Graph Auto-regressive model

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October 21, 2023

Auto-regressive (AR) model

Let it is given past p time steps $x_t^p = [x_t, x_{t-1}, \dots, x_{t-p+1}]$ So, the next observation is generated by this process:

$$x_{t+1} = f(x_t^p) + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2) \tag{1}$$

where $f(x_t^p)$ - AR function that could be parameterised somehow.
So, the prediction is given by $\hat{x}_{t+1} = \mathbb{E}_\epsilon [x_{t+1}] = f(x_t^p)$
However we want to predict next graph g_{t+1}, so lets generalize this to graph setting[1].

[1] Autoregressive Models for Sequences of Graphs

Graph Auto-regressive model

Firstly, lets generalize generation process.
We have graph space $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where

$$\mathcal{V} = \{v_i \in \mathbb{R}^F\}_{i=1}^N, \mathcal{E} = \{e_i \in \mathbb{R}^S\}_{v_i, v_j \in \mathcal{V}}$$

The past p time steps are $g_t^p = [g_t, g_{t-1}, \dots, g_{t-p+1}]$, where $\forall g \in \mathcal{G}$ So, the next observation is given by:

$$g_{t+1} = H\left(\phi(g_t^p), \eta\right), \eta \sim Q(g), H : \mathcal{G} \to \mathcal{G} \tag{2}$$

where H is function that effects noise on graph, η is noise graph and $Q(g)$ is a graph distribution defined on the Borel sets of space $(\mathcal{G}, \mathrm{d})$
So, the prediction is given by

$$\hat{g}_{t+1} = \arg\min_{g' \in \mathcal{G}} \int_{\mathcal{G}} \mathrm{d}(g', g_{t+1})^2 dQ(g) = \mathbb{E}_\eta^f\left[g_{t+1}\right] = \phi(g_t^p),$$

where $\mathbb{E}_\eta^f[\cdot]$ is Frechet mean, $\mathrm{d}(\cdot, \cdot)$ is pre-metric

Learning the AR function with a GNN

Authors[2] propose one of the possible architecture (Figure 1) that can parameterize AR function.

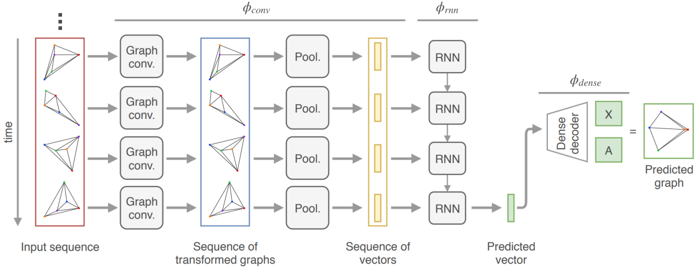

Figure: Proposed architecture

In this case by mapping graphs to a vector space, we go back to the numerical setting of (1)

[2] Autoregressive Models for Sequences of Graphs