Proposal

Yuanhao JIANG

Title: Extending Score-Based Diffusion Models for 3D Structure Generation.

Supervisor: Professor George Deligiannidis.

Brief description: Score-based diffusion models [4, 5] use SDEs to gradually add noise to data and then reverse the process to generate structured samples, requiring accurate score function estimation via neural networks trained with score matching.

Despite the success of it, the application of score-based diffusion models to 3D structure generation remains underexplored. 3D data pose unique challenges, including maintaining geometric consistency and handling non-Euclidean data. In applications such as 3D shape modeling or protein structure prediction, constraints such as smooth surfaces and structural integrity must be satisfied, necessitating methods that can generate constrained and structured data effectively. Building on the foundational work in SGMs [4, 5] and potentially intersection with constrained dynamics [1–3], this project seeks to extend score-based diffusion to 3D data, addressing these challenges with following objectives

1. Baseline Exploration for Standard Score-Based Diffusion.
2. Extension to 3D Data: Adapt score-based diffusion models for 3D structure generation, focusing on point clouds or voxel grids.
3. Manifold-Aware Generation: Investigate techniques for constraining the diffusion process to 3D manifolds, ensuring geometric consistency and structural validity.

Prerequisite courses/knowledge: Stochastic processes, differential equations, numerical solvers for SDEs, deep learning frameworks (PyTorch).

Data availability: A custom constrained dataset will be generated for trial, with extensions to opensource datasets CMU Mocap or Human3.6M later.

Computing: The project requires SRF GPUs at the later experimental stage for potential SDE simulations and training neural networks in score-based diffusion models.

References

[1] Hyungjin Chung, Byeongsu Sim, Dohoon Ryu, and Jong Chul Ye. Improving diffusion models for inverse problems using manifold constraints. *Advances in Neural Information Processing Systems*, 35:25683–25696, 2022.

[2] Valentin De Bortoli, Emile Mathieu, Michael Hutchinson, James Thornton, Yee Whye Teh, and Arnaud Doucet. Riemannian score-based generative modelling. *Advances in Neural Information Processing Systems*, 35:2406–2422, 2022.

[3] Chin-Wei Huang, Milad Aghajohari, Joey Bose, Prakash Panangaden, and Aaron C Courville. Riemannian diffusion models. *Advances in Neural Information Processing Systems*, 35:2750–2761, 2022.

[4] Yang Song, Conor Durkan, Iain Murray, and Stefano Ermon. Maximum likelihood training of score-based diffusion models. *Advances in neural information processing systems*, 34:1415–1428, 2021.

[5] Yang Song, Jascha Sohl-Dickstein, Diederik P Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations. *arXiv preprint arXiv:2011.13456*, 2020.