

Research notes on metrics for GNNs applied to biological problems

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Monday January 24, 2022

1 Generative modelling

1.1 Methods

1.1.1 Real-valued non volume-preserving used on images

2 Graph Neural Networks

2.1 Reviews

2.1.1 Graph neural networks:

A review of methods and applications Zhou et al mention several GNN approaches in use today Generative models popular today:

Sequential graph generation process

- GraphRNN - generates the adjacency matrix of a graph by generating the adjacency vector of each node step by step, with graph outputs with different number of nodes.
- Li 2018 - also generates nodes and edges sequentially uses the hidden state to decide what to do at the next step
- GraphAF - also a sequential process, Conducts a validity check of each molecule generated at each step to see if it's valid.

Non-sequential graph generation process

- MolGAN - to generate small molecules. Uses a permutation-invariant to solve the node adjacency matrix at once. Also implements an RL-based optimization toward desired chemical properties

- Ma et al 2018 - constrained VAE for semantic validity of generated graph
- GCPN similar to MolGAN, uses RL based methods to ensure validity of domain-specific rules
- Graph Normalizing Flows

This one has a fairly comprehensive website: <https://sites.google.com/view/graph-normalizing-flows>
Full architecture

6

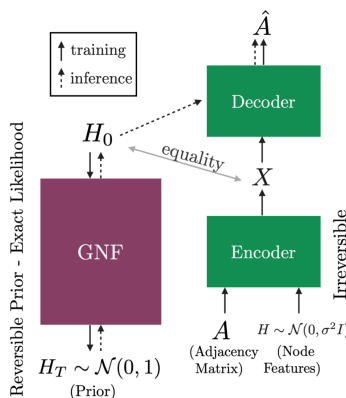


Figure 1: figure name

- Graphite isotropic gaussian for VAE + iterative refinement for decoding

2.2 Three most popular according to O’Bray 2021:

- GraphRNN, GRAN, Graph Score Matching.

3 Objective:

3.1 Generative graph dist close to the input graph dist

3.2 (pseudo)-metric to assess dissimilarity between G (generated graphs) and G^* (input graphs)

4 Criteria for good metrics:

1. Robust to noise
2. Expressive, if they don’t arise from the same dist, then metric should detect this.
3. Computationally efficient.

5 Problems with Frechet Inception Distance

- Used only for images.
- Perceived differences are not possible for graphs.
- How about LPIPS?

6 Why comparing graphs is hard:

- Metrics need to deal with spatial invariances such as cycles.
- Graph edit distance is NP-hard (Zeng 2009) and therefore does not satisfy efficiency criterion.

7 MMD - current accepted method to evaluate generative GNNs

- The MMD formula goes as follows:

$$\text{MMD}(X, Y) := \frac{1}{n^2} \sum_{i,j=1}^n k(x_i, x_j) + \frac{1}{m^2} \sum_{i,j=1}^m k(y_i, y_j) - \frac{2}{nm} \sum_{i=1}^n \sum_{j=1}^m k(y_i, y_j)$$

- use it for hypothesis/two-sample testing.
- In practice, we evaluate $d_{\text{MMD}}(\mathcal{G}, \mathcal{G}^*) := \text{MMD}(f(\mathcal{G}), f(\mathcal{G}^*))$ for a distribution \mathcal{G} . Given multiple distributions G_1, G_2, \dots , the values of d_{MMD} can be used to rank models, where smaller values are assumed to indicate a larger agreement with the original distribution \mathcal{G}^* .
- Commonly used kernels: first Wasserstein distance, total variation distance, radial basis function.
- Commonly used descriptor functions: degree distribution histogram, clustering coefficient, laplacian spectrum histogram.

7.1 Pitfalls of descriptors

- Degree distributions are ok seemingly
- Clustering does not distinguish fully connected vs disconnected cliques
- Spectral methods are not clearly expressive. Does not seem to be for certain classes of graphs.

8 MMD pitfalls

8.1 Parameters and descriptors are set a priori in the best case

8.2 Model performance is highly dependent on parameters and descriptor functions.

9 Computer Vision

9.1 Image-to-Image Translation

9.1.1 CycleGAN: Unpaired Image-to-Image Translation using

Cycle-Consistent Adversarial Networks citep:zhu2017CycleGAN.

This is one of my favorite papers. The authors extending some of the classic work done in Pix2Pix citep:isola2017pix2pix to *unpaired* sets of images. At the core of the CycleGAN procedure are two Generative Adversarial Networks that learn to map images between two domains. The key addition that makes this process work is an additional loss term, which enforces that images passed through both generators should be as close as possible to the input image. This has practical motivation: if we translate one way and then translate back, we should expect the input to be unchanged. The results are impressive and eye catching. This work inspired a paper of mine: GeneSIS-RT.

References