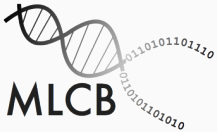
Progress update

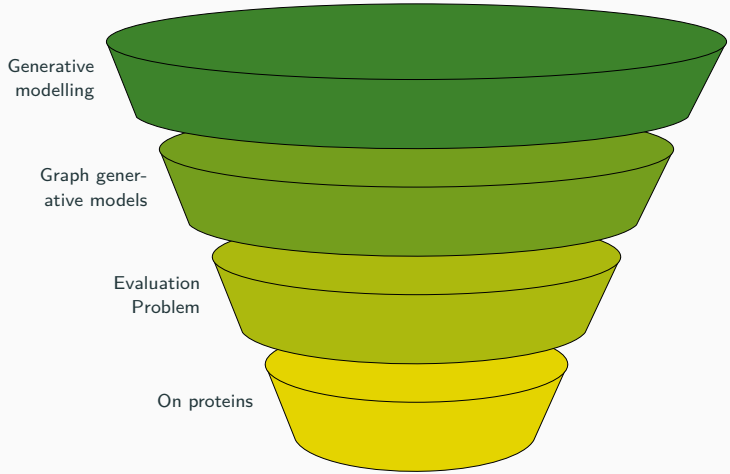
Philip Hartout

April 15, 2022

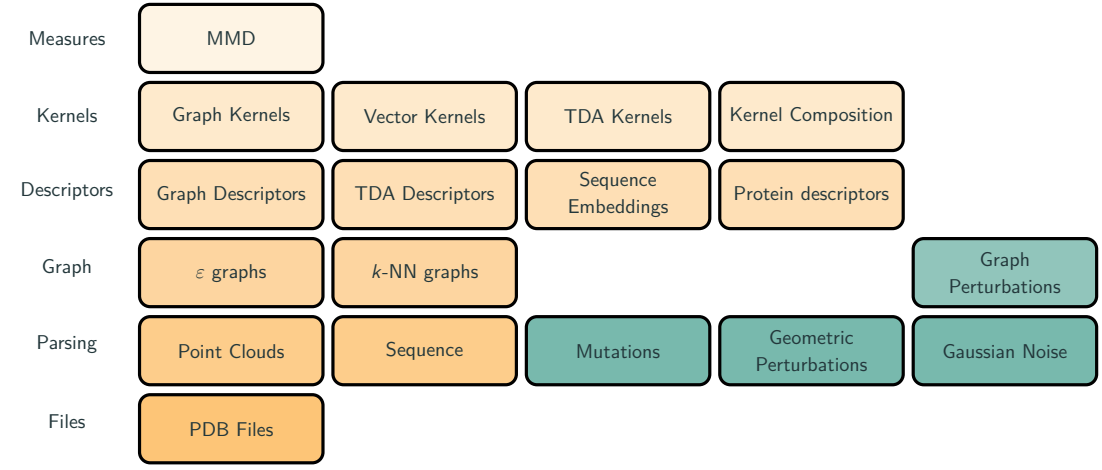


D BSSE

ETH zürich


Generative modelling
Graph generative models
Evaluation Problem
On proteins

Overview



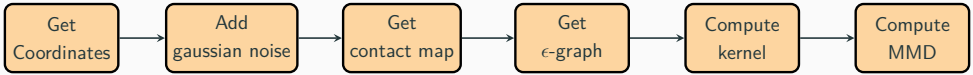
orange: modules; green: perturbations

Composable transformations & using `sklearn` API standards sensibly


```
base_feature_pipeline = pipeline.Pipeline(
    [
        ("coordinates", Coordinates(granularity="CA", n_jobs=12),),
        ("contact map", ContactMap(metric="euclidean", n_jobs=12,),),
        ("epsilon graph", EpsilonGraph(epsilon=epsilon, n_jobs=12),),
    ]
)

proteins = base_feature_pipeline.fit_transform(paths_to_pdb_files)
```

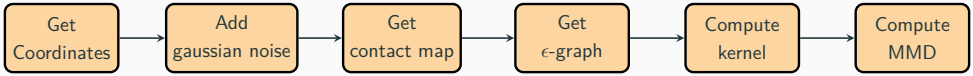
Composable transformations & using `sklearn` API standards sensibly




```
base_feature_pipeline = pipeline.Pipeline(
    [
        ("coordinates", Coordinates(granularity="CA", n_jobs=12),),
        (
            "add gaussian noise",
            GaussianNoise(
                random_seed=42, noise_mean=0, noise_variance=10, n_jobs=12,
            ),
        ),
        ("contact map", ContactMap(metric="euclidean", n_jobs=12,),),
        ("epsilon graph", EpsilonGraph(epsilon=epsilon, n_jobs=12),),
    ]
)

proteins_perturbed = base_feature_pipeline.fit_transform(paths_to_pdb_files)
```

Composable transformations & using `sklearn` API standards sensibly




```
base_feature_pipeline = pipeline.Pipeline(
    [
        ("coordinates", Coordinates(granularity="CA", n_jobs=12),),
        (
            "add gaussian noise",
            GaussianNoise(
                random_seed=42, noise_mean=0, noise_variance=10, n_jobs=12,
            ),
        ),
        ("contact map", ContactMap(metric="euclidean", n_jobs=12,),),
        ("epsilon graph", EpsilonGraph(epsilon=epsilon, n_jobs=12),),
    ]
)

proteins_perturbed = base_feature_pipeline.fit_transform(paths_to_pdb_files)
```

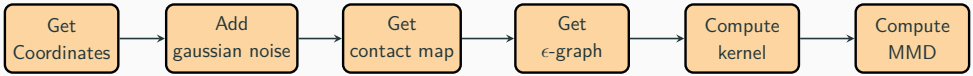
```
graphs = load_graphs(proteins, graph_type="eps_graph")
graphs_perturbed = load_graphs(proteins_perturbed, graph_type="eps_graph")

mmd = MaximumMeanDiscrepancy(
    biased=True,
    squared=True,
    kernel=WeisfeilerLehmanKernel(
        n_jobs=12, n_iter=5, normalize=True, biased=True,
    ),
).compute(graphs, graphs_perturbed)
```

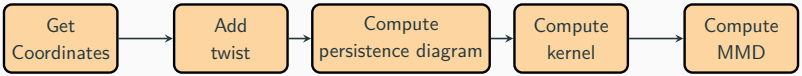
Reusable Components

But I want results!

MMD experiments informs the best representation to use for proteins



TDA captures morphological perturbations of proteins



1-sentence takeway

Parametrize your MMD sensibly.

Backup slides

Detailed breakdown of modules

Point clouds:

- Granularity can be set to α-Carbon, β-Carbon, entire backbone or all-atom setting.

Graph Descriptors:

- Degree Histogram
- Clustering Histogram
- Laplacian spectrum

Topological Descriptors

- Persistence diagrams
- Persistence landscape
- Persistence image
- Betti Curves

Sequence Embeddings (ESM, different sizes)

Protein Descriptors

- Ramachandran angles
- Interactomic clashes

Graph Kernels (Weisfeiler-Lehman Kernel)
Vector kernels (Linear, Gaussian)
TDA Kernel (Persistence Fisher Kernel)
Kernel composition ($\times$, $+$)
MMD (Squared, biased)

Perturbations
Graph level (rewire, add/remove edge)
Point cloud perturbations (twist, taper, shear)
Protein perturbations (mutate)
All modules work on multiple proteins simultaneously

The admin stuff

Message through slack for follow-up Qs

Extensive GitHub documentation & up-to-date codebase at

https://github.com/pjhartout/msc_thesis

Private repo a.t.m., message me to request access.

Temporary page!

LaTeX was unable to guess the total number of pages correctly. As there was some unproces
data that should have been added to the final page this extra page has been added to receiv

If you rerun the document (without altering it) this surplus page will go away, because LaTeX
now knows how many pages to expect for this document.