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Supervisor Review of the Bachelor Thesis of Nikita Kolesnichenko

This work is about the application of Generative Adversarial Networks (GANs) in the area of bioinformatics. Specifically, it is concerned with de novo protein design based on protein contact maps. Contact maps contain the pairwise distance between alpha-carbons on the protein backbone. To design novel proteins a GAN is trained to generate novel contact maps on the basis of an existing dataset.

Since this topic exceeds the scope of a bachelor thesis, it was subdivided into two parts.

1) In the practical part, Nikita had to compare two GAN variants on the CIFAR10 dataset. Here, he had to implement the models as well as the evaluation method, a hyperparameter search had to be performed and the results had to be compared and presented in a scientific way.
2) In the theoretical part, Nikita had to discuss how GANs can be applied to generate novel protein structures. This comprises a description of the principle behind GANs and a description of contact maps and their underlying biology.

In the course of this thesis, Nikita underwent an extremely positive development, both in terms of practical skills as well as in terms of personality. A lack of specific knowledge or skills that might have hampered him in the beginning became a source of motivation. He started to acquire knowledge beyond the specific topic and developed solid programming skills in the respective domain language. Under our guidance he implemented neural networks as well as the necessary code for the evaluation. He conducted an extensive

hyperparameter search to determine if one of the GAN variants consistently outperforms the other and compared the results.

Nikita showed a deep interest in machine learning in general and independently laid the foundation for a solid understanding thereof. He regularly discussed the current status of his work with us and sought and valued our feedback. His work meets what is commonly expected from a bachelor student. We can state with confidence that Nikita is worthy of the Bachelor of Science degree, given the work he performed for this thesis.

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