Optimizer and LR Schedule

Outline

Introduction

Why?

- **Core component** of deep learning
  - Drives the entire training process
  - Determines how models learn from data
  - Critical for model convergence
- **Impact**
  - Training speed
  - Model performance
  - Final accuracy
  - Generalization

Challenges

- Complex loss landscapes
  - Non-convex optimization
  - Multiple local minima and Saddle points
- Training
  - Vanishing/exploding gradients
  - Slow convergence
  - Unstable
  - Overfitting

Optimizer vs Schedulers

Optimizer

- How parameters update
- adapt learning based on gradients

Learninig rate schedule

- Manage learning rate dynamics
- Balance exploration vs exploitation
- Convergence speed
- Final model perormance

Evolution

- Traditional
  - Basic Gradient Descent
  - Batch Gradient Descent
  - Stochastic Gradient Descent (SGD)
  - mini-batch
- Modern
  - Momentum
  - Adaptive learning rates
  - Combined strategies

Optimizer

Common Optimizers Family

- First Generation
  - SGD
  - SGD with momentum
  - Nesterov accelerated gradient
- Adaptive methods
  - AdaGrad
  - RMSprop
  - AdaDelta
  - Adam
- Modern
  - AdamW
  - Lion
  - Lamb
  - ...

Gradient Descent

$$\theta = \theta - \eta * \nabla J(\theta) \tag{1}$$

Where,

- θ: model parameters
- η: learning rate
- $\nabla J(\theta)$: gradient of loss function

Batch Gradient Descent

- Uses entire dataset for each update
- Slow
- High memory
- Deterministic updates

For a dataset with n sample, $i \in [1, n]$:

$$
\begin{aligned}
L &= \left(\frac{1}{n}\right) * \sum L(\theta; x_i, y_i) \\
\theta &= \theta - \eta * \left(\frac{1}{n}\right) * \sum \nabla L(\theta; x_i, y_i)
\end{aligned}
\tag{2}
$$

Batch Gradient Descent Pseudo code

```
for epoch in epochs:
  grads = grad(loss_fn(weights, all_n_samples))
  weights = weights - learning_rate * grads
```

SGD and Mini-batch

- Update parameters for each sample or a m-size batch

$$
\begin{aligned}
L &= \left(\frac{1}{m}\right) * L(\theta; x_i, y_i) \\
\theta &= \theta - \eta * \left(\frac{1}{m}\right) * \nabla L(\theta; x_i, y_i)
\end{aligned} \tag{3}
$$

```
for epoch in epochs:
  for batch in get_batches(dataset, size=m):
    grads = grad(loss_fn(weights, batch))
    weights = weights - learning_rate * grads
```

AdaGrad (Adaptive Gradient)

- Adaptive learning rate for each parameter
- Larger updates for infrequent parameters
- Smaller updates for frequent parameters

$$\begin{aligned} r_t &= r_{t-1} + \nabla J(\theta_{t-1})^2 \\ \theta_t &= \theta_{t-1} - \left(\frac{\eta}{\sqrt{r_t + \varepsilon}}\right) * \nabla J(\theta_{t-1}) \end{aligned} \tag{4}$$

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$$

- Learning rate will decrease over time

Momentum

- Inpire by physics momentum
- Accumulate gradients history
- Helps overcome local minima
- Reduce training oscillations

$$\begin{aligned} v_t &= \beta v_{t-1} + (1-\beta)\nabla J(\theta_{t-1}) \\ \theta_t &= \theta_{t-1} - \eta v \end{aligned} \tag{5}$$

- v: velocity (momentum)
- β: momentum coefficient (0.9 in practice)

```
Without momentum (oscillating):

  /\    /\/\/\
 /  \/\/
/

With momentum (smooth):

  /^^^^^
 /
/
```

Weight Decay

- Prevents model overfitting
- Penalize large weights
- Encourage simpler models
- Reduces model's dependency on single features

Weight Decay

L2 norm in the loss function

$$L = L + \left(\frac{\lambda}{2}\right) \|\theta\|^2 \tag{6}$$

Standard Weight Decay in optimizer

$$\theta_t = \theta_{t-1} - \eta \nabla J(\theta_{t-1}) - \lambda \theta_{t-1} \tag{7}$$

Weight Decay pseudo code

```
for params, grad in zip(params, grads):
  param = param - lr * (grad + wd * param)
  # or
  param = param - lr * grad - lr * wd * param
```

Some Typical values for λ

Dataset Size	λ Value
Small ($<$ 10k sample)	1e-3
Medium (10k - 1M)	1e-4
Large ($>$ 1M)	1e-5

Architecture Type	λ Adjustment
CNN	Base λ
Transformer	0.1 × Base λ
ResNet	0.5 × Base λ

Some Typical values for λ

Data Type	**λ Adjustment**
Simple/Linear	$2 \times$ Base λ
Complex/Nonlinear	$0.5 \times$ Base λ

Training Length	**λ Adjustment**
Short (< 20 epochs)	$0.5 \times$ Base λ
Long (> 100 epochs)	$2 \times$ Base λ

SGD with Momentum

Add momentum term to vanilla SGD

$$\begin{aligned} v_t &= \beta * v_{t-1} + \nabla J(\theta_{t-1}) \\ \theta_t &= \theta_{t-1} - \eta * v_t \end{aligned} \tag{8}$$

Nesterov Accelerated Gradient

- Momentum: Current → Gradient → Momentum → Update
- Nesterov: Current → Look-ahead → Gradient → Momentum → Update

$$\begin{aligned} v_t &= \beta * v_{t-1} + \nabla J(\theta_{t-1} + \beta * v_{t-1}) \\ \theta_t &= \theta_{t-1} - \eta * v_t \end{aligned} \tag{9}$$

RMSprop

- Improves AdaGrads' declining learning rate with exponential moving average (EMA)

Before

$$
\begin{aligned}
r_t &= r_{t-1} + \nabla J(\theta_{t-1})^2 \\
\theta_t &= \theta_{t-1} - \left(\frac{\eta}{\sqrt{r_t + \varepsilon}}\right) * \nabla J(\theta_{t-1})
\end{aligned} \tag{10}
$$

After

$$
\begin{aligned}
r_t &= \beta * r_{t-1} + (1 - \beta) * \nabla J(\theta_{t-1})^2 \\
\theta_t &= \theta_{t-1} - \left(\frac{\eta}{\sqrt{r_t + \varepsilon}}\right) * \nabla J(\theta_{t-1})
\end{aligned} \tag{11}
$$

Adam

- Adds momentum to RMSprop
- Maintains moving averages of gradients (momentum) and squared gradients (LR)

$$
\begin{aligned}
m_t &= \beta_1 * m_{t-1} + (1 - \beta_1) * \nabla J(\theta_{t-1}) \\
v_t &= \beta_2 * v_{t-1} + (1 - \beta_2) * \nabla J(\theta_{t-1})^2 \\
m_t &= \frac{m_t}{1 - \beta_1^t} \\
v_t &= \frac{v_t}{1 - \beta_2^t} \\
\theta_t &= \theta_{t-1} - \left(\frac{\eta}{\sqrt{v_t + \varepsilon}} \right) * m_t
\end{aligned}
\tag{12}
$$

AdamW

- Add weight decay to Adam

$$\theta_t = \theta_{t-1} - \left(\frac{\eta}{\sqrt{v_t + \varepsilon}}\right) * m_t - \lambda * \theta_{t-1} \tag{13}$$

Lion (Google in 2023)

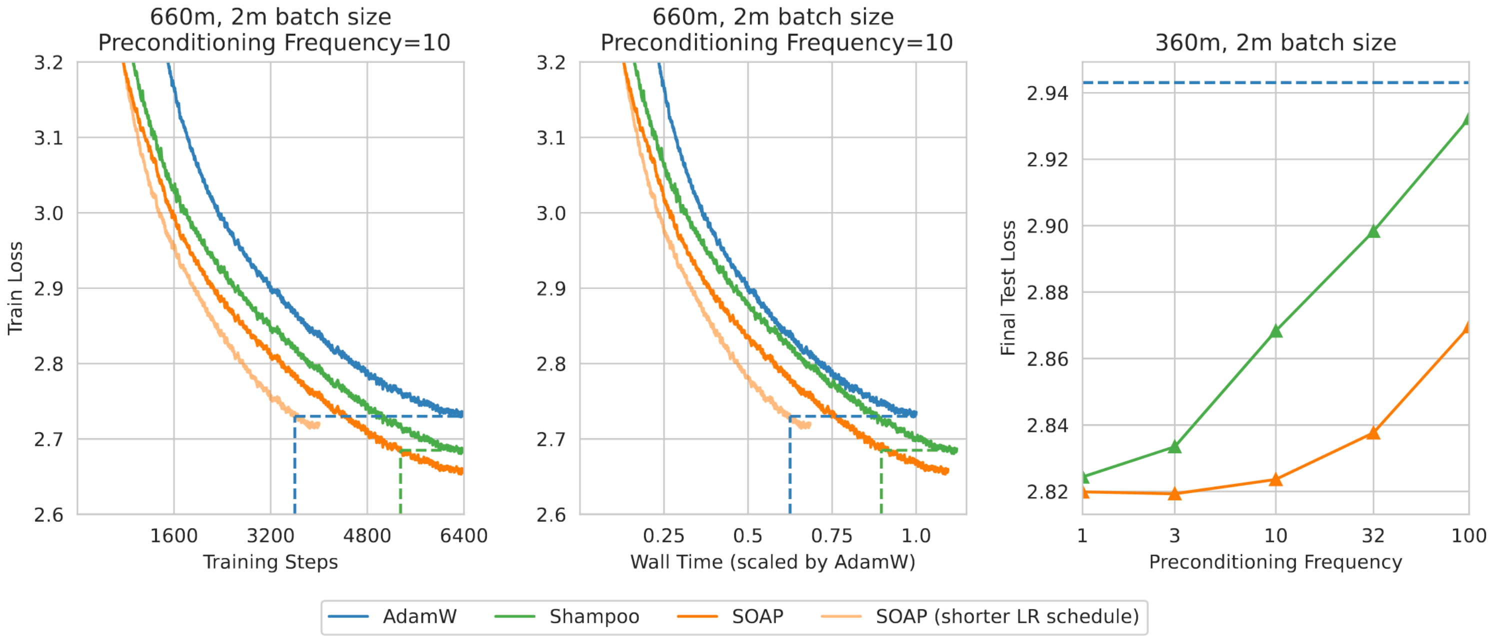
- Use sign gradient instead of raw gradient
- Reduce memory usage

$$\begin{aligned} m_t &= \beta_1 * m_{t-1} + (1 - \beta_1) * \mathrm{sign}(\nabla J(\theta_{t-1})) \\ \theta_t &= \theta_{t-1} - \eta * \mathrm{sign}(m_t) \end{aligned} \tag{14}$$

1. Chen, X. *et al.* Symbolic Discovery of Optimization Algorithms. (2023) doi:10.48550/arXiv.2302.06675

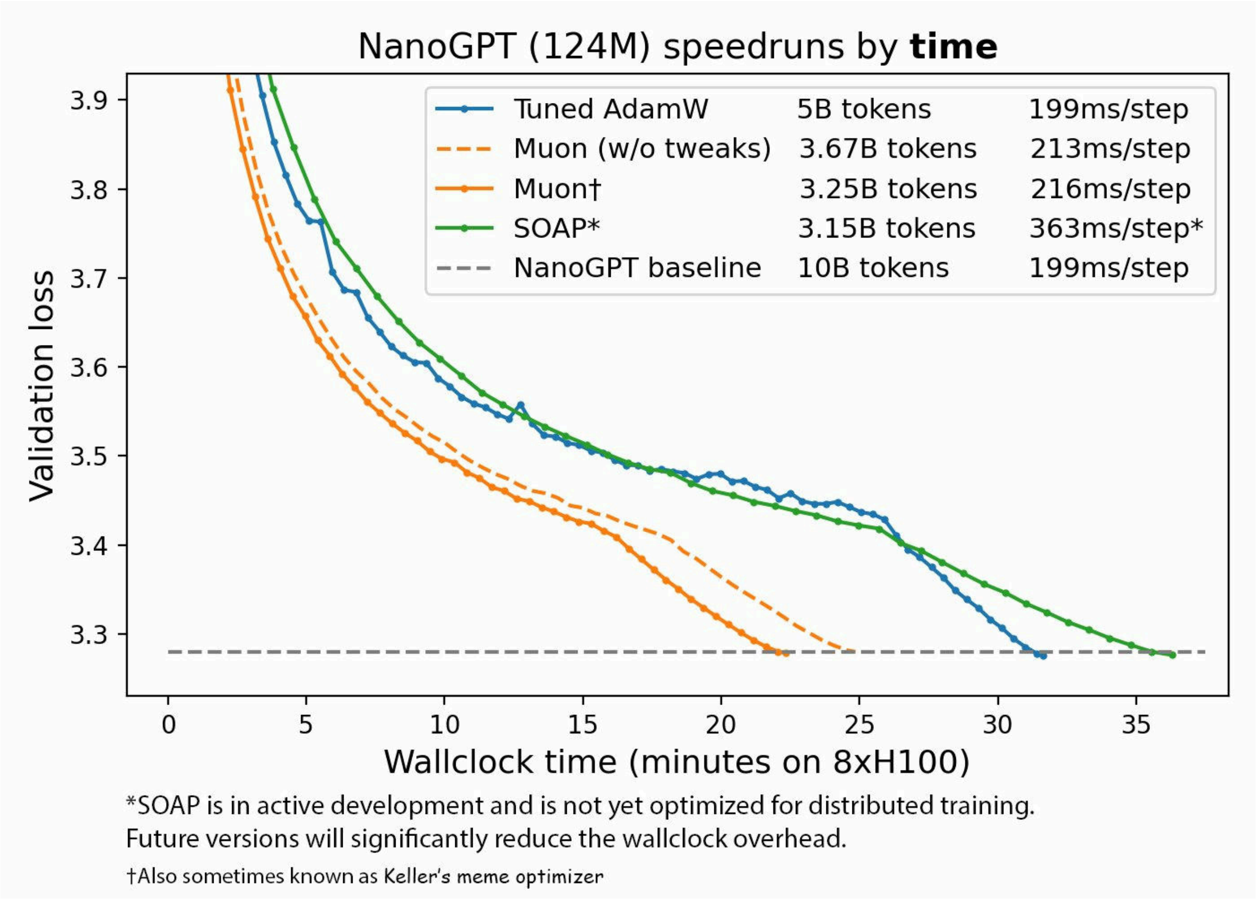
SOTA Optimizers

SOAP[2]



2. Vyas, N. *et al.* SOAP: Improving and Stabilizing Shampoo Using Adam. (2024) doi:10.48550/arXiv.2409.11321

Muon[3]



3. Jordan, K. KellerJordan/Modded-Nanogpt. (2024)

Schedule

Why?

Problems with fixed LR

- Large: training unstable
- Small: slow convergence

Common Schedules

- Step Decay
- Cosine Annealing
- Warm-up
- One Cycle
- Reduce on Plateau
- …

Step Decay

$$\eta = \eta_{\text{init}} \gamma^{\left\lfloor \frac{\text{epoch}}{\text{step\_size}} \right\rfloor} \tag{15}$$

Where γ is the decay factor and **step_size** is the number of epochs to decay.

```
lr = [
  0.1,  # epoch 0-30
  0.01,  # epoch 30-60
  0.001,  # epoch 60-90
  ...
]
```

Cosine Annealing

$$\eta_t = \eta_{\min} + \left(\frac{1}{2}\right) * (\eta_{\max} - \eta_{\min}) * \left(1 + \cos\left(\frac{T_{\text{cur}}}{T_{\max}}\pi\right)\right) \tag{16}$$

Where t is the current epoch, T_{cur} is the current step, and $T_{\max}$ is the total number of steps.

4. Loshchilov, I. & Hutter, F. SGDR: Stochastic Gradient Descent with Warm Restarts. (2017) doi:10.48550/arXiv.1608.03983

Warm-up Strategy

- Stabilizes early training
- Prevents early divergence

```
if step < warmup_steps:
  lr = warmup_schedule(step)
else:
  lr = normal_schedule(step)
```

One Cycle

1. Linearly increase LR to max lr (warmup)
2. Linearly decrease LR to min lr
   - Optionally, use other annealing (like cosine) to decrease LR further

```
if step < warmup_steps:
  lr = linear_increase(step, lr)
else:
  lr = cosine(step - warmup_steps, total_steps - warmup_steps)
```

Reduce on Plateau

Adaptize Learning Rate Strategy

```python
def update(current_metric):
  # Check if we should change the learning rate or not by comparing the metrics
  is_better = compare(current_metric, best_metric)

  # Change the best metric
  if is_better:
    best_metric = current_metric
    num_bad_epochs = 0
  else:
    num_bad_epochs += 1

  # Change the learning rate if necessary
  if num_bad_epochs >= patience:
    lr = max(lr * factor, min_lr)
    num_bad_epochs = 0
```

Hyperparameter suggestion in LR Schedules

Step Decay

Parameter	Common Values
step_size	2000-4000 steps
gamma	0.1-0.5

Warm-up

Model Type	Warmup Steps
CNN	5% steps
Transformer	10% steps
Fine-tuning	6% steps
Large batch size > 1000	15% - 20%

Model Type	**Warmup Steps**
Transfer learning	3-5%
Small datasets	3-5%
Unstable training	Increase 5%

Learning Rate Range Suggestions

LR Range

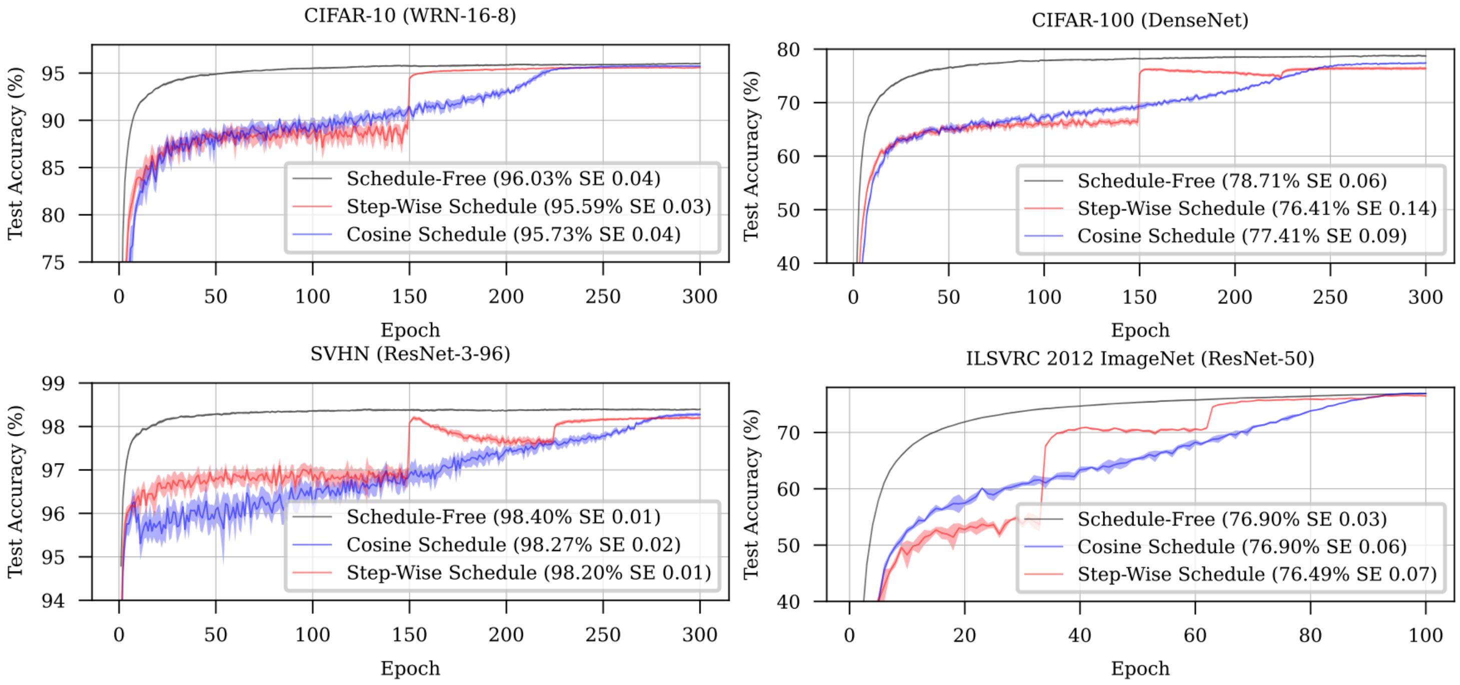
Optimizer	Learning Rate Range
SGD (no momentum)	0.1 - 1.0
SGD with Momentum	0.01 - 0.1
Adam/AdamW	1e-4 - 1e-3
RMSprop	1e-4 - 1e-3
AdaGrad	0.01 - 0.1
Lion	1e-4 - 3e-4

Learning Rate Range Suggestions

Adjustments

Scenario	LR Adjustment
Batch size doubled	LR × $\sqrt{2}$
Deeper network	LR × 0.5
Fine-tuning	LR × 0.1
Unstable training	LR × 0.1

SOTA Schedule The Road Less Scheduled[5]



5. Defazio, A. *et al.* The Road Less Scheduled. (2024) doi:10.48550/arXiv.2405.15682

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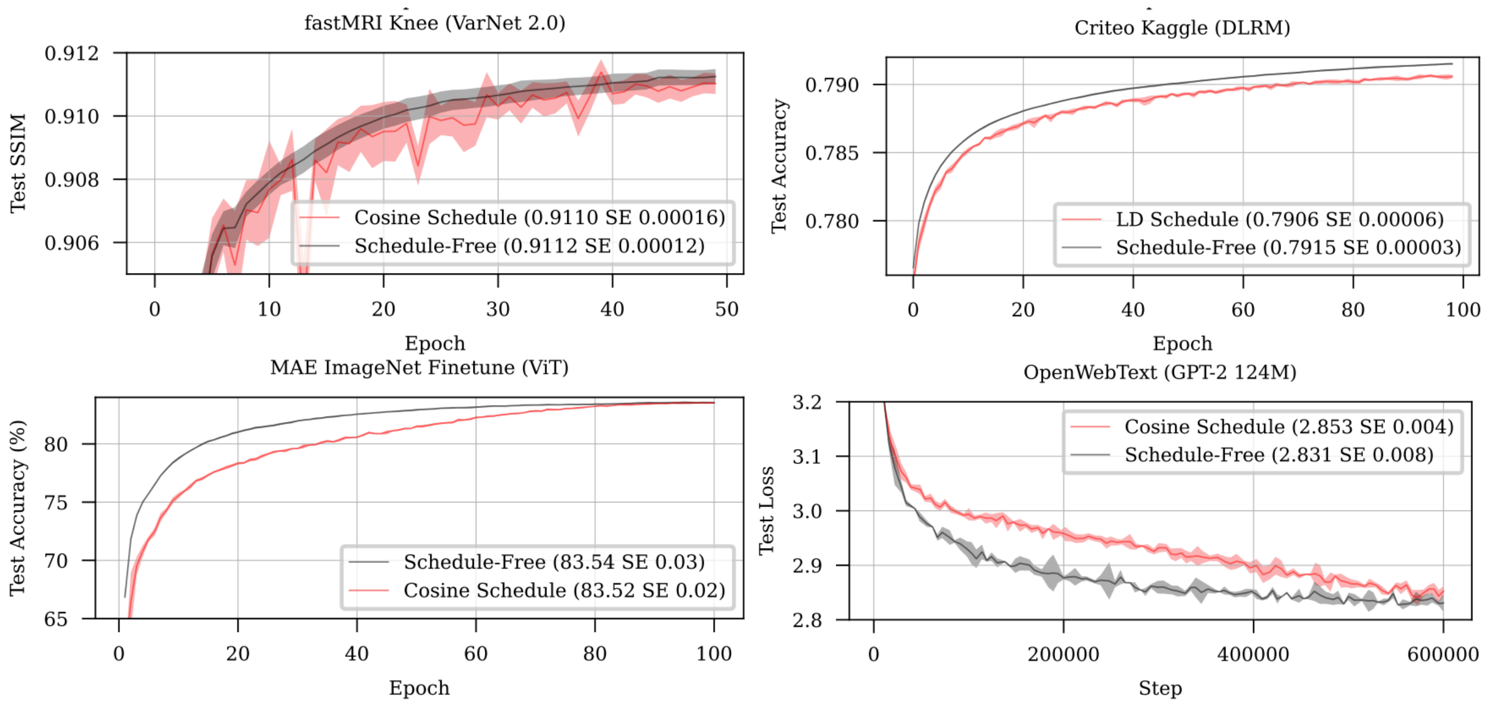

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