Conformal Inductive Graph Neural Networks

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TLDR

- Conformal Prediction (CP) produces prediction **sets** guaranteed to include the true label with high probability.
- In inductive GNNs the graph evolution breaks the CP guarantee.
- We restore the guarantee under node and edge exchangeablility.

Motivation

- Quantification of uncertainty is crucial yet hard for graphs.
- Model softmax is uncalibrated, therefore unreliable.
- Conformal sets are interpretable and reliable.

Standard Conformal Prediction

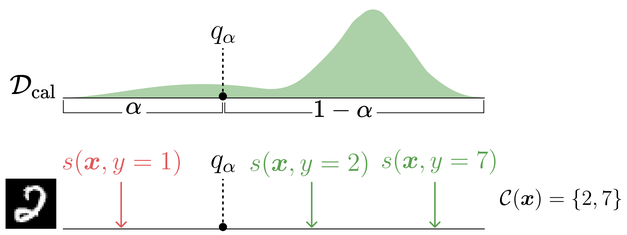
Given Black-box model $f(\cdot)$, holdout and exchangeable calibration set $\mathcal{D}_{\text{cal}} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$, user-specified $1-\alpha$, and new input $\boldsymbol{x}_{n+1}$.

Algorithm With $q_\alpha := \text{Quant}\left(\alpha; \{s(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}; 1\right)$, define prediction sets

$$\mathcal{C}_\alpha(\boldsymbol{x}_{\text{test}}) = \{y : \ s(\boldsymbol{x}_{\text{test}}, y) \geq q_\alpha\}$$

where $\text{Quant}\left(\cdot;\cdot;\cdot\right)$ is the quantile function, and $s(\cdot,\cdot)$ is the conformity score function capturing a heuristic notion of uncertainty (e.g. softmax outputs).

Guarantee $\text{Prob}\left[y_{\text{true}} \in \mathcal{C}(\boldsymbol{x}_{\text{test}})\right] \geq 1-\alpha$.



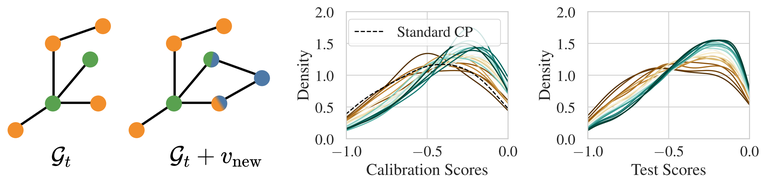
Conformal Prediction for GNNs

Transductive setting Permutation-equivariant GNN + Exchangeable calibration subset → Guarantee is valid.

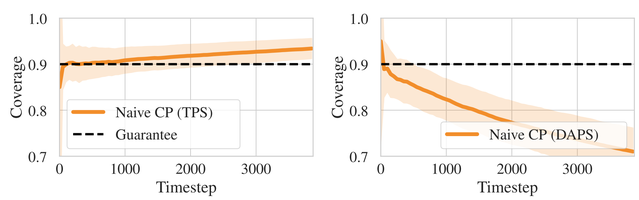
Inductive setting Message passing can break the exchangeability **of conformity scores** even with an exchangeable calibration set.

Conformal Prediction for Inductive GNNs

By introducing new nodes or edges, the embedding and scores will shift. This breaks the exchangeability and CP guarantee.

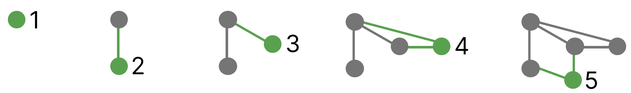


Coverage deviates from the desired level, resulting in over- or under-coverage (direction is unknown in practice).



Exchangeable Graph Sequences

Node-exchangeable Any node can appear at any time. Nodes come with all their edges to the existing nodes.



Node exchangeable generators result in dense or empty graphs.

Edge-exchangeable Any edge can appear at any time. Edges might connect new or existing nodes.

Our Results in Summary

Observation The shift in conformity scores is **symmetric**.

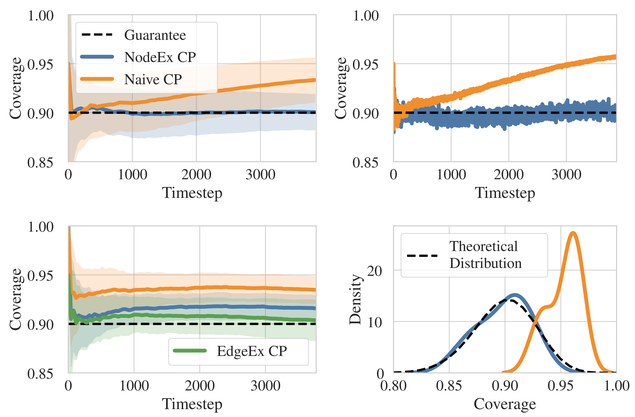
Solution Exact correction for the shift to recover the guarantee.

Results

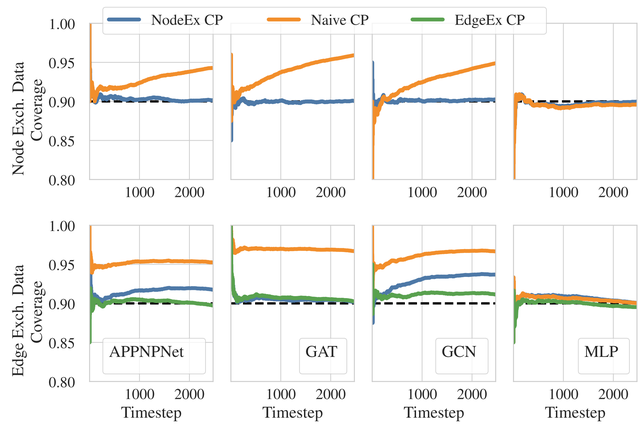
NodeEx CP **Recompute** all calibration scores given the current subgraph $\mathcal{G}_t$, **recalibrate** CP and predict.

$$\mathcal{C}^{(t)}(v_j) = \left\{y : s(v_j, y \mid \mathcal{G}_t) \geq \text{Quant}\left(\alpha; \{s(v_i, y_i \mid \mathcal{G}_t)\}_{i \in \mathcal{V}_{\text{cal}}}; w_i = 1\right)\right\}$$

EdgeEx CP Same as NodeEx CP but with weights $w_i = 1/\deg(v_i)$.



Recovers guarantee for all models.



Recovers guarantee for all scores.