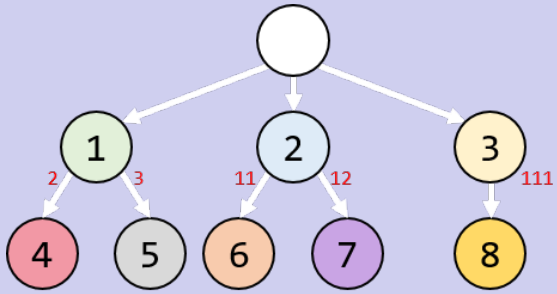


Master Thesis Seminar Talk

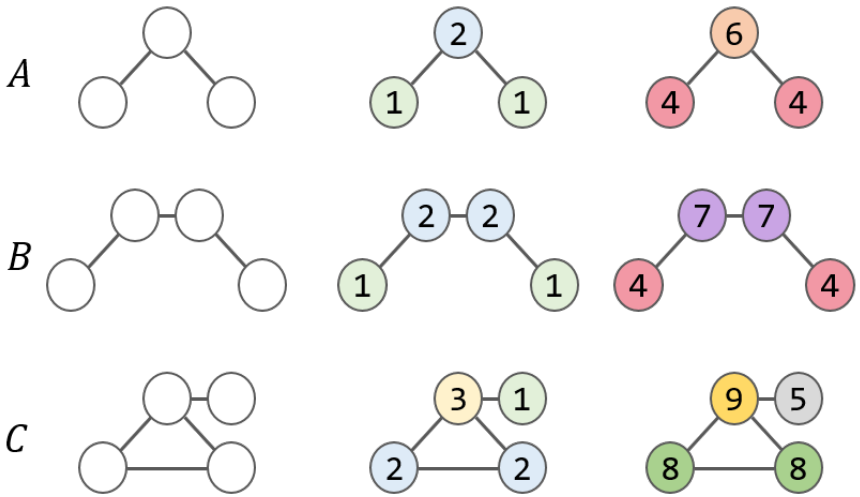
Progress Update

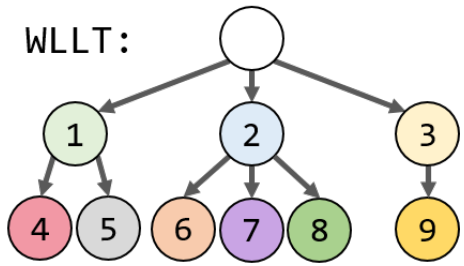
Fabrice Beaumont

Department of Information Systems and Artificial Intelligence - **Dr. Pascal Welke**

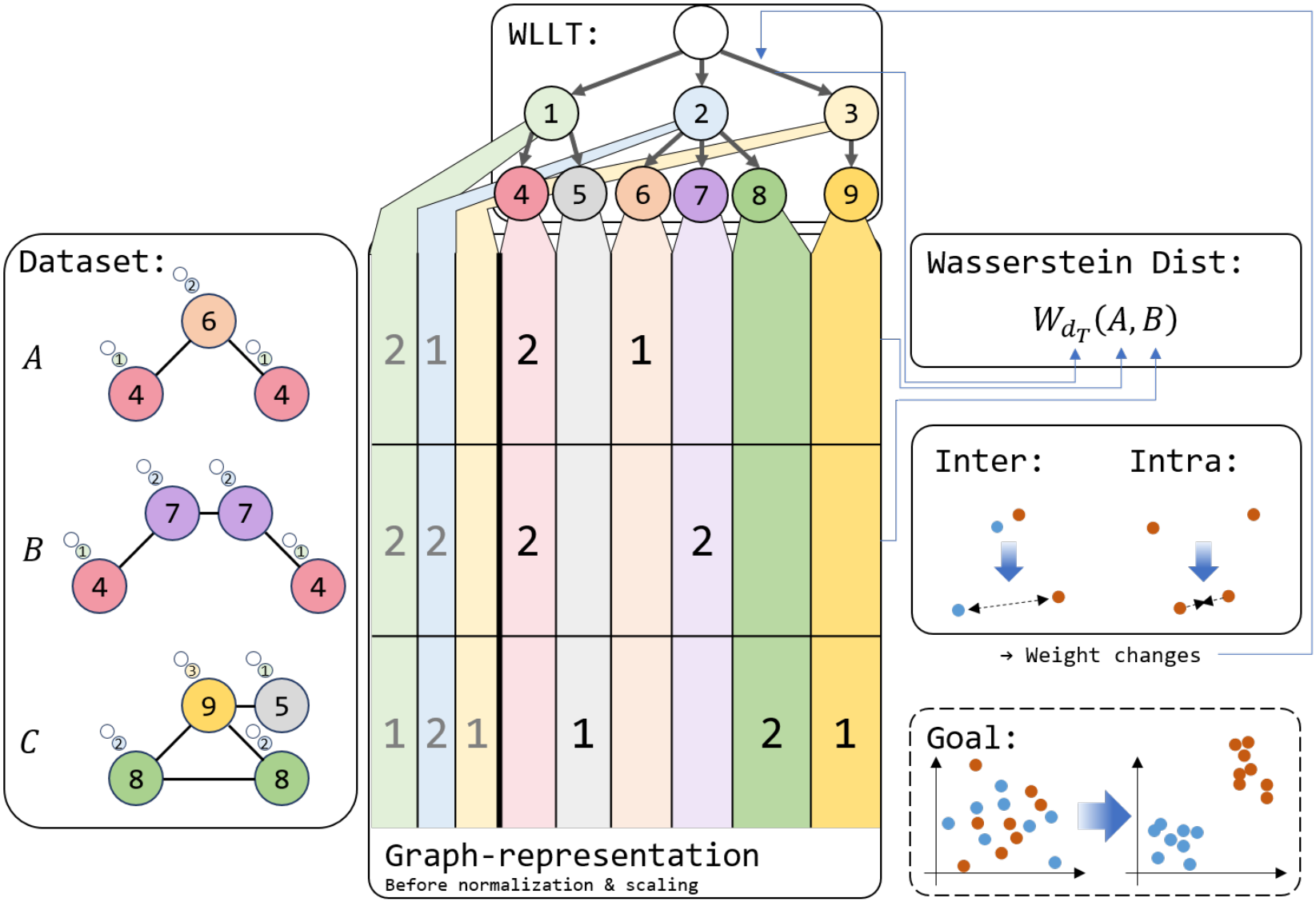
10. November 2022

Example of the whole procedure

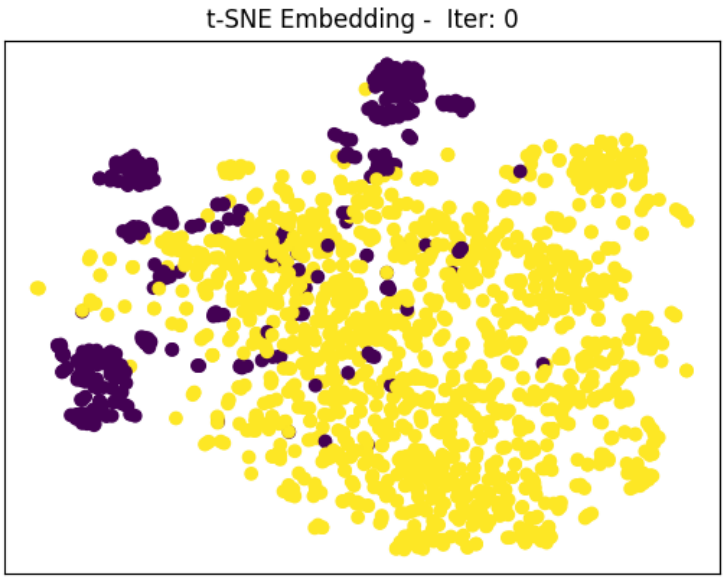


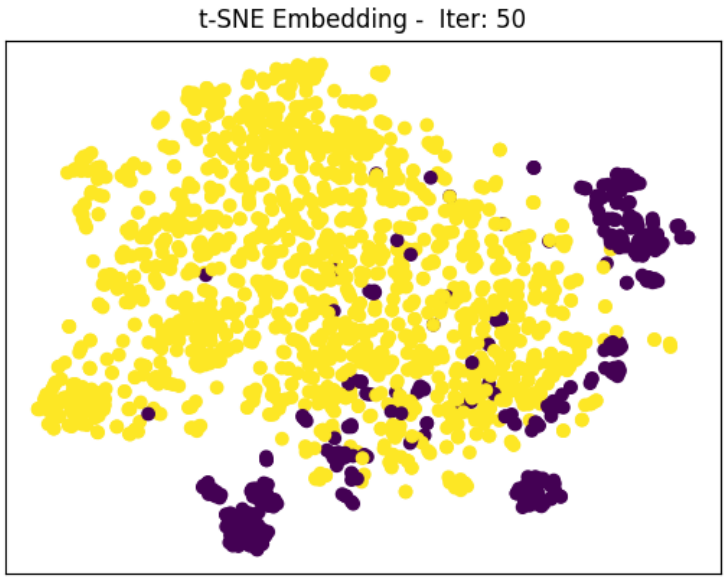


Example of the whole procedure



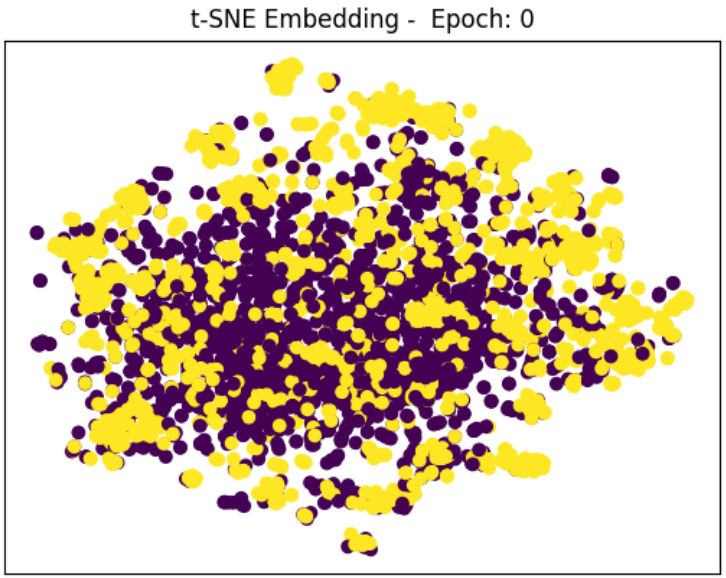
Example: AIDS t-SNE

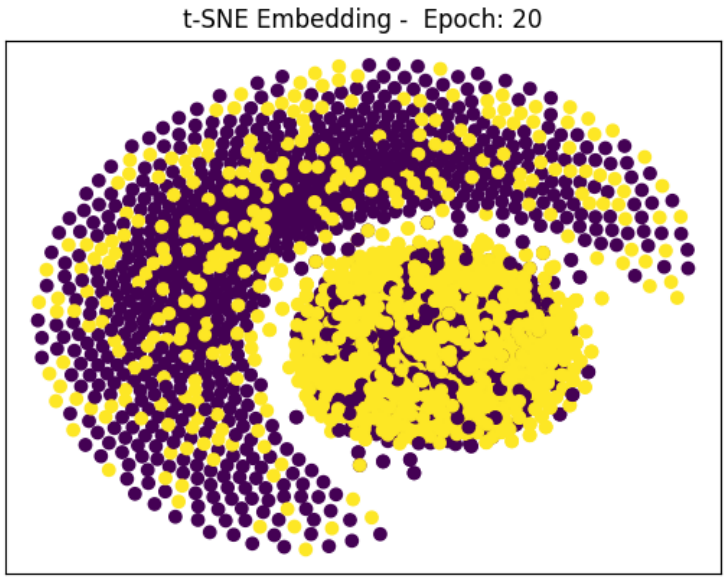




Bs: 5%, WLLT-d: 4, PP: 0.4, SVM-acc.: 80%

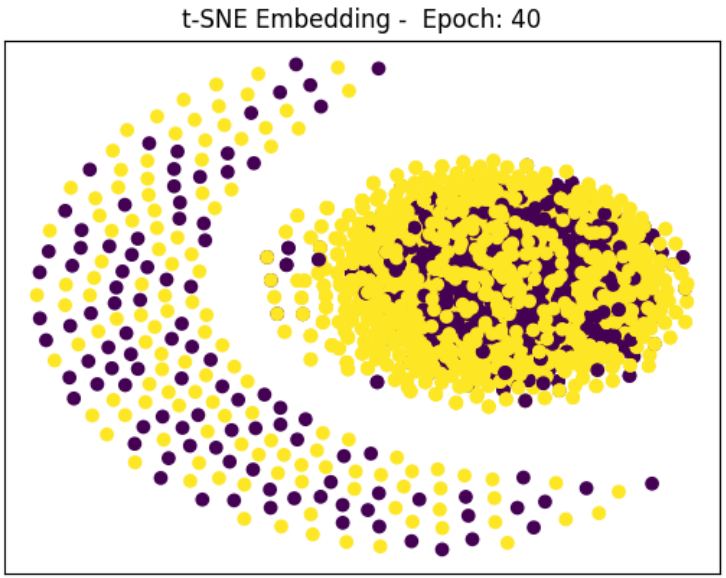
Example: NCI1 t-SNE

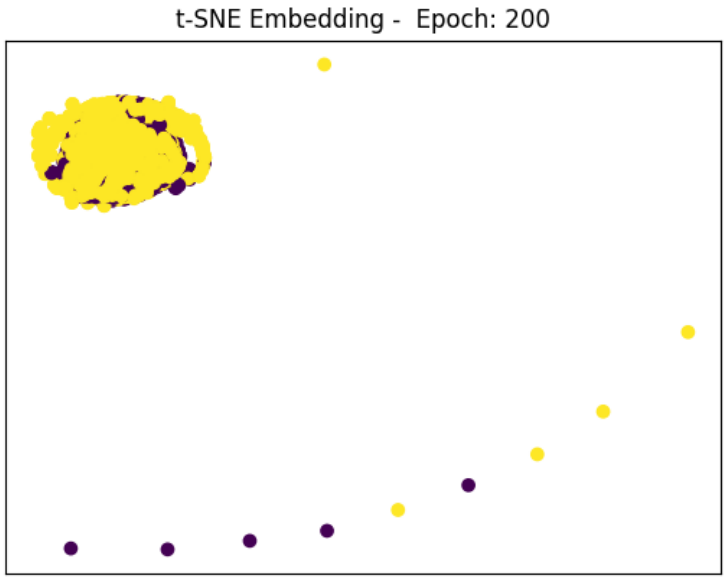




Bs: 5%, WLLT-d: 4, Pull: 1.0, Push: 0.1, SVM-acc.: 48%

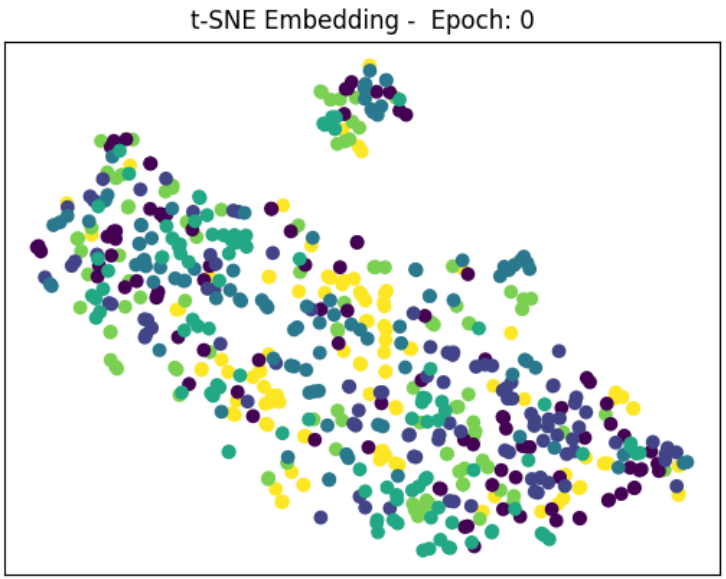
Example: NCI1 t-SNE

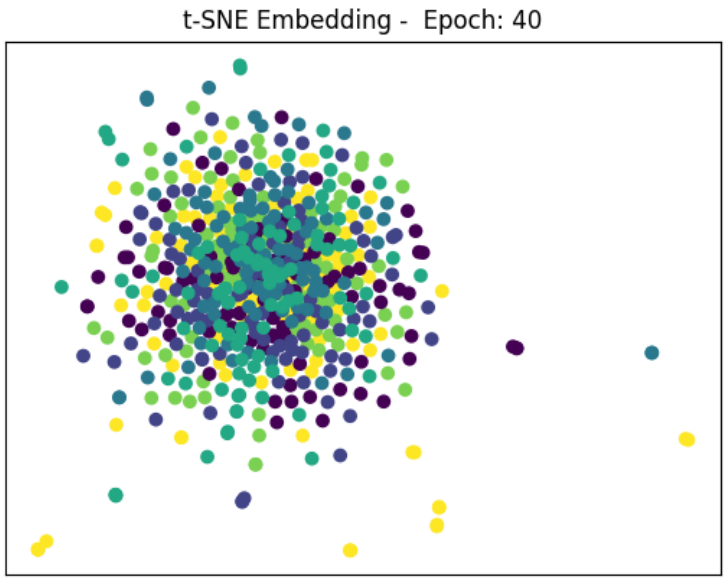




Bs: 5%, WLLT-d: 4, Pull: 1.0, Push: 0.1, SVM-acc.: 48%

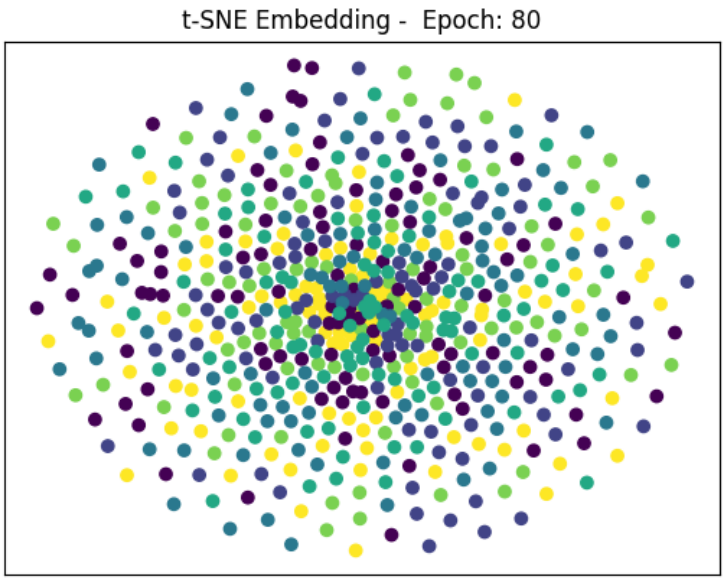
Example: ENZYMES t-SNE

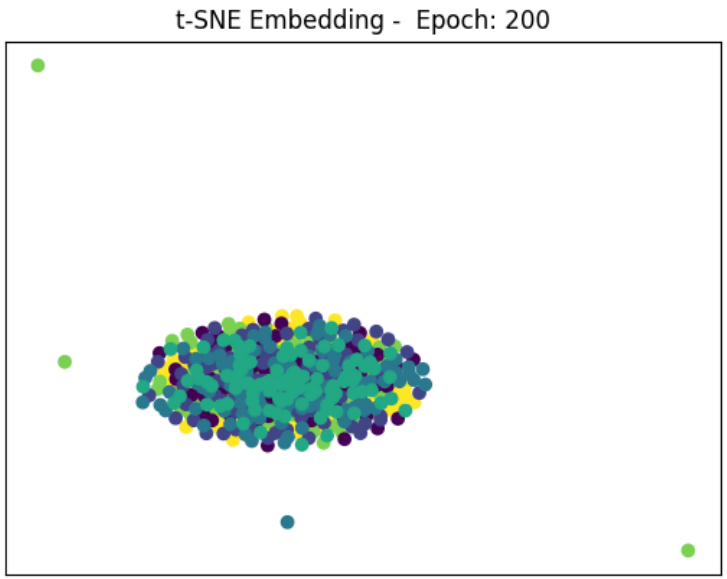




Bs: 5%, WLLT-d: 4, Pull: 1.0, Push: 0.1, SVM-acc.: 11%

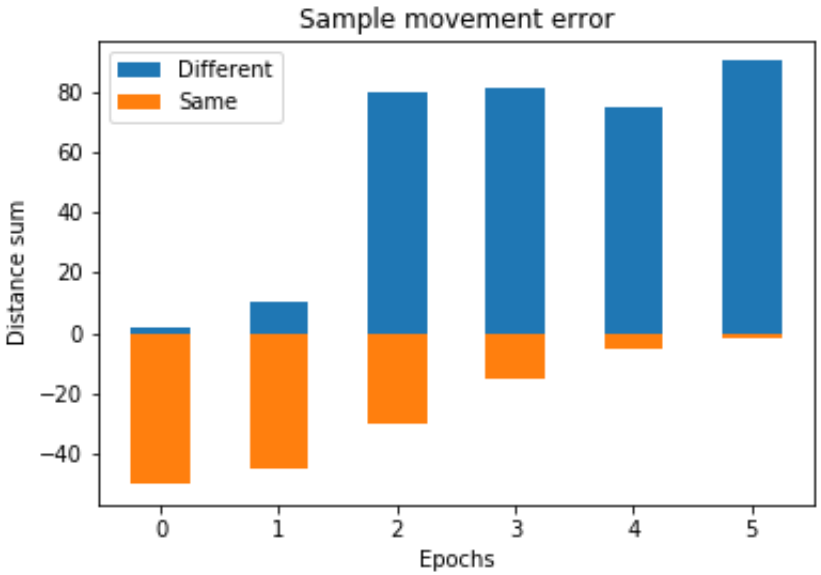
Example: ENZYMES t-SNE

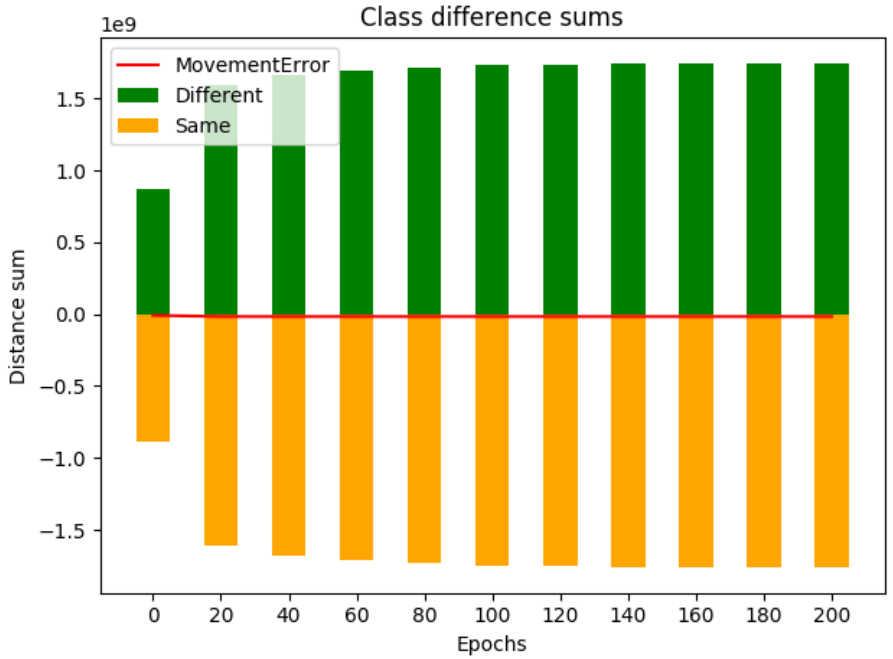




Bs: 5%, WLLT-d: 4, Pull: 1.0, Push: 0.1, SVM-acc.: 11%

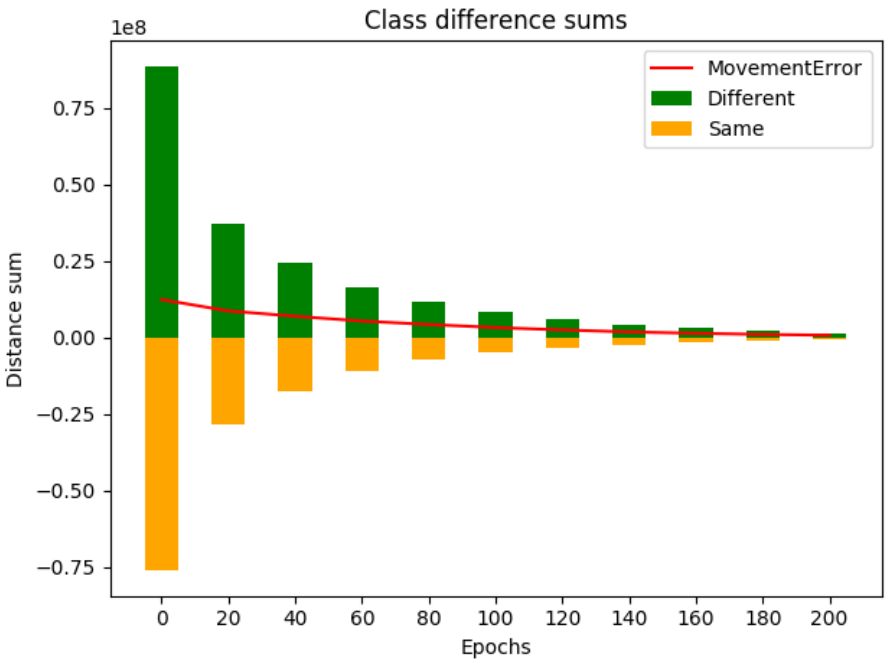
Example: Sample movement error

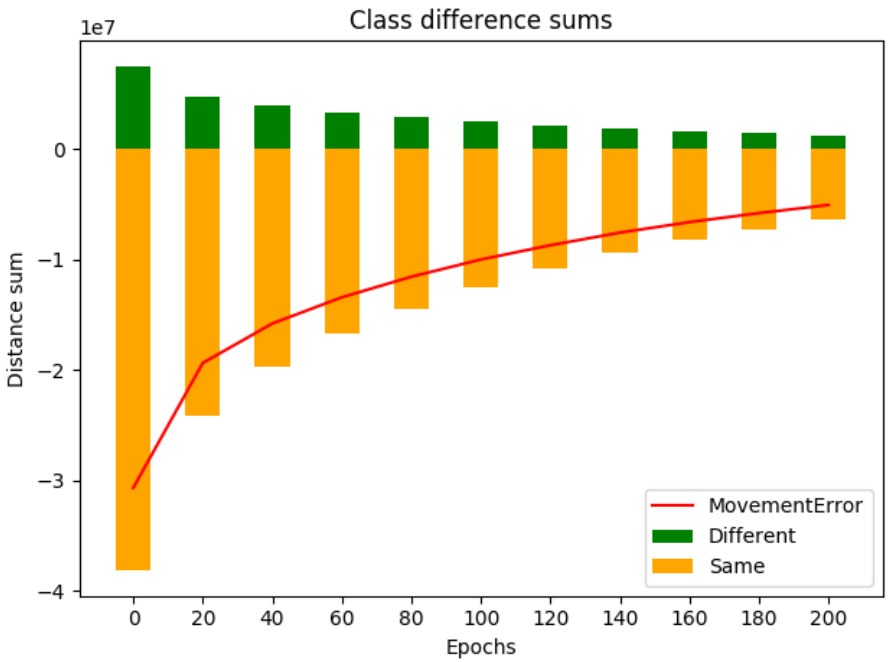




NCI1, Bs: 5%, WLLT-d: 4, Pull: 0.1, Push: 0.5, SVM-acc.: 48%

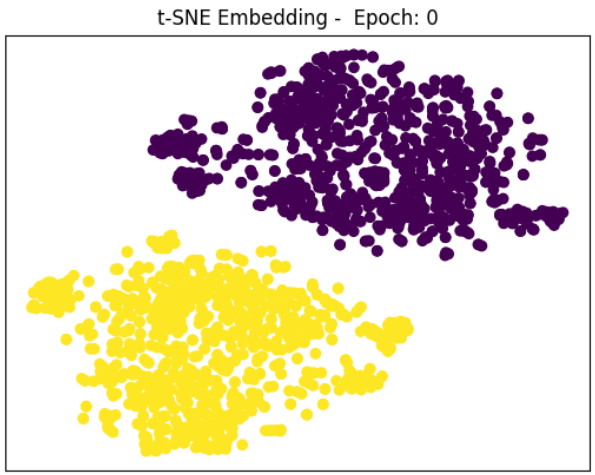
Example: Sample movement error

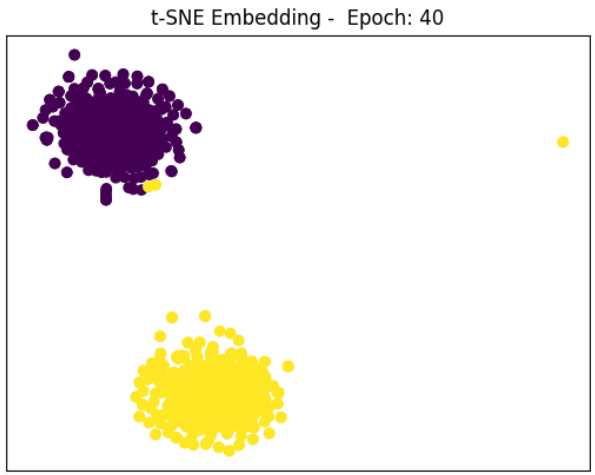


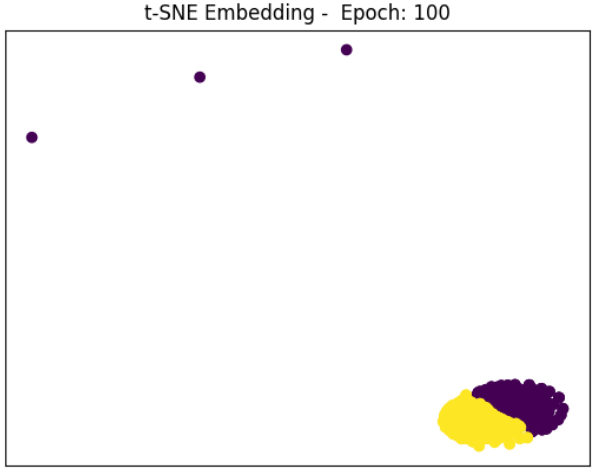


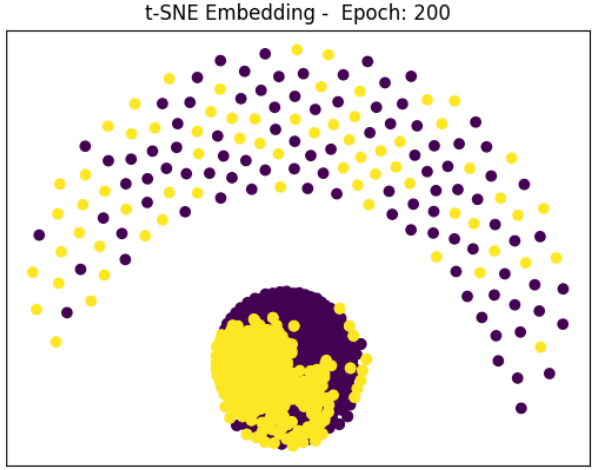
PROTEINS_c, Bs: 5%, WLLT-d: 4, Pull: 1.0, Push: 0.1, SVM-acc.: 64%
ENZYMES, Bs: 5%, WLLT-d: 4, Pull: 1.0, Push: 0.1, SVM-acc.: 11%

Example: Sample movement error









Example: AIDS_perfect

Separate clusters for:

WLLT-d=4, 100 epochs, Bs=5%, He_thdl=0.6, Pull=0.1, Push=0.1

And with changed:

- Bs=20%
- WLLT-d=2
- Lr=0.5

Assume that these parameters do not interfere with the cluster separation. Suspect instead the scaling effect of multiplicative updates. Thus try absolute updates.

Example: AIDS_perfect - SVM accuracy

Expected (almost) 100% for iteration 0. But got only 51%.

Testing the SVM with other **kernel lambdas** λ besides the standard 'scale' in the computation of the kernel matrix from the distance matrix D:

$$K := \exp(-\lambda D)$$

λ	scale	**auto**	0.1	0.5	1.0
Avg.Acc.	50.43	97.94	79.99	50.54	50.91
Std.dev.	3.69	2.53	1.26	0.93	0.55

Where:

- auto: $\lambda = 1/\big(\#\{\text{features}\} * \text{var}(D)\big)$
- scale: $\lambda = 1/(\#\{\text{features}\})$

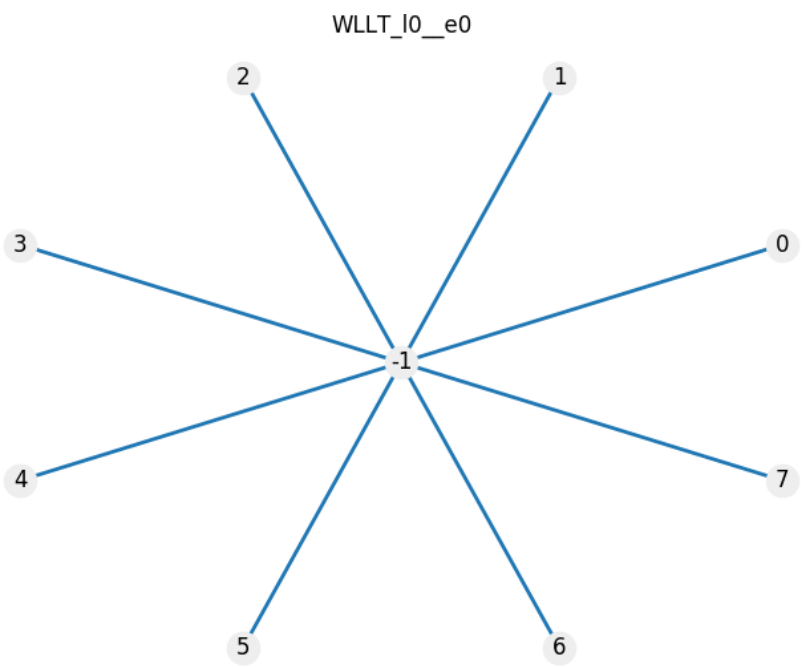
'scale' is the default of sklearn's svm implementation (since version 0.22).

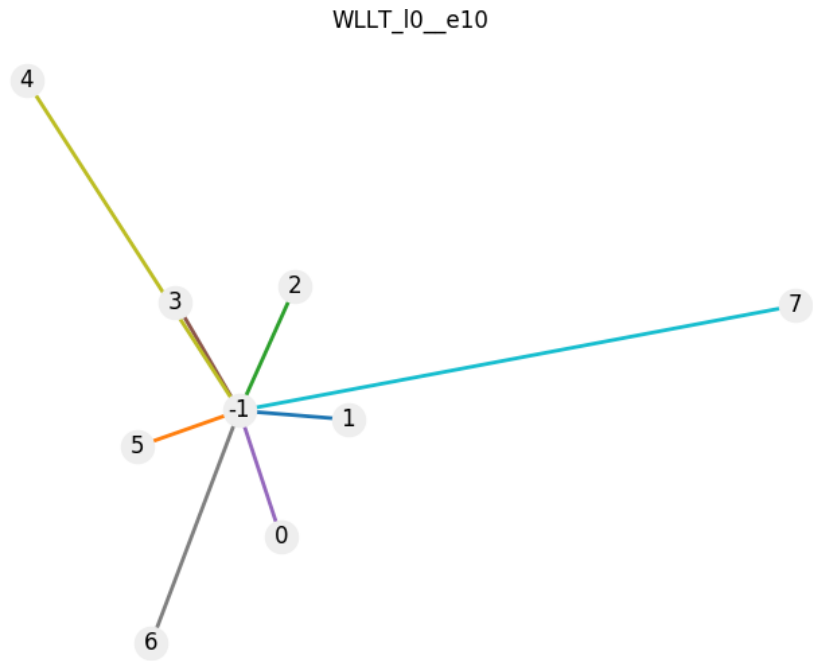
Outlook

- "Finish" experiments with `AIDS_perfect`
  (limits of push-pull, absolute weight update, single layer)
- Try to find more truly SME improving configuration for (normal) AIDS
  (Ideally increasing diff-cl distance **and** decreasing same-cl dist.)

- Besides this: **Terminate the evaluations** and report about the investigated parameter configurations.
  Outlook for improvement of the method: e.g. Layer gradient

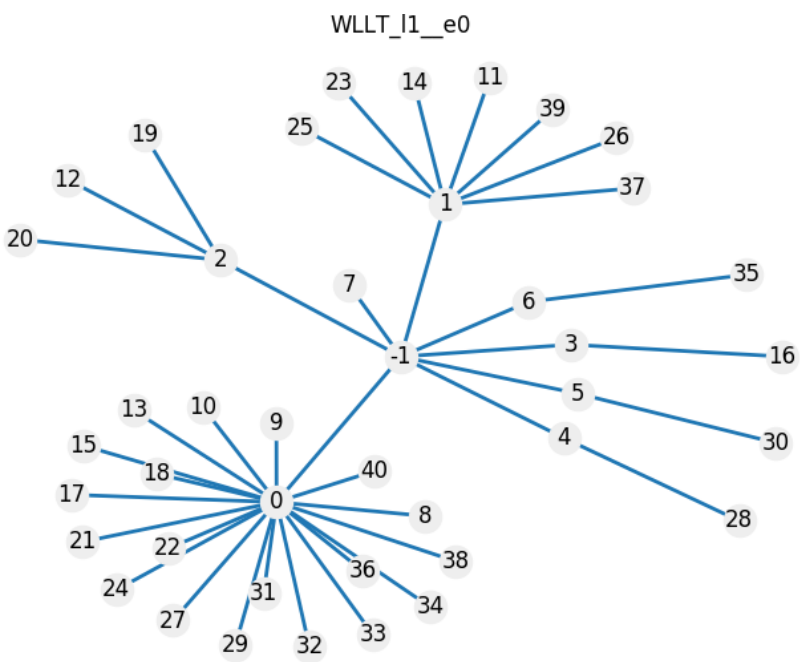
Example: MUTAG WLLT layer 0

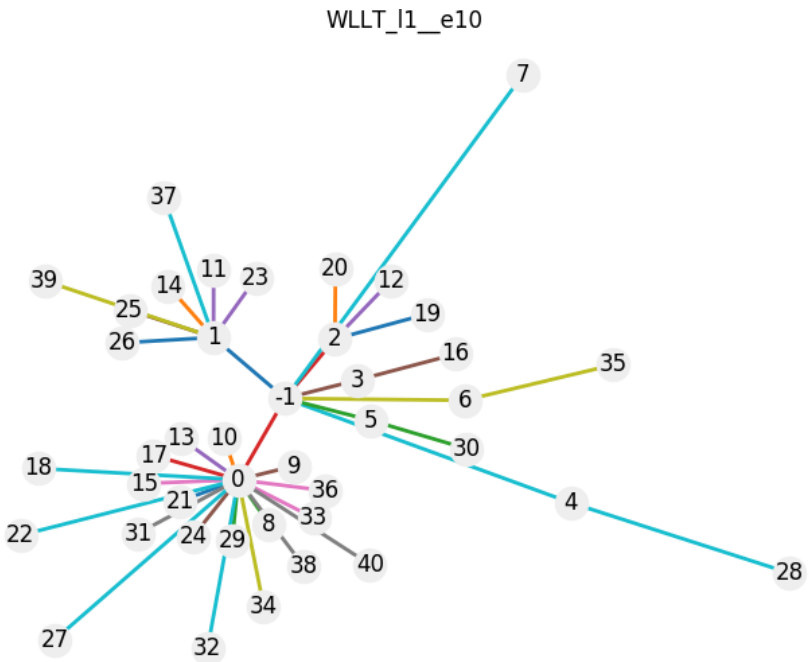




Bs: 20%, WLLT-d: 4, Pull: 0.3, Push: 0.1, SVM-acc.: 66%

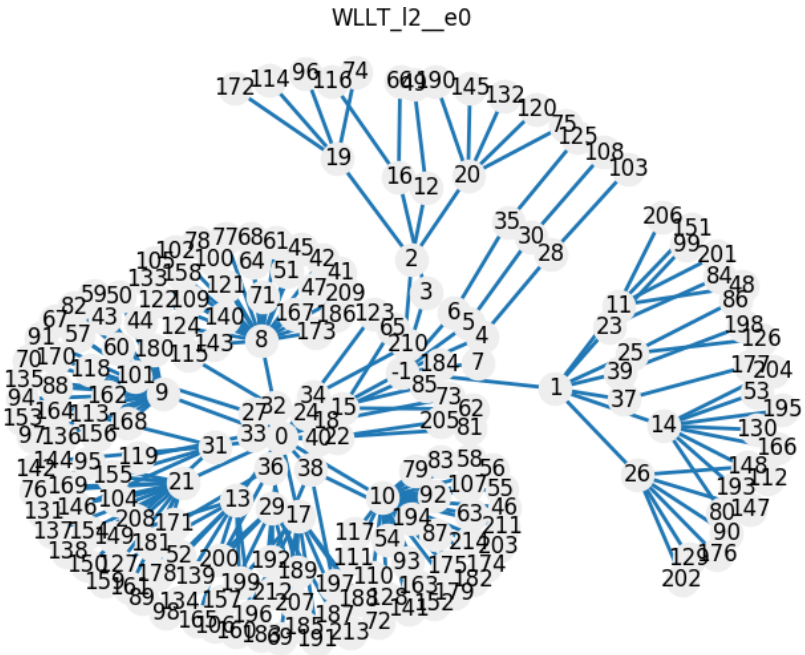
Example: MUTAG WLLT layer 1

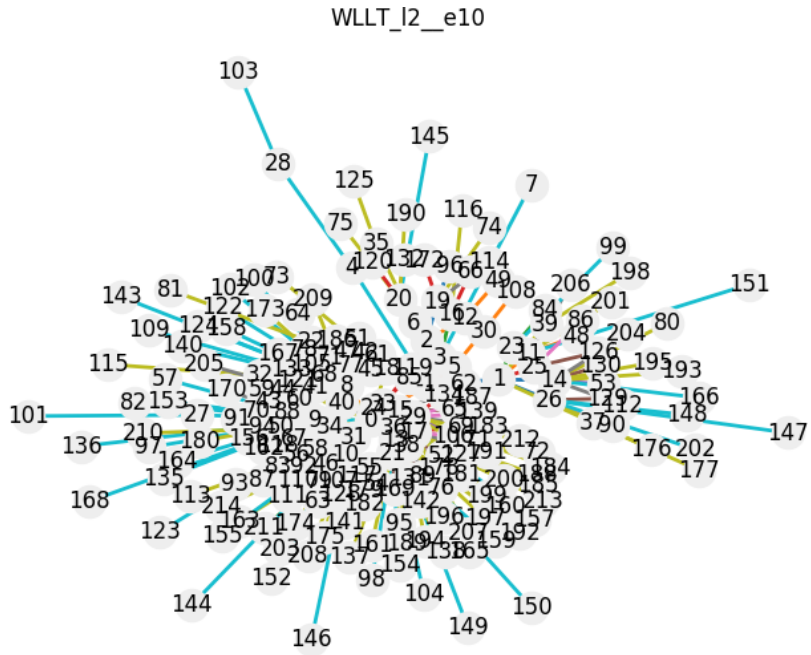




Bs: 20%, WLLT-d: 4, Pull: 0.3, Push: 0.1, SVM-acc.: 66%

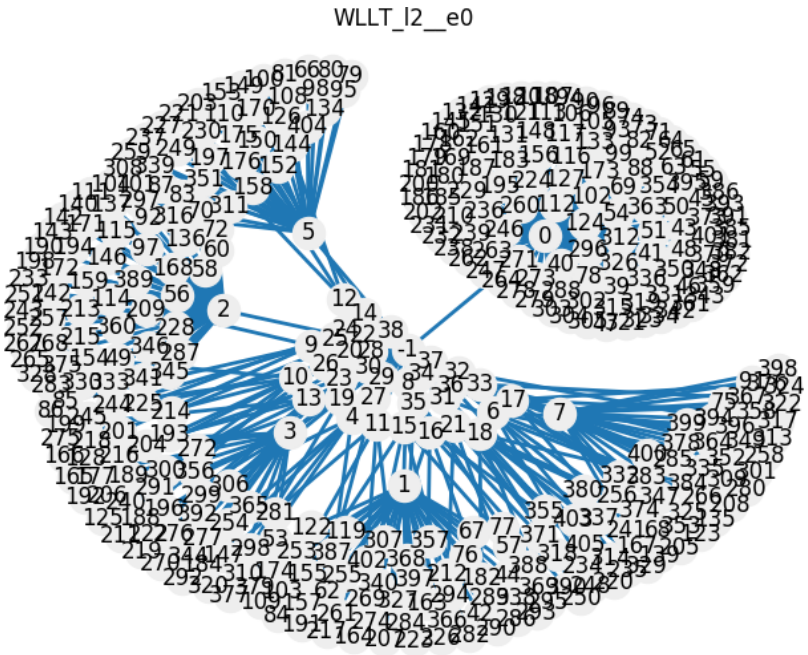
Example: MUTAG WLLT layer 2

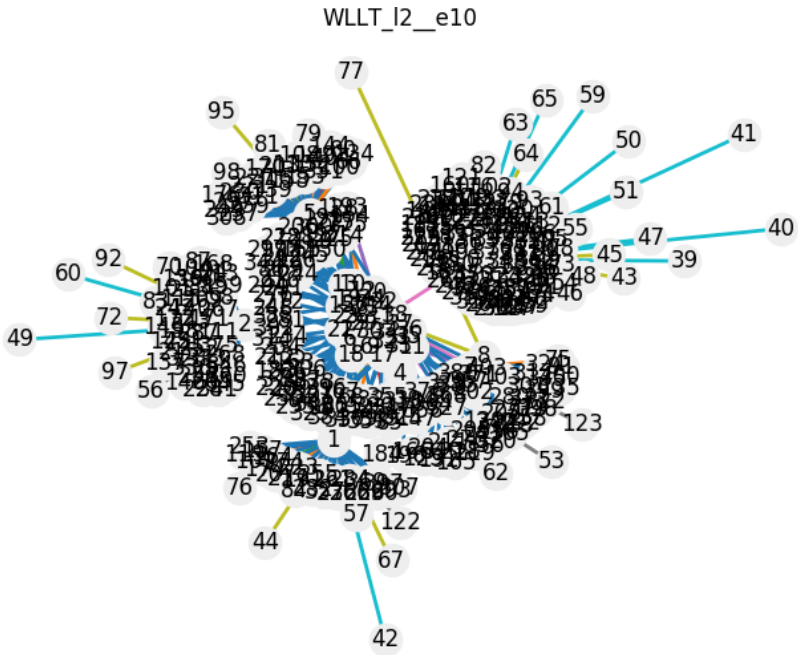




Bs: 20%, WLLT-d: 4, Pull: 0.3, Push: 0.1, SVM-acc.: 66%

Example: AIDS WLLT layer 2





Bs: 5%, WLLT-d: 4, PP: 0.4, SVM-acc.: 80%

Thank you all for listening.

I will be happy to answer any **questions** and hear your **comments**.

Preparation of the performance comparison

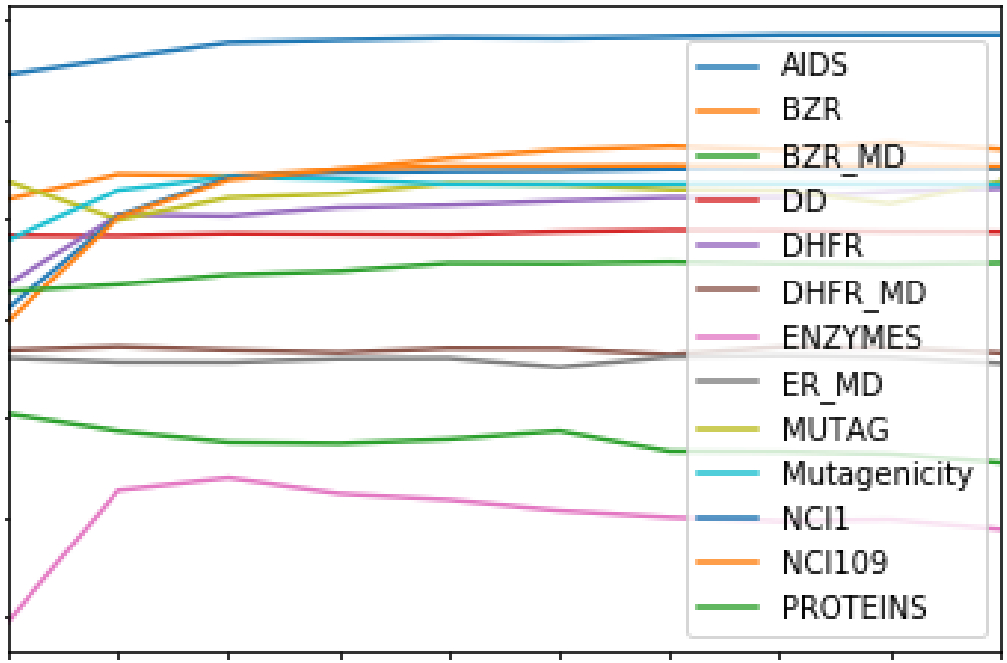


Figure: Classification accuracies on databases using Weisfeiler-Lehman.

```
grakel.kernels.WeisfeilerLehman(n_iter=[1-10], base=grakel.kernels.VertexHistogram, normalize=True)
grakel.utils.cross_validate_Kfold_SVM(K, y, n_iter=10)
```