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Over-squashing in Spatiotemporal Graph Neural Networks

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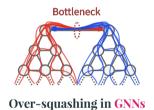
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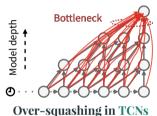


Over-squashing

GNNs suffer from over-squashing: information is compressed and lost through bottlenecks [1].

STGNNs introduce a temporal dimension, compounding the issue [2].





How does $\emph{spatiotemporal over-squashing}$ affect representation learning in STGNNs?

- [1] Alon et al., "On the bottleneck of graph neural networks and its practical implications", ICLR 2021.
- [2] Bengio et al., "Learning long-term dependencies with gradient descent is difficult", IEEE TNN 1994.

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Contributions

Formal characterization of spatiotemporal over-squashing.



② ...which amplifies the compression effects observed in static GNNs.

Proof that convolutional STGNNs are more sensitive to information far apart in time.

- © Counterintuitive behavior and opposite to graph over-squashing.
- © We outline architectural modifications that mitigate this imbalance when required.

Proof that spatiotemporal over-squashing affects T&S and TTS models to the same degree.

○ Theoretical support for scalable TTS designs.

Sensitivity analysis

Spatiotemporal over-squashing can be assessed via the spectral norm of the **STGNN**'s Jacobian:

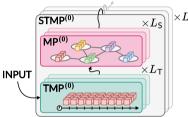
$$\left\|
abla_{i}^{u} oldsymbol{h}_{t}^{v(L)}
ight\| = \left\| rac{\partial oldsymbol{h}_{t}^{v(L)}}{\partial oldsymbol{h}_{t-i}^{u(0)}}
ight\|.$$

 \bigcirc How much features of u influence the output of v.

The Jacobian of the l-th disjoint layer factorizes as:

$$\frac{\partial \boldsymbol{h}_{t-j}^{v(l+1)}}{\partial \boldsymbol{h}_{t-i}^{u(l)}} = \underbrace{\frac{\partial \boldsymbol{h}_{t-j}^{v(l+1)}}{\partial \boldsymbol{z}_{t-j}^{u(l)}}}_{\text{space}} \underbrace{\frac{\partial \boldsymbol{z}_{t-j}^{u(l)}}{\partial \boldsymbol{h}_{t-i}^{u(l)}}}_{\text{time}}$$

We consider L disjoint STMP stacked layers:



 $LL_{\rm S}$ and $LL_{\rm T}$ are computational budgets.

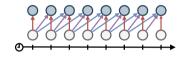
T&S
$$\longrightarrow$$
 TTS $L_S = L_T = 1$ $L = 1$

^[3] Topping et al., "Understanding over-squashing and bottlenecks on graphs via curvature", ICLR 2022.

Message-passing temporal convolutional networks

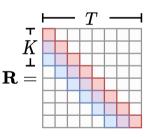
We focus on MPTCNs, where TMP is implemented using causal convolutions with K-sized filter τ :

$$m{h}_{t-i}^{(l+1)} = \sum_{k=0}^{K-1} m{ au}[k] \cdot m{h}_{t-i-k}^{(l)}$$



This can be written as a matrix multiplication using Toeplitz matrix ${f R}$:

$$oldsymbol{h}_{t-T:t}^{(l+1)} = \mathbf{R}^ op oldsymbol{h}_{t-T:t}^{(l)}$$



 ${f R}$ acts as a temporal topology matrix:

• $(\mathbf{R}^l)_{ij}$ is the number of paths from t-i to t-j after l layers.

Temporal sensitivity upper bound

We aim at studying $\left\| \nabla_{i} \boldsymbol{h}_{t}^{v(L)} \right\|$ in MPTCNs, starting from the temporal component: $\left\| \nabla_{i} \boldsymbol{h}_{t}^{v(L_{\mathsf{T}})} \right\|$

Theorem (4.1 — Over-squashing in TCNs)

Consider a TCN with L_T successive layers, all with kernel size K, and assume that $\|\mathbf{W}_k^{(l)}\| \leq w$ for all k < K and $l \leq L_T$, and that $|\sigma'| \leq c_\sigma$. For each nonnegative i < T, we have:

$$\left\| \nabla_{\stackrel{\boldsymbol{v}}{i}} \boldsymbol{h}_t^{\boldsymbol{v}(L_\mathsf{T})} \right\| \leq \underbrace{(c_\sigma \mathsf{w})^{L_\mathsf{T}}}_{\text{model}} \underbrace{\left(\mathbf{R}^{L_\mathsf{T}}\right)_{i0}}_{\text{temporal topology}}.$$

- Model and temporal topology have distinct and multiplicative effects on sensitivity.
- **60** R is a lower-triangular, Toeplitz, band matrix ($\mathbf{R}_{ii} = 0$ for $i \geq K$), so asymptotically we have...

Amplification of long-range temporal dependencies

Proposition (4.2 — Sink effect in causal TCNs)

Let $\mathbf{R} \in \mathbb{R}^{T \times T}$ be a lower-triangular Toeplitz matrix with lower bandwidth $K \geq 2$. For any i > j:

$$\left|rac{\left(\mathbf{R}^l
ight)_{j0}}{\left(\mathbf{R}^l
ight)_{i0}}
ight|
ightarrow 0$$
 as $l
ightarrow \infty$.

The final token receives considerably more influence from tokens positioned earlier in the sequence.

Counterintuitively, TCNs overemphasize earlier information when depth increases.

Sink effect: recent inputs vanish with depth, with all focus towards the first token.

Spatiotemporal sensitivity bound

Theoretical upper bound for common GNNs decomposed into model vs topology too (from [4]):

$$\left\| \nabla_{\boldsymbol{0}}^{\boldsymbol{u}} \boldsymbol{h}_{t}^{v(L)} \right\| \leq \underbrace{\left(c_{\xi} \boldsymbol{\theta}_{\mathsf{m}} \right)^{L} \left(\mathbf{S}^{L} \right)_{uv},}_{\text{topology}} \qquad \leftarrow \mathbf{S} \text{ is a function of } \mathbf{A}$$

We combine both results to analyze the spatiotemporal case.

 $[\]begin{tabular}{ll} \textbf{[4] Di Giovanni et al., "How does over-squashing affect the power of GNNs?", TMLR 2024.} \end{tabular}$

Spatiotemporal sensitivity bound

Theorem (5.1 - Over-squashing in MPTCNs)

Consider an MPTCN with L STMP layers, each consisting of L_T temporal (TMP) and L_S spatial (MP) layers. Then, for any $i, j \in \mathcal{V}$ and $p, q \in [0, T)$, the following holds:

$$\left\| \nabla_{i}^{u} \boldsymbol{h}_{t}^{v(L)} \right\| \leq \underbrace{\left(c_{\xi} \boldsymbol{\theta}_{\mathrm{m}} \right)^{LL_{\mathrm{S}}} \left(c_{\sigma} \mathbf{w} \right)^{LL_{\mathrm{T}}}}_{\text{model}} \underbrace{\left(\mathbf{S}^{LL_{\mathrm{S}}} \right)_{uv} \left(\mathbf{R}^{LL_{\mathrm{T}}} \right)_{i0}}_{\text{spatiotemporal topology}}.$$

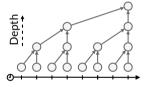
Again, the bound decomposes into model vs topology and time vs space. Two observations:

⚠ Improving only one dimension is insufficient if the other is bottlenecked.

Rewiring the temporal graph

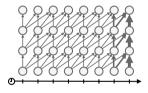
Two approaches to mitigate temporal over-squashing by *rewiring* the temporal graph.

Dilated convolutions



- © Exponentially expanding the receptive field reduces the paths from earlier tokens.
- Sink behavior after dilation resets.

Row-normalized convolutions



- Slowly converges to uniform attention distribution over the sequence.
- Has only effect on last token.

Assessment on real-world benchmarks

Empirical evaluation on traffic and weather data.

- T&S and TTS approaches perform comparably on average.
- Row-normalized convolutions improve accuracy.
- Findings remain valid even with more sophisticated architectures. (see Graph WaveNet [5])

Table 1: Forecasting error (MAE \pm std) with fixed computational budget.

| Models | | L | METR-LA | PEMS-BAY | EngRAD |
|-----------------------|-----------|---|-------------------|---|--------------------------------|
| MPTCN | R | 6 | 3.19±0.02 | $1.66 {\scriptstyle \pm 0.00}$ | 44.43±0.41 |
| | | 3 | 3.19±0.01 | $1.65{\scriptstyle\pm0.01}$ | 43.83 ±0.03 |
| | | 1 | 3.14 ±0.02 | $\textbf{1.63} {\scriptstyle \pm 0.01}$ | $44.47 \scriptstyle{\pm 0.42}$ |
| | ${f R}_N$ | 6 | 3.17±0.02 | $1.65{\scriptstyle\pm0.01}$ | 41.82±0.38 |
| | | 3 | 3.17±0.01 | $1.65{\scriptstyle\pm0.00}$ | $41.78 \scriptstyle{\pm 0.09}$ |
| | | 1 | 3.16±0.01 | 1.65±0.01 | 40.38±0.08 |
| Graph WaveNet (orig.) | | | 3.02±0.02 | 1.55±0.01 | 40.50±0.27 |
| Graph WaveNet (TTS) | | | 3.00±0.01 | $1.57{\pm \scriptstyle 0.00}$ | 40.64±0.29 |



References

- [1] Alon and Yahav. "On the bottleneck of graph neural networks and its practical implications". In: International Conference on Learning Representations. 2021.
- [2] Bengio, Simard, and Frasconi. "Learning long-term dependencies with gradient descent is difficult".

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- [3] Topping, Di Giovanni, Chamberlain, Dong, and Bronstein. "Understanding over-squashing and bottlenecks on graphs via curvature". In: International Conference on Learning Representations. 2022.
- [4] Di Giovanni, Rusch, Bronstein, Deac, Lackenby, Mishra, and Veličković. "How does over-squashing affect the power of GNNs?" In: *Transactions on Machine Learning Research* (2024). ISSN: 2835-8856.
- [5] Wu, Pan, Long, Jiang, and Zhang. "Graph WaveNet for Deep Spatial-Temporal Graph Modeling". In: Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI-19. International Joint Conferences on Artificial Intelligence Organization, July 2019 [URL].