Sequence modeling

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Sequence modeling

Basic ideas

- Sequences of vectors, e.g. frames in an audio stream
- Learn about subsequences

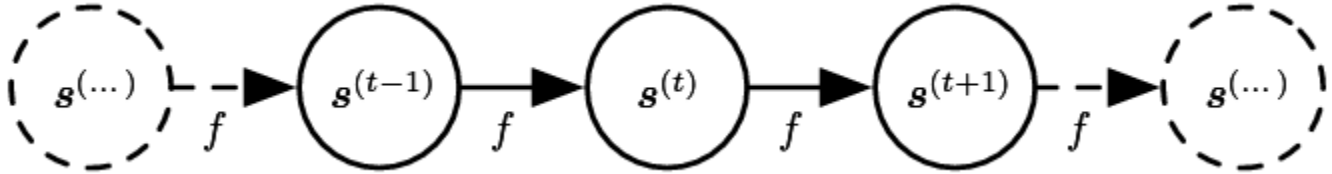
Unfolding computational graphs

- Consider a function that relies on previous state: $s^{(t)} = f(s^{(t-1)}|\theta)$
- Over time…

$$s^{(t)} = f(s^{(t-1)}|\theta)$$

$$s^{(t+1)} = f\left(s^{(t)}\middle|\theta\right) = f(f(s^{(t-1)}|\theta)|\theta)$$

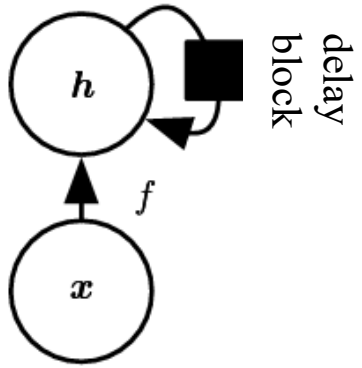
- We can think of this as a graph



Goodfellow et al. Fig 10.1

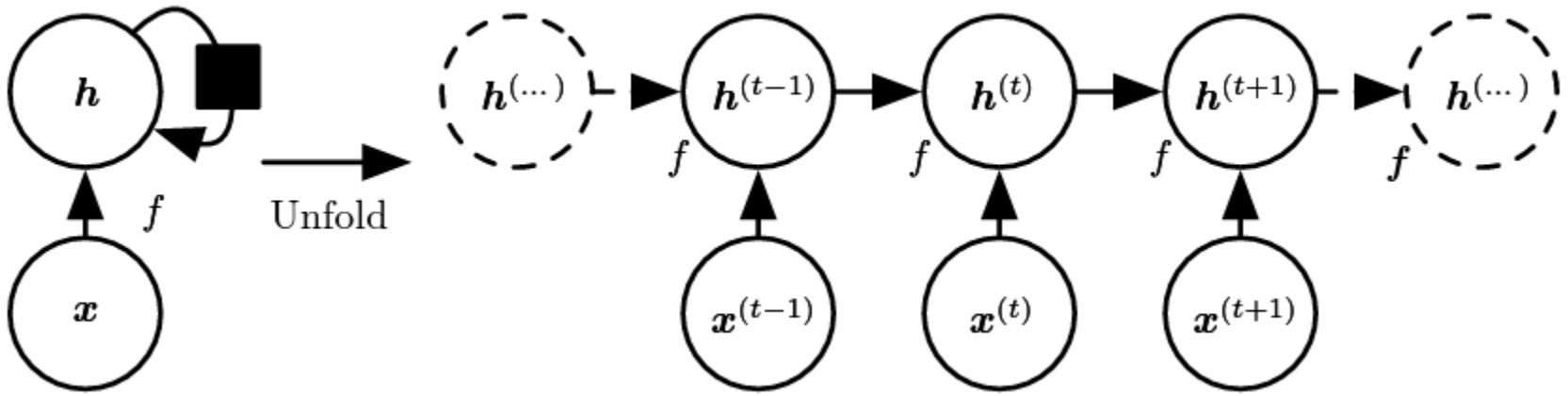
Add an input

- $s^{(t)} = f(s^{(t-1)}, x^{(t)}|\theta)$
- $s^{(t-1)}$ has history of input
- Consider this occurring in a hidden unit: $h^{(t)}=f(h^{(t-1)}, x^{(t)}|\theta)$



Goodfellow et al. Fig 10.2

Recurrent neural networks (RNNs)



Goodfellow et al. Fig 10.2

- Prior knowledge of $x^{(t)}$tends to be lossy, as one usually does not need the entire history

RNNs

RNNs take a sequence and output:

- a sequence
- or a single response

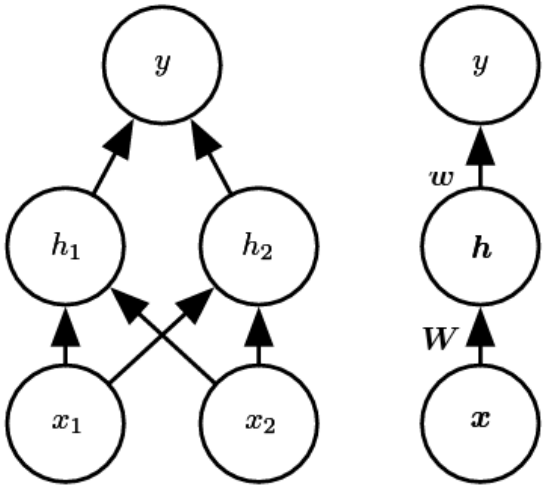
In addition to the current input, nodes can depend on:

- outputs of previous nodes
- previous outputs

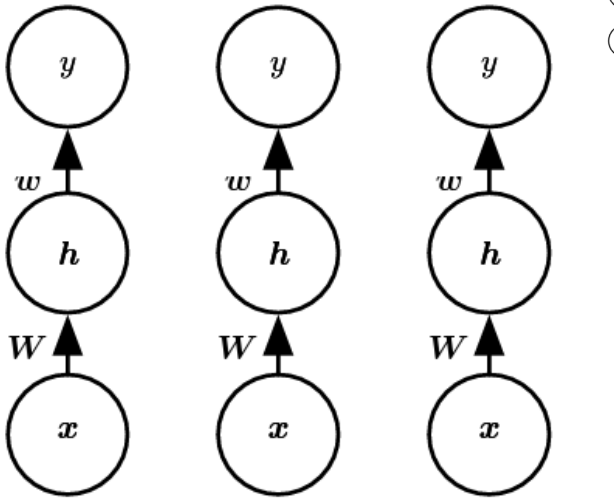
Recurrence in the hidden layers can result in Turing complete networks.

Notation

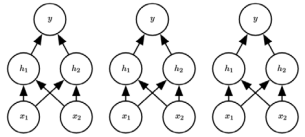
We are using compact network representation (chapter 6), networks can have breadth



Goodfellow et al. Fig. 6.2

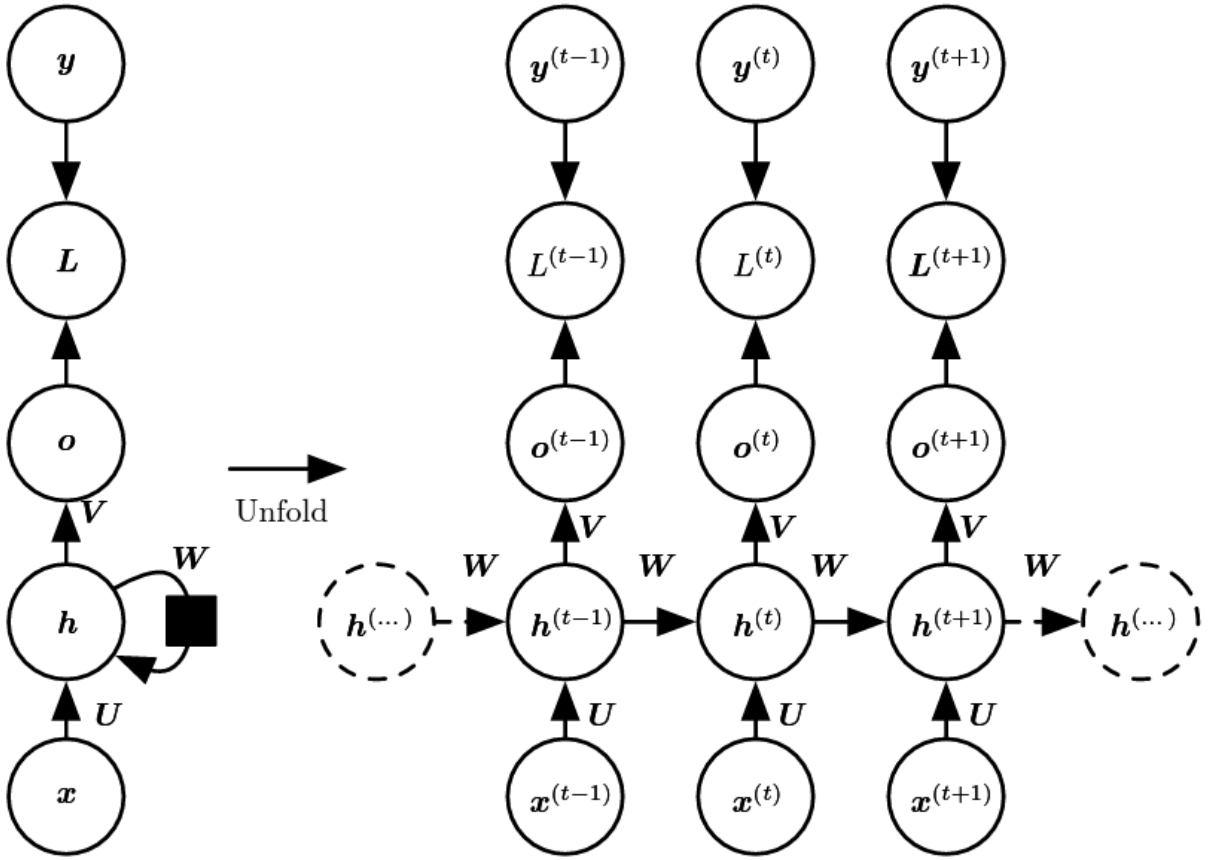


$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^{(1)} \quad \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^{(2)} \quad \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^{(3)}$$



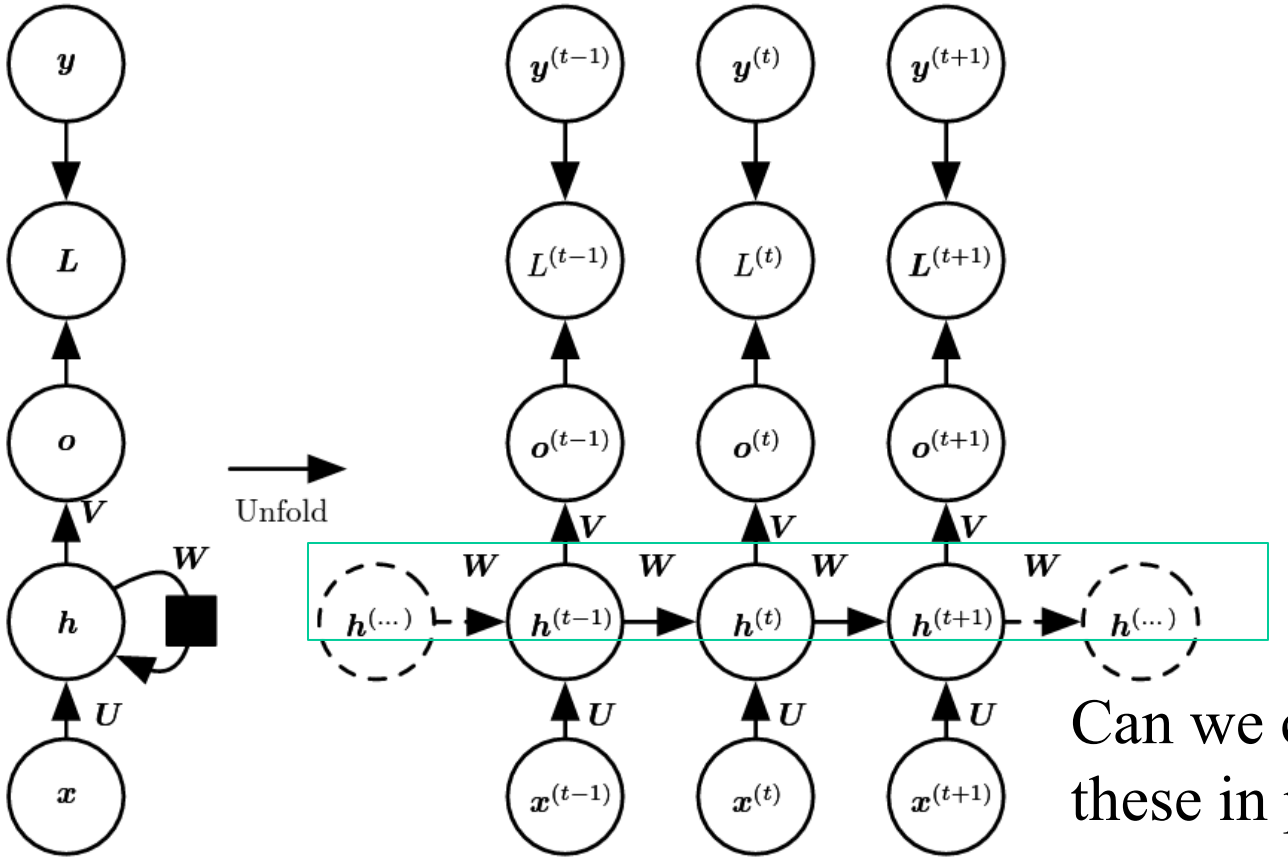
Case 1 example

one output/input, depends on previous inputs



Case 1 example

one output/input, depends on previous inputs

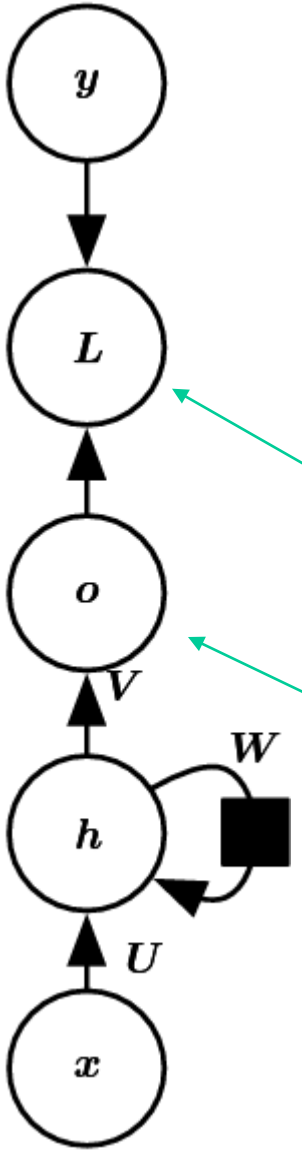


Can we compute these in parallel?

	GEFORCE RTX 3090	GEFORCE RTX 3080	GEFORCE RTX 3070
NVIDIA CUDA Cores	10496	8704	5888

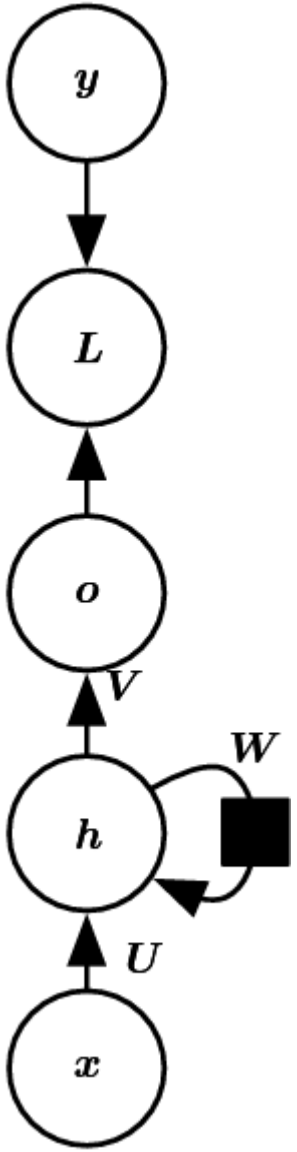
Case 1 example contd.

discrete (e.g. categorical) outputs



Loss(y,o) – Needed for training

output, e.g. unnormalized
log P(category|history)
For classification, can add a softmax layer for normalized probabilities, unnecessary for training



Case 1 example contd.

Forward propagation

Initialize state $h^{(0)}$

For each time t

$$\alpha^{(t)} = b + Wh^{(t-1)} + Ux^{(t)}$$

$$h^{(t)} = \tanh\left(\alpha^{(t)}\right)$$

$$o^{(t)} = c + Vh^{(t)}$$

$$\hat{y}^{(t)} = \text{softmax}(o^{(t)})$$ (postprocessing step)

Common RNN activation functions: sigmoid, tanh, & ReLU (be careful with ReLU - unbounded)

Loss of a sequence

- Sequence loss is sum of losses

$$L(\{x^{(1)}, x^{(2)}, \ldots, x^{(\tau)}\}, \{y^{(1)}, y^{(2)}, \ldots, y^{(\tau)}\}) = \sum_t L^{(t)}$$

- Suppose we use a negative log likelihood loss (e.g. MLE approach), this becomes

$$\sum_t L^{(t)} = -\sum_t \log P_{model}(y^{(t)} \mid x^{(1)}, x^{(2)}, \ldots, x^{(t)})$$

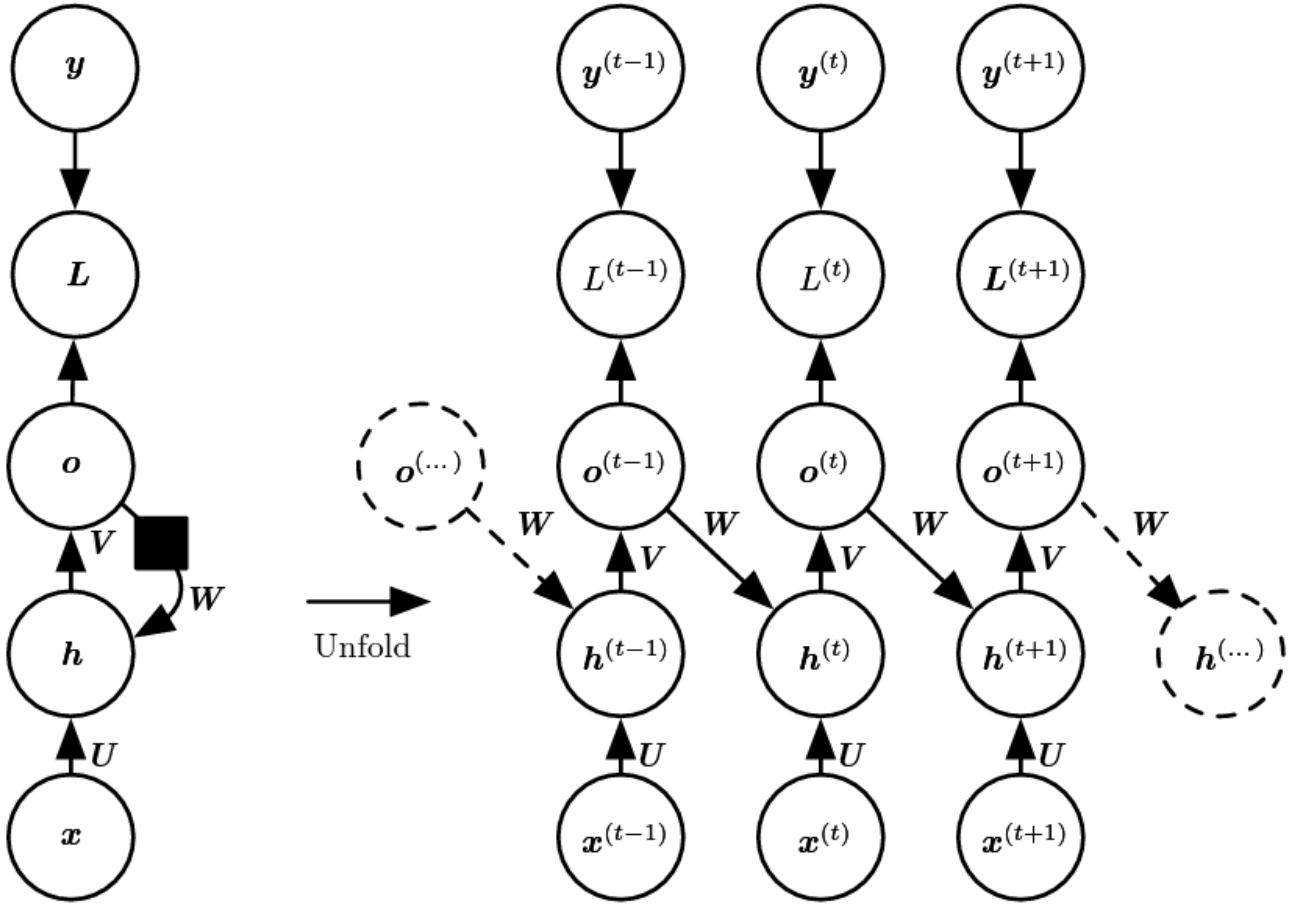
Gradient of sequence

(overview)

- Forward pass – Compute gradient of each step
- Backward pass – Use stored states and gradients to *back-propagate through time*
- Expensive in time and space

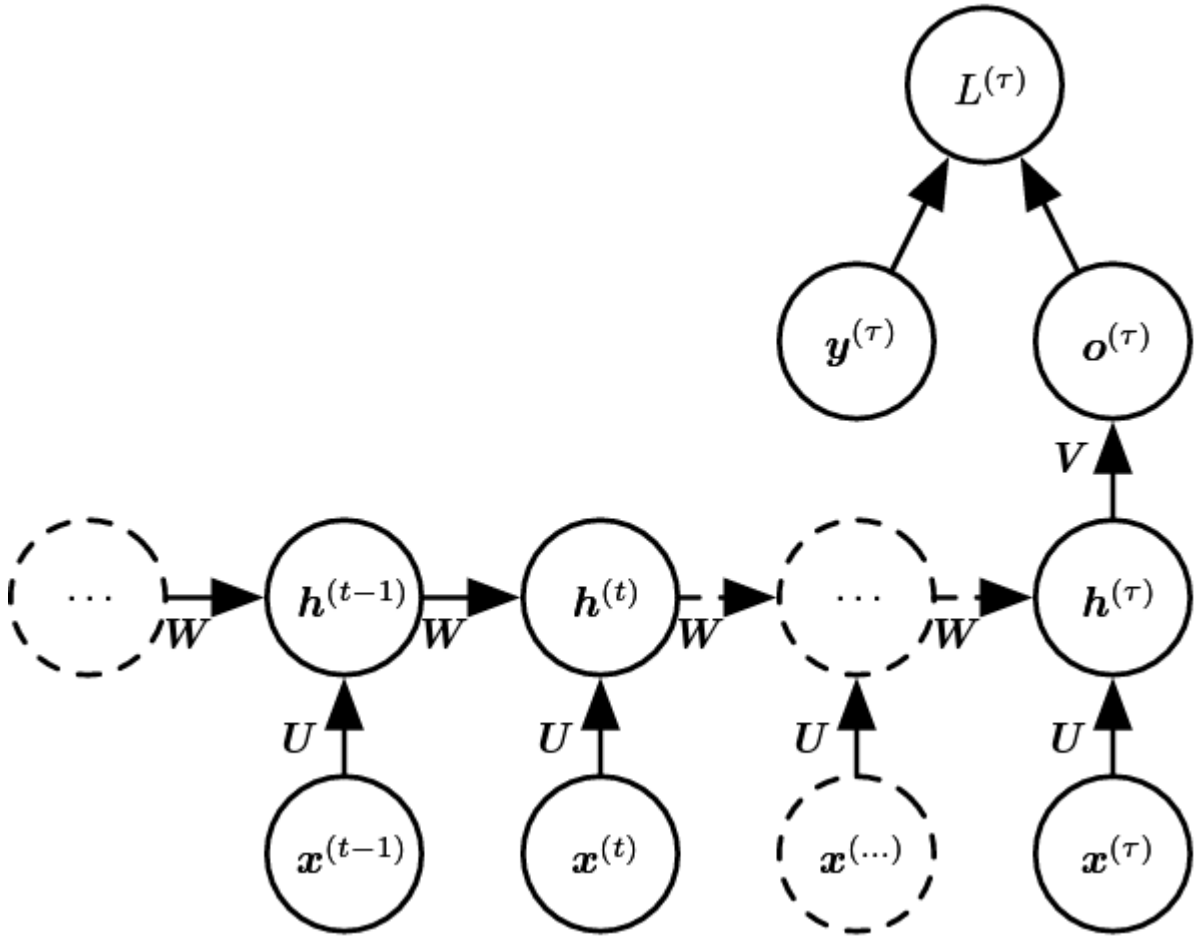
Case 2

output depends on previous output



Goodfellow et al. Fig. 10.4

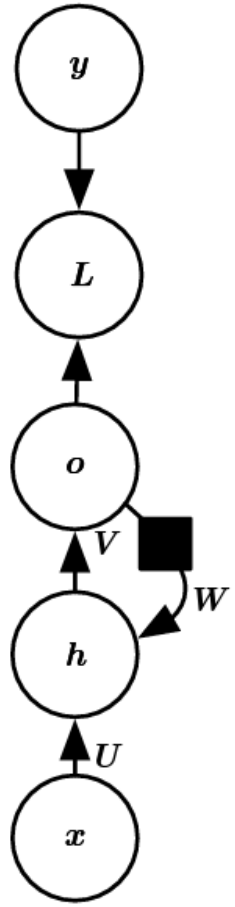
Case 3
labeling a sequence



Goodfellow et al. Fig. 10.5

More on output recurrences

- Dependence solely on output is not Turing complete
- Loss function minimizes difference between target and output; nothing will drive it to capture information about network state



Output recurrences: Teacher forcing

When training for output recurrences, we could use a MLE approach to find the model which maximizes:

$$\log P\left(y^{(1)}, y^{(2)} | x^{(1)}, x^{(2)}\right)$$

but we know first output should be: $y^{(1)}$

$$\log P\left(y^{(2)} | y^{(1)}, x^{(1)}, x^{(2)}\right) + \log P\left(y^{(1)} | x^{(1)}, x^{(2)}\right)$$

Teacher forcing

If we use the previous label instead of the previous prediction

$$\log P(y^{(1)}, y^{(2)} \mid x^{(1)}, x^{(2)})$$

we can parallelize the backpropagation as we don't need to compute the previous dependency.

Teacher forcing

We can rewrite the MLE target (Bayes rule):

$$\log P\left(y^{(1)}, y^{(2)} | x^{(1)}, x^{(2)}\right)$$

$$= \log\left(P(y^{(2)} | y^{(1)}, x^{(1)}, x^{(2)}) P(y^{(1)} | x^{(1)}, x^{(2)})\right)$$

$$= \log\left(P(y^{(2)} | y^{(1)}, x^{(2)}) P(y^{(1)} | x^{(1)})\right)$$

$y^{(t)}$ independent of $x^{(\tau)}$ where $t \neq \tau$

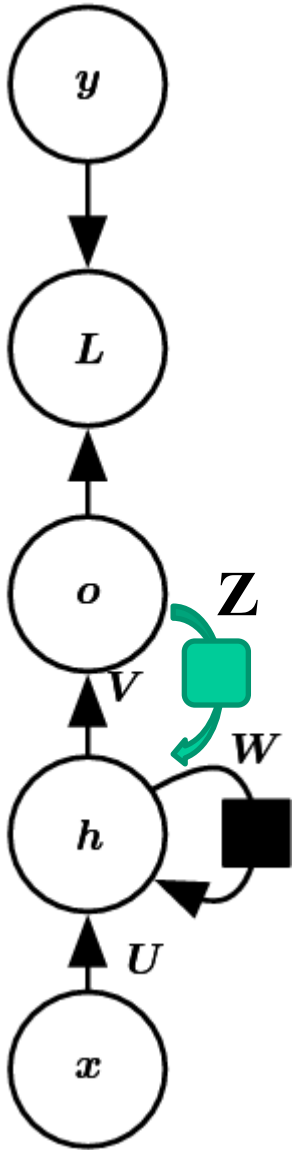
since there are no hidden recurrences

$$= \log P\left(y^{(2)} | y^{(1)}, x^{(2)}\right) + \log P\left(y^{(1)} | x^{(1)}\right)$$

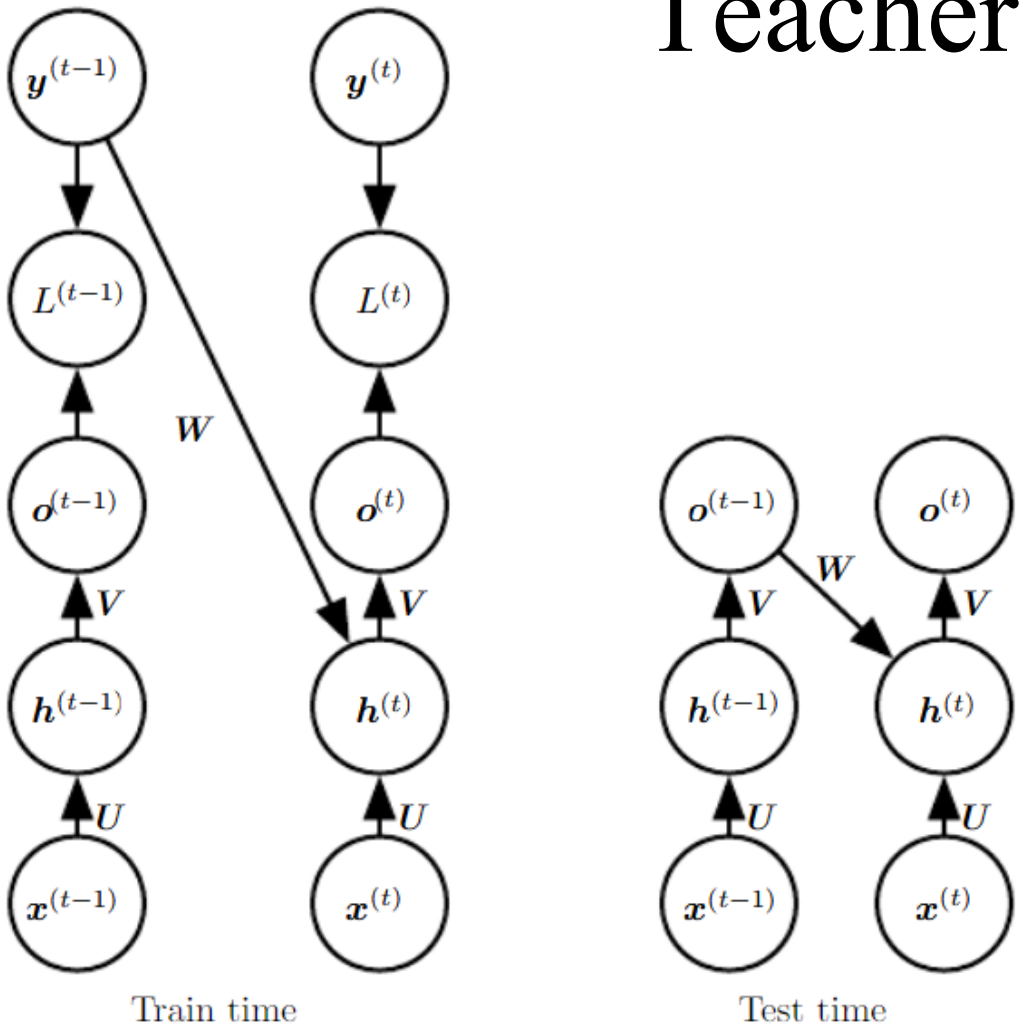
Teacher forcing

Teacher forcing can be used in networks with output and hidden layer recurrences, but…

we can no longer parallelize training and must use back-propagation through time



Teacher forcing



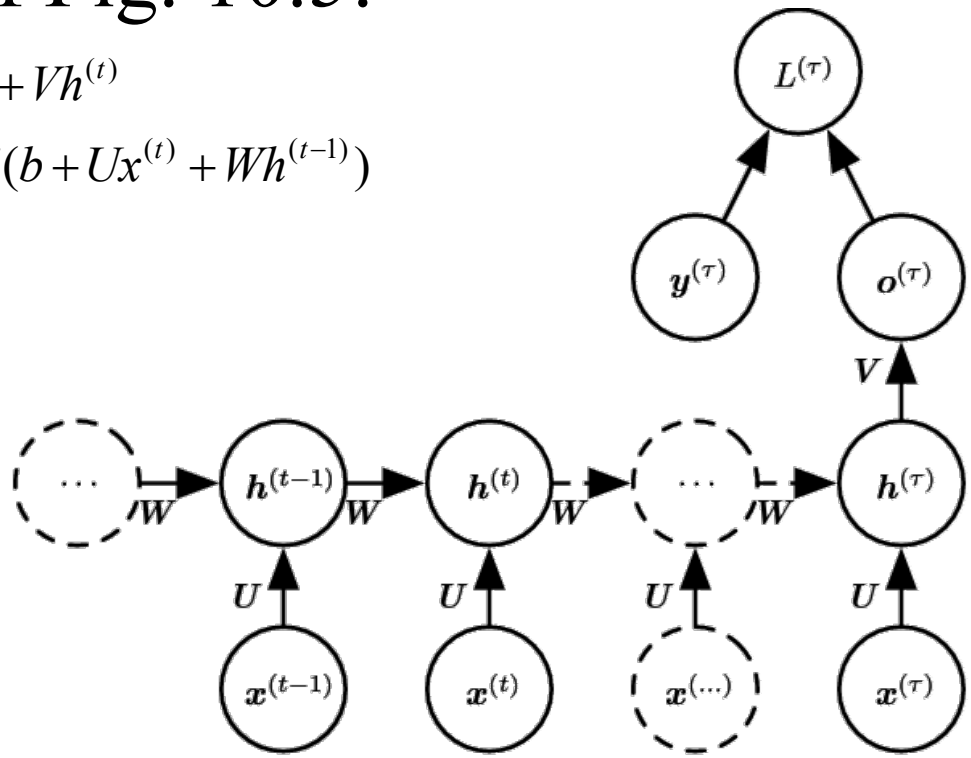
At test time, we do not Know $y^{(t-1)}$

Goodfellow et al. Fig 10.6

RNN gradient computation

- Assume loss at time t: $\partial L / \partial L^{(t)} = 1$
- Consider network of Fig. 10.5:

$$o^{(t)} = c + Vh^{(t)}$$
$$h^{(t)} = f(b + Ux^{(t)} + Wh^{(t-1)})$$



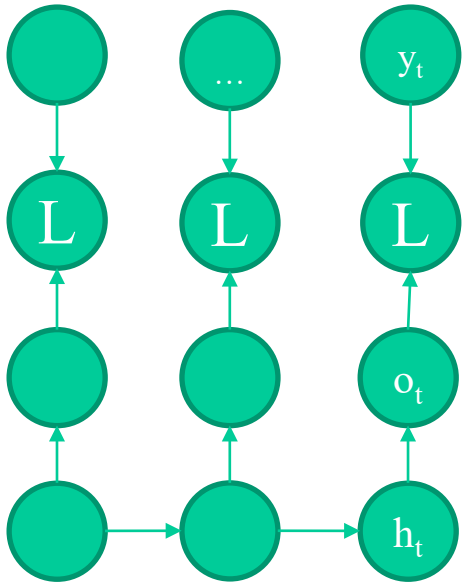
RNN gradient computation

- Assume output layer o feeds softmax layer $\hat{y}$
- In this example, we use negative log likelihood on each output $o_t(i)$ rather than cross entropy:

$$J(\theta) = -E_{x,y\sim\hat{p}_{data}} \log p_{model}(y|x)$$

$$= \frac{1}{2}\|y - \hat{y}\|^2 \text{ (eqns 6.12, 6.13)}$$

- We ignore the softmax layer in this discussion as it just produces probabilities and is not trainable.



RNN gradient computation

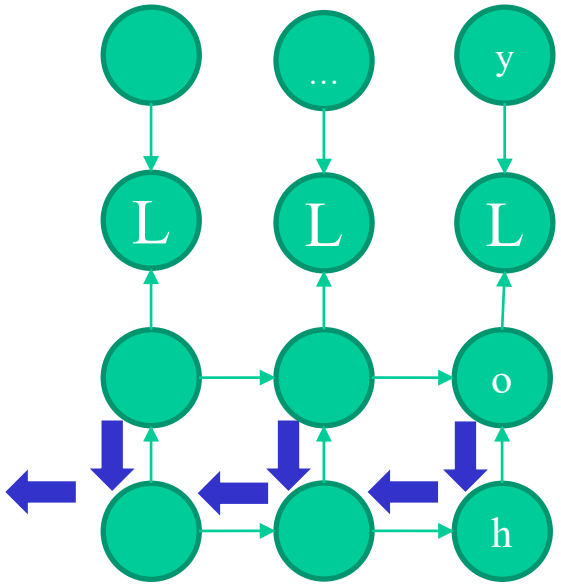
- Final loss: $\frac{\partial L}{\partial L^{(\tau)}} \triangleq 1$

- Consider arbitrary output time:

  Loss at h comes from two paths

  – Next h

  – Current output



RNN output layer gradient

- Outputs: only dependent on loss (if no output dependencies)

$$\left(\nabla_{o^{(t)}} L\right)_i = \frac{\partial L}{\partial L^{(t)}} \frac{\partial L^{(t)}}{\partial o_i^{(t)}} = 1 \frac{\partial L}{o_i^{(t)}}$$

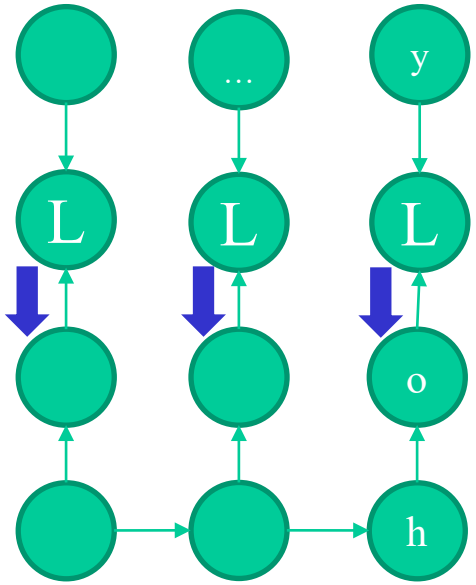
$$\frac{\partial L}{o_i^{(t)}} = \frac{\partial}{o_i^{(t)}} \frac{1}{2} \|y_i - \hat{y}_i\|^2$$

$$= \frac{\partial}{o_i^{(t)}} \frac{1}{2} \sqrt{(y_i - \hat{y}_i)^2}^2$$

$$= \frac{\partial}{o_i^{(t)}} \frac{1}{2} (y_i - \hat{y}_i)^2$$

$$= (y_i - \hat{y}_i)(-1)$$

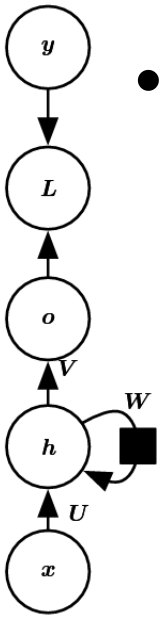
$$= \hat{y}_i^{(t)} - 1_{i,y^{(t)}} \text{ as } y_i \text{ is } 0/1$$



All y's are time dependent, notation dropped

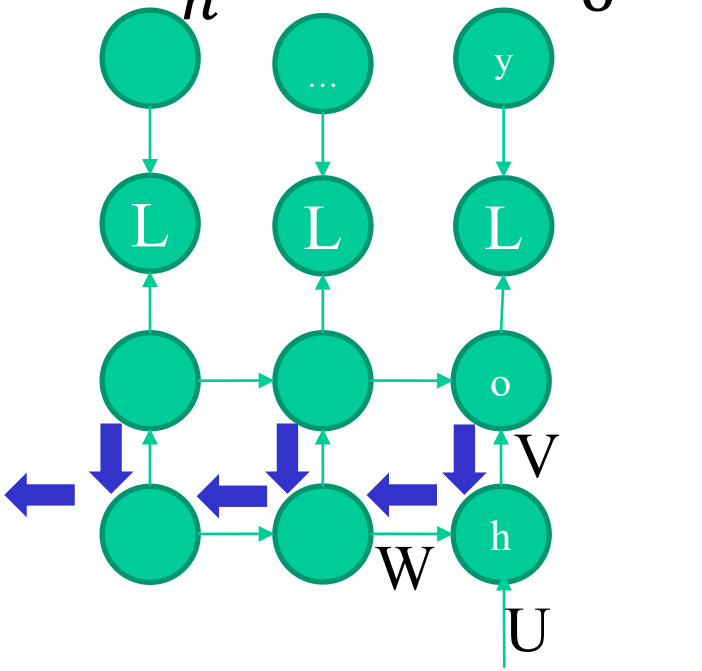
RNN hidden layer gradients

- Last step time τ: Only successor is loss: $\nabla_h^{(\tau)} L = V^T \nabla_{o^\tau} \mathrm{L}$
- Other times t: Loss at current step + loss from next h



$$\nabla_{h^{(t)}} L = \left(\frac{\partial h^{(t+1)}}{\partial h^{(t)}}\right)^T \nabla_{h^{(t+1)}} L + \left(\frac{\partial o^{(t)}}{\partial h^{(t)}}\right)^T \nabla_{o^{(t)}} L$$

Further simplification depends on activation function derivative (see text for an example)



Parameter updates

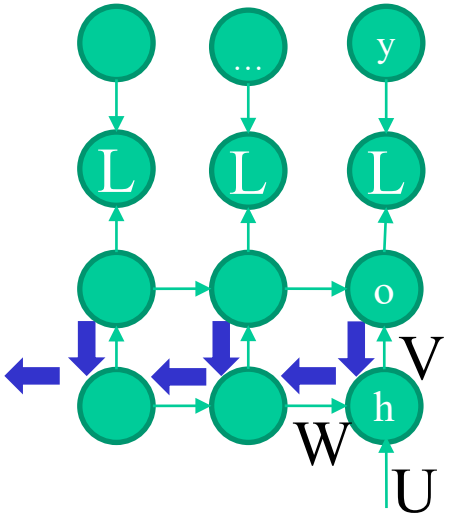
We need to learn how the loss should be applied to each of the parameters.

General idea:

- Create copies of parameters at each time step (avoids introducing dependencies)
- Statistic of gradient over time

Example:

$$\nabla_W L = \sum_t \sum_i \left(\frac{\partial L}{\partial h_i^{(t)}} \right) \nabla_{W^{(t)}} h_i^{(t)}$$



oh, oh…
rabbit hole

British Postal Service,
Graham Baker-Smith 2015

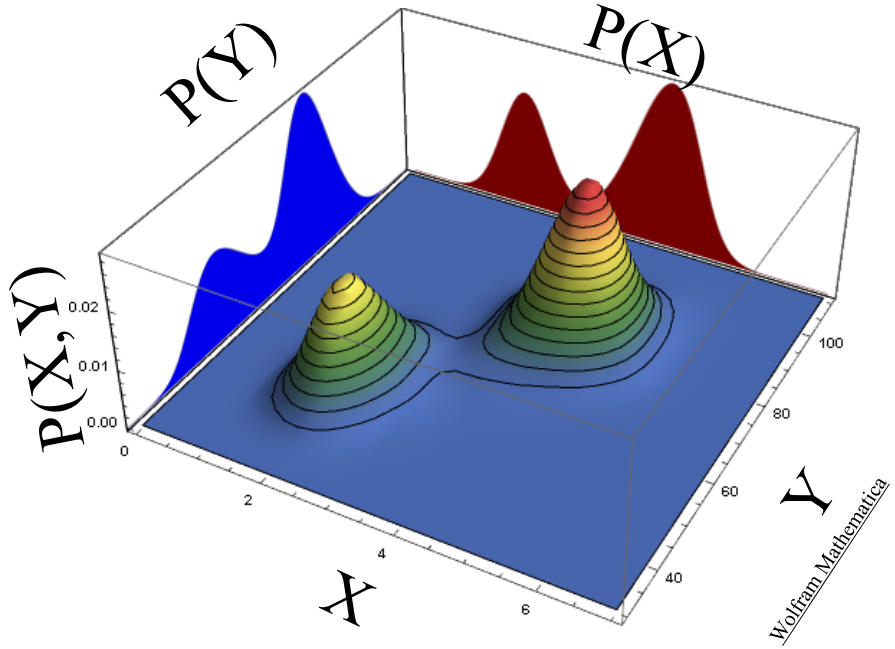
Marginal distributions

Integrate/sums over elements of a joint distribution to find P of desired random variable

$$X, Y \sim P(X, Y)$$

$$P(X = x) = \int_y P\,(x, y)dy$$

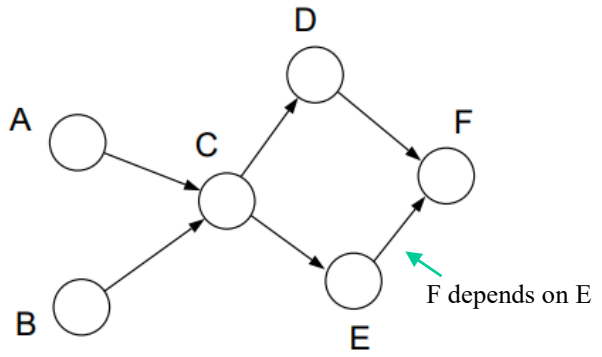
$$P(Y = y) = \int_x P\,(x, y)dx$$



Graphical models

- Networks of nodes can be used for inference/belief, frequently on latent (unobservable) variables
- Weights inform relationships between nodes
- Allows us to think about probabilities by marginalizing what we don't know

$$P(F \mid A,B) = \frac{\sum_{C}\sum_{D}\sum_{E} P(A,B,C,D,E,F)}{\sum_{C}\sum_{D}\sum_{E}\sum_{F} P(A,B,C,D,E,F)}$$



Jordan 1997 doi:10.1.1.116.7467

RNNs as directed graphical models

- Simple case: RNN of a sequence where only recursion is previous output and there are *no inputs*
- With a negative log likelihood loss,

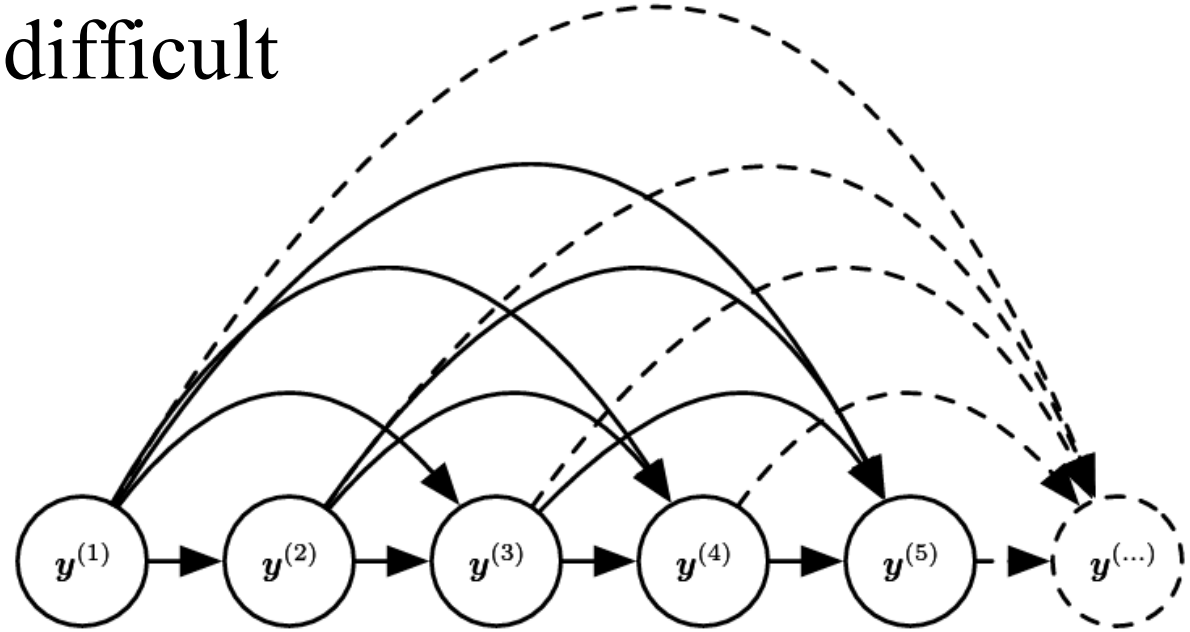
$$P(y^{(1)}, \ldots, y^{(\tau)}) = \prod_{t=1}^{\tau} P(y^{(t)} | y^{(t-1)}, \ldots, y^{(2)}, y^{(1)}) \quad \text{by chain rule of P}$$

$$L = \sum_{t} L^{(t)}$$

$$L^{(t)} = -logP(\hat{y}^{(t)} = y^{(t)} | y^{(t-1)}, y^{(t-2)}, \ldots, y^{(1)})$$

RNNs
as directed graphical models

- Graphical models with a long dependency require many edges
- These become difficult to estimate



Goodfellow et al. Fig. 10.7

RNNs
as directed graphical models

Ways to deal with large # of parameters

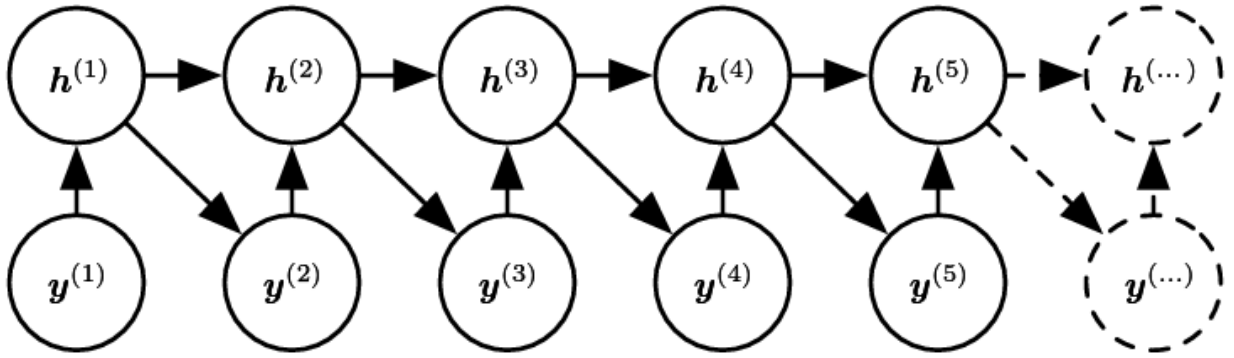
- Remove weak dependencies
- Assume a Markov property, values more than τ time steps in the past no longer matter, e.g. $\tau = 2$:

$$P(y^{(t)}|y^{(t-1)}, \ldots, y^{(2)}, y^{(1)})$$

$$= P(y^{(t)}|y^{(t-1)}, y^{(t-2)})$$

RNNs
as directed graphical models

- Introduce a state variable that captures the dependency



Goodfellow et al. Fig. 10.8

- Assumption: Relationship stationary, does not change over time

RNNs
as directed graphical models

Use as a sequence generator introduces a new problem: How to stop…

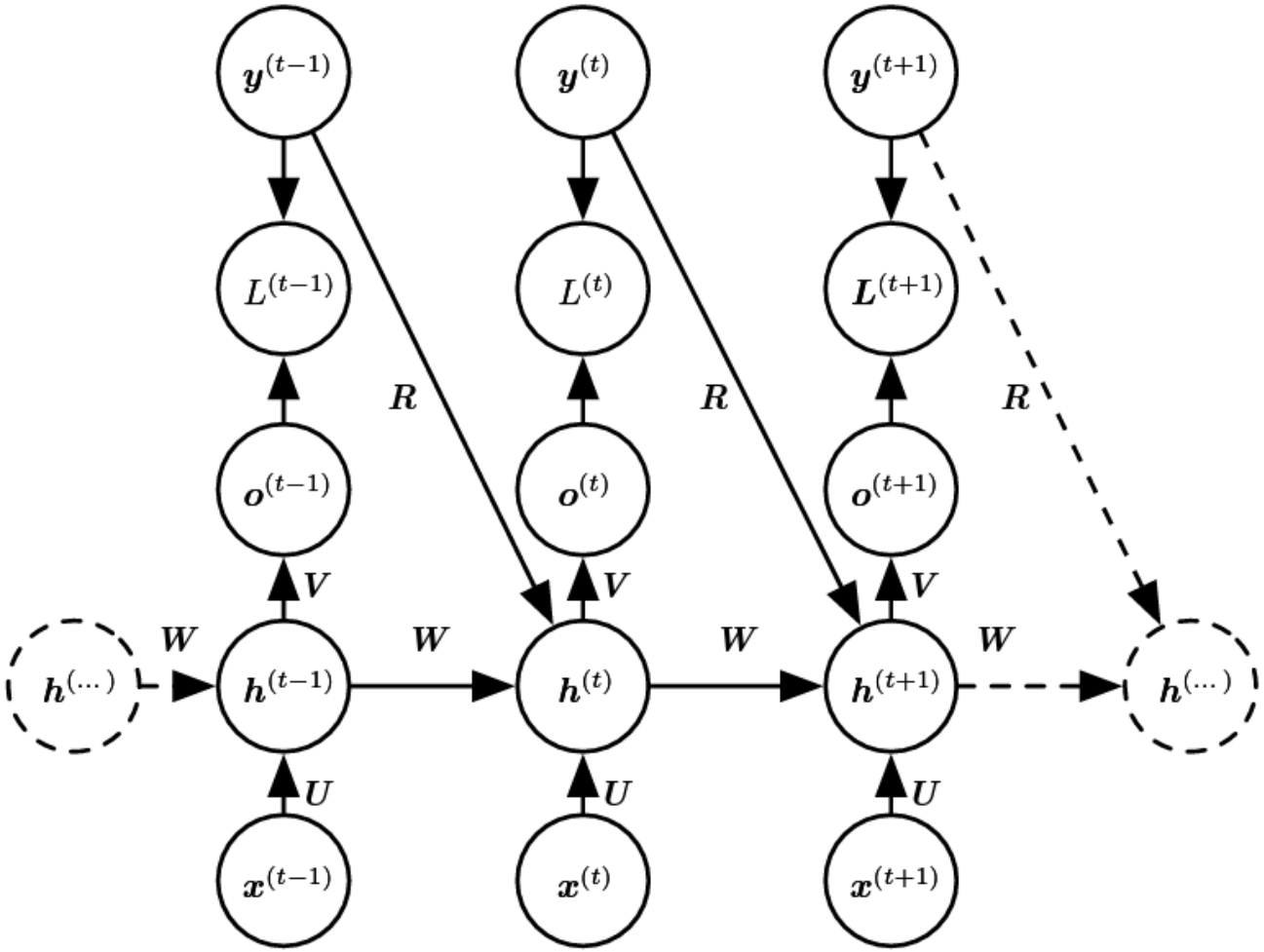
- Can introduce a stop symbol, or
- Train a node to predict end of sequence
- Train a node to predict sequence length

Sequences conditioned on context

- RNNs can serve as graphical models that depend on input & output history
- When the input sequence is of fixed size (usually not the case for speech) can provide
  - sequence as input to initial state
  - sequence as input at each time step

Input and output context example

(Fig. 10.10 Goodfellow et al.)



Bidirectional RNNs

- Sometimes, observing features in the future helps us know what occurred in the past…

$$P(x^{(2)} = e \mid x^{(1)} = b)$$

vs.

$$P(x^{(2)} = e \mid x^{(1)} = b, x^{(3)} = d)$$

- Very useful for speech recognition where coarticulation & phonotactics can play a large role

Bidirectional RNNs

- Compute two RNNs, one moving forward, the other backwards

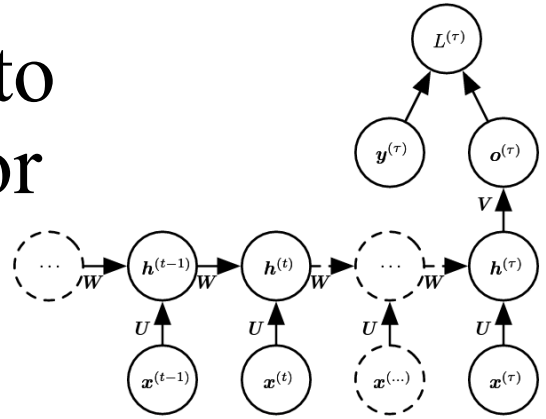
- Avoids need for fixed length window required for feed-forward nets or RNNs with a look-ahead buffer

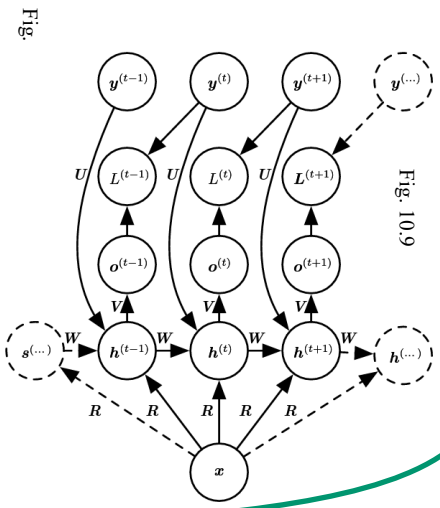
Bidirectional RNN Example

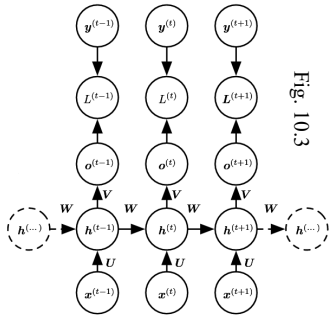
Fig. 10.11 Goodfellow et al.

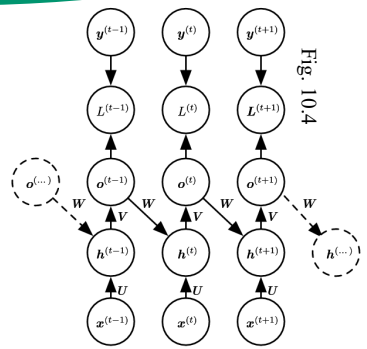
Recap so far

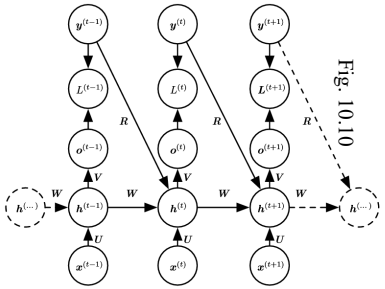
- Map sequence to fixed size vector
- Fixed vector to sequence
- N inputs to N outputs

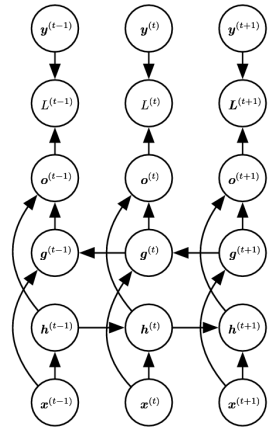








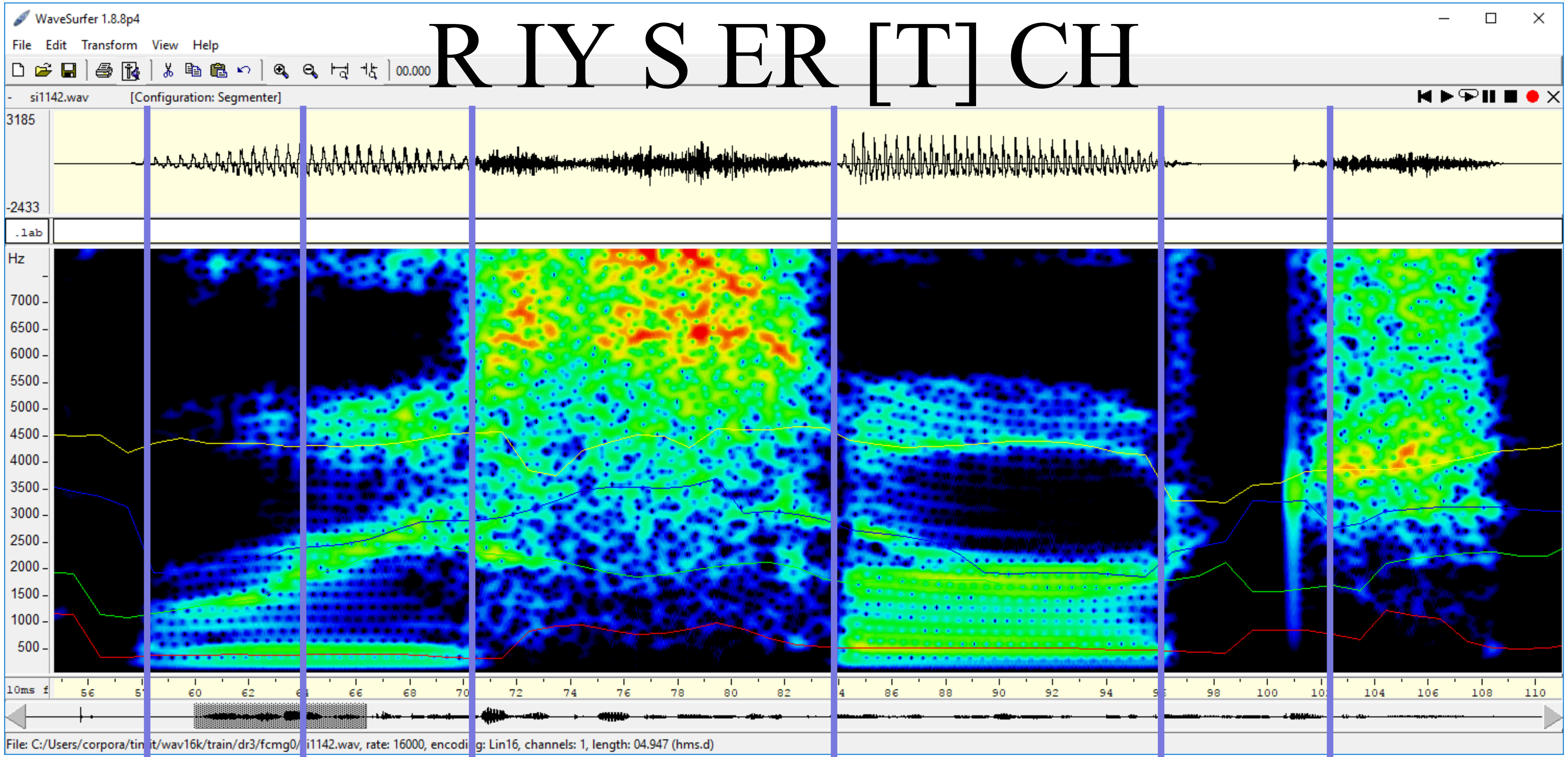




Networks from Goodfellow et al.

What about this?

R IY S ER [T] CH



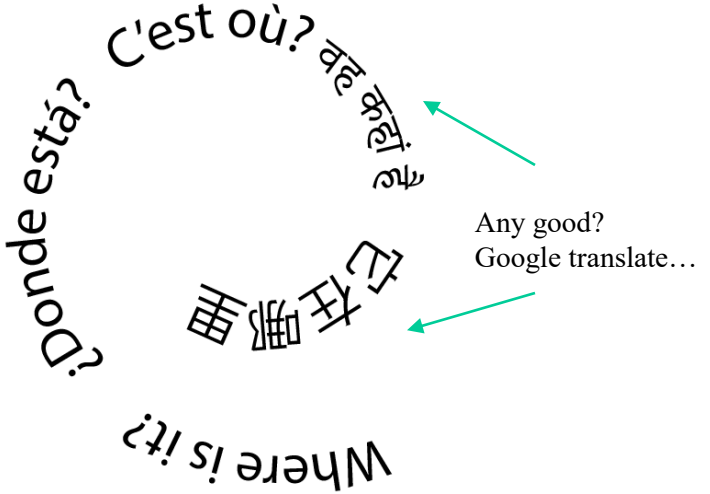
possible goals	R R R R R R	IY IY IY IY IY IY	S S S S S S S S S S S S S S S S S S	ER ER ER ER ER ER ER ER ER	T T T T T T T T	CH CH CH CH CH

10 ms advance

M to N sequences

Many applications require sequences of length M to be mapped to sequences of length N. e.g.

- speech recognition
- language translation



- query handling
  How can I get to Logan Heights?

M to N sequences

- Neural nets that handle this are known as *sequence to sequence*, or *encoder-decoder* architectures

- Basic idea:
  - Encoder RNN outputs a state or sequence representing the *concept*
  - Decoder RNN maps the concept onto another sequence

M to N sequences

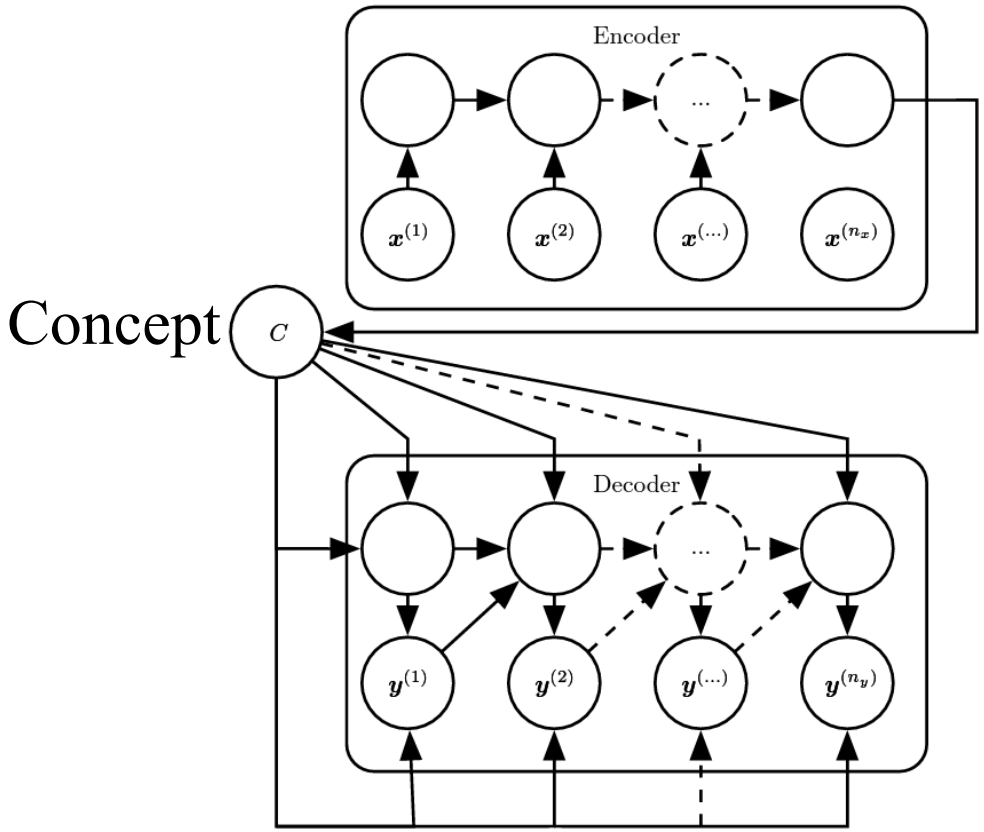


Fig. 10.12 Goodfellow et al.

Concept is typically final state or vector

Can use fixed vector to sequence architecture to generate new sequence

Deep recurrent networks

What happens when the recursions pass through multiple layers?

Layer n (could be multiple layers) serves the role of building a representation to feed into the hidden state layer h

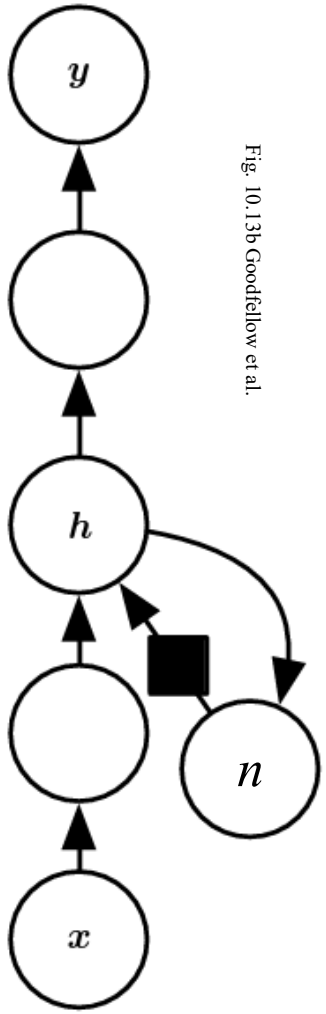


Fig. 10.13b Goodfellow et al.

Deep recurrent networks

- If layer n is deep, this creates a long path between h and the information that loops back through it
- Long paths make learning difficult

  (more on this next)
- Can introduce a delay loop to assist

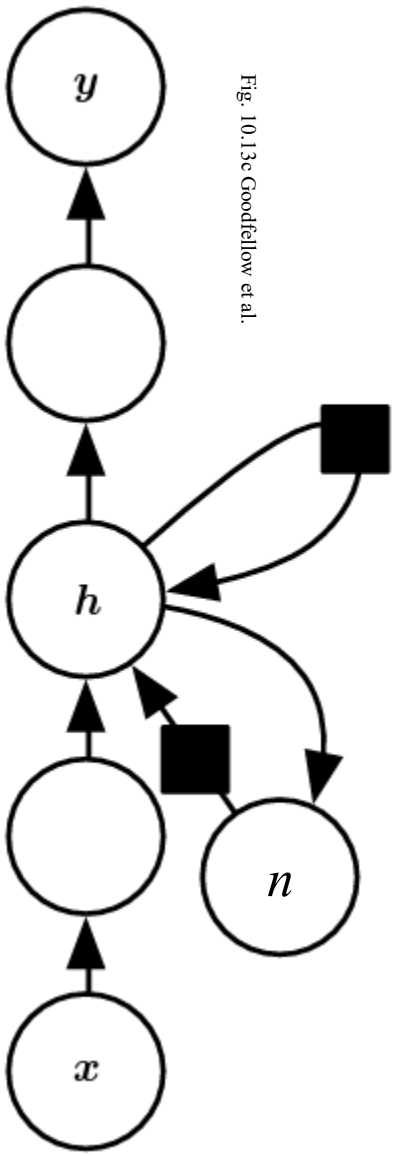


Fig. 10.13c Goodfellow et al.

Long-term dependencies

- Recurrence involves computing the same function over and over
- Let us simplify to think about implications
  - Use identity function as activation function
  - Recurrence becomes $h^{(t)} = W^T h^{(t-1)}$
  - Unwinding the recursion $h^{(t)} = (W^t)^T h^{(0)}$

Long-term dependencies

- Suppose W has an eigenvalue decomposition (2.7)
$$W = Q\Lambda Q^T$$
  - Q is a matrix of eigenvectors, $QQ^T = I$
  - Λ is a diagonal matrix of eigenvalues

Long-term dependencies

$$\mathrm{h} = (W^t)^T h^{(0)}$$

t is number of time steps

$$= (Q^T \Lambda Q)^t h^{(0)} \text{ as } W^T = (Q\Lambda \mathrm{Q}^T)^T = Q^T \Lambda Q$$

$$= Q^T \Lambda^t Q h^{(0)} \text{ as } Q^T \Lambda Q Q^T \Lambda Q = Q^T \Lambda \mathrm{I} \Lambda Q = Q^T \Lambda \Lambda \mathrm{Q}$$

What happens if eigen values are

- small?
- large?

Long-term dependencies

- In a non-recurrent net, weights will vary, but in RNNs the same weights are used over and over again.

- Techniques must be applied to be keep gradients from vanishing or exploding
(see references in Goodfellow et al 10.7 for further details)

Long-term dependence strategies

Skip connections

- Create networks with longer delays
- Reduces number of times weight is applied
- Delay of d reduces gradient vanishing by factor of $^1/_d$ (in our simplified example: $Q\Lambda^{t}/_{d}Q^T h^{(0)}$)
- Problems if what was skipped was important

Long-term dependence strategies

- Gated RNNs
  - Long-term dependence problem due to using the same weights at each step
  - What if the weights were dynamic?
  - Dynamic weights allow us to respond to input

Long short-term memory (LSTM)

- Popular gated architecture
- Weights are conditioned on context
- Can be interpreted as an attention mechanism

LSTM

LSTM adds one or more gates to control input and output as well as reset the state

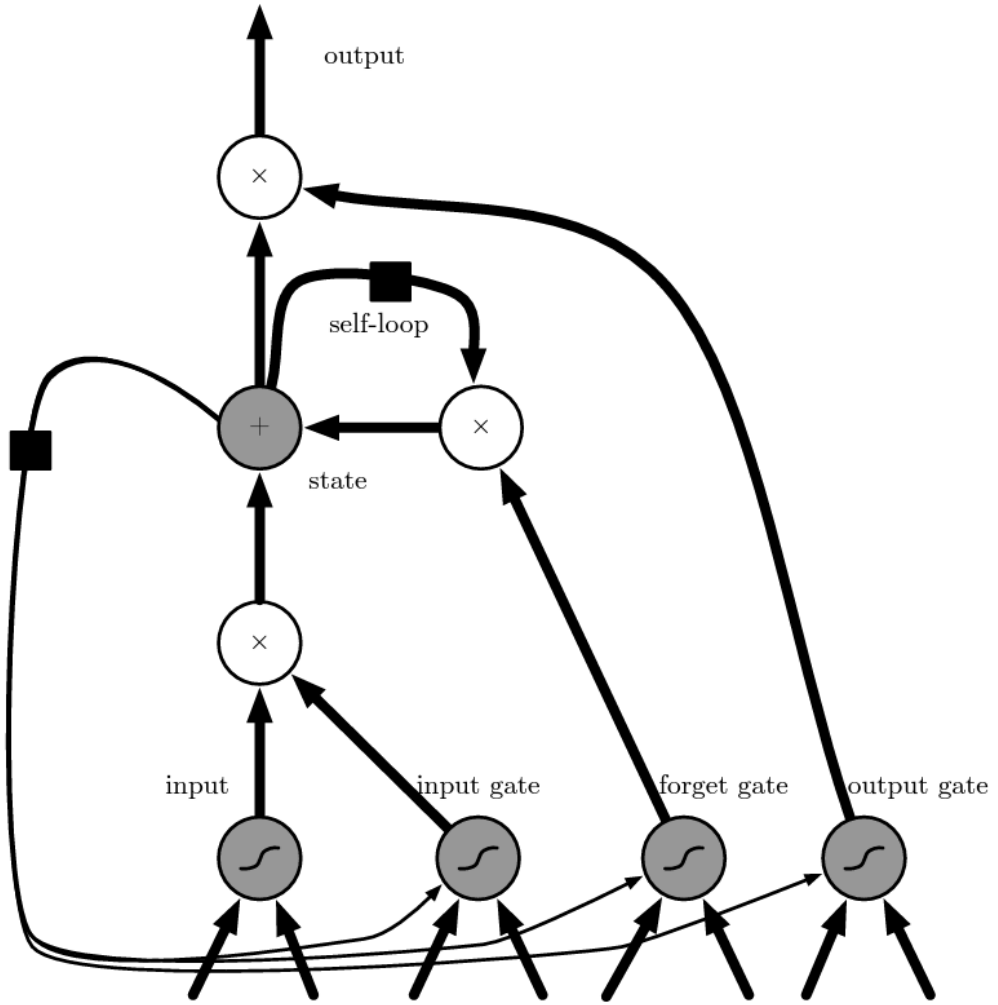


Fig. 10.16 Goodfellow et al.

LSTM forward propagation

forget gate

$$f_i^{(t)} = \sigma\left(b_i^f + \sum_j U_{i,j}^f x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right)$$

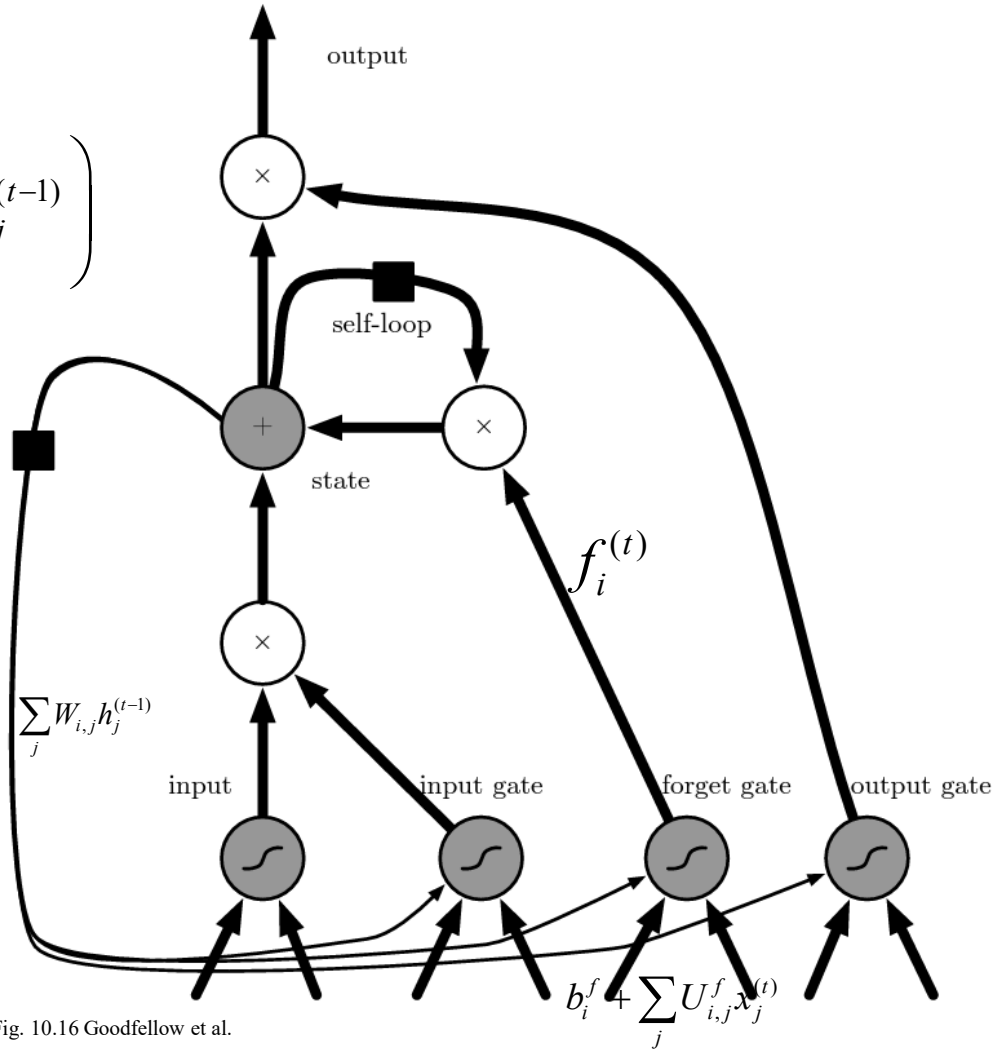


Fig. 10.16 Goodfellow et al.

LSTM forward propagation

external input gate

$$g_i^{(t)} = \sigma\left(b_i^o + \sum_j U_{i,j}^o x_j^{(t)} + \sum_j W_{i,j}^{(o)} h_j^{(t-1)} \right)$$

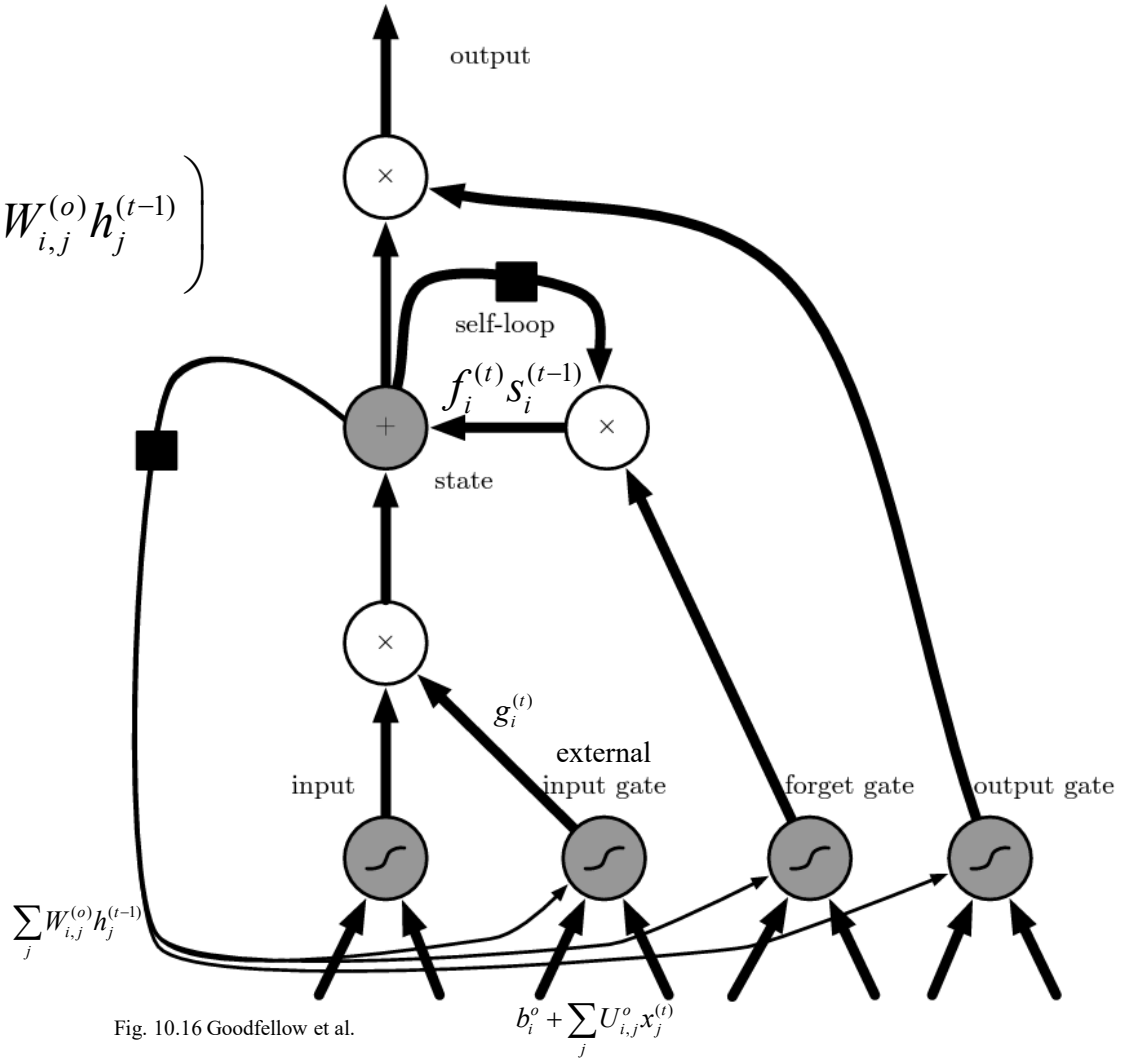


Fig. 10.16 Goodfellow et al.

LSTM forward propagation

state update

$$s_i^{(t)} = f_i^{(t)} s_i^{(t-1)} + g_i^{(t)} \sigma\left(b_i + \sum_j U_{i,j} x_j^{(t)} + \sum_j W_{i,j} h_j^{(t-1)} \right)$$

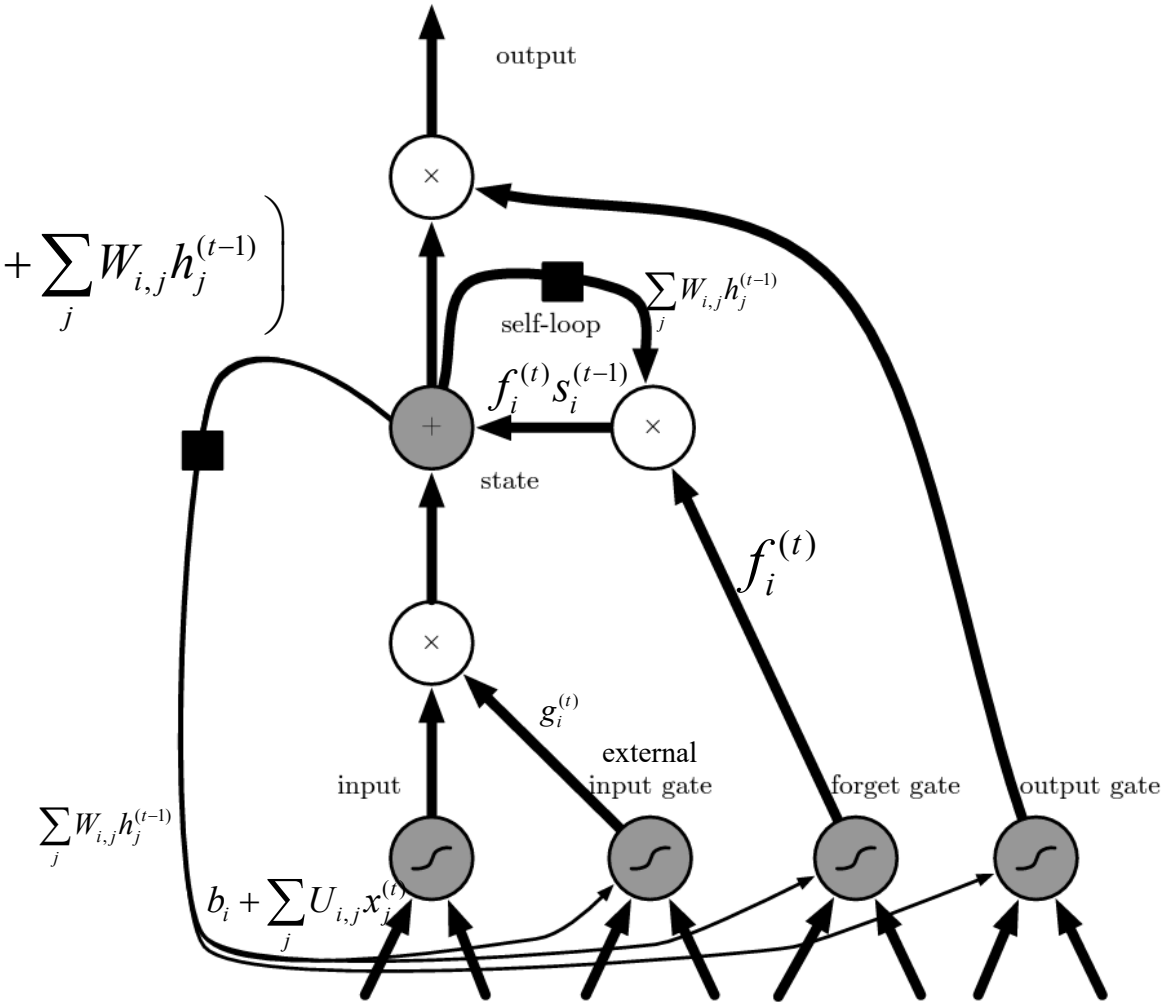


Fig. 10.16 Goodfellow et al.

LSTM forward propagation

output

$$h_i^{(t)} = \tanh(s_i^{(t)}) q_i^{(t)}$$

$$q_i^{(t)} = \sigma\left(b_i^o + \sum_j U_{i,j}^o x_j^{(t)} + \sum_j W_{i,j}^o h_j^{(t-1)} \right)$$

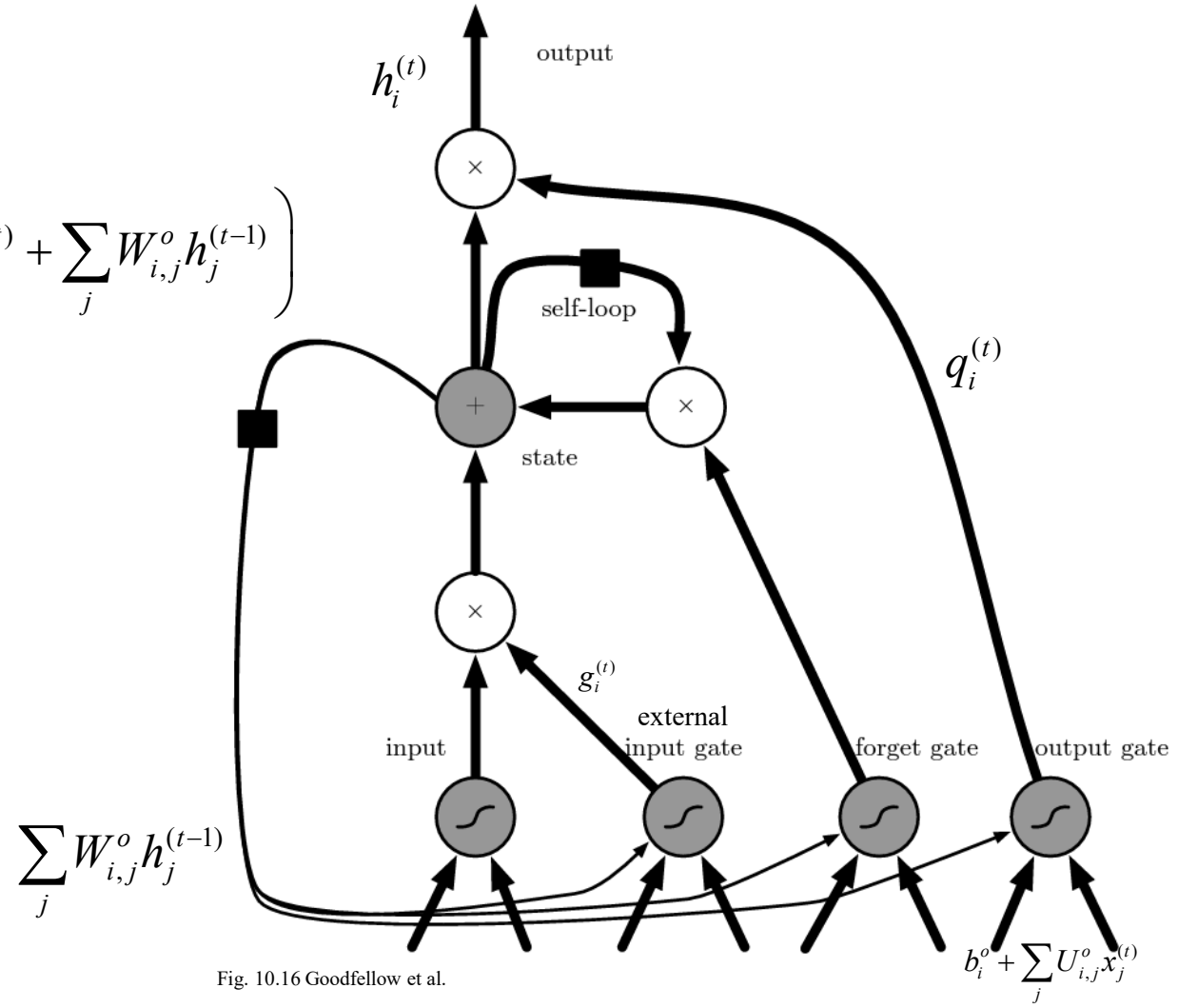


Fig. 10.16 Goodfellow et al.