

# Learning from Counterfactual Links for Link Prediction

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Course Project : CS768

October 26, 2023

# Running The Code

Due to computational requirements we resorted to running the code on Google Colab. However to satisfy the requirements we had to downgrade Colab's python version to 3.8.10 and CUDA to 10.2. These were required for torch v1.6.0 as higher versions of torch and corresponding PyG libraries had deprecation issues.

The accompanying Colab file is linked [CS768.ipynb](#)

# Datasets

The code was tested on 5 datasets namely

- Cora
- CiteSeer
- Facebook
- PubMed
- OBG-DDI

The primary metrics used were

- AUC Score
- Hits@20

# CiteSeer Dataset

	<b>Reported</b>	<b>Calculated (Frobenius)</b>	<b>Calculated (KL)</b>
AUC	$0.9212 \pm 0.0047$	$0.9336 \pm 0.0044$	$0.9328 \pm 0.0044$
AP	$0.9392 \pm 0.0041$	$0.9461 \pm 0.0038$	$0.9456 \pm 0.0035$
Hits@20	$0.6809 \pm 0.0149$	$0.6996 \pm 0.0278$	$0.6984 \pm 0.0181$
Hits@50	$0.7701 \pm 0.0192$	$0.7974 \pm 0.0149$	$0.7934 \pm 0.0135$
Hits@100		$0.8490 \pm 0.0135$	$0.8497 \pm 0.0120$
Best Val		$0.9474 \pm 0.0030$	$0.9464 \pm 0.0044$

# Cora Dataset

	<b>Reported</b>	<b>Calculated (Frobenius)</b>	<b>Calculated (KL)</b>
AUC	$0.9305 \pm 0.0024$	$0.9320 \pm 0.0036$	$0.9328 \pm 0.0031$
AP	$0.9424 \pm 0.0028$	$0.9440 \pm 0.0026$	$0.9441 \pm 0.0022$
Hits@20	$0.6557 \pm 0.0105$	$0.6383 \pm 0.0184$	$0.6293 \pm 0.0217$
Hits@50	$0.7549 \pm 0.0154$	$0.7537 \pm 0.0109$	$0.7510 \pm 0.0144$
Hits@100		$0.8360 \pm 0.0068$	$0.8364 \pm 0.0083$
Best Val		$0.9386 \pm 0.0027$	$0.9377 \pm 0.0035$

# Results and Inferences

The differences in reported and evaluated results can be attributed towards hardware differences. Google Colab used by us utilized Nvidia T4 GPU with 15 GB of system and GPU RAM. The original code was evaluated on a Linux server with Intel Xeon Gold 6130 Processor (16 Cores @2.1Ghz), 96 GB of RAM, and 4 RTX 2080Ti cards (11 GB of RAM each)

Calculated results were higher for all instances except Hits@20 and Hits@50 for Cora. for Cora, calculated value for Hits@50 were slightly less but well within the standard deviation reported. The mean for Hits@20 was deviated from the reported figure by more than 1 standard deviation.

# Results and Inferences

As part of our contributions we included KL Divergence Loss for  $\mathcal{L}_{disc}$ . There aren't significant differences in taking Frobenius norm and KL Divergence. Although train time for KL Divergence was lesser than Frobenius Norm by a factor of 16% for CiteSeer and 25% for Cora

	<b>Frobenius</b>	<b>KL</b>
Cora	62min.	46 min.
CiteSeer	92min.	77 min.

# Other Datasets

PubMed Dataset failed to load in Google Colab's memory due to a significantly higher count of nodes (19717 vs 3327 for CiteSeer) which led to significantly larger node embedding matrix. Hence the code was auto-killed.

For Facebook and OBG-DDI, Colab was able to load the data however computation was time-taking due to high number of links (88234 for Facebook, 1334889 for OBG-DDI vs 5278 for Cora) which led to Colab crashing on several accounts and running out of memory during execution



# Attempts Made

After communicating the problems faced with Colab we were allotted DGX9 server at IITB for computation. However we faced challenges with it. The server has CUDA 11.4 drivers and the code is compatible with torch v.1.6.0 and accompanying PyG libraries which required CUDA 10.2 or lower. Upgrading library versions to those compatible with CUDA 11.4 was infeasible due to dependency issues and deprecation issues

We tried downgrading to CUDA version but were unsuccessful due to lack of root access due to which we couldn't install CUDA 10.2