Machine Learning for Graphs and Sequential Data

Graphs – Generative Models

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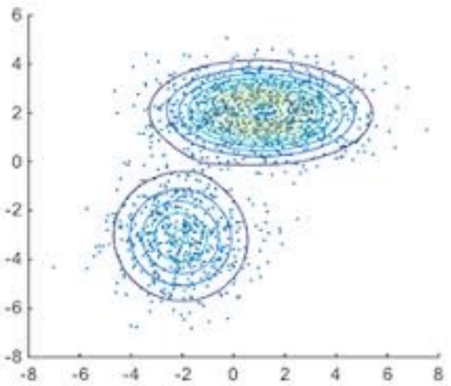
Data Analytics and
Machine Learning

Recap: Generative Models

- Generative model: statistical model to describe the data distribution
  - for unsupervised learning, e.g., $p(\boldsymbol{x})$
  - can also be used for generating data (hence the name)

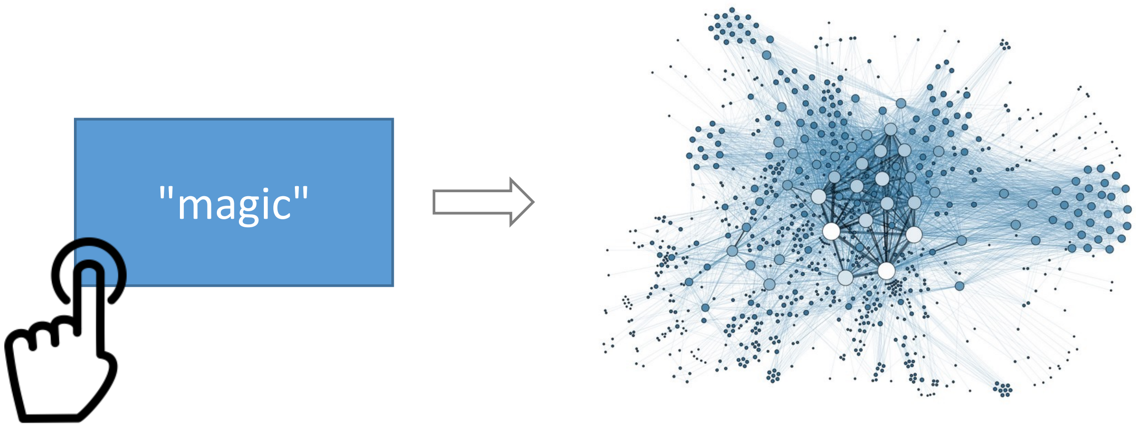


- Typical example: Gaussian Mixture Models (GMMs)

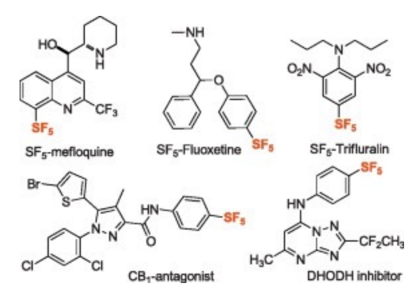
- Generative process of a GMM:
  1. Specify prior probability of each cluster k is $\pi_k > 0,\ \sum_k \pi_k = 1$
  2. For each sample i (you want to generate)
     a. Draw the cluster indicator $\mathrm{z_i} \sim Cat(\boldsymbol{\pi})$
        - $z_i = k$ means that the current datapoint i belongs to cluster k
     b. Draw the sample $\boldsymbol{x_i} \sim \mathcal{N}(\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i})$

Generative Models for Graphs

- How to artificially generate realistic graphs?
  - Generative models for graphs
  - Challenge: What are the latent factors influencing a graph?



- Applications: Forecast user behavior, large-scale analysis of algorithms, construct new molecules,…



Data Analytics and Machine Learning

Roadmap

- **Chapter: Graphs**
  1. Graphs & Networks
  2. **Generative Models**
     - **Models assuming (conditional) independent edges**
     - Preferential Attachment Models
     - Deep Generative Models
  3. Ranking
  4. Clustering
  5. Classification (Semi-Supervised Learning)
  6. Node/Graph Embeddings
  7. Graph Neural Networks (GNNs)

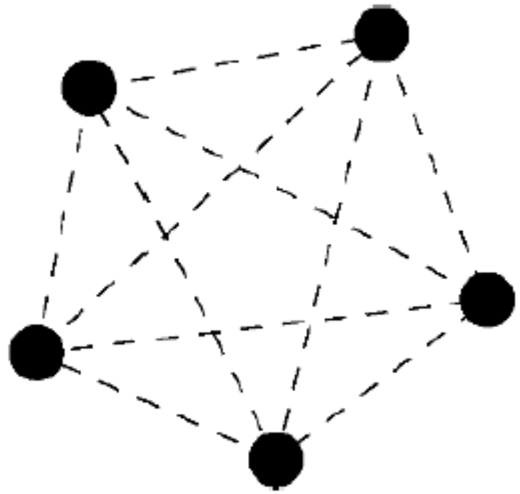
Generative Models for Graphs

- As you know, several laws apply for real world networks
- Goal: Generate synthetic graphs matching these criteria

- Seen before: Erdös-Renyi Random Graph Model

- Very simple generative process:
  Given $p \in [0,1]$ the edges are
  generated i.i.d. with

$$A_{ij} \sim Bernoulli(p)$$



Erdös-Renyi Random Graph Model: Properties

- **Degree distribution**
  - probability of a vertex having degree k is $p_k = \binom{N-1}{k} \cdot p^k \cdot (1-p)^{N-1-k} \approx \frac{z^k e^{-z}}{k!}$ $with\ z = p(N-1)$ → corresponds to a Poisson distribution
  - But: In real world data we observe power-law distributions ☹
- **Diameter**
  - The diameter concentrates around $\log(N)/\log(z)$, where z is the average node degree in the graph
  - → The diameter grows slowly with the number of nodes
  - But: In real data we observe small (constant) or even shrinking diameters ☹
- **Clustering Coefficient**
  - The clustering coefficient is equal to the connection probability $p = z/(N-1)$
  - → No community structure and dependent on number of overall nodes
  - But: Real world data looks totally different! ☹

Generative Model for Graphs with Communities

- How do we define a probabilistic model for graphs that captures community structure?

- Observation: In real graphs nodes from the same community are more likely to connect than nodes from different communities
  - using the same probability p for all edges doesn't make sense!

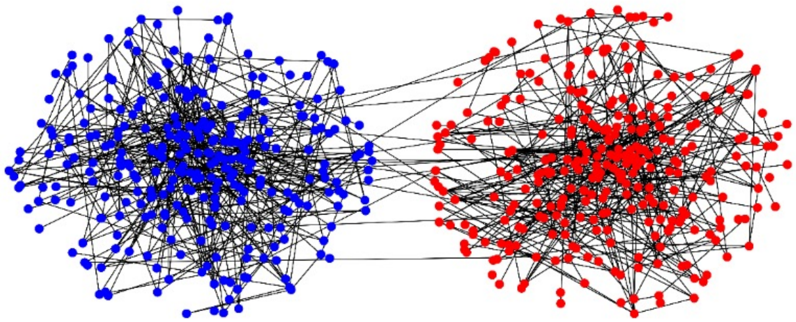
- Idea: Generalization of an Erdos-Renyi graph
  - nodes from the same community connect with probability p
  - nodes from different communities connect with probability q, where $p > q$

Planted Partition Model (PPM)

- We start with a set of nodes V, partitioned into 2 communities C_1, C_2
  - denote community assignment of node i as $z_i \in \{-1, 1\}$ – latent variables
- We generate an edge between every pair of nodes with probability

$$Pr\left(A_{ij} = 1 \middle| z_i, z_j\right) = \begin{cases} p & \text{if } z_i = z_j \\ q & \text{if } z_i \neq z_j \end{cases}$$

- Here we consider undirected, unweighted graphs, but the model can easily be extended to other cases as well.



Graph generated by a PPM with
$N = 600, p = 6/600, q = 0.1/600$
$z_i = -1$ for blue nodes, $z_i = 1$ for red nodes

Limitations of the PPM

- PPM is an improvement over ER graph generator, but we would like to
  - generate graphs with an arbitrary number of communities
  - generate communities with different edge densities
  - generate graphs with “more interesting” structure than just dense communities + few edges between communities

- Can we generalize PPM even further to achieve these properties?

Stochastic Block Model (SBM)

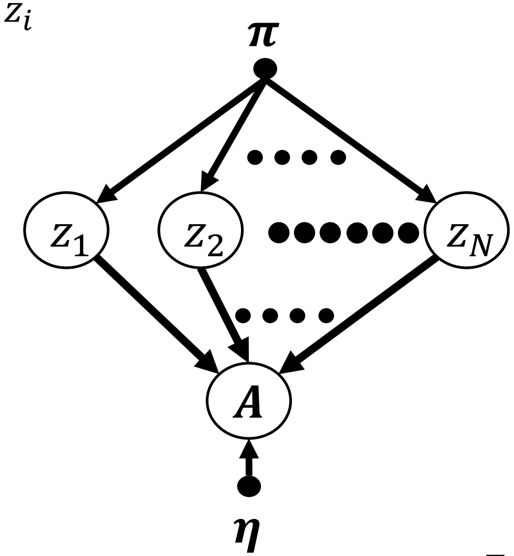
- **Stochastic block model** generalizes the PPM to graphs with arbitrary numbers and sizes of communities, and varying edge densities.

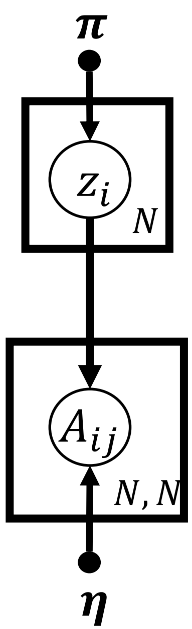
- Random variables:
  - $z_i \in \{1, \dots, K\}$: node i belongs to block/community z_i
  - $\boldsymbol{A} \in \{0,1\}^{N\times N}$: adjacency matrix

- Model parameters:
  - $\boldsymbol{\pi} = [\pi_1, \dots, \pi_K]$: community proportions
  - η_{uv}: edge probability between two nodes that are in communities u and v.

- Conditional distributions:
  - $\Pr(z_i = k) = \pi_k$
  - $\Pr\left(A_{ij} \middle| z_i, z_j\right) = \text{Bernoulli}(\eta_{z_i z_j})$

$$\boldsymbol{\pi} = [\pi_1, \pi_2, \dots, \pi_k]$$





$$\boldsymbol{\eta} = \begin{bmatrix} \eta_{11} & \cdots & \eta_{1K} \\ \vdots & \ddots & \vdots \\ \eta_{K1} & \cdots & \eta_{KK} \end{bmatrix}$$

Planted Partition Model as a Stochastic Block Model

- Planted partition model can be viewed as a special case of the stochastic block model with the following parameters

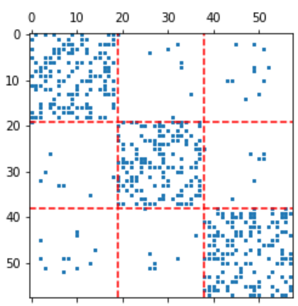
$$\boldsymbol{\pi} = [0.5, 0.5] \qquad \boldsymbol{\eta} = \begin{bmatrix} p & q \\ q & p \end{bmatrix}$$

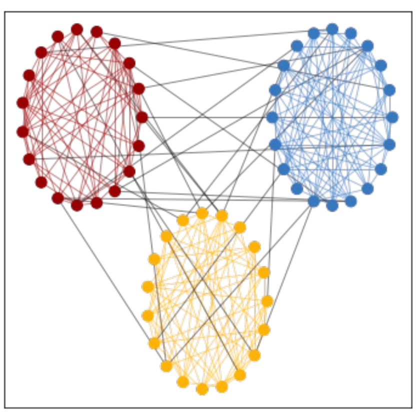
Some Types of Graphs Produced by SBM

Assortative

$$\boldsymbol{\eta} = \begin{bmatrix} 0.4 & 0.02 & 0.02 \\ 0.02 & 0.4 & 0.02 \\ 0.02 & 0.02 & 0.4 \end{bmatrix}$$

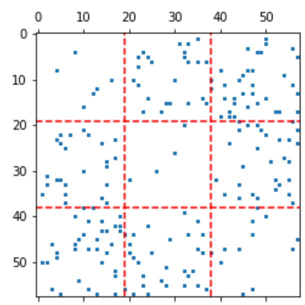
$\boldsymbol{A}$

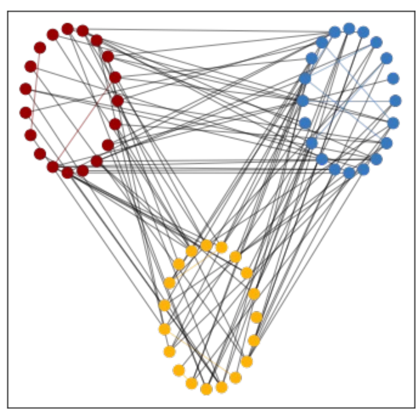




Disassortative

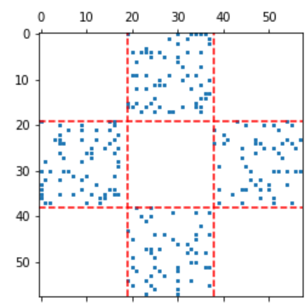
$$\begin{bmatrix} 0.02 & 0.08 & 0.08 \\ 0.08 & 0.02 & 0.08 \\ 0.08 & 0.08 & 0.02 \end{bmatrix}$$

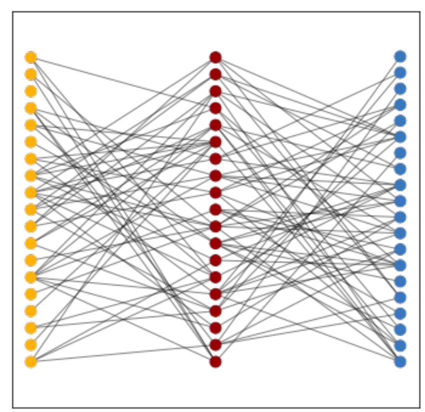




Ordered

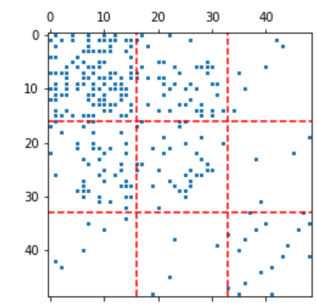
$$\begin{bmatrix} 0 & 0.15 & 0 \\ 0.15 & 0 & 0.15 \\ 0 & 0.15 & 0 \end{bmatrix}$$

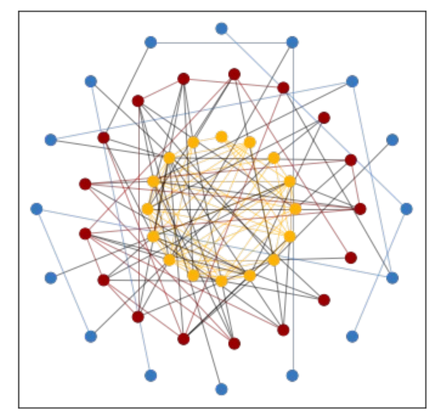




Core-periphery

$$\begin{bmatrix} 0.4 & 0.15 & 0.03 \\ 0.15 & 0.15 & 0.03 \\ 0.03 & 0.03 & 0.03 \end{bmatrix}$$





Limitations of SBM

- Stochastic block model is an elegant and well-studied model for graphs with communities, but it doesn't capture all patterns of real networks
  - real graphs have power-law degree distribution → Degree-Corrected SBM
    Karrer B. and Newman M. E. J.: Stochastic Blockmodels and Community Structure in Networks, in Physical Review E 83, 2011
  - real communities have more triangles → Geometric Block Model
    Galhotra S. et al.: The Geometric Block Model, in AAAI 2018
  - real communities are overlapping → Community-Affiliation Graph Model
    Yang J. and Leskovec J.: Overlapping Community Detection at Scale: A Nonnegative Matrix Factorization Approach, in WSDM 2013
- For an overview of recent advances in SBM see [Abbe2018]
  Abbe E.: Community Detection and Stochastic Block Models: Recent Developments, in JMLR 18, 2018

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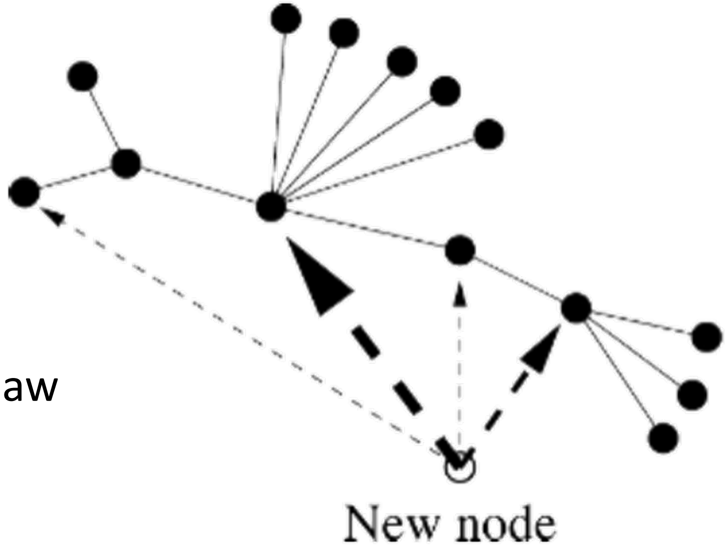
Preferential Attachment Models

- ER/PPM/SBM assume that the **edges** are generated **independently**
  - *all* nodes are given at the beginning; each potential edge corresponds to a Bernoulli distribution (independent of the others)

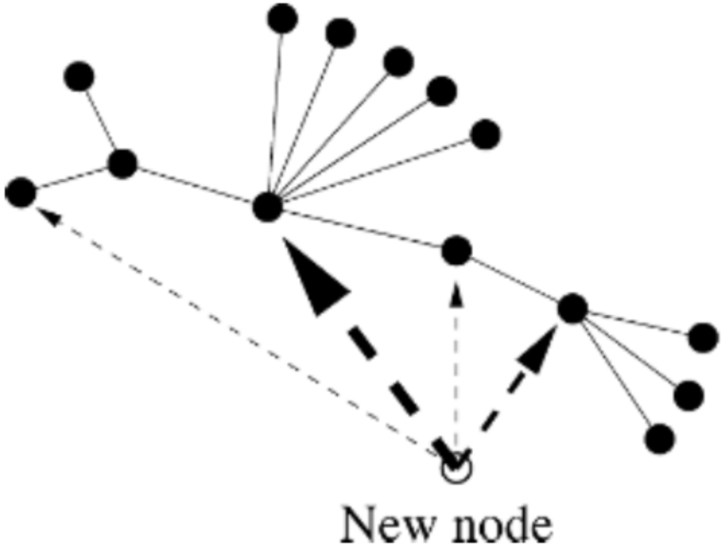
- Now: Generate network based on two processes
  - **Growth**: Instead of starting with all nodes, start with a small set of nodes and let the network grow over time by adding new nodes and edges
  - **Preferential attachment**:
    „rich get richer“ idea; probability of connecting nodes is proportional to the current degree of the nodes

→ „the rich get richer“ principle leads to a power law in the degree distribution



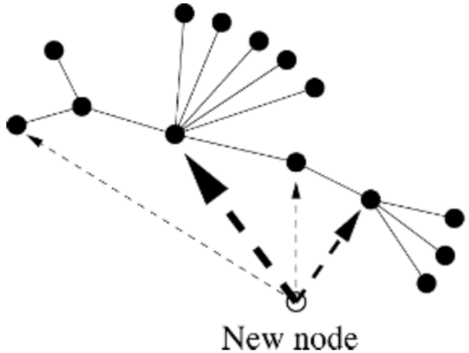
Preferential Attachment Models

- Prominent method: Initial Attractiveness (IA)
  - Extension of well-known BA model (Barabasi and Albert)
  - Allows to generate graphs following a power law degree distribution
  - Can realize a power law exponent γ in the range [2,infty)
    - BA model was stuck to exponent of γ=3



Initial Attractiveness [DMS2000]: Algorithm

1. Start with m_0 many nodes
2. Add a new node w
3. Simultaneously insert m directed edges (u, v)
   - **probability that the endpoint of an edge $(\mathbf{u}, \mathbf{v})$ corresponds to $\mathbf{v}$ is proportional to $\mathbf{A_v = A + indeg(v)}$**
     - A is the initial attractiveness of a node (same for all nodes)
     - $indeg(v)$ is the number of **currently** (!) incoming edges (**increases over time**)
   - Note: Not important where the edges (u, v) start
     - Example 1: all new edges start from w (like in the BA model)
     - Example 2: randomly select existing nodes
4. Goto step 2 until required number of nodes is obtained



[DMS2000] S. N. Dorogovtsev, J. F. F. Mendes and A. N. Samukhin, Structure of Growing Networks with Preferential Linking, Physical Review Letters

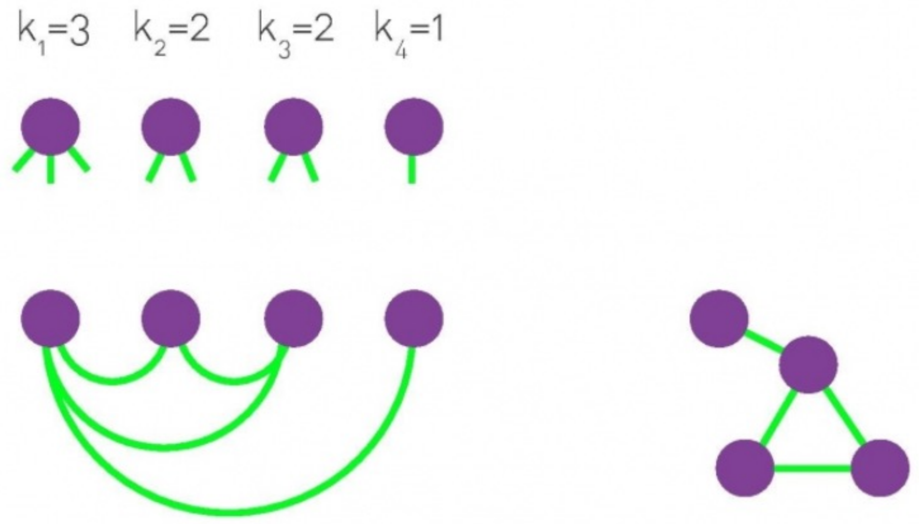
Initial Attractiveness: Properties

- Parameters: m (new edges per step) and A (initial attractiveness)
- **Degree distribution:**
  - The degree distribution follows a power law with exponent $\gamma = 2 + \frac{A}{m}$
  - Matches many real world data ☺
- **Diameter**:
  - For $m \geq 2$ the diameter grows as $O(\frac{\log N}{\log \log N})$
  - Matches the small world effect (diameter much smaller than number of nodes)
  - But: still slightly increasing in contrast to real world data 😐
- **Average degree:**
  - Remains constant over time
  - But: Increases for real world data; densification law ☹

Configuration Model

- Generating networks with arbitrary **specified** degree distribution
  1. Assign a degree to each node, represented as stubs or half-links
  2. Randomly select a stub pair and connect them
  – Depending on the order and way in which the stubs were chosen, we obtain different networks

- Preserves degree structure



Further Classical Graph Generators

- Many graph generators have been introduced
  - Overview presented in [CF2006]
  - Some further prominent methods:
    - Edge copying methods: realize community structure
    - Forest Fire Model: densification and shrinking diameter

[CF2006] Deepayan Chakrabarti, Christos Faloutsos: Graph mining: Laws, generators, and algorithms. ACM Comput. Surv. (CSUR) 38(1) (2006)

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Motivation

- All previously introduced generative models are "hand-crafted"
  - Observe properties (power law, triangles, communities, etc.) of real graphs → Build a generative model that generates them
  - Difficult to discover all relevant properties of real graphs
  - Difficult to "hand-craft" a single model capturing all properties simultaneously

- How can we find a model that captures all the complex (potentially even unknown) properties of real graphs?

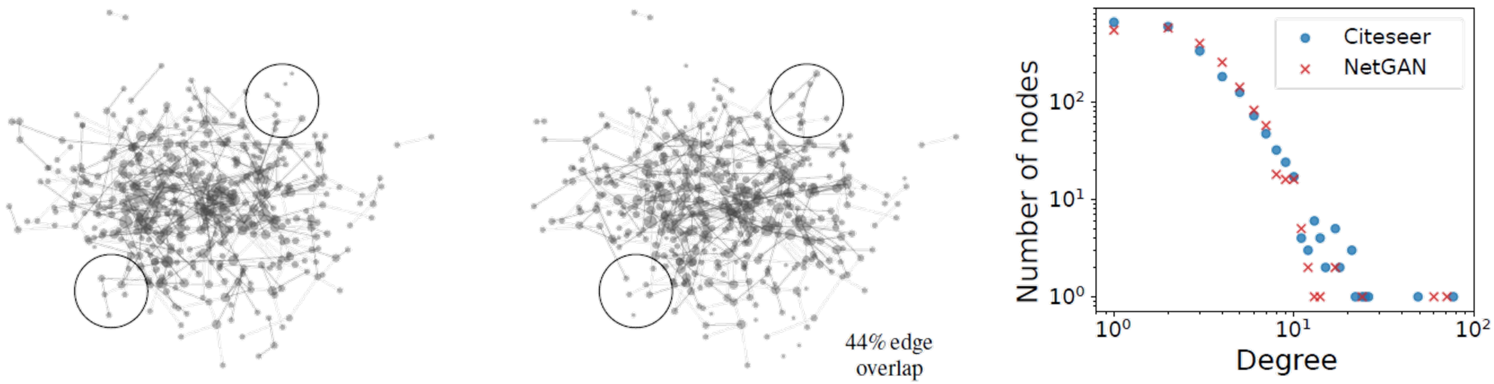
- Let us use the concept of deep generative models
  - i.e. *flexible* models that can be *learned* based on given data

Approaches

- Various deep generative modeling approaches have been applied to graphs.
  - Variational autoencoders
    - Variational Graph Autoencoders.
      Thomas Kipf, Max Welling. NeurIPS Workshop on Bayesian Deep Learning 2016
  - Generative adversarial networks
    - NetGAN: Generating Graphs via Random Walks.
      Aleksandar Bojchevski, Oleksandr Shchur, Daniel Zügner, Stephan Günnemann. ICML 2018
  - Normalizing flows
    - Graph Normalizing Flows.
      Jenny Liu, Aviral Kumar, Jimmy Ba, Jamie Kiros, Kevin Swerky. NeurIPS 2019
  - Score-based modeling
    - Permutation Invariant Graph Generation via Score-Based Generative Modeling.
      Chenhao Niu, Yang Song, Jiaming Song, Shengjia Zhao, Aditya Grover, Stefano Ermon. AISTATS 2020
  - Denoising diffusion
    - DiGress: Discrete Denoising Diffusion for Graph Generation.
      Clément Vignac, igor Krawczuk, Antoine Siraudin, Bohan Wang, Volkan Cevher, Pascal Frossard. ICLR 2023

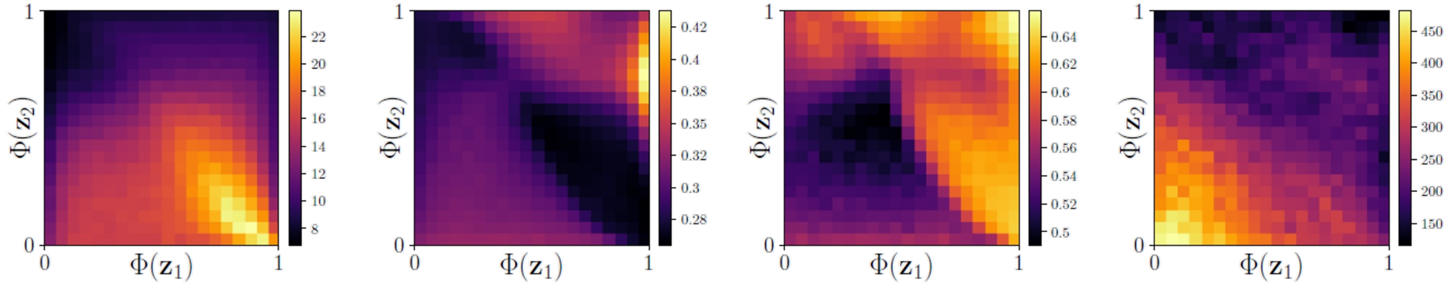
Example: NetGAN

- NetGAN learns properties of real graphs without manually specifying them
- Generate graphs that have the same structure but are not replicas



(a) Original graph (b) Graph generated by NetGAN (c) Degree distribution comparison

- Latent space interpolations produces smoothly changing graphs



(a) Avg. degree of start node (b) Avg. share of nodes in start community (c) Gini coefficient (input graph: 0.48) (d) Max. degree (input graph: 240)

Questions

- Can the Erdös-Renyi model generate all graphs that the Stochastic Block Model can generate?

- Is the Initial Attractiveness model equal to the Erdös-Renyi model as $A \to \infty$?

Summary

- Classic generative models for graphs are
  - (relatively) easy to analyze
  - but do not capture all important properties of real graphs

- Deep generative models learn to generate graphs that automatically capture the underlying laws and characteristics (e.g. power law, small world) without manually specifying them
  - though, theoretically analyzing such models is tricky
  - evaluation of generative models is hard in general, even harder for graphs

Reading Material

- [Jang2016] Jang, E., Gu, S., & Poole, B. (2016). Categorical reparameterization with gumbel-softmax. *arXiv preprint arXiv:1611.01144*.
- https://blog.evjang.com/2016/11/tutorial-categorical-variational.html
  Blog post by the author of [Jang2016] explaining their method with a tensorflow implementation
- [Bojchevski2018] Bojchevski, A., Shchur, O., Zügner, D., & Günnemann, S. (2018). Netgan: Generating graphs via random walks. *arXiv preprint arXiv:1803.00816*.

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