HOMEWORK 1
GENERATIVE MODELS OF TEXT *

10-423/10-623 GENERATIVE AI
http://423.mlcourse.org

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Instructions

- **Collaboration Policy**: Please read the collaboration policy in the syllabus.
- **Late Submission Policy:** See the late submission policy in the syllabus.
- **Submitting your work:** You will use Gradescope to submit answers to all questions and code.
  - **Written:** You will submit your completed homework as a PDF to Gradescope. Please use the provided template. Submissions can be handwritten, but must be clearly legible; otherwise, you will not be awarded marks. Alternatively, submissions can be written in LaTeX. Each answer should be within the box provided. If you do not follow the template, your assignment may not be graded correctly by our AI assisted grader and there will be a **2% penalty** (e.g., if the homework is out of 100 points, 2 points will be deducted from your final score).
  - **Programming:** You will submit your code for programming questions to Gradescope. We will examine your code by hand and may award marks for its submission.
- **Materials:** The data that you will need in order to complete this assignment is posted along with the writeup and template on the course website.

Question	Points
Recurrent Neural Network (RNN) Language Models	7
Transformer Language Models	13
Sliding Window Attention	10
Programming: RoPE and GQA	24
Code Upload	0
Collaboration Questions	2
Total:	56

*Compiled on Monday 9th September, 2024 at 21:25

1 Recurrent Neural Network (RNN) Language Models (7 points)

1.1. (3 points) **Numerical answer:** Consider an RNN (Elman Network) that takes inputs $\mathbf{x}_t \in \{0,1\}^2$, has hidden vectors $\mathbf{h}_t \in \mathbb{R}^2$, and output units $y_t \in \mathbb{R}$ for all $t \in \{1,\ldots,T\}$. Assume the recurrence is given by:

$$h_t = \text{slide}(W_{hh}h_{t-1} + W_{hx}x_t + b_h)$$
$$y_t = \text{slide}(W_{yh}h_t + b_y)$$

where $\text{slide}(a) = \min(1, \max(0, a))$ is the activation function. Let $W_{hh} \in \mathbb{R}^{2\times 2}$ be defined as follows:

$$W_{hh} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Define parameters $W_{yh} \in \mathbb{R}^{1\times 2}, b_h \in \mathbb{R}^2, b_y \in \mathbb{R}$ to satisfy the following condition: $y_t = 1$ if $\exists\, r, s \leq t$ such that $x_{r,0} = 1$ and $x_{s,1} = 1$ and $y_t = 0$ otherwise. Assume $h_0 = [0,0]^T$.

W_{hx}

b_h

W_{yh}

b_y

1.2. An autoregressive language model defines a probability distribution over sequences $\mathbf{x}_{1:T}$ of the form: $p(\mathbf{x}_{1:T}) = \prod_{t=1}^{T} p(x_t \mid x_1, \ldots, x_{t-1})$.

1.2.a. (2 points) **Short answer:** Suppose we are given an input $\mathbf{x}_{1:T}$ and we define a bidirectional RNN of the following form:

$$f_t = \sigma(W_{ff} f_{t-1} + W_{fx} x_t + b_f), \quad \forall t \in \{1, \ldots, T\}$$
$$g_t = \sigma(W_{gg} g_{t+1} + W_{gx} x_t + b_g), \quad \forall t \in \{1, \ldots, T\}$$
$$h_t = \sigma(W_{hf} f_t + W_{hg} g_t + b_g), \quad \forall t \in \{1, \ldots, T\}$$

(Notice that f_t builds up context from the left, g_t builds up context from the right, and h_t combines the two.) Can we define an autoregressive language model of the form $p(\mathbf{x}_{1:T}) = \prod_{t=1}^{T} p(x_t \mid h_{t-1})$? If so, define the probability distribution $p(x_t \mid \text{BiRNN}(\mathbf{x}_{1:t-1}))$. If not, why not? Assume that **no** weight matrix can be set to all zeros.

1.2.b. (2 points) **Short answer:** Suppose $\text{BiRNN}(\mathbf{x}_{1:t-1})$ computes a bidirectional RNN on the subsequence $\mathbf{x}_{1:t-1}$ and then returns h_{t-1}. Can we define an autoregressive language model of the form $p(\mathbf{x}_{1:T}) = \prod_{t=1}^{T} p(x_t \mid \text{BiRNN}(\mathbf{x}_{1:t-1})$? If so, define the probability distribution $p(x_t \mid \text{BiRNN}(\mathbf{x}_{1:t-1}))$. If not, why not?

2 Transformer Language Models (13 points)

2.1. Transformers use scaled-dot-product attention:

$$s_{t,j} = \mathbf{k}_j^T \mathbf{q}_t / \sqrt{|\mathbf{k}|}, \forall j, t$$
$$\mathbf{a}_t = \text{softmax}(\mathbf{s}_t), \forall t$$

where the values, queries, and keys are respectively given by: $\mathbf{v}_j = \mathbf{W}_v^T \mathbf{x}_j$, $\mathbf{q}_j = \mathbf{W}_q^T \mathbf{x}_j$, and $\mathbf{k}_j = \mathbf{W}_k^T \mathbf{x}_j$ for all j and $\mathbf{v}_j, \mathbf{q}_j, \mathbf{k}_j \in \mathbb{R}^{d_k}$.

2.1.a. (2 points) **Short answer:** Multiplicative attention instead defines the attention weights as:

$$\tilde{s}_{t,j} = \mathbf{k}_j^T \mathbf{W}_s \mathbf{q}_t / \sqrt{|\mathbf{k}|}, \forall j, t$$
$$\tilde{\mathbf{a}}_t = \text{softmax}(\tilde{\mathbf{s}}_t), \forall t$$

where $\mathbf{W}_s \in \mathbb{R}^{d_k \times d_k}$ is a parameter matrix. Could a Transformer with multiplicative attention learn a function that a Transformer with scaled dot product attention cannot?

Note: Two functions are equivalent if they produce the same output for every input in the domain.

2.1.b. (2 points) **Short answer:** Concatenated attention defines the attention weights as:

$$\hat{s}_{t,j} = \mathbf{w}_s^T [\mathbf{k}_j; \mathbf{q}_t], \forall j, t$$
$$\hat{\mathbf{a}}_t = \text{softmax}(\hat{\mathbf{s}}_t), \forall t$$

where $\mathbf{w}_s \in \mathbb{R}^{2d_k}$ is a parameter vector, and $[\mathbf{a}; \mathbf{b}]$ is the concatenation of vectors $\mathbf{a}$ and $\mathbf{b}$. Do there exist parameters $\mathbf{w}_s$ such that $s_{t,j}$ will approximately equal the angle θ between the two vectors $\mathbf{k}_j, \mathbf{q}_t$, or to $\cos(\theta)$? (Briefly justify your answer—a formal proof is not required.)

2.1.c. (2 points) **Short answer:** Additive attention defines the attention weights as:

$$\hat{s}_{t,j} = \mathbf{w}_s^T \tanh(\mathbf{W}_s[\mathbf{k}_j; \mathbf{q}_t]), \forall j, t$$
$$\hat{\mathbf{a}}_t = \text{softmax}(\hat{\mathbf{s}}_t), \forall t$$

where the parameters are $\mathbf{w}_s \in \mathbb{R}^{d_s}$ and $\mathbf{W}_s \in \mathbb{R}^{d_s \times 2d_s}$, dimensionality d_s is a hyperparameter, and $[\mathbf{a}; \mathbf{b}]$ is the concatenation of vectors $\mathbf{a}$ and $\mathbf{b}$. Do there exist parameters $\mathbf{w}_s, \mathbf{W}_s$ such that $s_{t,j}$ will approximately equal the angle θ between the two vectors $\mathbf{k}_j, \mathbf{q}_t$, or to $\cos(\theta)$? (Briefly justify your answer—a formal proof is not required.)

2.2. Self-attention is typically computed via matrix multiplication. Here we consider multi-headed attention without a causal attention mask.

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_N]^T$$
$$\mathbf{V}^{(i)} = \mathbf{X}\mathbf{W}_v^{(i)}$$
$$\mathbf{K}^{(i)} = \mathbf{X}\mathbf{W}_k^{(i)}$$
$$\mathbf{Q}^{(i)} = \mathbf{X}\mathbf{W}_q^{(i)}$$
$$\mathbf{S}^{(i)} = \mathbf{Q}^{(i)}(\mathbf{K}^{(i)})^T / \sqrt{d_k}$$
$$\mathbf{A}^{(i)} = \text{softmax}(\mathbf{S}^{(i)})$$
$$\mathbf{X}'^{(i)} = \mathbf{A}^{(i)}\mathbf{V}^{(i)}$$
$$\mathbf{X}' = \text{concat}(\mathbf{X}'^{(1)}, \ldots, \mathbf{X}'^{(h)})$$

where N is the sequence length, h is the number of attention heads, and each row involving i is defined $\forall i \in \{1, \ldots, h\}$.

2.2.a. (3 points) **Short answer:** Is the score matrix $\mathbf{S}^{(i)}$ always symmetric? If yes, show that it is. If not, describe a condition that would ensure it is symmetric.

2.2.b. (4 points) **Short answer:** Suppose we have two attention heads, $h = 2$, we let $d_k = d_m/h$, and we have a single input $\mathbf{X}$. Let $\mathbf{X}'$ be the output of multi-headed attention on $\mathbf{X}$ with the parameters:

$$\mathbf{W}_v^{(1)}, \mathbf{W}_k^{(1)}, \mathbf{W}_q^{(1)}, \mathbf{W}_v^{(2)}, \mathbf{W}_k^{(2)}, \mathbf{W}_q^{(2)} \in \mathbb{R}^{d_m \times d_k}$$

Now suppose we take those same parameters and concatenate along the rows to yield new parameters:

$$\mathbf{W}'_v = \text{concat}(\mathbf{W}_v^{(1)}, \mathbf{W}_v^{(2)}),\ \mathbf{W}'_k = \text{concat}(\mathbf{W}_k^{(1)}, \mathbf{W}_k^{(2)}),\ \mathbf{W}'_q = \text{concat}(\mathbf{W}_q^{(1)}, \mathbf{W}_q^{(2)}) \in \mathbb{R}^{d_m \times d_m}$$

And let $\mathbf{X}''$ be the output of single-headed attention on $\mathbf{X}$ with the parameters $\mathbf{W}'_v, \mathbf{W}'_k, \mathbf{W}'_q$.

In this case, does $\mathbf{X}'' = \mathbf{X}'$? Justify your answer.

3 Sliding Window Attention (10 points)

3.1. The simplest way to define sliding window attention is by setting the causal mask $\mathbf{M}$ to only include a window of $\frac{1}{2}w + 1$ tokens, with the rightmost window element being the current token (i.e. on the diagonal). Then our attention computation is:

$$\mathbf{X}' = \text{softmax}((\mathbf{Q}\mathbf{K}^T/\sqrt{d_k}) + \mathbf{M})\mathbf{V} \tag{1}$$

For example, if we have a sequence of length $N = 6$, and window size $w = 4$, then our mask matrix is:

$$\mathbf{M} = \begin{bmatrix} 0 & -\infty & -\infty & -\infty & -\infty & -\infty \\ 0 & 0 & -\infty & -\infty & -\infty & -\infty \\ 0 & 0 & 0 & -\infty & -\infty & -\infty \\ -\infty & 0 & 0 & 0 & -\infty & -\infty \\ -\infty & -\infty & 0 & 0 & 0 & -\infty \\ -\infty & -\infty & -\infty & 0 & 0 & 0 \end{bmatrix}$$

3.1.a. (1 point) **Short answer:** If we implement sliding window using the matrix multiplications described in Equation 1, what is the time complexity in terms of N and w? Let d_k be a constant that does not need to be included in your answer. (For this and subsequent questions, assume that the cost of multiplying two matrices $\mathbf{X} \in \mathbb{R}^{m \times n}$ and $\mathbf{Y} \in \mathbb{R}^{n \times p}$ is $O(mnp)$.)

3.1.b. (1 point) **Short answer:** If we implement sliding window using the matrix multiplications described in Equation 1, what is the space complexity in terms of N and w? Let d_k be a constant that does not need to be included in your answer.

3.2. **Pseudocode:** Fill in the blanks with pseudocode/math to create a function that takes in the queries, keys, and values and the window size w and computes the $\mathbf{X}'$ of Equation (1):

$$\text{SLIDINGWINDOWATTENTION}(\mathbf{Q}, \mathbf{K}, \mathbf{V}, w)$$

Your pseudocode/math must have lower asymptotic computational than the naive matrix multiplication approach described above. The function $\text{softmax}(\mathbf{x})$ applies softmax to a vector $\mathbf{x}$, and the function $\text{tensor}(\cdot)$ can be used to contruct vectors, matrices, tensors of arbitrary shape. In the pseudocode below, X_i means indexing into the vector / matrix X at index i.

```
def SlidingWindowAttention(Q, K, V, w):
    N, d_k = Q.shape()
    X' = tensor(N, d_k)
    w' =  __(1)__
    for j in 1 to N:
        a = tensor(__(2)__)
        for i in __(3)__:
            if __(4)__ :
                a_i = __(5)__

        a = softmax(a)
        for i in __(3)__:
            if __(4)__ :
                X'_j += __(6)__
    return X'
```

3.2.a. (1 point) Write psuedocode/math to fill in blank **(1)**.

3.2.b. (1 point) Write psuedocode/math to fill in blank **(2)**.

3.2.c. (1 point) Write psuedocode/math to fill in blank **(3)**. Note that both blanks will be filled with the same line.

3.2.d. (1 point) Write psuedocode/math to fill in blank **(4)**. Note that both blanks will be filled with the same line.

3.2.e. (1 point) Write psuedocode/math to fill in blank **(5)**.

3.2.f. (1 point) Write psuedocode/math to fill in blank **(6)**.

3.2.g. (1 point) **Short answer:** What is the space complexity of your pseudocode in terms of N and w?

3.2.h. (1 point) **Short answer:** What is the time complexity of your pseudocode in terms of N and w?

4 Programming: RoPE and GQA (24 points)

Introduction

In this section, you will take a run-of-the-mill GPT model and upgrade it to incorporate two of the key ingredients found in state-of-the-art large language models (LLMs), such as LLAMA-2.

The first ingredient are rotary position embeddings (RoPE). These will replace the existing absolute position embeddings with a relative position embedding that rotates small segments of each key and query vector.

The second ingredient is grouped-query attention (GQA). Although the GQA mechanism is fundamentally still causal attention, it enables the model to use less memory and run faster.

You will experiment with how these two model improvements lead to changes in model performance. And you will even evaluate how they perform in tandem.

Upon completion of this section, you will unfortunately not be able to claim to have trained a *large* language model, for the dataset we provide here (the complete works of Shakespeare) is rather small if not trite. However, you can reasonably claim to have built your own LLAMA-2 model.

Dataset

The dataset for this homework is a collection of the complete works of Shakespeare. The dataset file is `input.txt`, and is around 1.1MB in size.

Starter Code

The starter code was originally authored by Andrej Karpathy, of OpenAI fame, and released as minGPT. It offers a clear glimpse into the inner workings of a GPT model. We have simplified the codebase and provided to you a modified version. Ours contains the following files:

```
hw1/
   requirements.txt
   input.txt
   chargpt.py
   mingpt/
      model.py
      trainer.py
      utils.py
```

Here is what you will find in each file:

1. `requirements.txt`: A list of packages that need to be installed for this homework. This homework only requires 2 packages - `torch` and `einops`.
2. `input.txt`: The dataset—the works of Shakespeare.
3. `chargpt.py`: The main entry point used to train your transformer. It can be run with the command `python chargpt.py`. Append flags to this command to adjust the transformer configuration.
4. `mingpt/model.py`: The only file you need to modify for this homework. This file contains the construction of the GPT model. A vanilla, working transformer implementation

is already provided. You will implement the classes `RotaryPositionalEmbeddings` and `GroupedQueryAttention`. You will also need to make changes to the class `CausalSelfAttention` while implementing RoPE. (Hint: Locations in the code where changes ought to be made are marked with a **TODO**.)

5. `mingpt/trainer.py`: Code for the training loop of the transformer.
6. `mingpt/utils.py`: Helper functions for saving logs and configs.

Flags

All the parameters printed in the config can be modified by passing flags to `chargpt.py`. Table 1 contains a list of flags you may find useful while implementing HW1. You can change other parameters as well in a similar manner. Simply specify the config node (i.e. one of {system,data,model,trainer}), followed by a period '.', followed by the parameter you wish to modify.

Configuration Parameter	Example Flag Usage
Model sequence length	`--data.block_size=16` (`model.block_size` is autoset based on this flag)
Directory where model is stored	`--system.work_dir=out/new_chargpt`
Number of query heads (hyperparameter for GQA)	`--model.n_query_head=6`
Number of key-value heads (hyperparameter for GQA)	`--model.n_kv_head=3` (`n_query_head` must be divisible by `n_kv_head`) (For standard multi-head attention `n_query_head` = `n_kv_head`)
Directory from which to load a model trained in a previous run	`--model.pretrained_folder=out/chargpt3`
Whether to enable RoPE embeddings	`--model.rope=True`
Number of iterations to train the model	`--trainer.max_iters=200`
Device type (useful for debugging), one of	`--trainer.device=cpu`

Table 1: Useful flags for `chargpt.py`

Model

The default model in `chargpt.py` is a GPT model with 6 transformer layers. Each attention layer uses $h = 6$ attention heads. The maximum sequence length is $N = 16$. Because the vocabulary is comprised of only characters, the vocabulary size is only 65. The embedding dimension is $d_{model} = 192$ and the key/value/query dimension size is $d_k = d_{model}/h = 32$.

Rotary Position Embeddings (RoPE)

In this section, you will implement Rotary Position Embeddings (RoPE) (Su et al., 2021).

Background: Absolute position embeddings are added to the word embeddings in the first layer of a standard Transformer language model. Subsequent layers propagate position information up from the bottom.

Traditional attention is defined as below.

$$\begin{aligned}\mathbf{q}_j &= \mathbf{W}_q^T \mathbf{x}_j, \forall j \\ \mathbf{k}_j &= \mathbf{W}_k^T \mathbf{x}_j, \forall j \\ s_{t,j} &= \mathbf{k}_j^T \mathbf{q}_t / \sqrt{d_k}, \forall j, t \\ \mathbf{a}_t &= \text{softmax}(\mathbf{s}_t), \forall t\end{aligned}$$

where $d_k = |\mathbf{k}_j|$ is the size of the query/key/value vectors.

RoPE: Rotary Position Embeddings (RoPE) (Su et al., 2021) incorporate positional information directly into the attention computation, in every layer. If the input to the next attention layer is $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_N]^T$, then we introduce two functions $f_q(\mathbf{x}_j, j)$ and $f_k(\mathbf{x}_j, j)$, which compute the position-aware queries and keys respectively. Then the attention scores are computed as below:

$$\begin{aligned}\mathbf{q}_j &= \mathbf{W}_q^T \mathbf{x}_j, \forall j & \mathbf{k}_j &= \mathbf{W}_k^T \mathbf{x}_j, \forall j \\ \widetilde{\mathbf{q}}_j &= \mathbf{R}_{\Theta,j} \mathbf{q}_j & \widetilde{\mathbf{k}}_j &= \mathbf{R}_{\Theta,j} \mathbf{k}_j \\ s_{t,j} &= \widetilde{\mathbf{k}}_j^T \widetilde{\mathbf{q}}_t / \sqrt{d_k}, \forall j, t \\ \mathbf{a}_t &= \text{softmax}(\mathbf{s}_t), \forall t\end{aligned}$$

where $\mathbf{W}_k, \mathbf{W}_q \in \mathbb{R}^{d_{model} \times d_k}$. Herein we use $d = d_k$ for brevity.

To implement this efficiently in PyTorch, we want to construct a new matrix $\widetilde{\mathbf{Y}} = g(\mathbf{Y}; \Theta)$ such that $\widetilde{\mathbf{Y}}_{m,:} = \mathbf{R}_{\Theta,m} \mathbf{y}_m$ for a matrix of embeddings $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_N]^T \in \mathbb{R}^{N \times d_k}$, and $\Theta = \{\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, \ldots, d/2]\}$ (in practice this $\mathbf{Y}$ would be either the queries $\mathbf{Q}$ or the keys $\mathbf{K}$). We can construct the new matrix as follows:

$$\begin{aligned}\widetilde{\mathbf{Y}} &= g(\mathbf{Y}; \Theta) \\ &= \left[\begin{array}{ccc|ccc} Y_{1,1} & \cdots & Y_{1,\frac{d}{2}} & Y_{1,\frac{d}{2}+1} & \cdots & Y_{1,d} \\ \vdots & & \vdots & \vdots & & \vdots \\ Y_{N,1} & \cdots & Y_{N,\frac{d}{2}} & Y_{N,\frac{d}{2}+1} & \cdots & Y_{N,d} \end{array}\right] \otimes \left[\begin{array}{ccc|ccc} \cos 1\theta_1 & \cdots & \cos 1\theta_{\frac{d}{2}} & \cos 1\theta_1 & \cdots & \cos 1\theta_{\frac{d}{2}} \\ \vdots & & \vdots & \vdots & & \vdots \\ \cos N\theta_1 & \cdots & \cos N\theta_{\frac{d}{2}} & \cos N\theta_1 & \cdots & \cos N\theta_{\frac{d}{2}} \end{array}\right] \\ &+ \left[\begin{array}{ccc|ccc} -Y_{1,\frac{d}{2}+1} & \cdots & -Y_{1,d} & Y_{1,1} & \cdots & Y_{1,\frac{d}{2}} \\ \vdots & & \vdots & \vdots & & \vdots \\ -Y_{N,\frac{d}{2}+1} & \cdots & -Y_{N,d} & Y_{N,1} & \cdots & Y_{N,\frac{d}{2}} \end{array}\right] \otimes \left[\begin{array}{ccc|ccc} \sin 1\theta_1 & \cdots & \sin 1\theta_{\frac{d}{2}} & \sin 1\theta_1 & \cdots & \sin 1\theta_{\frac{d}{2}} \\ \vdots & & \vdots & \vdots & & \vdots \\ \sin N\theta_1 & \cdots & \sin N\theta_{\frac{d}{2}} & \sin N\theta_1 & \cdots & \sin N\theta_{\frac{d}{2}} \end{array}\right]\end{aligned}$$

Or more compactly:

$$
\begin{aligned}
\mathbf{C} &= \left[\begin{array}{ccc|ccc} 1\theta_1 & \cdots & 1\theta_{\frac{d}{2}} & 1\theta_1 & \cdots & 1\theta_{\frac{d}{2}} \\ \vdots & & \vdots & \vdots & & \vdots \\ N\theta_1 & \cdots & N\theta_{\frac{d}{2}} & N\theta_1 & \cdots & N\theta_{\frac{d}{2}} \end{array}\right] \\
\widetilde{\mathbf{Y}} &= g(\mathbf{Y};\Theta) \\
&= \left[\begin{array}{c|c} \mathbf{Y}_{\cdot,1:d/2} & \mathbf{Y}_{\cdot,d/2+1:d} \end{array}\right] \otimes \cos(\mathbf{C}) \\
&\quad + \left[\begin{array}{c|c} -\mathbf{Y}_{\cdot,d/2+1:d} & \mathbf{Y}_{\cdot,1:d/2} \end{array}\right] \otimes \sin(\mathbf{C})
\end{aligned}
$$

Now we can compute RoPE embeddings efficiently as below:

$$
\begin{aligned}
\mathbf{Q} &= \mathbf{X}\mathbf{W}_q & \mathbf{K} &= \mathbf{X}\mathbf{W}_k \\
\widetilde{\mathbf{Q}} &= g(\mathbf{Q};\Theta) & \widetilde{\mathbf{K}} &= g(\mathbf{K};\Theta) \\
\mathbf{S} &= \widetilde{\mathbf{Q}}\widetilde{\mathbf{K}}^T/\sqrt{d_k} \\
\mathbf{A} &= \text{softmax}(\mathbf{S})
\end{aligned}
$$

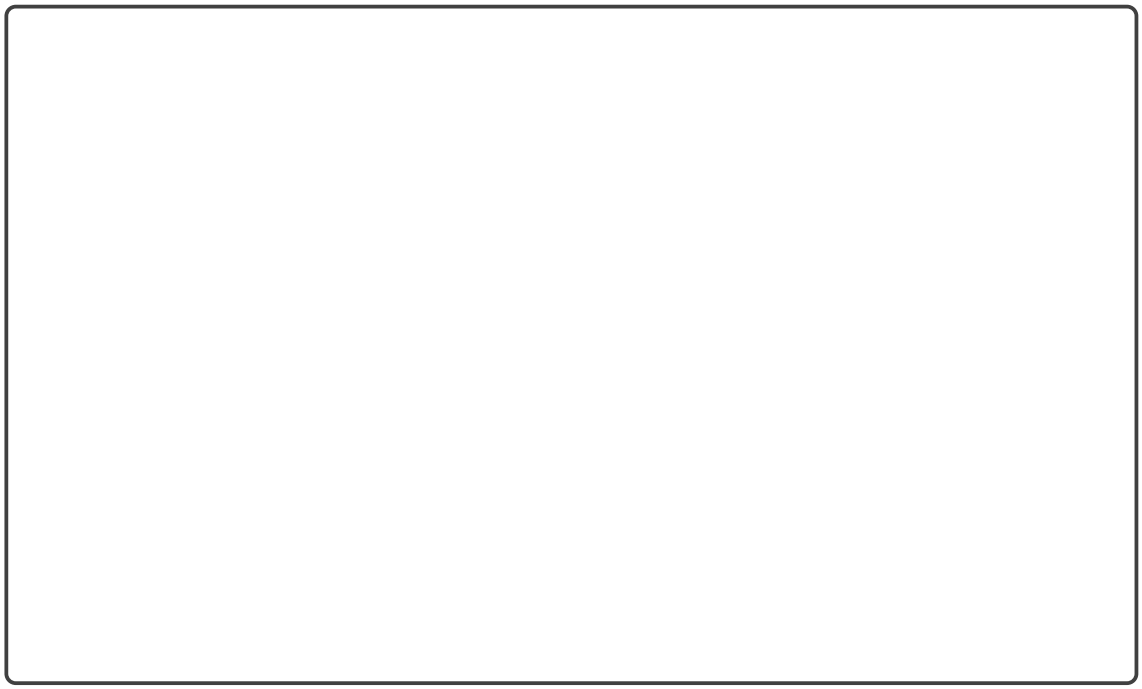
You do not have to understand all the math in the paper, but you may go through it to understand the intuition behind RoPE.

Implementation: You will implement RoPE within `minGPT`. To do so, you should make changes to the `RotaryPositionalEmbeddings` and the `CausalSelfAttention` classes in `mingpt/model.py`. Within `RotaryPositionalEmbeddings`, you will first implement `_build_cache`, and within the `forward` computation, your first steps should be building the cache if it has not been built yet.

RoPE Empirical Questions

4.1. (4 points) Plot the training loss for both your RoPE implementation and the vanilla minGPT over **1200 total training iterations** on the **same plot**: 600 iterations with a **sequence length of 16**, followed by 600 iterations with a **sequence length of 256**.

[Expected runtime on Colab T4 to run both: approximately 10 minutes]



4.2. (2 points) Provide a sample from your RoPE model after **600 iterations** of training with a **sequence length of 16**. Condition the sample on the first line of your favorite Shakespeare play.

[Expected runtime on Colab T4: approximately 3 minutes]

4.3. (2 points) Provide a sample from your RoPE model after **1200 iterations**, consisting of 600 iterations with a **sequence length of 16**, followed by 600 iterations with a **sequence length of 256**. Condition the sample on the first line of your favorite Shakespeare play.

[Expected runtime on Colab T4: approximately 5 minutes]

Grouped Query Attention (GQA)

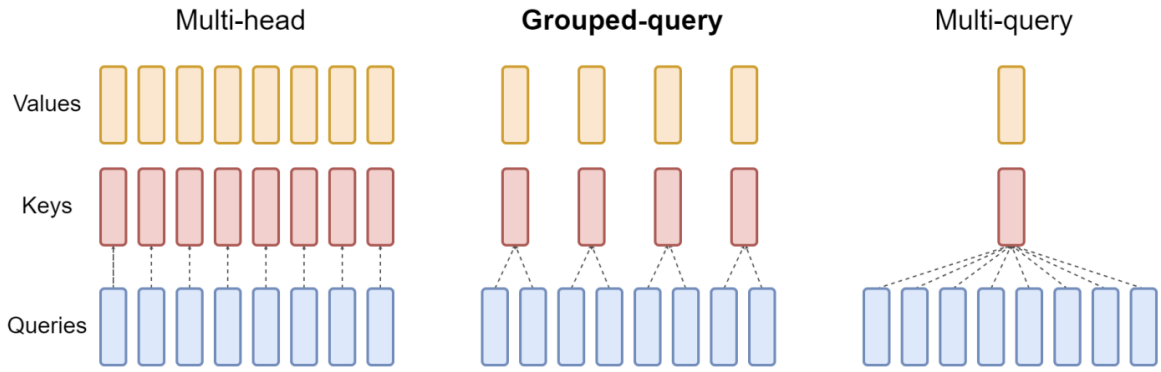


Figure 1: Schematic representation of attention mechanisms, showcasing Multi-head attention with individual keys and values for each head, Grouped-query attention with queries grouped to share common keys and values, and Multi-query attention utilizing a singular key and value for all queries.

In this section, you will implement Grouped Query Attention (GQA) (Ainslie et al., 2023).

GQA: Grouped Query Attention (GQA) is a technique in neural network architectures that modifies the attention mechanism used in models such as transformers. It involves dividing the query heads into groups, each sharing a single key head and value head. This approach can interpolate between Multi-Query Attention (MQA) and Multi-Head Attention (MHA), offering a balance between computational efficiency and model quality [Figure 1].

Let h_q denote the number of query heads and h_{kv} the number of key/value heads. We assume h_q is divisible by h_{kv} and $g = h_q/h_{kv}$ is the size of each group (i.e. the number of query vectors per key/value vector).

Our parameter matrices for GQA are all the same size: $\mathbf{W}_q^{(g,i)}, \mathbf{W}_k^{(g)}, \mathbf{W}_v^{(g)} \in \mathbb{R}^{d_{model} \times d_k}$ where $d_k = d_{model}/h_q$. However, we now have different numbers of query, key, and value heads:

$$
\begin{aligned}
\mathbf{X} &= [\mathbf{x}_1, \ldots, \mathbf{x}_T]^T \\
\mathbf{V}^{(i)} &= \mathbf{X}\mathbf{W}_v^{(i)}, \forall i \in \{1, \ldots, h_{kv}\} \\
\mathbf{K}^{(i)} &= \mathbf{X}\mathbf{W}_k^{(i)}, \forall i \in \{1, \ldots, h_{kv}\} \\
\mathbf{Q}^{(i,j)} &= \mathbf{X}\mathbf{W}_q^{(i,j)}, \forall i \in \{1, \ldots, h_{kv}\}, \forall j \in \{1, \ldots, g\}
\end{aligned}
$$

Above, we define g times more query vectors than key/value vectors. Then we compute the scaled dot-product between each query vector (i, j) and its corresponding key (i) and sum over the queries within each group to get the similarity scores. The similarity scores are used to compute an atten-

tion matrix, but with only h_{kv} heads:

$$\begin{aligned}
\mathbf{S}^{(i)} &= \sum_{j=1}^{g} \mathbf{Q}^{(i,j)} (\mathbf{K}^{(i)})^T / \sqrt{d_k}, \quad \forall i \in \{1, \ldots, h_{kv}\} \\
\mathbf{A}^{(i)} &= \text{softmax}(\mathbf{S}^{(i)}), \quad \forall i \in \{1, \ldots, h_{kv}\} \\
\mathbf{X}'^{(i)} &= \mathbf{A}^{(i)} \mathbf{V}^{(i)}, \quad \forall i \in \{1, \ldots, h_{kv}\} \\
\mathbf{X}' &= concat(\mathbf{X}'^{(i)}), \quad i \in \{1, \ldots, h_{kv}\} \\
\mathbf{X} &= \mathbf{X}' \mathbf{W}_o
\end{aligned}$$

where $\mathbf{W}_o \in \mathbb{R}^{(d_k * h_{kv}) \times d_{model}}$

Implementation Details: You will implement GQA in the `GroupedQueryAttention` class in `mingpt/model.py`. Much of your code will be similar to that in `CausalSelfAttention`.

Hint: You may find it easier to implement `GroupedQueryAttention` in a similar way to `CausalSelfAttention`.

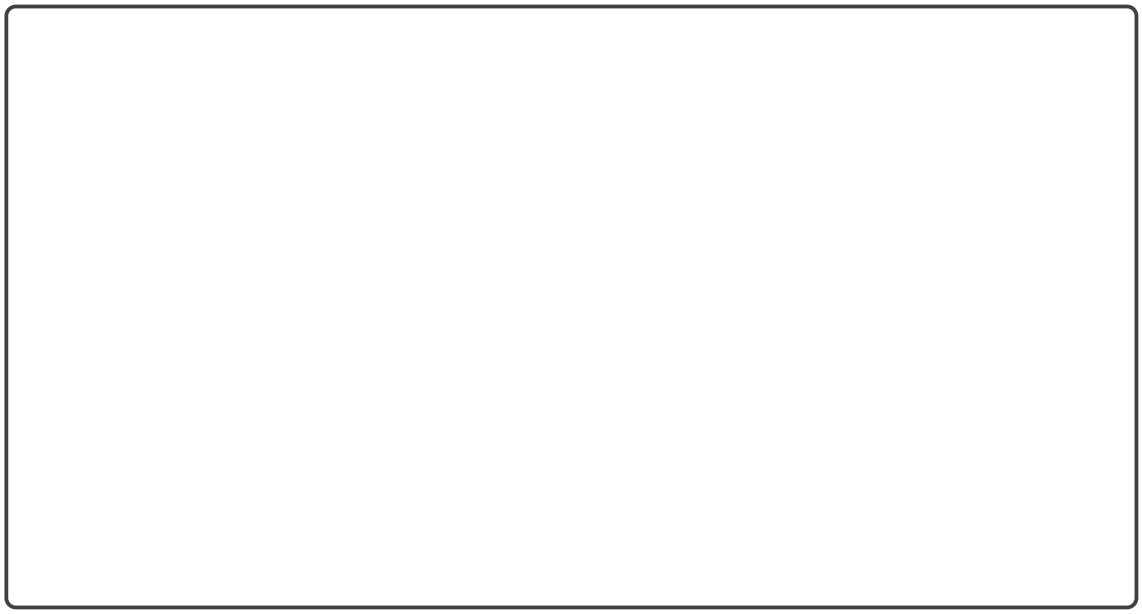
- **Initialization:**
  - Familiarize yourself with the configuration settings that initialize the attention mechanism, including the number of query heads, key/value heads, and embedding dimensions.
  - Ensure the embedding dimension is divisible by the number of query and key/value heads.
- **Regularization:**
  - Incorporate dropout layers for attention and residuals to prevent overfitting.
- **Dimensionality and Projections:**
  - Implement the linear projection layers for queries, keys, and values, considering the dimensionality constraints and the grouped nature of the mechanism.
- **Rotary Positional Embeddings:**
  - If rotary positional embeddings are enabled, integrate RoPE with query and key projections.
- **Forward Pass:**
  - In the forward method, transform the input according to the query, key, and value projections.
  - Apply the attention mechanism by computing grouped scaled dot-product attention
  - Mask the attention to ensure causality (preventing future tokens from being attended to).
  - Aggregate the attention with the values and project the output back to the embedding dimension.
- **Memory Efficiency:**
  - Monitor and record the CUDA memory allocation before and after the attention operation to analyze the memory efficiency of the GQA. A reference code to monitor memory is present in `CausalSelfAttention` class.

GQA Empirical Questions

The questions below assume you are using absolute position embeddings, not RoPE.

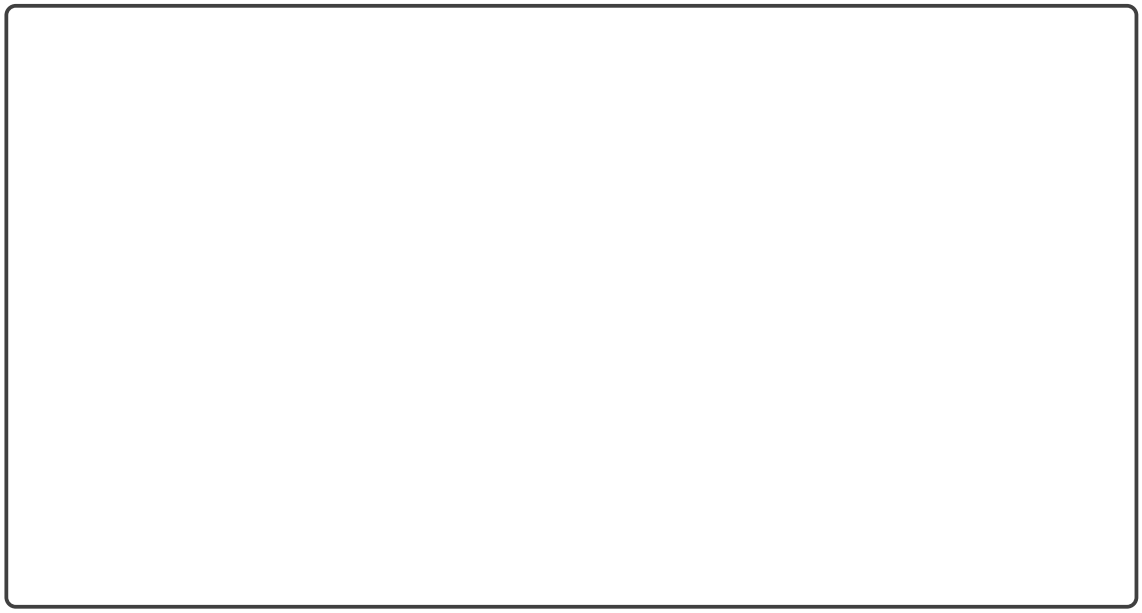
4.4. (4 points) Plot the **average time taken** to compute attention per iteration in milliseconds across $\{1, 2, 3, 6\}$ number of key heads with a **sequence length of 16** over **200 iterations**.

[Expected runtime on Colab T4: approximately 1 minute]



4.5. (4 points) Plot the **average memory consumption** in MB per iteration across $\{1, 2, 3, 6\}$ number of key heads with a **sequence length of 16** over **200 iterations**.

[Expected runtime on Colab T4: approximately 1 minute]

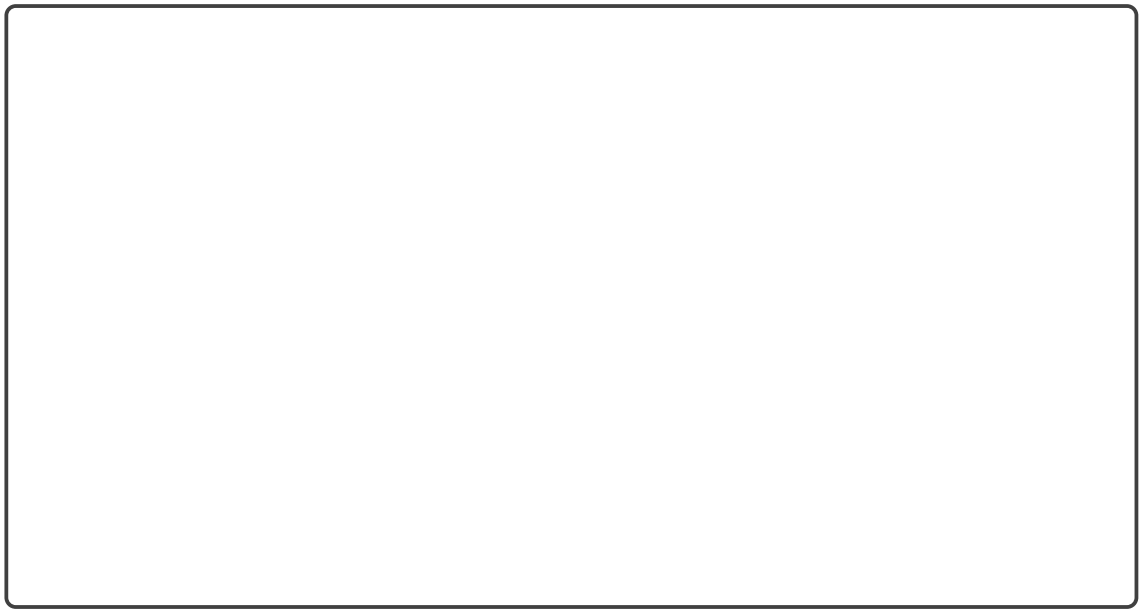


4.6. (4 points) Plot both the training loss of your GQA implementation with 2 key heads and the original (multi head attention) minGPT over **200 iterations** with a **sequence length of 16** on the **same plot**.

[Expected runtime on Colab T4 to run both: approximately 6 minutes]

4.7. (4 points) Plot the following four configurations on the **same plot**: 1. vanilla minGPT (no RoPE nor GQA), 2. RoPE only (no GQA), 3. GQA only (no RoPE), 4. RoPE and GQA. For each, plot the training loss over **1200 total training iterations**: 600 iterations with a **sequence length of 16**, followed by 600 iterations with a **sequence length of 256**.

[Expected runtime on Colab T4 to run all four: approximately 16 minutes]



5 Code Upload (0 points)

5.1. (0 points) Did you upload your code to the appropriate programming slot on Gradescope?
Hint: The correct answer is 'yes'.

- ◯ Yes
- ◯ No

For this homework, you should upload only `model.py`.

6 Collaboration Questions (2 points)

After you have completed all other components of this assignment, report your answers to these questions regarding the collaboration policy. Details of the policy can be found in the syllabus.

6.1. (1 point) Did you collaborate with anyone on this assignment? If so, list their name or Andrew ID and which problems you worked together on.

6.2. (1 point) Did you find or come across code that implements any part of this assignment? If so, include full details.