SeqGraph2Vec Proof

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Proposition 1 (Edge–sampling via random walks)**.** *Let $G = (V, E, W)$ be a connected, non-bipartite, undirected graph with $|V|$ nodes, symmetric non–negative edge–weight matrix $W \in \mathbb{R}^{|V|\times|V|}$, and*

$$\pi_{u\to v} = \begin{cases} \dfrac{W_{uv}}{\sum_{k\sim u} W_{uk}} & \textit{if } uv \in E, \\ 0 & \textit{otherwise.} \end{cases} \tag{1}$$

where $k \sim u$ denotes the set of one-hop neighbors of node u. Denote the (weighted) degree by $S_u := \sum_{k\sim u} W_{uk}$ and let $C := \sum_{u\in V} S_u$ (global constant). Then, the probability of traversing an undirected edge $uv \in E$ in a one-step random walk is given by:

(a) Equilibrium distribution:

$$P_{uv}^{\text{path}} = \frac{2W_{uv}}{C} \propto W_{uv} \tag{2}$$

(b) Uniform distribution:

$$P_{uv}^{\text{path}} = \frac{1}{|V|}\left(\frac{W_{uv}}{S_u} + \frac{W_{uv}}{S_v}\right) \tag{3}$$

Proof. Let $P_{ij}(t)$ be the occupation probability to find the random walker in the node j at time t, starting from i at $t = 0$. Then, P_{ij} obeys the master equation [**?**] and can be expressed as

$$P_{ij}(t+1) = \sum_{m\in V} P_{im}(t)\,\pi_{m\to j}. \tag{4}$$

Because W is symmetric,

$$S_u\,\pi_{u\to v} = W_{uv} = S_v\,\pi_{v\to u}. \tag{5}$$

Expanding Eq. (4) t times gives a path product representation

$$P_{ij}(t) = \sum_{j_1,\ldots,j_{t-1}} \pi_{i\to j_1}\cdot \pi_{j_1\to j_2}\cdots \pi_{j_{t-1}\to j}, \tag{6}$$

and inserting Eq. (6) into Eq. (5) repeatedly yields

$$S_i\,P_{ij}(t) = S_j\,P_{ji}(t) \qquad (\forall i, j,\, t \geq 0). \tag{7}$$

The relation in Eq. (7) allows to obtain the equilibrium probability distribution $P_j^\infty := \lim_{t\to\infty} P_{ij}(t)$, which is independent of i. Taking $t \to \infty$ in Eq. (7) and summing over i gives

$$P_j^\infty = \frac{S_j}{\sum_{u\in V} S_u} = \frac{S_j}{C}. \tag{8}$$

Starting from the equilibrium distribution, an undirected edge uv is traversed either $u \to v$ or $v \to u$:

$$\begin{aligned} P_{uv}^{\text{path}} &= P_u^\infty\,\pi_{u\to v} + P_v^\infty\,\pi_{v\to u} \\ &= \frac{S_u}{C}\cdot\frac{W_{uv}}{S_u} + \frac{S_v}{C}\cdot\frac{W_{uv}}{S_v} \\ &= \frac{2W_{uv}}{C} \propto W_{uv}. \end{aligned} \tag{9}$$

Under uniform node selection and one transition:

$$\begin{aligned} P_{uv}^{\text{path}} &= \frac{1}{|V|} \left(\pi_{u \to v} + \pi_{v \to u}\right) \\ &= \frac{1}{|V|} \left(\frac{W_{uv}}{S_u} + \frac{W_{uv}}{S_v}\right) \end{aligned} \tag{10}$$

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