
Improving Link Prediction on Citation Graphs using LLM Embeddings

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Abstract

1 Link prediction for citations of research papers is a key problem in analyzing
2 scholarly communication and predicting research trends. Typical methods have
3 relied on topological features or sparse textual representations, but these can
4 potentially miss the deeper semantic connections between papers. Our project
5 investigates the effectiveness of leveraging Large Language Models (LLMs) to
6 generate rich node embeddings for citation graph link prediction. We utilize the
7 `mistralai/Mistral-7B-v0.1` model to create embeddings from paper abstracts
8 obtained from the OpenAlex dataset. These generated embeddings serve as input
9 features for a Graph Neural Network (GNN) designed for link prediction. We
10 then compare the GNN's performance against standard baselines such as Common
11 Neighbors. Our experiments performed demonstrate that the GNN model trained on
12 Mistral-7B embeddings are able to significantly outperform the heuristic methods,
13 achieving a test AUC of approximately 0.93, which highlights the possibility of
14 LLM-derived semantic features for enhancing citation link prediction accuracy.

15 1 Introduction

16 Citation networks are graphical representations of scholarly communication, which is crucial for
17 understanding the development and evolution of academic research. In these citation networks, nodes
18 represent academic papers and directed edges represent citations, showing a map of knowledge flow
19 and influence. Predicting future links/citations has applications such as identifying potential research
20 collaborations, recommending relevant literature, and forecasting emerging research areas.

21 Traditional and typical solutions to the link prediction problem for paper citations often depend on
22 graph topology. This often leads to use of heuristic methods such as Common Neighbors (CN),
23 Adamic-Adar (AA), and the Katz index, which all quantify the likelihood of a link based on local
24 or global network structure of the graph. While these methods have proved to be somewhat useful,
25 they often fail to leverage the semantic content embedded in the papers themselves, or strictly use
26 metadata of papers (authors, publication venues, etc.), but still fail to capture semantic relationships.

27 LLMs have proved large advancements recently in demonstrating capabilities to understand and
28 represent complex textual information. At the same time, GNNs have also proven to be strong tools
29 for learning representations and performing tasks on graph-structured data. This project aims to
30 merge these two recent developments together by using an LLM to generate dense rich embeddings
31 from paper abstracts, which will then be used as node features for a GNN trained specifically for
32 citation link predictions.

33 Our hypothesis is that LLM-generated embeddings capture semantic similarity and conceptual
34 relatedness between papers more effectively than traditional features, leading to improved link
35 prediction performance when used with a GNN's ability to model graph structure. As aforementioned
36 above, we will be using the `mistralai/Mistral-7B-v0.1` model and applying it to a subset of the
37 large-scale OpenAlex citation dataset.

38 Our proposed distinctives and contribution are:

- 39 1. An end-to-end pipeline for generating LLM-based node embeddings from paper abstracts
40 and constructing a citation graph suitable for GNN-based link prediction
- 41 2. Demonstration of the effectiveness of Mistral-7B abstract embeddings as node features for
42 citation link prediction.
- 43 3. Comparison of our GNN model using the embeddings against heuristic link prediction
44 baselines (Common Neighbors and Adamic-Adar), showing forth significant performance
45 improvements.

46 2 Related Work

47 Citation link prediction, the task of forecasting future connections in scholarly networks, has been a
48 long-standing problem with approaches spanning various disciplines. Early methods predominantly
49 relied on the topological structure of the citation graph. Heuristics such as Common Neighbors
50 Adamic and Adar [2003], Adamic-Adar Adamic and Adar [2003], and the Katz index Katz [1953]
51 quantify the likelihood of a link based on shared neighbors or path counts. Other structural approaches
52 include matrix factorization techniques Menon and Elkan [2011] and probabilistic models Lü and
53 Zhou [2011]. While effective in capturing local or global network patterns, these methods inherently
54 ignore the semantic content of the papers themselves.

55 More advanced approaches started integrating textual information. Methods have explored using
56 keywords, topics derived from models like Latent Dirichlet Allocation (LDA) Blei et al. [2003], or
57 explicit textual similarity measures between paper abstracts or full texts Lü and Zhou [2011]. These
58 text-based features are often combined with topological features or used in isolation within traditional
59 machine learning models. However, these textual representations were typically sparse or based on
60 simpler embedding techniques compared to modern large language models.

61 With the rise of deep learning on graphs, Graph Neural Networks (GNNs) have become a powerful
62 tool for link prediction. GNNs learn node representations by aggregating information from their
63 neighbors, effectively capturing complex structural patterns. Standard GNN link prediction models
64 often use an encoder-decoder framework, where a GNN encoder learns node embeddings, and a
65 decoder (like a simple dot product or a multi-layer perceptron) predicts the link probability based on
66 pairs of node embeddings Zhou et al. [2020], Fey and Lenssen [2019]. While powerful in leveraging
67 graph structure, the quality of the node embeddings learned by the GNN is often dependent on the
68 initial node features.

69 The recent advancements in Large Language Models (LLMs) have opened new avenues for gener-
70 ating rich, contextualized text representations. Pre-trained transformer models have demonstrated
71 exceptional capabilities in capturing semantic nuances and relationships in text. Consequently, there
72 has been growing interest in leveraging LLM-generated embeddings as initial node features for
73 GNNs to enhance performance on various graph-based tasks Jin et al. [2023], He et al. [2023].
74 For scholarly graphs specifically, LLMs have been used for tasks like paper classification or topic
75 modeling, but their direct application to generate *node features for citation link prediction within
76 a GNN framework*, particularly using recent models like Mistral-7B, remains an active area of
77 exploration. Our work directly contributes to this emerging intersection, specifically demonstrating
78 the efficacy of using embeddings from intermediate LLM layers for this task compared to traditional
79 baselines and different embedding strategies.

80 3 Methodology

81 Our approach contains several stages: dataset acquisition and processing, node feature extraction
82 using an LLM, graph construction, definition of link prediction models, and finally the training and
83 evaluation setup.

84 3.1 Dataset: OpenAlex

85 We utilized the OpenAlex dataset Priem et al. [2022], which is a large-scale, publicly available
86 knowledge graph of scholarly communication. To manage our computation resources, we focused

87 running our model on a specific subset of papers relevant to computer science and published since
88 2020. We queried the OpenAlex API using the following filters:

- 89 • Primary location’s source ID: S4306400194 (likely corresponding to a specific CS source
90 like arXiv CS).
- 91 • Concept ID: C41008148 (Computer Science).
- 92 • Publication date: From 2020-01-01 onwards.

93 We used the API’s cursor pagination, limiting the retrieval to 100 pages at 200 papers
94 per page which resulted in a raw dataset of 20,000 papers. For each paper, we ex-
95 tracted its OpenAlex ID, its list of cited OpenAlex IDs (`referenced_works`), and its ab-
96 stract (from `abstract_inverted_index`). We then saved this data locally to `.json` files
97 (`openalex_papers_raw.json`, `openalex_citations_raw.json`) to avoid unnessecary API
98 calls.

99 3.2 Mistral-7B Node Feature Extractions

100 To capture the semantic content of each paper, we generated node embeddings using the
101 `mistralai/Mistral-7B-v0.1` model Jiang et al. [2023].

102 **Model Loading:** We loaded the Mistral-7B model using the Hugging Face transformers library.
103 To fit the model onto available GPU memory (NVIDIA Tesla T4 with 15GB), we employed 4-bit
104 quantization using the `bitsandbytes` library Dettmers et al. [2023], with NF4 quantization type
105 (`bnb_4bit_quant_type="nf4"`) and `float16` compute data type.

106 **Input Processing:** Each paper’s reconstructed abstract served as the input text. The abstracts were
107 tokenized using the Mistral-7B tokenizer, with left-padding applied. We set a maximum sequence
108 length of 512 tokens, truncating longer abstracts. Empty abstracts were represented by the tokenizer’s
109 padding token to ensure consistent batch processing.

110 **Embedding Strategy - Layer Choice:** Our initial approach involved extracting hidden states from
111 the final layer of the Mistral-7B model. However, when these embeddings were used as input features
112 for the GNN, we observed poor performance: the model tended to overfit quickly, and the resulting
113 validation AUC scores were close to random chance (0.5), indicating that these embeddings did not
114 effectively capture the semantic relationships required for citation prediction.

115 This observation motivated a change in strategy based on the understanding of LLM internal repre-
116 sentations. The final layer of a causal LLM like Mistral-7B is highly specialized for its pre-training
117 objective, that is, predicting the next token. This specialization might cause it to lose some broader
118 semantic information relevant for downstream tasks like semantic similarity. In contrast, intermediate
119 layers, such as the second-to-last layer, often retain more general contextual and semantic information
120 about the entire input sequence before the model narrows its focus to next-token prediction Jawahar
121 et al. [2019]. Therefore, we hypothesized that embeddings derived from an earlier layer might be
122 more suitable for our task.

123 Following this reasoning and common practices for obtaining sentence/document embeddings
124 from transformers, we switched to using the hidden states from the second-to-last layer
125 (`outputs.hidden_states[-2]`) for generating our node features.

126 **Pooling Strategy:** We processed the abstracts in batches (batch size of 8). For each abstract, we
127 obtained the hidden states from the chosen second-to-last layer. To derive a single fixed-size vector
128 representation, we applied **mean pooling** across the sequence length dimension of these hidden
129 states, using the attention mask to exclude contributions from padding tokens. This resulted in a
130 4096-dimensional embedding vector for each paper node, which formed the basis for our successful
131 GNN experiments.

132 3.3 Graph Construction

133 Using the fetched paper data and generated embeddings, we constructed a graph suitable for PyTorch
134 Geometric (PyG) Fey and Lenssen [2019].

- 135 1. **ID Mapping:** We created a mapping from the unique OpenAlex paper IDs in our 20,000-
136 paper set to contiguous integer indices (0 to N-1, where N=20,000).
- 137 2. **Node Features (x):** The 4096-dimensional Mistral-7B embeddings were ordered according
138 to the ID mapping and stacked into a feature matrix $X \in \mathbb{R}^{N \times 4096}$.
- 139 3. **Edge Index (*edge_index*):** We iterated through the citation data. For each paper u in our
140 set, we checked if any of its cited papers v (*referenced_works*) were also present in our
141 20,000-paper set. If both u and v were in the set, we added a directed edge (u, v) to our
142 edge list, represented by their corresponding integer indices. This resulted in 6,114 edges
143 within our subset. The edge list was converted into the PyG *edge_index* format (a tensor of
144 shape $[2, num_edges]$).
- 145 4. **Data Object:** The node features X and the *edge_index* were combined into a PyG ‘Data’
146 object. This object, containing $N = 20,000$ nodes and $E = 6,114$ edges, was saved to disk
147 (openalex_subset_mistral_base_graph.pt).

148 3.4 Link Prediction Models

149 **Heuristic Baselines:** We implemented two standard link prediction heuristics as baselines:

- 150 • **Common Neighbors (CN):** The score for a potential link (u, v) is $|\Gamma(u) \cap \Gamma(v)|$, where
151 $\Gamma(x)$ is the set of neighbors of node x .
- 152 • **Adamic-Adar (AA):** The score is $\sum_{w \in \Gamma(u) \cap \Gamma(v)} \frac{1}{\log |\Gamma(w)|}$, down-weighting common neigh-
153 bors with high degrees.

154 These scores were calculated based on the adjacency structure of the training graph (after splitting)
155 and evaluated on the validation and test edge sets.

156 **Graph Neural Network (GNN):** We defined a GNN model for link prediction using PyG, following
157 an encoder-decoder architecture.

- 158 • **Encoder:** A multi-layer GNN processes the input node features (Mistral embeddings
159 from the second-to-last layer) and the graph structure (*edge_index*) to produce final node
160 embeddings Z . We used GraphSAGE Hamilton et al. [2017], layers with mean aggregation.
161 The specific architecture trained consisted of 3 layers: Input(4096) \rightarrow SAGE(128) \rightarrow ReLU
162 \rightarrow LayerNorm \rightarrow Dropout(0.5) \rightarrow SAGE(64) \rightarrow ReLU \rightarrow LayerNorm \rightarrow Dropout(0.5) \rightarrow
163 SAGE(64). LayerNorm and Dropout were applied after intermediate layers.
- 164 • **Decoder:** An MLP decoder takes the concatenated embeddings of a source node u and a
165 target node v from the encoder output ($z_u || z_v$) and predicts a score (logit) for the edge (u, v) .
166 This involved projecting the concatenated dimension ($64 + 64 = 128$) to 1 via linear layers
167 (potentially with intermediate ReLU activations as defined in the full *LinkPredictorGNN*
168 class).

169 The model takes node features X , the message-passing *edge_index*, and the *edge_label_index*
170 (edges to be predicted) as input and outputs prediction logits for the edges in *edge_label_index*.

171 3.5 Training and Evaluation Setup

172 **Data Splitting:** We used PyG’s ‘RandomLinkSplit’ transform to partition the edges of our graph
173 (data) into training, validation, and test sets. We configured the split as follows:

- 174 • $num_val = 0.1, num_test = 0.1$: 10
- 175 • $is_undirected = False$: Citations are directed.
- 176 • $add_negative_train_samples = False$: We sample negative edges manually during the
177 training loop.
- 178 • $neg_sampling_ratio = 1.0$: For validation and test sets, *RandomLinkSplit* automati-
179 cally samples an equal number of negative edges (non-existing links).

180 This resulted in:

- *train_data*: Contains N nodes, 4892 message-passing edges (*edge_index*). Positive training edges are implicitly these 4892 edges.
- *val_data*: Contains N nodes, 4892 message-passing edges (used for GNN propagation during eval), 1222 edges to predict (*edge_label_index*), with 611 positive and 611 negative examples (*edge_label*).
- *test_data*: Contains N nodes, 5503 message-passing edges (training edges + validation positive edges), 1222 edges to predict (*edge_label_index*), with 611 positive and 611 negative examples (*edge_label*).

189 GNN Training:

- **Objective:** Binary classification using *torch.nn.BCEWithLogitsLoss*.
- **Negative Sampling:** In each training epoch, for every positive edge in the training message-passing graph (*train_data.edge_index*), we sampled one negative edge using PyG’s *negative_sampling* function (sparse method).
- **Optimizer:** Adam with a learning rate of 1×10^{-5} and weight decay of 5×10^{-4} .
- **Epochs & Early Stopping:** The model was trained for a maximum of 150 epochs. Early stopping was employed with a patience of 15 epochs based on the validation AUC score. Training halts if the validation AUC does not improve for 15 consecutive epochs. The model state corresponding to the best validation AUC was saved.

199 **Evaluation Metrics:** We evaluated the models using standard link prediction metrics:

- Area Under the ROC Curve (AUC)
- Precision
- Recall
- F1-Score
- Accuracy

205 For Precision, Recall, F1-Score, and Accuracy, a classification threshold is required. We determined
 206 the optimal threshold by maximizing the F1-score on the validation set predictions generated by the
 207 best saved GNN model. This optimized threshold was then applied to the test set predictions for final
 208 reporting. Heuristics were evaluated using their raw scores for AUC and an illustrative threshold for
 209 other metrics.

210 4 Experiments and Results

211 4.1 Experimental Setup

212 All experiments were conducted on a Google Colab instance equipped with an NVIDIA Tesla T4
 213 GPU (15 GB VRAM). Key software libraries included PyTorch (v2.6.0), PyTorch Geometric (v2.6.1),
 214 Transformers (v4.44.1, approx.), BitsAndBytes (v0.43.2, approx.), NumPy, and Scikit-learn. Key
 215 hyperparameters for the GNN training are listed in Section 3.5.

216 4.2 Baseline Results (Heuristics)

217 We evaluated the Common Neighbors (CN) and Adamic-Adar (AA) heuristics on the validation and
 218 test sets. The scores were calculated using the training graph structure (*train_data.edge_index*).
 219 Results are presented in Table. AUC provides the most reliable comparison, as other metrics depend
 220 heavily on threshold selection for heuristics.

221 4.3 GNN Model Performance

222 The GNN model using Mistral-7B second-to-last layer embeddings was trained with early stopping
 223 based on validation AUC. The training loss decreased steadily over the epochs, indicating successful
 224 optimization on the training data, as shown in Figure 2. The validation and test AUC scores improved

Table 1: Performance of Heuristic Baselines on Validation and Test Sets.

Set	Heuristic	AUC	Precision	Recall	F1-Score	Accuracy
Validation	CN	0.6113	0.5000	1.0000	0.6667	0.5000
Test	CN	0.6121	0.5000	1.0000	0.6667	0.5000
Validation	AA	0.5458	0.4831	0.9345	0.6369	0.4673
Test	AA	0.5516	0.4844	0.9394	0.6392	0.4697

rapidly in the initial epochs and then plateaued, as visualized in Figure 1. The model achieved the best validation AUC of 0.9288 at epoch 63. The corresponding test AUC at this epoch was 0.9298. Early stopping was triggered at epoch 78, as the validation AUC did not improve further for 15 consecutive epochs.

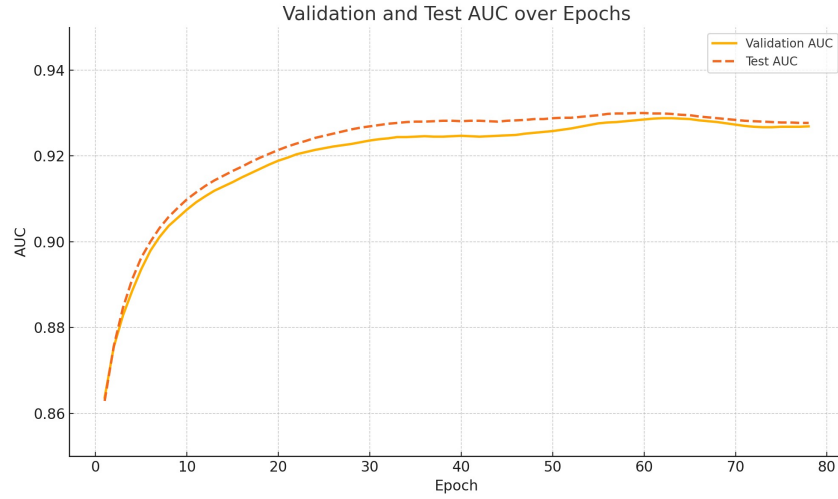


Figure 1: Validation and Test AUC scores over training epochs. The model reached peak validation performance around epoch 63.



Figure 2: Training loss (BCEWithLogitsLoss) over training epochs, showing consistent decrease.

The best saved model (from epoch 63) was evaluated on the test set. The optimal classification threshold determined on the validation set was 0.5918. Applying this threshold to the test set

231 predictions yielded the final performance metrics, summarized and compared with the baselines in
 232 Table 1.

Table 2: Final Link Prediction Performance Comparison on the Test Set.

Method	AUC	Precision	Recall	F1-Score	Accuracy
Common Neighbors (CN)	0.6121	0.5000*	1.0000*	0.6667*	0.5000*
Adamic-Adar (AA)	0.5516	0.4844*	0.9394*	0.6392*	0.4697*
GNN + Mistral-7B (L-1)	0.9298	0.8854	0.8347	0.8593	0.8633

*P/R/F1/Acc for heuristics based on an illustrative threshold; AUC is more reliable.

GNN results use embeddings from the second-to-last (L-1) layer of Mistral-7B.

GNN P/R/F1/Acc based on threshold optimized on validation set (0.5918).

233 4.4 Comparison and Discussion

234 The results clearly demonstrate the significant advantage of using the GNN model combined with
 235 appropriate LLM embeddings over the purely topology-based heuristic baselines. The GNN using
 236 second-to-last layer Mistral-7B embeddings achieved a test AUC of 0.930, dramatically exceeding
 237 the 0.612 AUC of the best heuristic (CN). This substantial improvement underscores the value of
 238 incorporating semantic information from paper abstracts.

239 Crucially, the choice of LLM layer for embedding extraction was vital. Our initial experiments
 240 using the final hidden layer yielded poor results (AUC roughly 0.5), likely because the final layer’s
 241 representations are overly specialized for next-token prediction and may lose broader semantic context
 242 valuable for similarity tasks. Switching to the second-to-last layer provided embeddings that were far
 243 more effective for the downstream link prediction task, aligning with observations that intermediate
 244 layers often capture more general semantics.

245 Our GNN leverages both the rich semantic features from the second-to-last LLM layer and the graph
 246 structure information learned through message passing. This two-fold approach allows it to identify
 247 potential citation links based on conceptual similarity, even in the absence of strong topological
 248 evidence like many shared neighbors. The balanced Precision (0.885) and Recall (0.835) further
 249 indicate the GNN’s superior ability to discriminate between true and false potential links compared
 250 to the baseline methods.

251 The need for careful hyperparameter tuning (low learning rate, weight decay) highlights the challenges
 252 of training GNNs on high-dimensional LLM features, but the final performance demonstrates the
 253 effectiveness of the approach when configured correctly.

254 5 Challenges Faced

255 5.1 Challenges Encountered

256 Several challenges were faced during this project:

- 257 • **Computational Cost & GPU Memory:** Generating embeddings using Mistral-7B, even
 258 quantized, was resource-intensive. Training the GNN on 4096-dimensional features also
 259 required significant GPU memory. Given our limited resources as undergraduate students,
 260 we felt a bit constrained and wished we could have scaled this implementation and project
 261 to a significant level.
- 262 • **Embedding Strategy Choice:** Selecting the optimal strategy for extracting embeddings
 263 from the LLM was non-trivial. Our initial failure using the final hidden layer necessitated
 264 experimentation and relying on insights about LLM layer representations, leading to the
 265 successful use of the second-to-last layer. Further exploration of layers or pooling methods
 266 could be beneficial but adds to the experimental overhead.
- 267 • **Data Handling & API Limitations:** Fetching and processing data from the large OpenAlex
 268 dataset required careful management of API calls, pagination, and data reconstruction.
 269 Subsetting was necessary for feasibility. Again, this refers back to computational cost;

270 ideally, with enough resources this would not have been necessary and moving forward wish
271 we could test on the entire dataset, or much more of it.

272 • **Hyperparameter Tuning:** Optimizing the GNN training process (learning rate, weight
273 decay) was crucial for achieving good performance and stability with the high-dimensional
274 LLM features. Given more time, we believe we could have optimized our model even more
275 to further demonstrate the capabilities of GNN paired with an LLM.

276 5.2 Future Improvements

277 The success of our approach using Mistral-7B embeddings and a GNN for citation link prediction
278 opens up several promising avenues for future research. A direct next step is to scale our method to a
279 significantly larger subset of the OpenAlex dataset or ideally, the entire dataset, provided sufficient
280 computational resources can be acquired. This would allow for training on a denser and more
281 representative graph, potentially revealing performance characteristics on a real-world scale.

282 Further exploration into the choice of LLM and embedding strategy is warranted. Experimenting with
283 different large language models (e.g., Llama, BERT variants, or models specifically fine-tuned for
284 scientific text) could yield even richer semantic representations. Investigating alternative methods for
285 deriving a fixed-size node embedding from the LLM’s output, such as using the CLS token equivalent,
286 different pooling strategies, or more sophisticated aggregation techniques across layers, could also
287 lead to performance improvements.

288 The GNN architecture itself can be further optimized. Testing different GNN layers (e.g., Graph
289 Attention Networks - GATs, Graph Convolutional Networks - GCNs), varying the number of layers,
290 hidden dimensions, and regularization techniques could enhance the model’s ability to leverage both
291 the semantic features and the graph structure. Additionally, exploring different decoder architectures
292 beyond simple concatenation and MLP could be beneficial.

293 A particularly interesting direction is to develop hybrid approaches that combine the LLM-derived
294 semantic embeddings with traditional topological features (like degree, clustering coefficient) or
295 metadata features (authors, venues, keywords) as initial node features for the GNN. This could allow
296 the model to benefit from multiple complementary sources of information.

297 Finally, incorporating temporal dynamics into the model is crucial for real-world citation prediction.
298 Future work could involve using time-aware GNN architectures or temporal graph sampling tech-
299 niques to model the evolving nature of the citation network and predict links based on the temporal
300 context of publications. Investigating the explainability of the model’s predictions – understanding
301 which semantic cues or structural patterns are most influential in predicting a citation – could also
302 provide valuable insights into scholarly communication.

303 6 Conclusion

304 This project successfully demonstrated the effectiveness of using Large Language Model embeddings
305 derived from an intermediate layer (second-to-last) of Mistral-7B as node features for improving
306 citation link prediction. The choice of embedding strategy was critical, as initial attempts using the
307 final layer embeddings failed to yield meaningful results. By combining the semantic understanding
308 captured by the appropriately chosen LLM layer with the structural learning capabilities of a Graph
309 Neural Network, our approach significantly outperformed standard topology-based heuristic methods,
310 achieving a test AUC of approximately 0.930 on a subset of the OpenAlex dataset. This highlights
311 the importance of both leveraging rich textual information via LLMs and carefully considering the
312 embedding extraction process for downstream graph learning tasks. While challenges remain, partic-
313 ularly concerning computational resources and optimal feature representation, this work confirms the
314 strong potential of integrating LLMs and GNNs for advancing our understanding and prediction of
315 scholarly communication networks.

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