# Locality-Aware Graph Rewiring in GNNs

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## Contents



## List of Acronyms

| | |
|---|---|
| GNN | Graph Neural Network |
| MPNN | Message Passing Neural Network |

## 1 Background

Let $G = (V, E)$ be an undirected graph with the adjacency matrix $\underline{\boldsymbol{A}} \in \mathbb{R}^{n \times n}$

$$\underline{\boldsymbol{A}}_{uv} = \begin{cases} 1 & (u, v) \in E \\ 0 & (u, v) \notin E \end{cases} \tag{1}$$

The diagonal degree matrix $\underline{\boldsymbol{D}} \in \mathbb{R}^{n \times n}$ is defined by

$$\underline{\boldsymbol{D}}_{uv} = \begin{cases} d_u & u = v \\ 0 & u \neq v \end{cases} \tag{2}$$

i.e. $\underline{\boldsymbol{D}}$ simply places all node degrees on the diagonal.

### 1.1 normalized adjacency and multi-hop propagation

**Definition 1.** The symmetrically normalized adjacency matrix is

$$\boxed{\hat{\underline{\boldsymbol{A}}} = \underline{\boldsymbol{D}}^{-1/2}\underline{\boldsymbol{A}}\underline{\boldsymbol{D}}^{-1/2}} \tag{3}$$

or, entrywise,

$$\hat{\underline{\boldsymbol{A}}}_{uv} = \begin{cases} \frac{1}{\sqrt{d_u d_v}} & (u,v) \in E \\ 0 & (u,v) \notin E \end{cases}$$

✍

**Proposition 1** (multi-hop propagation)**.** The entry $(\hat{\underline{\boldsymbol{A}}}^k)_{vu}$ can be computed explicitly as follows:

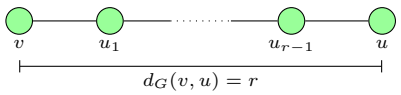
$$(\hat{\underline{\boldsymbol{A}}}^k)_{vu} = \sum_{\pi} \prod_{(x,y)\in\pi} \frac{1}{\sqrt{d_x d_y}} \tag{4}$$

where the sum is over all walks $\pi = (v, \ldots, u)$ of length $k$ from $v$ to $u$. ◁

**Corollary 2.** Let $v, u \in V$ with $r = d_G(v,u)$, where $d_G(\cdot,\cdot)$ denotes the shortest-path distance. Assume there is exactly one path

$$(v, u_1, \ldots, u_{r-1}, u)$$

of length $r$ between $v$ and $u$:




Then

$$\begin{aligned} (\hat{\underline{\boldsymbol{A}}}^r)_{vu} &= \frac{1}{\sqrt{d_v d_{u_1}}} \cdot \prod_{i=1}^{r-2} \frac{1}{\sqrt{d_{u_i} d_{u_{i+1}}}} \cdot \frac{1}{\sqrt{d_{u_{r-1}} d_u}} \\ &= \frac{1}{\sqrt{d_v d_u}} \prod_{i=1}^{r-1} \frac{1}{d_{u_i}} \end{aligned} \tag{5}$$

◁

#### 1.1.1 distance layers and layer degrees

**Definition 2.** For $\ell \in \mathbb{N}_0$, we define the distance-$(\ell+1)$ adjacency matrix $\underline{\boldsymbol{A}}_\ell \in \mathbb{R}^{n\times n}$ by

$$(\underline{\boldsymbol{A}}_\ell)_{uv} = \begin{cases} 1 & d_G(u,v) = \ell + 1 \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

where $d_G(u,v)$ is the shortest-path distance. The corresponding layer degree of a node $v$ at distance level $\ell$ is

$$d_{v,\ell} = \sum_{u\in V} (\underline{\boldsymbol{A}}_\ell)_{vu}, \tag{7}$$

i.e. the number of nodes at graph distance $\ell+1$ from $v$. Let $\underline{\boldsymbol{D}}_\ell$ be the diagonal matrix with $(\underline{\boldsymbol{D}}_\ell)_{vv} = d_{v,\ell}$. The normalized distance-$(\ell+1)$ adjacency is

$$\boxed{\hat{\underline{\boldsymbol{A}}}_\ell = \underline{\boldsymbol{D}}_\ell^{-1/2}\underline{\boldsymbol{A}}_\ell\underline{\boldsymbol{D}}_\ell^{-1/2}} \tag{8}$$

so that

$$(\hat{\underline{\boldsymbol{A}}}_\ell)_{uv} = \begin{cases} \frac{1}{\sqrt{d_{u,\ell} d_{v,\ell}}} & d_G(u,v) = \ell + 1 \\ 0 & \text{otherwise} \end{cases}$$

✍

Finally, we denote by

$$d_{\min} = \min_{v\in V} d_v \tag{9}$$

the minimum node degree in the graph.

## 1.2 graph Laplacian

**Definition 3.** The combinatorial graph Laplacian is

$$\underline{\boldsymbol{L}} = \underline{\boldsymbol{D}} - \underline{\boldsymbol{A}} \tag{10}$$

and the normalized graph Laplacian is

$$\boxed{\hat{\underline{\boldsymbol{L}}} = \underline{\boldsymbol{D}}^{-1/2}\underline{\boldsymbol{L}}\underline{\boldsymbol{D}}^{-1/2} \overset{(10)}{=} \underline{\boldsymbol{D}}^{-1/2}(\underline{\boldsymbol{D}} - \underline{\boldsymbol{A}})\underline{\boldsymbol{D}}^{-1/2} \overset{(3)}{=} \underline{\boldsymbol{I}}_n - \hat{\underline{\boldsymbol{A}}}} \tag{11}$$

It is symmetric and positive semidefinite, and its eigenvalues satisfy

$$0 = \lambda_0 \le \lambda_1 \le \cdots \le \lambda_{n-1}$$

$\lambda_1$ is called the spectral gap. The number of zero eigenvalues (i.e., the multiplicity of the 0 eigenvalue) equals the number of connected components of the graph. ✍

To understand Definition 3, consider a function $f\colon V \to \mathbb{R}$. Denote by $\vec{\boldsymbol{f}} \in \mathbb{R}^n$ the vector whose $v$-th entry is $f(v)$. Then

$$(\hat{\underline{\boldsymbol{L}}}\vec{\boldsymbol{f}})_v = f(v) - \frac{1}{\sqrt{d_v}} \sum_{(u,v)\in E} \frac{f(u)}{\sqrt{d_u}} \tag{12}$$

i.e., $(\hat{\underline{\boldsymbol{L}}}\vec{\boldsymbol{f}})_v$ is the value at $v$ minus a degree-normalized average of the neighbors. This is why the Laplacian is often viewed as a discrete second derivative on the graph: it measures how much $f$ at $v$ deviates from its neighborhood. Another important identity is the quadratic form

$$\vec{\boldsymbol{f}}^{\top}\underline{\boldsymbol{L}}\vec{\boldsymbol{f}} = \frac{1}{2}\sum_{(u,v)\in E} \big(f(u) - f(v)\big)^2 \tag{13}$$

which shows that $\underline{\boldsymbol{L}}$ (and hence also $\hat{\underline{\boldsymbol{L}}}$) is positive semidefinite, since the right-hand side is always nonnegative. Moreover, (13) is small exactly when $f$ varies slowly across edges, so the Laplacian encodes the smoothness of functions on the graph.

## 1.3 Cheeger inequality

The Cheeger inequality relates the spectral gap $\lambda_1$ to the Cheeger constant $h(G)$, which measures how difficult it is to separate the graph into two large pieces. It states, in particular, that

$$\tfrac{1}{2}h(G)^2 \le \lambda_1 \le 2h(G),$$

so a larger spectral gap implies that the graph is more "well-connected".

## 1.4 effective resistance

**Definition 4** (effective resistance)**.** View each edge $(u, v) \in E$ as an electrical resistor of resistance $1\,\Omega$. The resulting network has a well-defined resistance between any two nodes.

For two nodes $s, t \in V$, the effective resistance $R(s, t)$ is defined as the voltage difference needed to send one unit of electrical current from $s$ to $t$. It can be computed as

$$\boxed{R(s,t) = (\vec{\boldsymbol{e}}_s - \vec{\boldsymbol{e}}_t)^{\top}\underline{\boldsymbol{L}}^{\dagger}(\vec{\boldsymbol{e}}_s - \vec{\boldsymbol{e}}_t)} \tag{14}$$

where $\underline{\boldsymbol{L}}^{\dagger}$ is the Moore–Penrose pseudoinverse of $\underline{\boldsymbol{L}}$ and $\vec{\boldsymbol{e}}_v$ is the standard basis vector of vertex $v$. ✍

### 1.4.1 Interpretation

If the graph offers many short, parallel paths between $s$ and $t$, then current can flow easily, so $R(s, t)$ is small. If there are few or long paths, the current is "bottlenecked" and $R(s, t)$ is large. Thus, effective resistance measures how "well-connected" two nodes are inside the global geometry of the graph.

### 1.4.2 Connection to random walks

A random walk on $G$ is the Markov chain that, from a node $v$, moves to a uniformly random neighbor of $v$. Its transition matrix is

$$\underline{\boldsymbol{P}} = \underline{\boldsymbol{D}}^{-1}\underline{\boldsymbol{A}} \tag{15}$$

so $\underline{\boldsymbol{P}}_{vu} = 1/d_v$ if $(v,u) \in E$.

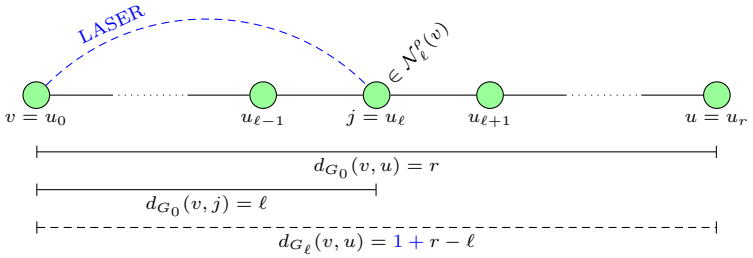
For two nodes $u, v$, the commute time $\texttt{CT}(u,v)$ is the expected number of steps for the random walk to start at $u$, reach $v$, and return to $u$ again. It can be related to the effective resistance via

$$\texttt{CT}(u,v) = 2|E|R(u,v) \tag{16}$$

giving a geometric interpretation of how "far apart" two nodes are in terms of random-walk behavior, i.e. two nodes have small commute time exactly when they have small effective resistance.

## 2 Theoretical analysis

### 2.1 Jacobian sensitivity




We have a unique path

$$(v = u_0, u_1, \ldots, u_{r-1}, u_r = u),$$

and we assume $j = u_\ell$. From Corollary 2, for the full path from $v$ to $u$:

$$(\hat{\underline{\boldsymbol{A}}}^{r})_{vu} = \frac{1}{\sqrt{d_v d_u}} \prod_{s=1}^{r-1} \frac{1}{d_{u_s}}$$

For the sub-path from $j = u_\ell$ to $u = u_r$ of length $r - \ell$, the same reasoning gives

$$(\hat{\underline{\boldsymbol{A}}}^{r-\ell})_{ju} = \frac{1}{\sqrt{d_j d_u}} \prod_{s=\ell+1}^{r-1} \frac{1}{d_{u_s}}.$$

Now we plug this into our expression:

$$\begin{aligned}
\frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}(\hat{\underline{\boldsymbol{A}}}^{r-\ell})_{ju}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{r-1}\frac{1}{d_{u_s}}} &= \frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}}} \cdot \frac{(\hat{\underline{\boldsymbol{A}}}^{r-\ell})_{ju}}{\prod_{s=\ell}^{r-1}\frac{1}{d_{u_s}}} \\
&\overset{(5)}{=} \frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}}} \cdot \frac{\frac{1}{\sqrt{d_j d_u}}\prod_{s=\ell+1}^{r-1}\frac{1}{d_{u_s}}}{\prod_{s=\ell}^{r-1}\frac{1}{d_{u_s}}} \\
&= \frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}}} \cdot \frac{1}{\sqrt{d_j d_u}} \cdot \frac{\prod_{s=\ell+1}^{r-1}\frac{1}{d_{u_s}}}{\frac{1}{d_{u_\ell}}\prod_{s=\ell+1}^{r-1}\frac{1}{d_{u_s}}} \\
&= \frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}}} \cdot \frac{1}{\sqrt{d_j d_u}} \cdot d_{u_\ell} \\
&= \frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}}} \cdot \sqrt{\frac{d_j}{d_u}}
\end{aligned}$$

So

$$\frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}(\hat{\underline{\boldsymbol{A}}}^{r-\ell})_{ju}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{r-1}\frac{1}{d_{u_s}}} = \frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}}} \cdot \sqrt{\frac{d_j}{d_u}} \tag{17}$$

Using

$$(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj} = \frac{1}{\sqrt{d_{v,\ell-1} d_{j,\ell-1}}}$$

and

$$\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}} \leq \frac{1}{d_{\min}^{\ell}}$$

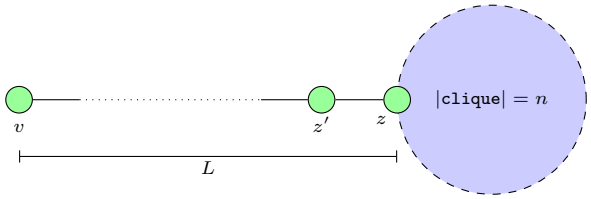
we obtain the bound

$$\frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{\ell-1}\frac{1}{d_{u_s}}} \geq \frac{(d_{\min})^{\ell}}{\sqrt{d_{v,\ell-1} d_{j,\ell-1}}} \tag{18}$$

Combining (17) and (18) yields

$$\boxed{\frac{(\hat{\underline{\boldsymbol{A}}}_{\ell-1})_{vj}(\hat{\underline{\boldsymbol{A}}}^{r-\ell})_{ju}}{\frac{1}{\sqrt{d_v d_u}}\prod_{s=1}^{r-1}\frac{1}{d_{u_s}}} \geq \frac{(d_{\min})^{\ell}}{\sqrt{d_{v,\ell-1} d_{j,\ell-1}}} \cdot \sqrt{\frac{d_j}{d_u}}} \tag{19}$$

### 2.2 Locality awareness




### 2.3 message passing paradigm

A common Graph Neural Network (GNN) family are Message Passing Neural Networks (MPNNs), which compute latent node representations by stacking $T$ layers of the form

$$\boxed{\vec{\boldsymbol{x}}_v^{(t)} = \mathtt{up}^{(t)}(\vec{\boldsymbol{x}}_v^{(t-1)}, \mathtt{agg}^{(t)}(\{\vec{\boldsymbol{x}}_u^{(t-1)} : (v,u) \in E\}))} \tag{20}$$

for $t = 1, \ldots, T$, where $\mathtt{agg}^{(t)}$ is some permutation-invariant aggregation function, while $\mathtt{up}^{(t)}$ updates the node's current state with aggregated messages from its neighbors.

### 2.4 over-squashing and long-range interactions

While the message-passing paradigm usually constitutes a strong inductive bias, it is problematic for capturing long-range interactions due to a phenomenon known as over-squashing. Given two nodes $u, v$ at distance $d_G(u,v) = r$, an MPNN will require $T \geq r$ layers to exchange messages between them. When the receptive fields of the nodes expand too quickly (due to volume growth properties characteristic of many real-world scale free graphs), the MPNN needs to aggregate a large number of messages into fixed-size vectors, leading to some corruption of the information. This effect on the propagation of information has been related to the Jacobian of node features decaying exponentially with $r$. More recently, it was shown that the Jacobian is affected by topological properties such as effective resistance.

### 2.5 graph rewiring

The main principle behind graph rewiring in GNNs is to decouple the input graph $G$ from the computational one. Namely, rewiring consists of applying an operation $\mathcal{R}$ to $G = (V, E)$, thereby producing a new graph $\mathcal{R}(G) = (V, \mathcal{R}(E))$ on the same vertices but with altered connectivity.

We begin by generalizing the MPNN formalism to account for the rewiring operation $\mathcal{R}$ as follows:

$$\vec{\boldsymbol{x}}_v^{(t)} = \mathtt{up}^{(t)}(\vec{\boldsymbol{x}}_v^{(t-1)}, \mathtt{agg}_G^{(t)}(\{\vec{\boldsymbol{x}}_u^{(t-1)} : (v,u) \in E\}), \mathtt{agg}_{\mathcal{R}(G)}^{(t)}(\{\vec{\boldsymbol{x}}_u^{(t-1)} : (v,u) \in \mathcal{R}(E)\})) \tag{21}$$

where a node feature is now updated based on information collected over the input graph $G$ and the rewired one $\mathcal{R}(G)$, through (potentially) independent aggregation maps. Many rewiring-based GNN models simply exchange messages over $\mathcal{R}(G)$, i.e., they take $\mathtt{agg}_G = 0$.

Ever since over-squashing was identified as an issue in MPNNs, several novel rewiring approaches have been proposed to mitigate this phenomenon.

## 3 A general paradigm: dynamic rewiring with local constraints

**Main idea** Anstead of considering a single rewired graph $\mathcal{R}(G)$, we use a sequence of rewired graphs $\{\mathcal{R}_\ell(G)\}_\ell$ such that for smaller $\ell$, the new edges added in $\mathcal{R}_\ell(G)$ are more 'local' (with respect to the input graph $G$) and sampled based on optimizing a connectivity measure.

In this Section, we discuss a general graph-rewiring paradigm that can enhance any MPNN and satisfies the criteria (i)–(iii) described above. Given a graph $G$, consider a trajectory of rewiring operations $\mathcal{R}_\ell$, starting at $G_0 = G$, of the form:

$$G = G_0 \xhookrightarrow{\mathcal{R}_1} G_1 \xhookrightarrow{\mathcal{R}_2} \cdots \xhookrightarrow{\mathcal{R}_L} G_L \tag{22}$$

Since we think of $G_\ell$ as the input graph evolved along a dynamical process for $\ell$ iterations, we refer to $G_\ell$ as the $\ell$-snapshot. For the sake of simplicity, we assume $\mathcal{R}_\ell = \mathcal{R}$, though it is straightforward to extend the discussion below to the more general case. In order to account for the multiple snapshots, we modify the layer form in (21) as

$$\vec{\boldsymbol{x}}_v^{(t)} = \mathtt{up}^{(t)}\left(\vec{\boldsymbol{x}}_v^{(t-1)}, \left(\mathtt{agg}_{G_\ell}^{(t)}(\{\vec{\boldsymbol{x}}_u^{(t-1)} : (v,u) \in E_\ell\})\right)_{0 \le \ell \le L}\right) \tag{23}$$

where, instead of aggregating messages over a single rewired graph, we now consider all the snapshots $G_\ell$ in the sequence.

Below we describe a rewiring paradigm based on an arbitrary connectivity measure $\mu : V \times V \to \mathbb{R}$ and locality measure $\nu : V \times V \to \mathbb{R}$. The measure $\mu$ can be any topological quantity that captures how easily different pairs of nodes can communicate in a graph, while the measure $\nu$ is any quantity that penalizes interactions among nodes that are 'distant' according to some metric on the input graph.

**Improving connectivity while preserving locality** The first property we demand of the rewiring sequence is that for all nodes $v, u$, we have $\mu_{G_{\ell+1}}(v,u) \ge \mu_{G_\ell}(v,u)$ and that for some nodes, the inequality is strict. If we connect all pairs of nodes with low $\mu$-value, however, we might end up adding non-local edges across distant nodes, hence quickly corrupting the locality of $G$. To avoid this, we constrain each rewiring by requiring the measure $\nu$ to take values in a certain range $\mathcal{I}_\ell \subset [0, \infty)$: an edge $(v,u)$ appears in the $\ell$-snapshot (for $1 \le \ell \le L$) according to the following rule:

$$(v,u) \in E_\ell \text{ if } \left(\mu_{G_0}(v,u) < \epsilon \text{ and } \nu_{G_0}(v,u) \in \mathcal{I}_\ell\right) \text{ or } (v,u) \in E_{\ell-1}. \tag{24}$$

To make the rewiring more efficient, the connectivity and locality measures are computed once over the input graph $G_0$. Since the edges to be added connect nodes with low $\mu$-values, the rewiring makes the graphs $G_\ell$ friendlier to message-passing as $\ell$ grows. Moreover, by taking increasing ranges of values for the intervals $\mathcal{I}_\ell$, we make sure that new edges connect distant nodes, as specified by $\nu$, only at later snapshots. By accounting for all the snapshots $G_\ell$ in (21), the GNN can access both the input graph, and more connected ones, at a much finer level than 'instantaneous' rewirings, defined next.