CS 520 Causal Inference and Learning

# Benchmarking Causal Discovery Algorithms on Medical Data

Colliders

Giuseppe Concialdi, Judhajit Roy, Vaibhav Jolly, Aditya R

# Motivation

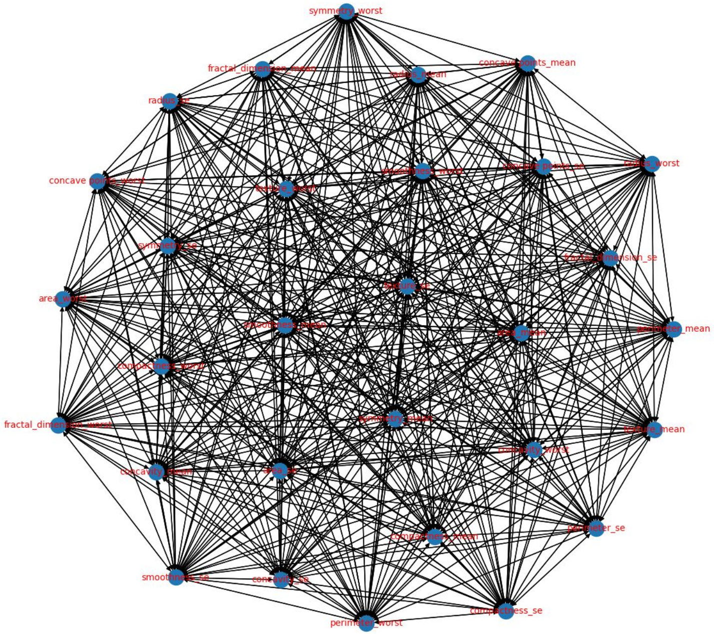
- Identify and validate the causal relationships between variables in medical datasets
- Benchmarking and assess the performance of several causal discovery algorithms
- Explore and compare classic causal discovery algorithms with recent deep-learning based approaches

## What is causal discovery?

Causal discovery is the task of identifying the causal relationships among a set of variables

# Proposed approach

- We explored several causal discovery algorithms:
    - **PC**
    - **GES**
    - **LiNGAM**
    - **NOTEARS**
    - **SAM**
    - **CGNN**
- Each algorithm perform some assumptions on the nature of the underlying data



# Proposed approach

Classic discovery algorithms

PC

GES

LiNGAM

- Conditional independence testing
- Greedy search of DAG space
- Exploiting asymmetry and linearity

- Hybrid techniques
- Few assumption about the data
- Requires large dataset

NOTEARS

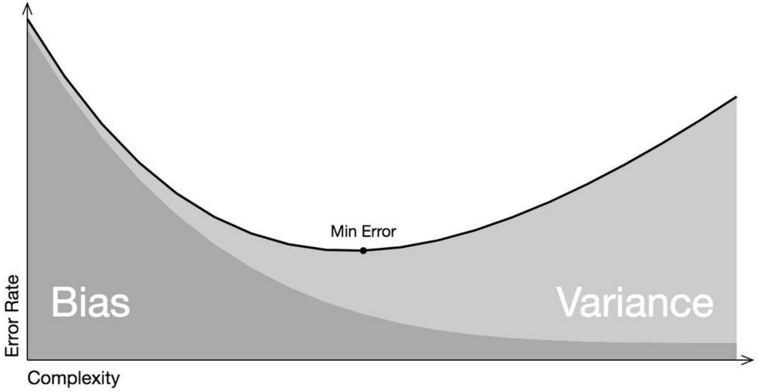
SAM

CGNN

Recent discovery algorithms

# Proposed approach

- **Unconstrained models**
  - The algorithm is applied directly on the data
  - Better predictions
  - Risk of overfitting the dataset
  - Slower evaluation
- **Constrained models**
  - The prediction is performed on top of the regularized data
  - Lower performance
  - Faster evaluation
  - Greater generalization



# Datasets

## Wisconsin Breast Cancer Dataset

- From UCI repository and contains 569 datapoints and 32 attributes.
- Features: Area, Texture and categorical columns like Diagnosis, which contains 357 Benign and 212 Malignant instances.

## Thyroid Dataset

- Also from UCI repository and contains 3500+ datapoints
- Features: hyperthyroid and hypothyroid conditions,  age, sex, sick, pregnant, tumor, TSH, T3, T4, etc

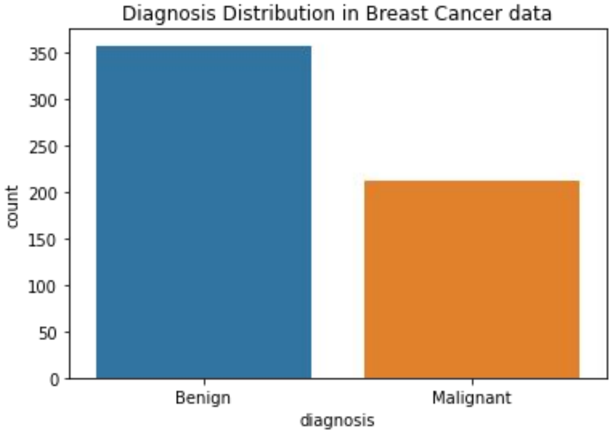
## Cardiovascular Disease Dataset

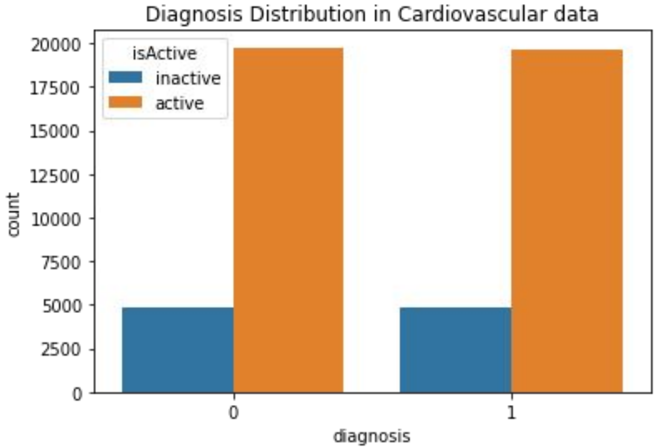
- Open-source large dataset on Kaggle. Contains 70,000 patient records and 11 features
- 34,979 patients are diagnosed with cardiovascular disease, and 35,021 are not.

# Data Exploration

Data pre-processed for all datasets:

- Irrelevant columns dropped, and missing data either replaced or removed
- Data was scaled in all datasets to ensure better graphical representation
- Labels encoded for categorical attributes like '*diagnosis*', '*gender*' and '*referral source*'

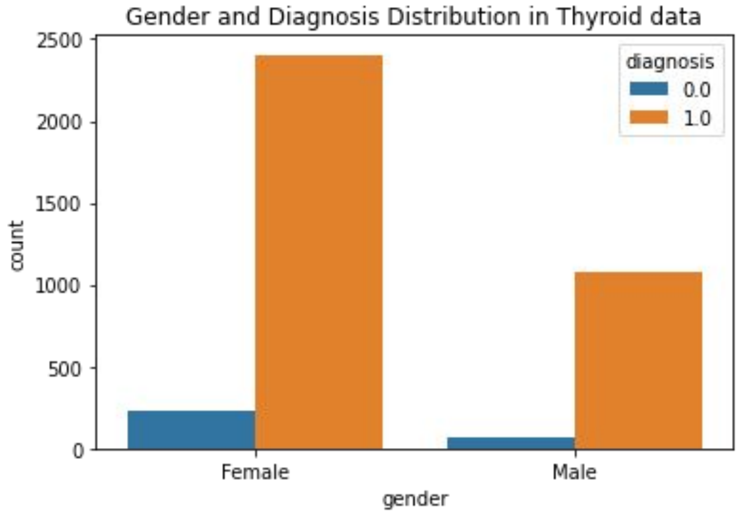


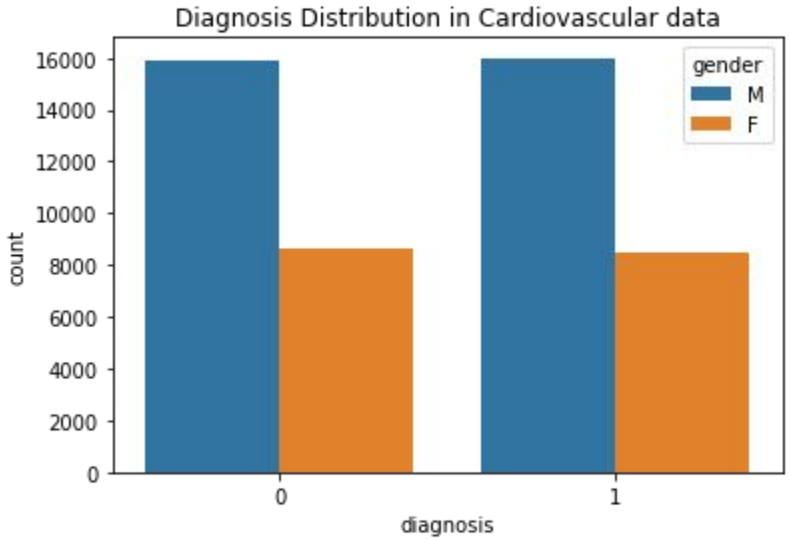



# Data Exploration

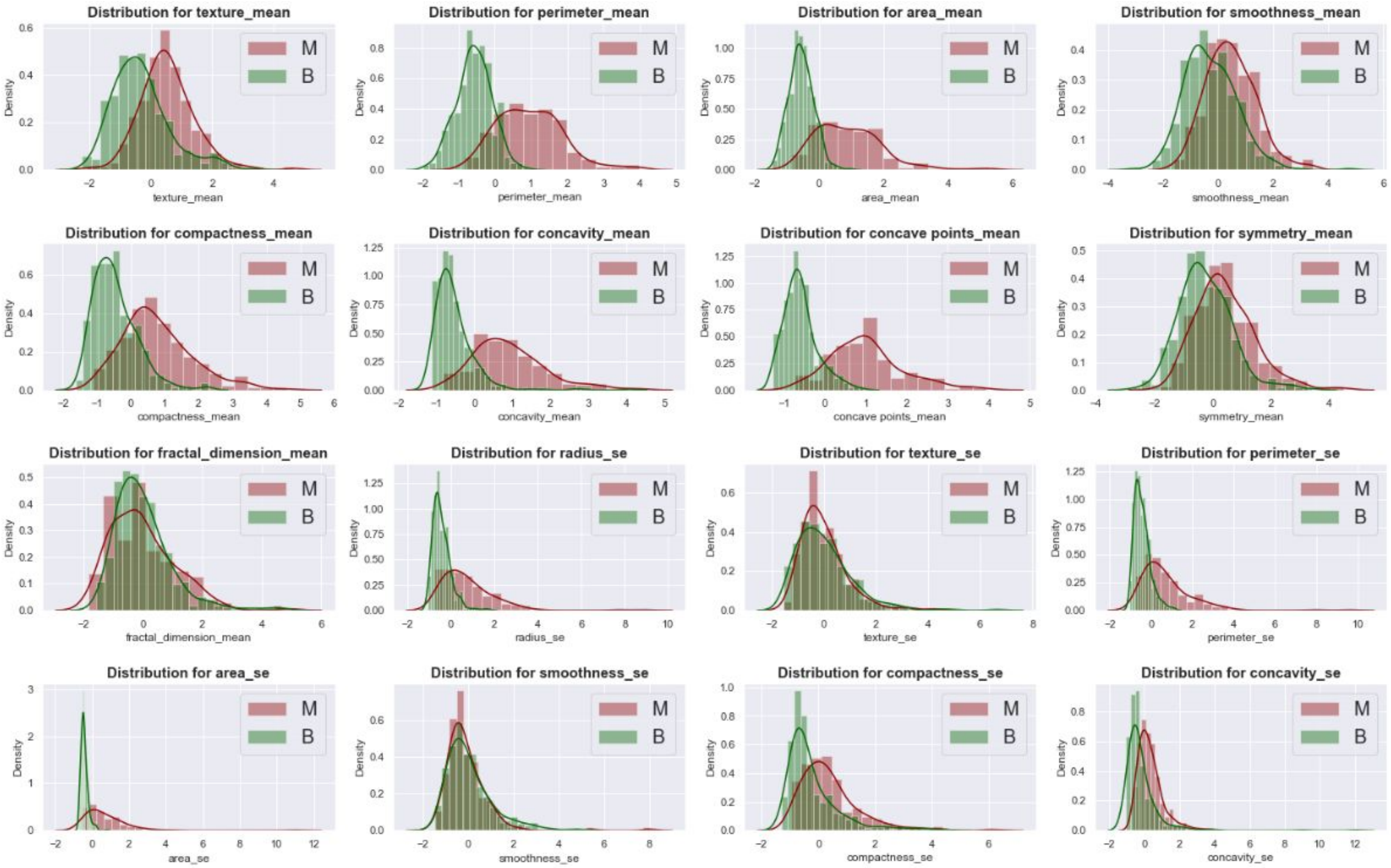
Interesting insights observed in each of the data sets:

- More positive thyroid outcomes observed among females than males
- The attributes in the cardiovascular data were mostly categorical/binary in nature
- There is no class imbalance in that dataset unlike the others

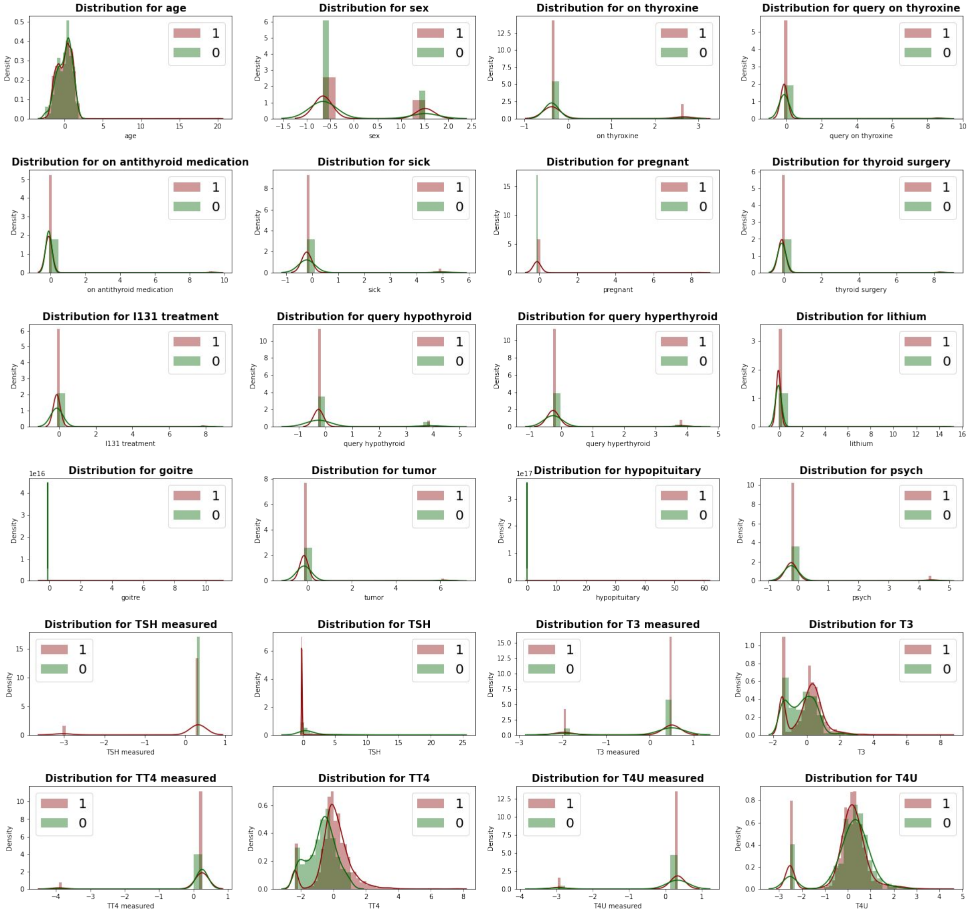


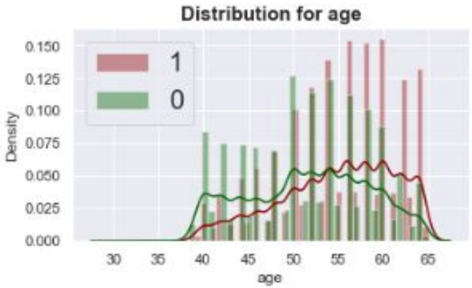
# Histogram of Attributes in Breast Cancer Dataset

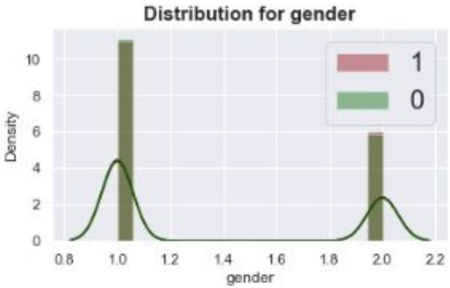


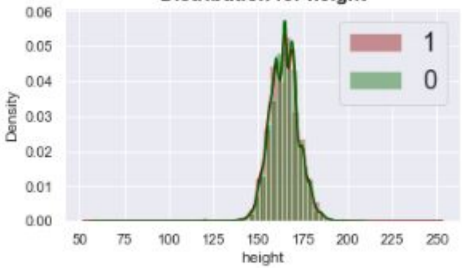
# Histogram of Attributes in Thyroid Dataset

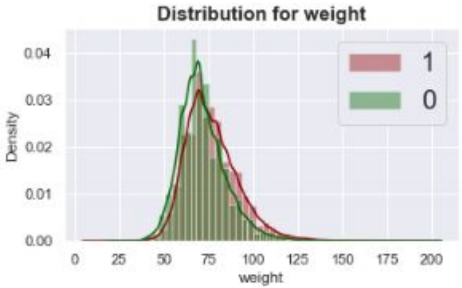


# Histogram of Attributes in Cardiovascular Disease Dataset



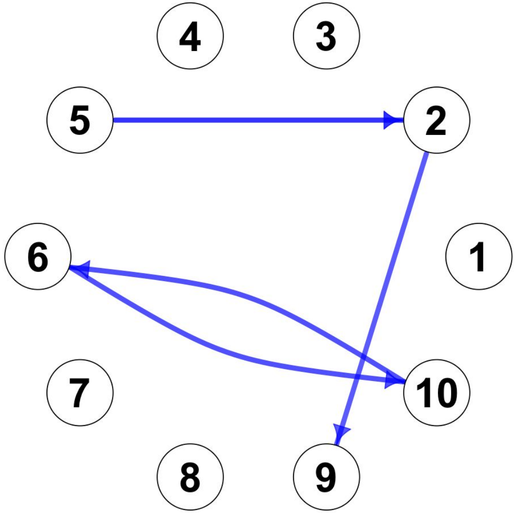



# Experiments

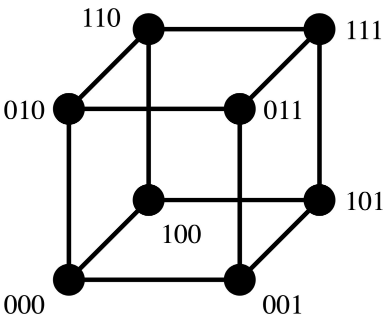
- Discovery of causal relations in medical-field datasets
- Validating causal structural models generated from various algorithms on medical data
- Understanding the relationships among the features and outcome
- Perform benchmarking using synthetic data on the various algorithms

# Synthetic data

- Data is generated in a controllable and flexible manner
- Easy to perform the evaluation of the causal algorithms
- Can misrepresent the complexity of the real-world data
- Inexpensive and easy to generate

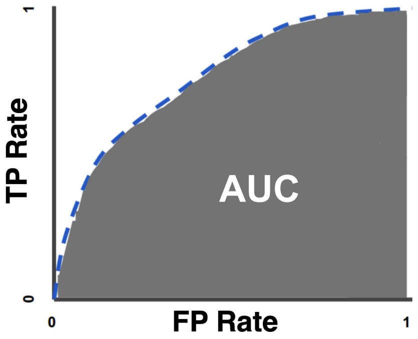


# Evaluation metrics



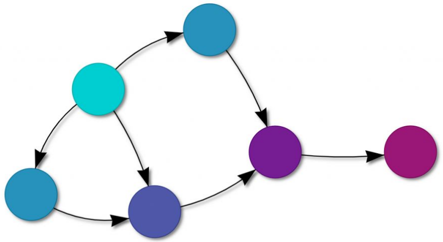

**Structural Hamming Distance**

This metric considers two directed acyclic graphs DAGs and counts how many edges do not coincide.




**Area Under ROC Curve**

Area under the curve of recall versus false positive rate (FPR) at different thresholds



**Bayesian Network Predictive Accuracy**

Models learned via causal discovery can be further used for multiple practical applications involving predictions

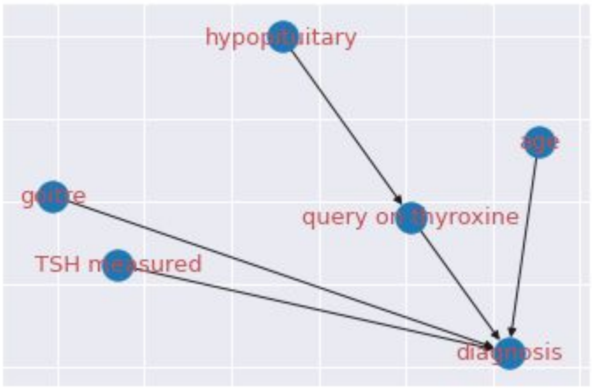
# Libraries and tools

- **Causal discovery toolbox** provides
  - A diverse pool of algorithms for causal discovery
  - Support for synthetic data generation
  - Several metrics for the evaluation of causal discovery
  - The API is entirely in Python
- **Causalnex** is a recent library that provides
  - Easy-to-use interface for causal discovery
  - Employs only the novel NOTEARS discovery algorithm

# Experiments on Medical Data

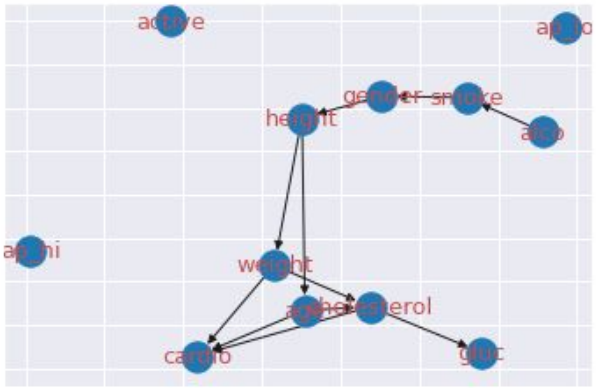
## Thyroid Dataset

- The most probable factors for **Thyroid** include: *Goitre, hypopituitary, thyroid surgery, TSH levels, pregnancy, age*
- The NOTEARS Causal Structure obtained show relationships between these factors and diagnosis



## Cardiovascular Dataset

- The most probable factors for **Cardiovascular** include: *Smoking, Alcohol Consumption, Inactivity, raised glucose levels*
- The Causal Structure is able to depict relationships for these factors

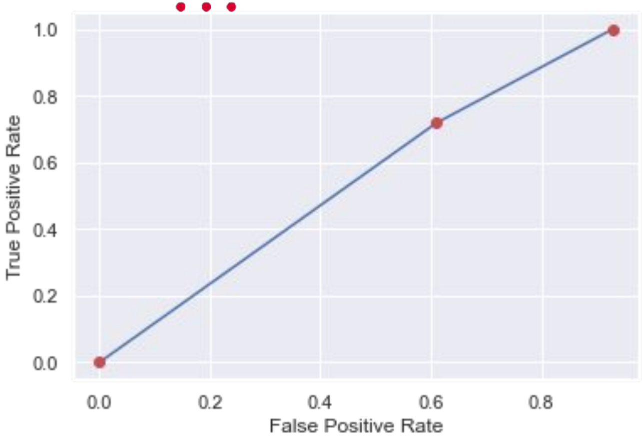


## Breast Cancer Dataset

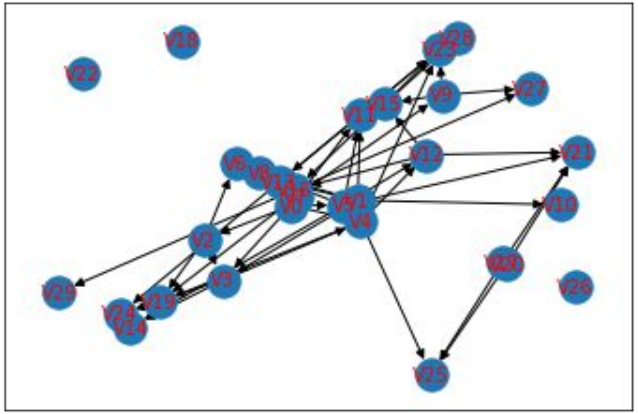
- Smaller dataset size affected causal inference
- Not many realistic relationships discovered

# Benchmark on Synthetic Data

- Causal Algorithms run on synthetic data and obtained Structure Hamming Distance and AUC
- SAM and CGNN, the deep learning based models have high hardware requirements
- This limited number of epochs for training

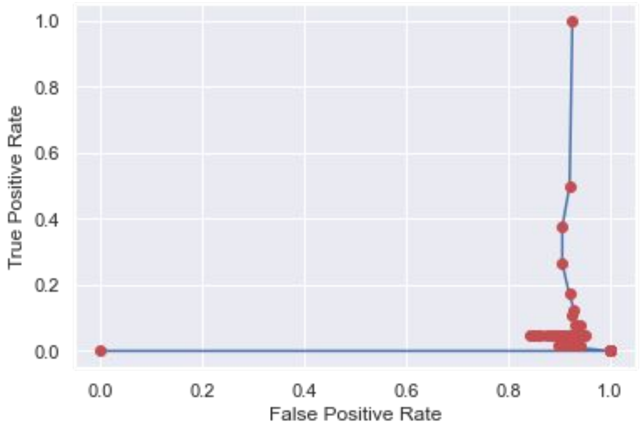


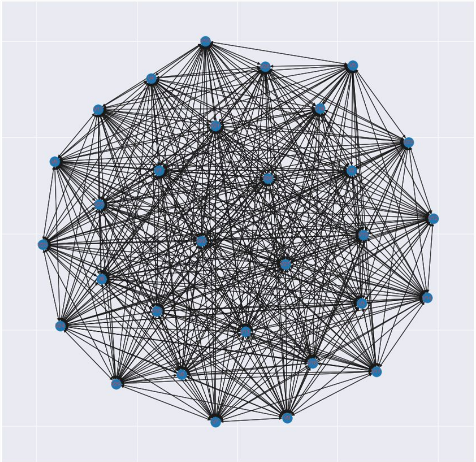

| Algorithm | SHD | AUC |
|---|---|---|
| **PC** | 75 | 0.367 |
| **GES** | 90 | 0.564 |
| **LiNGAM** | 127 | 0.289 |
| **SAM** | 806 | 0.080 |
| **NOTEARS** | 113 | 0.162 |
| **CGNN** | In progress | In progress |



# Benchmark on Synthetic Data

- Implemented the unconstrained versions of the algorithms to ensure fair experimental setup
- SAM shows the weakest performance due to model training for lesser epochs
- CGNN model was unable to converge due to stated hardware restrictions
- Edge threshold parameters needs to be explored in NOTEARS for better score



# Conclusions

From experiments using medical data, we infer and validate that:

- The Hybrid Causal Models perform better than the classical models in depicting representations

Through the benchmarking using synthetic data, we are able to show that

- GES gives the best model performance
- The model is able to draw a balance between the SHD and the AUC
- The SAM model shows potential in terms of performance with more training enough resources to compute the structure

# Challenges and Next Steps

- Limitations in hardware resources
- Difficulty in understanding causal structures due to large number of nodes and relations
- NN based models require more computation and training epochs to produce better results.
- Train/test CGNN and SAM for more epochs
- Validate results of medical causal structures, and implement constraints to reduce graph size and edges

# Thank you for your attention!

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