Machine Learning for Graphs and Sequential Data

Graphs – Node/Graph Embeddings

lecturer: Prof. Dr. Stephan Günnemann

Summer Term 23

Data Analytics and
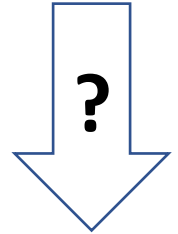Machine Learning
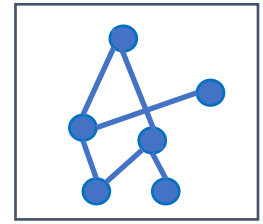
TUM

Roadmap

- **Chapter: Graphs**

  1. Graphs & Networks

  2. Generative Models

  3. Ranking

  4. Clustering

  5. Classification (Semi-Supervised Learning)

  6. **Node/Graph Embeddings**

  7. Graph Neural Networks (GNNs)

Data Analytics and
Machine Learning

Challenge of ML on Graphs

- So far, we have seen highly „specialized" ML methods for graphs

- Can we apply <u>traditional</u> ML methods to graphs?

    - Traditional ML approaches have no concept of graphs
      (they usually operate on i.i.d. vector data)

    - How to encode the graph structure (in vector form)?

- k-means
- SVM
- etc.

adjacency matrix

- Naive approaches violate basic properties and assumptions

    - Adjacency matrix as image is not invariant to node permutation

    - Concatenating features of neighbors produces variable length data
      (and we might even not have features - only structure)

   - $O(N^2)$ scaling in runtime

Data Analytics and
Machine Learning
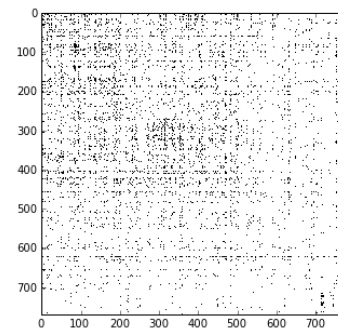
Learning Node Representations

General approach:

- Transform the graph such that each *vertex* is represented by a vector

  - Node embedding function $\Phi: V \rightarrow \mathbb{R}^d$ maps each node to a vector in $\mathbb{R}^d$ (e.g., the smallest d eigenvectors for spectral clustering).

  - Nodes close in the embedding space are "similar" w.r.t. graph structure
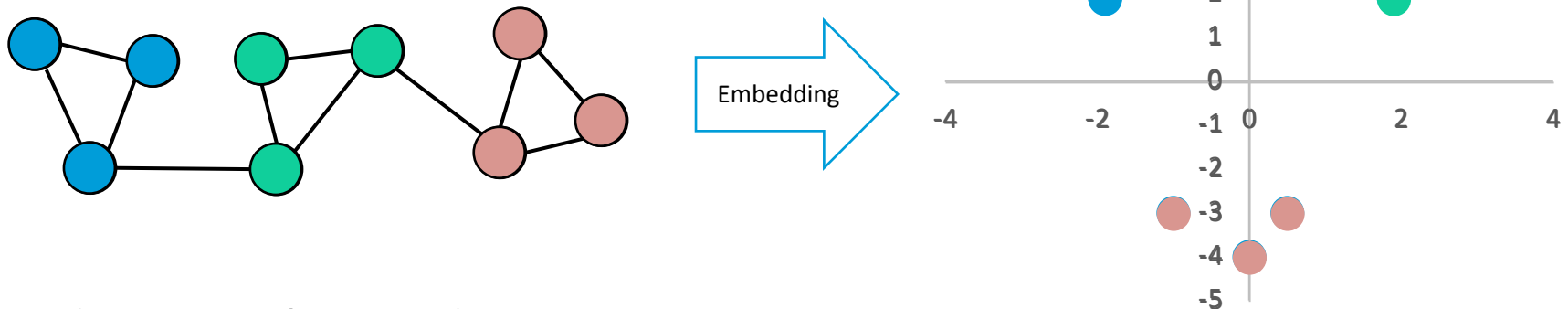
- We have transformed the **discrete nodes** into **vector data**.

  - We can now use **standard tools** for vector data to perform "downstream" tasks such as clustering or classification.

Applications

Embedding
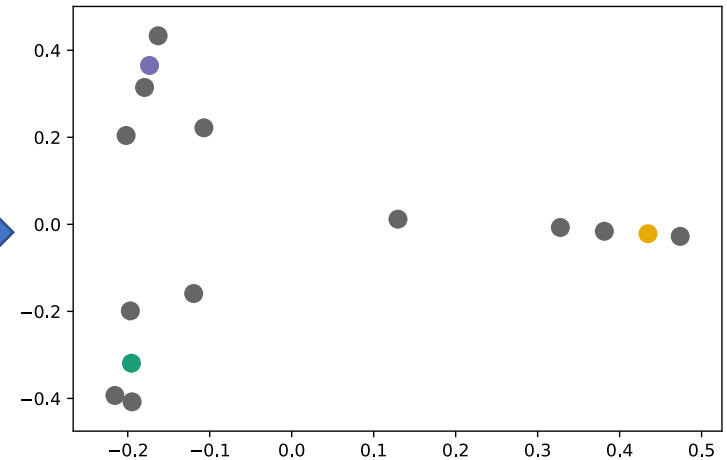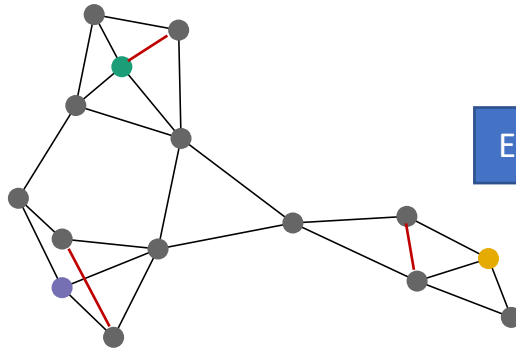
- **Clustering**

  Group the nodes into a set of clusters in an unsupervised way, e.g. using K-Means.

- **Semi-supervised classification**

  Given a small set of **labeled** nodes for which we know their class, classify the remaining nodes in the graph based on their representations.

- **Link prediction**

  – Predict likely (unobserved) links in the graph, e.g. friendship recommendation or "other users have watched/bought" lists.

  – $\Pr\big((i, j) \in E\big) \propto \Phi(v_i)^T \Phi(v_j)$

Data Analytics and
Machine Learning

Types of Embeddings

- Many possible ways to define an embedding

  - Differences come from how we define similarity between nodes in the embedding space and which properties of the graph we are trying to capture

  - For example in *role-based embeddings* nodes with similar role (e.g. hubs) should be close together in the embedding even if they are far in the graph

  - We will see an NLP inspired approach in the deep embeddings section

- Spectral embeddings → nodes are similar if they belong to the same clusters

- Deep embeddings → similarity depends on loss function and architecture

Data Analytics and
Machine Learning

Roadmap

- **Chapter: Graphs**

    1. Graphs & Networks

    2. Generative Models

    3. Ranking

    4. Clustering

    5. Classification (Semi-Supervised Learning)

    6. **Node/Graph Embeddings**

        – Motivation

        – **Selected Embedding Methods**

    7. Graph Neural Networks (GNNs)

Data Analytics and
Machine Learning

Recap: Spectral Clustering

- Construct the graph Laplacian L

- Compute the first k eigenvectors v_i of L in columns of H, i.e. $H_i^T = v_i$

- Represent the i-th node as the i-th row of H

- Cluster the vector representations, for example with k-means
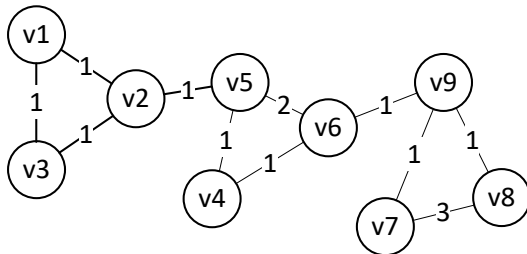
2	-1	-1	0	0	0	0	0	0
-1	3	-1	0	0	-1	0	0	0
-1	-1	2	0	0	0	0	0	0
0	0	0	2	-1	-1	0	0	0
0	-1	0	-1	4	-2	0	0	0
0	0	0	-1	-2	4	0	0	-1
0	0	0	0	0	0	4	-3	-1
0	0	0	0	0	0	-3	4	-1
0	0	0	0	0	-1	-1	-1	3

Graph Laplacian L

```
-0.3333   -0.4376    0.2939
-0.3333   -0.3370    0.0890
-0.3333   -0.4376    0.2939
-0.3333    0.0000   -0.5878
-0.3333   -0.0584   -0.3829
-0.3333    0.0584   -0.3829
-0.3333    0.4376    0.2939
-0.3333    0.4376    0.2939
-0.3333    0.3370    0.0890
```

Eigenvectors of L

- Smallest eigenvalues of L: 0 ; 0.23 ; 0.7

Data Analytics and
Machine Learning

Spectral Clustering: Embedding View

- Spectral embedding is based on the **eigenvectors of the graph Laplacian L**

  - L encodes the structural behavior of the graph G

  - $|V| \times |V|$ adjacency matrix is transformed and reduced to $|V| \times k$ matrix H

- Relation to PCA and dimensionality reduction

  - transformation is based on eigenvectors of the data-matrix and one retains only eigenvectors with smallest/largest eigenvalue
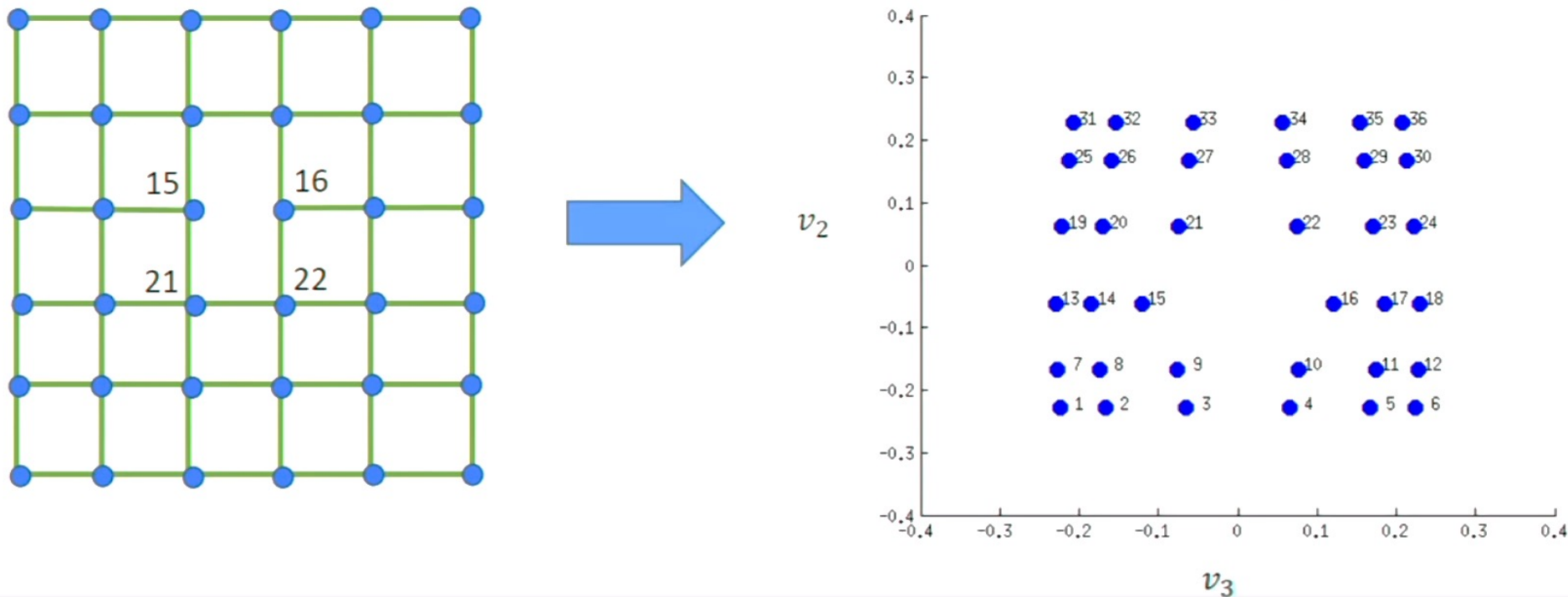
Data Analytics and
Machine Learning

Examples (I)

- Spectral embedding of a grid

Data Analytics and
Machine Learning
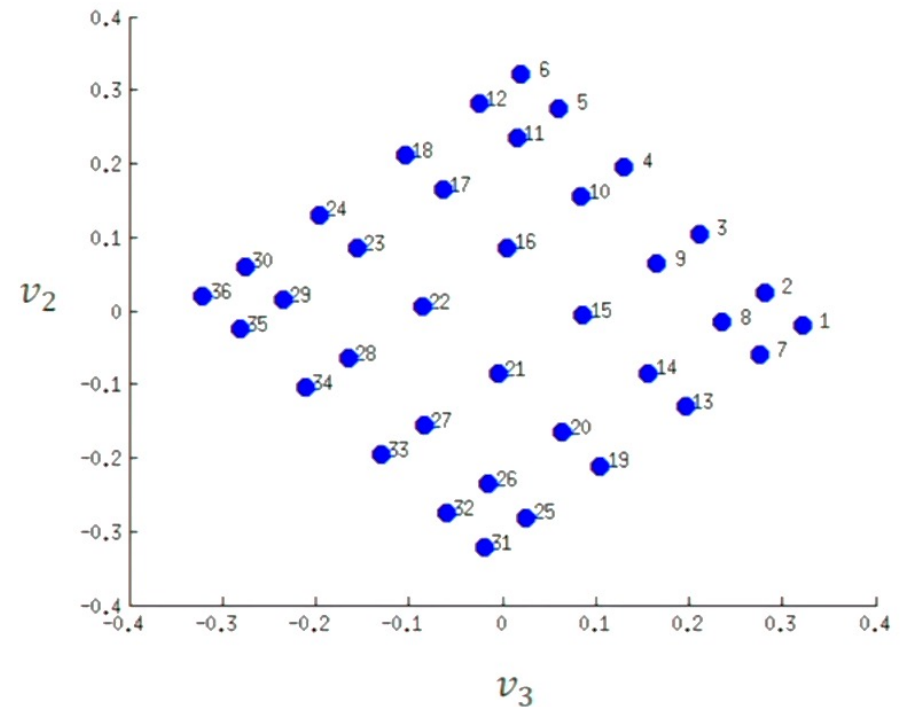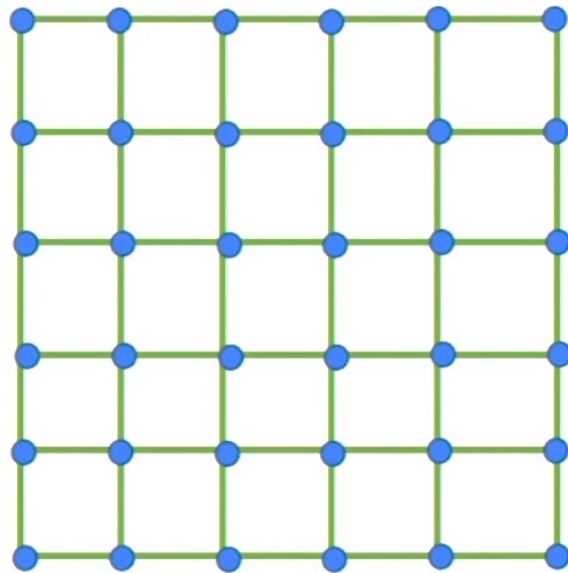
Examples (II)

- Spectral embedding of an incomplete grid with one edge removed

"Deep" Node Embedding Approaches

- Representation learning for graphs has become a very active field of research in recent years

  - specifically exploiting neural networks/deep learning etc.

- Goal: Try to capture more complex structure than spectral embeddings

  - thus, hopefully getting better results for specific downstream task

  - or capturing different notions of "similarity"

- Natural language processing (NLP) also deals with discrete data (words), and we can try to adapt successful techniques to graphs

  - **DeepWalk** [Perozzi2014] is a popular node embedding algorithm based on the word embedding model **word2vec** [Mikolov2013]

Data Analytics and
Machine Learning

DeepWalk

- **Idea**: transform the graph into a set of random walks and learn a **word2vec** model

- For every node v_i sample multiple random walks

- **Random walks** correspond to **sentences** in word2vec; both are sequences of discrete tokens (node-ids $\hat{=}$ words)

- Train word2vec on the collection of all these "sentences"

graph   sample   random walks   Train word2vec   embedding
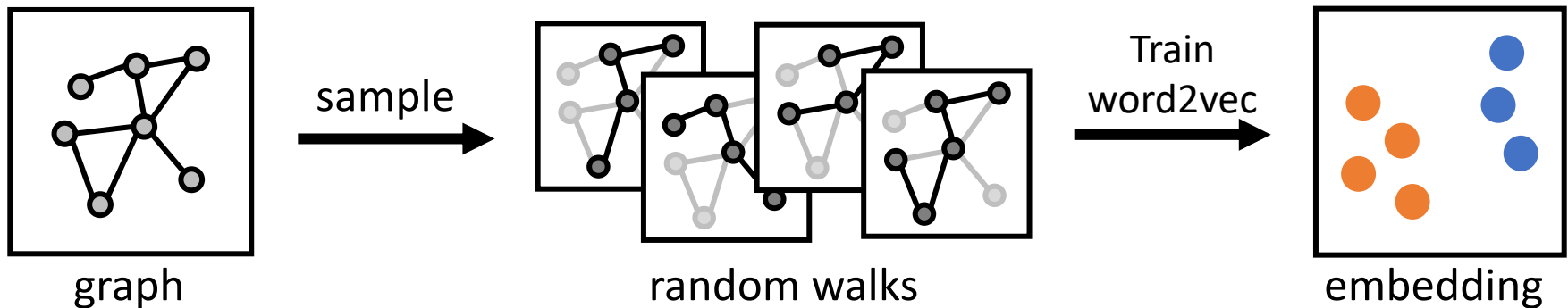
- **Result**: nodes that are close to each other in the graph and share many neighbors get similar vector representations (embeddings)

Data Analytics and Machine Learning

Graph2Gauss

- **Idea**: map each node v_i to a Gaussian distrib. in embedding space such that a node's 1st neighbors are closer than its 2nd neighbors and so forth (i.e. preserve ranking)

- Learn a mapping $f_\theta: v_i \mapsto \mathcal{N}\big(\mu_\theta(\boldsymbol{x}_i), \Sigma_\theta(\boldsymbol{x}_i)\big)$

  – For attributed graphs, $\boldsymbol{x}_i$ could represent the node feature of the vertex v_i

  – For plain graphs, $\boldsymbol{x}_i$ could represent the node id of v_i (e.g. via one hot encoding)

- For each node $\boldsymbol{u}$ define a loss $\sum_{(v,w)} E_{uv}^2 + e^{-E_{uw}}$ where $E_{uv} = KL(f_\theta(\boldsymbol{u})||f_\theta(\boldsymbol{v}))$ and $\boldsymbol{v}$ and $\boldsymbol{w}$ are all node pairs such that $\boldsymbol{v}$ is closer to $\boldsymbol{u}$ than $\boldsymbol{w}$ (ranking loss)

graph   *embedding*   *initial embeddings*   *training*   *final embeddings*
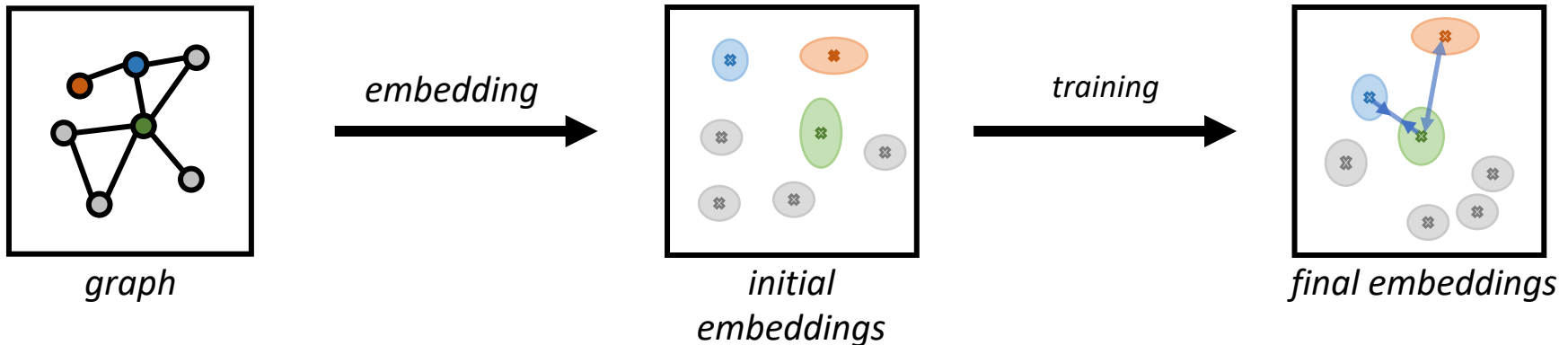
- **Result**: distances in embedding space correlate with distances in the graph and the Gaussian variances express how certain the model is about the embedding

- **Discussion:** Depending on the used input representation $\boldsymbol{x}_i$ (e.g. node features only), the connectivity might just be reflected in the loss function. This potential limitation, however, will allow for inductive learning, i.e. new nodes can easily by embedded [Bojchevski2018]

Data Analytics and
Machine Learning

Graph Embeddings (vs. Node Embeddings)

- Tasks such as predicting molecule properties work on the graph-level instead of with individual nodes

- **Idea**: Leverage node embeddings to embed graphs

- **Problem**: Graphs have different numbers of nodes

  – simple concatenation produces incompatible dimensionalities

- **Solution**: Aggregate all node embeddings into one graph embedding, for example with mean pooling

  – more advanced principles available

graph   node embeddings   graph embeddings

Data Analytics and
Machine Learning
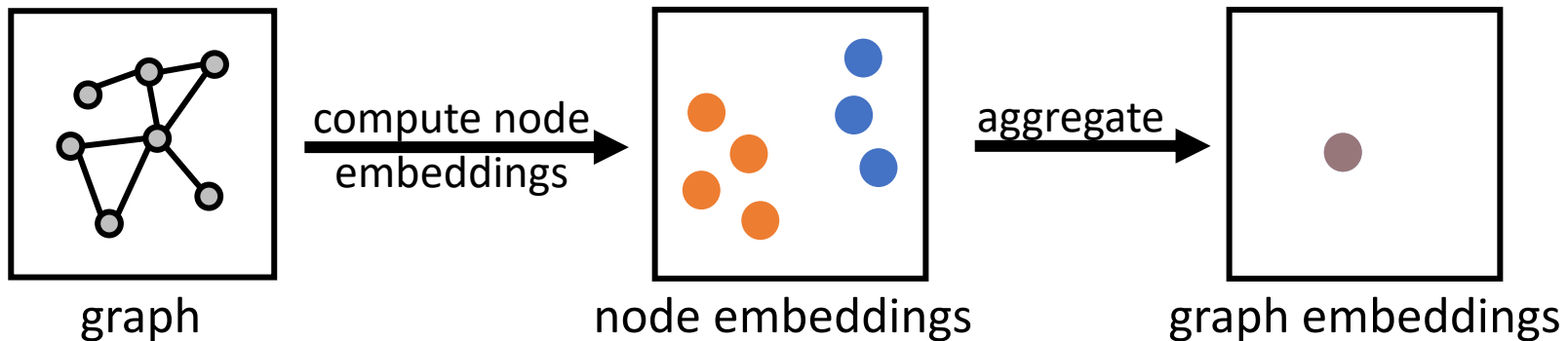
Summary

- Node embeddings translate discrete graph structure information into continuous data

- With node embeddings we can even find fixed-length representations for the graph as a whole

- Classic spectral methods only use graph structure, deep methods can easily combine structural and attribute information

- Embeddings can be fed into ML methods for vector data, e.g.

  - k-means

  - SVMs, NNs

  - visualization in 2D/3D

Data Analytics and
Machine Learning

Questions

- How can you use node embeddings to visualize the structure of a graph?

- Consider two nodes u and v in a graph that share the same node attributes x but are far apart in the graph. What can you say about the embeddings that Graph2Gauss would find for these nodes? How does this depend on the featurization of the nodes? Why do the other methods work better?

Data Analytics and
Machine Learning

Reading Material

- [Perozzi2014] Perozzi, B., Al-Rfou, R., & Skiena, S. (2014, August). Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 701-710)

- [Mikolov2013] Mikolov, T., Sutskever, I., Chen, K., Corrado, G. S., & Dean, J. (2013). Distributed representations of words and phrases and their compositionality. In *Advances in neural information processing systems* (pp. 3111-3119)

- [Bojchevski2018] Bojchevski, A., Günnemann, S. (2018). Deep Gaussian Embedding of Graphs: Unsupervised Inductive Learning via Ranking. In *International Conference on Learning Representations* (ICLR)

Data Analytics and
Machine Learning