EGNN for MI detection

Predicting and Interpreting Myocardial Infarction using Equivariant Graph Neural Networks

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Overview

1. **Introduction**
2. **Road to Equivariance**
3. **Interpretability**

The Problem

Predict Myocardial Infarction (MI)

- MI is a leading cause of death
- MI results from lesions in coronary arteries, but not all lesions lead to MI
- For patients suffering of cardio vascular disease, analyzing angiographies to predict MI is an expensive and time consuming task for experts

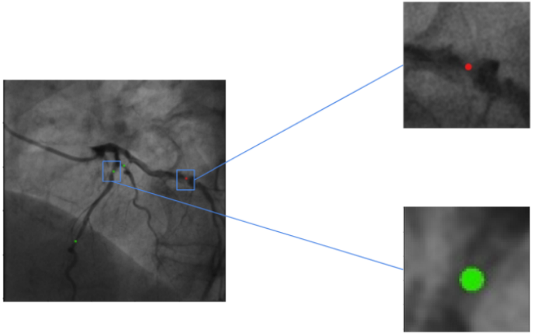

Figure: Example of patches (on the right) extracted from annotated angiography (on the left). Red and green color represents cultprit and non-culprit lesions respectively. Taken from [1].

Previous work at LTS4

- Using Deep Learning on images to predict MI [1]. Their method surpassed expert classification.
- Use of Graph Neural Networks to predict MI, also enriching data with computational fluid dynamics simulations. The model managed to fit the training data, but it overfitted a lot.

The Dataset

Personnalized 3D meshes

- 80 patients
- Reconstructions of up to three main arteries per patients
- Total of 188 data points, with 40% culprit, 60% non-culprit

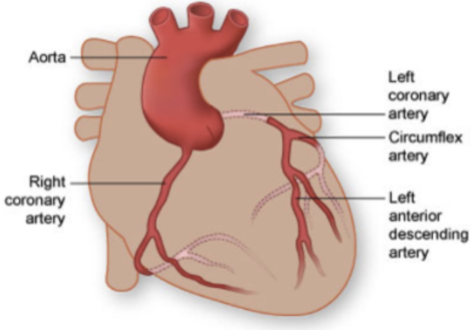

Figure: Model of a heart, with the three major arteries.

The Dataset (mathematical perspective)

Personnalized 3D meshes

- Each data point is a graph $G = (V, E)$ with triangles $T \subseteq E \times E \times E$
- Together with a coordinate map $c_G : V \to \mathbb{R}^3$

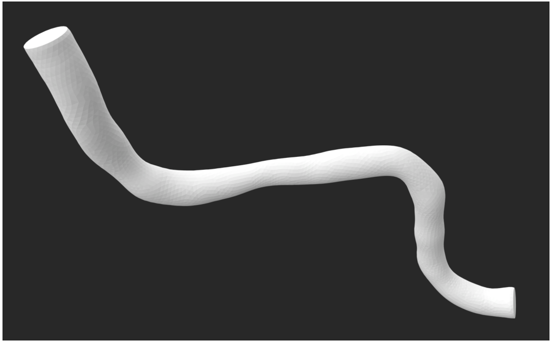

Figure: Example of a vessel reconstruction

Graph Neural Networks (GNNs)

Class of layers to treat signals on graphs
One GNN layer works as follows:

1. Each node receives a message from each of its neighbor
2. The received messages are aggregated (eg. summed)
3. The aggregate consists of the node's new feature

Equivariance

Why equivariance?

- Robustness: otherwise small rotations of the mesh can change the predicted class
- It is believed that equivariance fights the curse of dimensionality!
- GNNs equivariant to rotations and translations have recently been developed [2]

Definition

Let M be a $n \times n$ matrix, we say that $f : \mathbb{R}^n \to \mathbb{R}^n$ is *equivariant* with respect to M if $f(M \cdot \mathbf{x}) = M \cdot f(\mathbf{x})$ for all $x \in \mathbb{R}^n$.
It is invariant w.r.t. M if $f(M \cdot \mathbf{x}) = f(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^n$.
We say f is equi/in-variant to a set of matrices $\mathbb{T}$ if f is equi/in-variant w.r.t. M for all $M \in \mathbb{T}$

$E(n)$-Equivariant GNN

$$\mathbf{m}_{ij} = \phi_e \left(\mathbf{h}_i^l, \mathbf{h}_j^l, \left\|\mathbf{x}_i^l - \mathbf{x}_j^l\right\|^2, a_{ij}\right) \tag{3}$$

$$\mathbf{x}_i^{l+1} = \mathbf{x}_i^l + C \sum_{j \neq i} \left(\mathbf{x}_i^l - \mathbf{x}_j^l\right) \phi_x \left(\mathbf{m}_{ij}\right) \tag{4}$$

$$\mathbf{m}_i = \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij} \tag{5}$$

$$\mathbf{h}_i^{l+1} = \phi_h \left(\mathbf{h}_i^l, \mathbf{m}_i\right) \tag{6}$$

Figure: Equivariant layer defining equations from [2]

- at each stage, each node have an invariant feature (h), and an equivariant feature (x) (coordinates).
- (3) is the (invariant) message from i to j
- (4) is the (equivariant) coordinate update
- (5) is the aggregation
- (6) is the updated (invariant!) feature
- Each of ϕ_e, ϕ_x and ϕ_h are deep neural networks

Experiments

- Trained the original network using dataset augmented by 4 rotations ($\times 5$ dataset)
- Trained a model which has an equivariant architecture
- Augmented dataset with 5-nearest neighbour of each datapoint when considered as point cloud ($\times 2$ dataset)
- Augmented dataset with Gaussian noise at the coordinate level ($\times 2$ dataset)

Results

- Each model is trained with cross entropy loss, and Adam optimizer.
- We performed a 10-fold cross validation to tune hyper-parameters (including number of layers), and evaluated them on a test set 10 times with same train/validation split.

	Accuracy	Sensitivity	Specificity	f1-score
GIN	0.49 ± 0.05	0.47 ± 0.30	0.51 ± 0.40	0.38 ± 0.24
GIN_4Rot	0.63 ± 0.08	0.62 ± 0.13	0.65 ± 0.15	0.59 ± 0.10
Equiv_Gaussian	0.78 ± 0.10	0.85 ± 0.01	0.69 ± 0.14	0.72 ± 0.13
EquivGIN	0.81 ± 0.11	0.91 ± 0.12	0.66 ± 0.24	0.72 ± 0.18
Equiv_KNN5	0.82 ± 0.09	0.88 ± 0.07	$0.73 \pm 0.0.18$	0.76 ± 0.14

GNNExplainer

- GNNExplainer [3] is an interpretability framework that can be applied to any (graph) neural network
- It learns a mask of the graph, where important nodes are given high values
- It maximizes the mutual information:

$$I(Y, G_S) = H(Y) - H(Y|G = G_S), \tag{1}$$

  where Y is the target probability, G_S is a subgraph
- We compare this to the precise location of the lesion

GNNExplainer: Generating Explanations for Graph Neural Networks

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Results

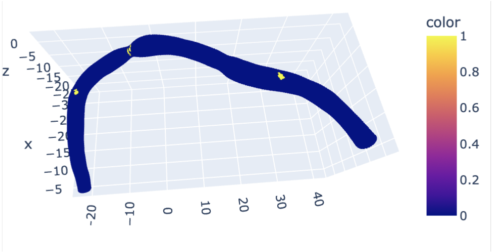

Figure: Importance mask output by GNNExplainer. 1 means important, 0 means unimportant

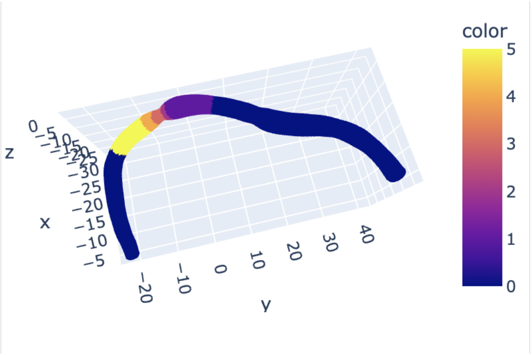

Figure: Expert mask, 1 is upstream from lesion, 2 is proximal part, 3 is mid part, 4 is distal part, 5 is downstream, 6 is rest of vessel

Results

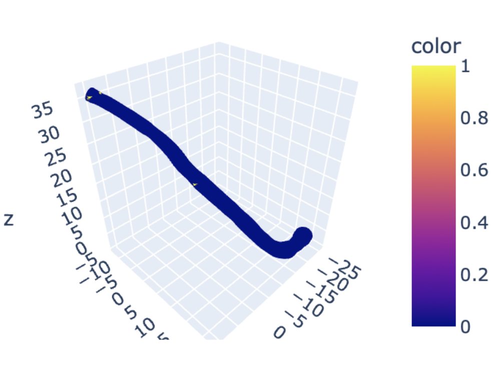

Figure: Importance mask output by GNNExplainer. 1 means important, 0 means unimportant

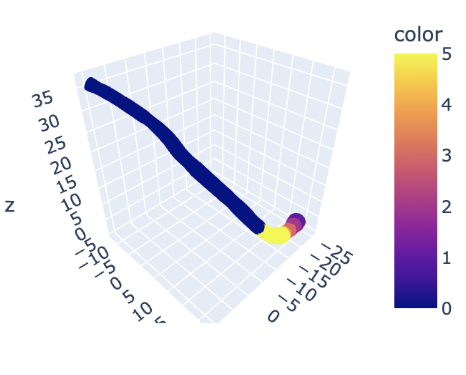

Figure: Expert mask, 1 is upstream from lesion, 2 is proximal part, 3 is mid part, 4 is distal part, 5 is downstream, 6 is rest of vessel

Results

- No statistically significant pattern was identified of the 18 (out of 19) positively predicted test samples
- 15 of them had an abnormal amount of important node in the 'rest' region. Many important nodes were in fact close to the boundary of the surface
- 10 of them had an abnormal amount of important nodes in the 'mid' part!

Conclusion and Future Work

- We demonstrated how graph neural networks and principles from geometric deep learning can provide robust and data efficient ways of solving medical problems that are hard and expensive for humans to do
- We tried to interprete our model
- There are many, many future directions this project can go into!

References

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The End