CIS 4190/5190: Applied Machine Learning

Spring 2025

## Homework 4

Handed Out: April 2nd

Due: 8 pm April 16th

- You are encouraged to format your solutions using LATEX. Handwritten solutions are permitted, but remember that you bear the risk that we may not be able to read your work and grade it properly we will not accept post hoc explanations for illegible work. You will submit your solution manuscript for written HW 4 as a single PDF file.
- The homework is **due at 8 PM** on the due date. We will be using Gradescope for collecting the homework assignments. Please submit your solution manuscript as a PDF file via Gradescope. Post on Ed Discussion and contact the TAs if you are having technical difficulties in submitting the assignment.
- Make sure to assign pages to each question when submitting homework to Gradescope. The TA may deduct 0.2 points per sub-question if a page is not assigned to a question.

## 1 Written Questions

Note: You do not need to show work for multiple choice questions. If formatting your answer in LATEX, use our LaTeX template hw4\_template.tex (This is a read-only link. You'll need to make a copy before you can edit. Make sure you make only private copies.).

1. [Text Generation/Language Modeling] (10 pts) Text generation is a popular application and area of research in NLP. In this problem, we will look at a specific yet common scenario of text generation, where you want to generate a sentence by sampling words from an autoregressive language model (such as GPT<sup>1</sup>). Given the first k prompt words  $\{w_1, w_2, ..., w_k\}$  from left-to-right order in a sentence, an autoregressive language model outputs the probability distribution of the next word conditioned on the prompt words:  $P(w_{k+1}|w_1, w_2, ..., w_k)$ . A complete sentence can be generated by iteratively sampling words from the next word probability distributions until an end-of-sentence indicator (such as period ".") is reached. But how should we sample the words from  $P(w_{k+1}|w_1, w_2, ..., w_k)$ ?

In this question, we will compare two different sampling strategies and learn the intuition behind them with a toy example. Suppose you are interested in generating a sentence that starts with the word "Alice". You are given an autoregressive language model with only 5 words in vocabulary - {Alice, enjoys, dislikes, apple, banana}. You tried the following three prompts, and here are the three conditional probability distributions of the next word you get. For all subquestions, assume that you only want to generate the next two words after "Alice".

<sup>&</sup>lt;sup>1</sup>Free web demo of a GPT-3 like model - https://6b.eleuther.ai/

Next Word	Probability
enjoys	0.45
dislikes	0.35
banana	0.10
apple	0.08
Alice	0.02

Table 1:  $P(w_1|\text{Alice})$ 

Next Word	Probability
banana	0.40
Alice	0.20
apple	0.35
dislikes	0.04
enjoys	0.01

Table 2:  $P(w_2|\text{Alice}, \text{enjoys})$ 

Next Word	Probability
apple	0.60
banana	0.25
Alice	0.10
enjoys	0.03
dislikes	0.02

Table 3:  $P(w_2|\text{Alice}, \text{dislikes})$ 

- (a) (1 pts) Suppose we use the greedy sampling strategy, that is, always sample the word with highest conditional probability as the next word. What will be the sentence you generated (i.e. "Alice" plus the next two words)?
- (b) (3 pts) Naturally, your goal with text generation is to generate the most probable sentence out of your vocabulary. In other words, you want to sample the sentence which maximizes the joint probability of  $P(w_1, w_2|w_0 = \texttt{Alice})$ . While deriving the exact probability distribution with RNN models is in most cases NP-hard <sup>2</sup>, people commonly use the natural log-sum of the next-word probability as an approximation to the log-likelihood of the sentence; In other words:

$$ln(P(w_1|w_0 = \texttt{Alice})) + ln(P(w_2|w_0 = \texttt{Alice}, w_1))$$

$$(1)$$

Use the above formula to estimate the log-likelihood of the following two sentences "Alice enjoys banana" and "Alice dislikes apple".

- (c) (2 pts) From the last question, do you think the greedy sampling strategy will always give you the most probable sentence? Why or why not?
  (*Hint: Let's take the reasonable assumption that sentences with higher estimated log-likelihood from Eq. 1 are more probable.*)
- (d) (4 pts) Let's consider an alternative sampling strategy called beam search. Instead of always taking the highest probability word, let's say we take the top-2<sup>3</sup> words instead. In our case for  $w_1$ , this would give us two beam hypotheses "Alice enjoys" and "Alice dislikes".

<sup>&</sup>lt;sup>2</sup>https://aclanthology.org/N18-1205.pdf

 $<sup>{}^{3}</sup>k=2$  for Top-k here is a tunable parameter, and the correct jargon for this is: beam search with beam size of two

For the  $w_2$ , we sample the top two words for the two beam hypotheses respectively, which gives us the following four hypotheses.

- Alice enjoys banana
- Alice enjoys apple
- Alice dislikes apple
- Alice dislikes banana

The next step would be estimating the log-likelihood of the four hypotheses, and we will be keeping the top-2 highest probability hypotheses and iteratively generate the next words. Which two hypotheses among the above four should we keep in this case? In other words, which two have the top-2 highest estimated log-likelihood among the above four? Show your computation (for the ones that you haven't computed before).

2. [Attention Mechanism] (10 pts) In this problem, we will walk through how dot-product attention weights we introduced in class are calculated. Suppose we have a Sequence-to-Sequence machine translation (MT) model from English to Dothraki, where the hidden states for the encoder and decoder RNNs have size of 4. We input the English sentence "Dragons eat apple too" into the MT model, and below are the values of the hidden states we get from the model in the encoder.

Name	Input Word	Hidden State
$h_1$	Dragons	$\left[0.7, 0.2, 0.3, 0.1 ight]$
$h_2$	eat	[0.2, 0.7, 0.3, 0.1]
$h_3$	apple	$\left[0.0, 0.6, 0.4, 0.3 ight]$
$h_4$	too	[0.1, 0.1, 0.0, 0.9]

Table 4: Encoder hidden state values  $h_1, ..., h_4$ 

Suppose the first word that the MT model generates in the decoder is "Zhavvorsa", and the hidden state value for the word is  $s_1 = [0.5, 0.2, 0.4, 0.1]$ . You are welcome (and encouraged!) to use electronic devices to help with calculations in this question.

(a) (3 pts) Calculate the dot-product attention scores  $\mathbf{E}^{1\ 4}$  for the word "Zhavvorsa". Recall that the definition of dot-product attention score is

$$\mathbf{E}^t = [s_t^T h_1, \dots, s_t^T h_N] \in \mathbb{R}^N \tag{2}$$

(b) (4 pts) Use the attention scores derived in (a), derive the attention distribution  $\alpha^1$  for "Zhavvorsa". Recall that

$$\alpha^{t} = softmax(\mathbf{E}^{t}) = \left[\frac{e^{s_{t}^{T}h_{1}}}{\sum_{k=1}^{N} e^{s_{t}^{T}h_{k}}}, \dots, \frac{e^{s_{t}^{T}h_{N}}}{\sum_{k=1}^{N} e^{s_{t}^{T}h_{k}}}\right]$$
(3)

<sup>&</sup>lt;sup>4</sup>Denoted lowercased  $e^1$  in lecture slides. Using uppercase here to avoid confusion with the Euler number e in 3

- (c) (3 pts) The attention distribution will be used as weights in a weighted summation when computing the attention output. With  $\alpha^1$  you derived in the last subquestion, take the weighted sum of the encoder hidden state to compute the attention output  $a^1$ .
- 3. [Transformers] (12 pts) Transformers is a model architecture that revolutionized the field of NLP, leading to remarkable improvements in language understanding tasks and is the building block of all current LLMs (e.g. BERT, GPT, etc.). A core component of the Transformer is the scaled dot-product attention mechanism, which computes attention as:

Attention
$$(Q, K, V) = \operatorname{softmax}\left(\frac{QK^{\top}}{\sqrt{d_k}}\right)V$$

We ignore the dot-product normalization part during the lecture for simplicity. This problem explores why the division by  $\sqrt{d_k}$  is necessary (and knowing this is important for a MLE interview :)). We encourage you to read the original paper.

- (a) (3 pts) Let x = [1, 2, 3]. Compute softmax(x). Then, compute softmax(10x) = softmax([10, 20, 30]). What do you observe about the distribution?
- (b) (2 pts) Describe or sketch the behavior of softmax as input values grow larger: [1,2,3], [10, 20, 30], [100, 200, 300]. How does this affect the output distribution?
- (c) (2 pts) What might be the consequence of this effect on gradients during training? What does this imply about learning when the logits are too large?
- (d) (2 pts) Sample two vectors  $q, k \in \mathbb{R}^{d_k}$  from  $\mathcal{N}(0, 1)$  with  $d_k = 2$  and compute  $q \cdot k$ . Now do the same with  $d_k = 64$ , and repeat a few times. What trend do you observe? (hint: you might want to write a simple python program for this, but we do not need you to submit that program).
- (e) (3 pts) Summarize why we divide the dot product by  $\sqrt{d_k}$  in the attention mechanism. Relate your explanation to training stability and optimization.
- 4. [Value Iteration] (10pts)

Let's imagine a graph navigation MDP with the following structure:

 $a \leftarrow b \leftrightarrow c \leftrightarrow d \leftrightarrow e \leftrightarrow f \leftrightarrow g \rightarrow h$ 

where each node is a state, and the arrows represent the possible action an agent can take to traverse the graph. States a, h are terminal states, so the episode ends upon reaching them.

The agent gets 100 reward for reaching a, 30 reward for reaching h, and 0 everywhere else.

$$R(s_t, a_t, s_{t+1}) = \begin{cases} 100 & \text{if } s_{t+1} = a \\ 30 & \text{if } s_{t+1} = h \\ 0 & \text{otherwise} \end{cases}$$

- (a) (1pts) The agent starts at state f, and the discount factor is 1.0. What is the optimal action at state f?
- (b) (1pts) The agent starts at state f, and the discount factor is 0.5. What is the optimal action at state f?
- (c) (2pts) The agent starts at state f. What discount factor would result in both actions being equally likely? Show your work and give the answer rounded to 2 decimal places (e.g. 0.98).
- (d) (2 pts) Follow the pseudo-code in Fig. 4.3 of this article to help your computation. Write out the V(s) of each state after one round of value iteration, i.e. one pass of the outer loop in Fig. 4.3. Loop over the states from left to right, initialize the values to 0, and use a discount factor of 1.
- (e) (2 pts) Write out the V(s) of each state after one round of value iteration. Loop over the states from *right to left*, initialize the values to 0, and use a discount factor of 1.
- (f) (2 pts) How many rounds of VI would it take for V to converge if we only did left to right updates? And how many rounds for convergence if we only did right to left updates?
- 5. [Reinforcement Learning] (7 pts) Consider a deterministic grid world shown in the figure 1 with an "absorbing" state G: any action performed at this state leads back to the same state. The immediate rewards are 10 for the labeled transitions and 0 for the unlabelled transitions. The discount factor  $\gamma = 0.8$ .
  - (a) (1.5 pts) Show the optimal policy by drawing arrows corresponding to optimal actions for each cell in the grid. Note that the optimal policy need not be unique.
  - (b) (1.5 pts) Compute the optimal V-value function  $V^*$  for the top left state (column 1, row 2) in this grid world.
  - (c) (4 pts) Now, consider applying the Q-learning algorithm to this grid world. Assume the table of Q-values is initialized to zero, and  $\alpha = 0.1$ . Assume the agent begins in the bottom left grid square and then travels clockwise along the perimeter of the grid until it reaches the absorbing goal state, completing the first training episode. Describe which Q-values are modified as a result of this episode, and give their revised values.

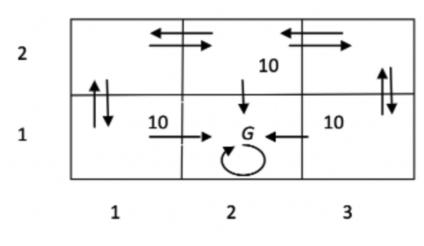


Figure 1: Gridworld