

# Reproducibility Project: CS598: Pre-training of Graph Augmented Transformers for Medication Recommendation (G-BERT)

Unnati Hasija / Prateek Dhiman Team 15 MCS DS - UIUC

## Content

- Key Tasks and Ablations
  - Replicating and Retraining G-BERT
  - Baseline Comparison
  - Transformer Architecture
  - Feasibility with GPT : New Model provided GGPT
- Achievements
- GGPT Approach and Architecture

# Key Tasks and Ablations

1. GBERT : Replication With as near accuracy and KPIs and Retraining On local machines and Azure VMs • Verify performance claims 2. Baseline Comparison With LR / LEAP/ RETAIN/GRAM / GAMENet 3. Transformer • Impact with changing graphs model and attention mechanism (GAT-> GCN and GAT->GTN) • Impact with Aggregation functions: (add-> mean) **Architecture** • Impact with change in hyperparameters 4. GGPT : Feasibility & • Initial research and feasibility of replacing BERT with GPT2 **Extension of GBERT** • Provision of new Model called GGPT.

## Achievements

- Successfully completed all tasks including hypotheses and ablations.
- Replication completed with Near accuracy with training on local CPU machine and Azure Virtual Machines.
- Verified GBERT Claims and the original ablations in the paper.
- Extended GBERT with GGPT in a matter of few weeks with a potential of fine-tuning and performance improvements.

#### **GBERT**: Replication and Retraining Success

After training and building a new model achieved:

- 99.46% of PR AUC
- 99.13% of F1 Score
- 99.13% of Jaccard Score

#### Baseline Comparison

- Gbert performs better with graphs and pre-training.
- Gbert performs better than Retain, GAMENet.

#### Transformer Architecture

- Working code for GCNConv and GTNConv to replace GAT for ablations.
- Working code aggregation and activation functions.
- Hyperparameter changing.
- Improved baseline GBERT KPIs F1 by 0.52%, PR AUC by 0.39%, Jaccard by 0.56% in our experimental setup via ablations

#### **GGPT**: Feasibility & Extension of GBERT

New Model built on similar lines as GBERT: GNN+ GPT2: GGPT

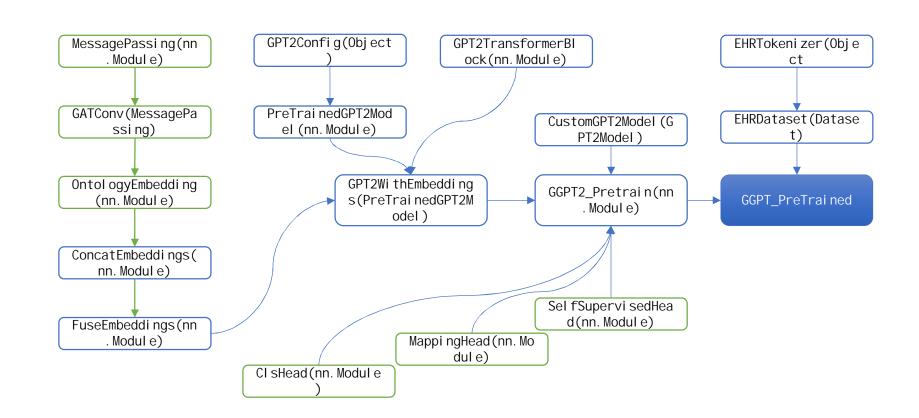
#### New proposed model:

# GGPT Approach and Architecture

Ontology Embedding

GPT2

Fine-Tuned Classifier

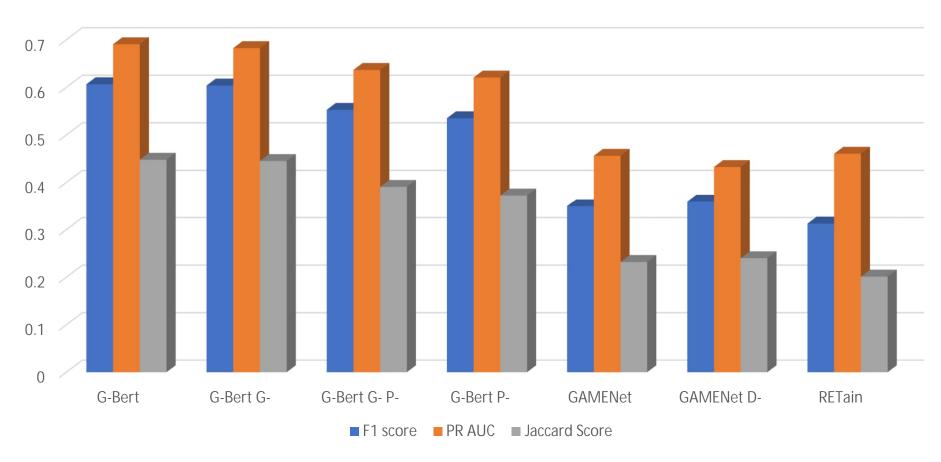


Original Code

Adapted / New Code

## Baselines





## Ablations to G-Bert

