CAP 5516
Medical Image Computing
(Spring 2025)

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Lecture 7: Introduction to Deep Learning (2)

Using optimization algorithms in PyTorch

```
optimizer = optim.SGD(model.parameters(), lr=0.01, momentum=0.9)
optimizer = optim.Adam([var1, var2], lr=0.0001)
```

1. optim.SGD: Specifies that you are using the SGD optimizer.
2. model.parameters(): Refers to the trainable parameters (weights and biases) of the model. These will be updated during training.
3. lr=0.01: The learning rate, which determines the step size for updating the parameters.
4. momentum=0.9:

- Momentum helps accelerate convergence in the relevant direction by considering past updates.
- It prevents oscillations in the loss landscape, particularly in regions with high curvature.

https://pytorch.org/docs/stable/optim.html

Using optimization algorithms in PyTorch

```
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optimizer = optim.Adam([var1, var2], lr=0.0001)
```

How it works:

- In each training iteration, SGD computes the gradient of the loss function with respect to the model's parameters.
- Parameters are updated as:

$$\theta_{t+1} = \theta_t - \eta \cdot g_t + \mu \cdot v_{t-1}$$

Where:

- θ_t: Parameter at step t.
- η: Learning rate (`lr`).
- g_t: Gradient at step t.
- μ: Momentum coefficient (`momentum`).
- v_{t-1}: Previous step's velocity.

Using optimization algorithms in PyTorch

```
optimizer = optim.SGD(model.parameters(), lr=0.01, momentum=0.9)
optimizer = optim.Adam([var1, var2], lr=0.0001)
```

Adam is an advanced optimizer that combines two key ideas:

- **Adaptive Learning Rates**
- **Momentum**

- 1. optim.Adam: Specifies that you are using the Adam optimizer.
- 2. [var1, var2]: A list of variables (e.g., tensors) you want to optimize. This is useful if you only want to optimize specific parts of the model or other variables.
- 3. lr=0.0001: The learning rate. Adam typically works well with smaller learning rates compared to SGD.

Which optimizer should I use?

https://www.lightly.ai/post/which-optimizer-should-i-use-for-my-machine-learning-project

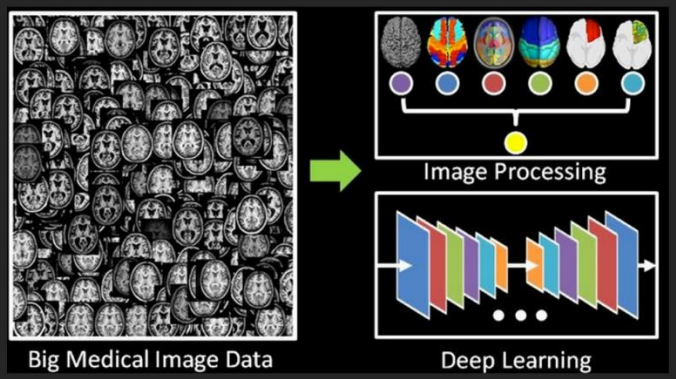
Optimizer	State Memory [bytes]	# of Tunable Parameters	Strengths	Weaknesses
SGD	0	1	Often best generalization (after extensive training)	Prone to saddle points or local minima Sensitive to initialization and choice of the learning rate α
SGD with Momentum	$4n$	2	Accelerates in directions of steady descent Overcomes weaknesses of simple SGD	Sensitive to initialization of the learning rate α and momentum β
AdaGrad	$\sim 4n$	1	Works well on data with sparse features Automatically decays learning rate	Generalizes worse, converges to sharp minima Gradients may vanish due to aggressive scaling
RMSprop	$\sim 4n$	3	Works well on data with sparse features Built in Momentum	Generalizes worse, converges to sharp minima
Adam	$\sim 8n$	3	Works well on data with sparse features Good default settings Automatically decays learning rate α	Generalizes worse, converges to sharp minima Requires a lot of memory for the state
AdamW	$\sim 8n$	3	Improves on Adam in terms of generalization Broader basin of optimal hyperparameters	Requires a lot of memory for the state
LARS	$\sim 4n$	3	Works well on large batches (up to 32k) Counteracts vanishing and exploding gradients Built in Momentum	Computing norm of gradient for each layer can be inefficient

Interpretability of Deep Neural Networks

Safety of AI models

Autonomous Driving

Trust of AI decision

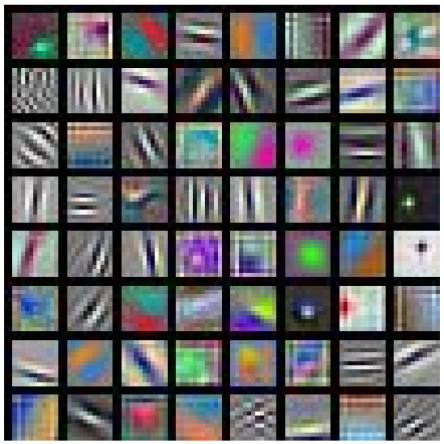


Medical Diagnosis

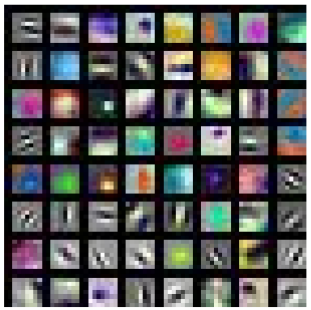
Policy and Regulation

Right to the explanation for algorithmic decisions

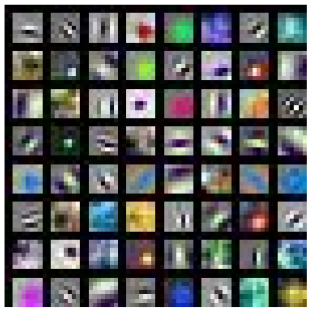
First Layer: Visualize Filters



AlexNet:
64 x 3 x 11 x 11

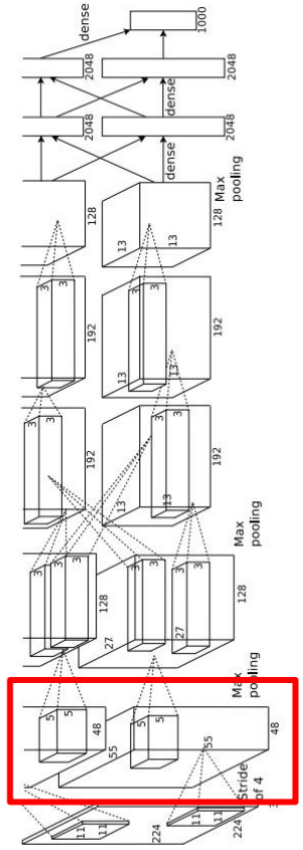


ResNet-18:
64 x 3 x 7 x 7



ResNet-101:
64 x 3 x 7 x 7

DenseNet-121:
64 x 3 x 7 x 7



Krizhevsky, "One weird trick for parallelizing convolutional neural networks", arXiv 2014
He et al, "Deep Residual Learning for Image Recognition", CVPR 2016
Huang et al, "Densely Connected Convolutional Networks", CVPR 2017

Visualize the filters/kernels (raw weights)

We can visualize filters at higher layers, but not that interesting

(these are taken from ConvNetJS CIFAR-10 demo)

Weights:

layer 1 weights

16 x 3 x 7 x 7

Weights:

layer 2 weights

20 x 16 x 7 x 7

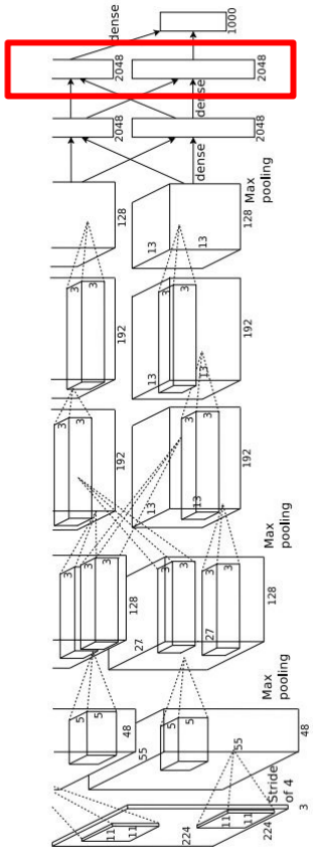
Weights:

layer 3 weights

20 x 20 x 7 x 7

Last Layer

FC7 layer

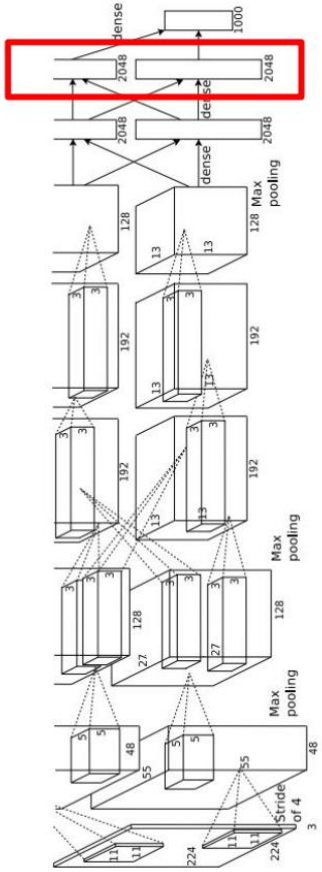


4096-dimensional feature vector for an image (layer immediately before the classifier)

Run the network on many images, collect the feature vectors

Last Layer: Nearest Neighbors

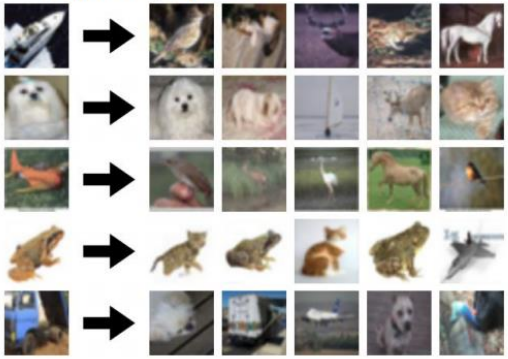
4096-dim vector



Test image

L2 Nearest neighbors in feature space

Recall: Nearest neighbors in pixel space



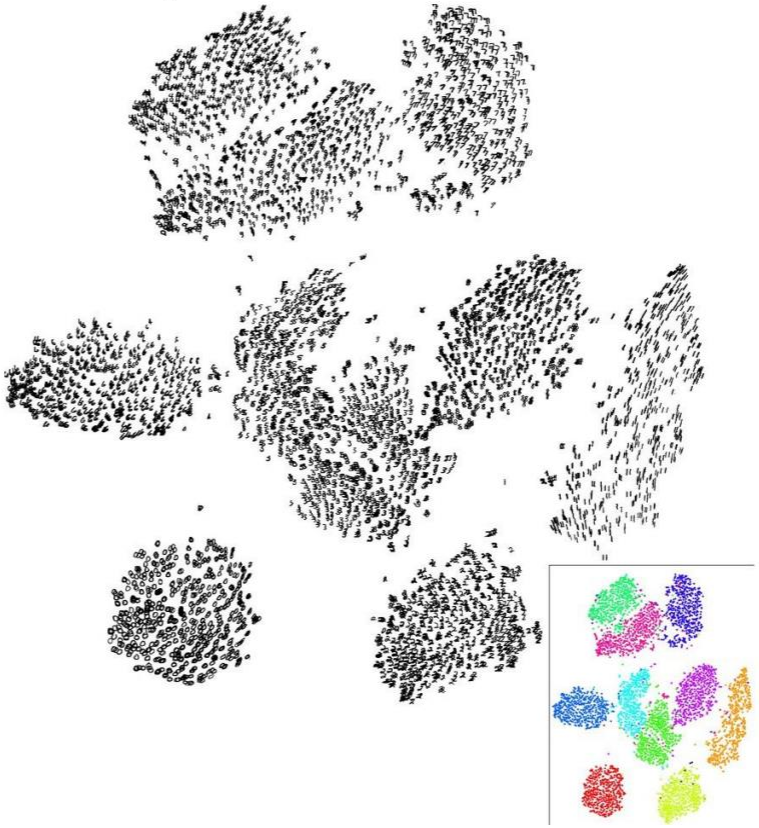
Krizhevsky et al, "ImageNet Classification with Deep Convolutional Neural Networks", NIPS 2012.
Figures reproduced with permission.

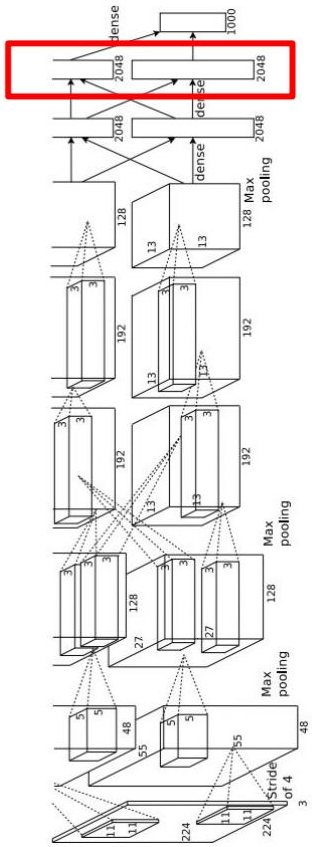
Last Layer: Dimensionality Reduction

Visualize the “space” of FC7 feature vectors by reducing dimensionality of vectors from 4096 to 2 dimensions

Simple algorithm: Principle Component Analysis (PCA)

More complex: **t-SNE**





Van der Maaten and Hinton, “Visualizing Data using t-SNE”, JMLR 2008

t-SNE

- A **non-linear dimensionality reduction** method that maps high-dimensional data to 2D/3D for **visualization**.

How does it work?

- Computes **pairwise similarities** in the original space (using Gaussian kernels).
- Maps points into a low-dimensional space, using a **Student-t distribution** to preserve **local neighborhoods**.
- Minimizes **Kullback–Leibler divergence** between high- and low-dimensional similarity distributions.

t-SNE

Why do we use t-SNE?

- **Visualizing Clusters**: It's often used in classification problems to see how **features separate different classes** in the model's learned representation space. If a model does a good job of separating classes, we might see distinct clusters in the 2D/3D t-SNE plot.

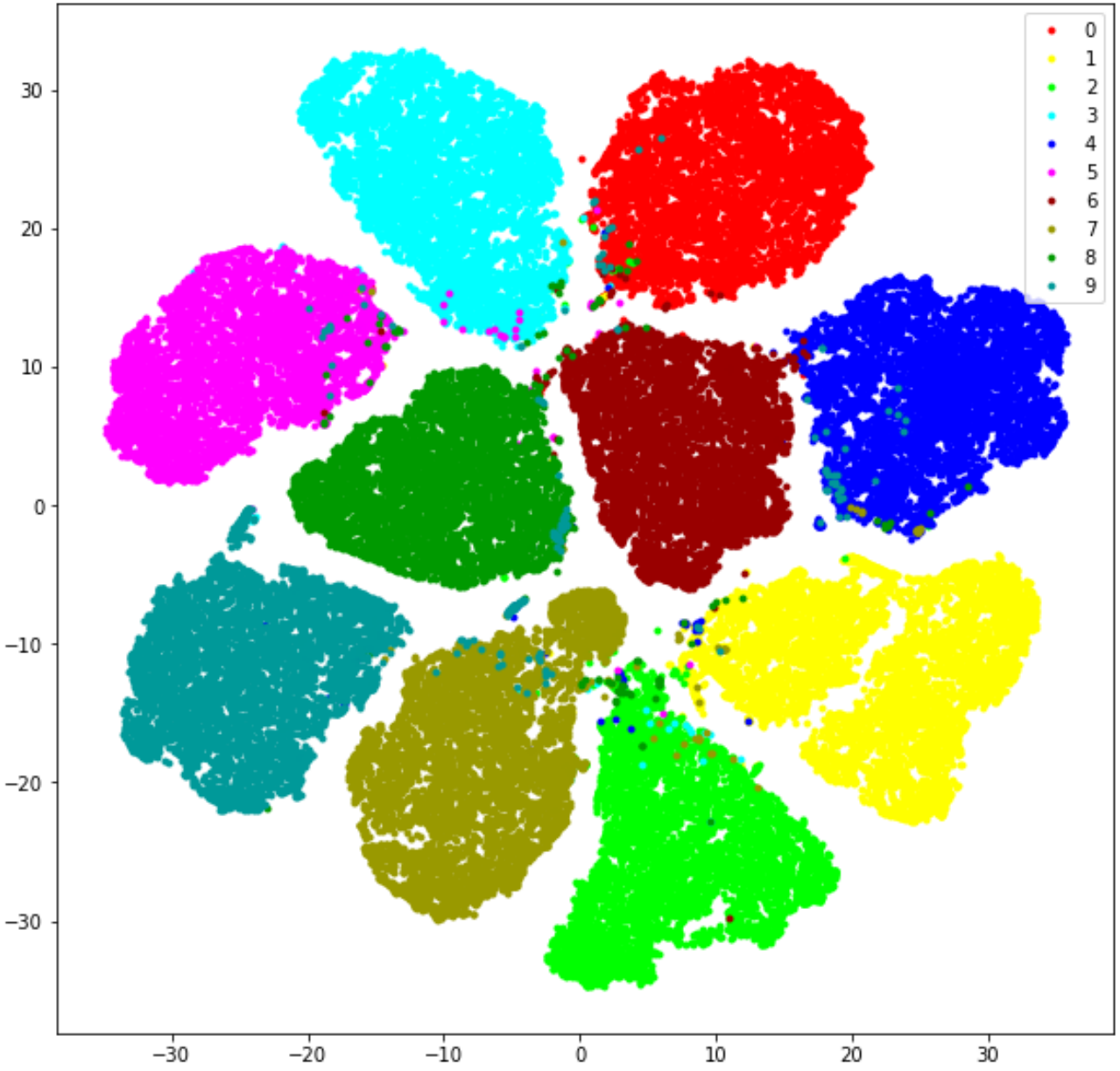
- **Preserving Local Similarities**: High-dimensional data often forms complex structures that simple methods (e.g., PCA) may not capture well. t-SNE attempts to preserve the "local" relationships: points that are *close* in the high-dimensional space are kept close in the low-dimensional space.

t-SNE

Example Use Case in Classification

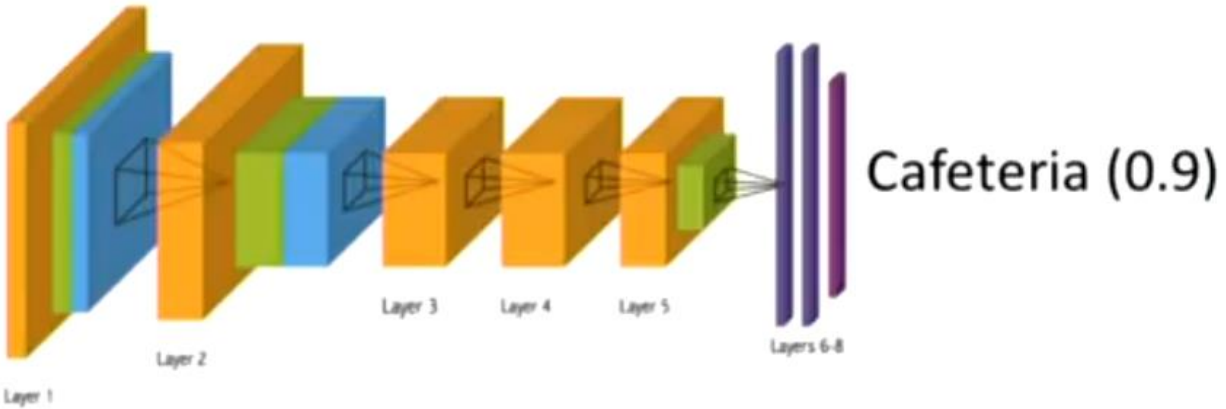
- Suppose you have a neural network that classifies images of handwritten digits (MNIST). You can:
- 1. Pass your dataset through the trained network and collect the final-layer embeddings (e.g., a 64-dimensional vector for each image).
- 2. Apply t-SNE to these 64-dimensional vectors to reduce them to 2D.
- 3. Plot each data point in 2D, color-coding them by their actual digit class (0–9).

t-SNE



An example of t-sne visualization of CNN learned feature

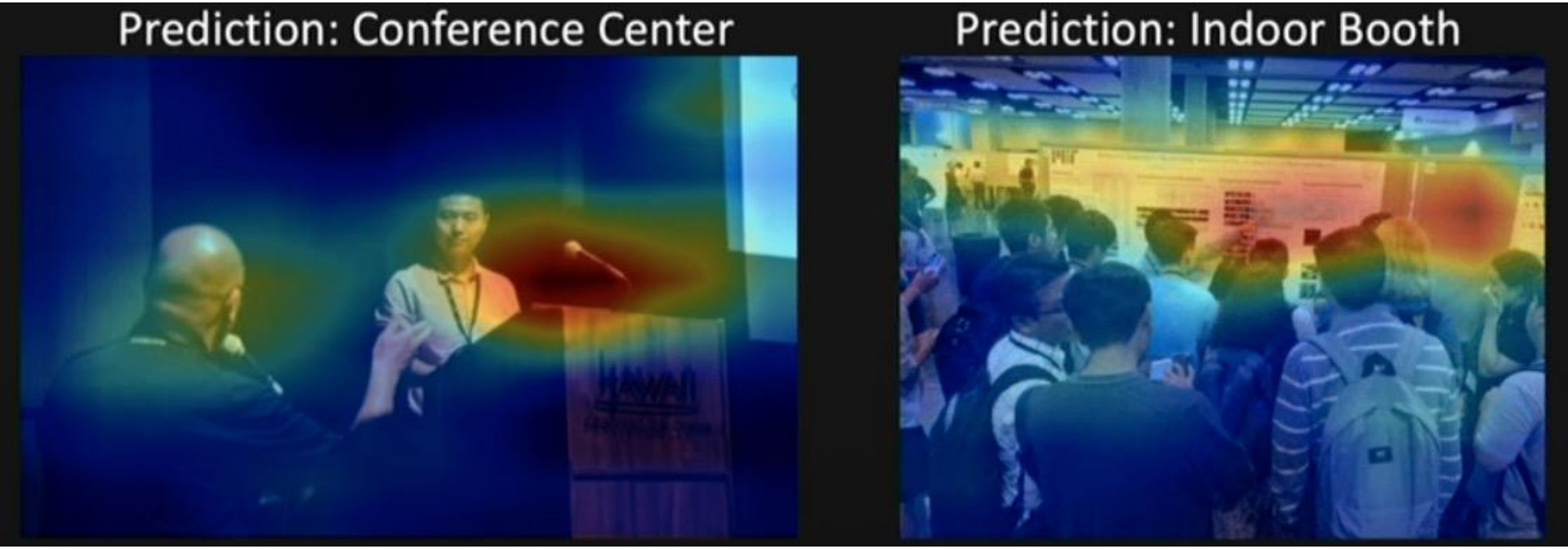
Why the network gives such prediction?



Credit: Bolei Zhou

Class Activation Map

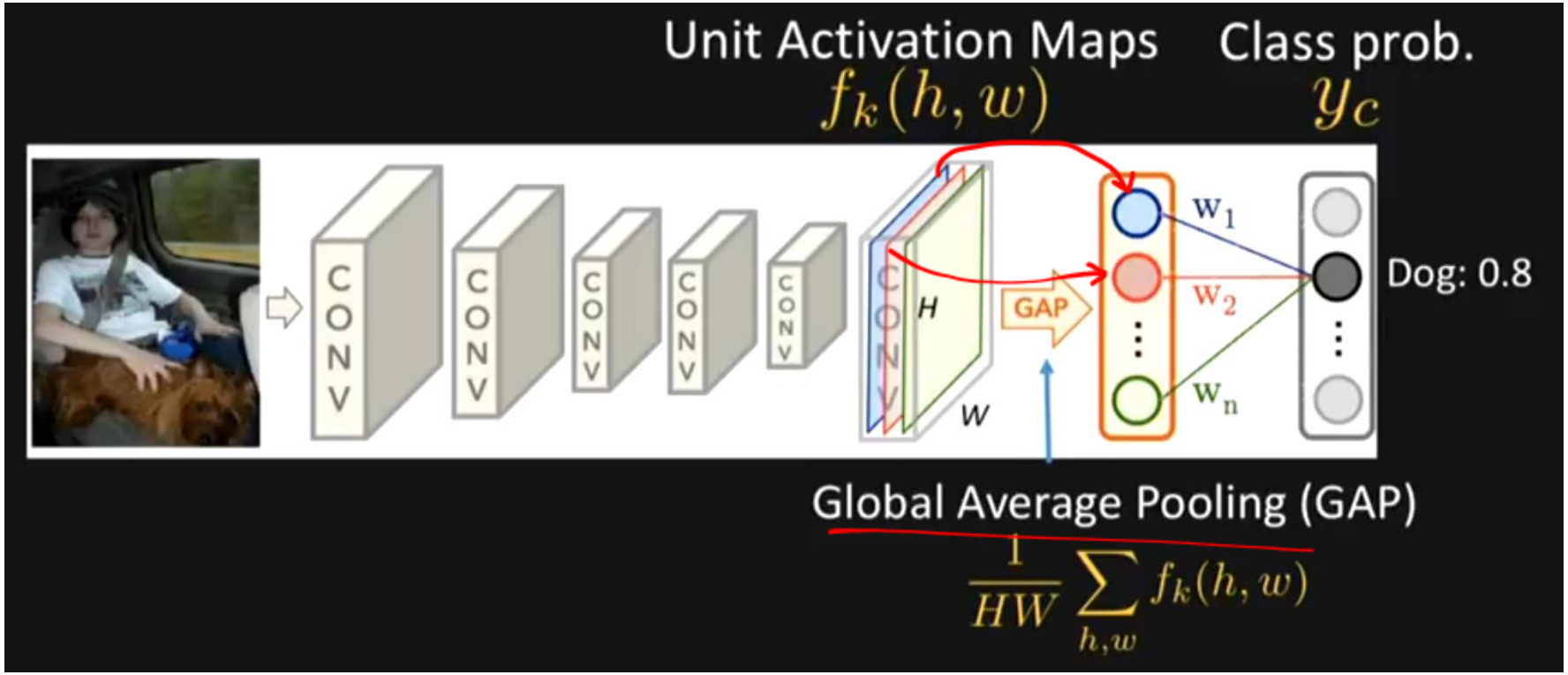
- Explain Prediction of Deep Neural Network



Credit: Bolei Zhou

Zhou, Bolei, et al. "Learning deep features for discriminative localization." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

What the CNN is looking



Credit: Bolei Zhou

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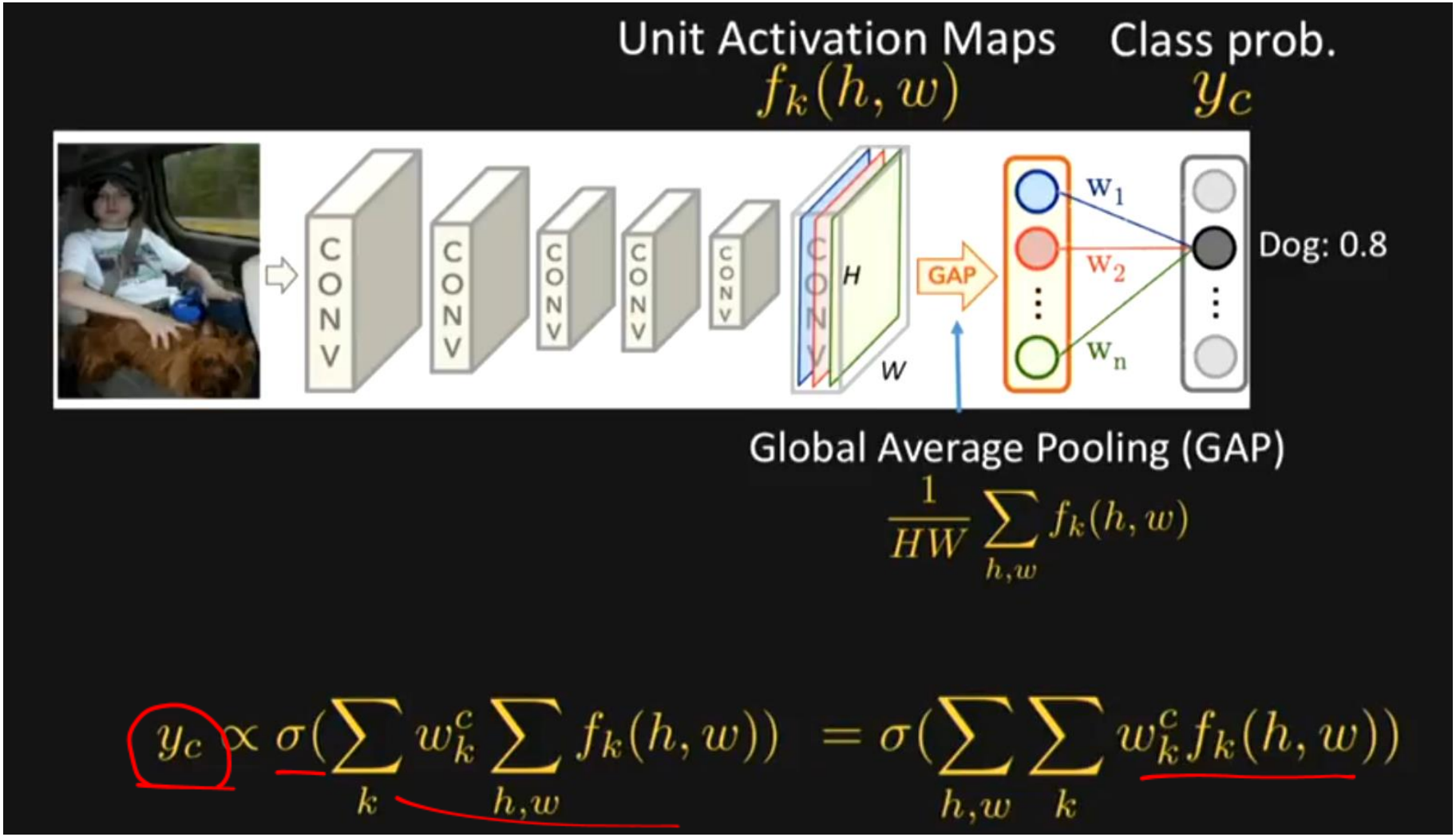
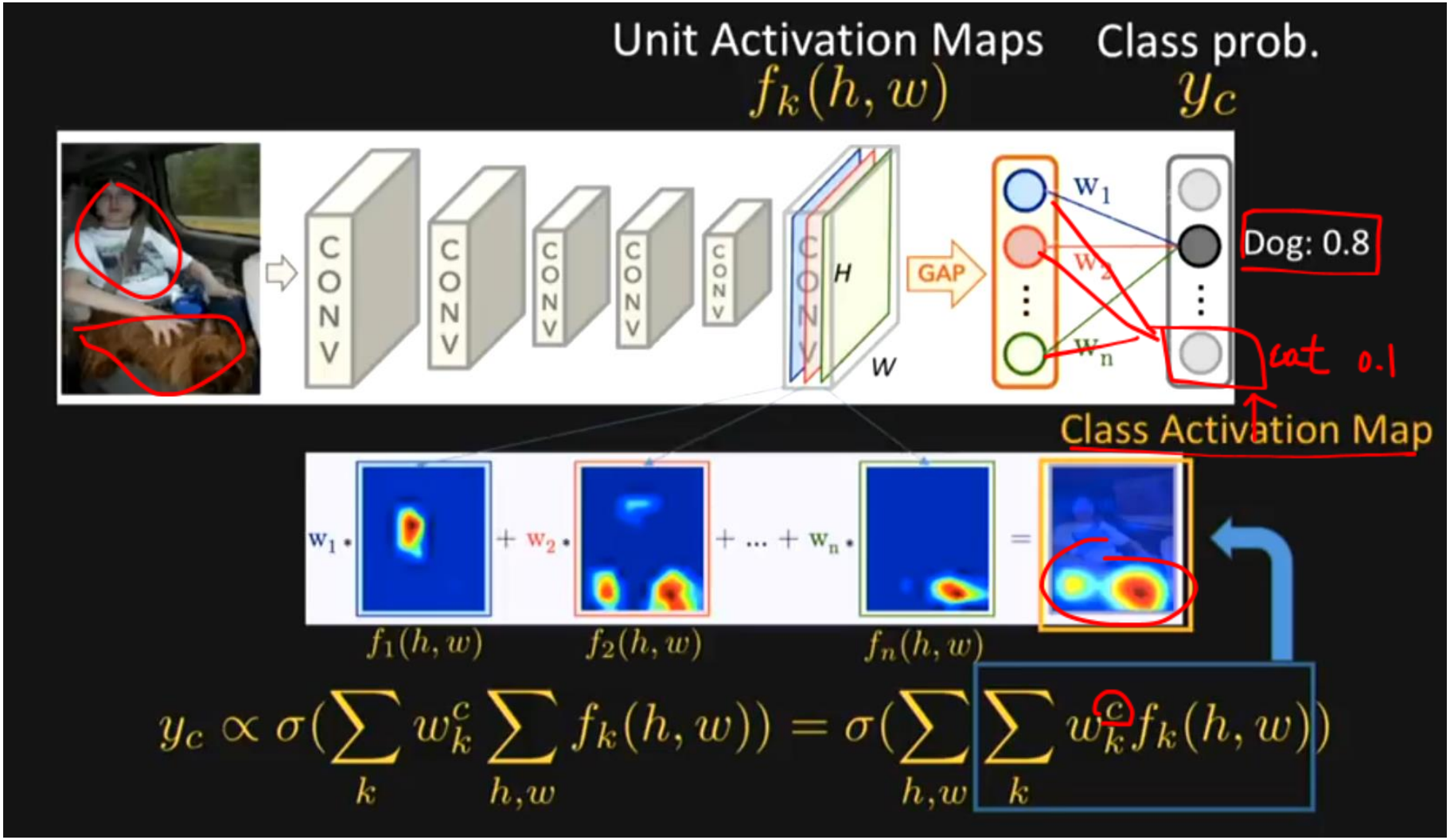


Zhou, Bolei, et al. "Learning deep features for discriminative localization." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

Credit: Bolei Zhou

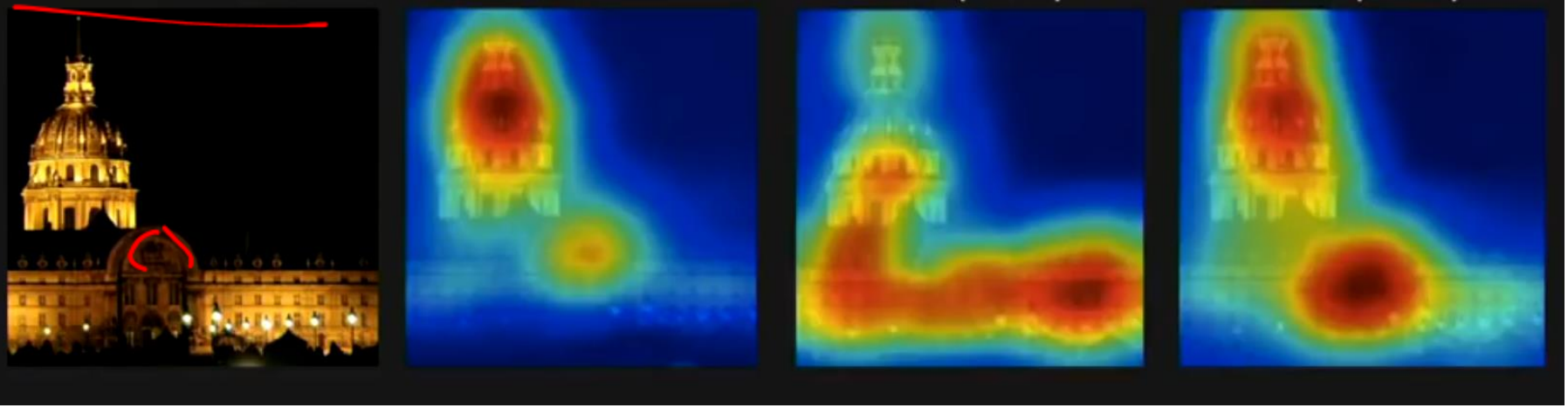
What the CNN is looking



Zhou, Bolei, et al. "Learning deep features for discriminative localization." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

Credit: Bolei Zhou

Class Activation Mapping: Explain Prediction of Deep Neural Network



Credit: Bolei Zhou

Credit: Bolei Zhou

Explain the failure cases

GT: House
Prediction: Sushi bar

Credit: Bolei Zhou

Explain the failure cases

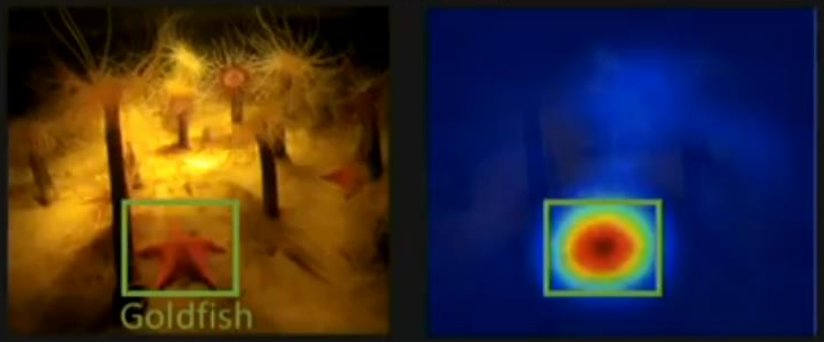
Credit: Bolei Zhou

What other applications can CAM serve beyond visualization?

Using CAM for localization

Evaluation on Weakly-Supervised Localization

Prediction: Starfish (0.83)



Prediction: Tricycle (0.92)

Method	Supervision	Localization Accuracy(%)
Backpropagation	weakly	53.6
Our method	weakly	**62.9**
AlexNet	full	65.8

Result on ImageNet Localization Benchmark

Credit: Bolei Zhou

Limitation of CAM

- To apply CAM, any CNN-based network must change its architecture, where GAP is a must before the output layer
  - i.e., architectural changes and hence re-training is needed

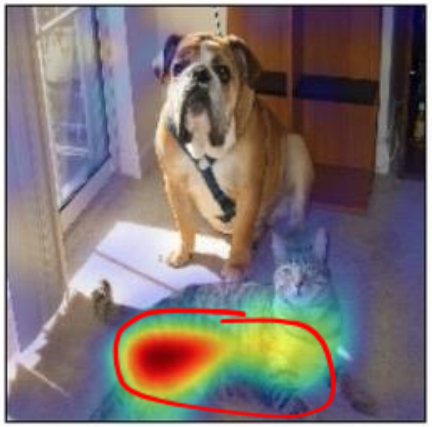
Grad-CAM (Gradient-weighted Class Activation Mapping)

- Grad-CAM (Gradient-weighted Class Activation Mapping) generalizes CAM for a wide variety of CNN-based architectures
  - i.e., without requiring architectural changes or re-training
- Uses the **gradients** (partial derivatives) flowing into a specific convolutional layer to produce a localization (heatmap) map.
- Essentially, for a given class, it calculates how changes in that layer's feature maps affect the class score and uses these gradients to weigh the feature maps.
- Summing the gradient-weighted feature maps yields a **heatmap** highlighting important regions contributing to the class prediction.

Selvaraju, Ramprasaath R., et al. "Grad-cam: Visual explanations from deep networks via gradient-based localization." Proceedings of the IEEE International Conference on Computer Vision. 2017.

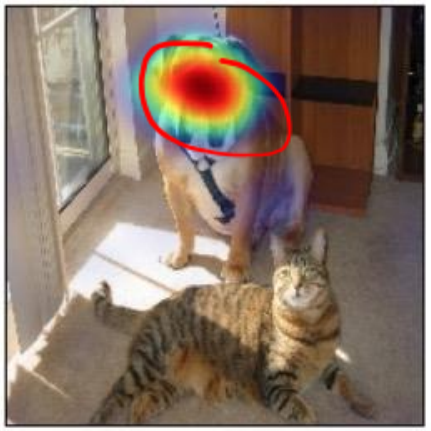
Grad-CAM

(a) Original Image



(c) Grad-CAM 'Cat'

(g) Original Image



(i) Grad-CAM 'Dog'

Selvaraju, Ramprasaath R., et al. "Grad-cam: Visual explanations from deep networks via gradient-based localization." Proceedings of the IEEE International Conference on Computer Vision. 2017.

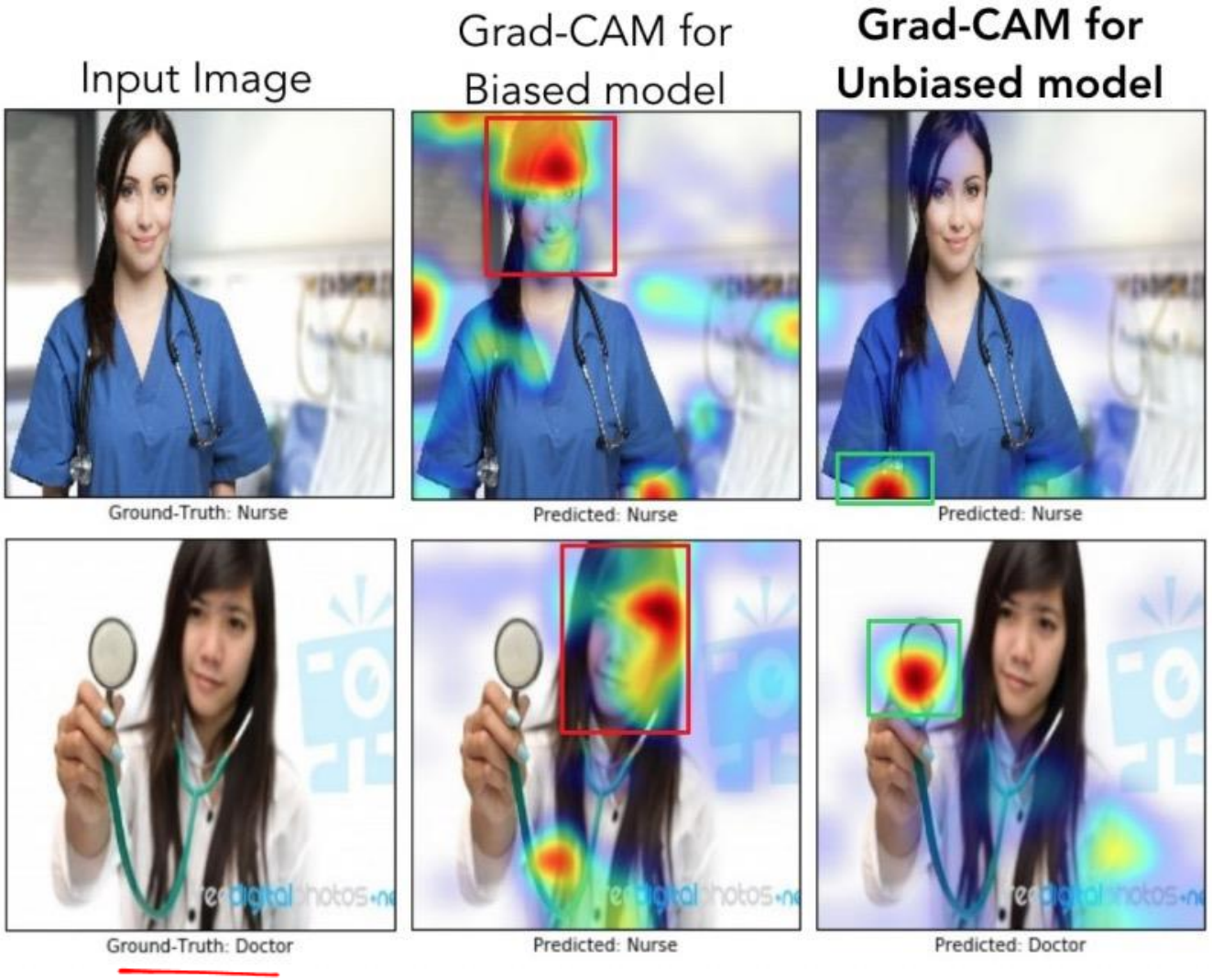
Grad-CAM for Weakly-supervised Localization

		Classification		Localization	
		Top-1	Top-5	Top-1	Top-5
VGG-16	Backprop [51]	30.38	10.89	61.12	51.46
	c-MWP [58]	30.38	10.89	70.92	63.04
	Grad-CAM (ours)	30.38	10.89	**56.51**	46.41
	CAM [59]	33.40	12.20	57.20	**45.14**
AlexNet	c-MWP [58]	44.2	20.8	92.6	89.2
	Grad-CAM (ours)	44.2	20.8	68.3	56.6
GoogleNet	Grad-CAM (ours)	31.9	11.3	60.09	49.34
	CAM [59]	31.9	11.3	60.09	49.34

Table 1: Classification and localization error % on ILSVRC-15 val (lower is better) for VGG-16, AlexNet and GoogleNet. We see that Grad-CAM achieves superior localization errors without compromising on classification performance.

Selvaraju, Ramprasaath R., et al. "Grad-cam: Visual explanations from deep networks via gradient-based localization." Proceedings of the IEEE International Conference on Computer Vision. 2017.

Grad-CAM for Identifying Bias in Dataset



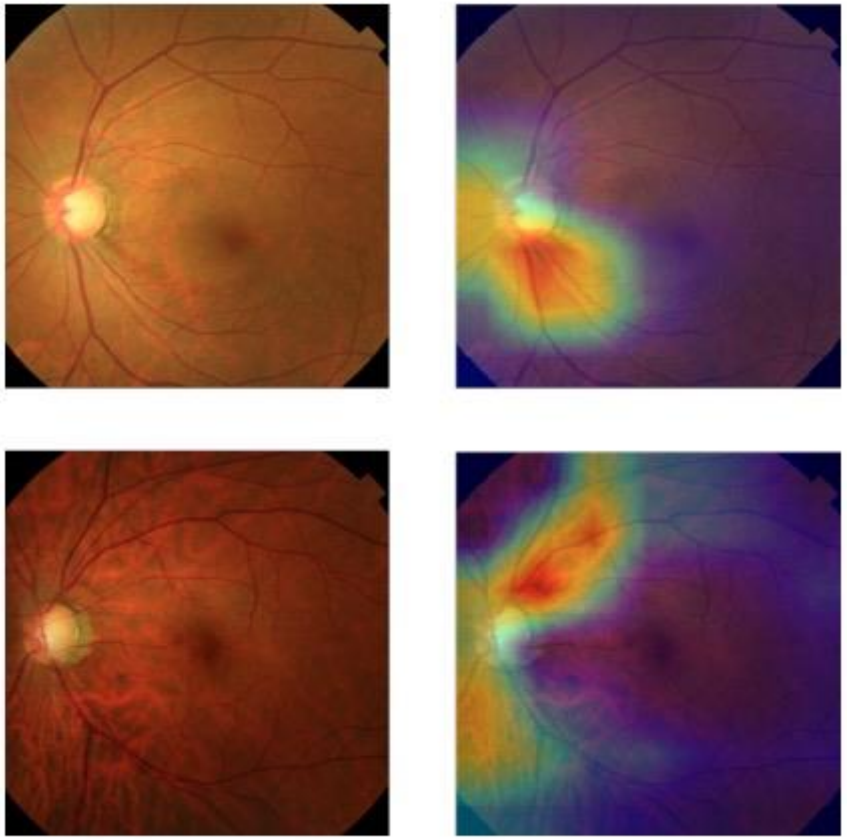
First row:
The biased model (model1) was looking at the face of the person to decide if the person was a nurse, whereas the unbiased model was looking at the short sleeves to make the decision.

Second row:
The biased model made the wrong prediction (misclassifying a doctor as a nurse) by looking at the face and the hairstyle, whereas the unbiased model made the right prediction looking at the white coat, and the stethoscope.

Selvaraju, Ramprasaath R., et al. "Grad-cam: Visual explanations from deep networks via gradient-based localization." Proceedings of the IEEE International Conference on Computer Vision. 2017.

Grad-CAM for Medical Image Analysis

- Grad-CAM for glaucoma diagnosis and localization



(a) Correctly localized suspicious areas.

Kim, Mijung, et al. "Web applicable computer-aided diagnosis of glaucoma using deep learning." arXiv preprint arXiv:1812.02405 (2018).

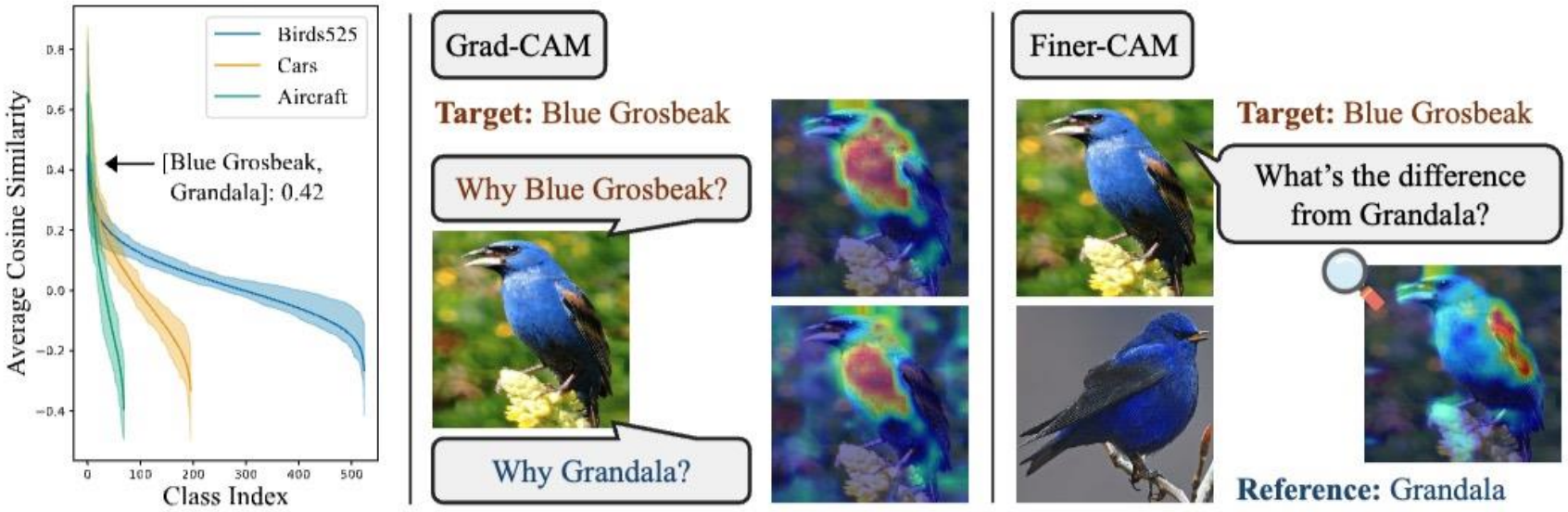


Figure 1. **Illustration of Finer-CAM. Left:** Sorted cosine similarity between the linear classifier weights of one class and the other classes, averaged across all classes. Many pairs of classes are highly similar, yet neural networks can effectively distinguish them to achieve high fine-grained classification accuracy. **Middle**: Standard CAM methods highlight main regions contributing to the target class's logit value, inadvertently including regions predictive of similar classes and overshadowing fine discriminative details. **Right**: We propose Finer-CAM to explicitly compare the target class with similar classes and spot the difference, enabling accurate localization of discriminative details.

Zhang et al. Finer-CAM: Fine-grained Visual Interpretability through Class-Specific Gradient Refinements
https://arxiv.org/pdf/2501.11309

More reading

- Bau, David, et al. "Network dissection: Quantifying interpretability of deep visual representations." *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*. 2017.

- Selvaraju, Ramprasaath R., et al. "Grad-cam: Visual explanations from deep networks via gradient-based localization." *Proceedings of the IEEE International Conference on Computer Vision*. 2017.

- Chattopadhay, Aditya, et al. "Grad-cam++: Generalized gradient-based visual explanations for deep convolutional networks." *2018 IEEE Winter Conference on Applications of Computer Vision (WACV)*. IEEE, 2018.

- Zhang et al. Finer-CAM: Fine-grained Visual Interpretability through Class-Specific Gradient Refinements https://arxiv.org/pdf/2501.11309

Implementation

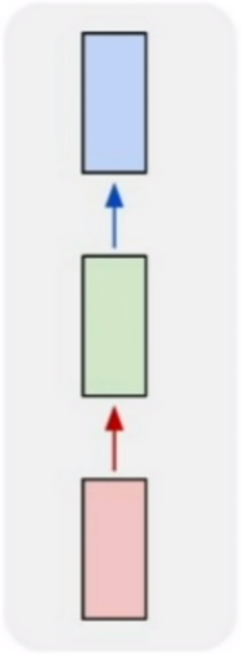
- CAM
  - https://github.com/zhoubolei/CAM
- Grad-CAM
  - https://github.com/ramprs/grad-cam/
  - Demo: http://gradcam.cloudcv.org/
- TorchCAM: class activation explorer
  - https://github.com/frgfm/torch-cam

Recurrent Neural Network (RNN)

Slides are adapted from Hung-yi Lee and Feifei Li

“Vanilla” Neural Network

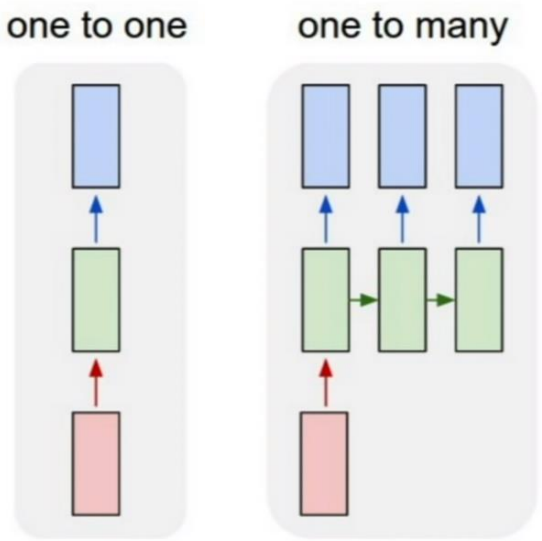
one to one



$f($  $)=$ “Cat”

Vanilla Neural Networks

Recurrent Neural Networks: Process Sequences



Example?

e.g. Image Captioning
Image -> sequence of words

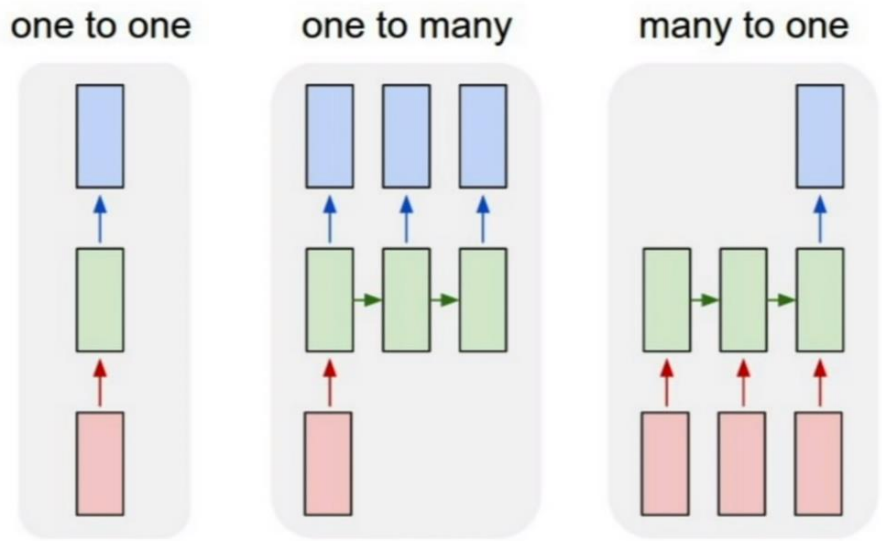

A person riding a motorcycle on a dirt road.

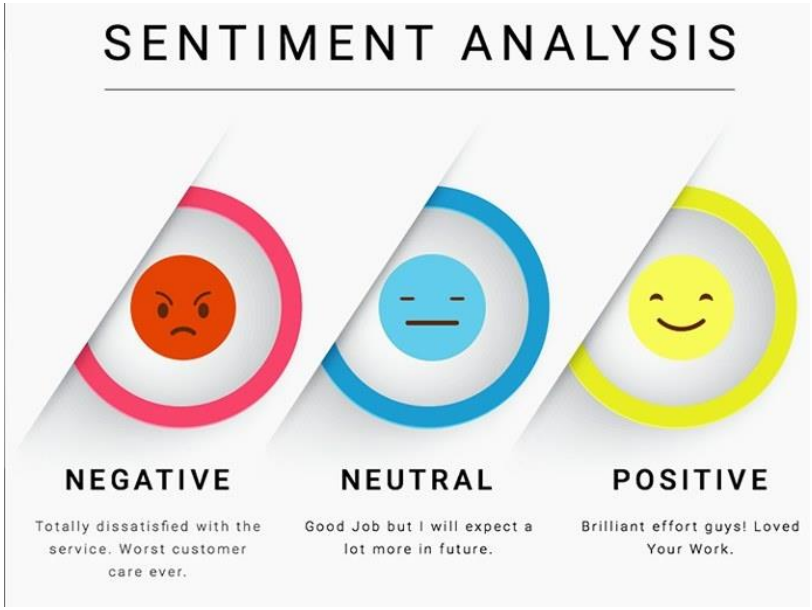

Two dogs play in the grass.


A group of young people playing a game of frisbee.


Two hockey players are fighting over the puck.

Recurrent Neural Networks: Process Sequences

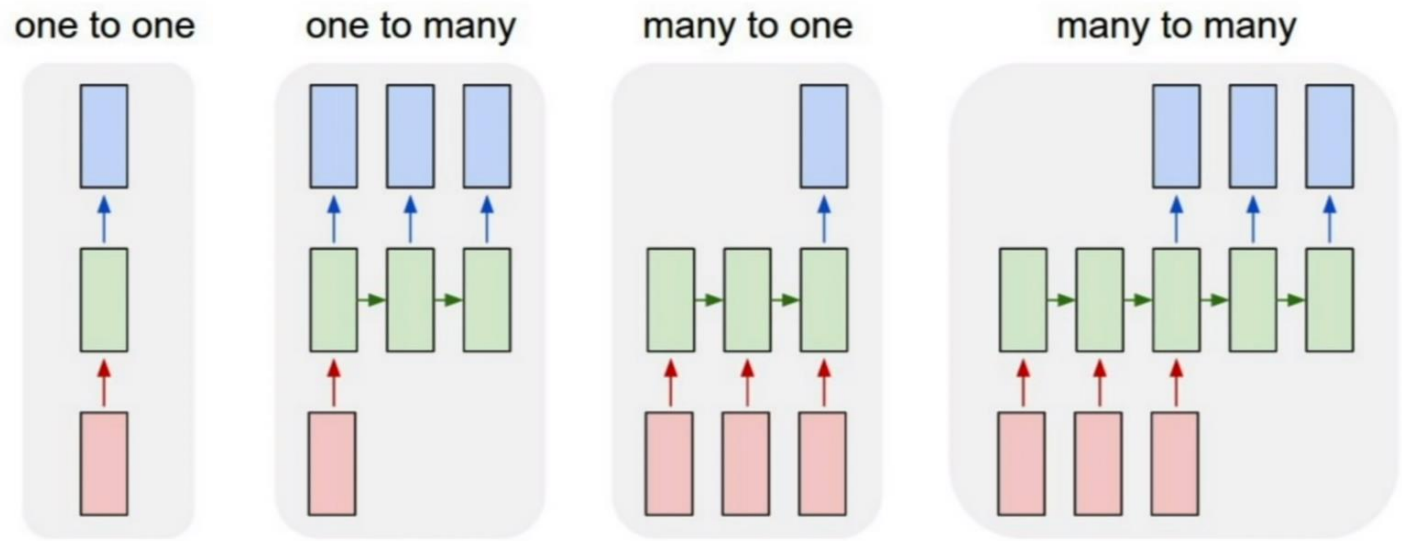




e.g. Sentiment Classification
Sequence of words -> sentiment

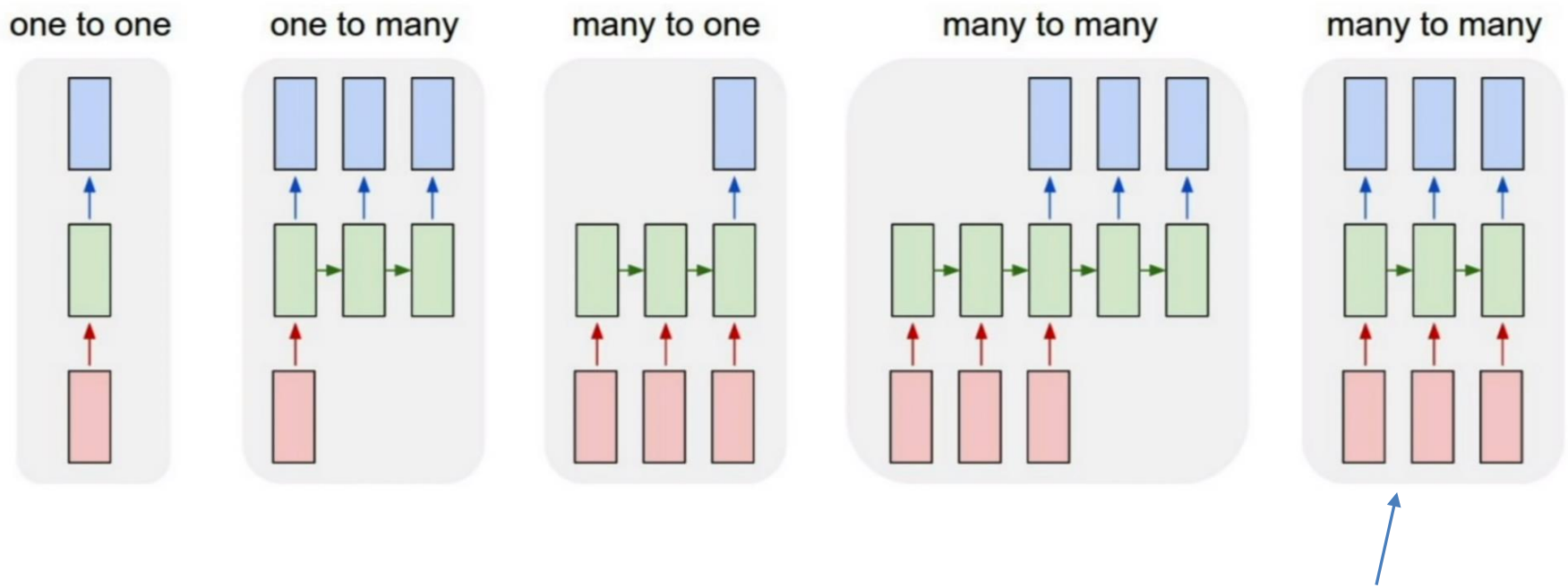
Video action recognition
(frames) -> action label

Recurrent Neural Networks: Process Sequences



e.g. Machine translation
Sequence of words ->
Sequence of words

Recurrent Neural Networks: Process Sequences



e.g. Video classification on frames

Sequences in the Wild

Audio

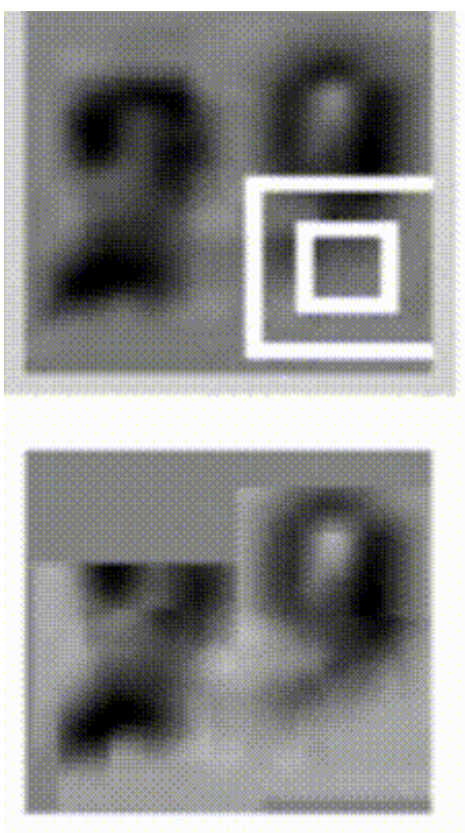
What are Sequences?

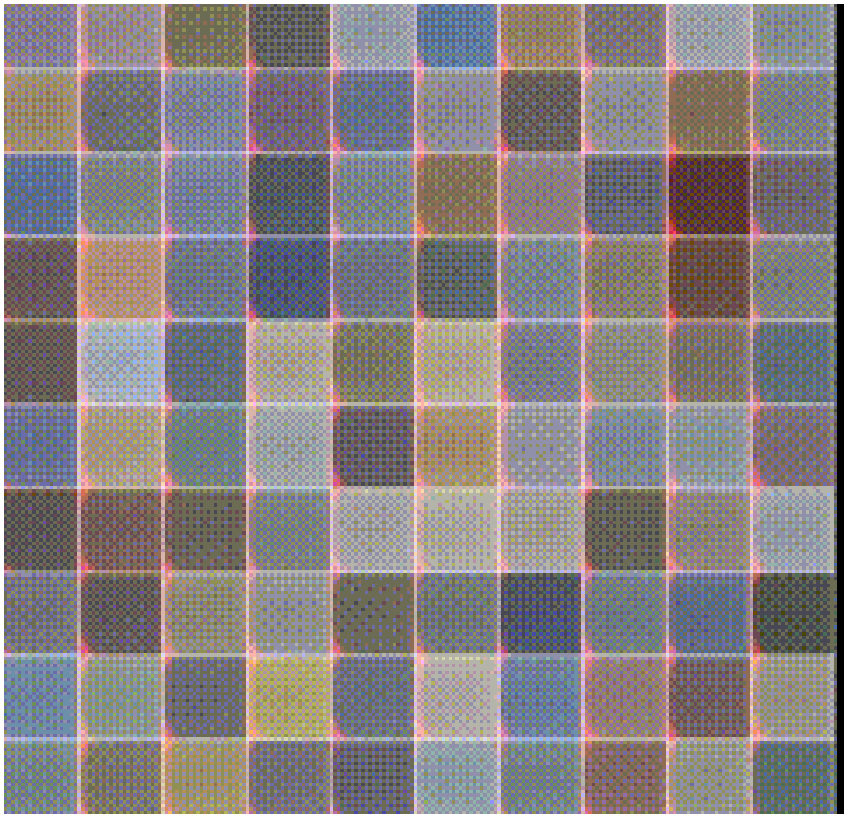
English: I love pickles and onions on my sandwich.

Stock Prediction: <date1, value1>, <date2, value2> ... <dateN, valueN>

- In general, It is a temporally ordered set of data points.

Recurrent Neural Network



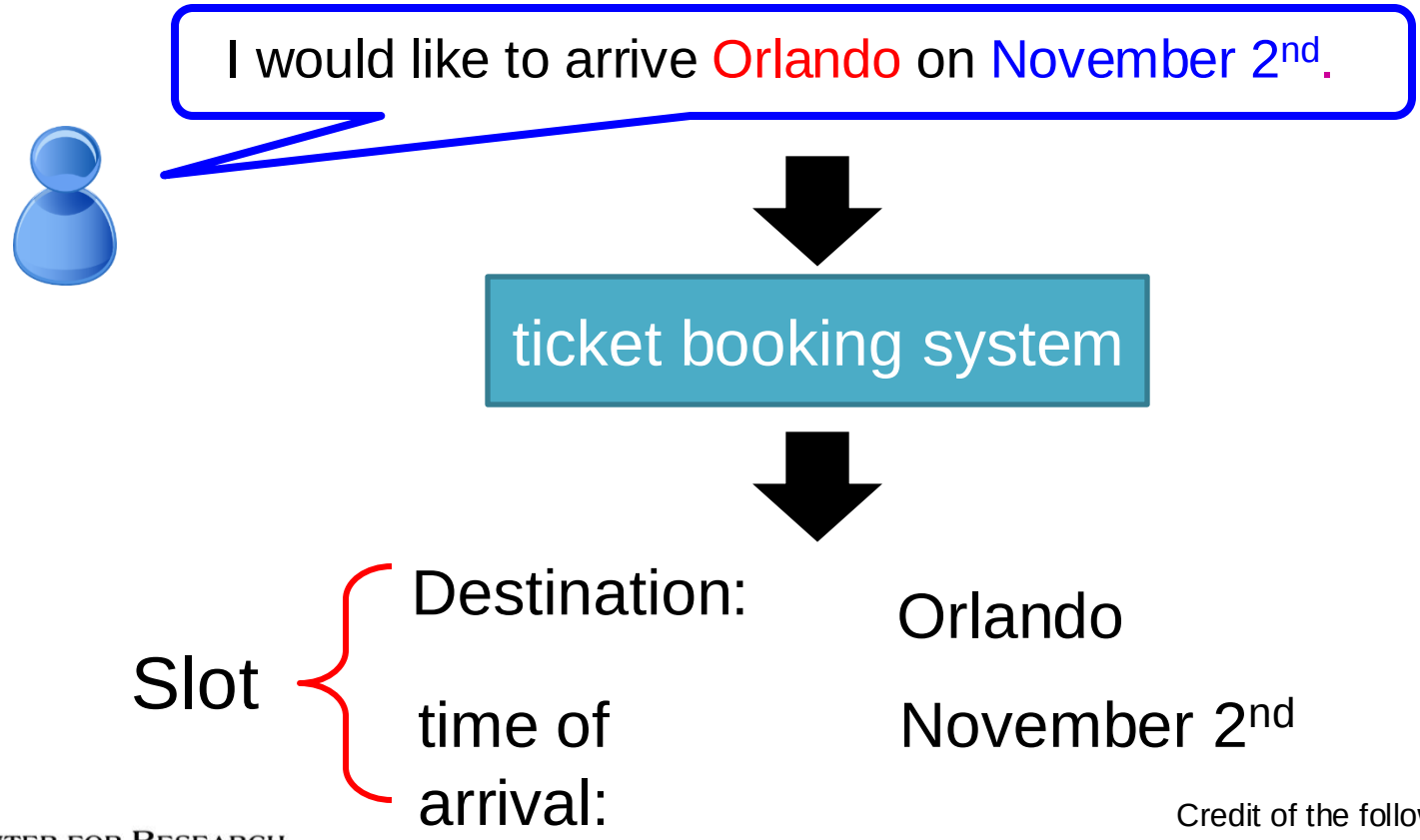


Left: RNN learns to read house numbers.
Right: RNN learns to paint house numbers.

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

Example Application

- Slot Filling



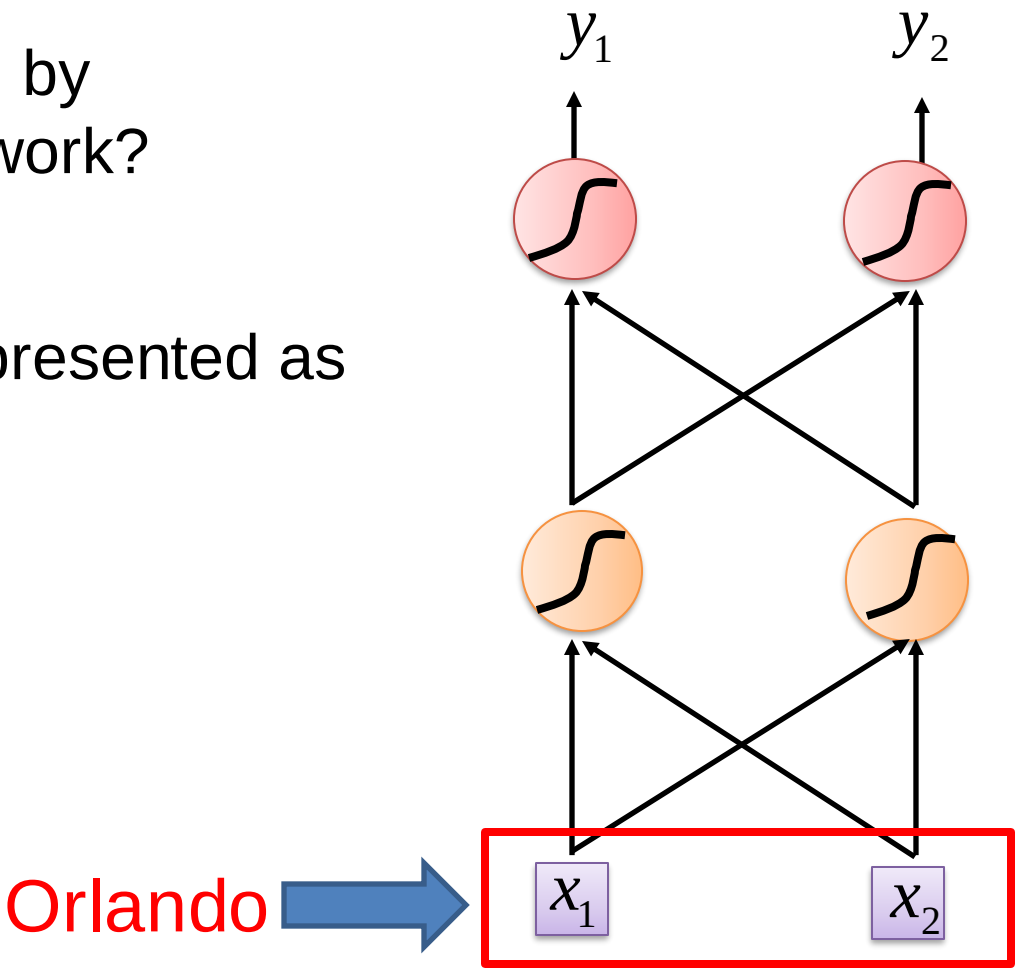
Credit of the following slides:
Dr. Hung-yi Lee

Example Application

Solving slot filling by Feedforward network?

Input: a word

(Each word is represented as a vector)



Example Application

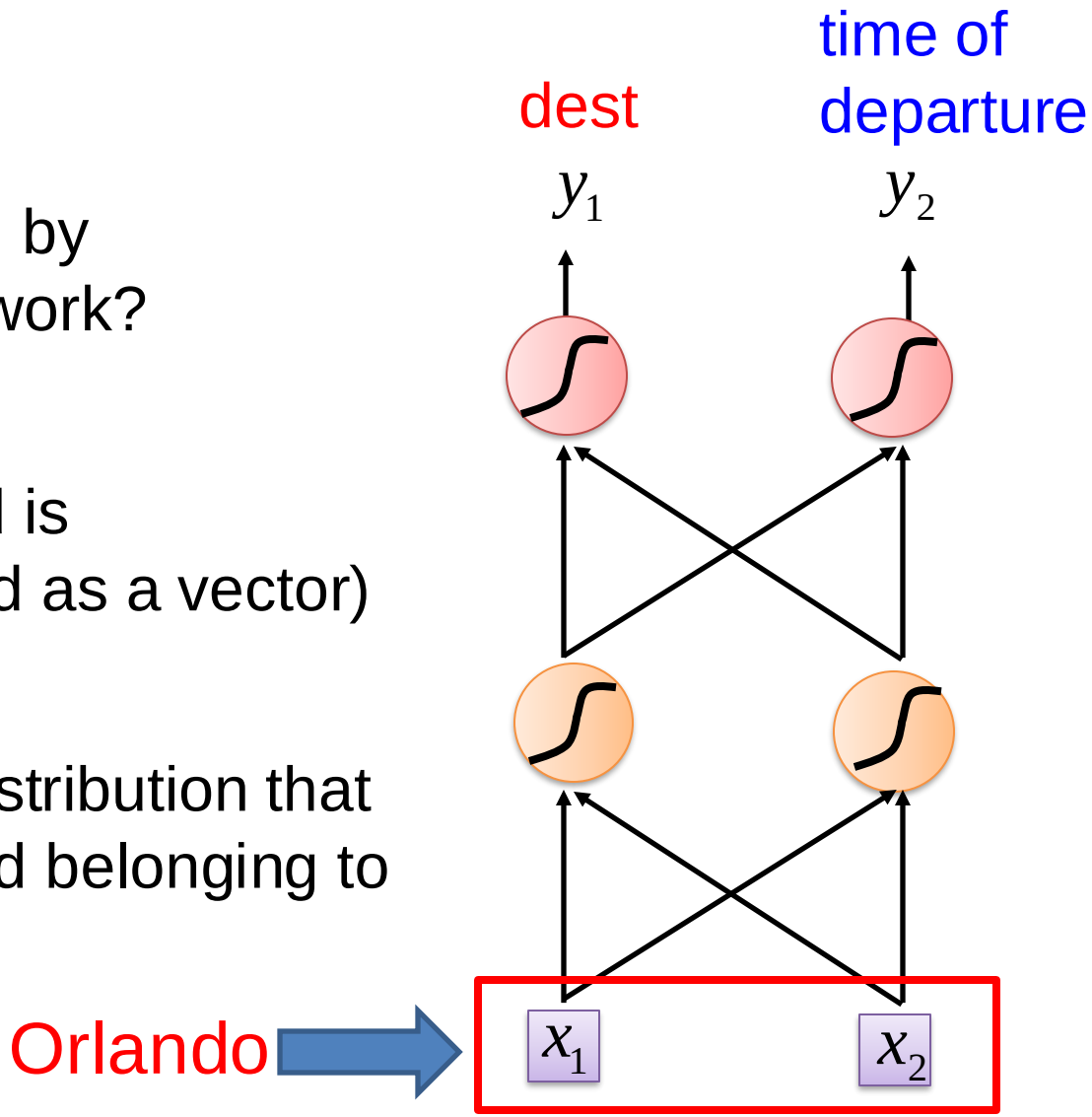
Solving slot filling by Feedforward network?

Input: a word

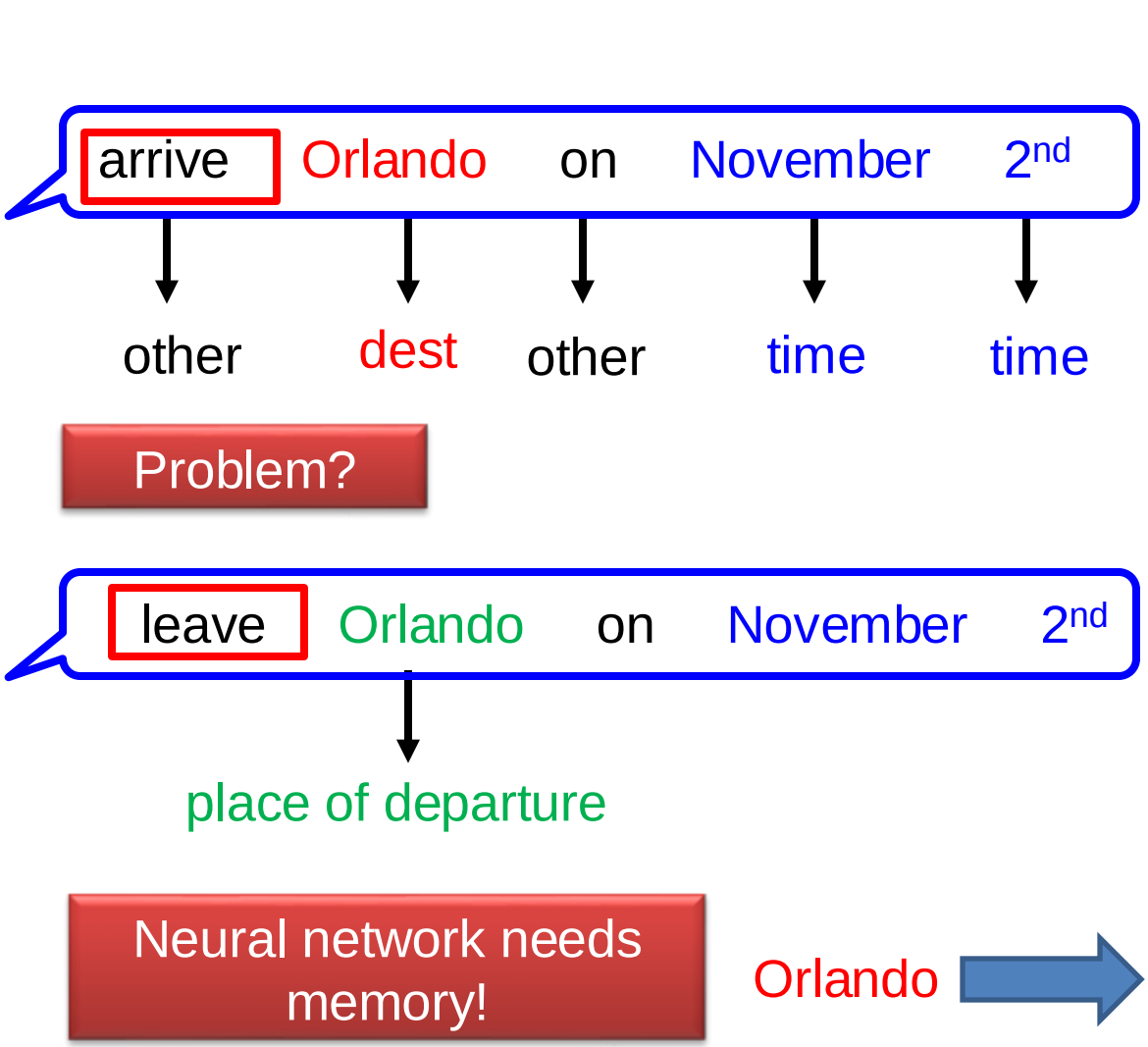
(Each word is represented as a vector)

Output:

Probability distribution that the input word belonging to the slots

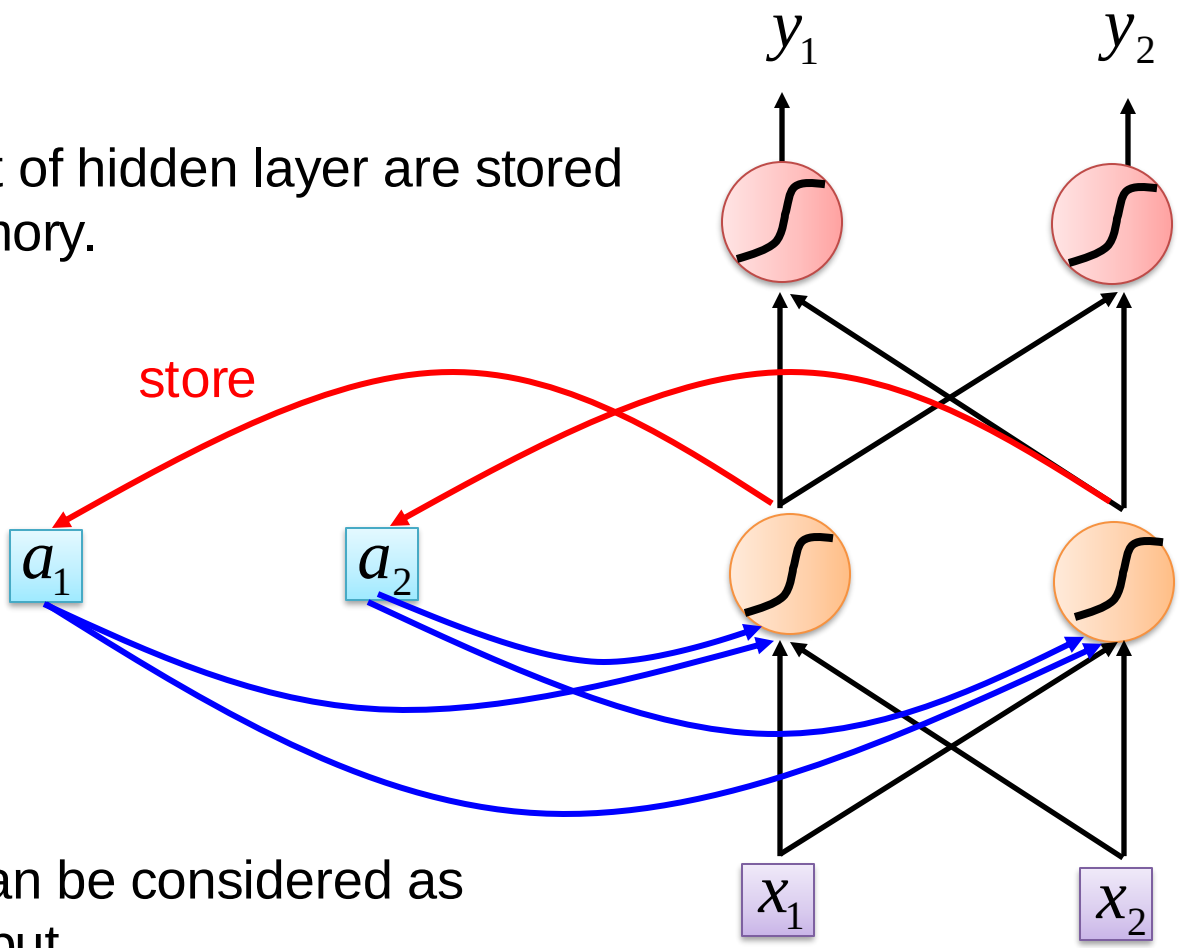


Example Application



Recurrent Neural Network (RNN)

The output of hidden layer are stored in the memory.

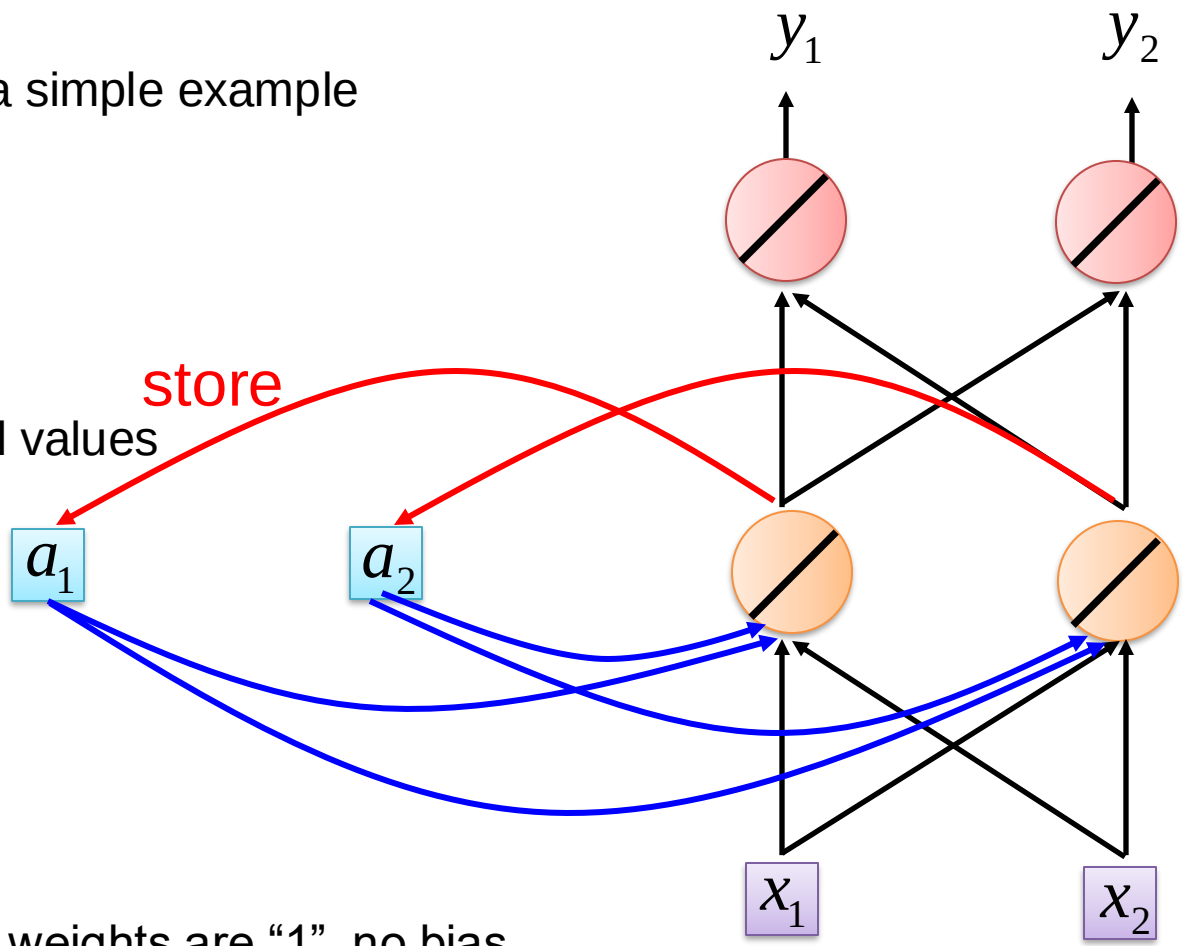


Memory can be considered as another input.

RNN

Input sequence: $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}2\\2\end{bmatrix}$ ……

Run a simple example



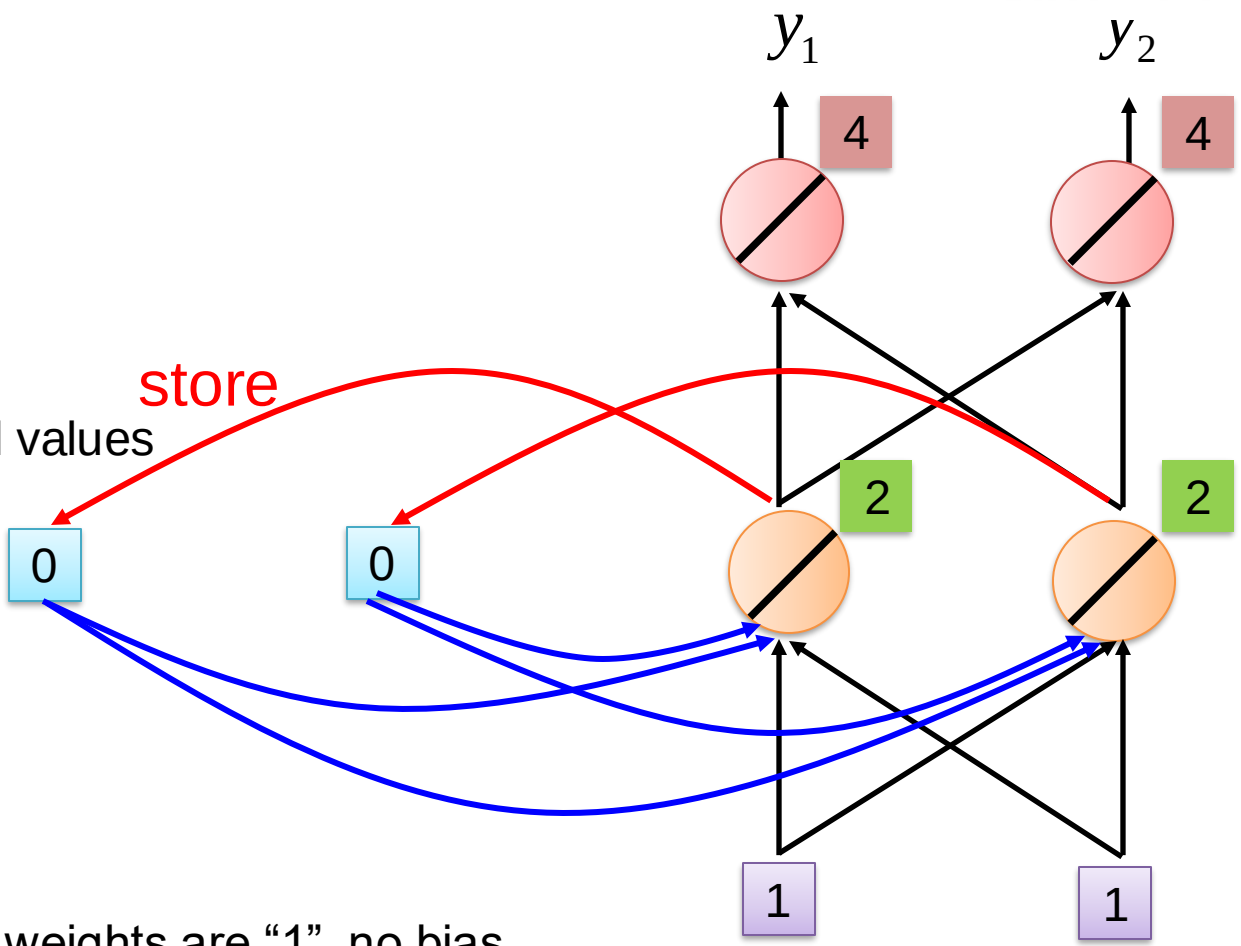
Given initial values to memory

All the weights are “1”, no bias
All activation functions are linear

RNN

Input sequence: $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}2\\2\end{bmatrix}$ ……

output sequence: $\begin{bmatrix}4\\4\end{bmatrix}$

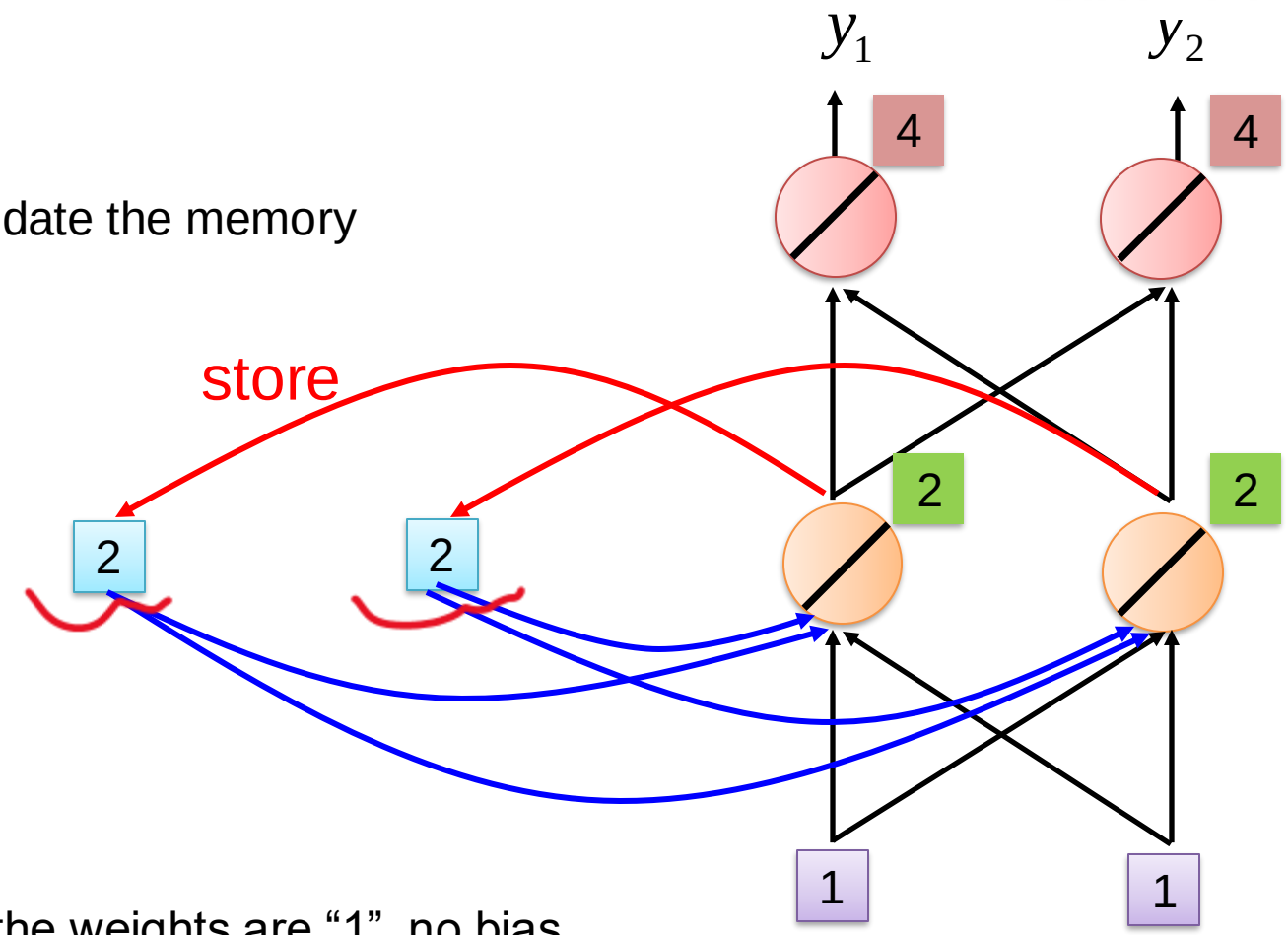


All the weights are “1”, no bias
All activation functions are linear

RNN

Input sequence: $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}2\\2\end{bmatrix}$ ……

output sequence: $\begin{bmatrix}4\\4\end{bmatrix}$



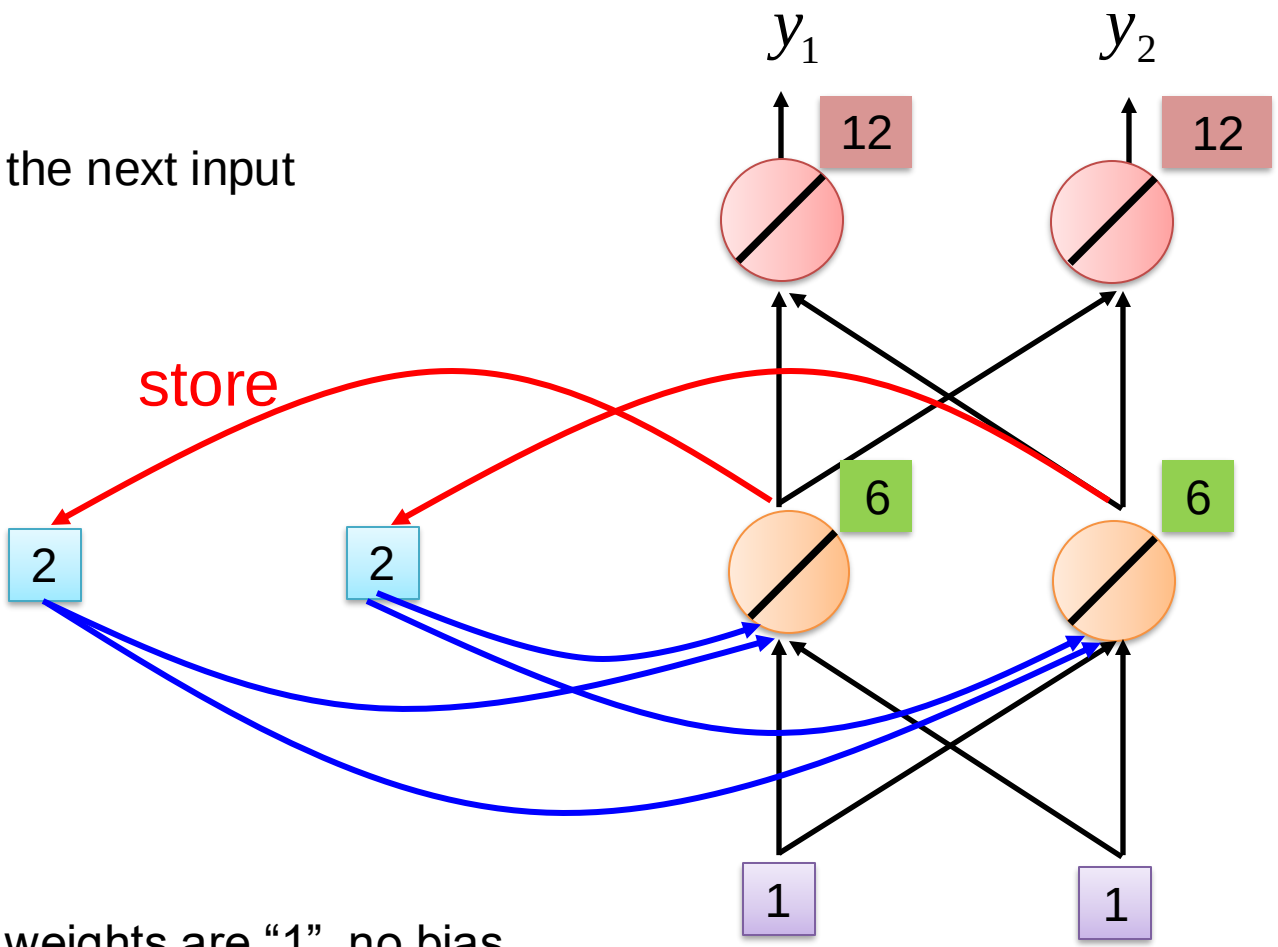
All the weights are “1”, no bias
All activation functions are linear

RNN

Input sequence: $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}2\\2\end{bmatrix}$ ……

output sequence: $\begin{bmatrix}4\\4\end{bmatrix}$ $\begin{bmatrix}12\\12\end{bmatrix}$

Take the next input

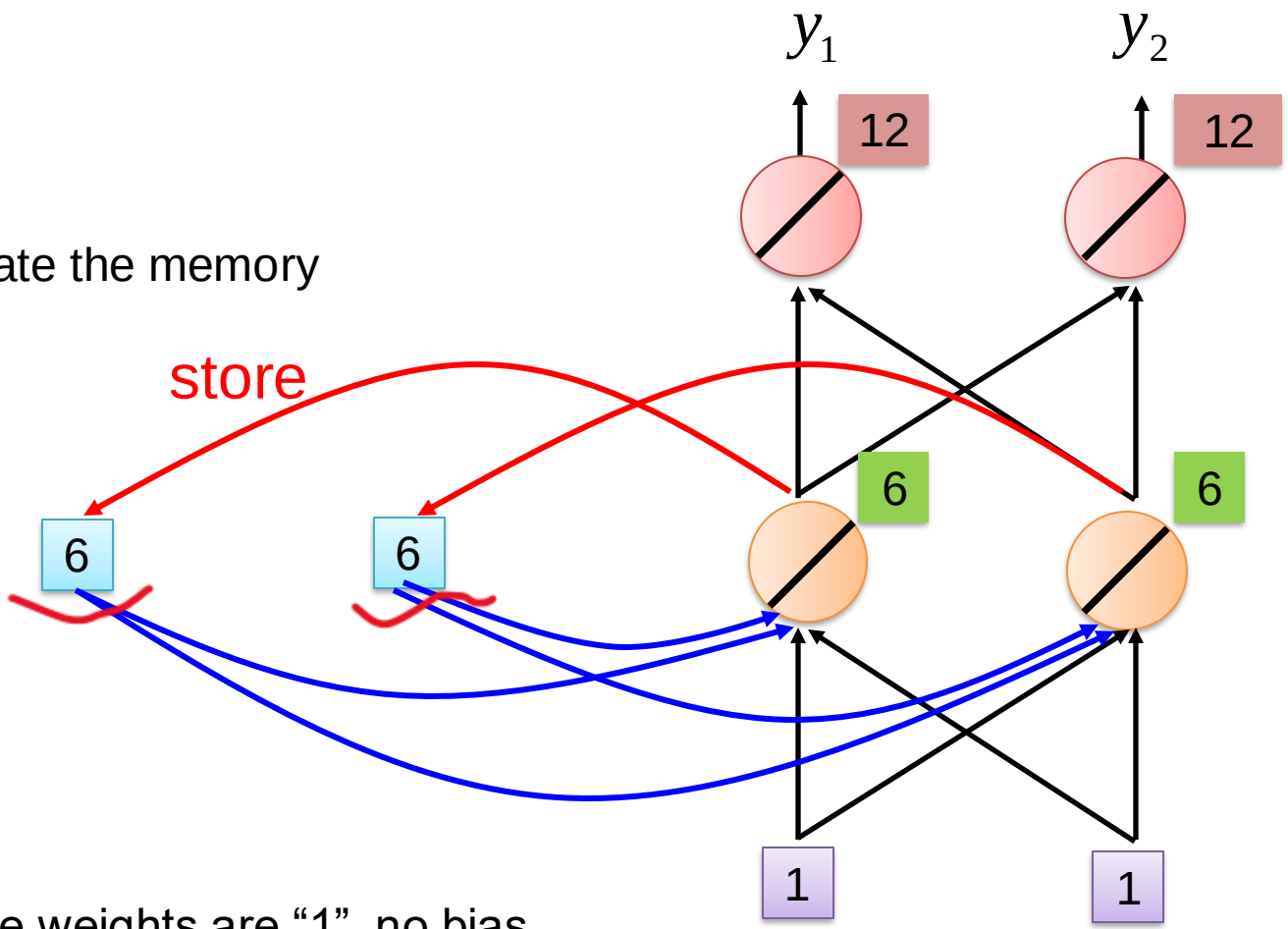


All the weights are “1”, no bias
All activation functions are linear

RNN

Input sequence: $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}2\\2\end{bmatrix}$ ……

output sequence: $\begin{bmatrix}4\\4\end{bmatrix}$ $\begin{bmatrix}12\\12\end{bmatrix}$



Update the memory

store

All the weights are “1”, no bias

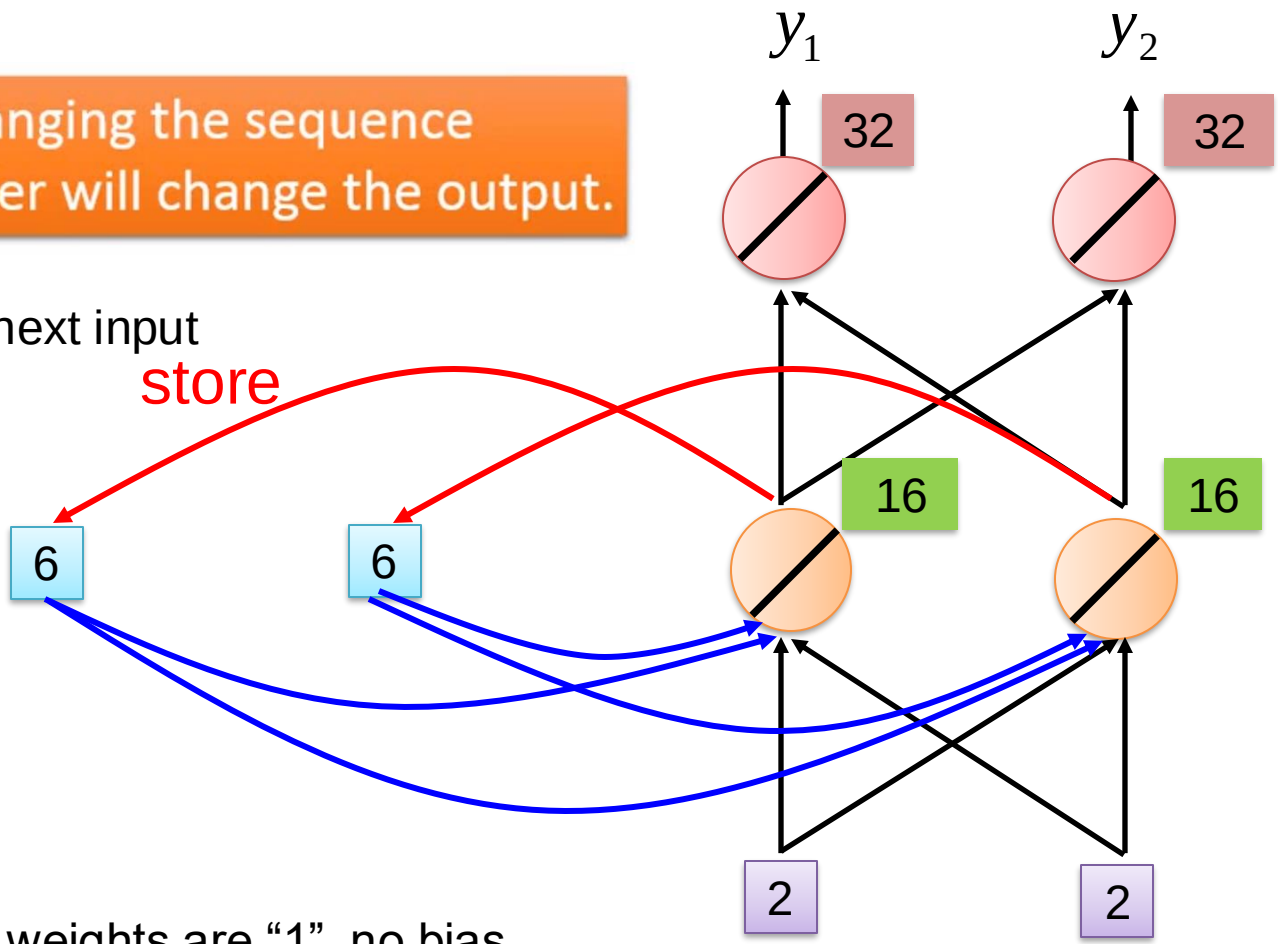
All activation functions are linear

RNN

Input sequence: $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}1\\1\end{bmatrix}$ $\begin{bmatrix}2\\2\end{bmatrix}$ ……

output sequence: $\begin{bmatrix}4\\4\end{bmatrix}$ $\begin{bmatrix}12\\12\end{bmatrix}$ $\begin{bmatrix}32\\32\end{bmatrix}$ ……

Changing the sequence order will change the output.



Take the next input

All the weights are “1”, no bias
All activation functions are linear

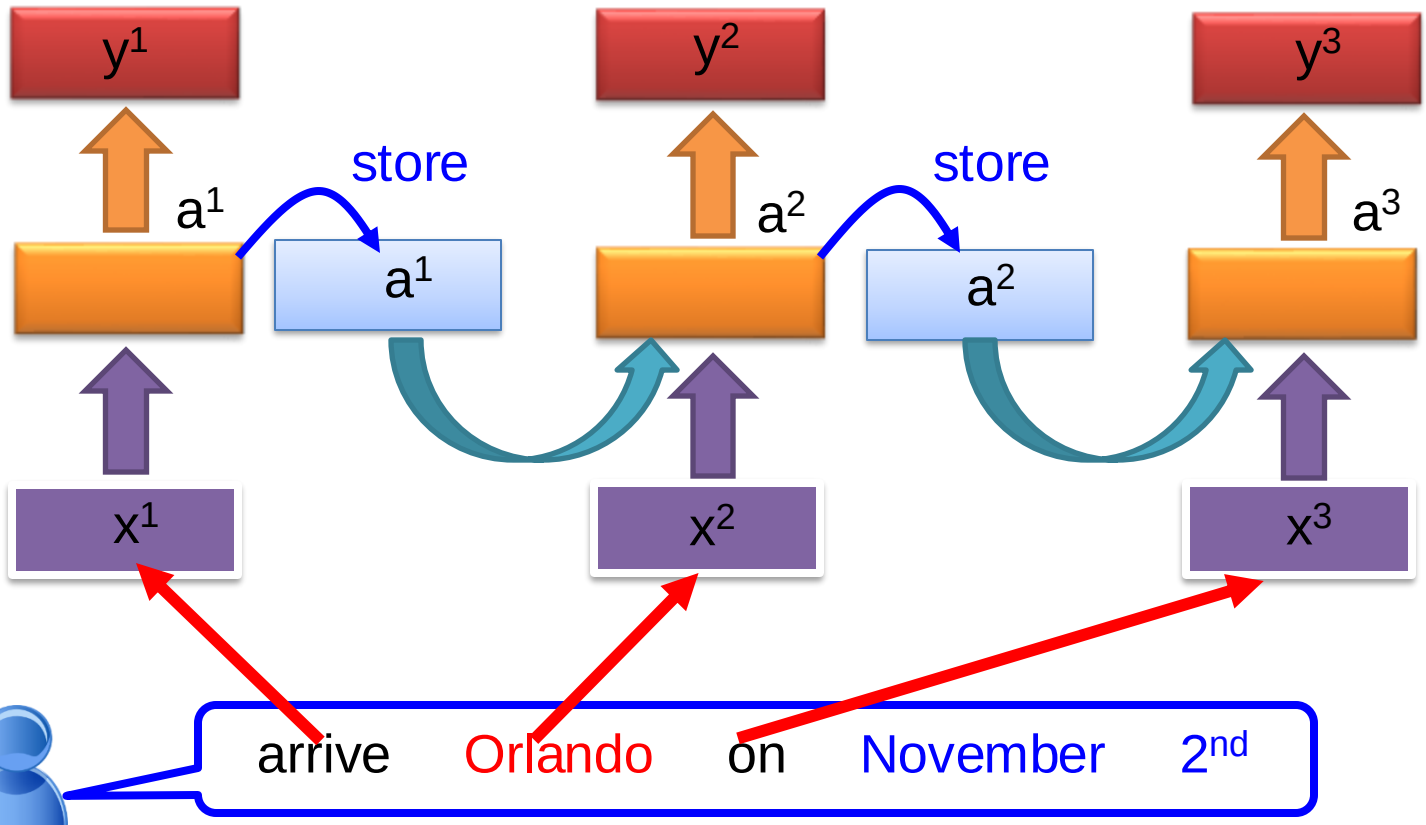
RNN

The same network is used again and again.

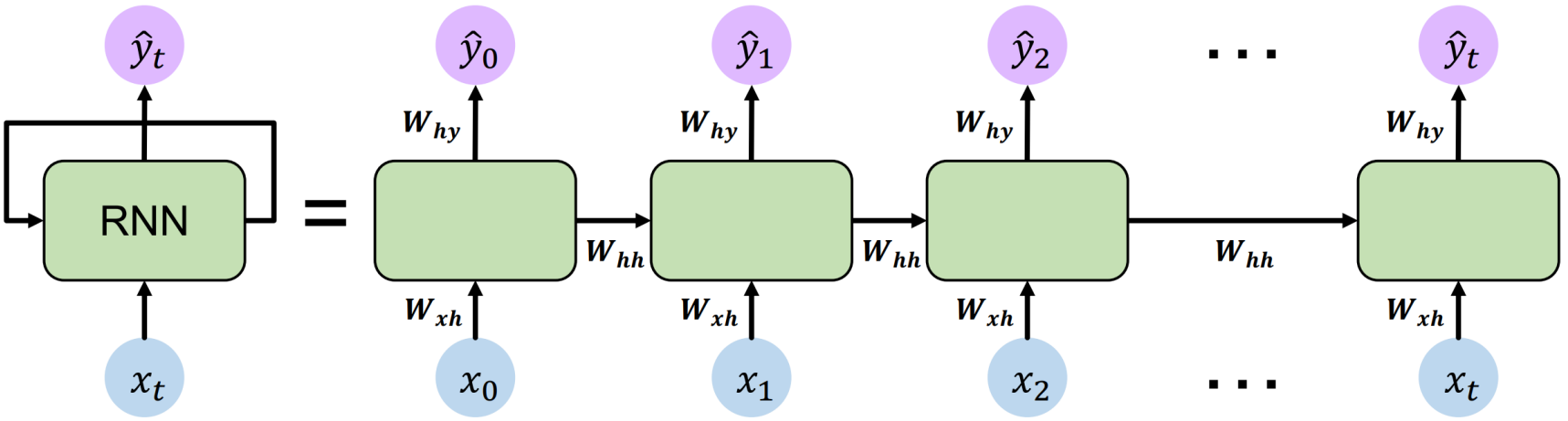
Probability of "arrive" in each slot

Probability of "Orlando" in each slot

Probability of "on" in each slot

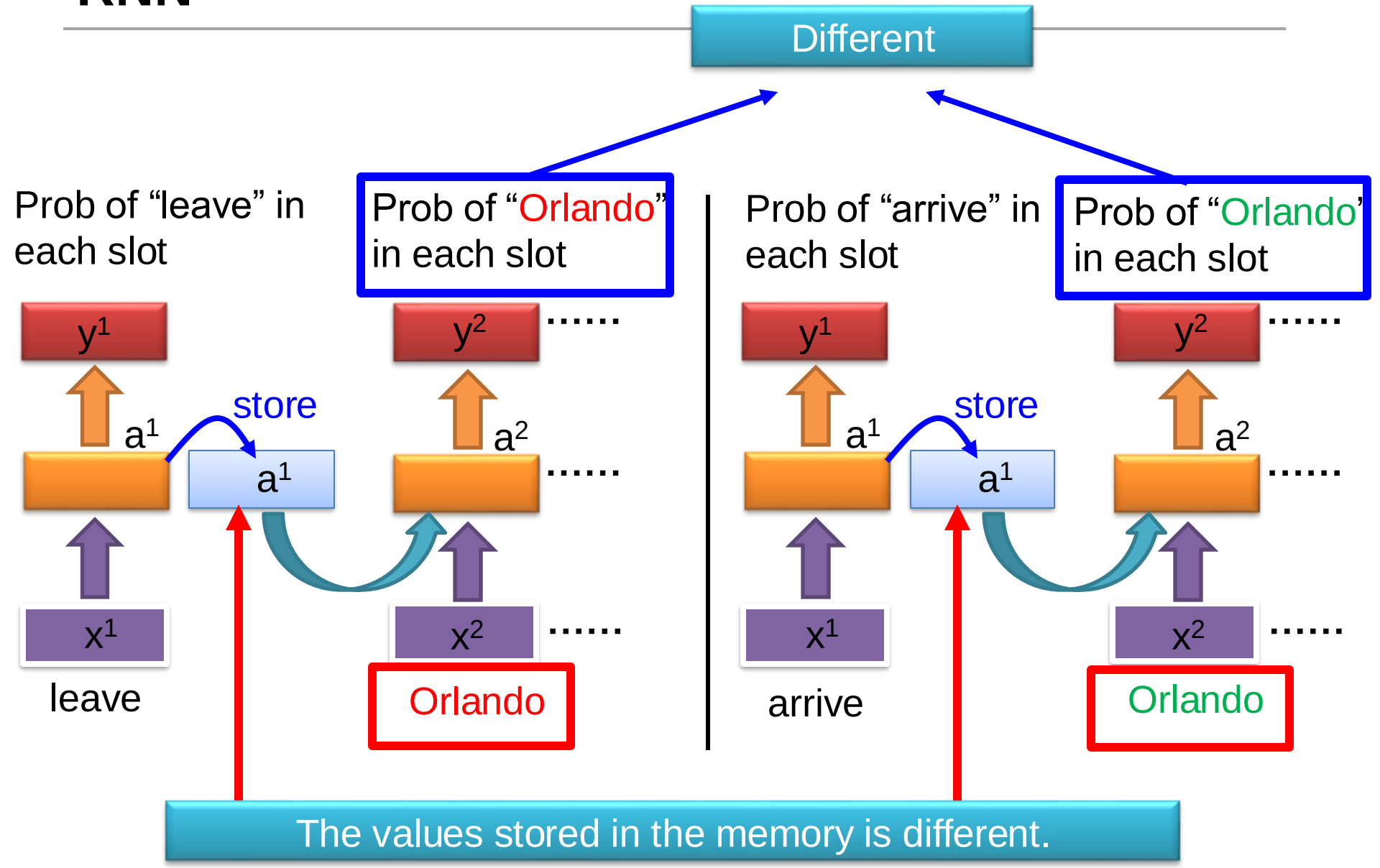


RNNs: computational graph across time

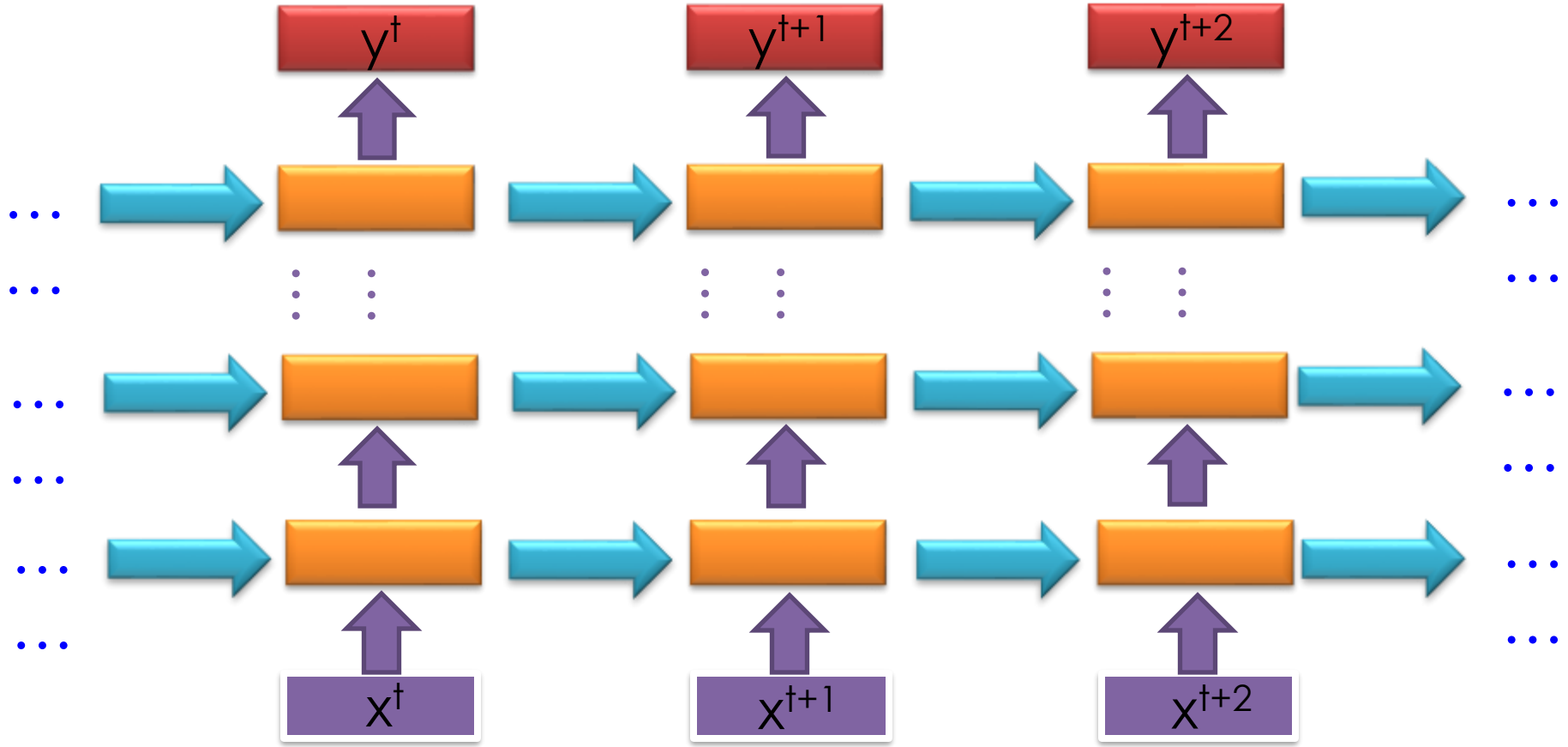


Unrolling

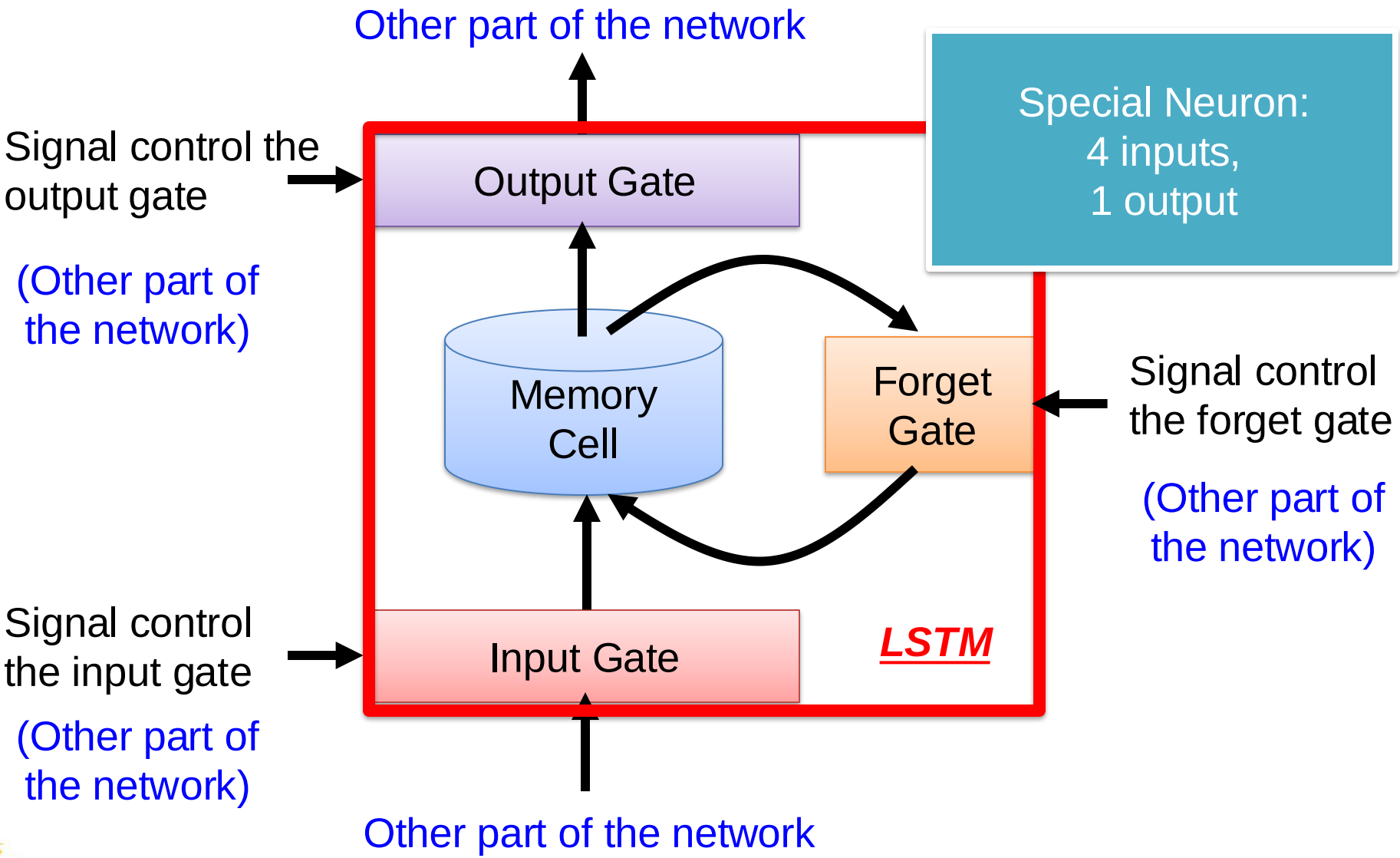
RNN


Different
Prob of "leave" in each slot
Prob of "Orlando" in each slot
Prob of "arrive" in each slot
Prob of "Orlando" in each slot
y1
y2
a1
a2
store
x1
x2
leave
Orlando
arrive
Orlando
The values stored in the memory is different.

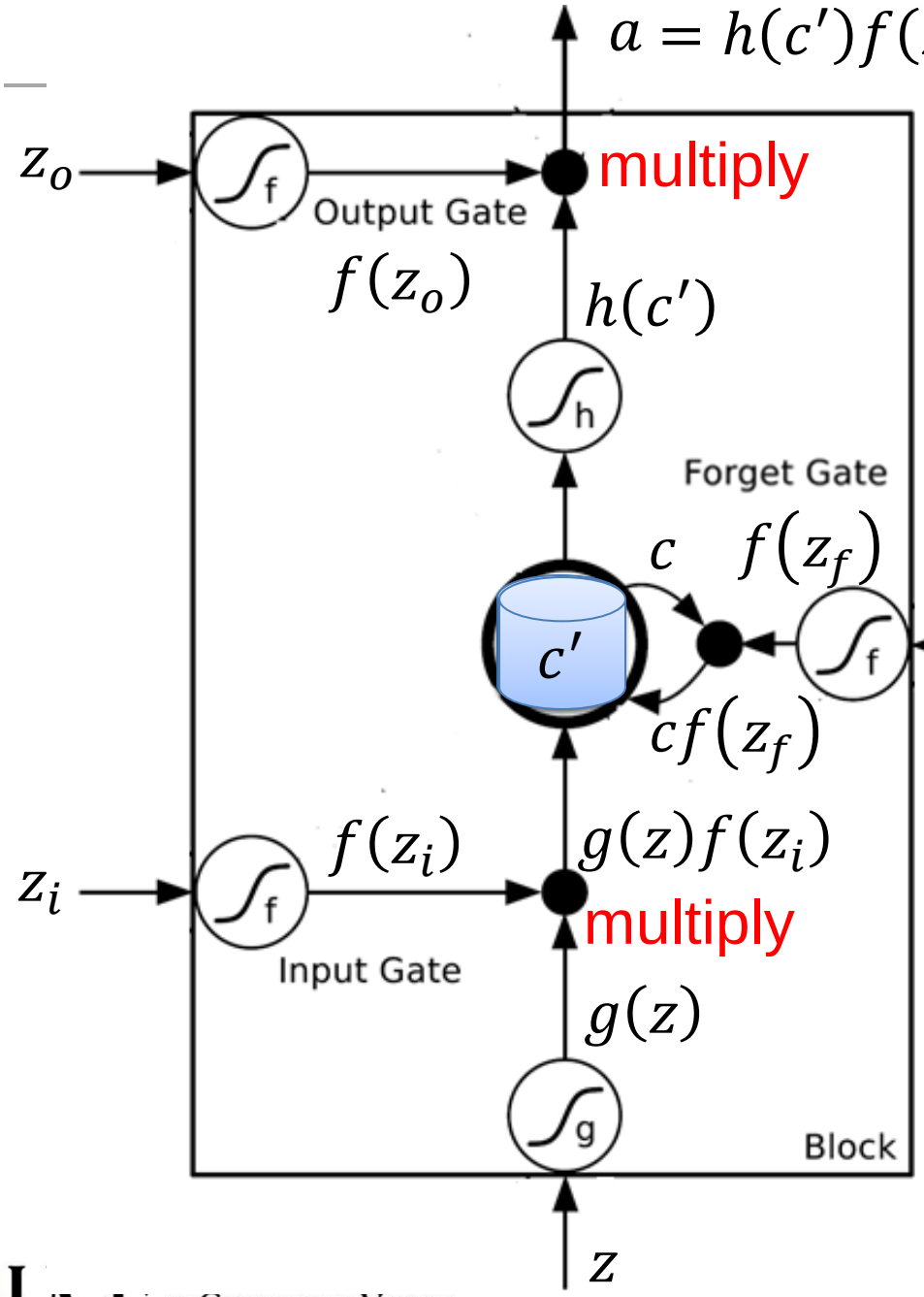
Of course, it can be deep …



Long Short-term Memory (LSTM)



Hochreiter, Sepp, and Jürgen Schmidhuber. "Long short-term memory." Neural computation 9.8 (1997): 1735-1780.



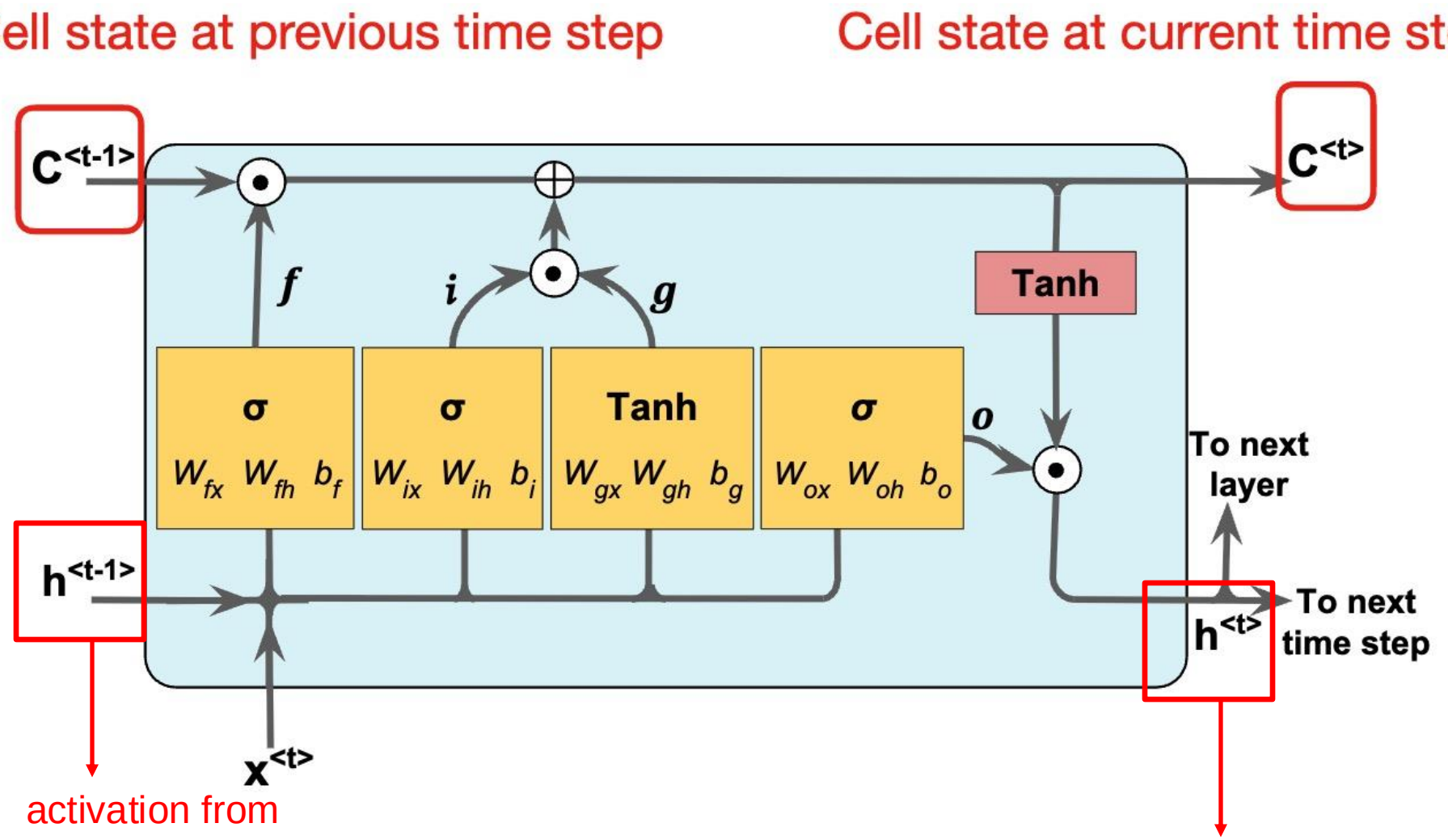
Activation function f is usually a sigmoid function

Between 0 and 1

Mimic open and close gate

$$c' = g(z)f(z_i) + cf(z_f)$$

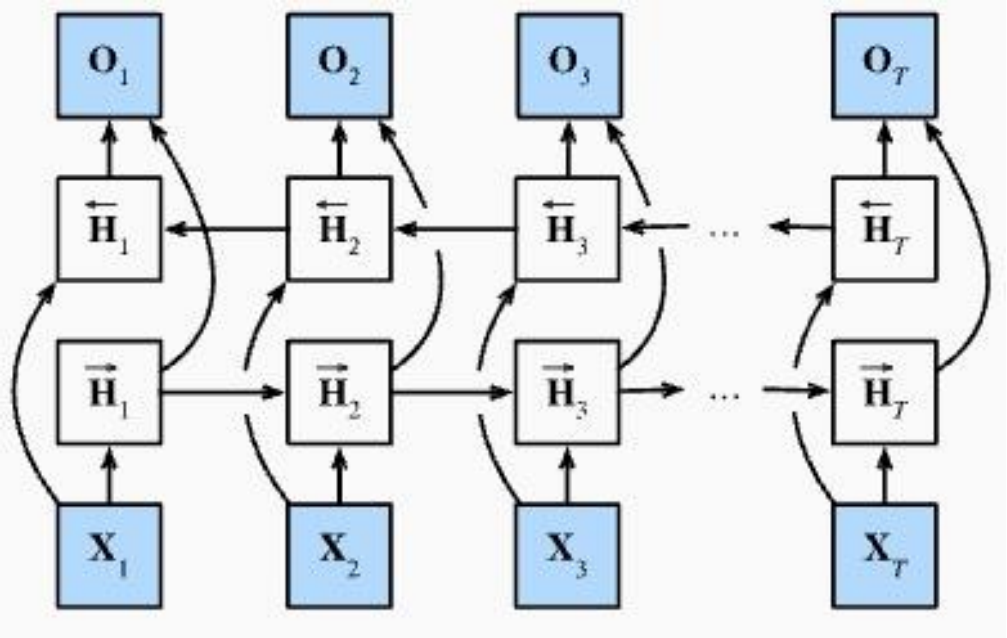
https://pytorch.org/docs/stable/generated/torch.nn.LSTM.html



Slide credit: Sebastian Raschka

Modern Recurrent Neural Nettworks

- Bidirectional Recurrent Neural Networks
  - a combination of two RNNs training the network in opposite directions.
  - It helps in analyzing the future events by not limiting the model's learning to past and present.
- Bidirectional LSTM



https://d2l.ai/chapter_recurrent-modern/bi-rnn.html

Limitations of RNNs

- Computations for over positions cannot be parallelized
- Long-range interactions are bottlenecked by a fixed size memory

Example applications

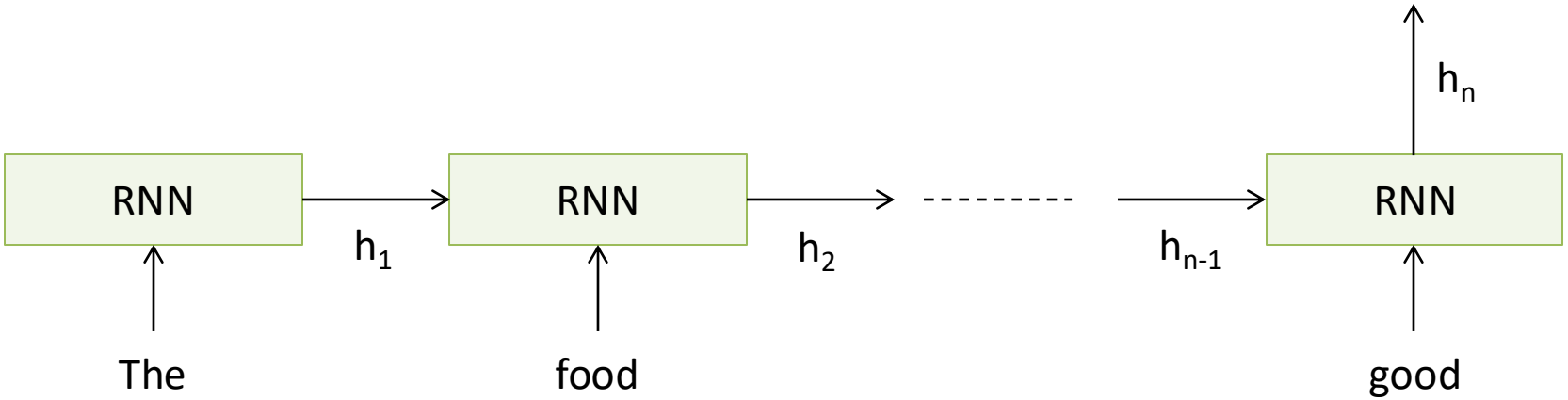
Sentiment Classification

- Classify a
  restaurant review from Yelp! OR
  movie review from IMDB OR
  …
  as positive or negative

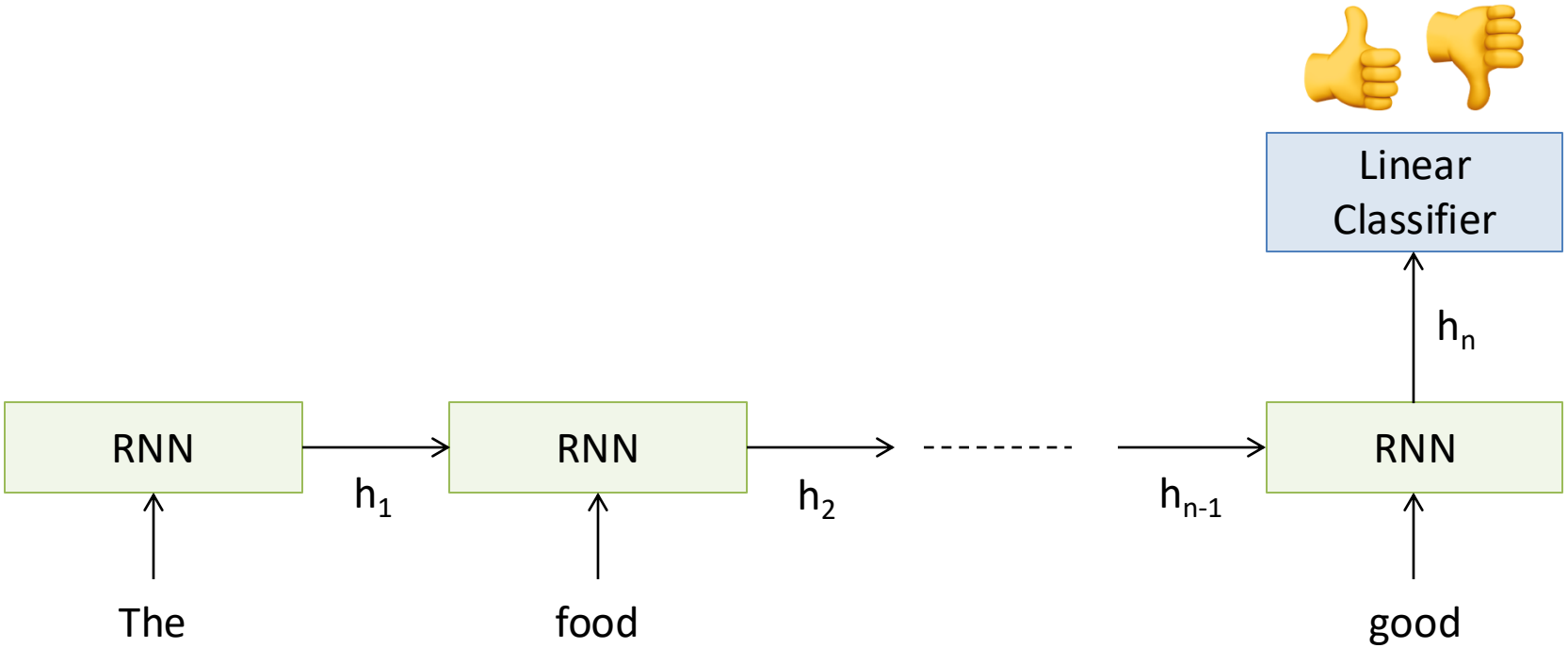
- Inputs: Multiple words, one or more sentences
- Outputs: Positive / Negative classification

- “The food was really good”
- “The chicken crossed the road because it was uncooked”

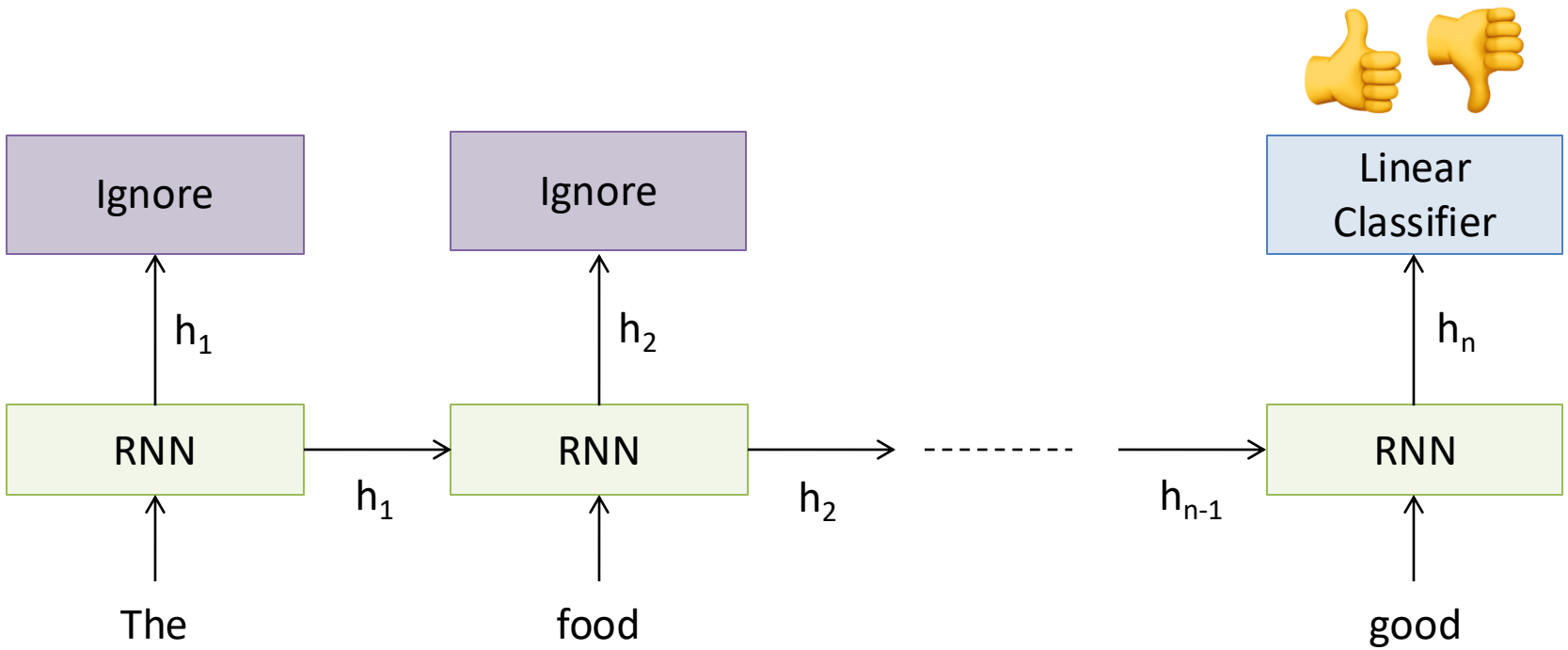
Sentiment Classification



Sentiment Classification



Sentiment Classification



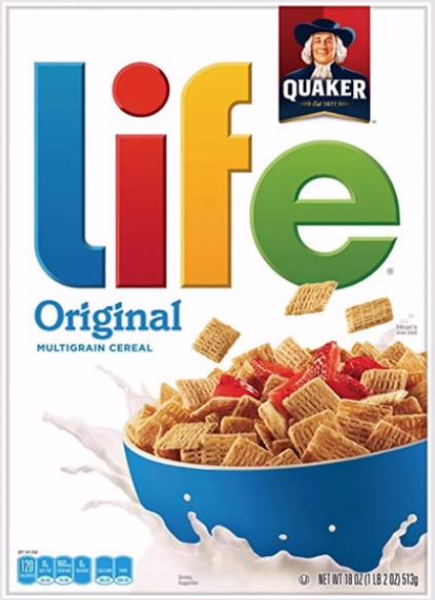
Customers Review 2,491

Thanos

September 2018

Verified Purchase

Amazing! This box of cereal gave me a **perfectly balanced breakfast**, as all things should be. I only ate half of it but **will definitely be buying again!**



A Box of Cereal

$3.99

Sequential inputs /outputs

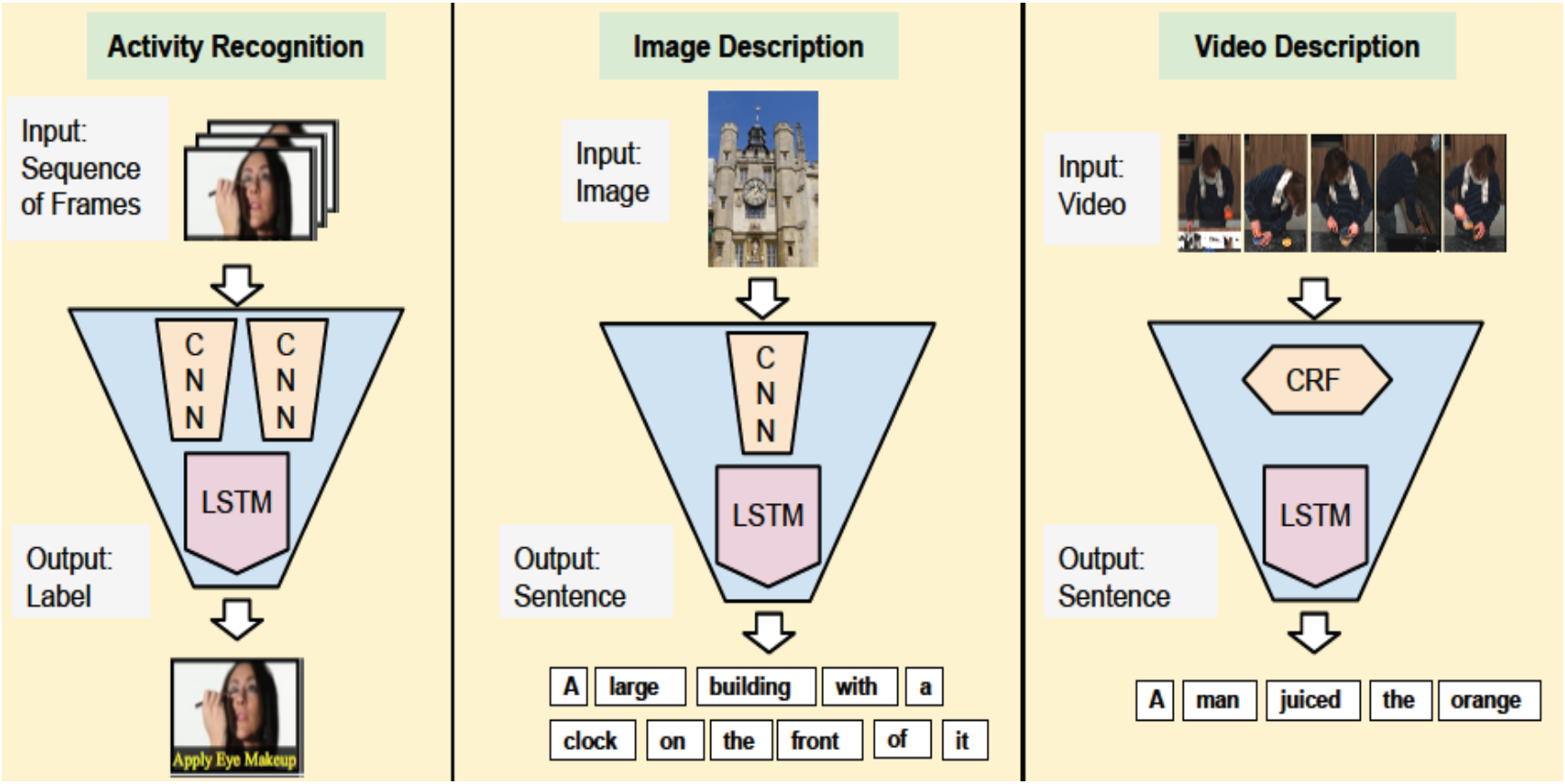


Image credit: main paper

Activity recognition

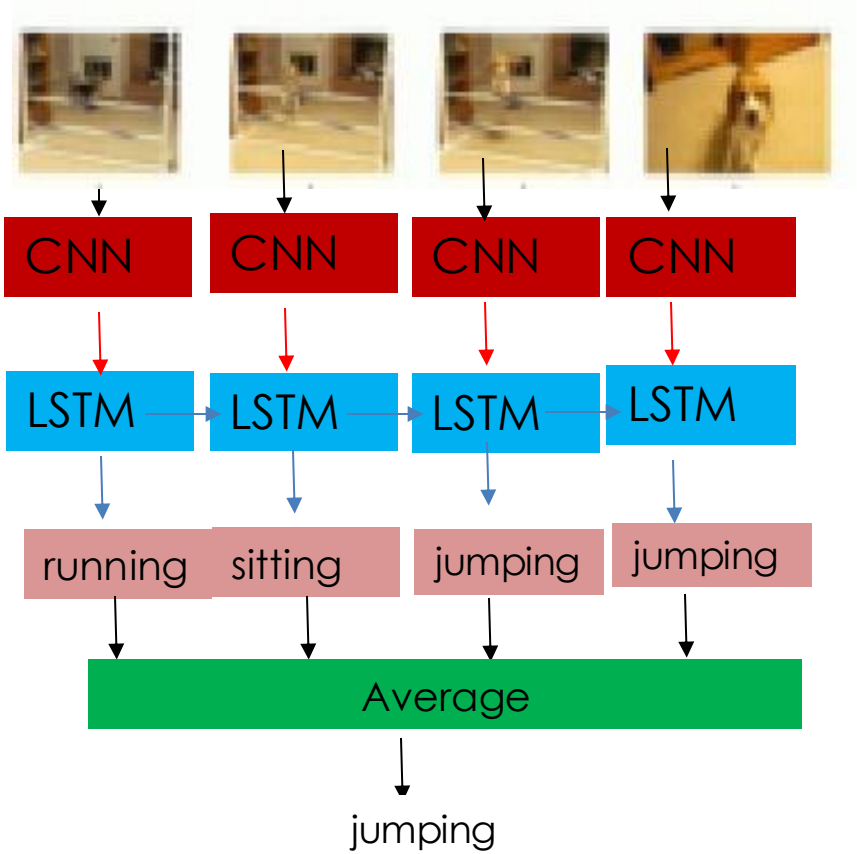
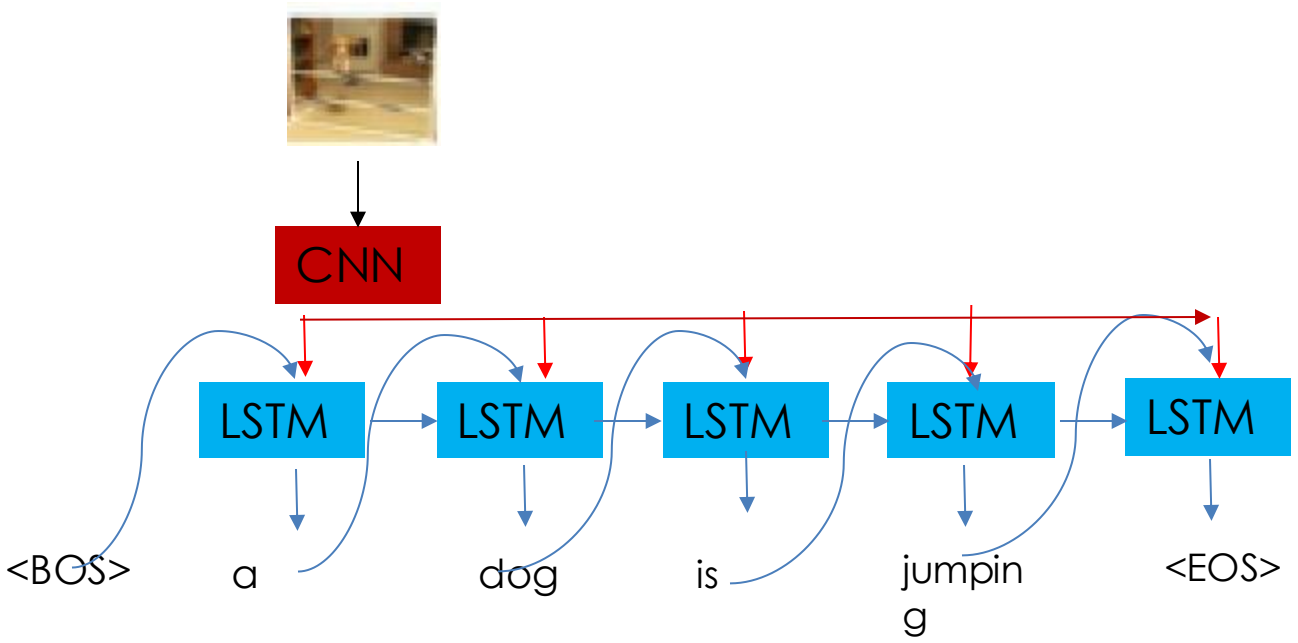


Image description



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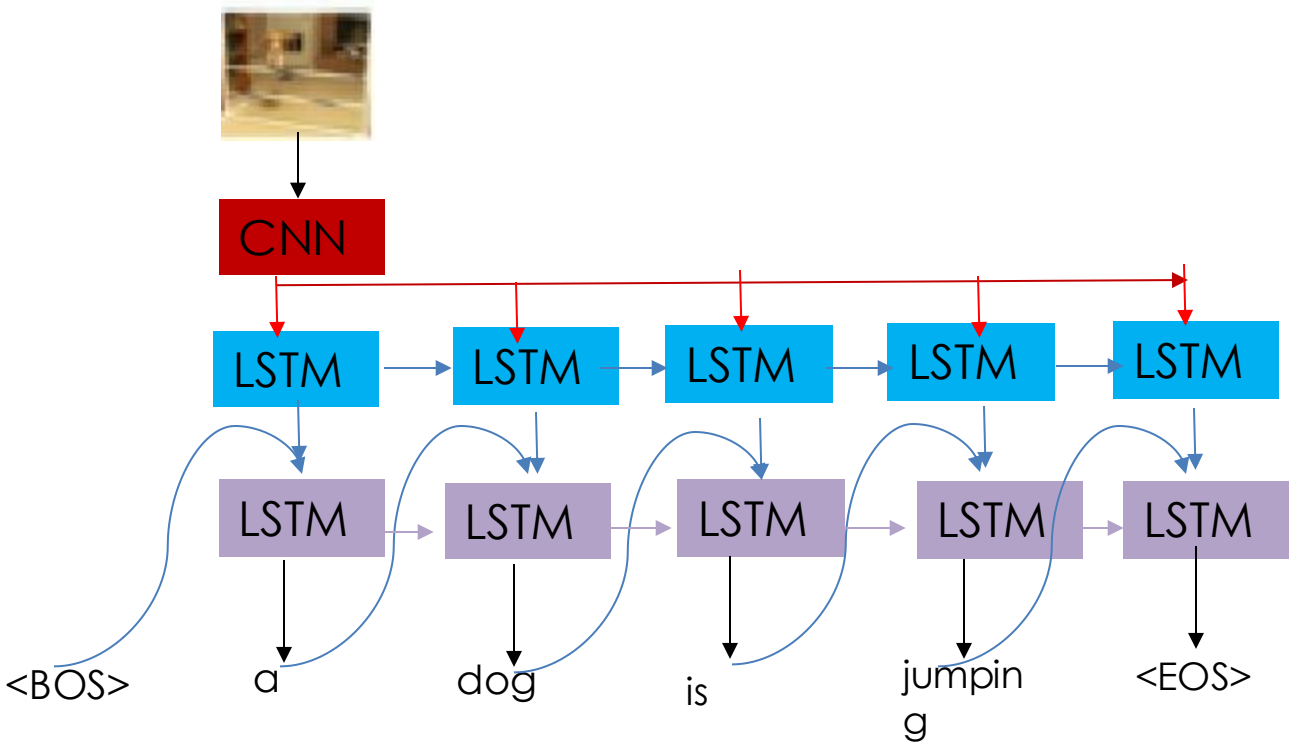

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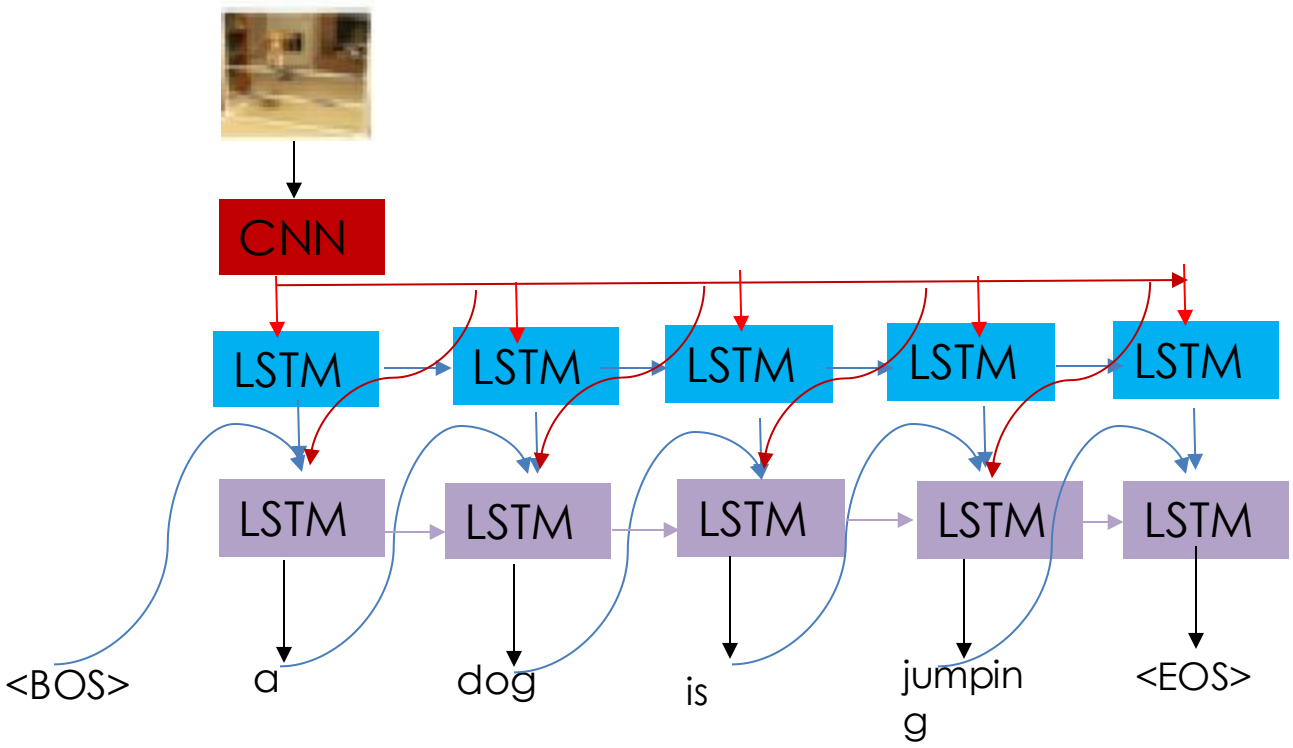
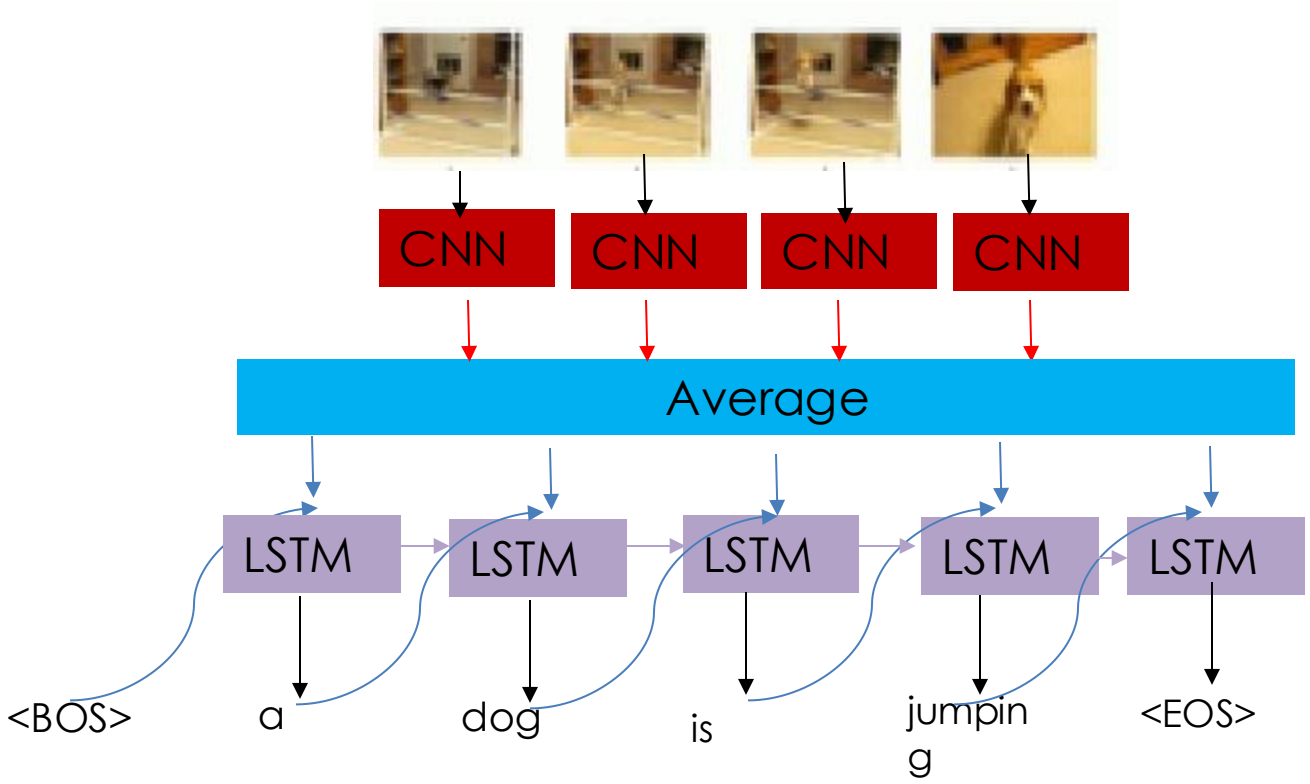
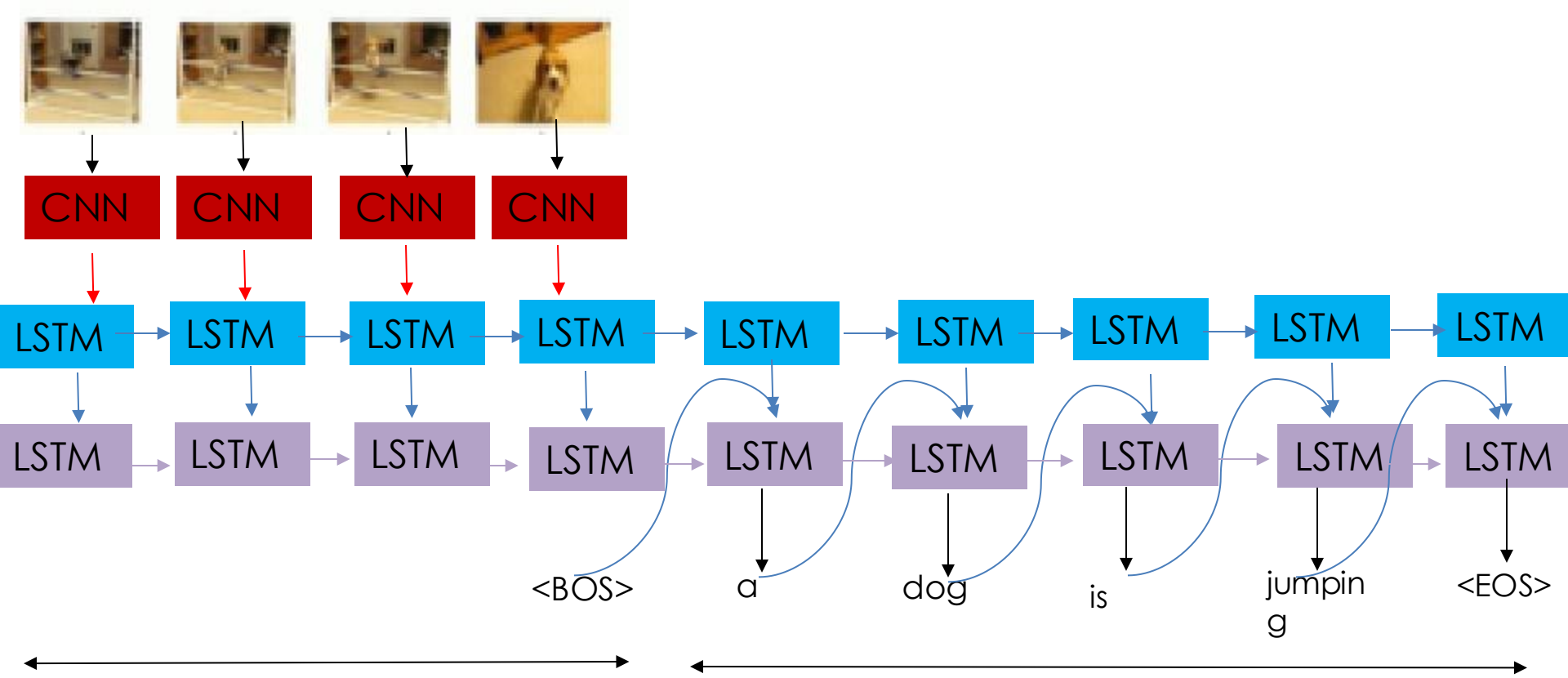


Video description



Video description



Thank you!

Question?

References and Slide Credits

- Many slides are adapted from the existing teaching or tutorial slides by Hung-yi Lee, Andrew Ng, Alexander Amini, Lex Fridman, and Stanford course - CS231n: Convolutional Neural Networks for Visual Recognition
- Special thanks to Dr. Hung-yi Lee for making his machine learning course slides and materials available
- Alexander Amini, MIT 6.S191 Introduction to Deep Learning: http://introtodeeplearning.com/
  - Youtube videos: https://www.youtube.com/watch?v=5tvmMX8r_OM&list=PLtBw6njQRU-rwp5__7C0oIVt26ZgjG9NI&index=1
- Lex Fridman, MIT Deep Learning and Artificial Intelligence Lectures: https://deeplearning.mit.edu/ https://www.youtube.com/watch?v=O5xeyoRL95U