Graph Neural Processes

Towards Bayesian Graph Neural Networks

Andrew Carr

Perception, Control, and Cognition Lab

Table of contents

Introduction

Problem

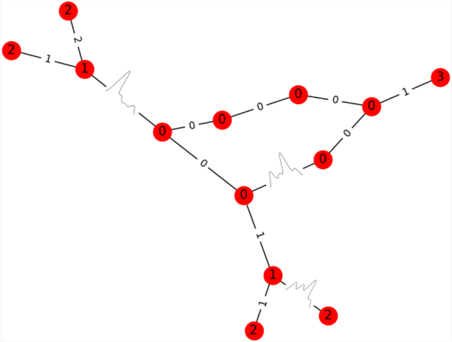
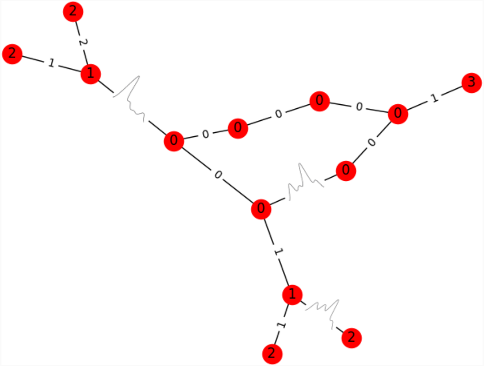


Figure 1: Graph with imputed edge distributions

Problem



$$G = (a, V, E)$$

$$V = \{v_i\}_{i=1:N^v}$$

$$E = \{e_k, v_k, u_k\}_{k=1:N^e}$$

Motivation

- Visual scene understanding
- Few-shot learning
- Learning dynamics of physical systems
- Traffic prediction
- Multi-agent systems
- Natural language processing
- semi-supervised text classification

Background

Graph Neural Networks

- Operate on Graph Structured Input

Graph Neural Networks

- Operate on Graph Structured Data
- Neural Operations on Graphs (e.g., spectral convolution)

Use Eigeninformation from traditional Graph Laplacian to perform convolution

$$L = D - A$$

Graph Neural Networks

- Operate on Graph Structured Input
- Neural Operations on Graphs (e.g., spectral convolution)
- Fixed sized input

Graph Neural Networks

- Operate on Graph Structured Input
- Neural Operations on Graphs (e.g., spectral convolution)
- Fixed sized input
- Difficult to scale

Graph Neural Networks

- Operate on Graph Structured Input
- Neural Operations on Graphs (e.g., spectral convolution)
- Fixed sized input
- Difficult to scale
- No measure of uncertainty

Conditional Neural Processes

$$P(Y_T|X_T, X_C, Y_C) \iff P(Y_T|X_T, r_C)$$

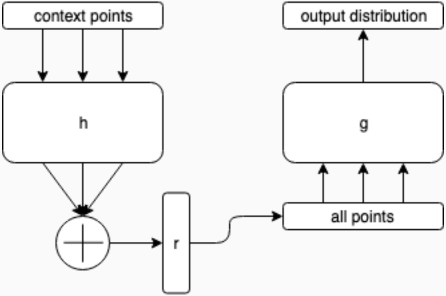
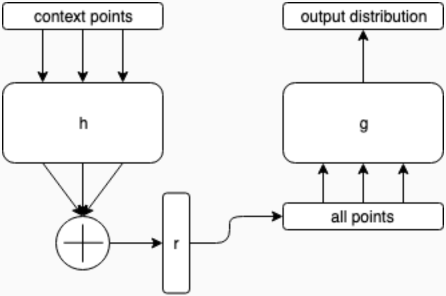


Figure 2: Conditional Neural Process Architecture

Conditional Neural Processes



$$r_i = h_\theta(\vec{x_i}) \qquad \forall \vec{x_i} \in X_C \tag{1}$$

$$r_C = r_1 \oplus r_2 \oplus r_3 \oplus \cdots \oplus r_n \tag{2}$$

$$z_i = g_\phi(\vec{y_i} | r_C) \qquad \forall \vec{y_i} \in X_T \tag{3}$$

Conditional Neural Processes

- Flexible

Conditional Neural Processes

- Flexible
- Scalable

Conditional Neural Processes

- Flexible
- Scalable
- Measures uncertainty

Our Method

Graph Neural Processes

- Conditional Neural Process on Graphs

Graph Neural Processes

- Conditional Neural Process on Graphs
- Edges are context points

Graph Neural Processes

- Conditional Neural Process on Graphs
- Edges are context points
- Spectral Features

Features

Normalized Symmetric Graph Laplacian

$$L = I_n - D^{-1/2} A D^{-1/2}$$

$$\Lambda = \sigma(L)$$

Features

Take the eigenvectors of the graph laplacian and select the first k to obtain the local spectral eigen features

$$\Lambda|_k = (\Lambda_{kj})_{\substack{k \in r \\ 1 \leq j \leq m}}$$

Features

Or, more clearly

$$\Lambda|_k = (\Lambda_{kj})_{\substack{k \in r \\ 1 \leq j \leq m}}$$

```
def get_local_spectral_eigen_features(G, ind, k):
    """
    G - graph (networkx graph)
    ind - location of the context point edge in the adjacency matrix
    k - hyperparameter tuned based on the size of the input graphs in X_C
    """
    A = nx.adjacency_matrix(G).toarray()
    N = A.shape[0]

    diags = A.sum(axis=1)**(-1/2)
    D = scipy.sparse.spdiags(diags.flatten(), [0], N, N, format='csr').toarray()

    L = np.eye(N) - D.dot(A).dot(D) # calculate normalized graph laplacian
    val, vec = np.linalg.eig(L)

    return vec[ind][:k]
```

Features

Additionally the value and degree of each node on the edge are used as features

Algorithm

How does it work?

Algorithm Walk Through

Let X input graphs
for $t = 0, \cdots, n_{\text{epochs}}$ **do**
  for x_i in X **do**
    Sample $p \leftarrow \text{unif}(p_0, p_1)$
    Assign $n_{\text{context points}} \leftarrow p \cdot |\text{Edges}(x_i)|$
    Sparsely Sample $x_i^{cp} \leftarrow x_i|_{n_{\text{context points}}}$
    Compute degree and adj matrix D, A for graph x_i^{cp}
    Compute $L \leftarrow I_{n_{\text{context points}}} - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$
    Define F^{cp} as empty feature matrix for x_i^{cp}
    Define F as empty feature matrix for full graph x_i
    for edge k in x_i **do**
      Extract eigenfeatures $\Lambda|_k$ from L
      Concatenate $[\Lambda|_k; v_k; u_k; d(v_k); d(u_k)]$ where v_k, u_k are the attribute values at the node, and $d(v_k), d(u_k)$ the degree at the node.
      if edge $k \in x_i^{cp}$ **then**
        Append features for context point to F^{cp}
      end if
      Append features for all edges to F
    end for
    Encode and aggregate $r_C \leftarrow h_\theta(F^{cp})$
    Decode $\tilde{x}_i \leftarrow g_\phi(F|r_C)$
    Calculate Loss $l \leftarrow \mathcal{L}(\tilde{x}_i, x_i)$
    Step Optimizer
  end for
end for

Experiments

16 Datasets

Dataset	$\|X\|$	$\|\bar{N}\|$	$\|\bar{E}\|$	$\|\cup \{e_k\}\|$
AIDS	2000	15.69	16.20	3
BZR_MD	306	21.30	225.06	5
COX2_MD	303	26.28	335.12	5
DHFR_MD	393	23.87	283.01	5
ER_MD	446	21.33	234.85	5
Mutagenicity	4337	30.32	30.77	3
MUTAG	188	17.93	19.79	4
PTC_FM	349	14.11	14.48	4
PTC_FR	351	14.56	15.00	4
PTC_MM	336	13.97	14.32	4
Tox21_AHR	8169	18.09	18.50	4
Tox21_ARE	7167	16.28	16.52	4
Tox21_aromatase	7226	17.50	17.79	4
Tox21_ARLBD	8753	18.06	18.47	4
Tox21_ATAD5	9091	17.89	18.30	4
Tox21_ER	7697	17.58	17.94	4

Table 1: Features of the explored data sets

Results

Results

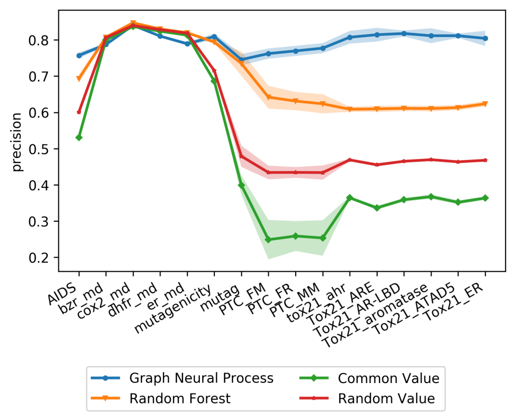


Figure 3: Experimental precision graph compared with baselines, we see our method performs achieves a $\sim .2$ higher precision on average.

Results

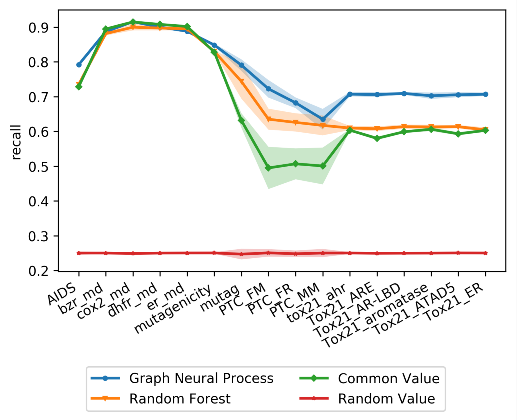


Figure 4: Experimental recall graph compared with baselines

Results

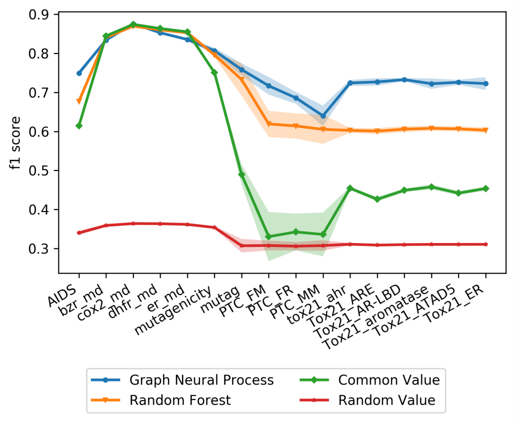


Figure 5: Experimental F1-score graph compared with baselines.

Results

Dataset	RF			RV			CV			GNP		
	P	R	F1	P	R	F1	P	R	F1	P	R	F1
AIDS	0.69	0.74	0.68	0.60	0.25	0.34	0.53	0.73	0.61	**0.76**	**0.79**	**0.75**
bzr_md	**0.81**	0.88	**0.84**	0.81	0.25	0.36	0.80	**0.89**	0.84	0.79	**0.89**	0.83
cox2_md	**0.85**	0.90	0.87	0.84	0.25	0.36	0.84	0.91	0.87	0.84	**0.92**	**0.88**
dhfr_md	**0.83**	0.90	0.86	**0.83**	0.25	0.36	0.82	**0.91**	0.86	0.81	0.90	**0.85**
er_md	0.82	**0.90**	0.85	0.82	0.25	0.36	0.81	**0.90**	**0.86**	0.79	0.89	0.84
mutagenicity	0.79	0.83	0.80	0.72	0.25	0.35	0.69	0.83	0.75	**0.81**	**0.85**	**0.81**
mutag	**0.73**	0.74	0.73	0.48	0.25	0.31	0.40	0.63	0.49	**0.75**	**0.79**	**0.76**
PTC_FM	0.64	0.64	0.62	0.43	0.25	0.31	0.25	0.50	0.33	**0.76**	**0.72**	**0.72**
PTC_FR	0.63	0.63	0.61	0.43	0.25	0.31	0.26	0.51	0.34	**0.77**	**0.68**	**0.69**
PTC_MM	0.62	0.62	0.61	0.43	0.25	0.31	0.25	0.50	0.34	**0.78**	**0.64**	**0.64**
tox21_ahr	0.61	0.61	0.60	0.47	0.25	0.31	0.36	0.60	0.45	**0.81**	**0.71**	**0.72**
Tox21_ARE	0.61	0.61	0.60	0.46	0.25	0.31	0.34	0.58	0.43	**0.81**	**0.71**	**0.73**
Tox21_AR-LBD	0.61	0.61	0.61	0.47	0.25	0.31	0.36	0.60	0.45	**0.82**	**0.71**	**0.73**
Tox21_aromatase	0.61	0.61	0.61	0.47	0.25	0.31	0.37	0.61	0.46	**0.81**	**0.70**	**0.72**
Tox21_ATAD5	0.61	0.61	0.61	0.46	0.25	0.31	0.35	0.59	0.44	**0.81**	**0.71**	**0.73**
Tox21_ER	0.62	0.60	0.60	0.47	0.25	0.31	0.36	0.60	0.45	**0.80**	**0.71**	**0.72**

Table 2: Experimental Results. RF=Random Forest; RV=Random edge label; CV=most common edge label; GNP=Graph Neural Process. P=precision; R=recall; F1=F1 score. Statistically significant bests are in bold with non-significant ties bolded across methods.

References i

See https://arxiv.org/abs/1902.10042 for complete list of references