Lab5 FlashAttention

Nov, 2024 Parallel Programming

Overview

- Platform Guide (NCHC CT)
- Attention
- FlashAttention
- Lab5 Assignment

Platform Guide (NCHC CT)

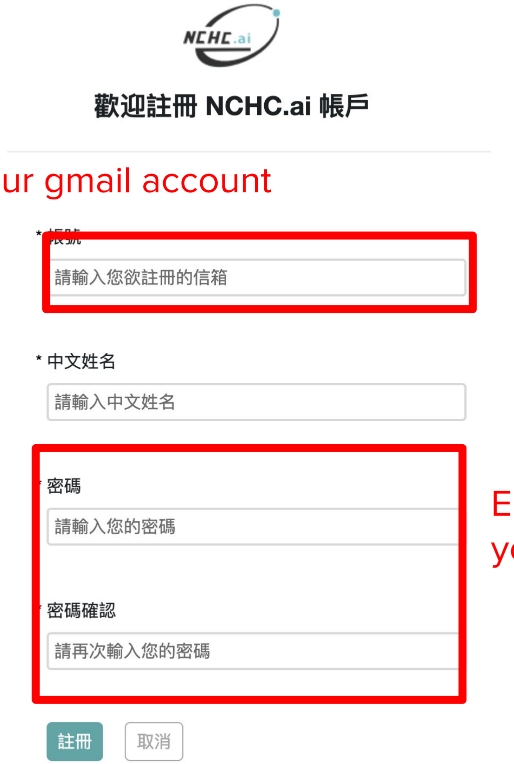
NCHC Container

- Webpage: https://portal.apps.edu-cloud.nchc.org.tw
- Register your account first
- GPU: RTX 3070
- Available time: Tuesday, Wednesday and Sunday 00:00-23:59
- Total available GPUs: 46
- Please stop your container if you aren't using it

Register

1

2



Your gmail account

Enter whatever you want

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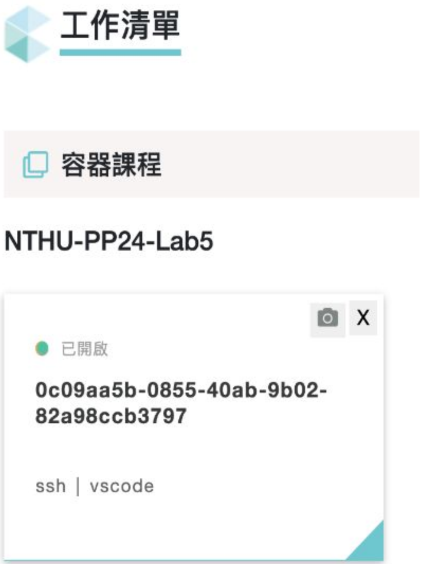
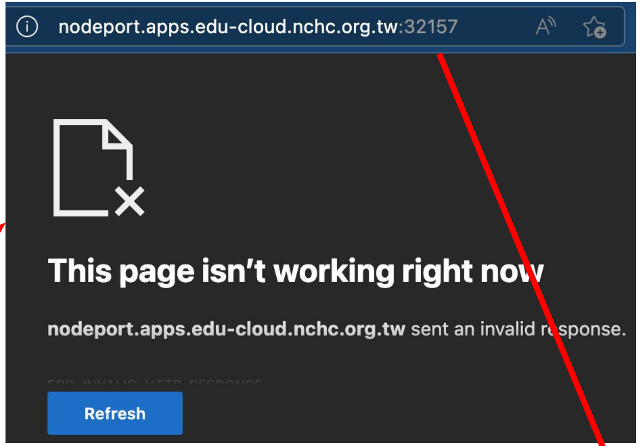
Start Container



Access the Container

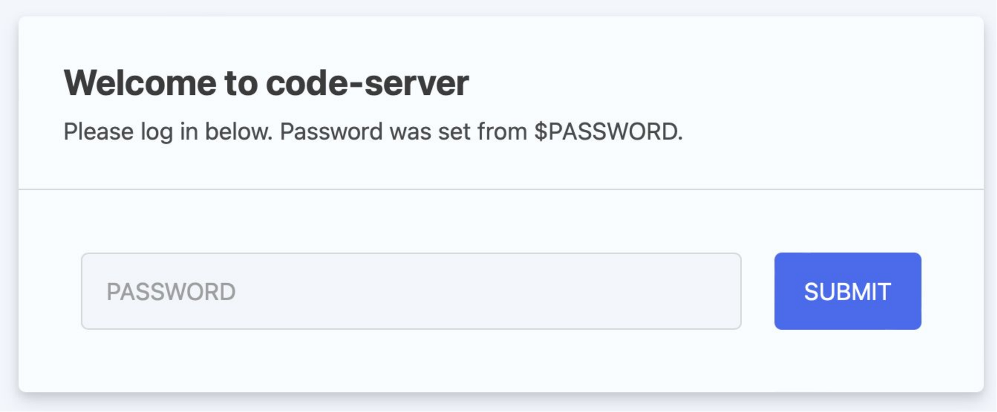
- SSH
  - The port number will be different
- Codeserver (the web version of vscode)
  - Click the “vscode” button



MobaXterm or Terminal:
ssh root@nodeport.apps.edu-cloud.nchc.org.tw -p 32157

User & Password

- User: root
- Password: student
  - The password of ssh and code-server is the same



First-time Setup Script

11/21 update

If you have already run this script, please run the new script again. If you haven't run it yet, make sure to run the new script as well. You must enter your Apollo CPU server username and password, not the GPU server credentials.

Open terminal in the container:

~~`bash <(curl -s https://apollo.cs.nthu.edu.tw/pp24/share/script/setup-remote.sh)`~~

```
bash <(curl -s https://apollo.cs.nthu.edu.tw/pp24/share/script/setup-remote-hw4.sh)
```

The script will execute the following commands:

- Set proper bash config for homework judger (e.g., hw4-remote-judge)
- Generate ssh key and install it on Apollo (you will be prompted to enter your Apollo account name and password)

Run this script only once, even you relaunched your container (since your personal data will be kept).

```
###############################
##     Installing SSH Key.    ###
###############################
Enter your username on apollo: pp24s085
/root/.ssh/id_rsa already exists.
Overwrite (y/n)? /usr/bin/ssh-copy-id: INFO: Source of key(s) to be installed: "/root/.ssh/id_rsa.pub"
The authenticity of host 'apollo-gpu.cs.nthu.edu.tw (140.114.91.189)' can't be established.
ED25519 key fingerprint is SHA256:5cV2dr2KzW4Iupn5g1e4xe+b0KV1T0UF1dEimOISCp4.
This key is not known by any other names
Are you sure you want to continue connecting (yes/no/[fingerprint])? yes
/usr/bin/ssh-copy-id: INFO: attempting to log in with the new key(s), to filter out any that are already installed
/usr/bin/ssh-copy-id: INFO: 1 key(s) remain to be installed -- if you are prompted now it is to install the new keys
(pp24s085@apollo-gpu.cs.nthu.edu.tw) Password:

Number of key(s) added: 1

Now try logging into the machine, with:   "ssh 'pp24s085@apollo-gpu.cs.nthu.edu.tw'"
and check to make sure that only the key(s) you wanted were added.

  % Total    % Received % Xferd  Average Speed   Time    Time     Time  Current
                                 Dload  Upload   Total   Spent    Left  Speed
100  3992  100  3992    0     0  48487      0 --:--:-- --:--:-- --:--:-- 48682
  % Total    % Received % Xferd  Average Speed   Time    Time     Time  Current
                                 Dload  Upload   Total   Spent    Left  Speed
100 18584  100 18584    0     0   216k      0 --:--:-- --:--:-- --:--:--  218k
###################################
##        Install completed      ###
## Please relogin the container ###
###################################
root@PP24:~#
```

Stop your container

- Please stop your container if you aren't using it; otherwise, other students may not have enough GPU resources
- Your files located under $HOME (/root/) will be preserved

NO MINING

Educational use only

Please cherish the computing resources we provided

Attention

Attention

- $\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$ $\mathbf{Q}, \mathbf{K}, \mathbf{V} \in \mathbb{R}^{N \times d}$

- Q: What we're focusing on.
- K: What features are available.
- V: What content is retrieved based on focus.

Attention

$$\boxed{\mathbf{S} = \mathbf{Q}\mathbf{K}^\top \in \mathbb{R}^{N\times N}}, \quad \mathbf{P} = \mathrm{softmax}(\mathbf{S}) \in \mathbb{R}^{N\times N}, \quad \mathbf{O} = \mathbf{P}\mathbf{V} \in \mathbb{R}^{N\times d},$$

$$\begin{bmatrix} \boxed{s_{11}} & s_{12} & s_{13} & s_{14} \\ s_{21} & s_{22} & s_{23} & s_{24} \\ s_{31} & s_{32} & s_{33} & s_{34} \\ s_{41} & s_{42} & s_{43} & s_{44} \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \\ q_{41} & q_{42} & q_{43} \end{bmatrix} \cdot \begin{bmatrix} k_{11} & k_{21} & k_{31} & k_{41} \\ k_{12} & k_{22} & k_{32} & k_{42} \\ k_{13} & k_{23} & k_{33} & k_{43} \end{bmatrix}$$

Attention

$$\mathbf{S} = \mathbf{Q}\mathbf{K}^\top \in \mathbb{R}^{N\times N}, \quad \boxed{\mathbf{P} = \mathrm{softmax}(\mathbf{S}) \in \mathbb{R}^{N\times N}}, \quad \mathbf{O} = \mathbf{P}\mathbf{V} \in \mathbb{R}^{N\times d},$$

$$\begin{bmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{21} & p_{22} & p_{23} & p_{24} \\ p_{31} & p_{32} & p_{33} & p_{34} \\ p_{41} & p_{42} & p_{43} & p_{44} \end{bmatrix} = \mathrm{softmax}\left(\begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ s_{21} & s_{22} & s_{23} & s_{24} \\ s_{31} & s_{32} & s_{33} & s_{34} \\ s_{41} & s_{42} & s_{43} & s_{44} \end{bmatrix}\right)$$

Attention

$$\mathbf{S} = \mathbf{Q}\mathbf{K}^\top \in \mathbb{R}^{N\times N}, \quad \mathbf{P} = \mathrm{softmax}(\mathbf{S}) \in \mathbb{R}^{N\times N}, \quad \boxed{\mathbf{O} = \mathbf{P}\mathbf{V} \in \mathbb{R}^{N\times d},}$$

$$\begin{bmatrix} \boxed{o_{11}} & o_{12} & o_{13} \\ o_{21} & o_{22} & o_{23} \\ o_{31} & o_{32} & o_{33} \\ o_{41} & o_{42} & o_{43} \end{bmatrix} = \begin{bmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{21} & p_{22} & p_{23} & p_{24} \\ p_{31} & p_{32} & p_{33} & p_{34} \\ p_{41} & p_{42} & p_{43} & p_{44} \end{bmatrix} \cdot \begin{bmatrix} v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \\ v_{31} & v_{32} & v_{33} \\ v_{41} & v_{42} & v_{43} \end{bmatrix}$$

Multi-Head Attention

- ❖ Rich Representations
- ❖ Efficient Parallelization
- ❖ E.g. emb_dim = 4096 -> num_heads = 32, head_size = 128

$$\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head_1}, ..., \mathrm{head_h})W^O$$
$$\text{where } \mathrm{head_i} = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

Causal Attention

❖ If you're predicting the next word in a sentence, the model shouldn't have access to future words beyond the current position.

$$\begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ s_{21} & s_{22} & s_{23} & s_{24} \\ s_{31} & s_{32} & s_{33} & s_{34} \\ s_{41} & s_{42} & s_{43} & s_{44} \end{bmatrix}$$

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

$$\text{Masked Scores}_{i,j} = \begin{cases} \frac{(QK^T)_{i,j}}{\sqrt{d_k}}, & \text{if } j \leq i \\ -\infty, & \text{if } j > i \end{cases}$$

$$\text{Masked Attention Weights}_{i,j} = \text{softmax}(\text{Masked Scores}_{i,j})$$

$$\text{Causal Attention}(Q, K, V) = \text{softmax}\left(\text{Mask}\left(\frac{QK^T}{\sqrt{d_k}}\right)\right)V$$

FlashAttention

FlashAttention - Overview

- Goal: avoid reading and writing the attention matrix to and from HBM.
  - Computing the softmax without access to the whole input.
  - Not storing the large intermediate attention matrix for the backward pass.

Algorithm 0 Standard Attention Implementation

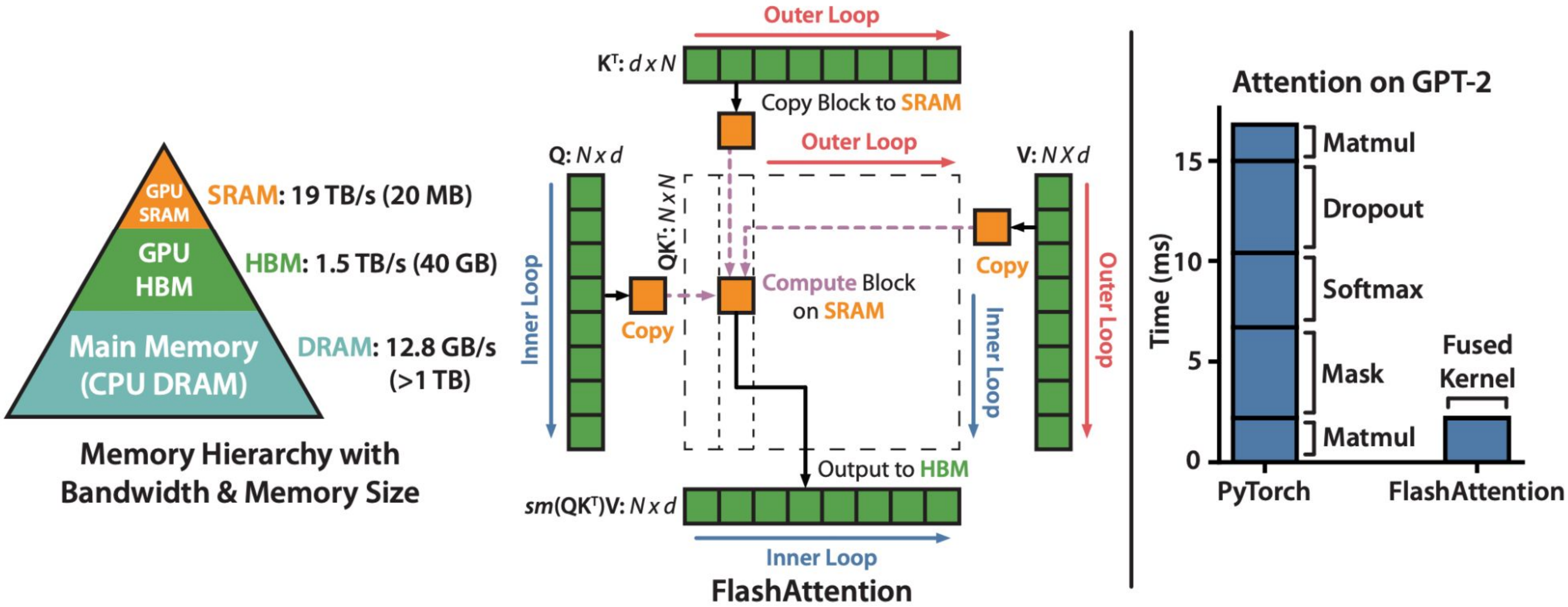
Require: Matrices $\mathbf{Q}, \mathbf{K}, \mathbf{V} \in \mathbb{R}^{N \times d}$ in HBM.

1: Load $\mathbf{Q}, \mathbf{K}$ by blocks from HBM, compute $\mathbf{S} = \mathbf{Q}\mathbf{K}^\top$, write $\mathbf{S}$ to HBM.
2: Read $\mathbf{S}$ from HBM, compute $\mathbf{P} = \mathrm{softmax}(\mathbf{S})$, write $\mathbf{P}$ to HBM.
3: Load $\mathbf{P}$ and $\mathbf{V}$ by blocks from HBM, compute $\mathbf{O} = \mathbf{P}\mathbf{V}$, write $\mathbf{O}$ to HBM.
4: Return $\mathbf{O}$.

FlashAttention - Method

- Tiling: split the input into blocks and make several passes over input blocks.
  - Matrix multiplication and pointwise operations are easy to handle.
  - SoftMax: need to maintain `m(x)`, `l(x)`.
- Recompute: store the softmax normalization factor in order to quickly recompute in the backward pass.

FlashAttention



FlashAttention - SoftMax

$$\operatorname{softmax}(x_i) = \frac{e^{x_i}}{\sum_{j=1}^{d} e^{x_j}}$$

$$m = \max_i (x_i); \quad \operatorname{softmax}(x_i) = \frac{e^{x_i - m}}{\sum_{j=1}^{d} e^{x_j - m}}$$

FlashAttention - SoftMax

$$m(x) := \max_i \quad x_i, \quad f(x) := \begin{bmatrix} e^{x_1 - m(x)} & \ldots & e^{x_B - m(x)} \end{bmatrix}, \quad \ell(x) := \sum_i f(x)_i, \quad \text{softmax}(x) := \frac{f(x)}{\ell(x)}.$$

For vectors $x^{(1)}, x^{(2)} \in \mathbb{R}^B$, we can decompose the softmax of the concatenated $x = \begin{bmatrix} x^{(1)} & x^{(2)} \end{bmatrix} \in \mathbb{R}^{2B}$ as:

$$m(x) = m(\begin{bmatrix} x^{(1)} & x^{(2)} \end{bmatrix}) = \max(m(x^{(1)}), m(x^{(2)})), \quad f(x) = \begin{bmatrix} e^{m(x^{(1)}) - m(x)} f(x^{(1)}) & e^{m(x^{(2)}) - m(x)} f(x^{(2)}) \end{bmatrix},$$

$$\ell(x) = \ell(\begin{bmatrix} x^{(1)} & x^{(2)} \end{bmatrix}) = e^{m(x^{(1)}) - m(x)} \ell(x^{(1)}) + e^{m(x^{(2)}) - m(x)} \ell(x^{(2)}), \quad \text{softmax}(x) = \frac{f(x)}{\ell(x)}.$$

FlashAttention - SoftMax

$$m_1 = max([1, 2]) = 2 \qquad m_2 = max([3, 4]) = 4 \qquad m = max(m_1, m_2) = 4$$

$$f_1 = [e^{1-2}, e^{2-2}] = [e^{-1}, e^0] \qquad f_2 = [e^{3-4}, e^{4-4}] = [e^{-1}, e^0] \qquad f = [e^{m_1 - m} f_1, e^{m_2 - m} f_2] = [e^{-3}, e^{-2}, e^{-1}, e^0]$$

$$l_1 = \sum f_1 = e^{-1} + e^0 \qquad l_2 = \sum f_2 = e^{-1} + e^0 \qquad l = e^{m_1 - m} l_1 + e^{m_2 - m} l_2 = e^{-3} + e^{-2} + e^{-1} + e^0$$

$$o_1 = \frac{f_1}{l_1} = \frac{[e^{-1}, e^0]}{e^{-1} + e^0} \qquad o_2 = \frac{f_2}{l_2} = \frac{[e^{-1}, e^0]}{e^{-1} + e^0} \qquad o = \frac{f}{l} = \frac{[e^{-3}, e^{-2}, e^{-1}, e^0]}{e^{-3} + e^{-2} + e^{-1} + e^0}$$

FlashAttention - Algorithm

Algorithm 1 FlashAttention

Require: Matrices $\mathbf{Q}, \mathbf{K}, \mathbf{V} \in \mathbb{R}^{N \times d}$ in HBM, on-chip SRAM of size M.

Set block sizes $B_c = \left\lceil \frac{M}{4d} \right\rceil, B_r = \min\left(\left\lceil \frac{M}{4d} \right\rceil, d\right)$.

Initialize $\mathbf{O} = (0)_{N \times d} \in \mathbb{R}^{N \times d}, \ell = (0)_N \in \mathbb{R}^N, m = (-\infty)_N \in \mathbb{R}^N$ in HBM.

Divide $\mathbf{Q}$ into $T_r = \left\lceil \frac{N}{B_r} \right\rceil$ blocks $\mathbf{Q}_1, \dots, \mathbf{Q}_{T_r}$ of size $B_r \times d$ each, and divide $\mathbf{K}, \mathbf{V}$ in to $T_c = \left\lceil \frac{N}{B_c} \right\rceil$ blocks $\mathbf{K}_1, \dots, \mathbf{K}_{T_c}$ and $\mathbf{V}_1, \dots, \mathbf{V}_{T_c}$, of size $B_c \times d$ each.

Divide $\mathbf{O}$ into T_r blocks $\mathbf{O}_i, \dots, \mathbf{O}_{T_r}$ of size $B_r \times d$ each, divide ℓ into T_r blocks $\ell_i, \dots, \ell_{T_r}$ of size B_r each, divide m into T_r blocks $m_1, \dots, m_{T_r}$ of size B_r each.

for $1 \le j \le T_c$ **do**

    Load $\mathbf{K}_j, \mathbf{V}_j$ from HBM to on-chip SRAM.

    for $1 \le i \le T_r$ **do**

        Load $\mathbf{Q}_i, \mathbf{O}_i, \ell_i, m_i$ from HBM to on-chip SRAM.

        On chip, compute $\mathbf{S}_{ij} = \mathbf{Q}_i \mathbf{K}_j^T \in \mathbb{R}^{B_r \times B_c}$.

        On chip, compute $\tilde{m}_{ij} = \mathrm{rowmax}(\mathbf{S}_{ij}) \in \mathbb{R}^{B_r}$, $\tilde{\mathbf{P}}_{ij} = \exp(\mathbf{S}_{ij} - \tilde{m}_{ij}) \in \mathbb{R}^{B_r \times B_c}$ (pointwise), $\tilde{\ell}_{ij} = \mathrm{rowsum}(\tilde{\mathbf{P}}_{ij}) \in \mathbb{R}^{B_r}$.

        On chip, compute $m_i^{\mathrm{new}} = \max(m_i, \tilde{m}_{ij}) \in \mathbb{R}^{B_r}$, $\ell_i^{\mathrm{new}} = e^{m_i - m_i^{\mathrm{new}}} \ell_i + e^{\tilde{m}_{ij} - m_i^{\mathrm{new}}} \tilde{\ell}_{ij} \in \mathbb{R}^{B_r}$.

        Write $\mathbf{O}_i \leftarrow \mathrm{diag}(\ell_i^{\mathrm{new}})^{-1}(\mathrm{diag}(\ell_i) e^{m_i - m_i^{\mathrm{new}}} \mathbf{O}_i + e^{\tilde{m}_{ij} - m_i^{\mathrm{new}}} \tilde{\mathbf{P}}_{ij} \mathbf{V}_j)$ to HBM.

        Write $\ell_i \leftarrow \ell_i^{\mathrm{new}}$, $m_i \leftarrow m_i^{\mathrm{new}}$ to HBM.

    end for

end for

Return $\mathbf{O}$.

Reference

- https://arxiv.org/pdf/2205.14135
- https://www.cvmart.net/community/detail/7943
- https://www.youtube.com/watch?v=eMlx5fFNoYc

Lab5 Assignment

Objective

- Evaluate the performance of attention mechanisms by comparing:
  - The original PyTorch implementation
  - The FlashAttention v2 implementation
- Analyze the benefits of FlashAttention and explore its advantages over the standard approach.
- Conduct benchmarking with varying parameters and compare the results to gain deeper insights.

Benchmark Script

- TA provide the Python benchmark script that does not require any modifications.
- Your task is to adjust only the parameters within the benchmark.
- The result will be outputted to a JSON file.
  - Execution time
  - FLOPs
  - Peak memory usage

{} benchmark_result.json ×

lab5 > {} benchmark_result.json > ...


```json
{
  "forward": {
    "time(s)": 0.007095515976349513,
    "FLOPS(TFLOPs/s)": 38.739664297876566
  },
  "backward": {
    "time(s)": 0.018877355754375456,
    "FLOPS(TFLOPs/s)": 36.40312638599925
  },
  "forward_backward": {
    "time(s)": 0.025972871730724968,
    "FLOPS(TFLOPs/s)": 37.04144402199095
  },
  "peak_memory_usage(MB)": 1288.00048828125
}
```

Benchmark Script

- Test following parameters and compare the results.
  - **batch_size**: int
  - **seq_len**: int
  - **num_heads**: int, (must be divisible by emb_dim)
  - **emb_dim**: int
  - **impl**: str, (choose between Pytorch and Flash2)
  - **causal**: bool

Preparation

- File are Located at `/tmp/lab5` on **NCHC**.
- The benchmark script is named `lab5.py`.
- Use `python lab5.py --help` to view detailed parameter descriptions.
- Important Notes:
  - Do not modify the source code.
  - Do not merge multiple tests into a single run, as this may result in incorrect output values.
- To run multiple tests, you can use a bash script for automation.

Workflow

- `cp -r /tmp/lab5 ~/lab5 && cd ~/lab5`
- `python lab5.py \`

```
    --batch_size 32 \
    --seq_len 1024 \
    --num_heads 32 \
    --emb_dim 2048 \
    --impl Flash2 \
    --causal \
    --repeats 30 \
    --output benchmark_result.json
```

Submission

- Plot the experimental data in a chart for better visualization.
- Analyze and explain your observations based on the collected data.
- Submit your report as a `lab5.pdf` file to eeclass before 11/28 23:59.
- Important Notes:
  - Get started as soon as possible since the NCHC platform is only accessible on Tuesday, Wednesday and Sunday.
  - Remember to stop your container when not in use.