Hot Topics Of Generative AI: LLMs and Diffusion Models
”Yang et al. - Directional diffusion models for graph representation learning“

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Chair 9 – Prof. Dr. Müller

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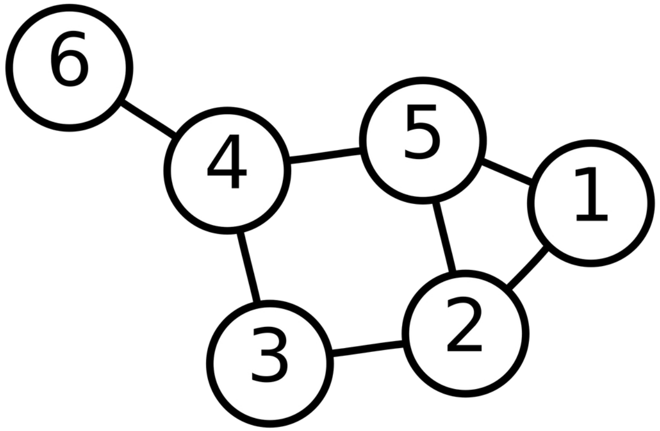
supervised by Tim Katzke

Agenda

1 What is Graph Representation Learning?

What is a graph?

- G = (V, E), vertices V and edges E
- Graphs can represent anything from molecules to road networks or social networks



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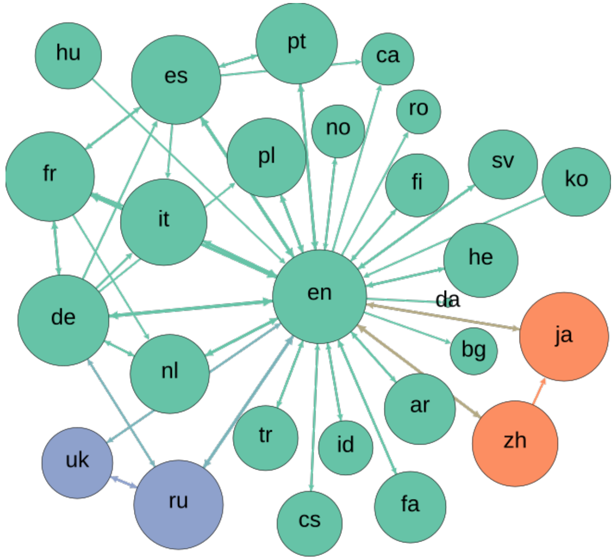

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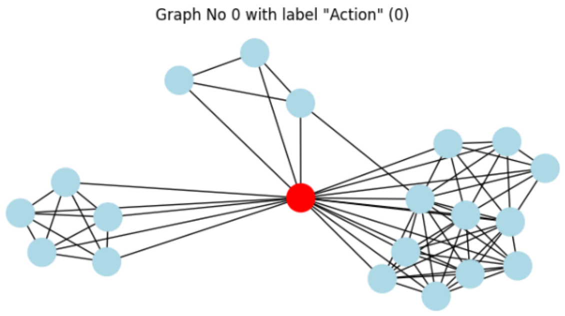
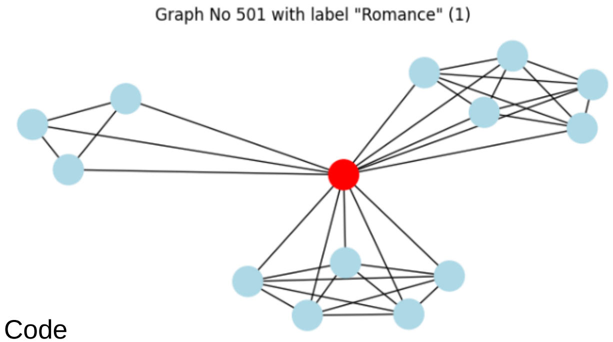
IMDB-Binary – A Graph Dataset

- Graph Learning on Graph Datasets enables the use of AI on those data structures
- IMDB-B contains ego-networks of actors from Action or Romance movies (Yanardag et al., 2015)
- From only the knowledge of which actors have co-starred, models can determine the genre with an accuracy of up to 95% (Nguyen et al., 2019)

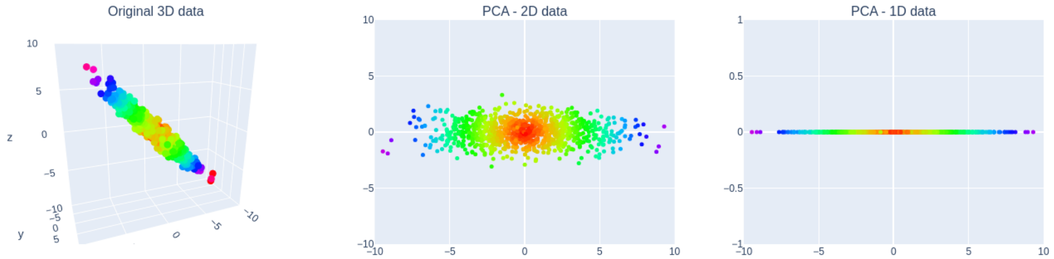




Presentation Code

Representation Learning

- RL is an important part of Machine Learning that converts data to a form that can be worked with more easily
- Here, there is also a difference between unsupervised and supervised learning
- Dimensionality Reduction is a prominent subfield



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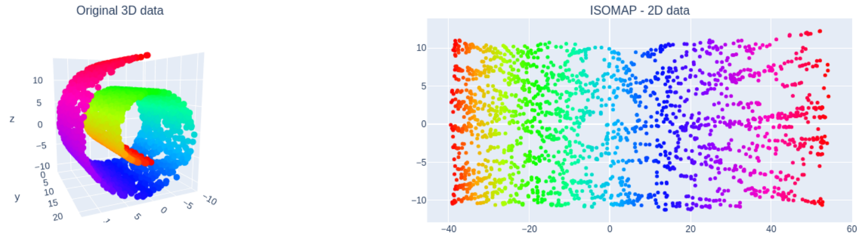

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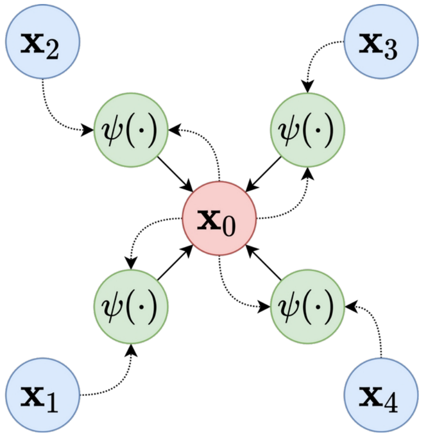
Graph Representation Learning - GNNs

- For RL on Graphs, Graph Neural Networks are often used
- They work similar to Convolutional Neural Networks (CNNs)
- Instead of using neighboring pixels, the adjacency matrix is used



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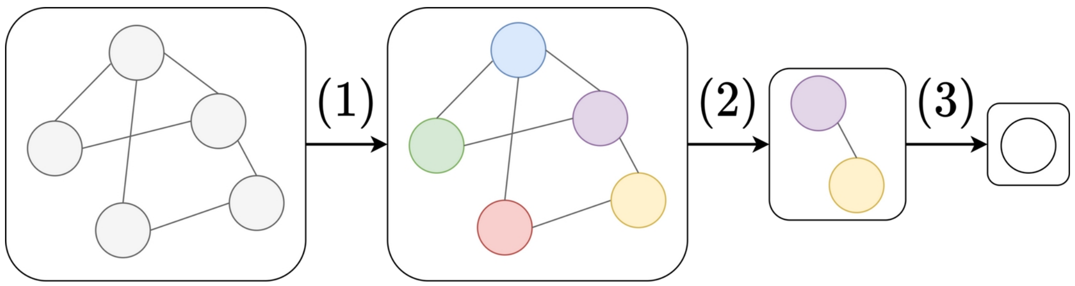

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2 The Successful Diffusion Model

Denoising Probabilistic Diffusion Models

- Originally from thermodynamics

- Introduced to Machine Learning only recently (Ho et al., 2020), but has become the standard for image generation beating former SOTA technology (Dhariwal et al., 2021)

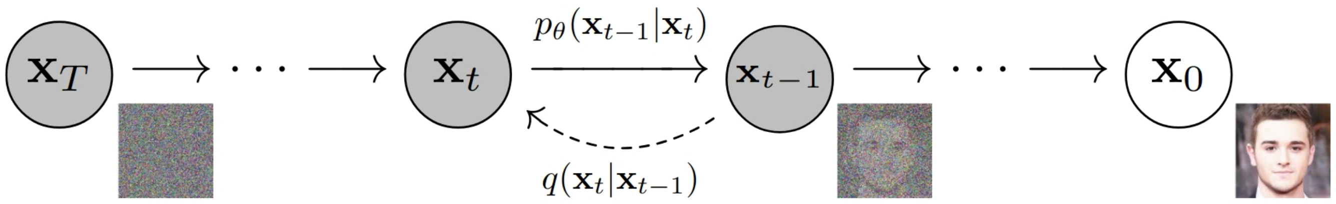
Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
6: **until** converged

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

Ho et al., 2020



Ho et al., 2020

The DM’s forward step

- To gradually add noise to the images, Diffusion Models add Gaussian noise in each step

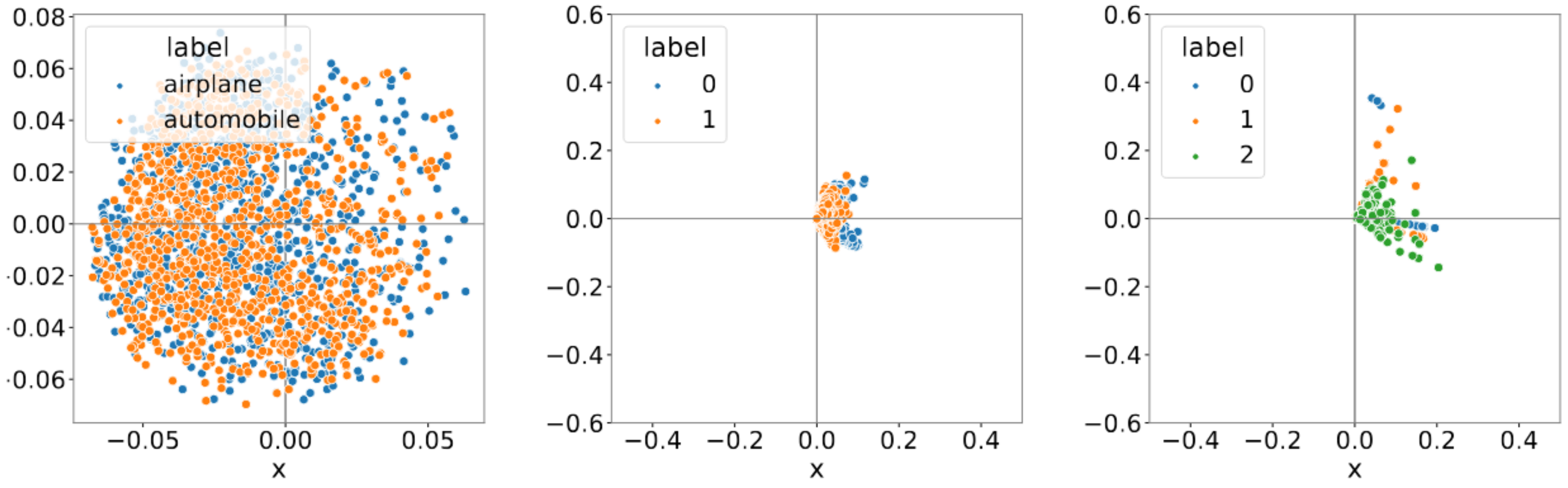
- Thus, all data is asymptotically converted to a standard Gaussian distribution (Ho et al., 2020)

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) := \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}) \qquad q(\mathbf{x}_t|\mathbf{x}_{t-1}) := \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

3 Graphs vs. Images

The Anisotropy of Graphs

- While images are naturally isotropic and euclidean, Graphs are anisotropic



(a) CIFAR-10 (b) Amazon-Photo (c) IMDB-M

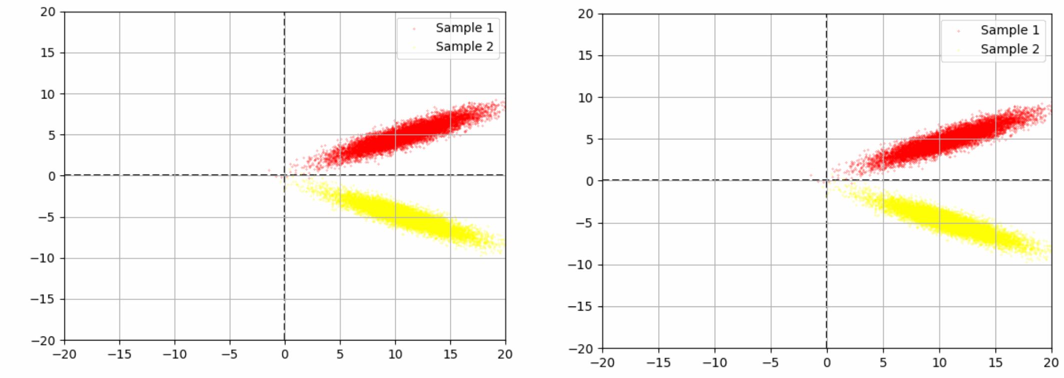
(Yang et al., 2023)

White Noise vs. Directed Noise

- The information density of a directed Gaussian declines quickly if White Noise is applied

- Hence, Yang et al. introduce “Directional Noise”:

$$x_{t,i} = \sqrt{\bar{\alpha}_t} x_{0,i} + \sqrt{1 - \bar{\alpha}_t}\epsilon',$$
$$\epsilon' = \operatorname{sgn}(x_{0,i}) \odot |\bar{\epsilon}|,$$
$$\bar{\epsilon} = \mu + \sigma \odot \epsilon \quad \text{where } \epsilon \sim \mathcal{N}(0, \mathbf{I})$$



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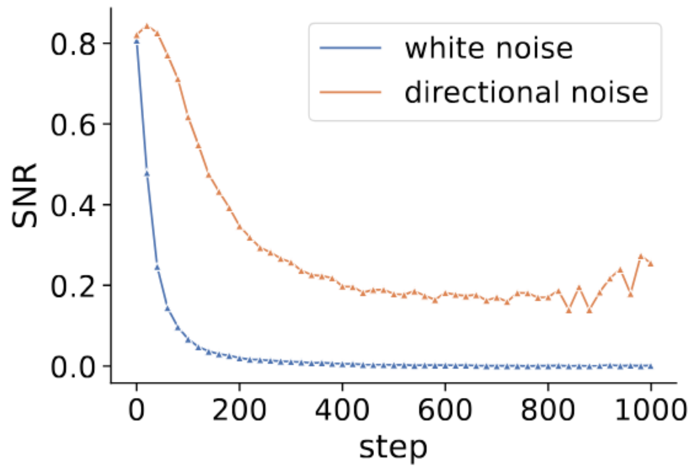
The effect on the Signal-To-Noise-Ratio

- The application of directional noise has a vital effect on the Signal-To-Noise-Ratio

- The SNR is fundamental for the learning process of Diffusion Models

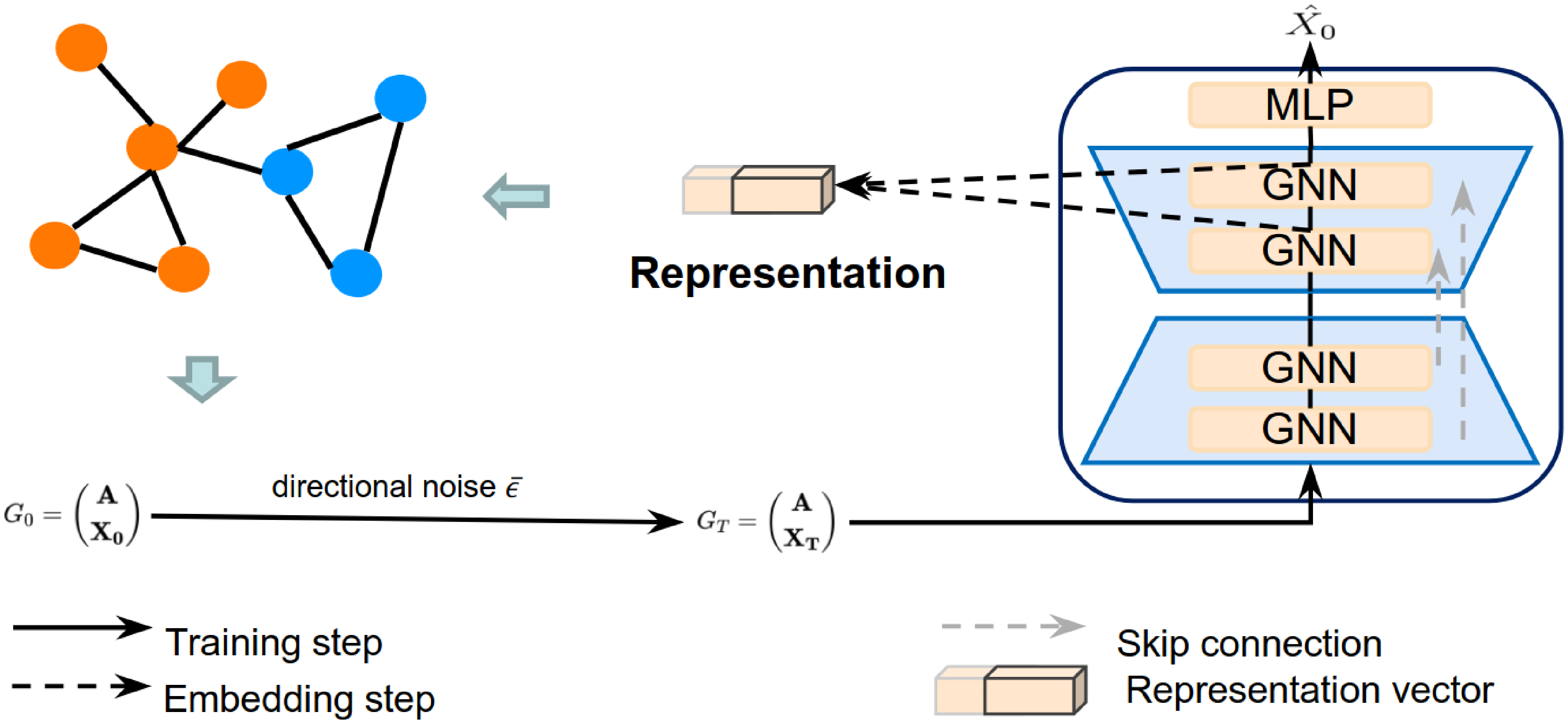


(a) Amazon-Photo

Yang et al., 2023

4 Directed Diffusion Models - Architecture

Components of the Model



Yang et al., 2023

The Algorithm

- The two algorithms work similar to Ho's algorithm
- Instead of generating an image, a representation is generated

Algorithm 1 The training algorithm.

Input: A batch of graphs $\mathcal{G} = \{G_1, \cdots G_B\}$
Output: The denoising network f_θ

Initialize: the denoising network f_θ
Compute μ, the mean of node features across batch $\mathcal{G}$
Compute σ, the standard deviation of node features across batch $\mathcal{G}$
while not convergence **do**
  for G_i in $\mathcal{G}$ **do**
    for $t = 1, \ldots, T$ **do**
      Sample directional noise ϵ' using equation (2)
      Take gradient descent step on
      $\nabla_\theta \left\| \mathbf{X}_0 - f_\theta(\sqrt{\bar{\alpha}_t}\mathbf{X_i} + \sqrt{1-\bar{\alpha}_t}\epsilon', \mathbf{A}, t) \right\|$
    end for
  end for
end while

Algorithm 2 Extracting representations.

Input: $G = (\mathbf{A}, \mathbf{X})$, forward step set $\{T_0, T_1, \ldots, T_K\}$, pre-trained denoising network f_θ
Output: $\mathbf{H}$, the representation of G

Compute μ the mean of node features
Compute σ the standard deviation of node features
for k in $\{T_0, T_1, \ldots, T_K\}$ **do**
  Sample directional noise ϵ' using equation (2)
  $\mathbf{X_k} \leftarrow \sqrt{\bar{\alpha}_k}\mathbf{X_0} + \sqrt{1-\bar{\alpha}_k}\epsilon'$
  $\mathbf{H}_k \leftarrow f_\theta(\mathbf{X_k}, \mathbf{A}, k)$
end for
Concatenate $\mathbf{H} = [\mathbf{H}_{T_0}, \mathbf{H}_{T_1}, \ldots, \mathbf{H}_{T_K}]$
return $\mathbf{H}$

Yang et al., 2023

5 Resulting Benchmarks

Graph Classification

- The paper compares multiple State-Of-The-Art models with DDMs
- The hyperparameters of the DDM were obtained by 10-fold cross validation
- SVMs are used on the learned representations
- While here only graph classification results are presented, the results from node classification are similarly promising

Results

Dataset	IMDB-B	IMDB-M	COLLAB	REDDIT-B	PROTEINS	MUTAG
GIN	75.1±5.1	52.3±2.8	80.2±1.9	92.4±2.5	76.2±2.8	89.4±5.6
DiffPool	72.6±3.9	-	78.9±2.3	92.1±2.6	75.1±2.3	85.0±10.3
Infograph	73.03±0.87	49.69±0.53	70.65±1.13	82.50±1.42	74.44±0.31	89.01±1.13
GraphCL	71.14±0.44	48.58±0.67	71.36±1.15	89.53±0.84	74.39±0.45	86.80±1.34
JOAO	70.21±3.08	49.20±0.77	69.50±0.36	85.29±1.35	74.55±0.41	87.35±1.02
GCC	72	49.4	78.9	89.8	-	-
MVGRL	74.20±0.70	51.20±0.50	-	84.50±0.60	-	89.70±1.10
GraphMAE	75.52±0.66	51.63±0.52	80.32±0.46	88.01±0.19	75.30±0.39	88.19±1.26
DDM	**76.40±0.22**	**52.53±0.31**	**81.72±0.31**	89.15 ±1.3	**75.47 ±0.50**	**91.51 ±1.45**

Yang et al., 2023

6 Conclusion

Research Outlook

- Yang et al. only introduce the idea, they admit that their hyperparameters are not optimal yet
- One open question is how the optimal set of diffusion steps can be determined
- Variants of DDMs could bring value to areas such as computer vision and natural language processing

What makes this paper special?

- The benchmarks are remarkable
- As mentioned, the technology introduced holds great potential for the future
- The researchers consider themselves „among the pioneers in the literature“ regarding the „exploration of anisotropic structure in graph data“

References & Weblinks

- Yang et al. (2023). Directional diffusion models for graph representation learning
- Yanardag et al. (2015). Deep Graph Kernels
- Nguyen et al. (2019). Universal Graph Transformer Self-Attention Networks
- Ho et al. (2020). Denoising Diffusion Probabilistic Model
- Dhariwal et al. (2021). Diffusion Models Beat GANs on Image Synthesis

- Presentation Code: https://github.com/JavaLangMarlon/ddm-proseminar-tu-dortmund