RNN Variants

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

CS540 Introduction to Artificial Intelligence Lecture 12

Young Wu Based on lecture slides by Jerry Zhu, Yingyu Liang, and Charles Dyer

July 5, 2021

 Recurrent Neural Network

RNN Variants

Midterm Reivew Session

- June 29 Dan will go through selected Homework questions and Past Exam questions, not recorded, notes will be posted.
- Dandi will go through the same questions this Thursday and Friday (June 18 and 19)12 : 30 to 1 : 45 for section 1, you can use the guest link to attend too.

RNN Variants

Special Bayesian Network for Sequences Motivation

- A sequence of features $X_1, X_2, ...$ can be modeled by a Markov Chain but they are not observable.
- A sequence of labels $Y_1, Y_2, ...$ depends only on the current hidden features and they are observable.
- This type of Bayesian Network is called a Hidden Markov Model.

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ● ●

HMM Applications Part 1 Motivation

- Weather prediction.
- Hidden states: $X_1, X_2, ...$ are weather that is not observable by a person staying at home (sunny, cloudy, rainy).
- Observable states: $Y_1, Y_2, ...$ are Badger Herald newspaper reports of the condition (dry, dryish, damp, soggy).
- Speech recognition.
- Hidden states: $X_1, X_2, ...$ are words.
- Observable states: $Y_1, Y_2, ...$ are acoustic features.

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ● ●

HMM Applications Part 2 Motivation

- Stock or bond prediction.
- Hidden states: X₁, X₂, ... are information about the company (profitability, risk measures).
- Observable states: $Y_1, Y_2, ...$ are stock or bond prices.
- Speech synthesis: Chatbox.
- Hidden states: $X_1, X_2, ...$ are context or part of speech.
- Observable states: $Y_1, Y_2, ...$ are words.

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● ● ●

Other HMM Applications

- Machine translation.
- Handwriting recognition.
- Gene prediction.
- Traffic control.

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Hidden Markov Model Diagram

Motivation

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ □ のQで

Transition and Likelihood Matrices

- An initial distribution vector and two-state transition matrices are used to represent a hidden Markov model.
- **1** Initial state vector: π .

$$\pi_i = \mathbb{P} \{ X_1 = i \}, i \in 1, 2, ..., |X|$$

2 State transition matrix: A.

$$A_{ij} = \mathbb{P}\left\{X_t = j | X_{t-1} = i\right\}, i, j \in \{1, 2, ..., |X|$$

Observation Likelihood matrix (or output probability distribution): B.

$$B_{ij} = \mathbb{P}\left\{Y_t = i | X_t = j\right\}, i \in 1, 2, ..., |Y|, j \in 1, 2, ..., |X|$$

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● ● ●

Markov Property Motivation

 The Markov property implies the following conditionally independent property.

$$\mathbb{P} \{ x_t | x_{t-1}, x_{t-2}, ..., x_1 \} = \mathbb{P} \{ x_t | x_{t-1} \}$$
$$\mathbb{P} \{ y_t | x_t, x_{t-1}, ..., x_1 \} = \mathbb{P} \{ y_t | x_t \}$$

RNN Variants

Evaluation and Training Motivation

- There are three main tasks associated with an HMM.
- Evaluation problem: finding the probability of an observed sequence given an HMM: y₁, y₂, ...
- Oecoding problem: finding the most probable hidden sequence given the observed sequence: x₁, x₂, ...
- Searning problem: finding the most probable HMM given an observed sequence: π, A, B, ...

RNN Variants

Expectation-Maximization Algorithm

- Start with a random guess of π , A, B.
- Compute the forward probabilities: the joint probability of an observed sequence and its hidden state.
- Compute the backward probabilities: the probability of an observed sequence given its hidden state.
- Update the model π , A, B using Bayes rule.
- Repeat until convergence.
- Sometimes, it is called the Baum-Welch Algorithm.

RNN Variants

▲□▶▲□▶▲≡▶▲≡▶ ≡ めぬぐ

Evaluation Problem

• The task is to find the probability $\mathbb{P}\{y_1, y_2, ..., y_T | \pi, A, B\}$.

$$\mathbb{P} \{ y_1, y_2, ..., y_T | \pi, A, B \}$$

= $\sum_{x_1, x_2, ..., x_T} \mathbb{P} \{ y_1, y_2, ..., y_T | x_1, x_2, ..., x_T \} \mathbb{P} \{ x_1, x_2, ..., x_T \}$
= $\sum_{x_1, x_2, ..., x_T} \left(\prod_{t=1}^T B_{y_t x_t} \right) \left(\pi_{x_1} \prod_{t=2}^T A_{x_{t-1} x_t} \right)$

• This is also called the Forward Algorithm.

Recurrent Neural Network

RNN Variants

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Evaluation Problem Example, Part 1

- Fall 2018 Final Q28 and Q29
- Compute $\mathbb{P} \{ X_4 = Y, X_5 = Z | X_3 = X \}.$
- Compute $\mathbb{P} \{ X_1 = X, X_2 = Z | Y_1 = A, Y_2 = B \}.$

Recurrent Neural Network

RNN Variants

Evaluation Problem Example, Part 2

Definition



Recurrent Neural Network

RNN Variants

Evaluation Problem Example, Part 3

Definition



Recurrent Neural Network

RNN Variants

Evaluation Problem Example, Part 4

Definition



Recurrent Neural Network

RNN Variants

◆□▶ ◆□▶ ◆□▶ ◆□▶ □ ● ●

Decoding Problem

- The task is to find $x_1, x_2, ..., x_T$ that maximizes $\mathbb{P} \{x_1, x_2, ..., x_T | y_1, y_2, ..., y_T, \pi, A, B\}.$
- Direct computation is too expensive.
- Dynamic programming needs to be used to save computation.
- This is called the Viterbi Algorithm.

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三 のへぐ

Viterbi Algorithm Value Function

• Define the value functions to keep track of the maximum probabilities at each time *t* and for each state *k*.

$$V_{1,k} = \mathbb{P} \{ y_1 | X_1 = k \} \cdot \mathbb{P} \{ X_1 = k \}$$

= $B_{y_1k} \pi_k$
 $V_{t,k} = \max_x \mathbb{P} \{ y_t | X_t = k \} \mathbb{P} \{ X_t = k | X_{t-1} = x \} V_{t-1,k}$
= $\max_x B_{y_tk} A_{kx} V_{t-1,k}$

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ □ のQで

Viterbi Algorithm Policy Function

• Define the policy functions to keep track of the x_t that maximizes the value function.

policy
$$_{t,k} = \arg \max_{x} B_{y_tk} A_{kx} V_{t-1,k}$$

• Given the policy functions, the most probable hidden sequence can be found easily.

$$x_{T} = \arg \max_{x} V_{T,x}$$
$$x_{t} = \text{ policy }_{t+1,x_{t+1}}$$

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Dynamic Programming Diagram

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Viterbi Algorithm Diagram

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Expectation-Maximization Algorithm (for HMM), Part 1

• Initialize the hidden Markov model.

$$\pi \sim \mathsf{D} \left(\left| X \right| \right), A \sim \mathsf{D} \left(\left| X \right|, \left| X \right| \right), B \sim \mathsf{D} \left(\left| Y \right|, \left| X \right| \right)$$

• Perform the forward pass.

$$\alpha_{i,t} \text{ represents } \mathbb{P} \{ y_1, y_2, ..., y_t, X_t = i | \pi, A, B \}$$

$$\alpha_{i,1} = \pi_i B_{y_1,i}$$

$$\alpha_{i,t+1} = \sum_{j=1}^{|X|} \alpha_{j,t} A_{ji} B_{y_{t+1}i}$$

RNN Variants

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Expectation-Maximization Algorithm (for HMM), Part 2

• Perform the backward pass.

$$\beta_{i,t} \text{ represents } \mathbb{P} \{ y_{t+1}, y_{t+2}, ..., y_T | X_t = i, \pi, A, B \}$$

$$\beta_{i,T} = 1$$

$$\beta_{i,t} = \sum_{j=1}^{|X|} A_{ij} B_{y_{t+1}j} \beta_{j,t+1}$$

RNN Variants

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Expectation-Maximization Algorithm (for HMM), Part 3 Algorithm

• Define the conditional hidden state probabilities for each training sequence *n*.

$$\gamma_{n,i,t} = \text{ represents } \mathbb{P} \{ X_t = i | y_1, y_2, ..., y_T, \pi, A, B \}$$

$$\gamma_{n,i,t} = \frac{\alpha_{i,t} \beta_{i,t}}{\sum_{j=1}^{|X|} \alpha_{j,t} \beta_{j,t}}$$

RNN Variants

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Expectation-Maximization Algorithm (for HMM), Part 4 Algorithm

• Define the conditional hidden state probabilities for each training sequence *n*.

$$\begin{aligned} \xi_{n,i,j,t} \text{ represents } \mathbb{P} \left\{ X_t = i, X_{t+1} = j | y_1, y_2, ..., y_T, \pi, A, B \right\} \\ \xi_{n,i,j,t} &= \frac{\alpha_{i,t} A_{ij} \beta_{j,t+1} B_{y_{t+1}j}}{\sum_{k=1}^{|X|} \sum_{l=1}^{|X|} \alpha_{k,t} A_{kl} \beta_{l,t+1} B_{y_{t+1}w}} \end{aligned}$$

Recurrent Neural Network

RNN Variants

Expectation-Maximization Algorithm (for HMM), Part 5

• Update the model.

$$\pi'_{i} = \frac{\sum_{n=1}^{N} \gamma_{n,i,1}}{N} \\ A'_{ij} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T-1} \xi_{n,i,j,t}}{\sum_{n=1}^{N} \sum_{t=1}^{T-1} \gamma_{n,i,t}}$$

▲□ > ▲圖 > ▲目 > ▲目 > ▲目 > ● ④ < ⊙

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ □ のQで

Expectation-Maximization Algorithm (for HMM), Part 6

• Update the model, continued.

$$B_{ij}' = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{1}_{\{y_{n,t}=j\}}\gamma_{n,i,t}}{\sum_{n=1}^{N} \sum_{t=1}^{T} \gamma_{n,i,t}}$$

• Repeat until π, A, B converge.

 RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● ● ●

Dynamic System Motivation

- The hidden units are used as the hidden states.
- They are related by the same function over time.

. . .

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

 $h_{t+2} = f(h_{t+1}, w)$
 $h_{t+3} = f(h_{t+2}, w)$

RNN Variants

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Dynamic System with Input Motivation

- The input units can also drive the dynamics of the system.
- They are still related by the same function over time.

. . .

$$\begin{split} h_{t+1} &= f(h_t, x_{t+1}, w) \\ h_{t+2} &= f(h_{t+1}, x_{t+2}, w) \\ h_{t+3} &= f(h_{t+2}, x_{t+3}, w) \end{split}$$

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

Dynamic System with Output Motivation

• The output units only depend on the hidden states.

$$y_{t+1} = f(h_{t+1})$$

 $y_{t+2} = f(h_{t+2})$
 $y_{t+3} = f(h_{t+3})$

...

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Dynamic System Diagram

RNN Variants

▲□▶ ▲□▶ ▲ □▶ ▲ □▶ □ のへぐ

Recurrent Neural Network Structure Diagram

RNN Variants

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Activation Functions

• The hidden layer activation function can be the tanh activation, and the output layer activation function can be the softmax function.

$$\begin{aligned} z_t^{(x)} &= W^{(x)} x_t + W^{(h)} a_{t-1}^{(x)} + b^{(x)} \\ a_t^{(x)} &= g\left(z_t^{(x)}\right), g\left(\vdots\right) = \tanh\left(\vdots\right) \\ z_t^{(y)} &= W^{(y)} a^{(1,t)} + b^{(y)} \\ a_t^{(y)} &= g\left(z_t^{(y)}\right), g\left(\vdots\right) = \text{ softmax } (\vdots) \end{aligned}$$

Recurrent Neural Network

RNN Variants

Cost Functions

• Cross entropy loss is used with softmax activation as usual.

$$C_t = H\left(y_t, a_t^{(y)}\right)$$
$$C = \sum_t C_t$$

RNN Variants

Multiple Sequential Data Notations

- There could multiple sequences in the training set index by *i* = 1, 2, ..., *n*. For one training instance, at time *t*, there are *m* features.
- x_{ijt} is the feature j of instance i at time t (position t of the sequence).
- y_{ijt} is the output *j* of instance *i* at time *t* (position *t* of the sequence).

RNN Variants

・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・

Multiple Sequential Activations Notations

- $z_{ijt}^{(x)}$ denotes the linear part of instance *i* unit *j* at time *t* in the hidden layer.
- $a_{ijt}^{(x)}$ denotes the activation of instance *i* unit *j* at time *t* in the hidden layer.
- $z_{ijt}^{(y)}$ denotes the linear part of instance *i* output *j* at time *t* in the output layer.
- a^(y)_{ijt} denotes the activation of instance i output j at time t in the output layer

・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・
 ・

Multiple Sequential Weights Notations, Part 1 Definition

- There are weights and biases between the input layer and the hidden layer, between the hidden layer and the output layer, as in usual neural networks.
- w_{j'j}^(x), j' = 1, ..., m, j = 1, ..., m^(h) denotes the weight from input feature j' to hidden unit j.

•
$$b_i^{(x)}, j = 1, ..., m^{(h)}$$
 denotes the bias of hidden unit j.

- w^(y)_{jj'}, j = 1, ..., m^(h), j' = 1, ..., K denotes the weight from hidden unit j to output unit j'.
- $b_{j'}^{(y)}, j' = 1, ..., K$ denotes the bias of output unit j'.

RNN Variants

Multiple Sequential Weights Notations, Part 2 Definition

- There are also weights between units within the hidden layer through time.
- $w_{j'j}^{(h)}, j, j' = 1, ..., m^{(h)}$ denotes the weight from hidden unit j' at time t to hidden unit j at time t + 1.

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

BackPropogation Through Time Definition

 The gradient descent algorithm for recurrent neural networks is called BackPropogation Through Time (BPTT). The update procedure is the same as standard neural networks using the chain rule.

$$w = w - \alpha \frac{\partial C}{\partial w}$$
$$b = b - \alpha \frac{\partial C}{\partial b}$$

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Unfolded Network Diagram

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Backpropagation Diagram 1

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Backpropagation Diagram 2

Recurrent Neural Network

RNN Variants

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへぐ

Backpropagation, Part 1 Definition

• The cost derivative is the same as softmax neural networks.

$$\frac{\partial C}{\partial C_t} = 1$$
$$\frac{\partial C_t}{\partial z_{ijt}^{(y)}} = z_{ijt}^{(y)} - \mathbb{1}_{\{y_{it}=j\}}$$

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

Backpropagation, Part 2

• The other derivatives are similar to fully connected neural networks.

$$\begin{aligned} \frac{\partial z_{ij't}^{(y)}}{\partial a_{ijt}^{(x)}} &= w_{jj'}^{(y)} \\ \frac{\partial z_{ij't}^{(y)}}{\partial w_{jj'}^{(y)}} &= a_{ijt}^{(x)} \\ \frac{\partial z_{ij't}^{(y)}}{\partial b_{j'}^{(y)}} &= 1 \end{aligned}$$

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

Backpropagation, Part 3

• The other derivatives are similar to fully connected neural networks.

$$\frac{\partial a_{ijt}^{(x)}}{\partial z_{ijt}^{(x)}} = g'\left(z_{ijt}^{(x)}\right) = 1 - \left(a_{ijt}^{(x)}\right)^2$$
$$\frac{\partial z_{ijt}^{(x)}}{\partial w_{j'j}^{(x)}} = x_{ij't}$$
$$\frac{\partial z_{ijt}^{(x)}}{\partial b_j^{(x)}} = 1$$

RNN Variants

Backpropagation, Part 4

• The chain rule goes through time, so each gradient involves a long chain of the partial derivatives between $a_t^{(x)}$ and $a_{t-1}^{(x)}$ for t = 1, 2, ..., T.

$$\frac{\partial a_{ijt}^{(x)}}{\partial z_{ijt}^{(x)}} = 1 - \left(a_{ijt}^{(x)}\right)^2$$
$$\frac{\partial z_{ijt}^{(x)}}{\partial a_{ij't-1}^{(x)}} = w_{j'j}^{(h)}$$

RNN Variants

Vanishing and Exploding Gradient

- If the weights are small, the gradient through many layers will shrink exponentially. This is called the vanishing gradient problem.
- If the weights are large, the gradient through many layers will grow exponentially. This is called the exploding gradient problem.
- Fully connected and convolutional neural networks only have a few hidden layers, so vanishing and exploding gradient is not a problem in training those networks.
- In a recurrent neural network, if the sequences are long, the gradients can easily vanish or explode.

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

Long Term Memory Discussion

- It is also very hard to detect that the current output depends on an input from many time steps ago.
- Recurrent neural networks have difficulty dealing with long-range dependencies.

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ □ のQで

Long Short Term Memory Discussion

- Long Short Term Memory (LSTM) network adds more connected hidden units for memories controlled by gates. The activation functions used for these gates are usually logistic functions.
- An LSTM unit usually contains an input gate, an output gate, and a forget gate, to keep track of the dependencies in the input sequence.

Recurrent Neural Network

RNN Variants

Long Short Term Memory Diagram

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

Gated Recurrent Unit

- Gated Recurrent Unit (GRU) does something similar to an LSTM unit.
- A GRU contains input and forget gates, and does not contain an output gate.

Recurrent Neural Network

RNN Variants

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Gated Recurrent Unit Diagram

Discussion