Variational Graph Auto-Encoders

Thomas N. Kipf
University of Amsterdam
T.N.Kipf@uva.nl

Max Welling
University of Amsterdam
Canadian Institute for Advanced Research (CIFAR)
M.Welling@uva.nl

1 A latent variable model for graph-structured data

We introduce the variational graph auto-encoder (VGAE), a framework for unsupervised learning on graph-structured data based on the variational auto-encoder (VAE) \[2, 3\]. This model makes use of latent variables and is capable of learning interpretable latent representations for undirected graphs (see Figure 1).

We demonstrate this model using a graph convolutional network (GCN) \[4\] encoder and a simple inner product decoder. Our model achieves competitive results on a link prediction task in citation networks. In contrast to most existing models for unsupervised learning on graph-structured data and link prediction \[5, 6, 7, 8\], our model can naturally incorporate node features, which significantly improves predictive performance on a number of benchmark datasets.

Definitions We are given an undirected, unweighted graph \( G = (V, E) \) with \( N = |V| \) nodes. We introduce an adjacency matrix \( A \) of \( G \) (we assume diagonal elements set to 1, i.e. every node is connected to itself) and its degree matrix \( D \). We further introduce stochastic latent variables \( z_i \), summarized in an \( N \times F \) matrix \( Z \). Node features are summarized in an \( N \times D \) matrix \( X \).

Inference model We take a simple inference model parameterized by a two-layer GCN:

\[
q(Z | X, A) = \prod_{i=1}^{N} q(z_i | X, A), \quad \text{with} \quad q(z_i | X, A) = \mathcal{N}(z_i | \mu_i, \text{diag}(\sigma_i^2)).
\]

(1)

Here, \( \mu = \text{GCN}_\mu(X, A) \) is the matrix of mean vectors \( \mu_i \); similarly \( \log \sigma = \text{GCN}_\sigma(X, A) \). The two-layer GCN is defined as \( \text{GCN}(X, A) = \tilde{A} \text{ReLU}(\tilde{A}XW_0)W_1 \), with weight matrices \( W_i \). \( \text{GCN}_\mu(X, A) \) and \( \text{GCN}_\sigma(X, A) \) share first-layer parameters \( W_0 \). \( \text{ReLU}(\cdot) = \max(0, \cdot) \) and \( \tilde{A} = D^{-\frac{1}{2}}AD^{-\frac{1}{2}} \) is the symmetrically normalized adjacency matrix.

Generative model Our generative model is given by an inner product between latent variables:

\[
p(A | Z) = \prod_{i=1}^{N} \prod_{j=1}^{N} p(A_{ij} | z_i, z_j), \quad \text{with} \quad p(A_{ij} = 1 | z_i, z_j) = \sigma(z_i^Tz_j),
\]

(2)

where \( A_{ij} \) are the elements of \( A \) and \( \sigma(\cdot) \) is the logistic sigmoid function.

Learning We optimize the variational lower bound \( \mathcal{L} \) w.r.t. the variational parameters \( W_i \):

\[
\mathcal{L} = \mathbb{E}_{q(Z | X, A)} \left[ \log p(A | Z) \right] - \text{KL} \left[ q(Z | X, A) \parallel p(Z) \right],
\]

(3)
We compare models based on their ability to correctly classify edges and non-edges. The validation set is used for optimization of hyperparameters. We compare against two popular baselines: spectral clustering (SC) [5] and DeepWalk (DW) [6]. Both SC and DW provide node embeddings \( Z \). We use Eq. (4) (left side) to calculate scores for elements of the reconstructed adjacency matrix. We omit recent variants of DW [7, 8] due to comparable performance. Both SC and DW do not support input features.

For VGAE and GAE, we initialize weights as described in [9]. We train for 200 iterations using Adam [10] with a learning rate of 0.01. We use a 32-dim hidden layer and 16-dim latent variables in all experiments. For SC, we use the implementation from [11] with an embedding dimension of 128. For DW, we use the implementation provided by the authors of [8] with standard settings used in their paper, i.e. embedding dimension of 128, 10 random walks of length 80 per node and a context size of 10, trained for a single epoch.

Discussion Results for the link prediction task in citation networks are summarized in Table [1]. GAE* and VGAE* denote experiments without using input features, GAE and VGAE use input features. We report area under the ROC curve (AUC) and average precision (AP) scores for each model on the test set. Numbers show mean results and standard error for 10 runs with random initializations on fixed dataset splits.

<table>
<thead>
<tr>
<th>Method</th>
<th>AUC</th>
<th>AP</th>
<th>AUC</th>
<th>AP</th>
<th>AUC</th>
<th>AP</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC [5]</td>
<td>84.6 ± 0.01</td>
<td>89.5 ± 0.00</td>
<td>80.5 ± 0.01</td>
<td>87.2 ± 0.01</td>
<td>84.2 ± 0.02</td>
<td>87.8 ± 0.01</td>
</tr>
<tr>
<td>DW [6]</td>
<td>83.1 ± 0.01</td>
<td>85.0 ± 0.00</td>
<td>80.5 ± 0.02</td>
<td>83.6 ± 0.01</td>
<td>84.4 ± 0.00</td>
<td>84.1 ± 0.00</td>
</tr>
<tr>
<td>GAE*</td>
<td>84.3 ± 0.02</td>
<td>88.1 ± 0.01</td>
<td>78.7 ± 0.02</td>
<td>84.1 ± 0.02</td>
<td>82.2 ± 0.01</td>
<td>87.4 ± 0.00</td>
</tr>
<tr>
<td>VGAE*</td>
<td>84.0 ± 0.02</td>
<td>87.7 ± 0.01</td>
<td>79.9 ± 0.03</td>
<td>84.1 ± 0.02</td>
<td>82.7 ± 0.01</td>
<td>87.5 ± 0.01</td>
</tr>
<tr>
<td>GAE</td>
<td>91.0 ± 0.02</td>
<td>92.0 ± 0.03</td>
<td>89.5 ± 0.04</td>
<td>90.9 ± 0.05</td>
<td>96.4 ± 0.00</td>
<td>96.5 ± 0.00</td>
</tr>
<tr>
<td>VGAE</td>
<td>91.4 ± 0.01</td>
<td>92.6 ± 0.01</td>
<td>90.8 ± 0.02</td>
<td>92.6 ± 0.02</td>
<td>94.4 ± 0.02</td>
<td>94.7 ± 0.02</td>
</tr>
</tbody>
</table>

Both VGAE and GAE achieve competitive results on the featureless task. Adding input features significantly improves predictive performance across datasets. A Gaussian prior is potentially a poor choice in combination with an inner product decoder, as the latter tries to push embeddings away from the zero-center (see Figure [1]). Nevertheless, the VGAE model achieves higher predictive performance on both the Cora and the Citeseer dataset.

Future work will investigate better-suited prior distributions, more flexible generative models and the application of a stochastic gradient descent algorithm for improved scalability.
Acknowledgments

We would like to thank Christos Louizos, Mart van Baalen, Taco Cohen, Dave Herman, Pramod Sinha and Abdul-Saboor Sheikh for insightful discussions. This project was funded by SAP Innovation Center Network.

References


