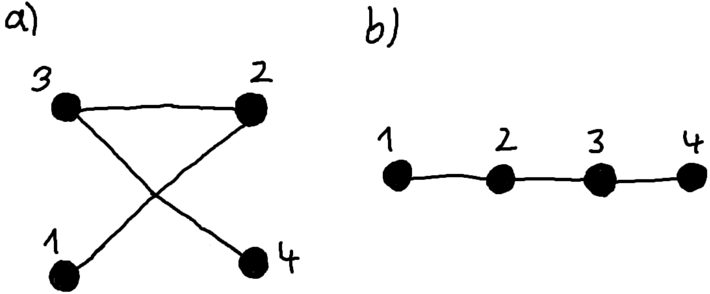
Graph Layouts and Contrastive Learning using Neighbour Embedding Algorithms

Hertie Institute for Artificial Intelligence in Brain Health, Berens Lab
supervised by Dr. Dmitry Kobak

presented by Alica Guzmán

23-02-2023

2D viszualizations of a graph



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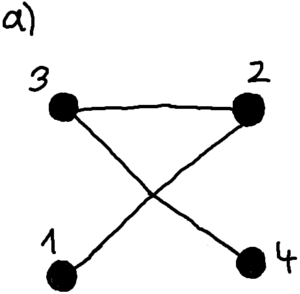

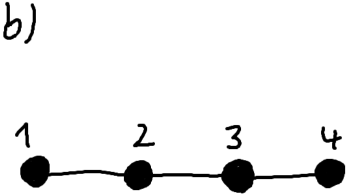

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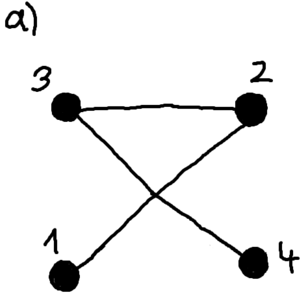

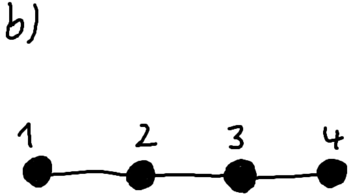

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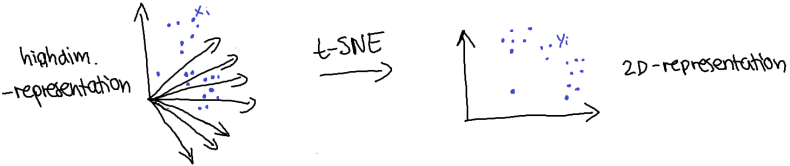
low-dimensional coordinates $\mathbf{y}_i$ with $i = 1, \ldots, 4$ (2-dim.)

Introduction to t-SNE

t-SNE



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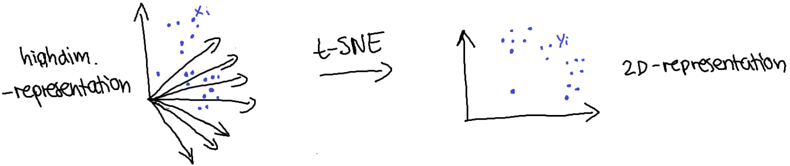

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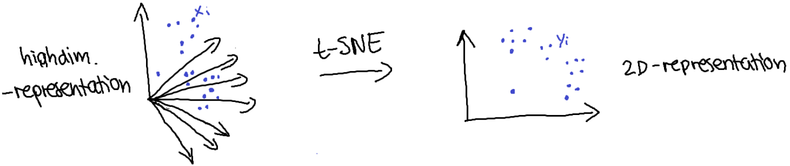

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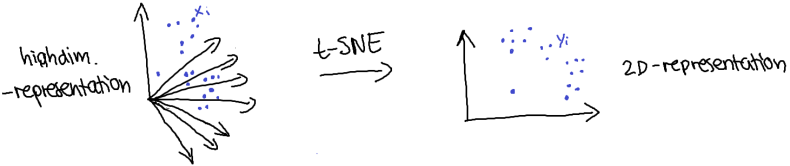

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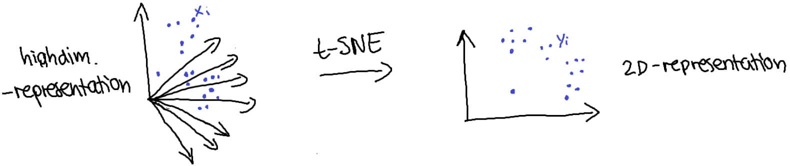

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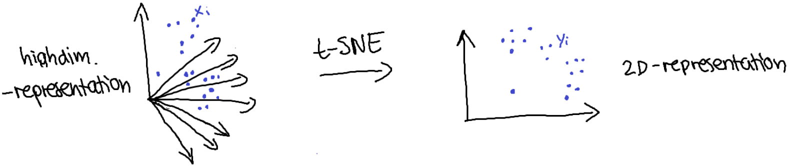

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$$\frac{\partial C_{KL}}{\partial y_i} \sim \underbrace{\sum_j p_{ij} N w_{ij}(y_i - y_j)}_{\text{attractive forces}} - \underbrace{\frac{N}{\sum_{k\neq l} w_{kl}} \sum_j w_{ij}^2 (y_i - y_j)}_{\text{repulsive forces}}.$$

(Maaten and Hinton 2008, Böhm, Berens and Kobak 2022)

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Same procedure...

Results

Graph t-SNE I

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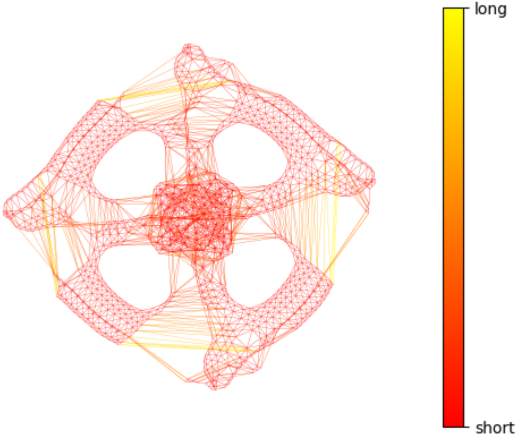
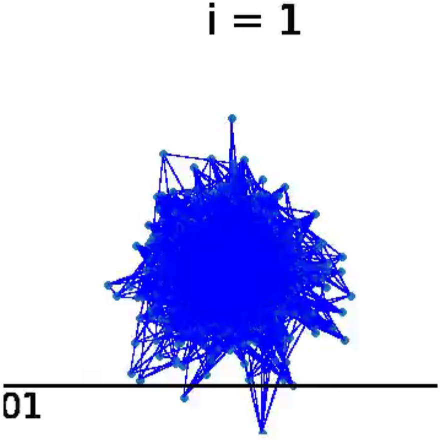


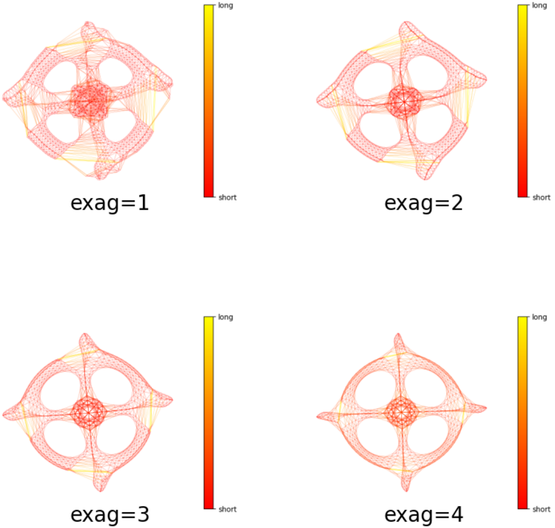
Standard t-SNE on dwt_1005. kNN recall = 0.79

Graph t-SNE I - Animation

show here animation



Graph t-SNE I - Exaggeration



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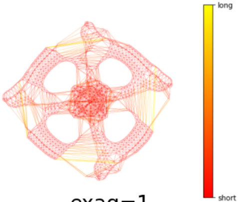
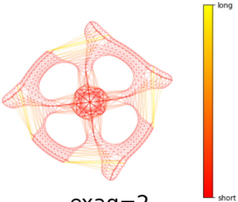


exag=1



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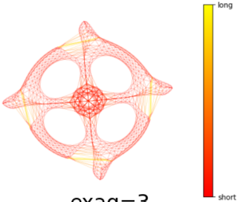

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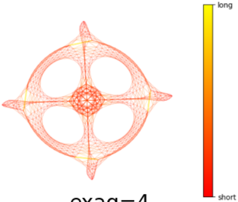
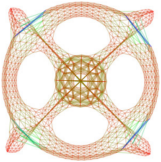


exag=4



dwt_1005 graph layout by tsNET* (Kruiger et al. 2017)

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    - segment of Amazon Co-Purchase Graph

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  - labeled by 10 subcategories
  - contains 767 node features, which are bag-of-words encoded product reviews

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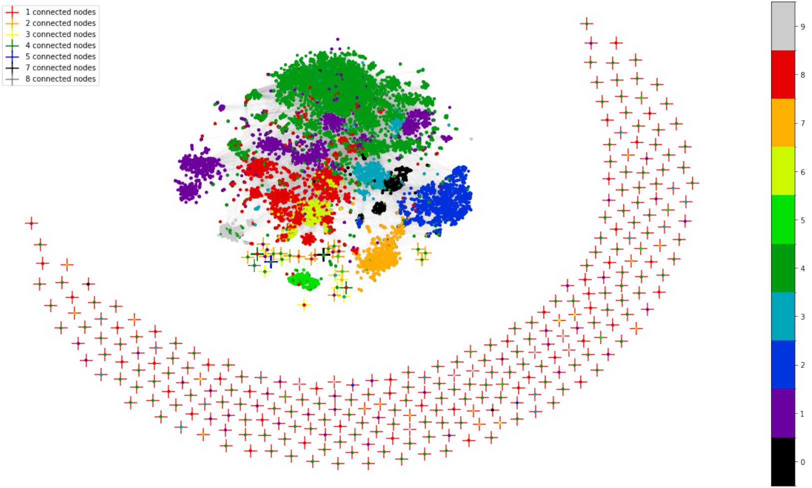

Standard t-SNE on Amazon Computer. Crosses indicate connected components. Coloured by Labels. kNN accuracy = 0.89

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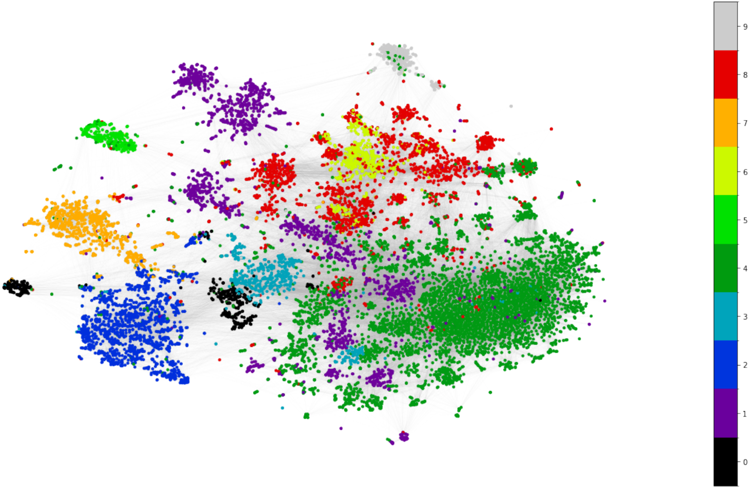

Standard t-SNE on the biggest connected component of Amazon Computer. Coloured by Labels. kNN accuracy = 0.93

Feature t-SNE

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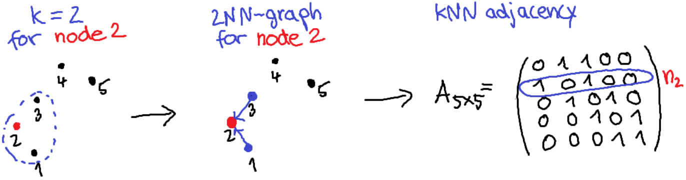

1. Find k nearest neighbours (default $k = 90$) in the feature space and construct a kNN adjacency matrix.

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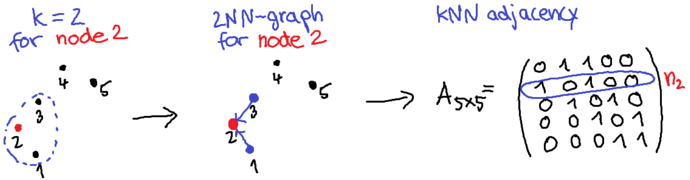

1. Find k nearest neighbours (default $k = 90$) in the feature space and construct a kNN adjacency matrix.
2. Construct an affinity matrix from the kNN adjacency.

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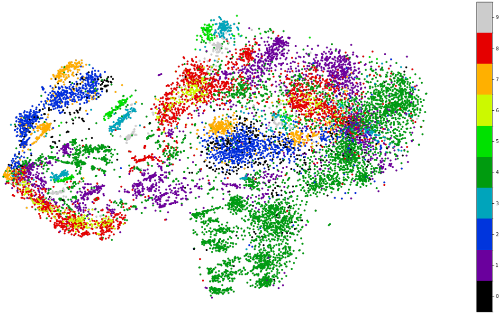
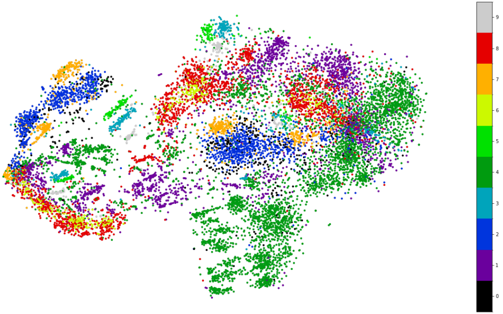
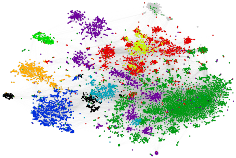


Standard t-SNE on features of biggest connected component of Amazon Computer. Coloured by Labels. kNN accuracy = 0.79

Feature t-SNE





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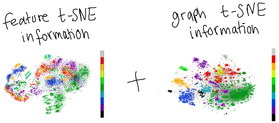
Contrastive Graph t-SNE Embedding - Concept

Idea: Combine



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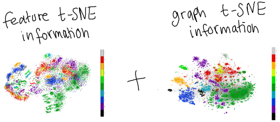
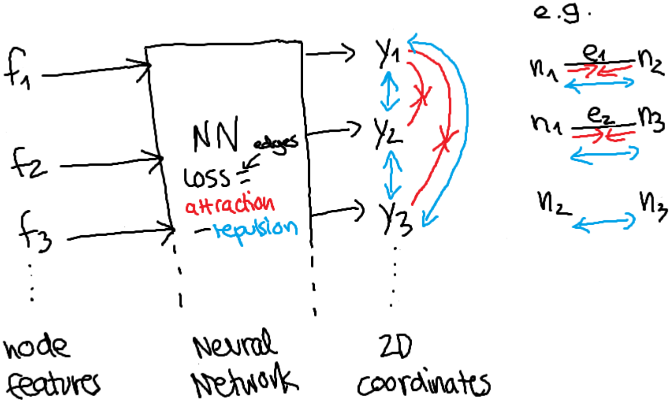
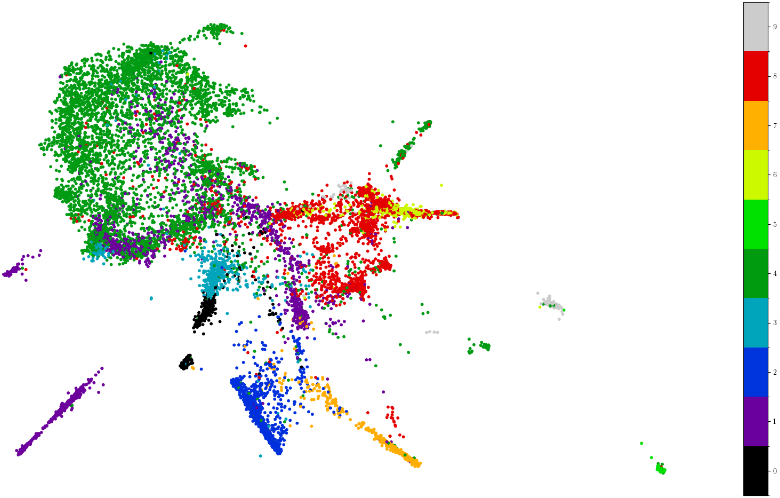




framework based on Damrich et al. 2022

Contrastive t-SNE Embedding



Contrastive t-SNE Embedding of biggest connected component of Amazon Computer. Coloured by label. kNN accuray = 0.84

Conclusion and Outlook

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- investigate Contrastive t-SNE Graph Embedding framework with different settings

Thank you!