AAAI-23 Main Track

Heterogeneous Graph Learning for Multi-modal Medical Data Analysis

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DSAIL Data Science & Artificial Intelligence

Problem definition

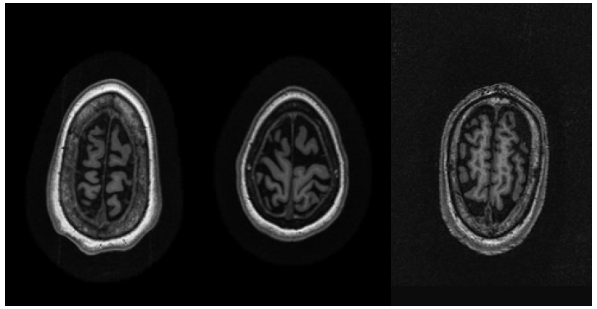


Image data

Patient	Age	DIG	TRA	ADA	MMS	City	APOE	RAV
1	42	34	-4	18.6	28	2	0	6
2	73	25	-15.8	31	20	9	1	4
3	80	38	-1.5	14.6	29	9	0	4
4	29	25	-9.4	21.3	27	4	1	4
5	65	34	-10.8	25.6	25	7	0	5

Non-image data

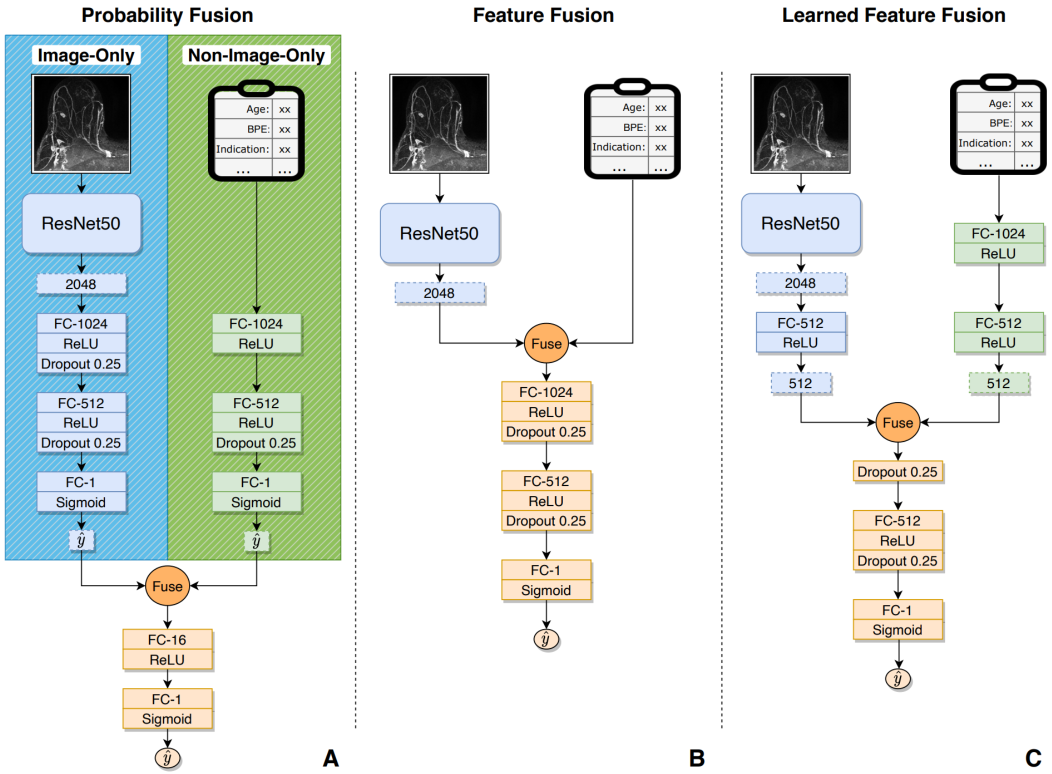
Fusing Method

(research goal)

Clinical Decision

- **Integrate** the multi-modal medical data (image and non-image data) for **more accurate clinical decisions**
- **Capture** important **information** from various aspects of the given data

Previous works



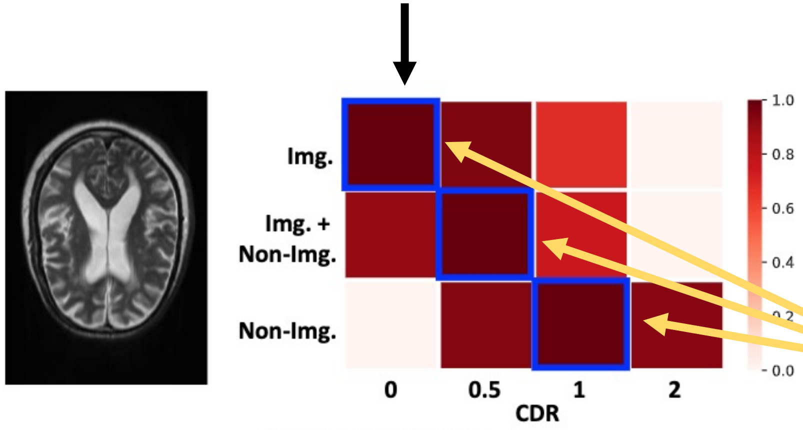
Naive multimodal fusion method

- Previous work demonstrates incorporating non-image data with images can significantly improve predictive performance
- But naïve integration of the modalities **cannot fully benefit from the complementary relationship** between the modalities.

G. Holste, S. C. Partridge, H. Rahbar, D. Biswas, C. I. Lee and A. M. Alessio, "End-to-End Learning of Fused Image and Non-Image Features for Improved Breast Cancer Classification from MRI," 2021 IEEE/CVF

Motivation Medical data is multi-modal in nature

Highest similarity value in each row



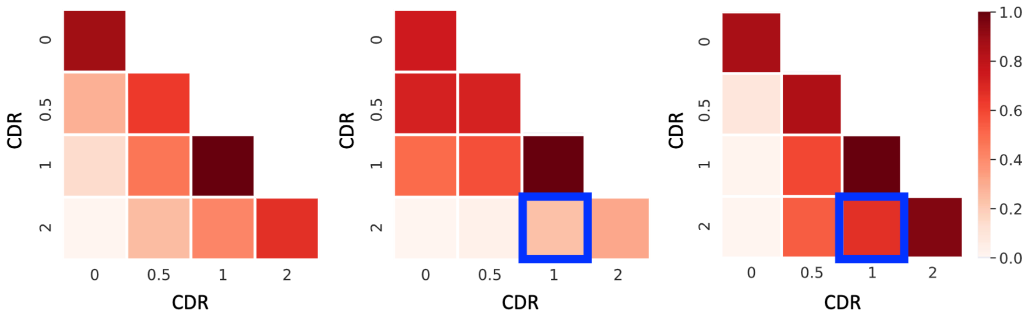
(a) Patient of CDR 0.5

- Routine clinical visits of a patient produce not only image data, but also non-image data (i.e., clinical information).

- Multiple modalities of medical data provide **different and complementary views** of the same patient.

Integration of diverse and complementary views from medical data can make **more informed** and **accurate** clinical decisions.

Motivation Diverse aspects of Clinical data provides rich information on patients



All non-image Features

Non-image Features type 1 (Family history)

Non-image Features type 2 (Cognitive Abilities)

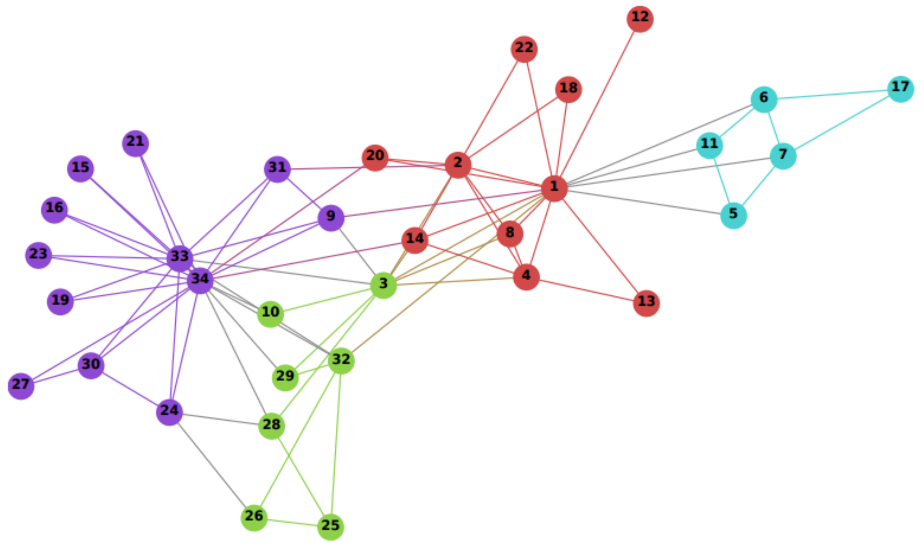
- Patients who suffer from the same disease share highly similar non-image data compared with those in different classes
- But diverse aspects of non-image data induce complex similarity relationships between patients

<u>Example</u>

- Type 1 feature fail to find connection between CDR 1 and 2
- Type 2 feature can make preemptive clinical decision on CDR 1

RQ1: How to incorporate complex similarity relationship between patients?

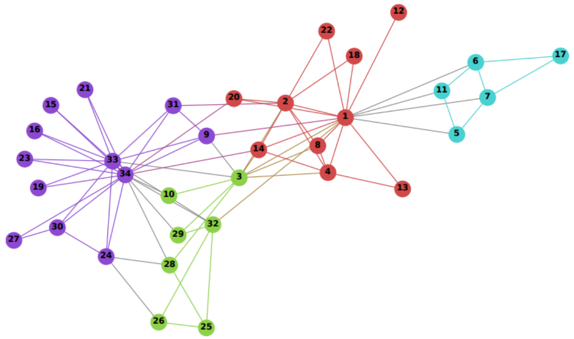
Methodology How can we capture the relationship between patients



- Graph structure provides a natural way of representing patients and their similarities
  - **Node**: multi-modal features including medical images and non-image data of the patient
  - **Edge**: represent the relationship between patient

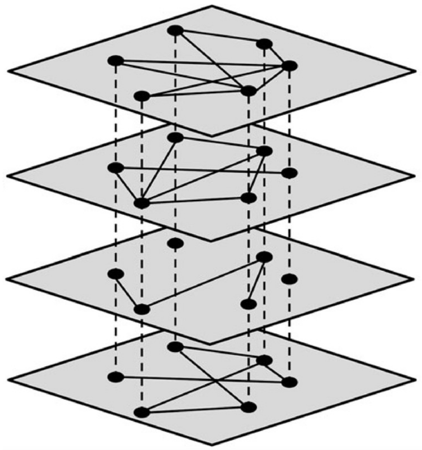
RQ2: Can single graph capture the complex relationship between patients ?

Methodology How can we capture the relationship between patients



Single Graph

- Single graph may miss the inherent complex relationships between patients
  - ➢ Single graph considers all relationships as the same
  - ➢ Whereas in reality, different relationships can have different characteristics and properties



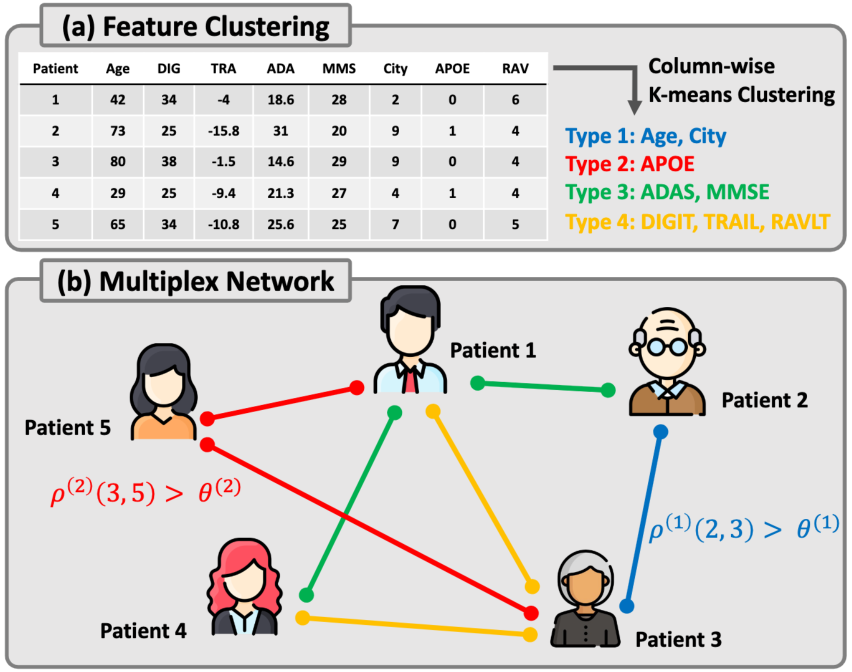
Multiplex Network

- <u>Multiplex network</u> considers the **multiple relationships** between nodes as different layers in the network
  - ➢ Each layer represents a specific type of relationship
  - ➢ Multiplex network can capture the complex relationships between patients, as it acknowledges the heterogeneity of relationships in the network

Goldblum, B.L., Reddie, A.W., Hickey, T.C. *et al.* The nuclear network: multiplex network analysis for interconnected systems. *Appl Netw Sci* **4**, 36 (2019).

Methodology

How can we capture the inherent complex relationship between patients ?



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$$\boldsymbol{C} \in \mathbb{R}^{|\mathcal{V}| \times F_{non-img}} \xrightarrow[\text{K-means}]{\text{Column-wise}} \boldsymbol{c}^{(1)}, \boldsymbol{c}^{(2)}, \cdots, \boldsymbol{c}^{(r)}, \cdots \boldsymbol{c}^{(K)}$$

$$\mathbf{A}^{(r)}(i,j) = \begin{cases} 1 & \text{if } \rho^{(r)}(i,j) > \theta^{(r)}, \\ 0 & \text{otherwise} \end{cases}$$

$$\rho^{(r)}(i,j) = \frac{\mathbf{c}_i^{(r)} \cdot \mathbf{c}_j^{(r)}}{\|\mathbf{c}_i^{(r)}\| \cdot \|\mathbf{c}_j^{(r)}\|}$$

- Using Column-wise K-means Clustering, divide non-image data into non-overlapping $|\mathcal{R}|$ types of features
- Using cosine-similarity and threshold for each type of non-image feature, construct multiplex network

Methodology Summarization research question

RQ1: How to incorporate complex similarity relationship between patients?

- Solution: Graph structure. More specifically, **multiplex network** which considers the **multiple relationships** between nodes as different layers in the network

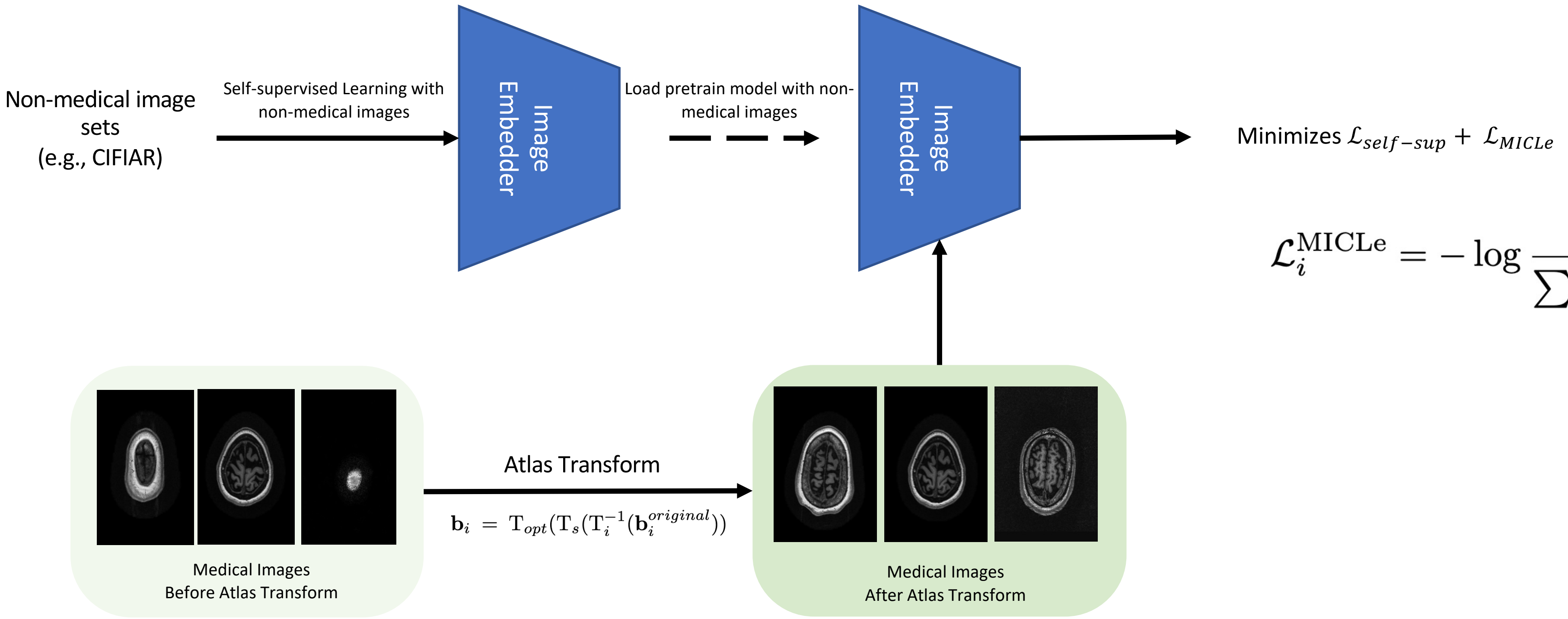
RQ2: Can single graph capture the complex relationship between patients ?

- Solution: Single graph is inadequate for depicting complex relationships. By utilizing a **multiplex network**, the complex relationships between patients can be captured, **recognizing the heterogeneity of relationships in the network**.

Methodology

Preparing Node Features

→ Node features: concatenate image features and non-image features



$$\mathcal{L}_i^{\mathrm{MICLe}} = -\log \frac{exp(sim(\mathbf{z}_i^1, \mathbf{z}_i^2)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} exp(sim(\mathbf{z}_i, \mathbf{z}_k)/\tau)}$$

- Train medical image on pretrained models (e.g., SimCLR, MoCo)
- The MICLe loss maximizes mutual information of images from same patient

Azizi, Shekoofeh, et al. "Big self-supervised models advance medical image classification." Proceedings of the IEEE/CVF International Conference on Computer Vision. 2021.

Methodology

Learn Multiplex Networks (HetMed is model-agnostic. We can adapt other multiplex network embedding models)

Adopt Deep Multiplex Graph Infomax (DMGI) [Park et al AAAI 2020]
-> Maximize the mutual information with relation-type specific summary vector

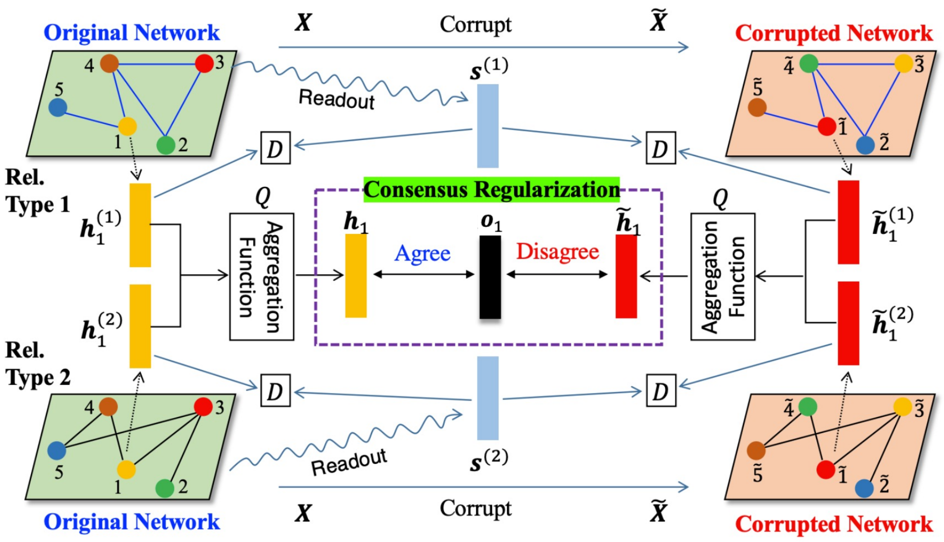


Figure from [Park et al AAAI 2020]

$$\mathcal{L}^{(r)} = \sum_{i=1}^{|\mathcal{V}|} \log \mathcal{D}(\mathbf{h}_i^{(r)}, \mathbf{s}^{(r)}) + \sum_{j=1}^{|\mathcal{V}|} \log \left(1 - \mathcal{D}(\tilde{\mathbf{h}}_j^{(r)}, \mathbf{s}^{(r)})\right)$$

Maximize the mutual information between relation-specific summary vector and relation-specific node embedding
Minimize the mutual information between relation-specific summary vector and relation-specific corrupted set

$$\ell_{cs} = \left[\mathbf{O} - \mathcal{Q}\left(\{\mathbf{H}^{(r)} | r \in \mathcal{R}\}\right)\right]^2 - \left[\mathbf{O} - \mathcal{Q}\left(\{\tilde{\mathbf{H}}^{(r)} | r \in \mathcal{R}\}\right)\right]^2$$

Consensus Regularization (Unify all the relation-specific node embeddings)
Maximize the agreement with the set of “real” node embedding
Minimize the agreement with the set of “fake” node embedding

$$\ell_{sup} = -\frac{1}{|\mathcal{Y}_L|} \sum_{l \in \mathcal{Y}_L} \sum_{i=1}^{c} Y_{li} \ln \hat{Y}_{li}$$

Semi-supervised loss

$$\mathcal{L} = \sum_{r \in \mathcal{R}} \mathcal{L}^{(r)} + \alpha \ell_{cs} + \beta \ell_{sup} + \gamma \|\mathbf{\Theta}\|^2$$

Park, Chanyoung, et al. "Unsupervised attributed multiplex network embedding." Proceedings of the AAAI Conference on Artificial Intelligence. Vol. 34. No. 04. 2020.

Methodology Overall Frameworks

Overall Frameworks of HetMed

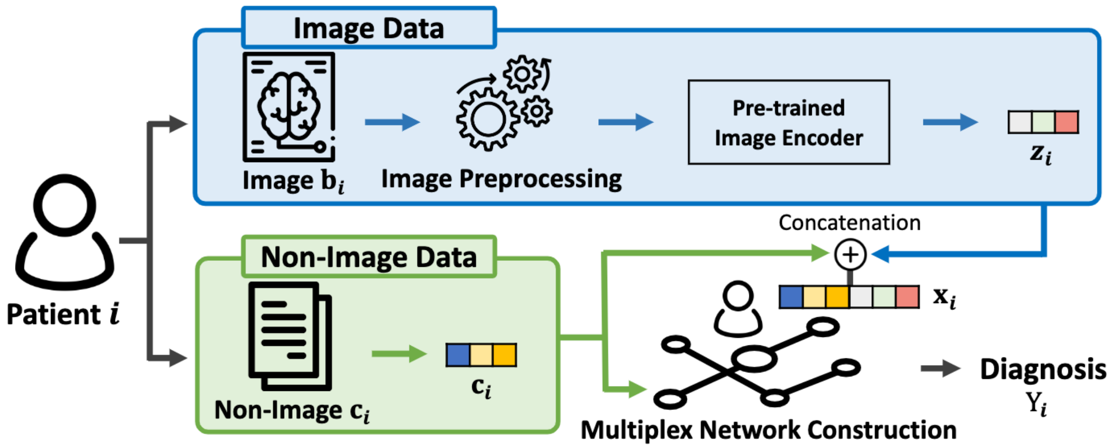


Image Data

- Image Preprocessing (atlas transform)
- Learn the image encoder (pre-trained with non-medical image)
- Extract embeddings of images

Non-image Data

- Column wise K-means Clustering
- Construct multiplex network via cosine similarity of each patient

Learn Multiplex Network

- Node feature = Concatenate (image embedding, non-image data)
- Learn consensus embedding
- Diagnosis

Experiments Dataset

Three brain dataset / Two breast cancer dataset

- ADNI (Alzheimer’s Disease Neuroimage Initiative)
  135 cognitive normal / 203 late mild cognitive impairment / 79 Alzheimer’s disease
- OASIS-3 (Open Access Series of Imaging Studies)
  670 cognitive normal / 189 very mild impairment / 38 mild impairment / 82 moderate dementia (Alzheimer’s disease)
- ABIDE (Autism Brain Imaging Data Exchange)
  473 autism spectrum disorder / 504 healthy controls
- Duke-Breast
  44 tumor grade 1.0 / 105 tumor grade 2.0 / 465 tumor grade 3.0
- CMMD (Chinese Mammography Dataset)
  481 benign patients / 1293 malignant patients

Petersen, R. C.; Aisen, P.; Beckett, L. A.; Donohue, M.; Gamst, A.; Harvey, D. J.; Jack, C.; Jagust, W.; Shaw, L.; Toga, A.; et al. 2010. Alzheimer’s disease neuroimaging initiative (ADNI): clinical characterization. Neurology, 74(3): 201–209.
LaMontagne, P. J.; Benzinger, T. L.; Morris, J. C.; Keefe, S.; Hornbeck, R.; Xiong, C.; Grant, E.; Hassenstab, J.; Moulder, K.; Vlassenko, A. G.; et al. 2019. OASIS-3: longitudinal neuroimaging, clinical, and cognitive dataset for normal aging and Alzheimer disease. MedRxiv
Di Martino, A.; O’connor, D.; Chen, B.; Alaerts, K.; Anderson, J. S.; Assaf, M.; Balsters, J. H.; Baxter, L.; Beggiato, A.; Bernaerts, S.; et al. 2017. Enhancing studies of the connectome in autism using the autism brain imaging data exchange II. Scientific data, 4(1): 1–15.
Xiao, J., Rahbar, H., Hippe, D.S. *et al.* Dynamic contrast-enhanced breast MRI features correlate with invasive breast cancer angiogenesis. *npj Breast Cancer* **7**, 42 (2021). https://doi.org/10.1038/s41523-021-00247-3
Cai, H.; Huang, Q.; Rong, W.; Song, Y.; Li, J.; Wang, J.; Chen, J.; and Li, L. 2019. Breast microcalcification diagnosis using deep convolutional neural network from digital mammograms. Computational and mathematical methods in medicine, 2019.

Experiments Settings

- Image pretrain models
  - SimCLR, MoCo

- End-to-End fusion models [G. Holste et al]
  - Feature fusion, Probability fusion, Learned fusion
  - For fair comparison, we train image embedder in end-to-end manner within other approaches

- Graph based fusion models
  - Spec. [Parisot, Sarah, et al], GCN

Chen, Ting, et al. "A simple framework for contrastive learning of visual representations." International conference on machine learning. PMLR, 2020.
He, Kaiming, et al. "Momentum contrast for unsupervised visual representation learning." Proceedings of the IEEE/CVF conference on computer vision and pattern recognition. 2020.
G. Holste, S. C. Partridge, H. Rahbar, D. Biswas, C. I. Lee and A. M. Alessio, "End-to-End Learning of Fused Image and Non-Image Features for Improved Breast Cancer Classification from MRI," 2021 IEEE/CVF
Parisot, Sarah, et al. "Spectral graph convolutions for population-based disease prediction." International conference on medical image computing and computer-assisted intervention. Springer, Cham, 2017.

Experiments Main results

Model	ADNI		OASIS-3		ABIDE		Duke-Breast		CMMD	
	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1
Feat. (=MLP)	0.521 (0.017)	0.562 (0.020)	0.216 (0.008)	0.625 (0.022)	0.407 (0.015)	0.753 (0.020)	0.466 (0.031)	0.712 (0.032)	0.667 (0.021)	0.75 (0.017)
Prob.	0.509 (0.009)	0.522 (0.020)	**0.230** (0.022)	0.639 (0.025)	0.385 (0.034)	0.761 (0.031)	0.407 (0.028)	0.688 (0.025)	0.564 (0.013)	0.665 (0.026)
Learned	0.576 (0.012)	0.598 (0.022)	0.199 (0.009)	0.647 (0.010)	0.649 (0.021)	0.776 (0.023)	**0.484** (0.022)	0.625 (0.024)	0.714 (0.032)	0.773 (0.020)
Spec.	0.628 (0.009)	0.788 (0.018)	0.202 (0.011)	0.679 (0.014)	0.696 (0.032)	0.717 (0.037)	0.427 (0.010)	0.701 (0.025)	0.681 (0.036)	0.742 (0.024)
GCN	0.606 (0.022)	0.795 (0.015)	0.201 (0.021)	0.670 (0.033)	0.768 (0.019)	0.770 (0.017)	0.430 (0.016)	0.671 (0.020)	0.683 (0.028)	0.745 (0.016)
HetMed	**0.774** (0.037)	**0.813** (0.024)	0.205 (0.005)	**0.697** (0.011)	**0.778** (0.035)	**0.784** (0.033)	0.432 (0.024)	**0.794** (0.057)	**0.716** (0.008)	**0.785** (0.010)

Performance on End-to-End Learning

Pretrain	Model	ADNI		OASIS-3		ABIDE		Duke-Breast		CMMD	
		Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1
SimCLR	MLP	0.561 (0.022)	0.781 (0.031)	0.219 (0.017)	0.646 (0.016)	0.703 (0.023)	0.735 (0.022)	0.430 (0.019)	0.652 (0.019)	0.523 (0.027)	0.751 (0.014)
	GCN	0.611 (0.019)	0.816 (0.014)	**0.235** (0.025)	0.685 (0.026)	0.751 (0.016)	0.756 (0.018)	0.440 (0.017)	0.698 (0.019)	0.625 (0.014)	0.745 (0.022)
	HetMed	**0.851** (0.009)	**0.857** (0.012)	**0.235** (0.020)	**0.686** (0.017)	**0.833** (0.005)	**0.842** (0.004)	**0.447** (0.011)	**0.765** (0.021)	**0.720** (0.025)	**0.781** (0.022)
MoCo	MLP	0.547 (0.012)	0.757 (0.020)	**0.247** (0.014)	0.669 (0.013)	0.708 (0.012)	0.739 (0.014)	0.439 (0.020)	0.699 (0.027)	0.531 (0.033)	0.748 (0.021)
	GCN	0.616 (0.016)	0.825 (0.018)	0.238 (0.013)	0.679 (0.021)	0.734 (0.022)	0.749 (0.030)	0.445 (0.026)	0.716 (0.024)	0.611 (0.019)	0.752 (0.021)
	HetMed	**0.832** (0.011)	**0.842** (0.020)	0.242 (0.030)	**0.690** (0.022)	**0.855** (0.006)	**0.858** (0.006)	**0.446** (0.011)	**0.753** (0.027)	**0.706** (0.018)	**0.764** (0.024)

Performance on Pretraining strategies on Medical image

HetMed outperforms other baselines because it considers **multiple types of features** of medical data

Experiments Main results

Model	ADNI		OASIS-3		ABIDE		Duke-Breast		CMMD	
	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1
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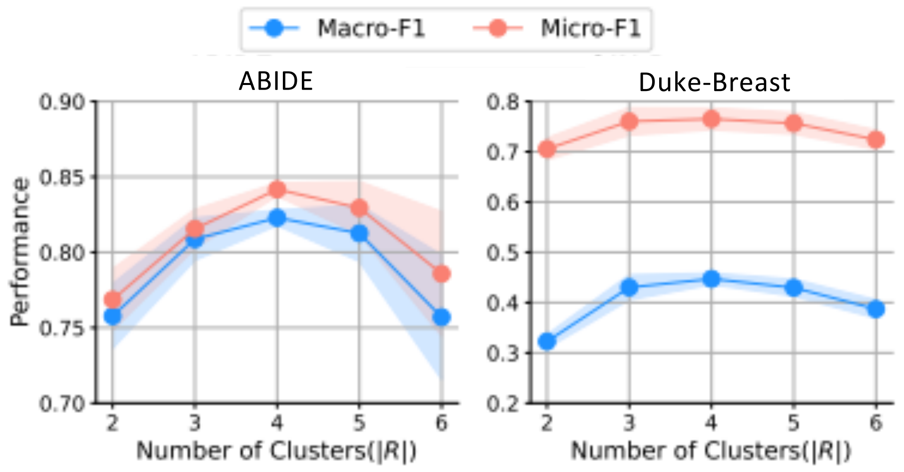
Performance on Pretraining strategies on Medical image

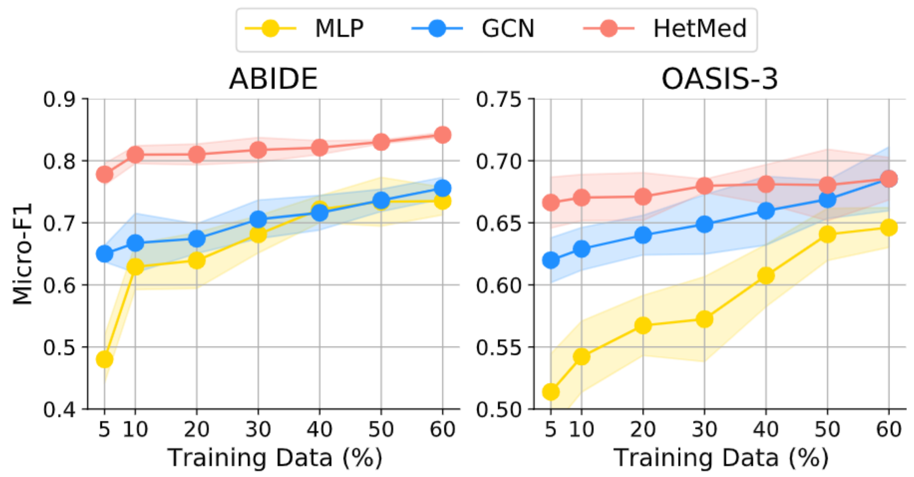
- **Graph based** model perform **better than the naïve fusion** method
- Moreover, **HetMed outperforms** GCN, which considers **various relationships** between patients

Experiments Model Analysis



Number of Clusters

- The number of relation types between patients ($|R|$) determines how complex the relationship between patients is to be modeled
  - **Too few** clusters → **lack of capability** to model the complex relationship between patients.
  - **Too many** clusters → # of clusters can get larger than the number of relation types inherent in the data → leads to **redundant information** between multiple types of relationship.



Number of Training Data

- HetMed **consistently produces accurate predictions** even under the lack of labeled data.
- By modeling complex relationship into a multiplex network, HetMed becomes **more robust** than single relationship network (GCN) or naïve fusion methods (MLP).

Experiments Model analysis

Model	ABIDE		OASIS-3	
	Ma-F1	Mi-F1	Ma-F1	Mi-F1
Random	0.757 (0.042)	0.766 (0.041)	0.231 (0.013)	0.672 (0.018)
HetMed (Clustering-based)	0.833 (0.005)	0.842 (0.004)	0.235 (0.007)	0.686 (0.011)
Domain Knowledge	**0.851** (0.005)	**0.853** (0.006)	**0.295** (0.020)	**0.717** (0.017)

Non-Image Features Splitting Strategy

- Multiplex network was constructed based on non-overlapping $|R|$ types of non-image features by K-means clustering
- Compare the performance of HetMed with
  - Splitting features **randomly**
  - Splitting features on **domain knowledge**

- Clustering-based strategy outperforms the random splitting strategy
- Splitting based **on domain knowledge outperforms**
  → These are clinically more meaningful, which leads to capture complex relationship between patients that is clinically more meaningful
- With some help of clinicians, the performance can be further improved
  → HetMed can serve as a clinical decision support tool

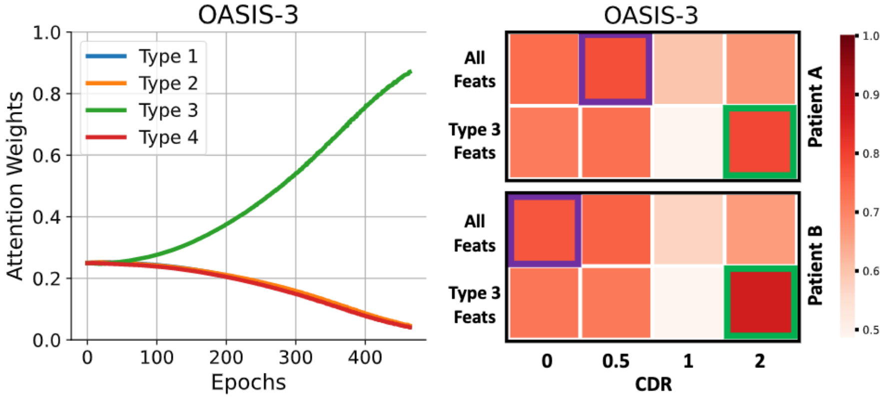
Experiments Other multiplex network embedding

Model	ADNI		OASIS-3		ABIDE		Duke-Breast		CMMD	
	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1
MLP	0.561 (0.022)	0.781 (0.031)	0.219 (0.017)	0.646 (0.016)	0.703 (0.023)	0.735 (0.022)	0.430 (0.019)	0.652 (0.019)	0.523 (0.027)	0.751 (0.014)
GCN	0.611 (0.019)	0.816 (0.014)	**0.235** (0.025)	0.685 (0.026)	0.751 (0.016)	0.756 (0.018)	0.440 (0.017)	0.698 (0.019)	0.625 (0.014)	0.745 (0.022)
HAN	0.801 (0.015)	0.823 (0.023)	0.221 (0.014)	0.677 (0.017)	0.829 (0.022)	0.834 (0.031)	0.434 (0.028)	0.745 (0.034)	0.719 (0.019)	0.779 (0.027)
GATNE	0.812 (0.018)	0.820 (0.014)	0.226 (0.008)	0.669 (0.020)	0.799 (0.023)	0.802 (0.018)	0.423 (0.010)	**0.785** (0.032)	0.705 (0.019)	0.767 (0.015)
DMGI	**0.851** (0.009)	**0.857** (0.012)	**0.235** (0.020)	**0.686** (0.017)	**0.833** (0.005)	**0.842** (0.004)	**0.447** (0.011)	0.765 (0.021)	**0.720** (0.025)	**0.781** (0.022)

HetMed is a model-agnostic framework: Can adopt various multiplex network embedding methods

- Adopt recent multiplex network embedding methods (i.e., HAN, GATNE)
- The **multiplex network** embedding methods **outperforms simple fusion methods** (i.e., MLP, GCN)
  → Due to complex relationship between patients
- **DMGI** outperforms **all other multiplex network embedding methods**
  → Consensus regularization and attentive mechanism can capture relationship between patients

Experiments Model Practicality - Explainability



(a) Type-specific attention weights (b) Case Study

Explainability

- Attentive pooling mechanism in HetMed

→ Captures the importance of each relation type for medical diagnosis

Case Study on OASIS-3 Dataset

- Alzheimer's disease (CDR: 2) : Patient A, Patient B
- Most important relation type: Type 3
- Compare average cosine-similarity of non-image feature between A (or B) and other patients
- Based on all features → **fail to predict** correct disease
- Based on type 3 features → **correct** prediction

HetMed can infer the importance of each feature type, which can be used to explain the model prediction.

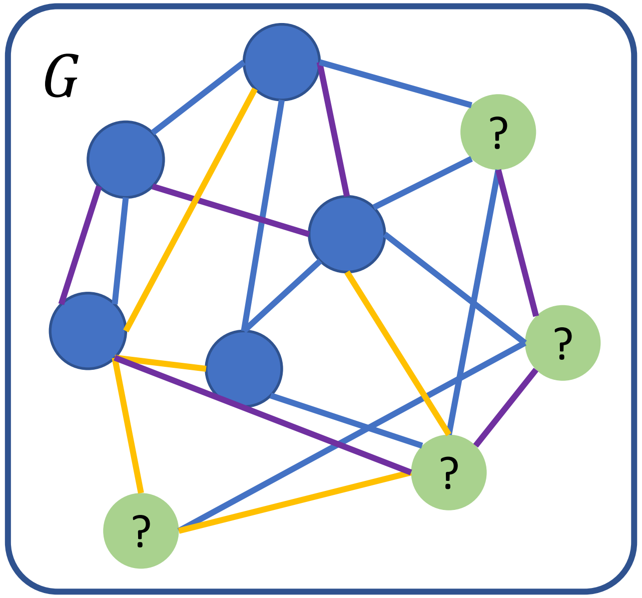
Experiments Model Practicality - Generalizability

In the real-world, new patients arrive at the hospital (= adding new node and edges)

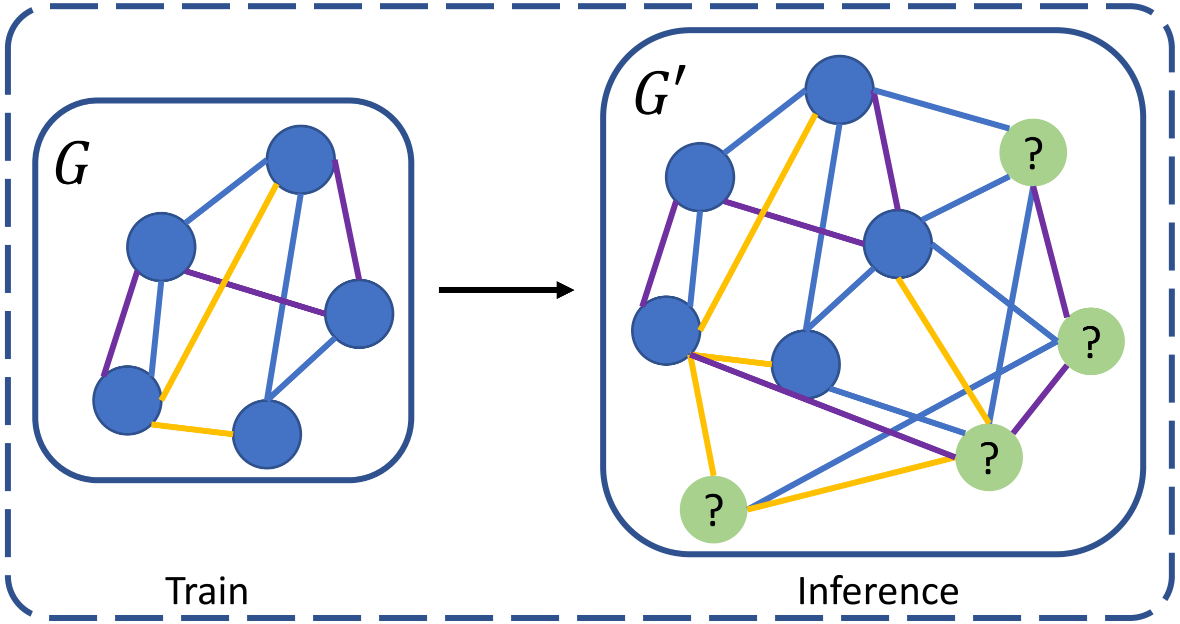
Predict disease of new patients using information of existing patients graphs (= inductive setting of graph)

Inductive Setting

- first train on a training set of nodes and edges, and then make predictions for new nodes and edges that were **not part of the original training set**



Transductive Setting
Train G / Inference “?” in G



Inductive Setting
Train G / Inference “?” In G'

Experiments Model Practicality - Generalizability

In the real-world, new patients arrive at the hospital (= adding new node and edges)

Model	OASIS-3		Duke-Breast		CMMD	
	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1
MLP	0.197 (0.017)	0.646 (0.029)	0.359 (0.011)	0.622 (0.023)	0.484 (0.028)	0.642 (0.053)
GCN	0.203 (0.016)	0.674 (0.015)	0.360 (0.023)	0.653 (0.006)	0.592 (0.018)	0.670 (0.027)
HetMed	**0.217** (0.009)	**0.684** (0.012)	**0.362** (0.012)	**0.742** (0.032)	**0.631** (0.014)	**0.748** (0.013)

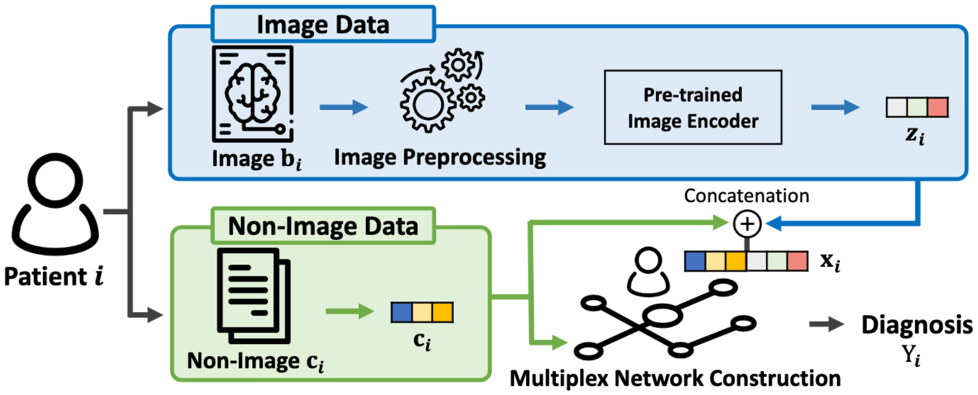
Inductive Setting

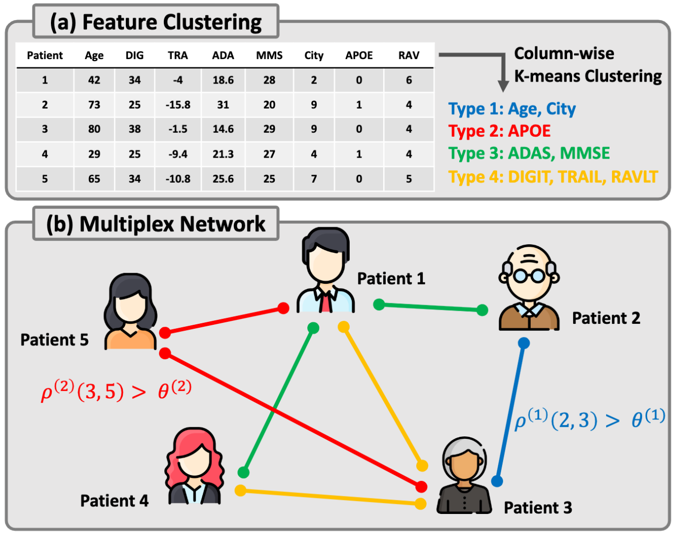
- **Graph based methods** (i.e., GCN and HetMed) perform **better than non graph-based method** (i.e., MLP)
- Moreover, **HetMed outperforms** which again verifies that considering various relationships between patients is crucial and also show the practicality of HetMed

Conclusion

Propose a general framework for fusing multiple modalities of medical data

Fuse multiple modalities into a multiplex network that contains complex relational information between patients





By doing so, HetMed captures important information for clinical decision by considering various aspects of given data

Extensive experiments show
1) Improvement of performance on patient diagnosis
2) Robustness on training data
3) Practicality: Explainability and Generalizability

Thank you!

[Full Paper] https://arxiv.org/abs/2211.15158

[Source Code] https://github.com/Sein-Kim/Multimodal-Medical

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