Machine Learning and Physics
Winter Semester 2024/2025

Exercise Sheet #9

Due: 07.01.24 14h00

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General Regulations.

- Please hand in your solutions in groups of two (preferably from the same tutorial group). Submissions by a single person alone will not be corrected.
- Your solutions to theoretical exercises can be either handwritten notes (scanned), or typeset using LaTeX. For scanned handwritten notes please make sure that they are legible and not too blurry.
- For the practical exercises, the data and a skeleton for your jupyter notebook are available at `https://github.com/sciai-lab/mlph_w24`. Always provide the (commented) code as well as the output, and don't forget to explain/interpret the latter. Please hand in your notebook (`.ipynb`), as well as an exported pdf-version of it.
- Submit all your files in the Übungsgruppenverwaltung, only once for your group of two. Specify all names of your group in the submission.

1 Pretraining LLMs

(a) The encoder-only LLM BERT was pretrained with two tasks: Masked Language Modeling (MLM) and Next Sentence Prediction (NSP). Suggest two other possible pretraining tasks and explain why they could be meaningful. (3 pts)

(b) The decoder-only LLM GPT was pretrained with Causal Language Modeling (CLM) a.k.a. next token prediction. Give two alternative pretraining tasks and explain why they could be meaningful. For each task, discuss its computational complexity and how well it can be parallelized across training samples. (3 pts)

2 Under the hood of LLMs: Llama 2.7B

In the provided jupyter notebook, you will find code that loads the weights of the Llama 2.7B model trained by meta. The jupyter notebook demonstrates how one can interact with an LLM first hand if one has full access to it.

(a) Add comments to explain the code you find in the jupyter notebook. You are not expected to run the code, which requires an access token. (4 pts)

(b) Bonus: Create a HuggingFace account (`https://huggingface.co/`), request an access token and execute the code to investigate the inner workings of the LLM yourself. Investigate what the LLM will return if you prompt it with an empty string and use probabilistic decoding. (4 pts)

3 Flow-based modeling

(a) Let X, Y be two random variables and X follow the uniform distribution on the interval $[0, 1]$. Let $Y' = g(X) = \mathrm{CDF}_Y^{-1}(X)$ be the inverse of the cumulative distribution function of Y (a.k.a. quantile function). Show that the probability density function (pdf) of Y and Y' are identical. (2 pts)

Hint: Relate the cumulative distribution functions for the random variables X and Y'.

(b) Explain how you can use the result from (a) to transform a general 1D pdf p_X into any pdf p_Y. Apply your idea to find the transformation to transform the samples which follows a pdf of $p_X(x) = 1/2x,\ x \in [0, 2]$ into samples which follow a pdf of $p_Y(y) = -1/2y + 1,\ y \in [0, 2]$. Test it in the provided jupyter notebook. (4 pts)

(c) Use the relation which you proved in part (a) to derive basic form of the Box-Muller transform to convert samples uniformly sampled from $[0, 1]$ into samples from a standard normal distribution. (3 pts)

Hint: Use that a sample from a 2D standard normal can be obtained as $(x_1, x_2) = r(\cos\phi, \sin\phi)$ *by sampling* r *from the marginal radial distribution and uniformly sampling an angle* $\phi \in [0, 2\pi]$.

(d) Explain why the procedure derived in (a) cannot be generalized straightforwardly to arbitrary multivariate distributions. (2 pts)

(e) Let X be a 1D random variable with pdf $p_X(x)$. Show that the 1D random variable $Y = h(X)$ follows a pdf of

$$p_Y(y) = \left(p_X(x) \left| \frac{dh}{dx}(x) \right|^{-1} \right) \Bigg|_{x=h^{-1}(y)},$$

assuming that h is differentiable and monotonous. (2pts)