# Dimensionality reduction using graphs

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# #19: Dimensionality reduction using graphs

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## Problem statement

- **Dimensionality reduction**
  - Reduce dimension of data while preserving the structure of data, such as clustering or closeness of points
  - Can be used for
    - Visualisation (reduction to 2D or 3D)
    - Preprocessing for ML algorithms
  - State of the art algorithms
    - PCA – powerful and fast, cannot capture complex manifolds
    - UMAP, t-SNE – powerful and fast, complex to understand



## Our goal

- **Our research question**
  - Can we capture the structure of data in graph?
    - Use graph as a compact representation of the data
    - Can be used to compress data
  - Can we use the obtained graph to reduce dimensionality?
    - We can use graph embedding methods
- **Advantages of our approach**
  - Easy to understand algorithm
  - Able to capture complex manifolds



## Graph building

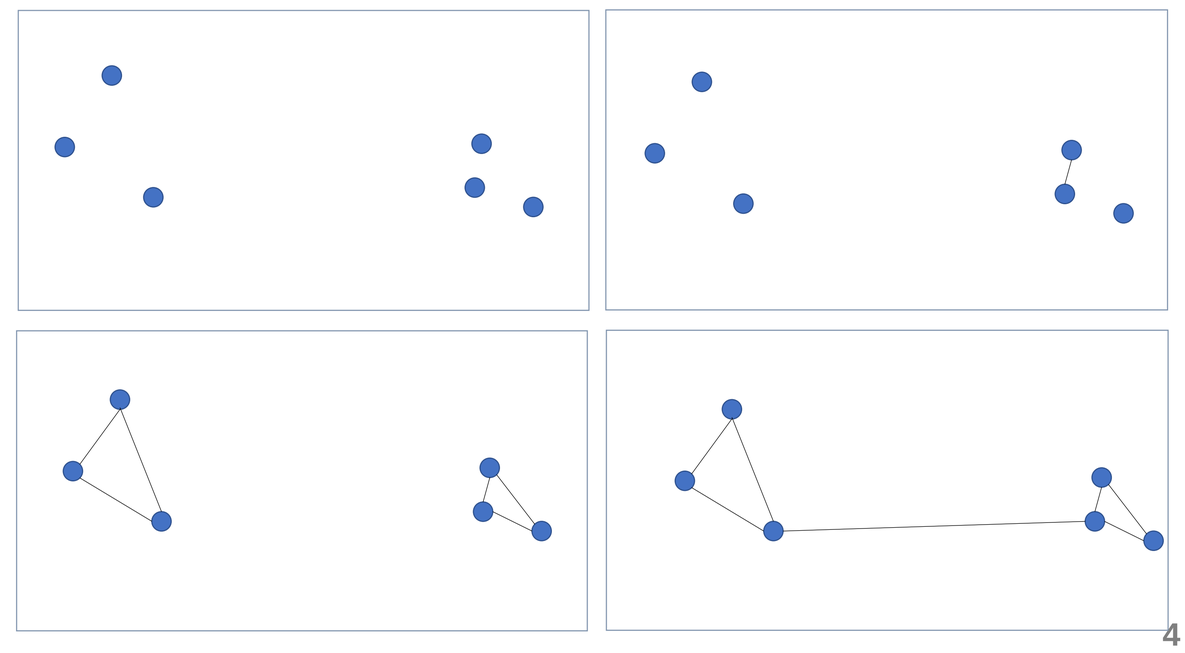
- **Cheapest builder**
  - Every datapoint is represented by node
  - We compute pairwise distances between all datapoints
  - Points with the shortest distances are connected by edges, edges added one by one until the graph is connected
  - Edge weights are added using the distances as

$$w = \frac{1}{d^k}$$

  - k is a hyperparameter
- **Spanning tree**
  - We can use spanning tree, weights same as cheapest builder



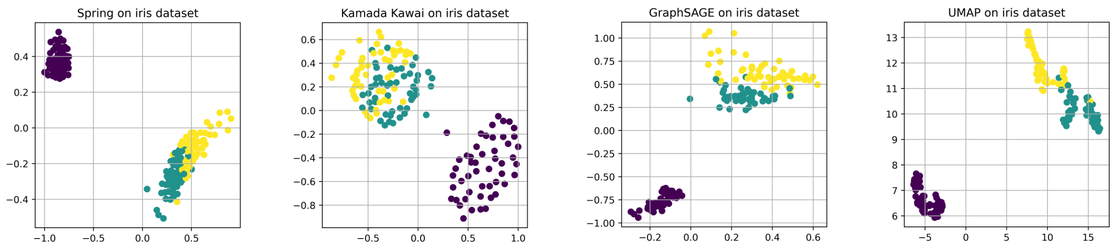
## Graph building – cheapest builder



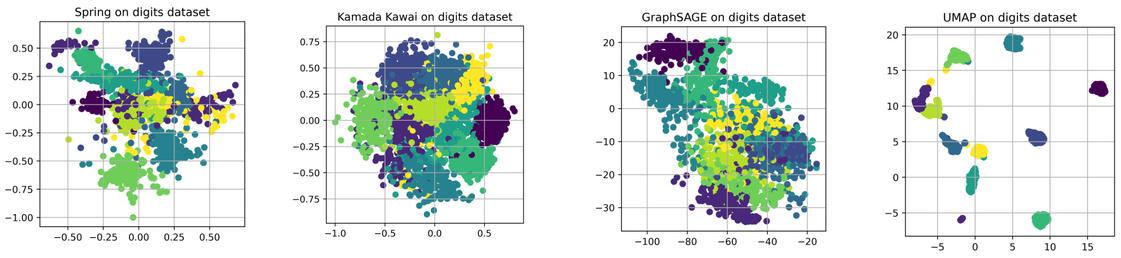


## Visual results

Iris – 150 datapoints, dimensionality 4, 3 classes



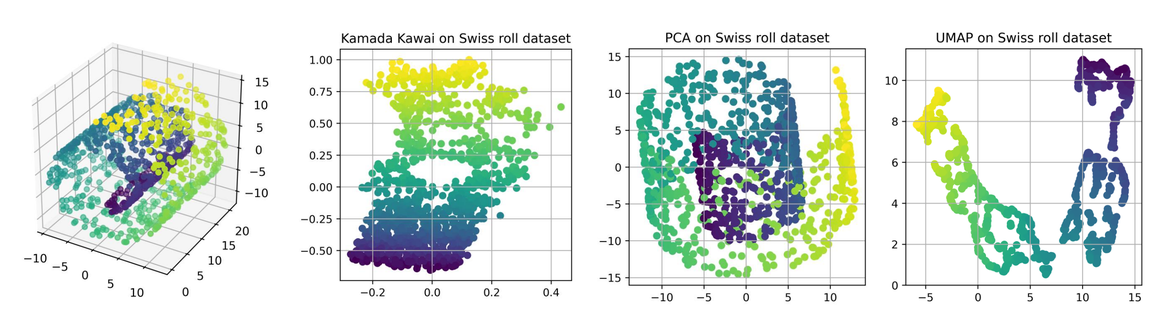

Digits - 1797 datapoints, dimensionality 64, 10 classes



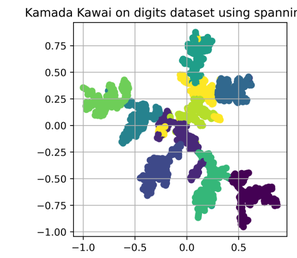



## Visual results

Can we unroll the Swiss roll?




How do the embeddings look using spanning tree?






## Quantitative results – digits dataset

| Algorithm | Dimension | Trustworthiness | Continuity | Computation time |
|---|---|---|---|---|
| Cheapest + Spring | 2 | 0.9182 | 0.9784 | 1m 49.7s |
| Cheapest + Kamada Kawai | 2 | 0.8728 | 0.9661 | 8m 39.0s |
| Spanning + Kamada Kawai | 2 | **0.9875** | **0.9859** | 2m 5.0s |
| Cheapest + GraphSAGE | 2 | 0.8462 | 0.9530 | 34m 22.6s |
| PCA | 2 | 0.8591 | 0.9646 | 0.2s |
| UMAP | 2 | **0.9913** | **0.9927** | 7.2s |
| Cheapest + Kamada Kawai | 10 | 0.9949 | 0.9937 | 11m 8.1s |
| Spanning + Kamada Kawai | 10 | **0.9951** | **0.9867** | 57m 38.1s |
| Cheapest + GraphSAGE | 10 | 0.9611 | 0.9774 | 24m 40.5s |
| PCA | 10 | **0.9979** | **0.9990** | 0.3s |
| UMAP | 10 | 0.9961 | 0.9944 | 7.8s |



## Summary

- We used simple algorithms for graph building and still obtained great results
- Our algorithm is able to compete with state-of-the-art algorithms in terms of trustworthiness and continuity
- However, we can not compete in computational time
- Also, we use all pairwise distances, which is not feasible for big datasets
- None of our methods is universally best on every dataset
- That creates a room for improvements