Progress update

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Introduction

- TDA stuff
- Perturbations
- Next steps?

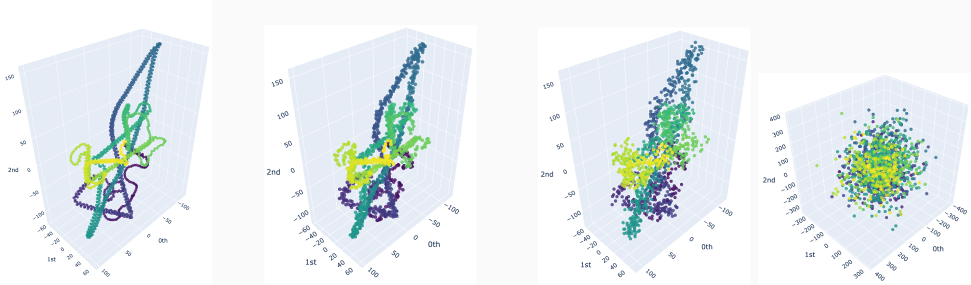
Kernels on persistence diagrams

Implemented properly from GUDHI [2].
A number of kernels are available:

- The sliced Wasserstein kernel (approximates Wasserstein similarity between PDs and is p.s.d.). [1]
- The persistence weighted Gaussian kernel (slower to compute + approximates). [3]
- The persistence scale space kernel [5] (approximates, is slower as well). [5] proves that the p-Wasserstein distance is not n.s.d.
- The persistence Fisher kernel [4]. Looks the fastest and does not approximate any other distance to be p.s.d.

Perturbations

Nice visualizations



(a) No noise **(b)** 2 **(c)** 6 **(d)** 99

Figure 1: Progressive injection of Gaussian Noise

Single experiment

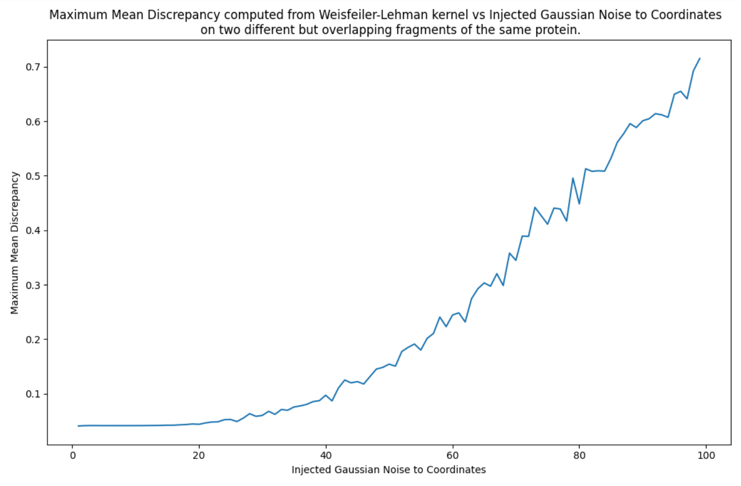


Figure 2: What happens to the MMD for $\varepsilon = 20$?

Multiple experiments varying ε for the ε-graphs

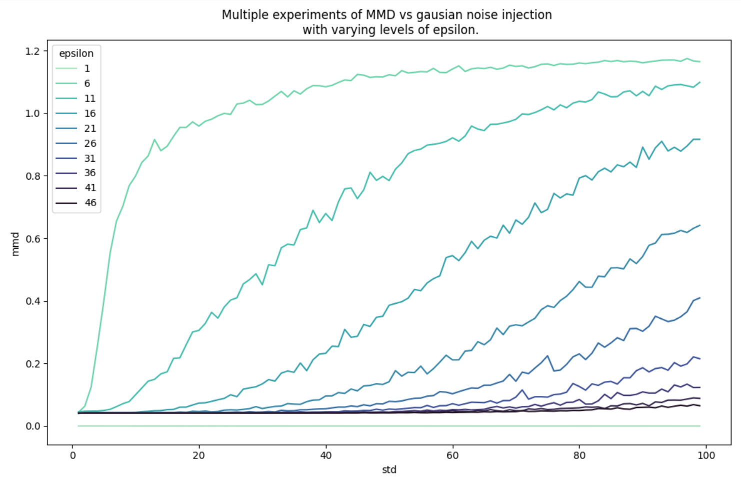


Figure 3: What happens to the MMD if ε varies?

Compressed representations

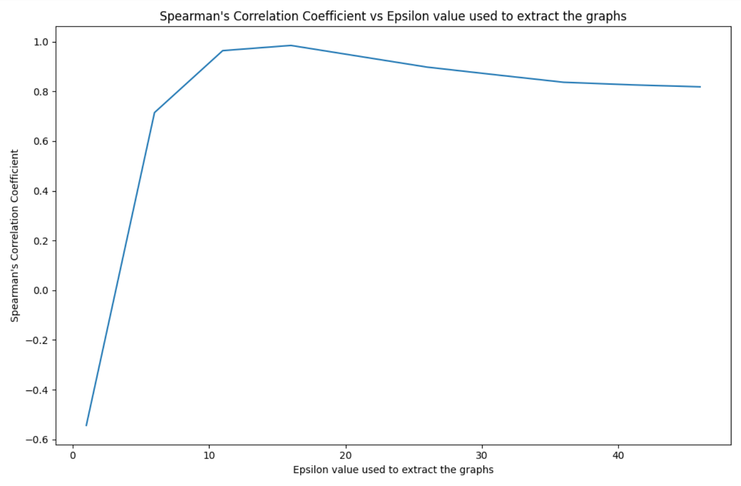


Figure 4: How can we represent the previous plot in a more compressed way?

Next steps

- Data version control and better pipelining using dvc
- Apply perturbations to subdomain (apply rotation to part of protein)
- Clashing descriptors, Ramachandran angles
- Non-MMD based meaure. [6]
- TDA experiments using aforementioned kernel
- Actually make progress on background

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