Leveraging Knowledge Graphs for Enhancing Machine Learning-based Heart Disease Prediction

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Outline

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- Introduction and motivation
- Knowledge graph construction
- Infusing KG into ML pipeline
- Results
- Conclusion and future work

Introduction & Motivation

- ML algorithms widely used across various domains for predictive tasks.
- However the effectiveness of ML models is constrained by the scarcity of annotated datasets needed for training accurate models.
- The challenge of limited annotated datasets for training ML models is particularly critical in domains where accuracy is crucial, such as medical diagnosis.

Knowledge Graphs

- Use of KGs to enrich the data - enhance the performance.
- KGs provide a structured representation of domain-specific knowledge.
- By utilizing existing ontologies and KGs, we can infuse our datasets with rich, contextual information that goes beyond raw data.

Preprocessing Knowledge Graphs

- Heart disease domain:

  age, chest pain type, resting blood pressure, heart rate…

- Ontologies that describe the dataset’s features

- Three different ontologies in the heart disease domain:
  - *Small* ontology - existing ontology from Trepan Reloaded [1]
  - *Extended* ontology - extended HFO ontology [2]
  - *SNOMED* ontology - extracted from SNOMED [3]

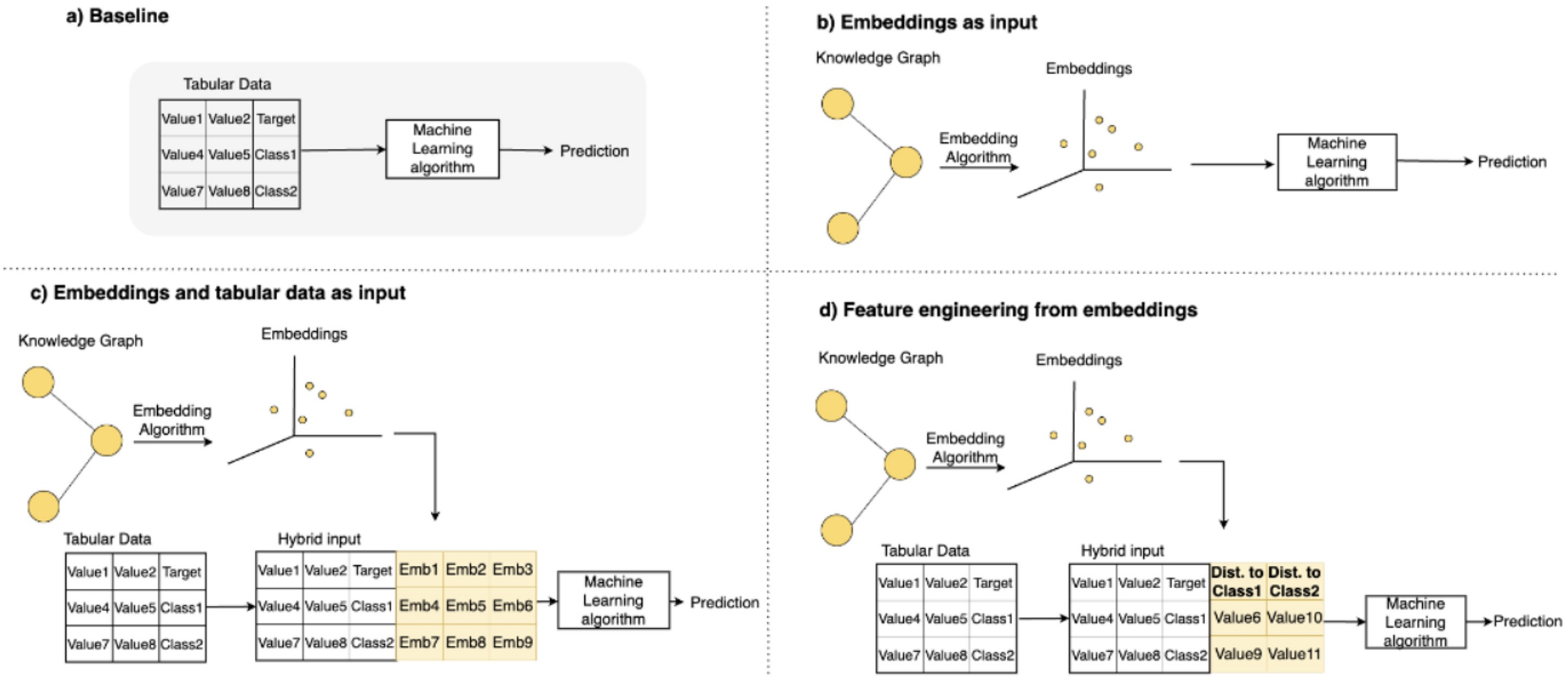
Preprocessing Knowledge Graphs

- Mapped the features of the dataset to the concepts/relations
- KGs construction - population of the ontologies with dataset instances

Table 1: Details of the KGs for heart disease domain.

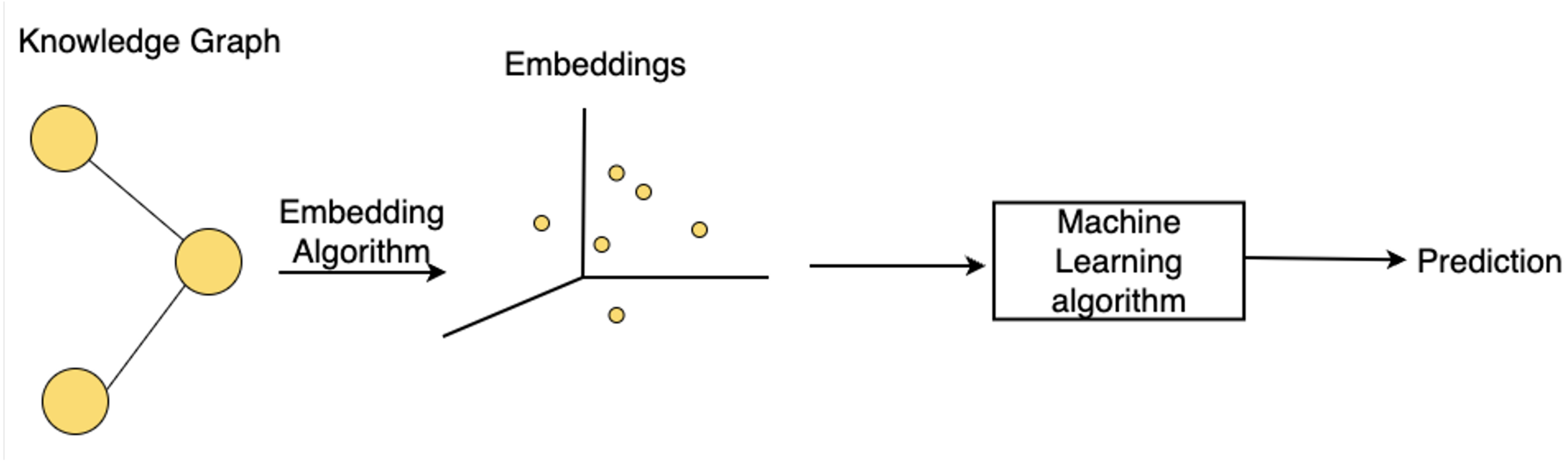
KG	Logical Axioms	Classes	Object prop.	Data prop.
Small	4637	29	6	10
Extended	6682	1664	6	10
Snomed	1963	80	24	10

Knowledge Graphs infusion into ML pipeline



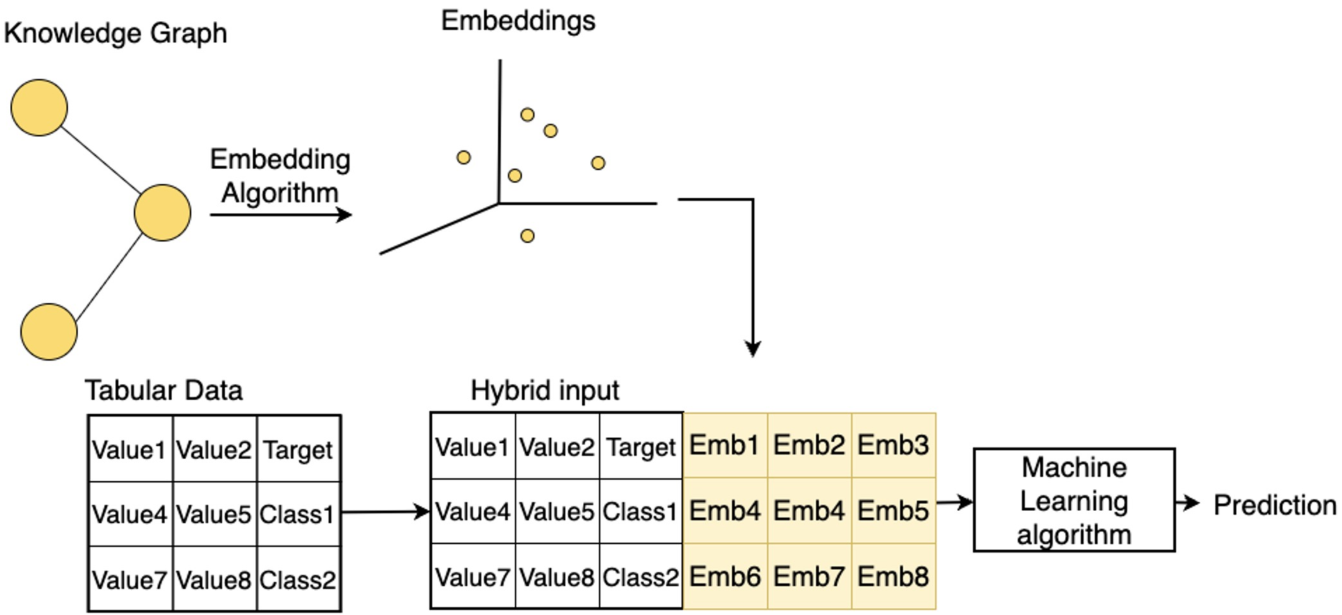
Embedding as input

- Training ML learning with embeddings from KG only.
- Embeddings represent patients in vector space



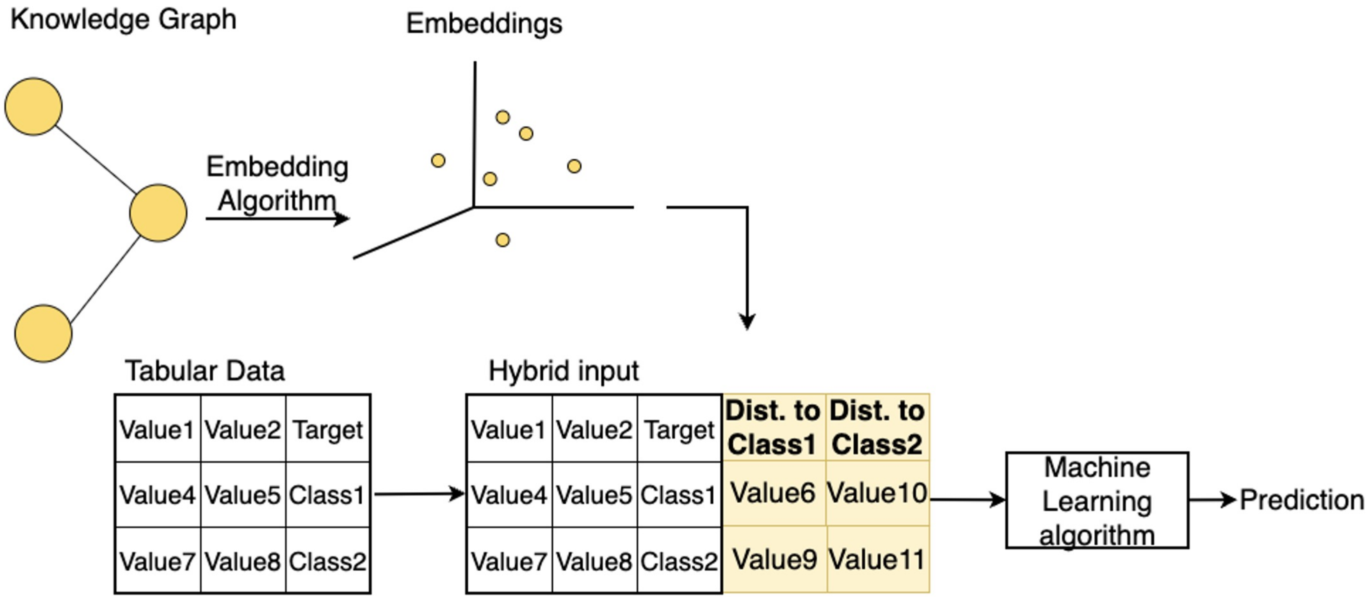
Enriching tabular data with embeddings

- For each patient, embedding vectors are added as extra columns.



Feature Engineering from embeddings

- For each patient in the embedding space, their Euclidean distance to ‘disease’ and ‘no disease’ class is added.



Experiment Setup

- Dataset: Heart disease prediction from Kaggle (303 patients)
- ML models:
  - KNN, SVM, XGBoost, FFNN
- Metrics used :
  - Accuracy, F2 Score
- Embedding algorithms:
  - RDF2Vec, Node2vec

age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	label
63.0	Male	TypicalAngina	145.0	233.0	Yes	LeftVentricularHypertrophy	150.0	No	2.3	Downsloping	Zero	FixedEffect	0
67.0	Male	Asymptomatic	160.0	286.0	No	LeftVentricularHypertrophy	108.0	Yes	1.5	Flat	Three	Normal	1
67.0	Male	Asymptomatic	120.0	229.0	No	LeftVentricularHypertrophy	129.0	Yes	2.6	Flat	Two	ReversableEffect	1
37.0	Male	NonAnginalPain	130.0	250.0	No	Normal	187.0	No	3.5	Downsloping	Zero	Normal	0
41.0	Female	AtypicalAngina	130.0	204.0	No	LeftVentricularHypertrophy	172.0	No	1.4	Upsloping	Zero	Normal	0
56.0	Male	AtypicalAngina	120.0	236.0	No	Normal	178.0	No	0.8	Upsloping	Zero	Normal	0
62.0	Female	Asymptomatic	140.0	268.0	No	LeftVentricularHypertrophy	160.0	No	3.6	Downsloping	Two	Normal	1

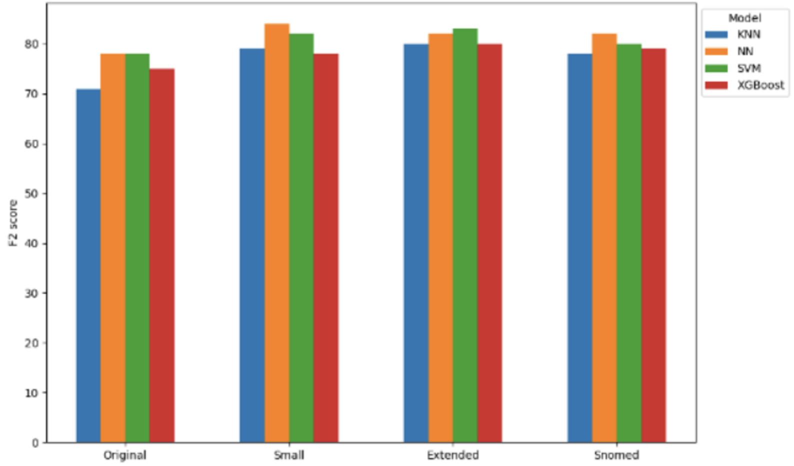
Results

Table 3: Comparison of Accuracy and F2 Scores Across Models using various KG Inputs.

Model	Original Acc.	Original F2	Rdf2Vec Acc.	Rdf2Vec F2	Node2Vec Acc.	Node2Vec F2	Comb-R2V Acc.	Comb-R2V F2	Comb-N2V Acc.	Comb-N2V F2	FE-R2V Acc.	FE-R2V F2	FE-N2V Acc.	FE-N2V F2
Small KG														
KNN	0.81	0.71	0.51	0.34	0.72	0.59	0.81	0.71	0.81	0.71	0.65	0.53	**0.83**	**0.79**
NN	0.82	0.78	0.53	0.04	0.81	0.79	0.82	0.78	0.82	0.77	0.73	0.69	**0.85**	**0.84**
SVM	0.82	0.78	0.54	0.00	0.81	0.78	0.82	0.78	0.83	0.81	0.74	0.65	**0.84**	**0.82**
XGB	0.79	0.75	0.50	0.40	0.73	0.67	0.80	0.75	0.81	0.75	0.65	0.57	**0.80**	**0.78**
Snomed KG														
KNN	0.81	0.71	0.54	0.34	0.76	0.66	0.81	0.71	0.81	0.72	0.65	0.53	**0.83**	**0.78**
NN	0.82	0.78	0.57	0.29	0.79	0.75	0.82	0.78	0.82	0.77	0.70	0.65	**0.84**	**0.82**
SVM	0.82	0.78	0.54	0.00	0.80	0.75	0.82	0.78	0.82	**0.80**	0.69	0.62	**0.83**	**0.80**
XGB	0.79	0.75	0.58	0.48	0.76	0.70	**0.82**	0.77	**0.81**	0.77	0.64	0.58	**0.81**	**0.79**
Extended KG														
KNN	0.81	0.71	0.53	0.37	0.80	0.72	0.81	0.71	0.81	0.72	0.52	0.24	**0.84**	**0.80**
NN	0.82	0.78	0.54	0.05	0.80	0.78	0.82	0.79	0.83	0.80	0.55	0.26	**0.84**	**0.82**
SVM	0.82	0.78	0.54	0.00	0.79	0.76	0.82	0.78	0.83	0.80	0.56	0.22	**0.84**	**0.83**
XGB	0.79	0.75	0.53	0.43	0.77	0.73	0.82	0.77	0.81	0.77	0.54	0.41	**0.82**	**0.80**

Results - Impact of KG Size and Structure

- Different algorithms favor different KG characteristics
- NN best performance - Small KG
- KNN and XGB best performance - Extended KG



Conclusion

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- Using RDF2Vec and Node2Vec embeddings from KGs improves the accuracy and F2 scores - especially when distances to the classes are added as additional features
- The performance of ML algorithms is affected by the size and structure of KGs, with different algorithms favoring different KG characteristics.
- Adding KG information to ML algorithms enhances performance across all models without altering their inherent performance hierarchy.

Future work

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- Apply this approach in various domains beyond heart disease.
- Investigate different embedding algorithms and use different ML algorithms.
- Measure data-dependency of ML algorithms and compare this with the complementary contributions from KGs.

Questions?

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