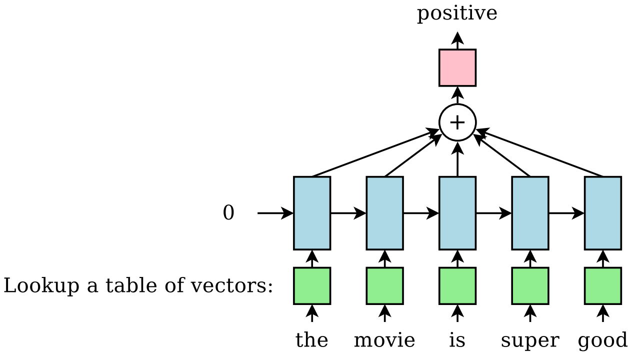
Word embeddings



- To process a sequence of words
  - Store a dictionary that maps words to vectors in $\mathbf{R}^D$
  - Use these $\mathbb{R}^D$ vectors as inputs to an RNN.
- Work by: Yoshua Bengio et al (2003). Drove people crazy in 2013.

Outline

Adding a Softmax head



- You can sum over the $\mathbf{h}_t$ and hook up a softmax head to make a prediction about your sequence
  - Example: sentiment analysis

Multiple softmax heads

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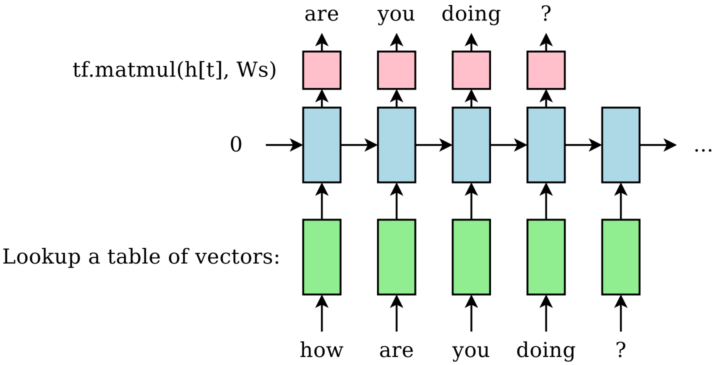

- You can use the $\mathbf{h}_t$ as to predict the next word in your sequence
  - It's called *language model*
  - Because it can model $p(w_t|w_{<t})$

Sequence to Sequence models

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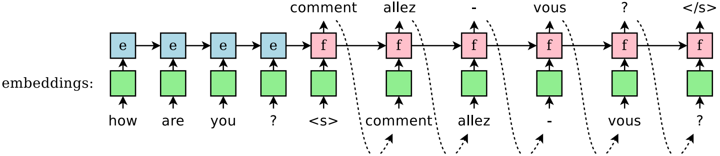

- Only use the softmax heads where you want to generate a translated word
  - It's called *neural machine translation*
  - Because it can model $p(\mathbf{t}_t|\mathbf{t}_{<t}, \mathbf{s})$

Attention

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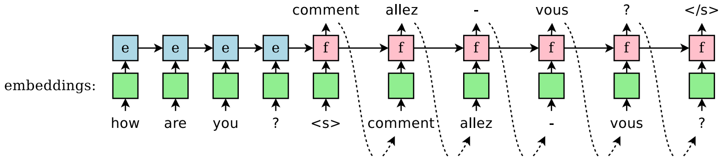

- Yet another way to manipulate your $\mathbf{h}_t$ states.
- $\mathbf{e}_i$, $\mathbf{f}_j$ are your blue and red states

$$
\begin{aligned}
\alpha_{j,i} &= g(\mathbf{f}_j, \mathbf{e}_i) \\
a_{j,i} &= \text{Softmax}(\alpha_{j,1}, \alpha_{j,2}, ..., \alpha_{j,|\mathbf{s}|}) \\
c_j &= \sum_{i=1}^{|\mathbf{s}|} a_{j,i}\mathbf{e}_i
\end{aligned} \tag{3}
$$

Outline

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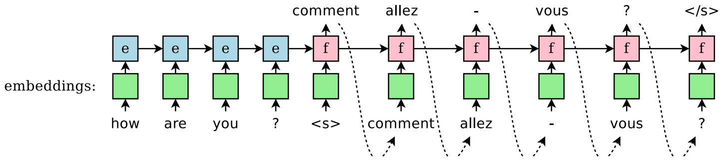
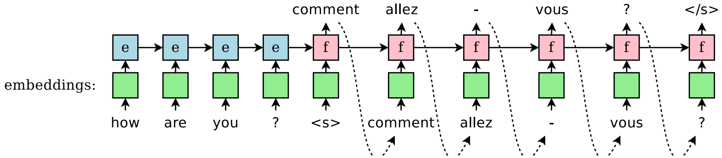
The Picture So Far



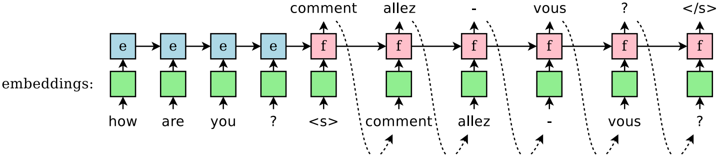
- We have a sequence of hidden vectors
  - In general: $\mathbf{h}_i \in \mathbf{R}^H$ for any input sequences
  - In this case: $\mathbf{e}_i, \mathbf{f}_j \in \mathbf{R}^H$ are the blue and red states
- Can hook up softmax heads to these $\mathbf{h}_i$, $\mathbf{e}_i$, $\mathbf{f}_j$ to make predictions.
- How can we train the RNN to make such predictions?

The Computational Pipeline: Hidden States



- **Inputs:** the words. You need *both* English and French words.
  - $\texttt{how}, \texttt{are}, \texttt{you}, \texttt{?}, \langle \texttt{s} \rangle, \texttt{comment}, \texttt{allez}, \texttt{-}, \texttt{vous}, \texttt{?}, \langle \texttt{s} \rangle$
- **Word embeddings:** look up the words in a saved dictionary
  - $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, \mathbf{y}_4, \mathbf{y}_5, \mathbf{y}_6 \in \mathbb{R}^D$
- **Recurrent Computations:** f is your chosen RNN function
  - Encoder: $\mathbf{e}_0 = 0; \mathbf{e}_t = f(\mathbf{x}_t, \mathbf{e}_{t-1})$
  - Decoder: $\mathbf{f}_0 = \mathbf{e}_4; \mathbf{f}_t = f(\mathbf{y}_t, \mathbf{f}_{t-1})$

The Computational Pipeline: Loss Function



- **Predictions:** Let $\mathbf{W}_{\text{soft}} \in \mathbb{R}^{D \times \text{vocab\_size}}$ be trainable parameters

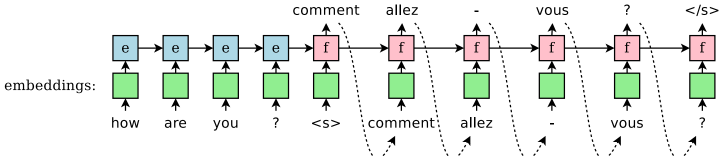
$$p(y_t | y_{<t}, \mathbf{x}) = \text{Softmax}(\mathbf{f}_{t-1} \cdot \mathbf{W}_{\text{soft}}), \text{ for } t = 2, 3, ..., |\mathbf{y}| \tag{4}$$

$$p(\mathbf{y}|\mathbf{x}) = \prod_{t=2}^{|\mathbf{y}|} p(y_t | y_{<t}, \mathbf{x}) \tag{5}$$

- **Loss function:** The canonical cross-entropy loss

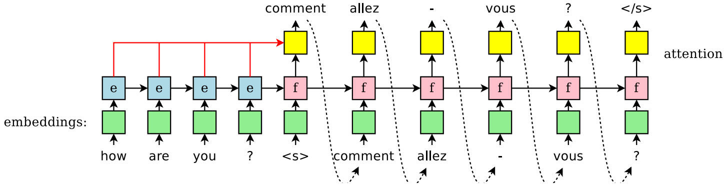
$$\mathcal{L} = -\log p(\mathbf{y}|\mathbf{x}) = -\sum_{t=2}^{|\mathbf{y}|} \log p(y_t | y_{<t}, \mathbf{x}) \tag{6}$$

The Computational Pipeline: Training



- We have defined *a computational graph*
  - which is a composite of *many* functions
- Thus we can use back-propagation to compute the gradients
  - which is just the chain rule
- Model parameters consist of:
  - Relevant word embeddings
  - $\mathbf{W}_{\text{soft}}$
  - Any parameters of the recurrent function f

The Computational Pipeline: Attention



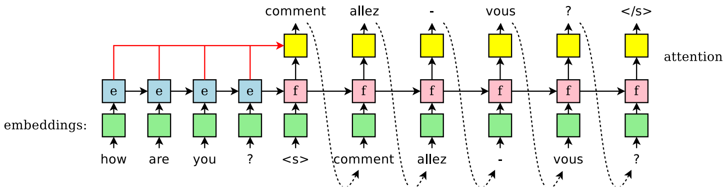
- **Recurrent Computations:** f is your chosen RNN function
  - Encoder: $\mathbf{e}_0 = 0; \mathbf{e}_t = f(\mathbf{x}_t, \mathbf{e}_{t-1})$; Decoder: $\mathbf{f}_0 = \mathbf{e}_4; \mathbf{f}_t = f(\mathbf{y}_t, \mathbf{f}_{t-1})$
- **Predictions:** previously *without attention*

$$p(y_t | y_{<t}, \mathbf{x}) = \text{Softmax}(\mathbf{f}_{t-1} \cdot \mathbf{W}_{\text{soft}}), \text{ for } t = 2, 3, ..., |\mathbf{y}| \tag{7}$$

- **Predictions:** now *with attention*

$$p(y_t | y_{<t}, \mathbf{x}) = \text{Softmax}(\mathbf{a}(\mathbf{f}_{t-1}, \mathbf{e}_{1 \cdots |\mathbf{x}|}) \cdot \mathbf{W}_{\text{soft}}) \tag{8}$$

The Computational Pipeline: Attention



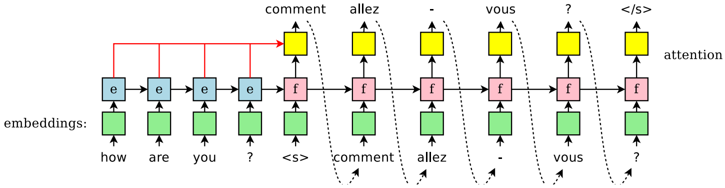
- **Predictions:** now *with attention*

$$p(y_t|y_{<t}, \mathbf{x}) = \text{Softmax}(\mathbf{a}(\mathbf{f}_{t-1}, \mathbf{e}_{1\ldots|\mathbf{x}|}) \cdot \mathbf{W}_{\text{soft}}) \quad (9)$$

- **Attention:** how is $\mathbf{a}(\mathbf{f}, \mathbf{e}_{1\ldots|\mathbf{x}|})$ computed?

$$\alpha_i = g(\mathbf{f}, \mathbf{e}_i);\ a_i = \text{Softmax}(\alpha_{1\ldots|\mathbf{x}|});\ \mathbf{a}(\mathbf{f}, \mathbf{e}_{1\ldots|\mathbf{x}|}) = \sum_{i=1}^{|\mathbf{x}|} a_i \mathbf{e}_i \quad (10)$$

The Computational Pipeline: Attention

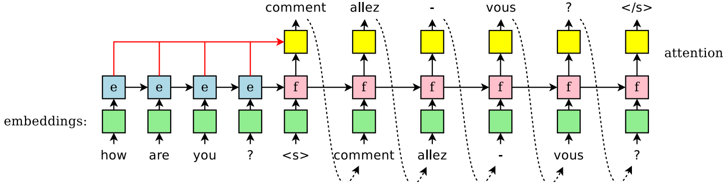


- **Attention:** how is $\mathbf{a}(\mathbf{f}, \mathbf{e}_{1\ldots|\mathbf{x}|})$ computed?

$$\alpha_i = g(\mathbf{f}, \mathbf{e}_i);\ a_i = \text{Softmax}(\alpha_{1\ldots|\mathbf{x}|});\ \mathbf{a}(\mathbf{f}, \mathbf{e}_{1\ldots|\mathbf{x}|}) = \sum_{i=1}^{|\mathbf{x}|} a_i \mathbf{e}_i \quad (11)$$

- Choices of g:
  - Bahdanau attention: $g(\mathbf{f}, \mathbf{e}_i) = \tanh\left(\mathbf{f} \cdot \mathbf{w}_f + \mathbf{e}_i \cdot \mathbf{w}_e\right) \cdot \mathbf{v}$, where $\mathbf{w}_f, \mathbf{w}_e \in \mathbf{R}^{H \times H}$ and $\mathbf{v} \in \mathbb{R}^{H \times 1}$ are trainable parameters
  - Luong attention: $g(\mathbf{f}, \mathbf{e}_i) = \mathbf{f} \cdot \mathbf{e}_i^\top$

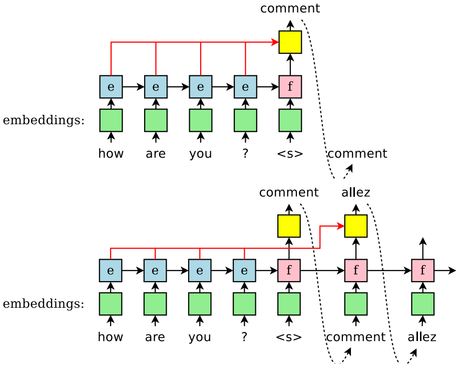
The Computational Pipeline: Attention



- Even with attention, the overall RNN is still a composite of functions
- The training procedure stays the same

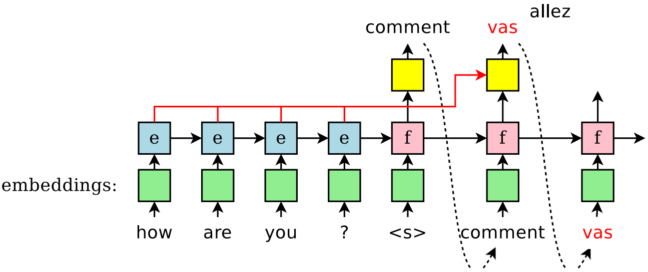
Outline

How to Translate with a Trained RNN?



- Goes step-by-step, based on *your own predictions*

What If You Are Wrong?



- You live with your mistakes...
- Yes, it is bad. Therefore many people are finding a fix
  - Reinforcement Learning: Data as Demonstrator; MIXER, etc.
  - Reward-Augmented Maximum Likelihood

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General Regularization Strategy: Dropout

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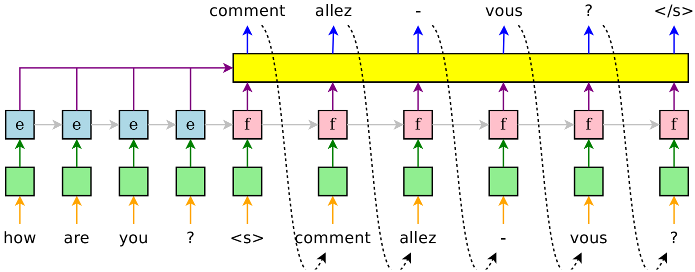
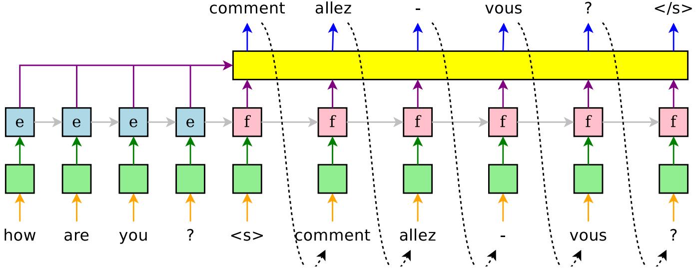


- Each colored arrowed can be dropped using *the same mask*.
  - Word embeddings dropout mean to remove *the whole word*

Other Strategies: ℓ_p



- ℓ_2 norm of all or some parameters
- ℓ_2 norm of all or some hidden states: $\sum_i \|\mathbf{e}_i\|^2$, $\sum_j \|\mathbf{f}_j\|^2$
- ℓ_2 difference of all or some hidden states: $\sum_i \|\mathbf{e}_i - \mathbf{e}_{i-1}\|^2$, $\sum_j \|\mathbf{f}_j - \mathbf{f}_{j-1}\|^2$