Maincode

Skill Assessment

LLM training and optimisation

Teddy Lo
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Contents

Abstract

In this project, I optimise a large language model (LLM) by minimizing its validation loss using the GPT architecture. I study the impact of batch size on validation performance and implement variants of the attention layer, including Sparse Attention. The baseline model achieves a validation loss of 1.754, while the best-optimized model reaches 0.94398. Additionally, I implement various functions to streamline and improve the model development process, including experiment tracking with Weights & Biases, automated training offload using GitHub Actions, and a structured system for model development, tracking, and analysis.

Introduction

This project began with a simple Python training script for an autoregressive text generation model, using GPT as a template and trained on the julien040/hacker-news-posts dataset from Hugging Face. The dataset consists of Hacker News titles, which were split into training and validation sets using a fixed seed and ratio. The model was trained to predict the next token in the titles and evaluated on the validation set.

During the initial iteration of development, several challenges emerged that limited both efficiency and model performance:

1. **CPU-Only Computation & Manual Environment Constraints** *(see Appendix A for information)*
    - Training a ~27-million-parameter model on CPU required ~1 hours per run, restricting the ability to perform multiple experiments or hyperparameter sweeps.
    - Manual environment setup (configuring paths, Docker containers, and hyperparameters) added overhead and increased the risk of errors.
2. **Suboptimal Model Performance** *(see Appendix A for information)*
    - Both the GPT-2-based architecture and the training pipeline required further optimization to reduce validation loss, improve predictive accuracy, and ensure efficient convergence.
3. **Non-Modular Codebase**
    - The existing code lacked structure and modularity, complicating the integration of new components, architectures, or attention mechanisms.
4. **Inefficient Hyperparameter Exploration** *(see Appendix B for information)*
    - Long runtimes and manual setup made systematic evaluation of different hyperparameter configurations impractical.

5. **Absence of Monitoring and Logging Mechanisms** *(see Appendix B for information)*
   - The training process lacked a standardized monitoring system, reducing visibility into metrics, loss curves, and experiment reproducibility.

Related Work

Training Paradigm of Language Models

To optimise the performance of a language model, it is essential to understand the **training paradigm**. This includes how performance scales with **model size**, **dataset size**, and **compute resources**, as well as the influence of **batch size** on training dynamics. Mastery of these concepts provides the foundation for systematically exploring and testing model parameters.

Scaling Laws for language model [1]

This study examines the impact of several key factors on model performance using the WebText dataset:

- Model size(N)
- Dataset size (D)
- Compute (C) [Approximately $\approx 6 \times N \times Batch\_Size \times Number\_of\_optimisation\_steps$]

The key findings are:

1. **Performance depends strongly on scale, weakly on model shape**
   - Increasing model size and dataset size significantly reduces test loss, while adjusting model shape (depth vs. width) has less effect.
2. **Smooth power-law relationships**
   - Test loss decreases predictably according to power-law scaling with respect to model size (N), dataset size (D), and compute (C).
3. **Joint scaling of model and data**
   - To maximize performance, model size (N) and dataset size (D) must be scaled together. Scaling only, one leads to diminishing returns.
4. **Sample efficiency of larger models**
   - Larger models achieve the same loss levels in fewer optimization steps, making them more sample efficient.

5. **Compute efficiency**
    - When neither model size nor dataset size is the bottleneck, additional compute (C) yields predictable improvements in test loss.

Key takeaway: Model performance is governed by scaling laws. For any fixed dataset size and compute, there exists an **optimal model size**, too small underfits, too large wastes capacity, which can be found by systematic sweeps

An Empirical Model of Large-Batch Training [2]

A complementary study on the training paradigm of language models emphasizes the **empirical law of large-batch training**:

- **Gradient noise scale:** Batch size directly influences the variance (noise) in gradient estimates.
- **Exploration vs. convergence:**
    - Smaller batch sizes introduce more noise, encouraging the model to explore local minima.
    - Larger batch sizes reduce noise, allowing faster convergence but at the cost of potentially poorer generalization.
- **Dataset dependence:** The optimal batch size depends primarily on dataset size rather than model size.

In this project, these insights motivated systematic exploration of batch size under hardware constraints. Although the mathematical tools from the paper to precisely estimate optimal batch size were not applied, an initial **sweep test of batch size** was conducted as the first attempt at optimization.

Attention Variants

Speaking of current LLM architectures, Mixture-of-Experts (MoE) models are widely used, with examples including DeepSeek R1 and Grok. Sparse attention is commonly applied in MoE models, as it can **maintain or even improve performance** compared to full causal attention. By leveraging **sparse factorization**, sparse attention significantly **reduces memory and computation costs**, making it more efficient for large-scale models.

Generating Long Sequences with Sparse Transformers [3]

Sparse Attention [3] is a mechanism that reduces memory and computation costs to $O(n\sqrt{n})$. Two factorized schemes are commonly used: **strided** and **fixed**. In strided attention, one head attends to a local window of the previous l tokens, while another head attends to every l-th token further back, capturing both short- and long-range dependencies. In fixed attention, one head focuses on tokens within the same block of size l, while the other attends to a fixed set of "summary" positions in each block, efficiently summarizing local context. These mechanisms allow the model to retain important information without the quadratic cost of full self-attention. According to the paper, **fixed attention is particularly beneficial for text generation tasks**, improving efficiency while maintaining or enhancing performance.

Sparser is Faster and Less is More: Efficient Sparse Attention for Long-Range Transformers [4]

The core idea of this paper, SparseK Attention Layer, is to select a **constant number of key-value (KV) pairs** per query, resulting in **linear time complexity** and a **constant memory footprint** during generation.

Key components:

- **Scoring Network:** output the importance score of each KV pair without needing access to all queries.
- **Differentiable Top-k Mask Operator (SPARSEK):** Produces a soft, differentiable mask over KV pairs, enabling gradient-based optimization for efficient, learnable attention.

Although SPARSEK Attention theoretically supports a fully linear-time formulation, my current implementation only realizes a reduced-complexity variant with $O(m\ log(m)\ )$ efficiency, where m is the number of key–value pairs.

Experiment

Data Analysis [6]

Before training, the dataset was thoroughly explored to understand its structure, tokenization behaviour, and potential challenges. Key steps and findings are summarized below:

Dataset Inspection

- Loaded both training and validation titles.
- Checked dataset lengths before and after tokenization.
- Verified the first 10 training IDs to ensure correct loading.

Longest Title Strings

- **Training set:** Longest string = 98 characters, at index 6099:
  "Rough silicon nanowires potentially allow much more efficient waste-heat to electricity conversion"
- **Validation set:** Longest string = 91 characters, at index 229:
  "Official Google Blog: 'This site may harm your computer' on every search result??"

Longest Tokenized Titles

- **Training set:** Maximum token length = 68, title: *"ZalgoScript"*
- **Validation set:** Maximum token length = 44, title: *"Bangladeshi model Farhana Akhtar Nisho (ফারহানা আখতার নিশু) hot and sexy photo"*
- **Observation:** Titles with non-English or visually obfuscated characters are harder to encode with BPE, resulting in longer token sequences.

Vocabulary and Token Statistics

	Unique words	Unique tokens
Training	25,516	14,403
Validation	4,177	4,669
Combined	27,707	14,751

Note:

- The number of unique words in combined is slightly higher than training alone since BPE concatenates characters rather than recognizing full words.
- The number of unique tokens is just below the defined vocabulary size parameter (**16,000**), which corresponds to the output dimension of the model's final layer.
- Tokens in validation not seen in training: **348**.

Result

Initial Iteration: (see Appendix C)

Observing the training loss graph, there is **noticeable noise**, indicating variability in gradient estimates likely caused by a relatively small batch size for this dataset. While this is not inherently problematic for training neural networks, given the limited number of epochs, the current batch size may not be optimal. Therefore, the first step is to determine the optimal batch size for this dataset, motivating a systematic sweep over different batch sizes.

Secondly, the validation loss is slightly above the baseline, suggesting that there is room for improvement in the current architecture. The validation loss generally follows the same trend as the training loss; however, it is important to note **that the training loss ends at 8.32, while the validation loss is 1.78**, indicating a substantial gap between the two.

Second Iteration: (see Appendix D)

After sweeping the batch size, the validation loss decreases as the batch size increases. This suggests that **an ideal batch size for this dataset is 256 with validation loss 1.594,** which was subsequently included as a sweep parameter in later GPT experiments alongside other hyperparameters. Larger batch sizes make it easier for the model to approach a global minimum, as the model can consider more information at each step and better estimate the general direction of the gradient. Notably, the validation loss for batch size 256 starts around 1.8, compared to approximately 2 for smaller batch sizes. Additionally, the noisiness observed in the training loss decreases as the batch size increases, reflecting a lower gradient noise ratio.

Third Iteration: (see Appendix E)

In this GPT parameters sweep, the validation loss reached **1.27**, a significant improvement over the original **1.78**. The sweep tested batch sizes of 128 and 256, but only the runs with batch size 128 appeared in the dashboard, as all runs with batch size 256 crashed due to GPU out-of-memory errors. Scaling up the GPT model improved performance, supporting a key finding from the scaling laws: performance scales strongly with model size. The top 30 runs achieved parameter counts between **3,667,200 and 12,059,648**, with the best performance observed at **6–8 layers**. Models with either higher or lower numbers of layers performed worse, illustrating another central point of the scaling laws: under a fixed dataset size, increasing model size beyond a certain point lead to a performance bottleneck unless the dataset is also scaled accordingly.

Fourth Iteration: (see Appendix F)

Based on experience from previous runs, I attempted to reduce memory usage by adopting variable dimensions in a GPT-UNet–like architecture, aiming to decrease the number of parameters and enable a batch size of 256. However, this approach was unsuccessful. To diagnose the issue, I implemented memory estimation functions to monitor GPU usage and confirmed that the model's memory footprint itself was within bounds. While the **n_layer depth remained within 6–8**, consistent with earlier findings, the variable-dimension design significantly degraded performance, with the best validation loss plateauing around **1.55**. Overall, this sweep neither provided useful insights nor resolved the memory bottleneck observed in earlier experiments.

Fifth Iteration: (see Appendix G)

During exploratory data analysis (EDA) of the dataset and task, it became evident that full causal self-attention was not always necessary for this text generation problem. Key observations included:

- **Local dependencies dominate** – Predictions mainly rely on relationships among nearby tokens within a title.
- **End-of-sequence classification** – Generation largely reduces to deciding whether to end the sequence or extend it, which does not require global context.
- **Independence across samples** – Each title is independent, so modelling long-range dependencies across samples is unnecessary.

Given these properties, full causal self-attention introduces **quadratic complexity** without meaningful performance benefits. In contrast, **sparse attention focuses compute on relevant local dependencies,** offering a more efficient solution.

A parameter sweep on sparse attention was conducted using a not-yet fully optimized GPT model. Validation losses **ranged between 1.25 and 1.285**, demonstrating a measurable improvement in efficiency and performance. The best results were obtained with **an intermediate dimension of 64 and 8 attention heads**, even though these values were not at the edges of the tested parameter ranges.

Based on these results, the best-performing sparse attention configuration was integrated into the GPT configuration for subsequent training runs.

Sixth Iteration: (see Appendix H)

Building on the success of sparse attention in the unoptimized GPT runs, I selected one of the top-performing parameter configurations and integrated it into the GPT architecture. By sweeping both **model parameters** and **batch sizes**, I achieved a validation loss of **0.94 with a batch size of 256**, a measurable improvement over previous run.

However, some attempts with a batch size of **256** frequently failed due to **out-of-memory (OOM) errors**. This highlighted that the **fundamental memory constraint remained unresolved**, even with sparse attention providing computational efficiency.

To investigate, I analysed inference and training memory usage. During the analysis, I consulted the Ultrascale Playbook (Hugging Face Spaces) which indicates that in many large-scale training setups, the majority of GPU memory is taken up by optimizer state rather than the model's parameter storage. This insight guided my decision to focus on mixed precision, optimizer-level tweaks, and limiting batch size to avoid OOM errors.

As a result, I adopted a **batch size of 128** for stable runs while continuing to explore **optimizer-level techniques** (e.g., state sharding, memory-efficient optimizers, mixed precision) to further reduce memory usage and unlock larger-scale consistent training.

Seventh Iteration: (see Appendix I)

During training, **out-of-memory (OOM) errors** initially constrained the feasible model size and batch configuration. To address this, I investigated and applied two effective strategies:

1. **Environment configuration** – Setting PYTORCH_CUDA_ALLOC_CONF=expandable_segments:True allowed CUDA memory segments to grow dynamically, reducing fragmentation.
2. **Automatic mixed precision (AMP)** – Enabling torch.amp lowered memory requirements by storing activations in lower precision while maintaining numerical stability.

Together, these techniques **alleviated the OOM bottleneck** and **enabled stable training of a 3M-parameter model with a batch size of 256**. With these optimizations in place, I was also able to scale up to ~4M parameters at the same batch size without encountering OOM issues.

Additional: (see Appendix J)

To improve performance, I implement an attention layer with lower memory and time complexity. **SparseK Attention** further reduces memory complexity to $O(m \log(m))$. By employing a linear projection and the SparseK operation,a dynamic masking function that produces a differentiable top-k mask—this approach makes attention less dense while remaining efficient. Intuitively, it can improve performance and accelerate training by focusing computation on the most relevant elements while reducing memory overhead.

Implementing SparseK Attention is challenging because no reference code is available. By carefully following the paper and leveraging assistance from AI, I was able to successfully implement this method. Additionally, this process enhanced my understanding of transformer architectures and the potential of gradient-based masking operators. While the improvement in task performance is not drastic, this is mainly due to the relatively small size of the model used in this experiment.

Code Design

Abstract Level Overview:

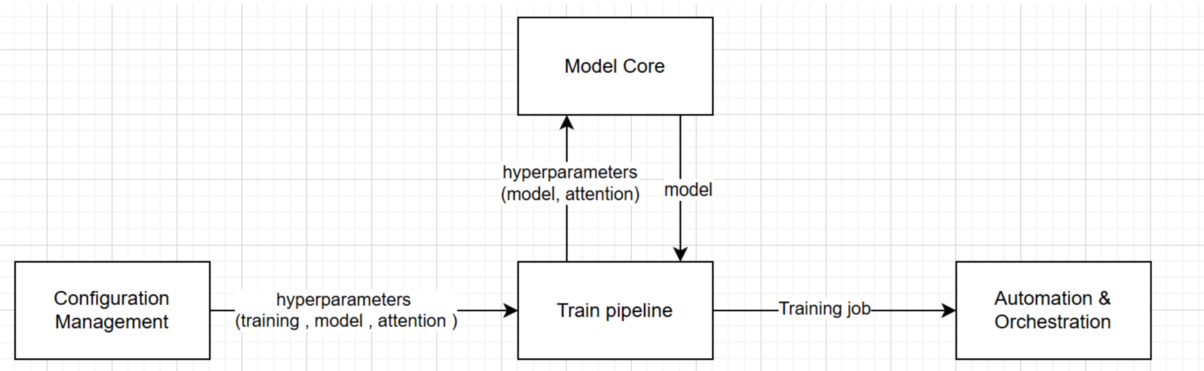
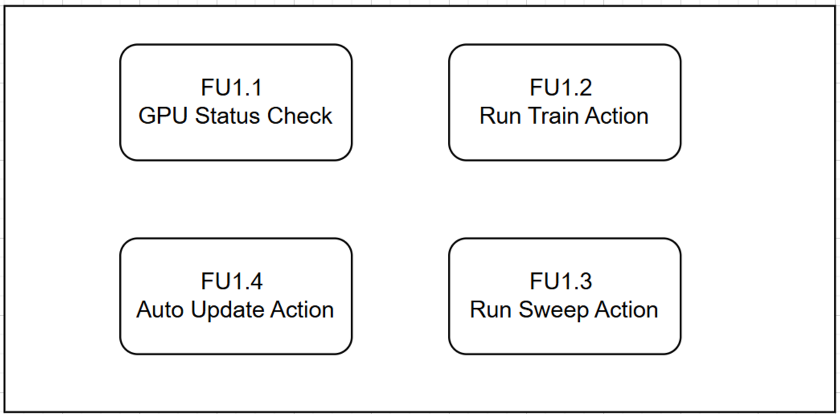


Figure 1 functional flow diagram of the training and optimisation system

Functional Unit 1: Automation & Configuration

Problem addressed: CPU-Only Computational & Manual Environment Constraints



Short summary:

This unit automates and manages the execution of training and experimentation workflows. By leveraging **GitHub Actions, Docker, and GPU acceleration**, it ensures **reproducible environments, streamlined setup, and efficient monitoring**, effectively serving as a **lightweight MLOps** layer for rapid iteration and reliable experiment orchestration.

Subunits:

- GPU Status Check *(See Appendix K for code and output)* – monitors GPU availability and memory usage to ensure resources are ready for training.
- Training Functions *(See Appendix L for code)* – executes model training in a reproducible, containerized environment.
- Sweep Functions *(See Appendix L for code)* – automates hyperparameter tuning through W&B sweeps with full logging and tracking.
- Update Mechanism *(See Appendix M for code)* – keeps the self-hosted runner synchronized with the latest codebase, enabling smoother CI/CD workflows.

Functional Unit 2: Configuration Management

Problem addressed: Inefficient Hyperparameter Exploration

Short Summary:

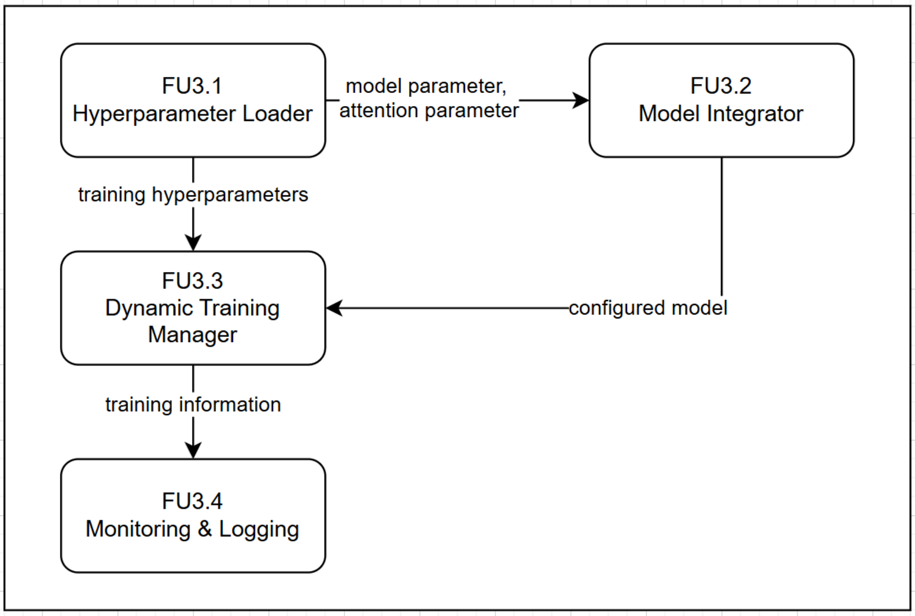
This unit **centralizes all experiment settings**, including base hyperparameters, sweep configurations, and best-performing (SOTA) configurations, ensuring reproducibility, clarity, and easy management of training experiments without relying on manual flags or ad-hoc changes.

Subunits:

- All experiment settings *(see Appendix N for hierarchy and code sample)*, including:
  - Sweep configurations, Base hyperparameters configuration, SOTA configuration

Functional Unit 3: Train pipeline

Problem addressed: Absence of Monitoring and Logging Mechanisms, Non-Modular Codebase



Short Summary:

This unit **orchestrates end-to-end training by reading hyperparameters from YAML configuration files and setting up runs accordingly**. It dynamically interacts with the **Model Core** to build models with the requested architecture and attention layers. The pipeline supports flexible schedules, optimizers, and training optimization techniques, while **integrating monitoring library for monitoring and logging,** making training modular, reproducible, and adaptable to new experiments.

Subunits:

- Configurable Training Framework *(see Appendix O for code)* – Reads base hyperparameters, sweep configurations, and SOTA configs from YAML files and passes configuration to Model Core to build the appropriate architecture and attention layers.
- Monitoring and Logging *(see Appendix P for code)* – Supports multiple schedulers, optimizers, and mixed-precision training.

Functional Unit 4: Model Core

Problem address: Non-Modular Codebase, Suboptimal Model Performance

Short Summary:

The Model Core contains the system's fundamental components—architecture, attention mechanisms, and tokenizer. It functions as the computational engine, **dynamically building models according to configurations provided by the Training Pipeline**. A modular design is critical, enabling flexible integration of new architectures, attention variants, and tokenization strategies.

Subunits:

- Memory Estimation *(see Appendix Q for code)* – Estimates memory usage per layer and overall model, helping detect and prevent out-of-memory errors.
- Configurable Models and Layers *(see Appendix Q for code)* – Provides flexible configuration classes that control architecture parameters and manage dependencies across layers.
- Model Organisation *(see Appendix Q for code)* – Establishes a clear class hierarchy to structure models, making the codebase easier to extend and maintain.

References

[1] Kaplan, J., McCandlish, S., Henighan, T., Brown, T. B., Chess, B., Child, R., Gray, S., Radford, A., Wu, J., & Amodei, D. (2020). Scaling Laws for Neural Language Models. *arXiv preprint arXiv:2001.08361*. https://arxiv.org/abs/2001.08361

[2] McCandlish, S., Kaplan, J., & Amodei, D. (2018). *An Empirical Model of Large-Batch Training*. arXiv preprint arXiv:1812.06162. https://www.alphaxiv.org/abs/1812.06162

[3] Child, R., Gray, S., Radford, A., and Sutskever, I. (2019). Generating Long Sequences with Sparse Transformers. *arXiv preprint arXiv:1904.10509*.

[4] Chao Lou, Zixia Jia, Zilong Zheng, and Kewei Tu. "Sparser is Faster and Less is More: Efficient Sparse Attention for Long-Range Transformers." *arXiv preprint arXiv:2406.16747*, 2024.

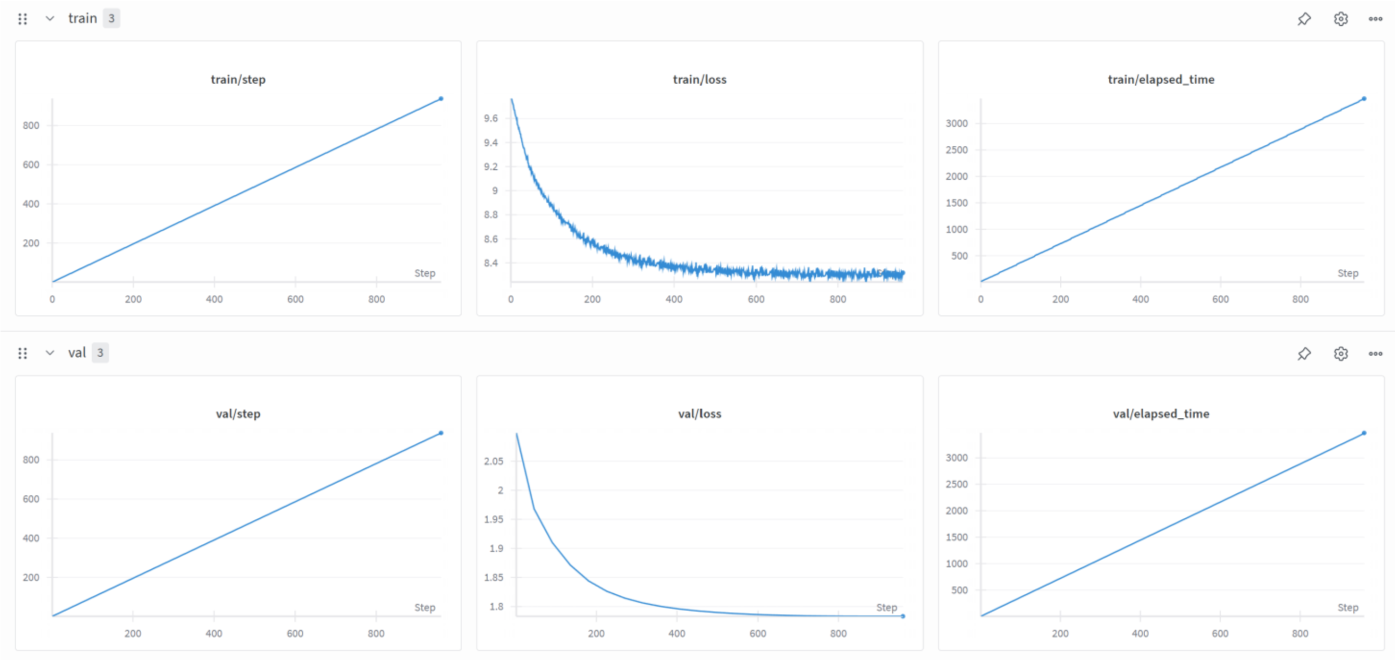
[6] https://github.com/tedasdf/mainrun/blob/main/mainrun/EDA.ipynb

Appendix

Appendix A

https://github.com/tedasdf/mainrun/actions/runs/17524976010/job/49774162371

hyperparameters_configured: seed=1337, epochs=7, val_frac=0.1, num_titles=100000, vocab_size=16000, context_length=128, log_file=./logs/mainrun.log, model_architecture=gpt, batch_size=64, lr=0.005, weight_decay=0.1, scheduler=cosine, optimizer=sgd, evals_per_epoch=3, amp_bool=False, device=cpu device_info: device=cpu ,[938/938] validation_step: loss=1.783221 time=3473.00s



Appendix B

https://github.com/MaincodeHQ/mainrun/blob/main/mainrun/train.py

Inefficient Hyperparameter Exploration

```
@dataclass
class Hyperparameters:
    block_size: int = 128
    batch_size: int = 64
    vocab_size: int = 16_000
    n_layer: int = 6
    n_head: int = 8
    d_model: int = 512
    dropout: float = 0.1
    lr: float = 6e-3
    weight_decay: float = 0.0
    evals_per_epoch: int = 3

    epochs: int = 7
    seed: int = 1337
    num_titles: int = 100_000
    val_frac: float = 0.10
    log_file: str = "./logs/mainrun.log"
```

Absence of monitoring and visualisation

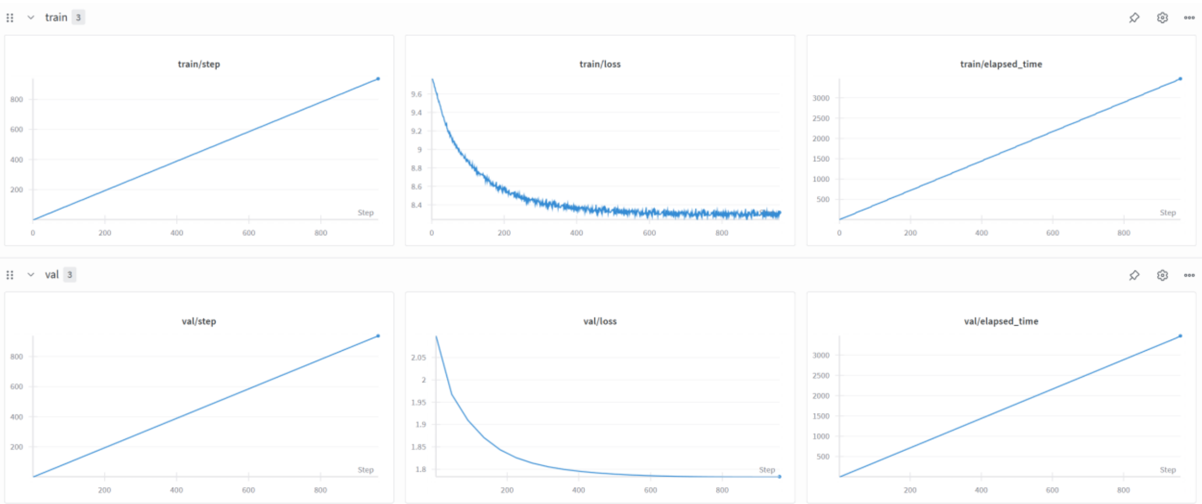
```python
def configure_logging(log_file: str):
    Path(log_file).parent.mkdir(parents=True, exist_ok=True)

    file_handler = open(log_file, 'w')

    structlog.configure(
        processors=[
            structlog.stdlib.filter_by_level,
            structlog.stdlib.add_logger_name,
            structlog.stdlib.add_log_level,
            structlog.stdlib.PositionalArgumentsFormatter(),
            structlog.processors.TimeStamper(fmt="iso"),
            structlog.processors.StackInfoRenderer(),
            structlog.processors.format_exc_info,
            structlog.processors.UnicodeDecoder(),
            structlog.processors.JSONRenderer()
        ],
        context_class=dict,
        logger_factory=structlog.stdlib.LoggerFactory(),
        cache_logger_on_first_use=True,
    )

    class DualLogger:
        def __init__(self, file_handler):
            self.file_handler = file_handler
            self.logger = structlog.get_logger()

        def log(self, event, **kwargs):
            log_entry = json.dumps({"event": event, "timestamp": time.time(), **kwargs})
            self.file_handler.write(log_entry + "\n")
            self.file_handler.flush()

            if kwargs.get("prnt", True):
                if "step" in kwargs and "max_steps" in kwargs:
                    tqdm.write(f"[{kwargs.get('step'):>5}/{kwargs.get('max_steps')}] {event}: loss={kwargs.get('loss', 'N/A'):.6f} time={kwargs.get('elapsed_time', 0):.2f}s")
                else:
                    parts = [f"{k}={v}" for k, v in kwargs.items() if k not in ["prnt", "timestamp"]]
                    if parts:
                        tqdm.write(f"{event}: {', '.join(parts)}")
                    else:
                        tqdm.write(event)

    return DualLogger(file_handler)

logger = None
```

Appendix C

Configuration

https://github.com/tedasdf/mainrun/blob/main/mainrun/config/hyperparameter_config/hyperparams.yaml

Wandb display

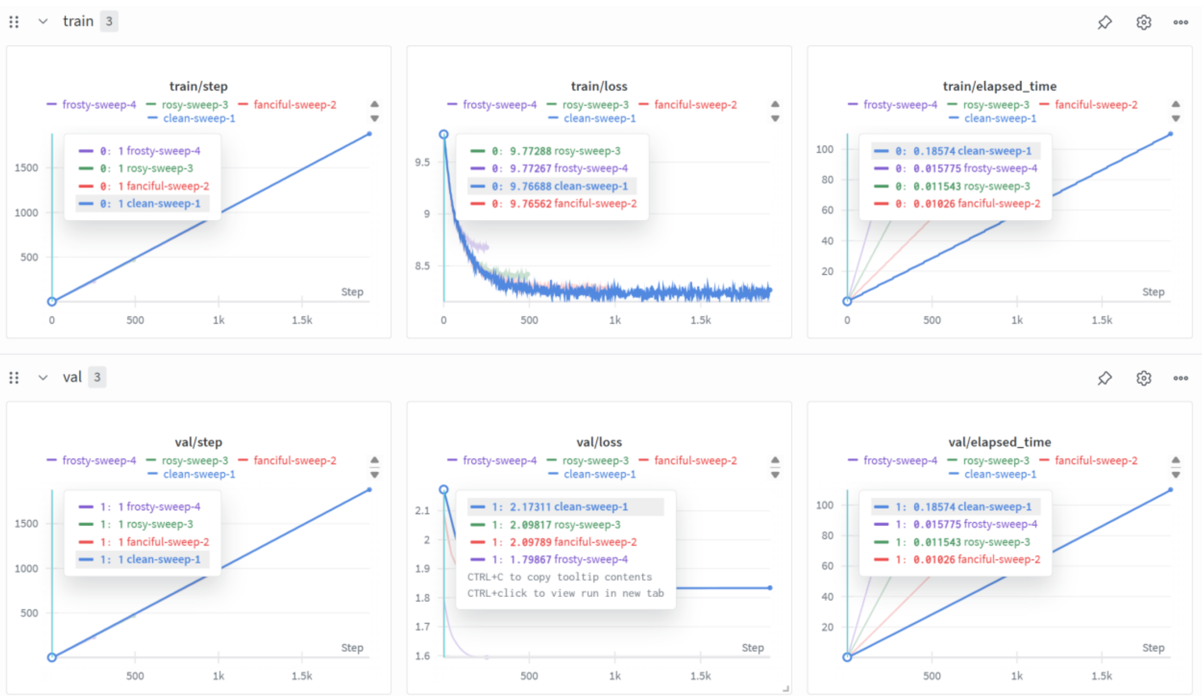


Model validation loss: [938/938] validation_step: loss=1.783221 time=3473.00s

Appendix D

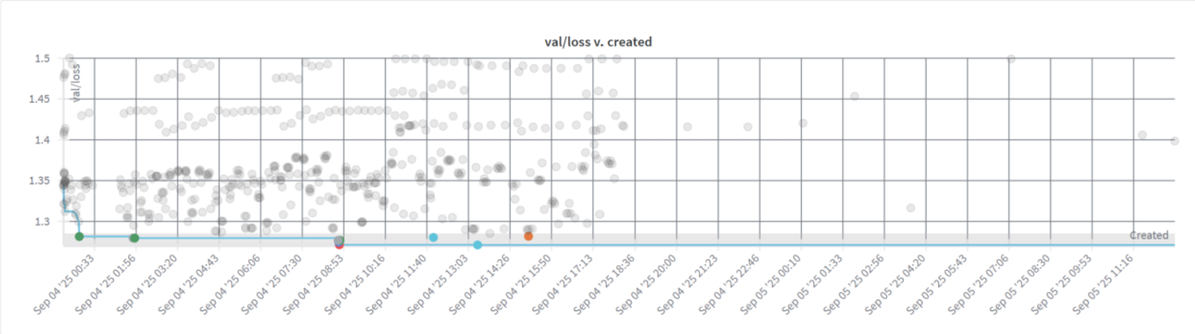
	Batch size	Model Validation loss
young-sweep-1	32	1.834
eager-sweep-2	64	1.778
noble-sweep-3	148	1.805
icy-sweep-4	256	1.594

Initial Validation loss

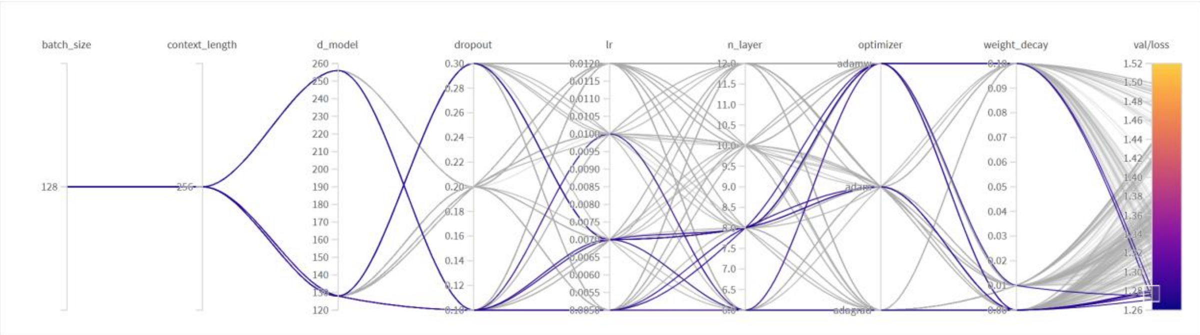


Appendix E

Validation loss distribution



Sweep distribution diagram

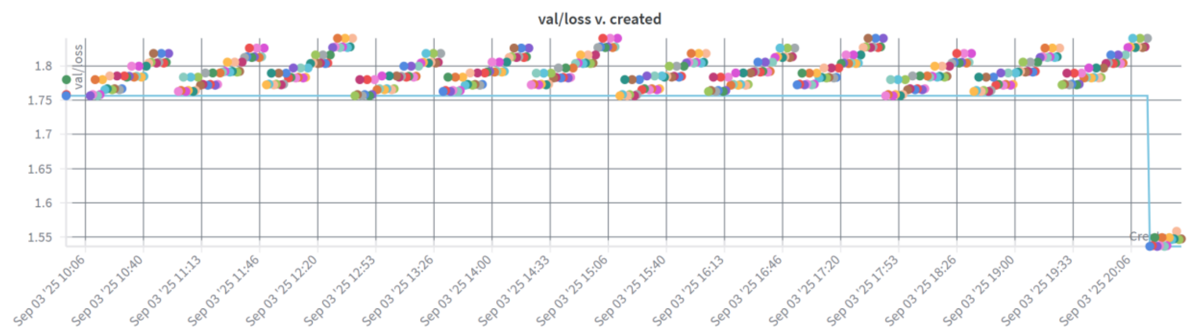


Sweep Configuration

https://github.com/tedasdf/mainrun/blob/main/mainrun/config/sweep_config/sweep_gpt_old.yaml

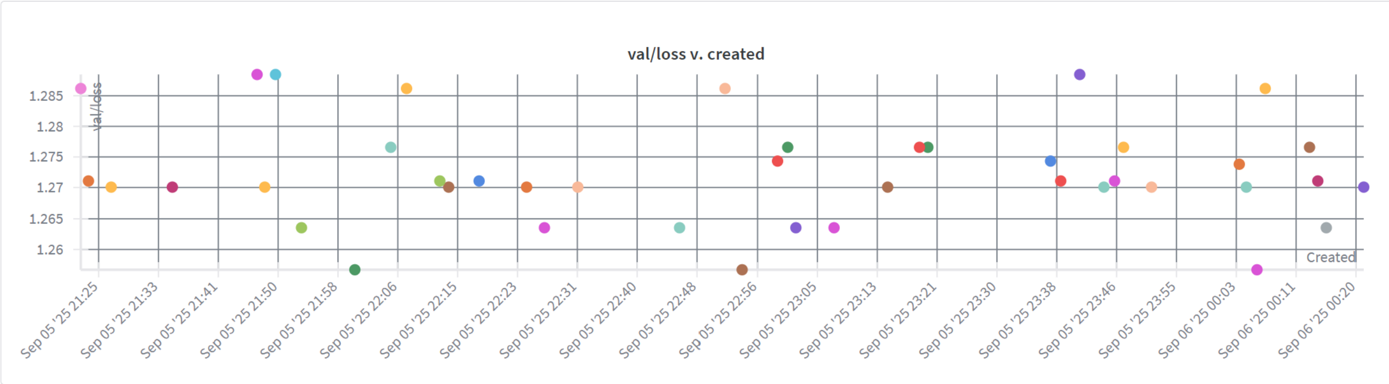
Appendix F

https://github.com/tedasdf/mainrun/blob/main/mainrun/config/sweep_config/sweep_unet_old.yaml



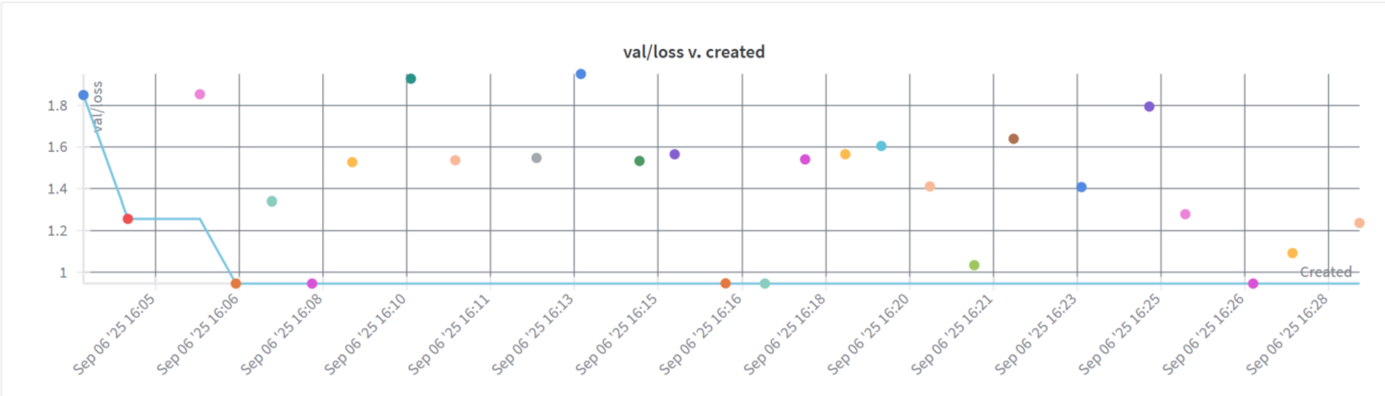
Appendix G

Configuration :https://github.com/tedasdf/mainrun/blob/main/mainrun/config/sweep_config/sweep_gpt_sparse.yaml



Appendix H

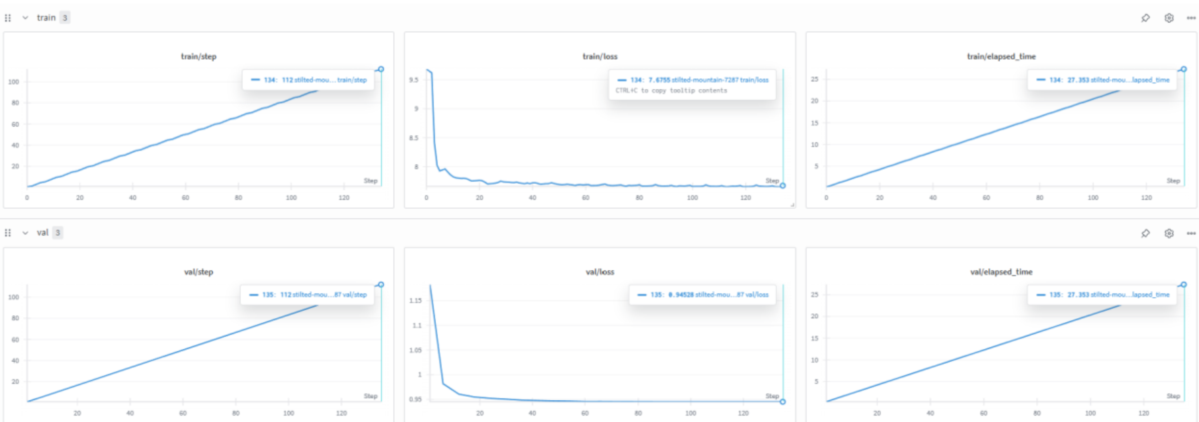
Configuration:https://github.com/tedasdf/mainrun/blob/main/mainrun/config/sweep_config/sweep_gpt_new.yaml



Appendix I

Configuration:

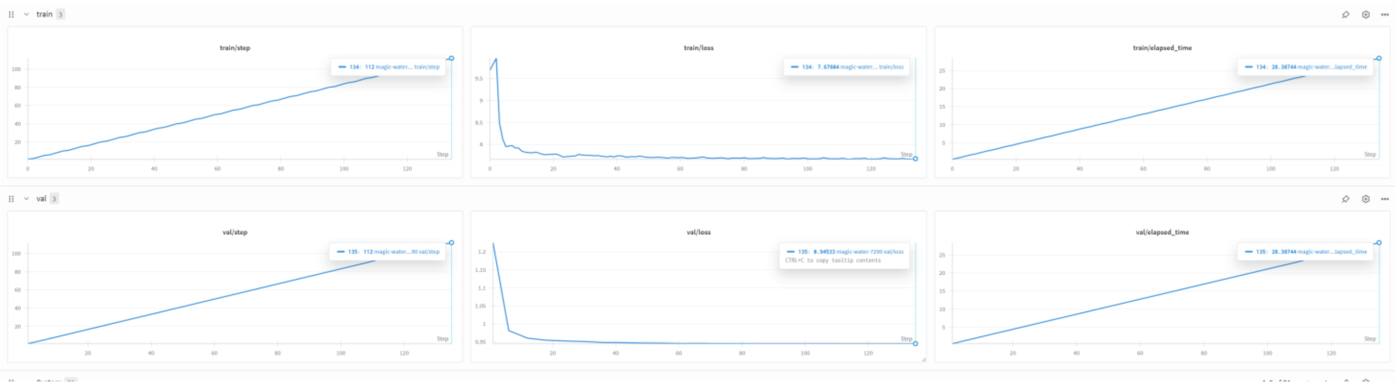
https://github.com/tedasdf/mainrun/blob/main/mainrun/config/training.yaml



Appendix J

Configuration:

Train log : https://github.com/tedasdf/mainrun/actions/runs/17572561402/job/49911287854

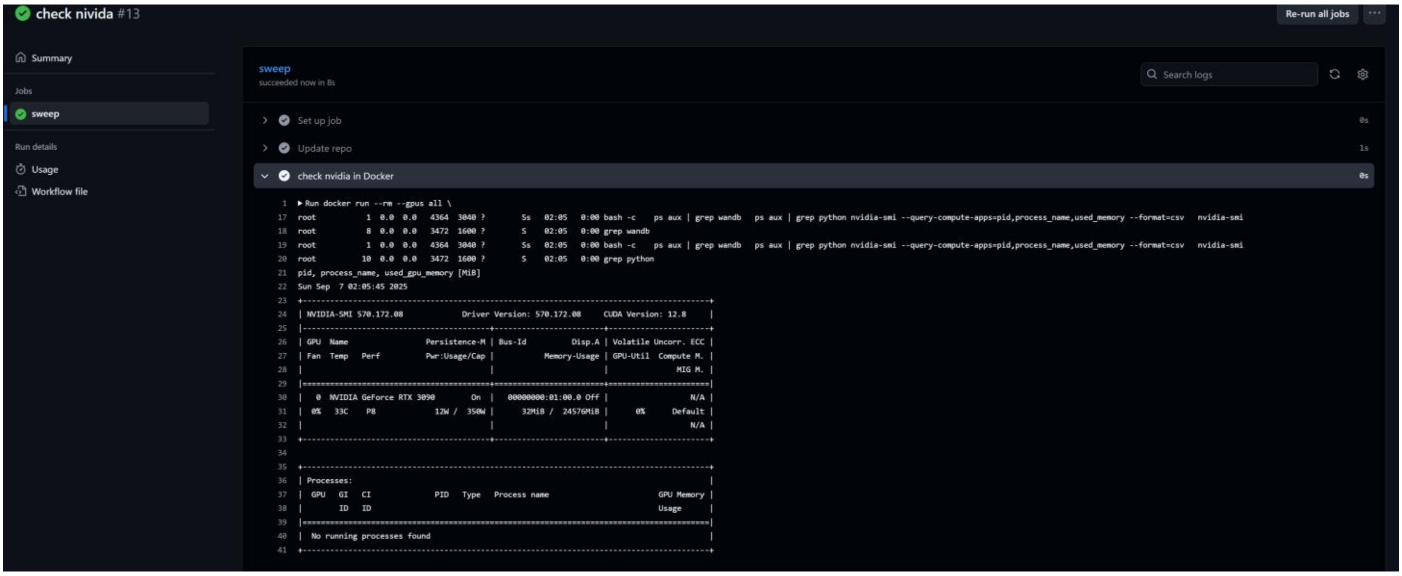


Appendix K

Code for check nvidia (.github/workflows/checknvidia.yml)

```
name: check nivida

on:
  workflow_dispatch:   # Trigger manually

jobs:
  sweep:
    runs-on: [self-hosted, x64, linux, docker]

    steps:
      - name: Update repo
        run: |
          cd /home/labadmin/Documents/mainrun
          git reset --hard
          git pull origin main

      - name: check nvidia in Docker
        run: |
          docker run --rm --gpus all \
          -v /home/labadmin/Documents/mainrun:/workspace \
          -w /workspace/mainrun \
          --env-file /home/labadmin/Documents/mainrun/.env \
          -e WANDB_PYTHON_EXECUTABLE=/usr/bin/python3 \
          -e PYTHONPATH=/workspace/mainrun \
          mainrun-env \
          bash -c "
            ps aux | grep wandb
            ps aux | grep python
          nvidia-smi --query-compute-apps=pid,process_name,used_memory --format=csv


          nvidia-smi"
```

Workflow page



Check Nvidia Action: https://github.com/tedasdf/mainrun/actions/workflows/checknvidia.yml

Appendix L

Code for Train Model (.github/workflows/train.yml , github/workflows/sweep.yml)

- due to the similarity of the code of both sweep and train, only code of train model is displayed.

```yaml
name: Train Model

on:
  workflow_dispatch:    # Run manually

jobs:
  train:
    runs-on: [self-hosted, x64, linux, docker]

    steps:
      - name: Update repo
        run: |
          cd /home/labadmin/Documents/mainrun
          git reset --hard
          git pull origin main

      - name: Run training in Docker
        run: |
          docker run --rm --gpus all \
            -v /home/labadmin/Documents/mainrun:/workspace \
            -w /workspace \
            --env-file /home/labadmin/Documents/mainrun/.env \
            -e PYTORCH_CUDA_ALLOC_CONF=expandable_segments:True \
            mainrun-env-new \
              bash -c " git config --global --add safe.directory /workspace && \
                       git config --global user.email 'teedsingyau@gmail.com' && \
                       git config --global user.name 'Ted Lo' && \
                       task train"
```

Train Model Action: https://github.com/tedasdf/mainrun/actions/workflows/train.yml

Sweep Action: https://github.com/tedasdf/mainrun/actions/workflows/sweep.yml

Appendix M

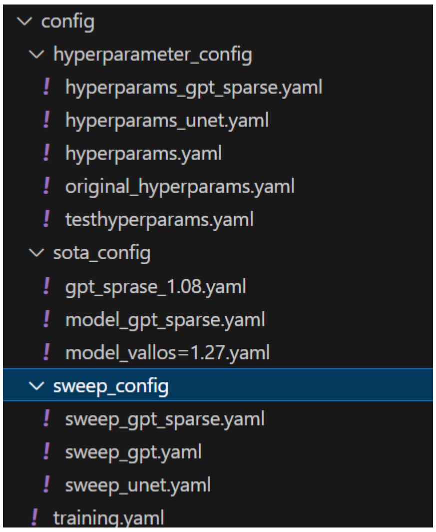
Code for Auto Update Code (.github/workflows/update.yml)

```yaml
name: Auto Update Code

on:
  push:
    branches:
      - main   # run only when you push to main

jobs:
  update:
    runs-on: [self-hosted, x64, linux, docker]   # your self-hosted runner
    steps:
      - name: Pull latest code safely using PAT
        env:
          GITHUB_TOKEN: ${{ secrets.PAT_TOKEN }}  # PAT stored as secret
        run: |
          cd /home/labadmin/Documents/mainrun
          git remote set-url origin https://$GITHUB_TOKEN@github.com/tedasdf/mainrun.git
          git fetch origin
          git reset --hard origin/main
          git clean -fd -e .env
```

Auto Update Code Action: https://github.com/tedasdf/mainrun/actions/workflows/update.yml

Appendix N

Hierarchy of Configuration Management



Sample Sweep configuration

```yaml
program: train.py
method: random   # or grid, or bayes
metric:
  name: val/loss
  goal: minimize
parameters:
  hyperparams.lr:
    values: [ 0.02 , 0.017, 0.012]
  hyperparams.batch_size:
    values: [ 64, 128 , 256]
  hyperparams.context_length:
    values:  [256]
  hyperparams.optimizer:
    values: ["adamw", "adagrad"]
  hyperparams.weight_decay:
    values: [ 0.1  , 0.15, 0.3, 0.5]
  model_configs.gpt.dropout:
    values: [0.1, 0.3 , 0.4]
  model_configs.gpt.d_model:
    values: [ 128, 256]
  model_configs.gpt.n_layer:
    values: [ 6, 8]

  model_configs.gpt.init_method:
    values: ['xavier' , 'normal' , 'kaiming', 'uniform']
```

Hyperparameter sample

```yaml
hyperparams:
  #############################################
  # FIXED hyperparameters
  #############################################
  seed: 1337
  epochs: 7
  val_frac: 0.10
  num_titles: 100000
  vocab_size: 16000 # Vocabulary size of the tokenizer
  context_length: 256
  ##############################################
  # CHANGEABLE hyperparameters
  ##############################################
  model_architecture: "gpt" # gpt, unet_gpt
  log_file: "./logs/mainrun.log"
  ###############################################
  # Training hyperparameters
  ###############################################
  batch_size: 256
  lr: 0.02
  weight_decay: 0.5
```

```yaml
  scheduler: "cosine" # none, linear, cosine
  optimizer: "adamw"
  evals_per_epoch: 3
  amp_bool: True



model_configs:
  gpt:
    d_model: 128
    hidden_layer: 128
    n_layer: 8
    dropout: 0.1
    init_method: 'xavier'
    attention_layer: 'sparse'
  unet_gpt:
    d_model: 512
    hidden_layer: 128
    n_layer: 6
    dropout: 0.1
    init_method: 'normal'
    attention_layer: 'causal'
    bottleneck_sizes: [512, 256, 256, 128, 128, 256]

attn_configs:
  causal:
    n_head: 8
    intermediate_dim : 0 # if 0 , normal , elif > 0 , bottleneck
  sparse:
    attn_type: 'fixed'  # 'all', 'fixed', 'local'. 'strided'
    n_head: 8
    num_verts: 16   #
    local_attn_ctx: 32
    sparseblocksize: 128
    vertsize: 128
    n_bctx: 4
    intermediate_dim : 64 # if 0 , normal , elif > 0 , bottleneck


      #   UNET d_model: 512
  #   n_head: 8
  #   n_layer: 6
  #   dropout: 0.1
  #   bottleneck_size: 256
  # unet_gpt:
```

Appendix O:

Parser Argument:

```
import torch

    torch.cuda.empty_cache()
    load_dotenv(dotenv_path=".env")


    parser = argparse.ArgumentParser()
    parser.add_argument("--test", action="store_true", help="Run test")
    parser.add_argument("--sweep", action="store_true", help="Run hyperparameter sweep")
    parser.add_argument("--sweep_config", type=str, help="Path to sweep YAML config")
    parser.add_argument("--orig_yaml", type=str, default="config/hyperparams.yaml")
    args = parser.parse_args()
```

--sweep and **--original_yaml** specify configuration YAMLs:

- **Sweep configuration:** Path for parameter sweeping.
- **Original YAML:** Path for base hyperparameters, usually updated with results from sweeps to improve performance over time.

--test and **--sweep** specify the type of run:

- **Testing:** Allows dynamic import or removal of training-monitoring and Docker-related functionality.
- **Sweep:** Activates W&B sweep functionality for hyperparameter optimization.

Selection of optimizer and scheduler

```
 ### Optimizer and Scheduler
    if args.optimizer == "sgd":
        opt = torch.optim.SGD(model.parameters(), lr=args.lr,
weight_decay=args.weight_decay)
    elif args.optimizer == "adamw":
        opt = torch.optim.AdamW(model.parameters(), lr=args.lr,
weight_decay=args.weight_decay)
    elif args.optimizer == "adam":
        opt = torch.optim.Adam(model.parameters(), lr=args.lr,
weight_decay=args.weight_decay)
    elif args.optimizer == "adagrad":
        opt = torch.optim.Adagrad(model.parameters(), lr=args.lr,
weight_decay=args.weight_decay)
    elif args.optimizer == 'RMSprop':
        opt = torch.optim.RMSprop(model.parameters(), lr=args.lr ,
weight_decay=args.weight_decay)
    else:
        raise ValueError(f"Unsupported optimizer: {args.optimizer}")

    if args.scheduler == "cosine":
        scheduler = torch.optim.lr_scheduler.CosineAnnealingLR(opt, T_max=max_steps)
    elif args.scheduler == "linear":
```

```
        scheduler = torch.optim.lr_scheduler.LinearLR(opt, start_factor=1.0,
end_factor=0.0, total_iters=max_steps)
    elif args.scheduler == "step":
        scheduler = torch.optim.lr_scheduler.StepLR(opt, step_size=args.step_size,
gamma=args.gamma)
    elif args.scheduler == "none":
        scheduler = torch.optim.lr_scheduler.LambdaLR(opt, lr_lambda=lambda step: 1.0)
    else:
        raise ValueError(f"Unsupported scheduler: {args.scheduler}")
```

Selection of attention layer and architecutre

```
### Attention setup
    if modelparams['attention_layer'] == 'causal':
        attn = AttnConfig(
            d_model=modelparams['d_model'],
            block_size=args.context_length,
            dropout=modelparams['dropout'],
            **attnparams
        )

    elif modelparams['attention_layer'] == 'sparse':
        attn = SparseAttnConfig(
            d_model=modelparams['d_model'],
            block_size=args.context_length,
            dropout=modelparams['dropout'],
            **attnparams
        )



    #### Model setup
    if args.model_architecture == "gpt":
        cfg = GPTConfig(
                vocab_size=args.vocab_size,
                block_size=args.context_length,
                attn_config = attn,
                activation_function = 'gelu',
                **modelparams
            )
        model = GPT(cfg).to(device)
    elif args.model_architecture == "unet_gpt":
        cfg = UnetGPTConfig(
            vocab_size=args.vocab_size,
            block_size=args.context_length,
            attn_config = attn,
            activation_function='gelu',
            **modelparams
        )
        model = GPUnetT(cfg).to(device)
    else:
        raise ValueError(f"Unsupported model architecture: {args.model_arhitecture}")
```

Training optimization technique sample

```
ptr = 0
    step = 0
    t0 = time.time()

    scaler = GradScaler()
    for epoch in range(1, args.epochs + 1):
        for _ in tqdm(range(1, batches + 1), desc=f"Epoch {epoch}/{args.epochs}"):
            step += 1
            xb, yb, ptr = get_batch(train_ids, ptr, args.context_length, args.batch_size,
device)


            if args.amp_bool:
                with autocast():  # enables float16 for eligible ops
                    _, loss = model(xb, yb)

                # Backward with gradient scaling
                scaler.scale(loss).backward()

                # Gradient clipping (scale before unscale!)
                scaler.unscale_(opt)  # important for clip_grad_norm_

                torch.nn.utils.clip_grad_norm_(model.parameters(), 1.0)

                # Optimizer step
                scaler.step(opt)
                scaler.update()

                # Scheduler step (unchanged)
                scheduler.step()
            else:
                _, loss = model(xb, yb)

                # l1_norm = sum(p.abs().sum() for p in model.parameters())
                # l2_norm = sum(p.pow(2).sum() for p in model.parameters())

                # loss = loss + l1_norm * L1 + l2_norm * L2
                opt.zero_grad(set_to_none=True)
                loss.backward()
                torch.nn.utils.clip_grad_norm_(model.parameters(), 1.0)
                opt.step()
                scheduler.step()
```

Appendix P:

Wandb sweep

```
def sweep_train():
        orig_cfg = OmegaConf.load(args.orig_yaml) # defaults
        cfg = copy.deepcopy(orig_cfg)  # create a separate copy to modify

        with wandb.init() as run:
            print("RUNCONFIG")
            print(dict(run.config))

            print("Before")
            print(cfg)

            for key, val in dict(run.config).items():
                parts = key.split(".")  # split by all dots
                d = cfg
                # traverse down to the last dictionary
                for p in parts[:-1]:
                    d = d[p]
                d[parts[-1]] = val  # set the value

            print("After applying sweep")
            print(cfg)
            main(cfg , False)


    if not args.test:
        wandb.login(key=os.getenv("WANDB_API_KEY"))
        import utils

    if args.sweep:

        cfg = OmegaConf.load(args.sweep_config)
        # Convert to a plain dictionary
        cfg_dict = OmegaConf.to_container(cfg, resolve=True)

        sweep_id = wandb.sweep(cfg_dict, project="gpt-from-scratch", entity="arc_agi")
        wandb.agent(sweep_id, function=sweep_train , count=50)
```

Wandb logging

```
if not test:
        wandb.init(
            project="gpt-from-scratch",
            entity="arc_agi",
            config=hparams   # <--- pass hyperparams to W&B
        )
```

```python
logger.log("training_step",
                      step=step,
                      max_steps=max_steps,
                      loss=loss.item(),
                      elapsed_time=elapsed,
                      prnt=False)
            if not test:
                wandb.log({
                    "train/loss": loss.item(),
                    "train/step": step,
                    "train/elapsed_time": elapsed
                })

            if step == 1 or step % eval_interval == 0 or step == max_steps:
                val_loss = evaluate()
                logger.log("validation_step",
                          step=step,
                          max_steps=max_steps,
                          loss=val_loss,
                          elapsed_time=elapsed)

                if not test:
                    wandb.log({
                        "val/step" : step,
                        "val/loss": val_loss,
                        "val/step": step,
                        "val/elapsed_time": elapsed
                    })
    if not test:
        artifact = wandb.Artifact("logs" , type="log")

        artifact.add_file(args.log_file)
        wandb.log_artifact(artifact)
        wandb.finish()
```

Appendix Q

```python
@dataclass
class ModelConfig:
    vocab_size: int
    context_length: int
    batch_size: int
    embed_dim: int
    dropout: float
    n_layers: int



@dataclass
class GPTConfig:
    vocab_size: int
    block_size: int
    n_layer: int
    d_model: int
    dropout: float
    attn_config : AttnConfig
    hidden_layer : int
    attention_layer: str
    norm_type: str  = 'pre' # 'pre' or 'post'
    activation_function: str = 'gelu'  # 'relu' or 'gelu'
    init_method: str = 'xavier'

class GPT(nn.Module):
    def __init__(self, cfg: GPTConfig):

@dataclass
class UnetGPTConfig(GPTConfig):
    hidden_layer_list: List[int] = None




class GPUnetT(GPT):
    def __init__(self, cfg: UnetGPTConfig):
```

```python
@dataclass
class AttnConfig:
    d_model: int
    n_head: int
    block_size: int
    dropout: float
    intermediate_dim: int  # must be specified for bottleneck attention
```

```python
@dataclass
class SparseAttnConfig(AttnConfig):
    attn_type: str  # 'fixed_sparse' or 'strided_sparse'
    num_verts: int
    local_attn_ctx: int
    sparseblocksize: int
    vertsize: int
    n_bctx: int


class CausalSelfAttention(nn.Module):


class SparseCausalSelfAttention(CausalSelfAttention):
```

memory function

```python
def memory_before_inference(self, dtype=torch.float32):
        elem_size = torch.tensor([], dtype=dtype).element_size()
        total_mem = 0

        # Token embedding
        total_mem += self.token_emb.weight.numel() * elem_size

        # Positional embedding
        total_mem += self.pos_emb.numel() * elem_size

        # Dropout has no persistent parameters

        # Blocks
        for i, block in enumerate(self.blocks):
            if hasattr(block, "memory_before_inference"):
                block_mem = block.memory_before_inference(dtype)
            else:
                block_mem = sum(p.numel() * elem_size for p in block.parameters())
            print(f"Block {i+1} memory: {block_mem / (1024**2):.3f} MB")
            total_mem += block_mem

        # Final LayerNorm
        total_mem += sum(p.numel() * elem_size for p in self.ln_f.parameters())

        # Head
        total_mem += self.head.weight.numel() * elem_size

        print(f"Total GPT memory before inference: {total_mem / (1024**2):.3f} MB")
        return total_mem / (1024**2)  # MB
```

example of configurable setting (weight initialisation)

```python
@staticmethod
    def _init_weights(module, cfg):
        """Initialize weights based on cfg.init_method."""
        if isinstance(module, (nn.Linear, nn.Embedding)):
            if cfg.init_method == "normal":
                nn.init.normal_(module.weight, mean=0.0, std=0.02)
            elif cfg.init_method == "xavier":
                nn.init.xavier_normal_(module.weight)
            elif cfg.init_method == "kaiming":
                nn.init.kaiming_normal_(module.weight, mode='fan_in', nonlinearity='relu')
            elif cfg.init_method == "uniform":
                bound = 1.0 / (cfg.d_model ** 0.5)  # Scaled by sqrt(d_model)
                nn.init.uniform_(module.weight, -bound, bound)
            else:
                raise ValueError(f"Unknown init_method: {cfg.init_method}")

            if isinstance(module, nn.Linear) and module.bias is not None:
                nn.init.zeros_(module.bias)
```