

# Disease Outcome Prediction Using Graph Auto-encoders

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# Motivation



Head and Neck Cancer<sup>1</sup>



Breast Cancer<sup>2</sup>



Cardiovascular disease<sup>3</sup>



Colorectal Cancer<sup>4</sup>



Lung Cancer<sup>5</sup>



Alzheimer's Disease<sup>6</sup>

<sup>1</sup> Reproduced from "Head and Neck Cancer is not Just a Smoker's Disease Anymore", Mount Sinai News. <sup>2</sup> S. Roan, "Early Stage Breast Cancer: Do You Really Need Your Lymph Nodes Removed?", Everyday Health. <sup>3</sup> "Conquering Cardiovascular Disease", NIH. <sup>4</sup> "Colorectal Cancers", Dr. Fuhrman. <sup>5</sup> K. O'Sullivan, "New drug approved for advanced lung cancer by HSE", The Irish Times. <sup>6</sup> M. Casalino, "Alzheimer's Association Offers Virtual Dementia Tour", Patch

## Motivation

- ▶ Traditionally: risk calculator for possibility of disease development.
- ▶ Framingham study: prediction for hospitalization for long-term cardiovascular disease

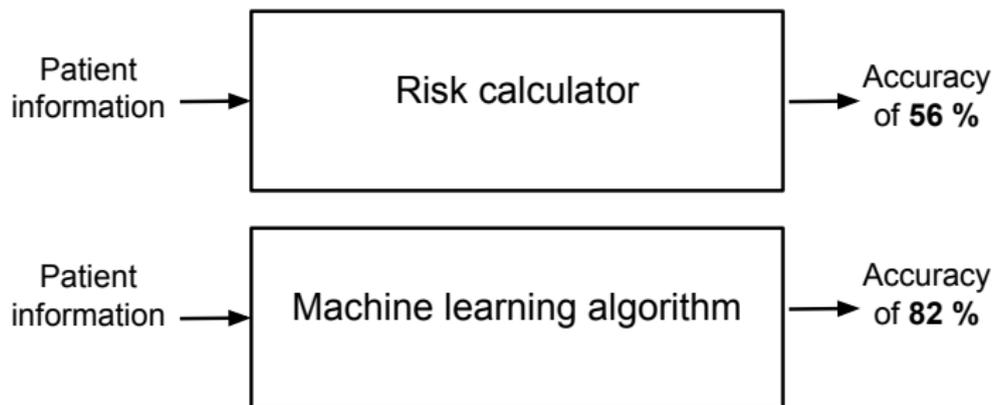
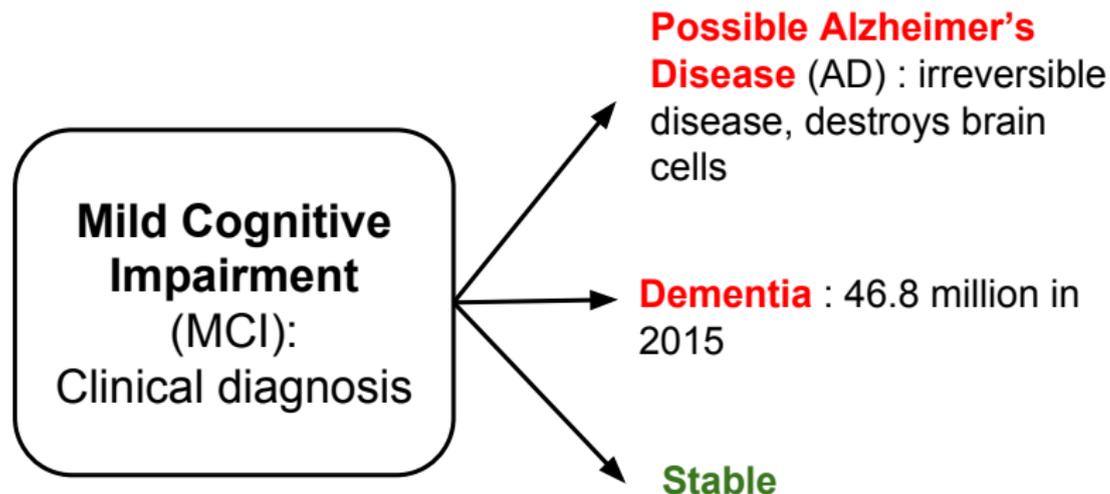


Figure 2: Comparison of a risk calculator and a machine learning algorithm<sup>7</sup>

<sup>7</sup>W. Dai et al., "Prediction of hospitalization due to heart diseases by supervised learning methods" Int. J. medical informatics, vol. 84, no. 3, pp. 189–197, 2015.

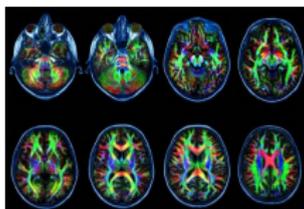
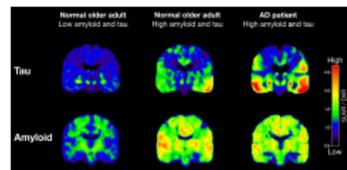
## Motivation



→ **Early and accurate diagnosis** for an early treatment to improve the quality of life for some time

# Goal

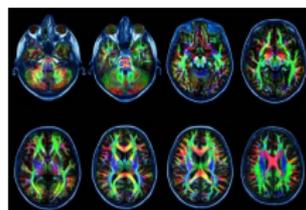
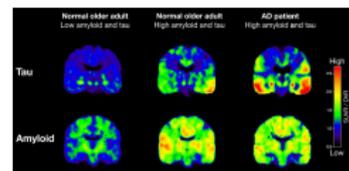
- ▶ Predict conversion from MCI to AD
- ▶ Multimodal data with missing values

(a) MRI<sup>8</sup>(b) DTI<sup>9</sup>(c) PET<sup>10</sup>

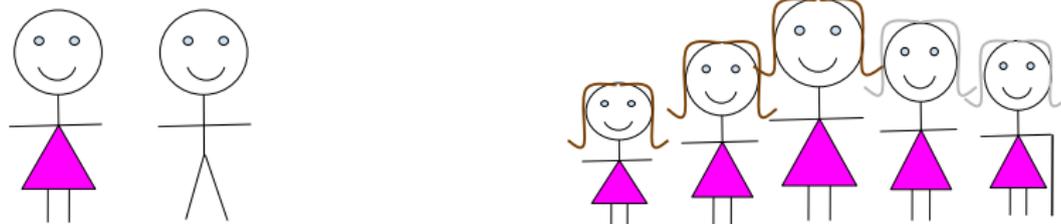
<sup>8</sup> Clinica developers, "Volume pre-processing - Clinica Documentation". <sup>9</sup> Rachel VanCott, "NOVA — scienceNOW — Diagnosing Damage image 3 — PBS". <sup>10</sup> University of California - Berkeley, "PET scans reveal key details of Alzheimer's protein growth in aging brains"

## Goal

- ▶ Predict conversion from MCI to AD
- ▶ Multimodal data with missing values

(a) MRI<sup>8</sup>(b) DTI<sup>9</sup>(c) PET<sup>10</sup>

- ▶ Use characteristics of subjects



<sup>8</sup> Clinica developers, "Volume pre-processing - Clinica Documentation". <sup>9</sup> Rachel VanCott, "NOVA — scienceNOW — Diagnosing Damage image 3 — PBS". <sup>10</sup> University of California - Berkeley, "PET scans reveal key details of Alzheimer's protein growth in aging brains"

# Problem formulation

- Deal with **missing values**
- Perform **classification**

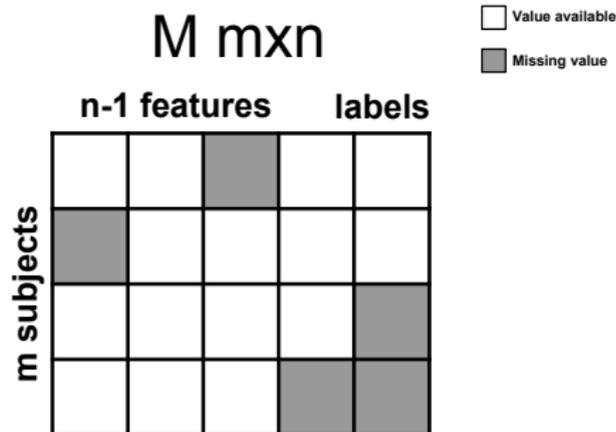
## Problem formulation

- Deal with **missing values**
- Perform **classification**
- Matrix completion
- Label as feature

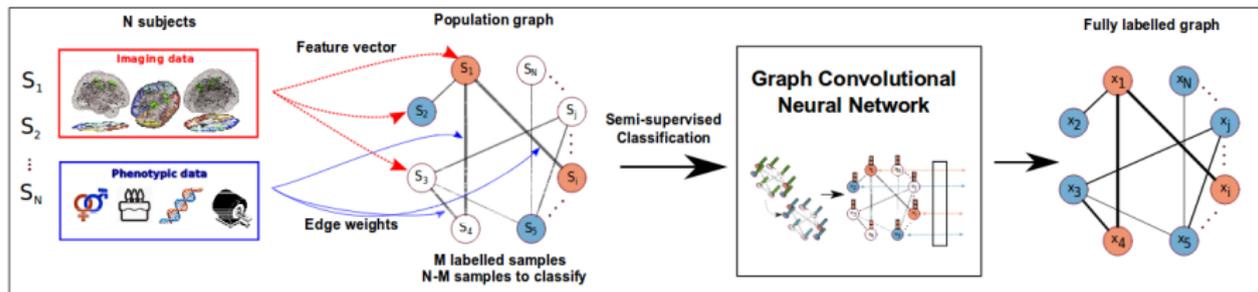
# Matrix completion

- ▶ Recover missing values by solving optimization problem
- ▶ Loss function :

$$l = \|\Omega * (M - \tilde{M})\| + \gamma l_{\Omega_b}(M, \tilde{M}) + \beta \sum_{i=1}^q W_i \quad (1)$$



# Graph methods for the prediction of MCI to AD conversion



**Figure 5:** Overview of the pipeline used for classification of population graphs using Graph Convolutional Networks. Reproduced from Parisot et al. [1]

- ▶ No missing data
- ▶ One graph

# Graph methods for the prediction of MCI to AD conversion

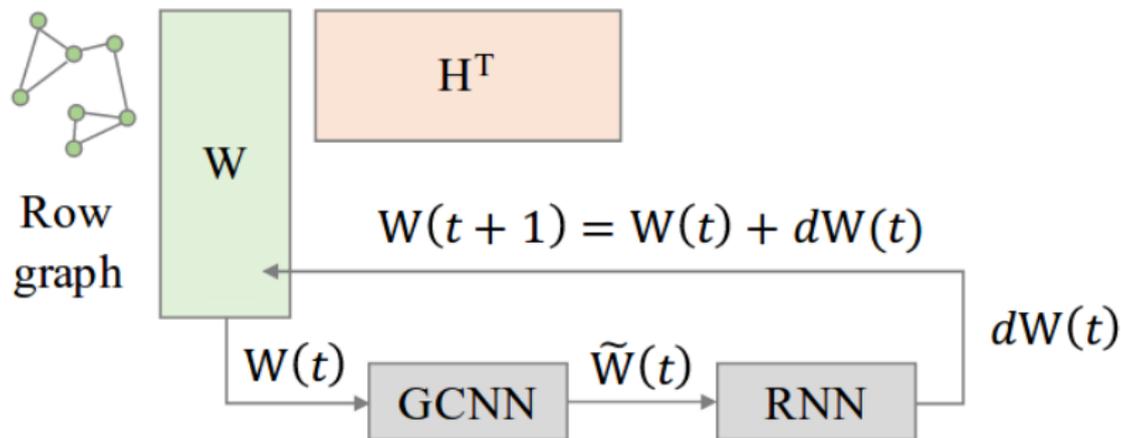


Figure 6: Vivar et al. [2]

- ▶ Matrix completion
- ▶ Missing data
- ▶ One graph

# A novel graph-based method for the prediction of MCI to AD conversion

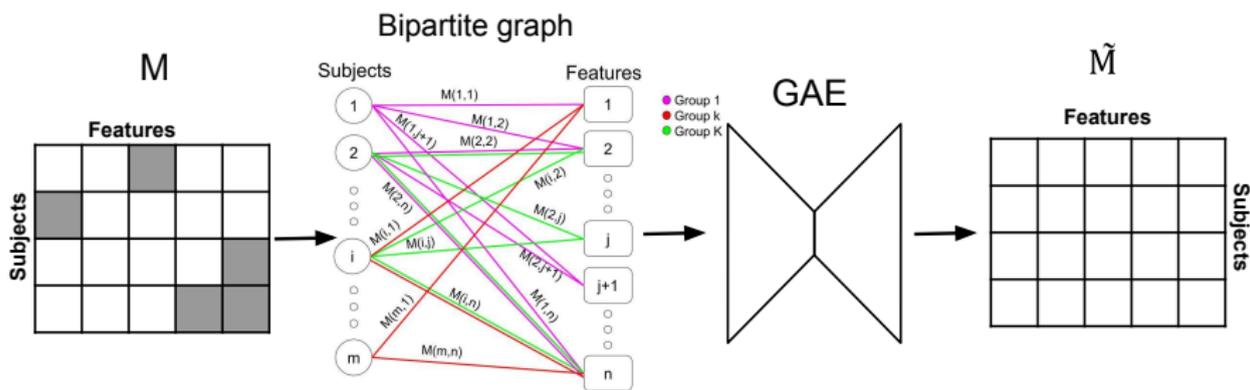
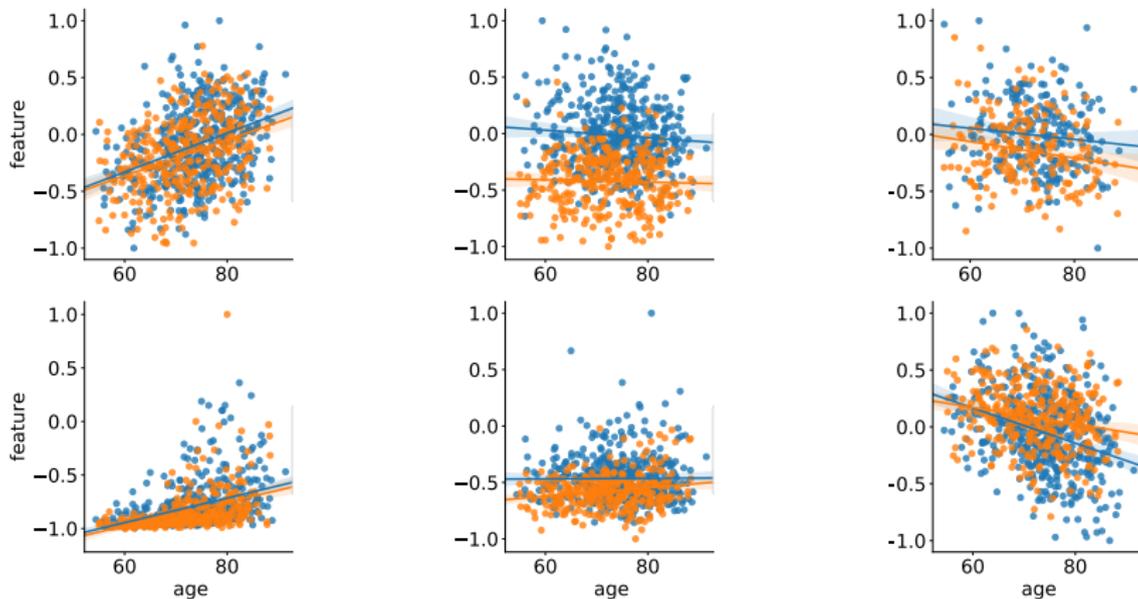


Figure 7: Proposed architecture

- ▶ Matrix completion : Van den Berg et al. [3]
- ▶ Missing data
- ▶ Multiple graphs

## Defining the feature dependencies



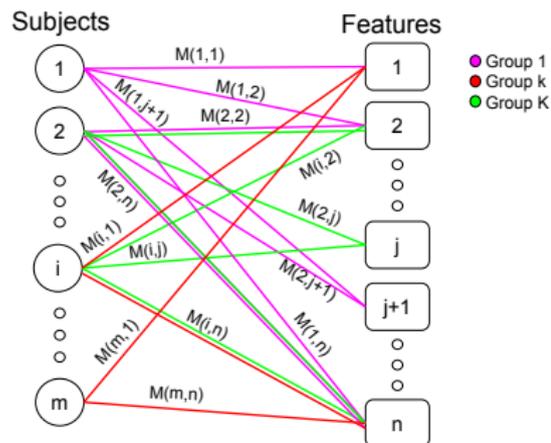
**Age-related features.**

**Sex-related features.**

**Age & Sex features.**

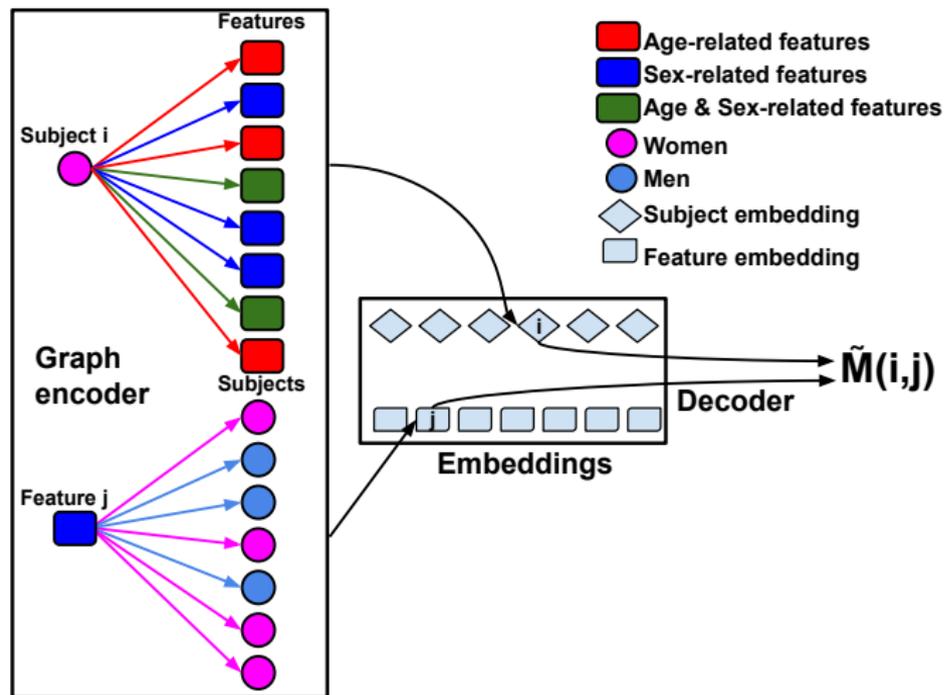
**Figure 8:** Relationships of age and sex (Men and Women) with six different features in the case of Alzheimer's disease.

# Bipartite graph



- Relationship between a group of subjects and a group of features

## Graph Auto-encoder



# Datasets

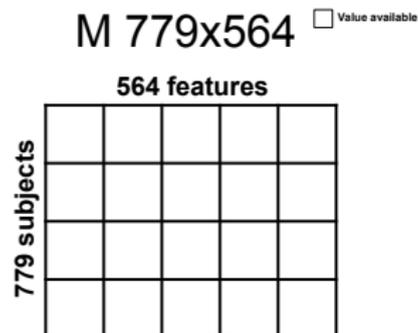
## TADPOLE dataset

- ▶ 779 subjects
- ▶ 564 features
- ▶ 21 % missing data

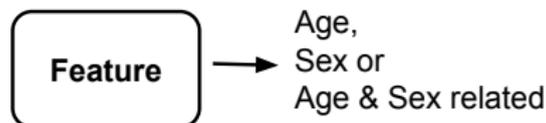
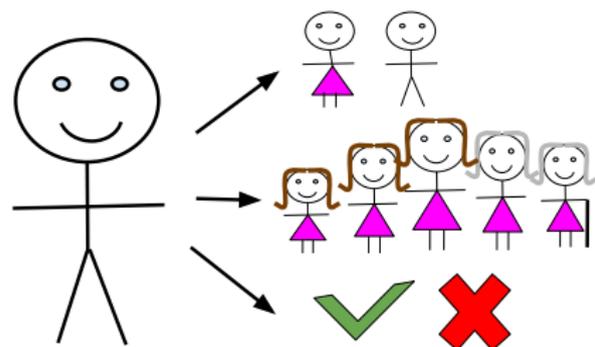


## Creation of a synthetic dataset

- ▶ 779 subjects
- ▶ 564 features
- ▶ No missing data



## Creation of the synthetic dataset



$$M(i, j) = m_j f_{ij} + i_j + \epsilon_{ij} + v_j * y_i \quad (2)$$

$$f_{ij} = x_i \text{ if age} \quad (3)$$

$$= s_i \text{ if sex} \quad (4)$$

$$= s_i x_i \text{ if age \& sex} \quad (5)$$

$$m_j \sim \mathcal{U}[-m, m] \quad (6)$$

$$i_j \sim \mathcal{U}[a, b] \quad (7)$$

$$\epsilon_{ij} \sim \mathcal{N}(0, \sigma) \quad (8)$$

$$v_j \sim \mathcal{U}[c, d] \quad (9)$$

## Evaluation measure for performance

- ▶ Chosen Metrics: Integral of ROC : AUC (Area Under the Curve)
- ▶ ROC measures the true positive rate, relative to the number of false positives
- ▶ Integral of ROC ranges from 0 to 1, with 1 being the best

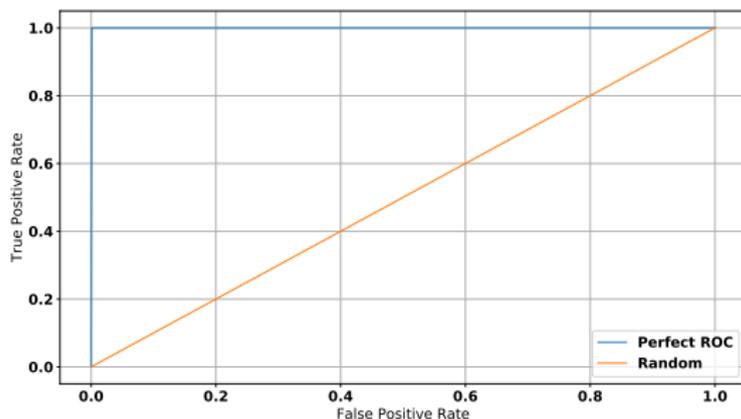
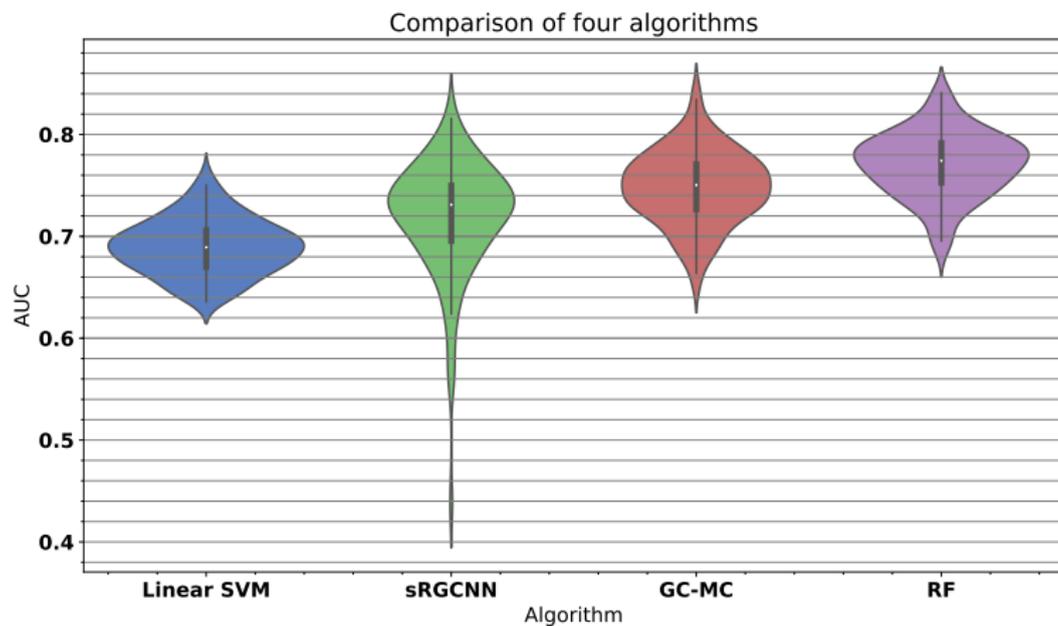
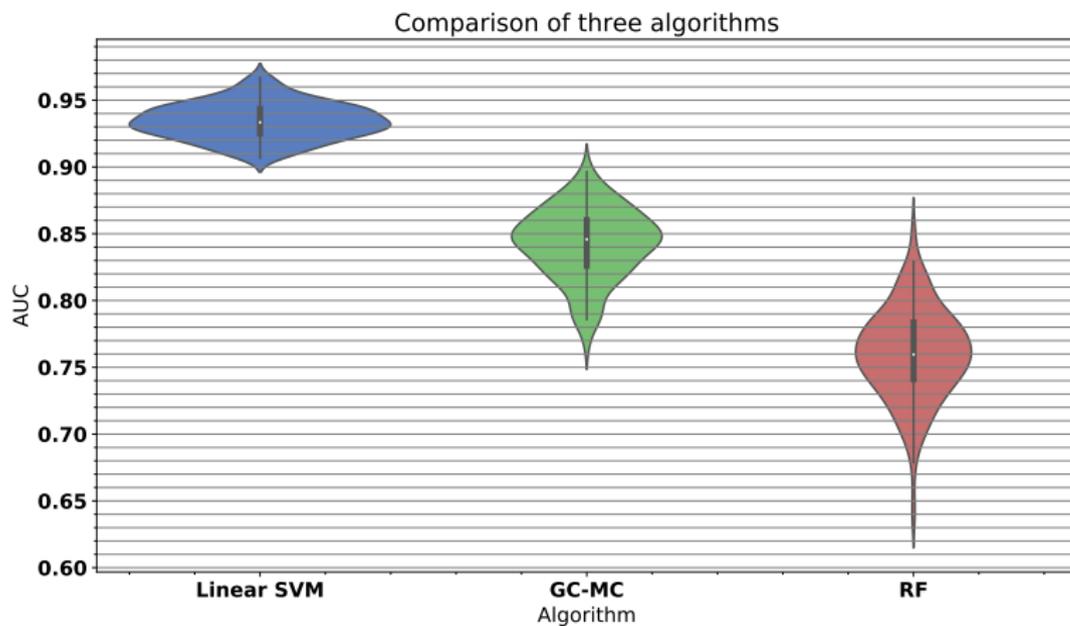


Figure 9: Perfect and random ROC curve

# Results on the real dataset



# Results on the synthetic dataset



## Conclusion

- ▶ Better than baseline methods linear SVM and MLP
- ▶ Better performance than sRGNN by 2.9 %
- ▶ Random Forest performs better

Future work:

- ▶ Remove missing values in the dataset