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Due: 21.11.2023 23:59 CET

Points: 16 + 2 bonus

To get access to this week's code use the following link: https://classroom.github.com/a/V-x00Lms

General constraints for submissions: Please adhere to these rules to make our and your life easier! We will deduct points if you fail to do so.

- Your code should work with Python 3.8.
- You should only fill out the TODO-gaps and not change anything else in the code.
- Add comments to your code, to help us understand your solution.
- Your code should adhere to the PEP8 style guide. We allow line lengths of up to 120.
- While working on the exercise, push all commits to the dev branch (details in assignment 1). Only push your final results to the master branch, where they will be automatically tested in the cloud. If you push to master more than 3 times per exercise, we will deduct points.
- All provided unit tests have to pass: In your *GitHub* repository navigate to *Actions* → your last commit → Autograding → education/autograding to see which tests have passed. The points in autograding only show the number of tests passed and have nothing to do with the points you get for the exercise.
- for loops can be slow in Python, use vectorized numpy operations wherever possible (see assignment 1 for an example).
- Submit a single PDF named submission.pdf. Include your matriculation numbers on the top of the sheet. Add the answers and solution paths to all non-coding questions in the exercise. Do not leave answers to any questions as comments in the code. You can use Latex with the student template (provided in exercise 1 / ILIAS) or do it by hand.
- Please help us to improve the exercises by filling out and submitting the feedback.md file.
- We do not tolerate plagiarism. If you copy from other teams or the internet, you will get 0 points. Further action will be taken against repeat offenders!
- Passing the exercises ($\geq 50\%$ in total) is a requirement for passing the course.

How to run the exercise and tests

- See the setup.pdf in exercise 1 / ILIAS for installation details.
- We always assume you run commands in the root folder of the exercise repository.
- If you use miniconda, do not forget to activate your environment with conda activate mydlenv
- Install the required packages with pip install -r requirements.txt
- Python files in the *root folder* of the repository contain the scripts to run the code.
- Python files in the tests/ folder of the repository contain the tests that will be used to check your solution.
- Test everything at once with python -m pytest
- Run a single test with python -m tests.test_something (replace something with the test's name).
- To check your solution for the correct code style, run pycodestyle --max-line-length 120 .
- The scripts runtests.sh (Linux/Mac) or runtests.bat (Windows) can be used to run all the tests described above. If you are on Linux, you need execution rights to run runtests.sh.

This exercise focuses on optimization, we will:

- Calculate update steps of SGD with momentum by hand
- Implement the Adam optimizer
- Compare Adam, SGD, SGD with momentum
- Implement and analyze some learning rate schedules

1. Pen and Paper tasks

1) [3 points] Perform three update steps of SGD with momentum to the weights $\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$ of the linear function $\hat{\mathbf{y}} = \mathbf{w}^\top X$ optimizing the mean squared error (MSE). Thus, the loss for one sample is given by $(\hat{y} - y)^2$ and according to slide 43 in the optimization lecture, the per-sample losses are summed and divided by the batch size.

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Given:

the initial state
$$\mathbf{w} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
, velocity $\mathbf{v} = \begin{bmatrix} 0 & 0 \end{bmatrix}$, data $X = \begin{bmatrix} 2 \\ -1 \end{bmatrix} \begin{bmatrix} -1 \\ 3 \end{bmatrix}$, target $\mathbf{y} = \begin{bmatrix} 3 & 1 \end{bmatrix}$, learning rate $\alpha = 0.2$, momentum strength $\beta = 0.8$ and batch size $B = 2$.

2) [2 points] Prove that bias corrected first order moment s (i.e., \hat{s}) is equal to the gradient for every step in Adam when that gradient remains constant.

Hint: This can be done using mathematical induction.

2. Coding Tasks

In this coding exercise, you will implement an Adam optimizer and compare it with SGD and SGD with momentum. You will also implement two learning rate schedulers - one which uses piecewise constants and another which uses cosine annealing.

Please note that we extended the Module class in lib/network_base.py with a state (self.training = True) to determine whether we're training or evaluating the module. We also added two methods to toggle this state - def train() and def eval(). You will see these methods being used in the train function in lib/training.py.

- 1) [2 points] **Todo:** Implement the step function of the adam optimizer (class Adam in file lib/optimizers.py) **Hint:** We provide an implementation of SGD in the same file.
- 2) [2 points] **Todo:** Train three models, one with Adam, one with SGD and one with SGD with momentum, for 10 epochs each. Each model should have one hidden layer with 30 hidden units followed by relu activation. Start by implementing the create_and_train_model function and use it in compare_optimizers in file lib/training.py afterwards. Run train_models.py to run your code.
- 3) [2 points] **Todo:** Compare Adam vs SGD vs SGD with Momentum.

Create two plots, one for training loss curves and one for training accuracies curves, for each of the three models above (function plot_learning_curves in file lib/plot.py).

Run plot_trained_models.py to run your code.

4) [4 points] Todo: Implement the learning rate scheduler PieceWiseConstantLR and CosineAnnealingLR. You can use the provided LambdaLR class for this, which works analogously to the PyTorch LambdaLR. (class PiecewiseConstantLR and CosineAnnealingLR in file lib/lr_schedulers.py).

PyTorch implements learning rate schedules as wrappers for the optimizer and requires the user to call scheduler.step() after each epoch. We've already done this for you in the training loop in function train in lib/training.py.

5) [1 point] **Todo:** Plot learning rate schedules.

To verify your implementation, plot the learning rate schedules with number of epochs on the x-axis and learning rate on the y-axis (function plot_lr_schedules in file lib/plot.py).

Run plot_lr_schedules.py to run your code.

3. [1 bonus point] Code Style

On every exercise sheet, we will also make use of pycodestyle to adhere to a common python standard. Your code will be automatically evaluated on submission (on push to master). Run pycodestyle --max-line-length=120. to check your code locally.

4. [1 bonus point] Feedback

Todo: Please give us feedback by filling out the feedback.md file.

- Major Problems?
- Helpful?
- Duration (hours)? For this, please follow the instructions in the feedback.md file.
- Other feedback?

This assignment is due on 21.11.2023 23:59 CET. Submit your solution for the tasks by uploading (git push) the PDF, txt file(s) and your code to your group's repository. The PDF has to include the name of the submitter(s). Teams of at most 3 students are allowed.