GGUN: Global Graph Understanding via Graph Neural Network Explanation for Identification of Influential Nodes in Healthcare

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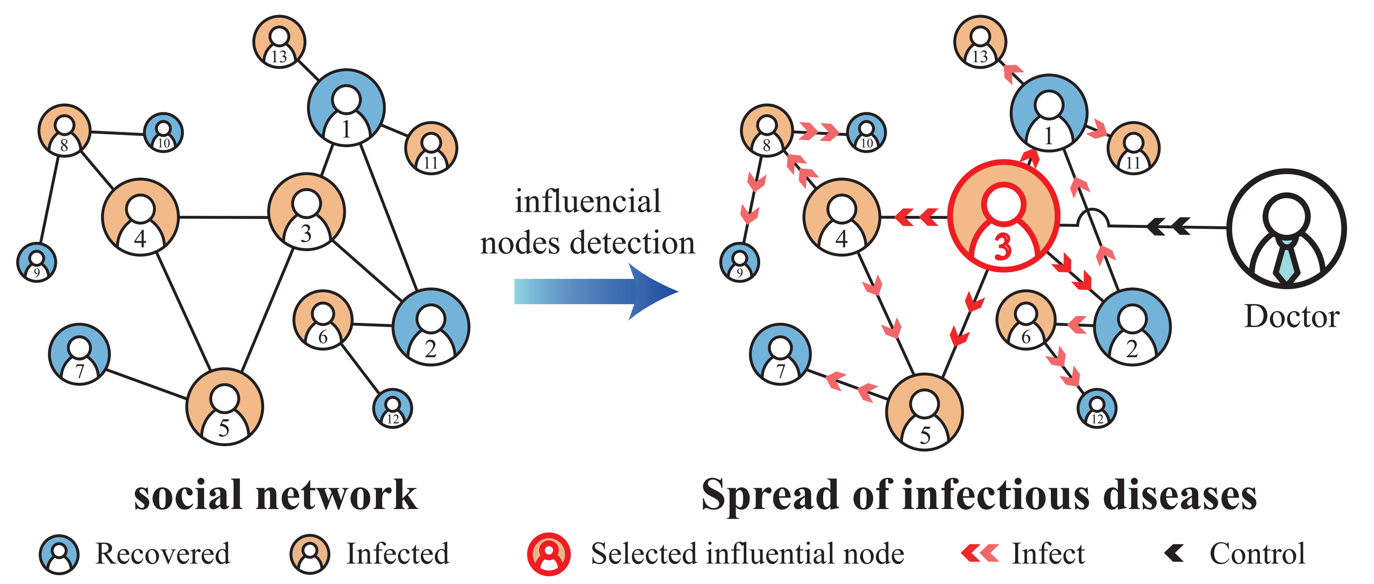
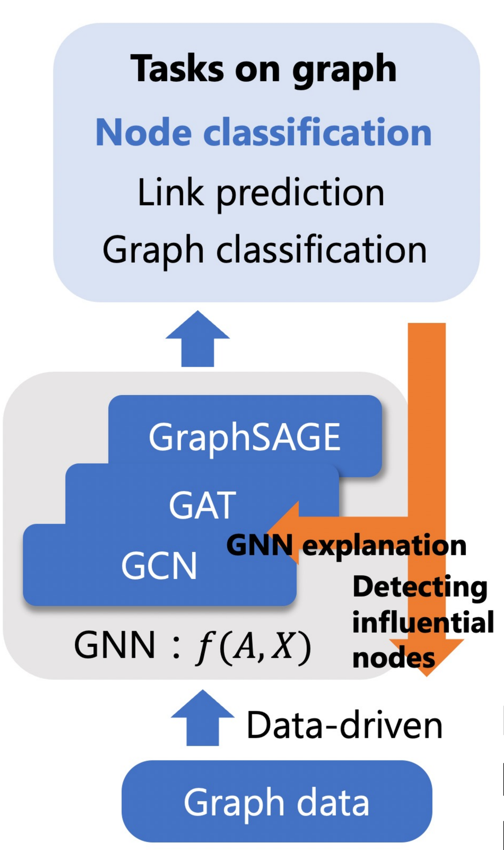
Introduction



Detecting influential individuals in social network to locating those highly infectious person

Data-driven approach: leveraging the power of GNN



Node classification employing GNN

$\hat{A}$	Symmetric normalized adjacency matrix.
X	Attribute matrix.
W	Weight parameter.

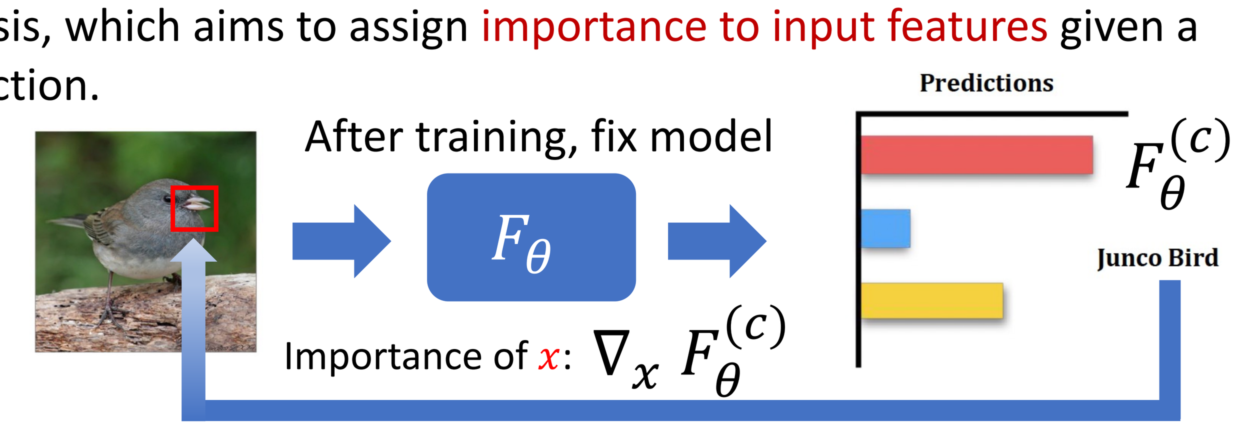
Following [1], we consider a GCN with a single hidden layer:

$$\mathrm{softmax}(\hat{A}\sigma(\hat{A}XW^{(1)})W^{(2)})$$

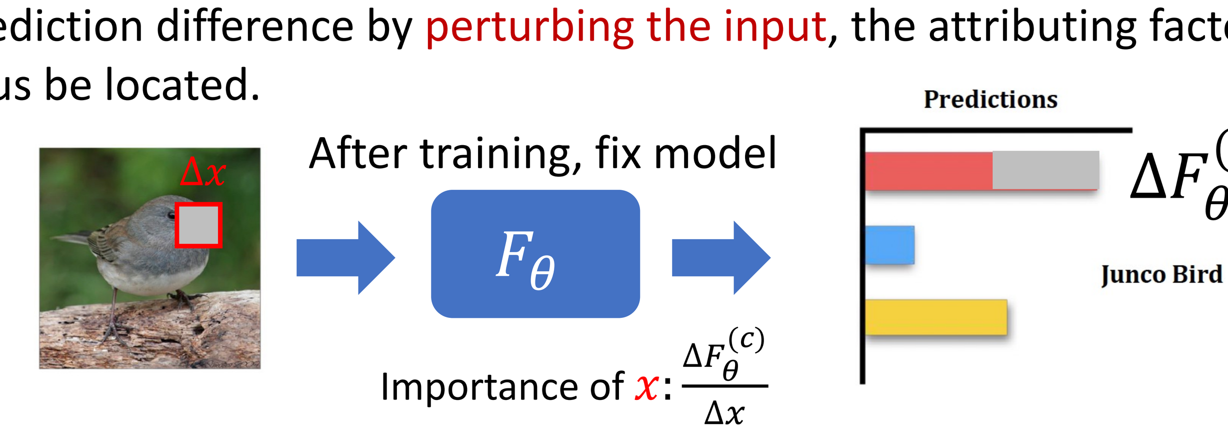
Model parameter $\theta = (W^{(1)}, W^{(2)})$ is optimized by minimizing the cross-entropy loss towards health-related predictions(infected or recovered)

Perturbation-based explanation

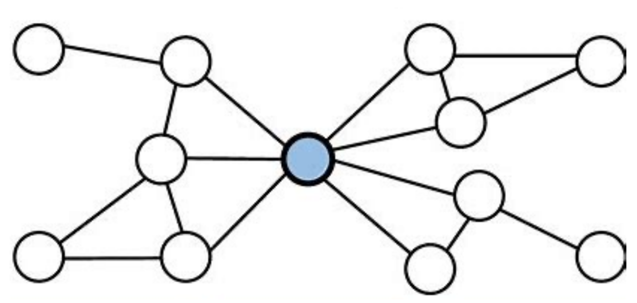
A large fraction of existing explanation methods are based on sensitivity analysis, which aims to assign importance to input features given a prediction.



However, gradient calculation can not be applied to graph data. Breaking the discreteness of adjacency matrix results in useless explanations. Perturbation-based explanation is another choice[2]. Through measuring the prediction difference by perturbing the input, the attributing factors can thus be located.



Centrality-based methods



Degree centrality, Eigenvector centrality, Betweenness centrality …

Oversimplify: nodes are homogenous

High-centrality nodes ≠ influential nodes

GGUN leverage attribute and structure simultaneously

GGUN: Global Graph Understanding via Graph Neural Network Explanation

We aim to select a set of important nodes from an attributed graph dataset. We design the proposed method GGUN: 1) Global explanation method in a data-driven manner. We utilize the explanatory prediction power of GNN by first training a model on origin graph. Following the idea of perturbation-based explanation, i.e. final predictions will change significantly once important features are perturbed. 2) Relaxing the infeasible bi-level combinatorial optimization into trainable convex optimization problem.

Primal problem: Finding K nodes that minimize unchanged predictions on G' when removing nodes set S from G:

$$\underset{\mathcal{S}\subset\mathcal{V}}{\operatorname{argmin}} \sum_{v\in\mathcal{V}} \mathbf{1}\left(y_v^G = y_v^{G'}\right) \quad s.t.\ |\mathcal{S}| < K$$

This is a Combinatorial Optimization problem with unfeasible $O(N^K)$ search space!

Greedy search: still computational-challenging; local optimum

We use 2 strategies:

1. Approximating the loss function

Convert deterministic prediction to continuous probabilistic form.

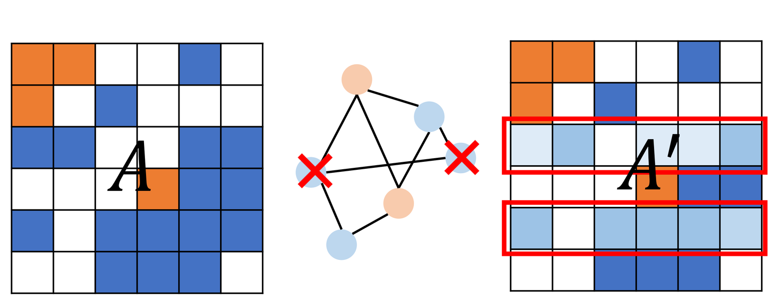
$$\underset{\mathcal{S}\subset\mathcal{V}}{\operatorname{argmin}} \sum_{v\in\mathcal{V}} \left(P'_{v,c_{\text{old}}} - \max_{c\neq c_{\text{old}}} P'_{v,c}\right)$$

Assumption: the class with the second largest probability is is always an ideal target[3].

$$\underset{c\neq c_{\text{old}}}{\operatorname{argmax}}\, P'_{v,c} = \underset{c\neq c_{\text{old}}}{\operatorname{argmax}}\, P_{v,c} = c^*$$

2. Relaxing discrete constraint

Convert discrete variable into continuous form: $S \rightarrow A$



Removing node: full-zero row/column

Lagrange: full zero Sparsity

$$\mathcal{R}(A') = \lambda_1 \|A'\|_{2,1} + \lambda_2 \|A - A'\|_F$$

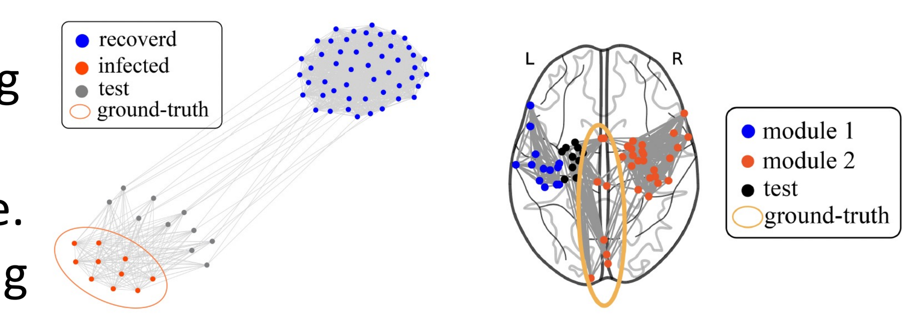
Final formulation of GGUN: $\underset{\mathcal{S}\subset\mathcal{V}}{\operatorname{argmin}} \sum_{v\in V} \left(P'_{v,c_{\text{old}}} - P'_{v,c^*}\right) + \mathcal{R}(A')$

Experiment Evaluation

We aim to support two claims: **Claim 1:** The nodes selected by GGUN influence the predictions in the graph more significantly than baselines. **Claim 2:** Explanations provided by GGUN are closer to the ground-truth.

Synthetic dataset generation

The rules of dataset generating can be regarded as ground-truths. **Case 1:** infected people. **Case 2:** critical hubs connecting 2 modules of neurons.



(a) **Case 1**: Disease spread (b) **Case 2**: Brain network

Quantitative analysis

Fidelity(F-prob) defines the difference between the original and the new predictions on the perturbed graph. GGUN achieve the best of F-Prob obviously.

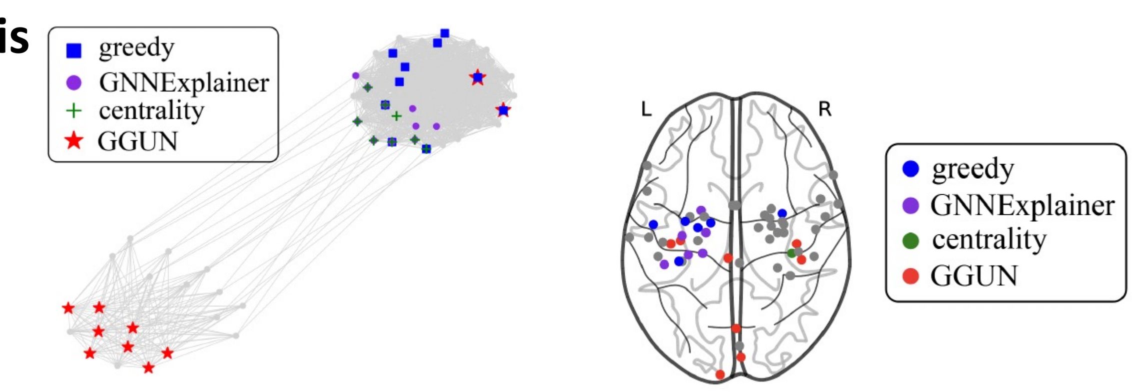
Accuracy(Acc) defines the selected node as a percentage of ground-truths. GGUN obtain 8/10 and 4/10 accuracy, while accuracy of baselines equal to 0.

	Synthetic 1		Synthetic 2	
Metrics	F-Prob	Acc	F-Prob	Acc
Ground-truth	0.7657	–	0.7443	–
Centrality	−0.6369	0/10	<u>0.5991</u>	0/8
CCM-Greedy	<u>0.1072</u>	0/10	−0.5226	0/8
GNNExplainer	−0.6396	0/10	0.5917	0/8
GGUN	**0.4288**	**8/10**	**0.6681**	**4/8**

- GNNExplainer is a well-established local explanation method, i.e., explain for one specific node
- CCM-Greedy is the greedy search of primal problem

Qualitative analysis

Only GGUN captures ground-truths successfully, while baselines fall into local optimum.



(a) **Case 1** result (b) **Case 2** result

Future work

In this work, we propose GGUN, a global graph understanding framework for identification of influential nodes in healthcare. Experimental results with visualizations on two synthetic datasets validate the superior explanatory performance of GGUN. In the near future, we plan to conduct experiments on more real world datasets with expert-annotated influential nodes. We should verify that GGUN is trustworthy before applying it to high-stakes healthcare cases.

References

[1] *KIPF, T. N., AND WELLING, M. Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907 (2016).*
[2] *RIBEIRO, M. T., SINGH, S., AND GUESTRIN, C. " why should i trust you?" explaining the predictions of any classifier. In Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining (2016), pp. 1135–1144.*
[3] *ZÜGNER, D., AKBARNEJAD, A., AND GÜNNEMANN, S. Adversarial attacks on neural networks for graph data. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (2018), pp. 2847–2856.*
[4] *YING, R., BOURGEOIS, D., YOU, J., ZITNIK, M., AND LESKOVEC, J. Gnnexplainer: Generating explanations for graph neural networks. Advances in neural information processing systems 32 (2019), 9240.*