#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

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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

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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

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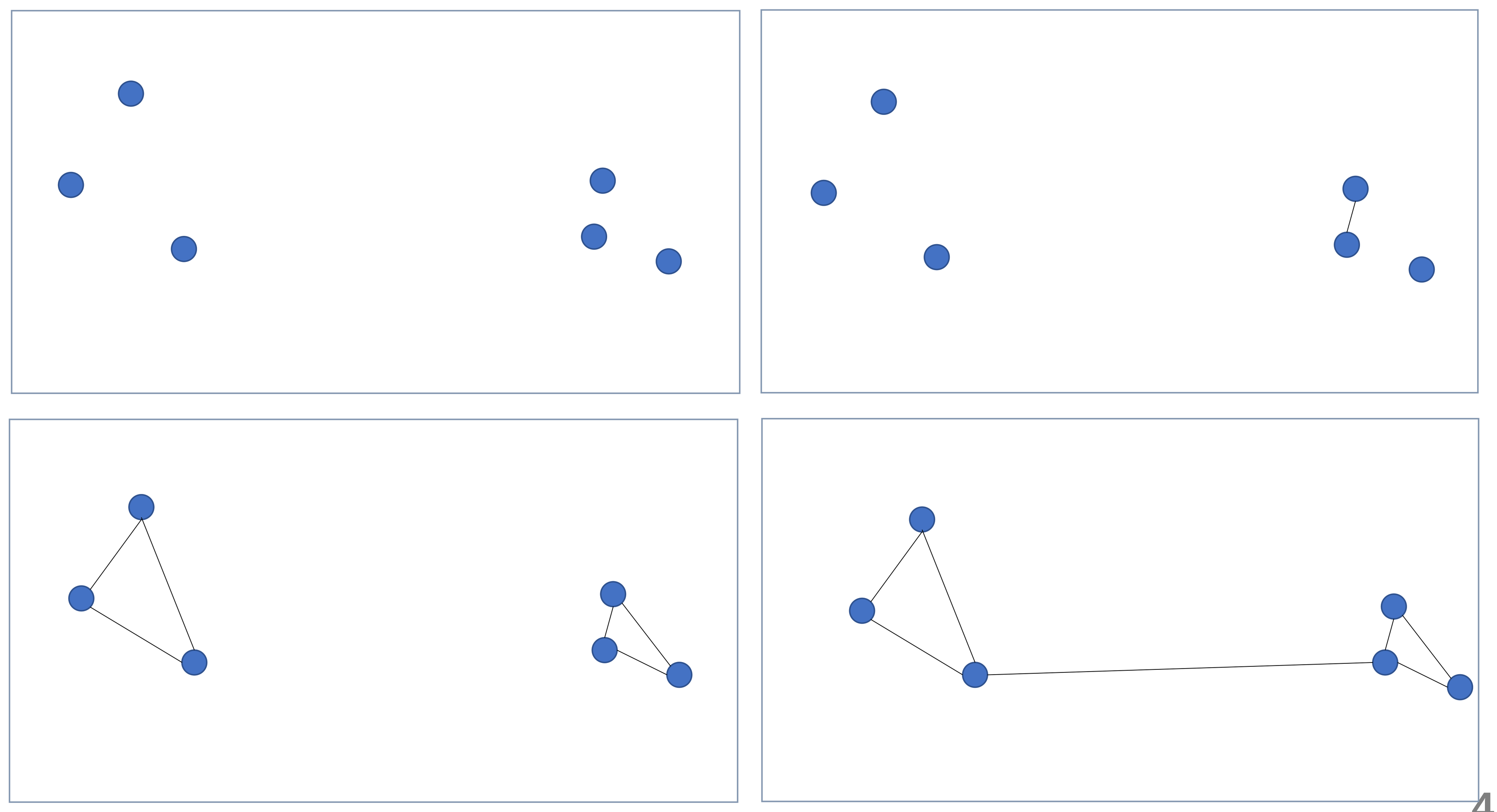
Graph building – cheapest builder



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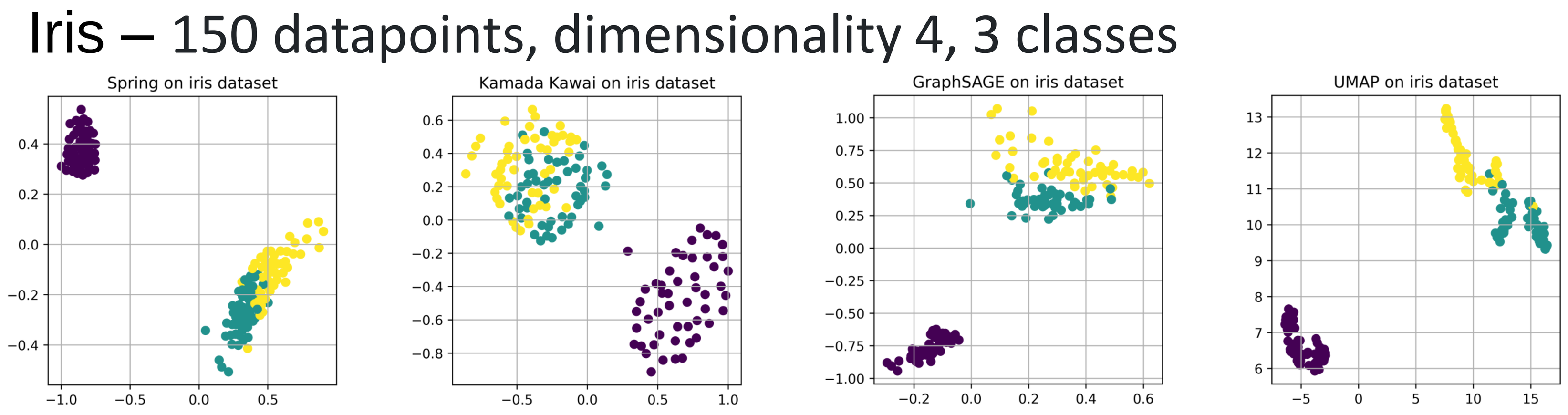
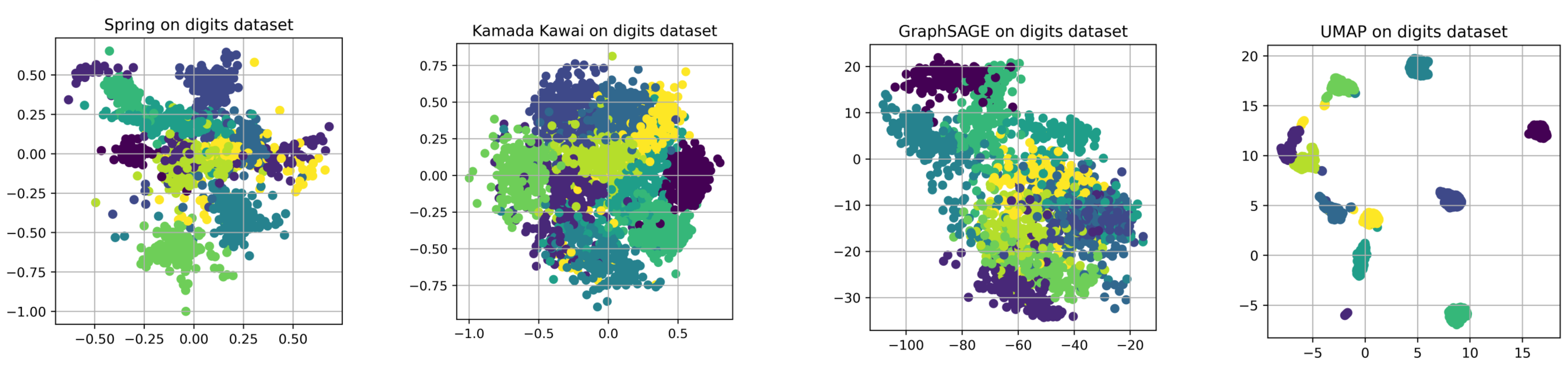
Visual results

Iris – 150 datapoints, dimensionality 4, 3 classes



Digits - 1797 datapoints, dimensionality 64, 10 classes



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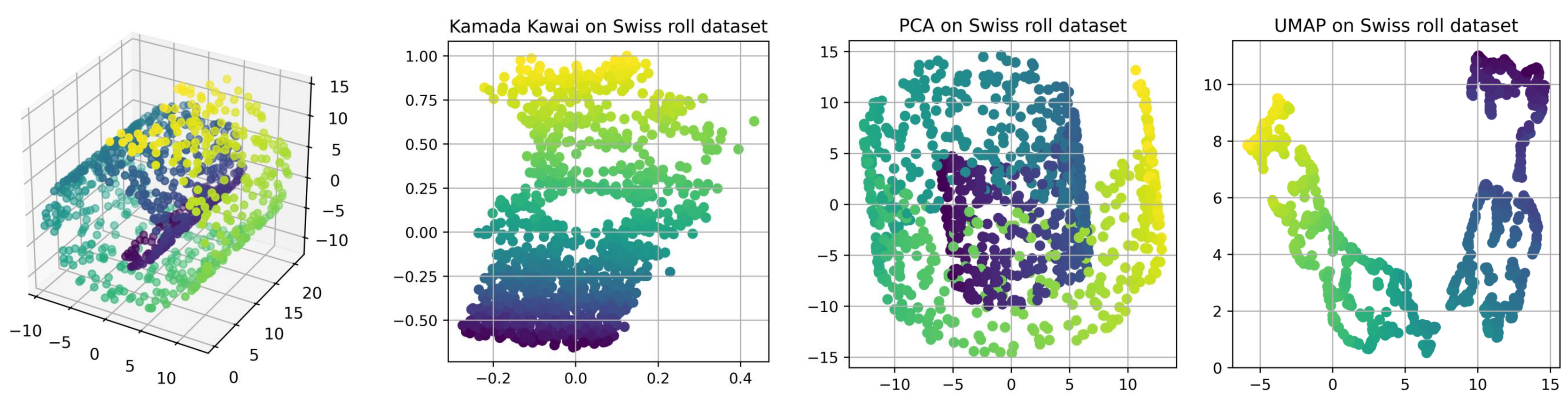
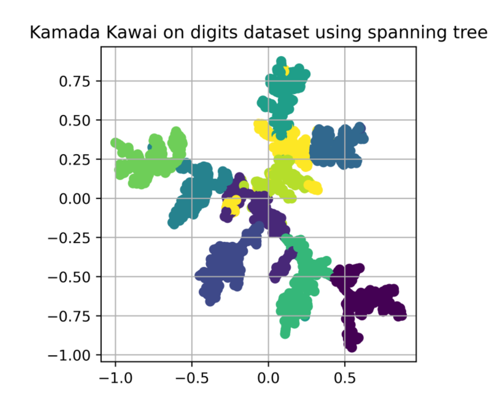
Visual results

Can we unroll the Swiss roll?



How do the embeddings look using spanning tree?



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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

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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

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