Delaunay Graph: Addressing Over-Squashing and Over-Smoothing Using Delaunay Triangulation

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Graph Neural Networks

- Graph Neural Networks operate on the Message Passing Neural Networks (MPNNs) paradigm. This paradigm involves iteratively applying AGGREGATE and UPDATE functions to enhance node representations. The process updates the representations by utilizing the information contained in the neighbors.

$$m_i^{(\ell)} = \text{AGGREGATE}^{(\ell)}\left(h_i^{(\ell-1)}, \{h_j^{(\ell-1)} \mid j \in \mathcal{N}(i)\}\right)$$

$$h_i^{(\ell)} = \text{UPDATE}^{(\ell)}\left(h_i^{(\ell-1)}, m_i^{(\ell)}\right)$$

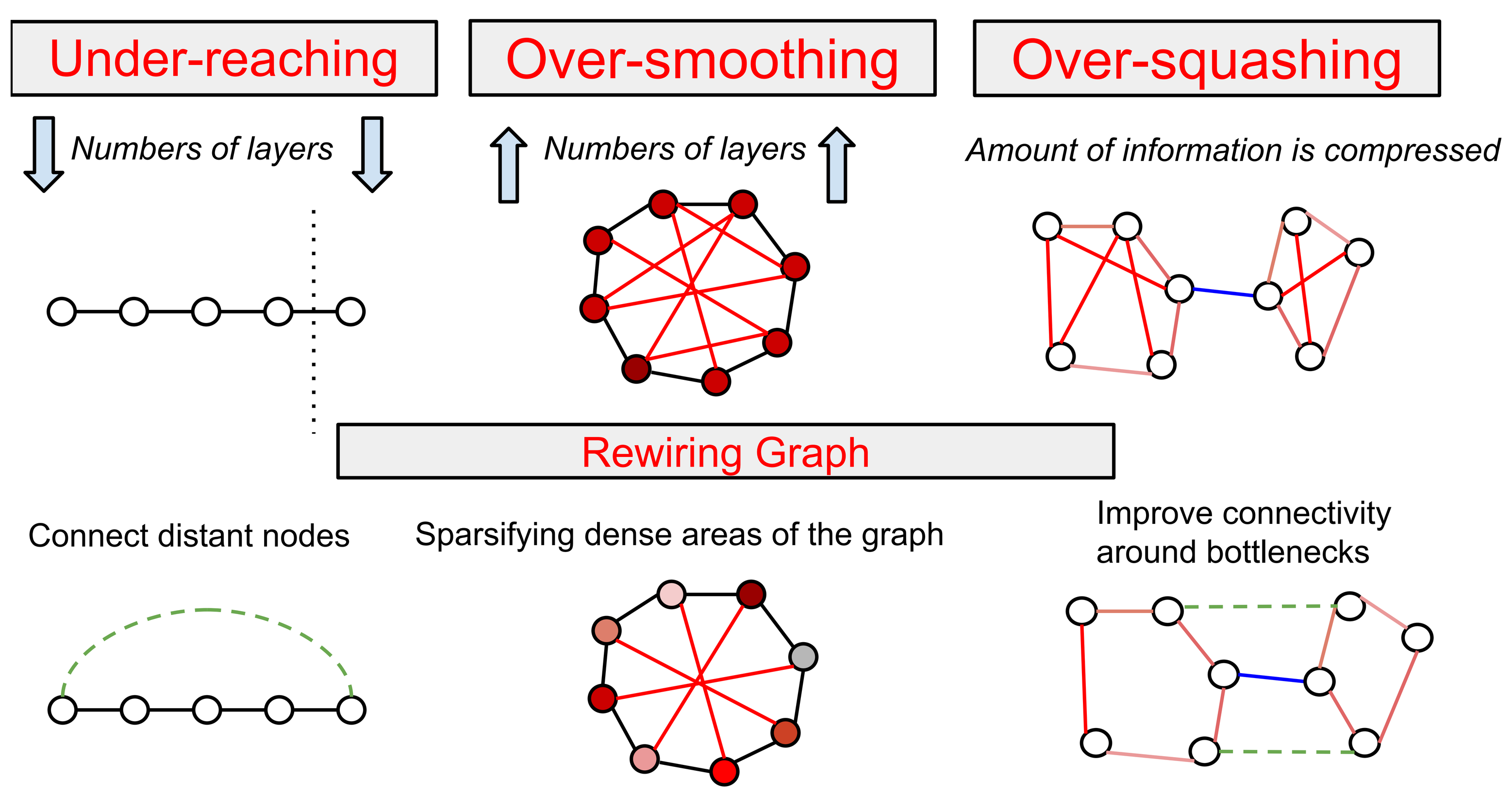
- Local operation => it takes k layers to exchange information between two nodes at a distance of k => difficulties to fetch long-term information.

<u>Increasing the number of layers is not a good idea because it causes :</u>

- Over-smoothing => As the number of layers increases, the message passing becomes excessively intensive => the features of the nodes gradually become more similar.
- Over-squashing => At each stage, node representations are aggregated with others before being passed on to the next node. Since the size of node feature vectors does not change, they quickly run out of representation capacity to preserve all previously combined information.

Rewiring

A common approach to mitigate Over-Squashing and Over-Smoothing is by rewiring the input graph.



Curvature on graph

As for a manifold, the notion of curvature is a good way to caraterize the local behavior of a graph.

[1] $c_{ij} = 4 - d_i - d_j + 3m$

[2] $c_{ij} = \dfrac{2}{d_i} + \dfrac{2}{d_j} - 2 + 2\dfrac{m}{\max\left\{d_i, d_j\right\}} + \dfrac{m}{\min\left\{d_i, d_j\right\}} + \dfrac{(\Gamma_{\max})^{-1}}{\max\left\{d_i, d_j\right\}}(\gamma_i + \gamma_j)$

where m is the number of triangles that contain e_{ij}

<u>[3] Positive curvature => dense areas=> Accentuates Over-Smoothing</u>

<u>[2] Negatives curvature => Bottleneck => Accentuates Over-Squashing</u>

Motivation

How can you avoid negative-curvature edges while avoiding dense areas in the graph?

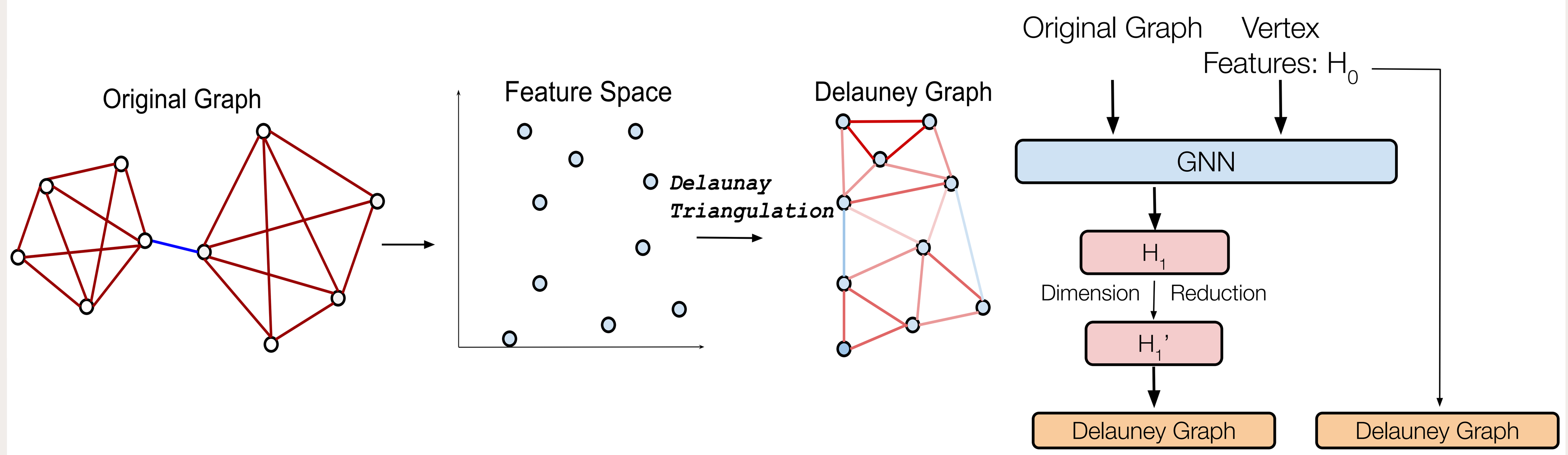
<u>Applying a Delaunay triangulation allows to maximize the number of triangle in the graph while ensuring a maximum clique size of 3.</u>

Delaunay Graph

While the majority of the rewiring methods modify the original graph structure, we propose a complete rebuild of the graph, based only on the features of the nodes, ignoring the edges of the original graph. We choose to introduce the new edges of the rewired graph by applying a Delaunay triangulation on the node features.

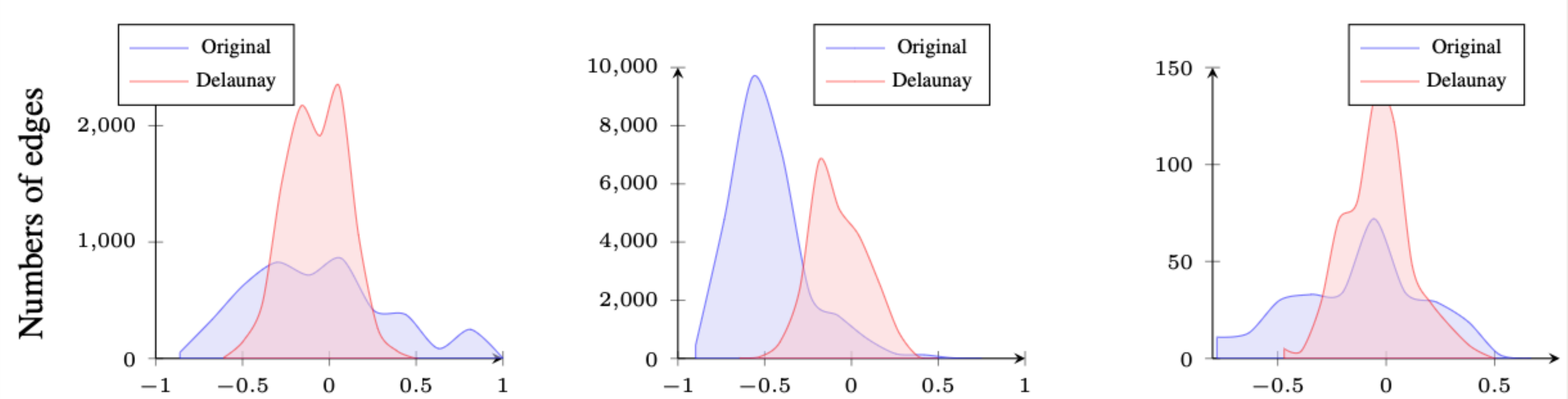
Delaunay Triangulation [4]

A Delaunay triangulation, denoted as DT(P), for a set P of points in the d-dimensional Euclidean space, is a triangulation where no point in P resides within the circum-hypersphere of any d-simplex in DT(P).



<u>In dimension 2, Delaunay triangulation has particularly interesting properties for graph construction.</u>

Delaunay Graph properties



<u>Avoid strongly negatively curved edges=> Mitigate over-squashing</u>

<u>Size of largest clique is 3.</u>
<u>Avoid strongly positively curved edges => Mitigate over-smoothing</u>

Type	Dataset	# Nodes	# C	# O-Edges	# O-Homo	# D-Edges	# D-homo	# Homo gain
Heterophilic	Squirrel	5021	5	217073	0.22	31170	0.59	168%
	Chameleon	2277	5	36101	0.25	13630	0.69	176%
	Texas	181	5	309	0.06	1072	0.63	950%
	Wisconsin	251	5	499	0.06	1470	0.55	817%
	Cornell	181	5	295	0.11	1064	0.67	509%
	Roman-empire	22662	18	32927	0.06	135922	0.58	1060%
	Actor	7600	5	33544	0.24	45520	0.40	33%
Homophilic	Citeseer	3 312	6	4 715	0.71	19923	0.78	10%
	Cora	2 708	7	5 429	0.83	16214	0.88	6%
	Pubmed	19 717	3	44348	0.77	118192	0.86	9%

<u>Good degree distribution</u>

<u>Improve graph homophily</u>

Experiments

	Base (GCN)	DIGL	FA	SRDF	FOSR	BORF	GTR	**DR**
Cham.	65.35±0.54	54.82 ±0.48	26.34 ±0.61	63.08 ±0.37	67.98 ±0.40	65.35 ±0.51	<u>68.03</u> ±0.61	**74.28** ±0.48
Squir.	51.30±0.38	40.53 ±0.29	22.88 ±0.42	49.11±0.28	52.63 ±0.30	$\geq$ 24h	<u>53.32</u> ±0.44	**65.25** ±0.26
Actor	30.02±0.22	26.75 ±0.23	26.03±0.30	<u>31.85</u> ±0.22	29.26±0.23	31.36 ±0.27	31.08 ±0.28	**41.36** ±0.20
Texas	56.19 ±1.61	45.95 ±1.58	55.93 ±1.76	<u>59.79</u> ±1.71	61.35 ±1.25	56.30±1.61	57.18 ±1.64	**70.46** ±1.61
Wisc.	55.12±1.51	46.90 ±1.28	46.77±1.48	<u>58.49</u> ±1.23	55.60 ±1.25	55.37 ±1.47	57.22 ±1.50	**70.98**±1.50
Corn.	44.78 ±1.45	44.46 ±1.37	45.33±1.55	<u>47.73</u> ±1.51	45.11 ±1.47	46.81 ±1.56	47.57 ±1.52	**67.22** ±1.48
R-emp.	51.66 ±0.17	53.93 ±0.14	OOM	<u>52.53</u> ±0.13	52.38 ±0.21	<u>58.58 ±0.14</u>	53.31 ±0.23	**61.99** ±0.14
Cora	87.73 ±0.25	<u>88.31</u> ±0.29	29.86 ±0.28	87.73 ±0.31	87.94 ±0.26	87.72±0.27	87.86 ±0.28	**91.39** ±0.24
Citeseer	76.01 ±0.25	76.22 ±0.34	22.31 ±0.34	76.43 ±0.32	76.34 ±0.27	<u>76.49</u> ±0.28	76.12 ±0.28	**81.14** ±0.34
Pubmed	88.20 ±0.10	<u>88.51</u> ±0.10	OOM	88.16 ±0.11	88.42 ±0.10	88.34 ±0.10	88.44 ±0.10	**88.69** ±0.10

	Base (GAT)	DIGL	FA	SRDF	FOSR	BORF	GTR	**DR**
Cham.	65.07 ±0.41	56.34 ±0.43	27.11 ±0.56	63.15±0.44	66.61 ±0.45	<u>66.92</u> ±0.51	65.97 ±0.54	**72.04** ±0.37
Squi.	50.87 ±0.56	41.65 ±0.68	21.49 ±0.71	50.36 ± 0.38	52.02 ±0.43	$\geq$ 24h	<u>52.72</u> ±0.48	**61.47** ±0.29
Actor	29.92 ±0.23	31.22 ±0.47	28.20 ±0.51	<u>31.47</u> ±0.25	29.73 ±0.24	29.64 ± 0.33	30.13 ±0.31	**40.25** ±0.23
Texas	56.84 ±1.61	46.49 ±1.63	56.17 ±1.71	57.45 ±1.62	<u>61.85</u> ±1.41	56.68 ± 1.49	57.88 ±1.65	**74.30** ±1.38
Wisc.	53.58 ±1.39	46.29 ±1.47	46.95 ±1.52	<u>56.80</u> ±1.29	54.06±1.27	55.39 ± 1.23	56.53±1.64	**74.33** ±1.24
Cornell	46.05 ±1.49	44.05 ±1.44	44.60 ±1.74	48.03 ±1.66	48.30±1.61	48.57 ± 1.56	<u>48.70</u> ±1.63	**68.03** ±1.62
R-Emp.	49.23 ±0.33	<u>53.89</u> ±0.16	OOM	50.75 ±0.17	49.54 ±0.31	51.03 ± 0.26	50.60 ±0.24	**61.80** ±0.16
Cora	87.65 ±0.24	<u>88.31</u> ±0.29	30.44 ±0.26	88.11 ±0.28	88.13 ±0.27	87.72±0.27	87.94±0.23	**91.37** ±0.23
Citeseer	76.20 ±0.27	76.22 ±0.34	23.11 ±0.32	76.26 ±0.31	75.94±0.32	<u>76.44</u> ±0.44	76.35 ±0.28	**81.61** ±0.25
Pubmed	87.39 ±0.11	<u>87.96</u> ±0.10	OOM	87.44 ±0.12	87.56 ±0.11	87.61 ±0.12	87.31 ±0.12	**89.14** ±0.09

<u>On average, Delaunay Rewiring demonstrated a substantial increase of 21.8% in performance when compared to the basic GCN and GAT.</u>

Complexity and running time

Models	Input Graphs	Type of Rewiring	Complexity	Hyperparameters
DIGL	Required	Structural Rewiring	$\mathcal{O}(N)$	Grid-search
SDRF	Required	Structural Rewiring	$\mathcal{O}(\lvert\mathcal{E}\rvert d_{\max}^2)$	Grid-search
FOSR	Required	Structural Rewiring	$\mathcal{O}(N^2)$	Grid-search
BORF	Required	Structural Rewiring	$\mathcal{O}(\lvert\mathcal{E}\rvert d_{\max}^3)$	Grid-search
GTR	Required	Structural Rewiring	$\mathcal{O}(\lvert\mathcal{E}\rvert \text{ poly } \log N + N^2 \text{ poly } \log N)$	Grid-search
DR (Ours)	Not necessary	Feature Rewiring	$\mathcal{O}(N\log(N))$	Heuristic

Number of data	Time (in sec)
100 000.	≤ 1
1 000 000	15
5 000 000	200

<u>Delaunay Rewiring is highly scalable for large datasets.</u>

<u>The input graph is not necessary</u>

Conclusion

- Our approach involves utilizing node features to induce a new graph structure based on Delaunay triangulation.
- The structural properties of the Delaunay graph allow for good information diffusion by reducing Over-Smoothing and Over-Squashing.
- Our extensive experimentation conducted on homophobic and heterophillic graphs demonstrates that our method consistently outperforms existing graph rewiring methods.

References

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