

Enhancing Future Link Prediction in Quantum Computing Semantic Networks through LLM-Initiated Node Features

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Abstract

Quantum computing is rapidly evolving in both physics and computer science, offering the potential to solve complex problems and accelerate computational processes. The development of quantum chips necessitates understanding the correlations among diverse experimental conditions. Semantic networks built on scientific literature, representing meaningful relationships between concepts, have been used across various domains to identify knowledge gaps and novel concept combinations. Neural network-based approaches have shown promise in link prediction within these networks. This study proposes initializing node features using LLMs to enhance node representations for link prediction tasks in graph neural networks. LLMs can provide rich descriptions, reducing the need for manual feature creation and lowering costs. Our method, evaluated using various link prediction models on a quantum computing semantic network, demonstrated efficacy compared to traditional node embedding techniques. The code and data are available at: <https://github.com/boxorange/QC-LinkPrediction>

1 Introduction

Quantum computing is an active area of research in both physics and computer science, due to its potential to solve complex quantum physics problems and significantly accelerate certain computational processes (Shor, 1997; Montanaro, 2016; Arute et al., 2019). However, the current limitations of hardware hinder the practical application of quantum computers (Krantz et al., 2019; Kjaergaard et al., 2020), and the further development of robust quantum processors involves an increasingly wide range of conditions (Huang et al., 2021; Martinis, 2021), material characteristics (Murray, 2021; Place et al., 2021), and physical phenomena. Understanding the correlations among these variables and predicting their potential interconnections in

the future is crucial for experimental progress. Scientific literature serves as a vital resource for acquiring this knowledge, as it encompasses a vast array of research work.

A semantic network represents meaningful relationships between concepts, and researchers constructed a semantic network based on co-occurring concepts from scientific literature, utilizing it to identify knowledge gaps, missing connections between concepts, and novel combinations not previously considered (Rzhetsky et al., 2015; Krenn and Zeilinger, 2020). In recent years, Graph Neural Networks (GNNs) demonstrated promising predictive capabilities for link prediction within the graph forms of semantic networks (Zhang and Chen, 2018; Li et al., 2023). A significant challenge in creating semantic networks is the provision of sufficient initial features for nodes within a graph. In many real-world graph datasets, node features are often either missing or insufficient, potentially hindering link prediction models for effective learning and prediction (Zhao et al., 2017).

This study aims to initialize node features using Large Language Models (LLMs). LLMs have demonstrated exceptional performance across various question-answering tasks and information retrieval systems in zero-shot conditions (Kamalloo et al., 2023; Zhu et al., 2023), significantly improving text embeddings (Wang et al., 2023). These embeddings serve as initial node representations for link prediction tasks in GNNs. The rationale behind this approach is that LLMs, trained on extensive datasets from diverse literature and online sources, can provide rich descriptions of relevant concepts. This method enhances the feature set available for GNN training and reduces the reliance on human-curated feature creation. Additionally, it has the potential to produce more reliable node representations compared to traditional connectivity-based embeddings, particularly when connectivity data is lacking. In cold-start link prediction

problems (Sedhain et al., 2014; Zhang and Wang, 2015; Tang and Wang, 2022), where nodes lack edges, informative node features become critical (Zhao et al., 2017), contributing to the generation of structural information and facilitating link formation (Müller et al., 2024). Our approach offers a straightforward yet impactful method for node feature initialization using LLMs, without the need for external resources or dependency on graph structure. We evaluated this method through various link prediction models, conducting a comparative analysis with widely-used node embedding techniques within a quantum computing semantic network.

2 Creation of Semantic Network for Quantum Computing

The construction of a concept network from scratch necessitates significant human resources and time. As an alternative, we utilize the pre-existing semantic network of quantum physics. SEMNET (Krenn and Zeilinger, 2020) was developed to forecast future research trends in quantum physics. It is based on scientific publications in the field of quantum physics and includes a list of human-compiled quantum physics concepts derived from books and Wikipedia. In SEMNET, nodes represent physical concepts, and edges indicate the co-occurrence of two concepts in an article’s title or abstract.

Our domain experts in quantum physics have scrutinized the list of concepts, selecting those that have a high correlation with quantum computing research. Certain concepts were revised, and additional ones that appeared to be pertinent to quantum computing research, such as "quasiparticle poisoning," were incorporated. This process resulted in a compilation of 3,001 quantum computing concepts.

Given the lack of a corpus upon which SEMNET was created, we scraped all articles under the quantum physics category on arXiv that contained at least a pair of quantum computing concepts. This resulted in a total of 136,122 papers spanning from 2007 to 2024 (as of June 15, 2024). Appendix A illustrates the number of quantum computing papers published on arXiv over time.

3 LLM-powered Concept Feature Embedding

We derived quantum computing concept features from LLMs using a question-answering prompt. For this purpose, we employed a selection of state-of-the-art LLMs, specifically Gemini-1.0-pro

(Gemini-Team et al., 2023), Mixtral (Jiang et al., 2024), and LLaMA 3 (Meta-AI, 2024). The following example illustrates a query prompt and the corresponding answer generated by an LLM.

Query: What are the features of quasiparticle in quantum computing?

Answer:

1. **Wave-Particle Duality:** Quasiparticles exhibit both wave-like and particle-like behavior. They can be described by a wave function, which determines their quantum state and allows them to interfere with each other. At the same time, they can also behave as localized particles with well-defined energy and momentum.
 2. **Collective Behavior:** Quasiparticles often arise from the collective behavior of many interacting particles. They emerge as excitations of a quantum system, such as a solid or a liquid, and represent the quantum mechanical description of these collective modes.
 3. **Quasiparticle Energy and Momentum:** Quasiparticles have a well-defined energy and momentum, which are related to their wave-like properties. The energy and momentum of a quasiparticle are typically not the same as the energy and momentum of the individual particles that make up the system.
- ...

We utilized the Google AI Text Embedding model (Google-AI, 2024), text-embedding-004, to generate text embeddings from the concept features produced by the LLMs. Figure 1 illustrates the node features derived from the LLMs, which are used in the link prediction models.

4 Experiments

We evaluated the initial node representations generated by LLMs in a transductive experimental setup, where models predict edges between existing nodes in the graph. The models were trained on historical concept connections and tasked with predicting future, unknown connections. The evaluation was performed using various link prediction algorithms.

4.1 Experiment Setup

Dataset An undirected homogeneous (binary) graph, also known as a single relational graph, was constructed for the purpose of link prediction. The dataset was divided into three subsets based on specific time intervals, a common approach for time series data in link prediction tasks (chronological splitting). The training set encompassed the period from 2007 to 2021 and included 428,079 edges. The validation set corresponded to the year 2022 and contained 25,011 edges. The test set covered

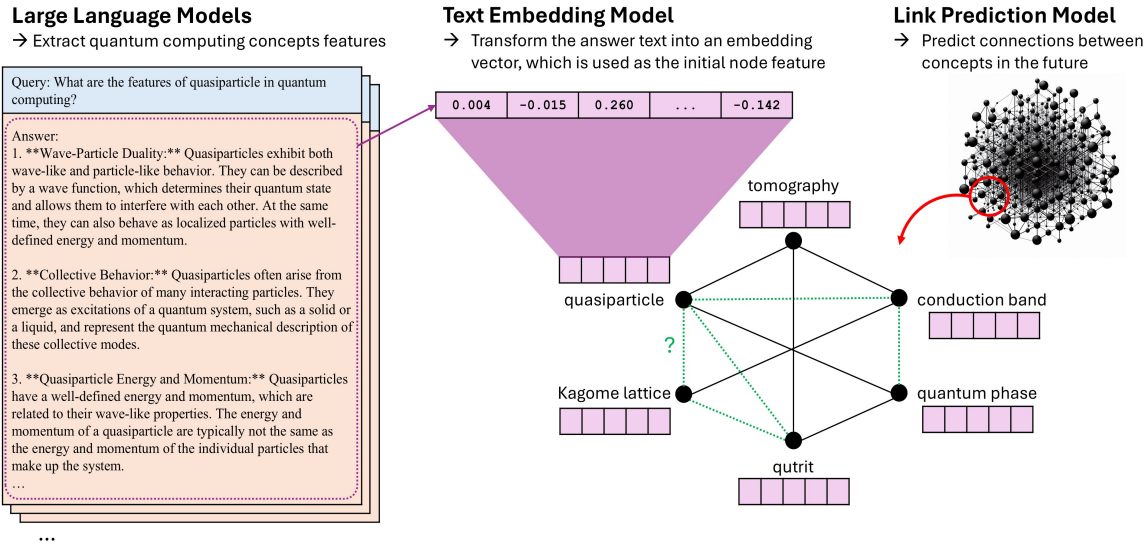


Figure 1: The overview of future link predictions in the quantum computing semantic network using LLM-generated initial node features. In the example graph, solid lines indicate past established connections, while dotted lines represent a subset of potential future connections to be predicted by the model for relevance.

the most recent year, from 2023 to 2024, comprising 50,063 edges. The dataset was distributed with an approximate ratio of 85:5:10 for training, validation, and testing, respectively.

Link Prediction Models & Baselines We conducted an evaluation of the proposed node features across three classes of link prediction models: (1) Multi-layer Perceptron (MLP), (2) message-passing mechanism-based GNNs including GraphSAGE (Hamilton et al., 2017), GCN (Kipf and Welling, 2016a), and GAE (Kipf and Welling, 2016b), and (3) GNNs with pair-wise information methods, specifically NCN (Wang et al., 2024b) and BUDDY (Chamberlain et al., 2023) that leverage common neighbor information and sub-graph features to further capture the relation between the nodes for potential links respectively. The selection of these GNN models was based on their high ranking in recent comprehensive evaluations of link prediction methods (Li et al., 2023).

We conducted a comparative analysis of the embeddings generated by LLMs with those produced by widely recognized node embedding methods, including DeepWalk (Perozzi et al., 2014), LINE (Tang et al., 2015), and node2vec (Grover and Leskovec, 2016). These methods were employed in previous studies comparing node feature initialization techniques (Duong et al., 2019; Zhu et al., 2021; Berahmand et al., 2021; Cui et al., 2022).

Implementation Details & Evaluation Setting

The experiments were conducted using $4 \times$ NVIDIA A100 80GB GPUs. Specifically, the Mixtral-8x7B-Instruct (46B) and LLaMA-3 (70B) models were executed on $4 \times$ NVIDIA A100 80GB GPUs to generate concept features. All link prediction methods were performed on a single NVIDIA A100 80GB GPU. The Google Gemini-1.0-pro and text-embedding-004 models were accessed via the Gemini APIs. The maximum number of generated tokens per query was set to 512 for all models, and the default embedding size of 768, as produced by the Google text embedding model, was employed. To maintain consistency, node embeddings of size 768 were also generated using the baseline methods. In terms of latency, the Gemini-pro model required approximately 3 hours, the Mixtral model 6 hours, and the LLaMA-3 (70B) model 8 hours to generate features related to quantum computing concepts. The text embedding process was completed in less than 2 minutes.

We followed the hyper-parameter ranges for the models employed in the comprehensive link prediction evaluation (Li et al., 2023). For the model evaluation, we measured the area under the receiver operating characteristic curve (AUROC) and average precision (AP), which are commonly used metrics for link prediction tasks in homogeneous graphs. These metrics provide a robust and comprehensive assessment of the model’s performance (Yang et al., 2015; Zhu et al., 2021). Each experi-

Node Embedding	MLP		GCN		GraphSAGE	
	AUROC	AP	AUROC	AP	AUROC	AP
DeepWalk	82.48 ± 0.19	80.72 ± 0.12	88.98 ± 0.14	87.80 ± 0.17	86.40 ± 0.21	84.51 ± 0.24
LINE	83.92 ± 0.48	81.94 ± 0.52	86.95 ± 0.03	85.51 ± 0.02	83.25 ± 2.62	80.48 ± 4.11
node2vec	84.82 ± 0.20	82.75 ± 0.25	88.27 ± 0.18	86.76 ± 0.28	87.06 ± 0.14	85.31 ± 0.20
Gemini-1.0-pro	86.56 ± 0.20	84.62 ± 0.26	89.63 ± 0.05	88.39 ± 0.05	88.79 ± 0.12	87.33 ± 0.14
LLaMA3 (70B)	86.15 ± 0.24	84.18 ± 0.29	89.52 ± 0.06	88.29 ± 0.07	88.67 ± 0.09	87.16 ± 0.11
Mixtral-8x7B (46B)	87.02 ± 0.22	85.14 ± 0.27	89.61 ± 0.08	88.38 ± 0.11	88.87 ± 0.10	87.45 ± 0.18

Node Embedding	GAE		NCN		BUDDY	
	AUROC	AP	AUROC	AP	AUROC	AP
DeepWalk	86.18 ± 0.10	84.39 ± 0.10	88.92 ± 0.17	87.52 ± 0.21	87.84 ± 0.07	86.31 ± 0.10
LINE	86.56 ± 0.01	85.13 ± 0.01	88.83 ± 0.06	87.42 ± 0.08	87.63 ± 0.02	86.13 ± 0.02
node2vec	81.89 ± 0.44	80.12 ± 0.43	88.98 ± 0.12	87.66 ± 0.15	88.55 ± 0.08	87.18 ± 0.08
Gemini-1.0-pro	87.27 ± 0.12	85.35 ± 0.13	89.07 ± 0.25	87.46 ± 0.28	88.79 ± 0.07	87.35 ± 0.09
LLaMA3 (70B)	86.89 ± 0.11	85.03 ± 0.11	88.90 ± 0.24	87.33 ± 0.27	88.55 ± 0.04	87.09 ± 0.06
Mixtral-8x7B (46B)	86.77 ± 0.15	84.91 ± 0.14	88.99 ± 0.27	87.44 ± 0.25	88.87 ± 0.06	87.40 ± 0.08

Table 1: Comparison of LLM-generated node embeddings with other node embeddings in link prediction methods on a homogeneous, undirected graph representing quantum computing concept relations in a transductive setting. **Bold** indicates the best score among all initial node embeddings in the model.

ment was repeated ten times with different random seeds to ensure the reliability of the results.

4.2 Node Embedding Comparison Results

Table 1 presents the link prediction results using baseline and LLM-powered node embeddings. The majority of models initialized with LLM-generated embeddings demonstrated higher performance than their baseline counterparts. Among the methods evaluated, Gemini and Mixtral typically emerged as the top performers, although no clear winner was identified, while Llama showed slightly weaker performance. Notably, the LLM-generated features resulted in more significant improvements in MLP and message passing GNNs (GCN, GraphSAGE, GAE) than in the GNN with pair-wise information methods (NCN, BUDDY). This can be attributed to the fact that MLP and GNNs relying on message passing mechanisms are generally more impacted by the initial node embeddings compared to those models that incorporate additional link specific information. Message passing aggregates information from a node’s neighborhood, and if the initial embedding already captures substantial information, it can have a stronger influence on the final embedding.

We further compared node feature initialization methods on isolated (zero-degree) nodes, which pose significant challenges for GNNs (Ahn and Kim, 2021; Zanardini and Serrano, 2024). We identified 30 isolated nodes in the training data and

1,382 connections to these in the test data. The evaluation results are presented in Appendix B. Although the baseline methods exhibited higher performance in certain instances, particularly with the GCN in conjunction with LINE, the representations produced by LLMs were generally more effective in identifying previously unseen connections to isolated nodes. Furthermore, they yielded a more consistent performance in comparison to the baseline methodologies. For these isolated nodes, the content of the node features is crucial for the link prediction task due to the absence of connectivity information. The baseline models typically generate node embeddings based on the connectivity information of a graph, which may result in inadequate embeddings for isolated nodes. In contrast, embeddings generated by LLMs are robust against the absence of link connectivity information and can thus produce reliable representations for isolated nodes.

4.3 Merging LLM embeddings

We conducted an evaluation incorporating features from various models. To merge conceptual features derived from multiple LLMs, we employed mean- and max-pooling on the embeddings, and we extracted concise conceptual features from the outputs of three LLMs using the Gemini-pro model. The prompt used was: "Summarize this text about the features of {KEYWORD}. Text: {CONCATENATED FEATURES FROM THE LLMs}."

Models	Embedding	AUROC	AP
MLP	Mixtral	87.02 ± 0.22	85.14 ± 0.27
	Mean pool	86.95 ± 0.17	4.96 ± 0.19
	Max pool	87.06 ± 0.18	85.16 ± 0.19
	LLM-Blender	86.71 ± 0.17	84.70 ± 0.17
	Summarized	86.72 ± 0.14	84.81 ± 0.21
GCN	Gemini Pro	89.63 ± 0.05	88.39 ± 0.05
	Mean pool	89.68 ± 0.08	88.45 ± 0.09
	Max pool	89.58 ± 0.06	88.33 ± 0.09
	LLM-Blender	89.60 ± 0.04	88.37 ± 0.08
NCN	Gemini Pro	89.07 ± 0.25	87.46 ± 0.28
	Mean pool	89.08 ± 0.22	87.64 ± 0.23
	Max pool	88.96 ± 0.24	87.47 ± 0.25
	LLM-Blender	88.96 ± 0.22	87.40 ± 0.20
	Summarized	88.84 ± 0.23	87.29 ± 0.25

Table 2: Comparison of different merging methods of LLM-generated feature embeddings. **Bold** indicates the best score in the model, and *italic* denotes performance degradation relative to the standalone embedding.

Furthermore, we evaluated a method to select the optimal response for each query from three distinct models, utilizing LLM-Blender (Jiang et al., 2023). This ensembling framework chooses the top score answer from multiple LLMs through a specialized pairwise comparison technique and a generative fusion module. These merged embeddings were compared against the leading LLM node embeddings across different models, including MLP, GCN (top performance among message-passing models), and NCN (the highest scorer in GNNs with pairwise information). The comparative analysis, presented in Table 2, highlights that simple techniques such as mean or max pooling can effectively merge embeddings. While these methods reduce the need for more complex approaches, certain pooling strategies exhibited performance degradation compared to standalone embeddings.

4.4 Time Decayed Embedding

Additionally, we incorporated time-decay information from the dataset. In future trend predictions involving time series data, time-decayed information can be important for maintaining the relevance of recent data and highlighting recent changes. To leverage the time-decay information of concept pairs over time, we developed time-decayed node representations based on co-occurrence matrices by year. These representations can be integrated with the LLM feature embeddings to enhance the

Models	Embedding	AUROC	AP
MLP	Gemini	86.56 ± 0.20	84.62 ± 0.26
	Gemini + TD	87.85 ± 0.24	86.25 ± 0.35
	LLaMA3	86.15 ± 0.24	84.18 ± 0.29
	LLaMA3 + TD	87.26 ± 0.20	85.62 ± 0.27
	Mixtral	87.02 ± 0.22	85.14 ± 0.27
	Mixtral + TD	87.94 ± 0.28	86.33 ± 0.32
GCN	Gemini	89.63 ± 0.05	88.39 ± 0.05
	Gemini + TD	89.65 ± 0.09	88.46 ± 0.09
	LLaMA3	89.52 ± 0.06	88.29 ± 0.07
	LLaMA3 + TD	89.61 ± 0.04	88.40 ± 0.07
	Mixtral	89.61 ± 0.08	88.38 ± 0.11
NCN	Mixtral + TD	89.65 ± 0.05	88.47 ± 0.05
	Gemini	89.07 ± 0.25	87.46 ± 0.28
	Gemini + TD	89.14 ± 0.27	87.75 ± 0.27
	LLaMA3	88.90 ± 0.24	87.33 ± 0.27
	LLaMA3 + TD	89.08 ± 0.20	87.61 ± 0.19
	Mixtral	88.99 ± 0.27	87.44 ± 0.25
Mixtral + TD	89.04 ± 0.24	87.51 ± 0.22	

Table 3: Link prediction performance using Time-Decayed (TD) embedding concatenation. **Bold** indicates the best score among all embeddings.

model’s capabilities. The time-decayed embeddings serve as optional auxiliary data in time series analyses, as they cannot function as standalone embeddings due to the potential lack of connections between concepts, which would result in non-informative embeddings. A comprehensive explanation of the time-decayed embedding generation process is available in the Appendix C. Table 3 shows the performance of MLP, GCN, and NCN models with concatenated node embeddings with LLM features and time-decayed representations. The incorporation of time-decayed information in the node representation enhanced all models predictive capability, with the MLP model demonstrating the greatest improvement.

5 Implications of Model Predictions: An Analytical Review by Domain Scientists

Our domain scientists examined the connections commonly predicted correctly by the top three models. While many of the link predictions correspond to fundamental concept connections that have existed within the field of quantum information science for many years (e.g., “nonlinear oscillator” and “transmon,” “Hilbert space” and “quantum information,” etc.), some of the emerging connections within the test set seem timely and point towards recent trends and scientific breakthroughs

within the field. Two examples relevant to quantum engineering that were observed within the data set are listed below.

The models accurately predicted a breakthrough in the coherent control of magnons (Xu et al., 2023). Methods for coupling classical magnons to photon cavities have been in development for the past decade (Huebl et al., 2013; Tabuchi et al., 2015; Boventer et al., 2018, 2020), and the recent development of nonclassical coherent control of magnons built on this prior work. Therefore, it can be concluded that the models recognized the trend toward coherently controlled quantum magnonics for its prediction.

Likewise, the models recognized the importance of phonon engineering to the performance of superconducting qubits (Kitzman et al., 2023). This concept connection, which emerged naturally with the field of superconducting technologies, has been vitally important within the context of recent studies (Wilén et al., 2021; Yelton et al., 2024) on gamma and muon ray impacts on superconducting quantum devices, wherein phonons serve as the mediating particle for qubit decoherence from such high-energy particles. Indeed, phonon engineering will likely prove to be an essential component of quantum engineering in the coming years.

6 Related Work

LLMs have shown impressive performance across numerous NLP tasks, particularly in node classification on graphs (Fatemi et al., 2024; Chen et al., 2024). However, they struggle to capture graph structural information (Wang et al., 2024a) and face scalability issues (Hu et al., 2020) due to higher prediction costs compared to GNNs. Despite this, LLMs provide valuable semantic knowledge, particularly for node feature initialization, enhancing GNN performance in link prediction. In this study, we employed three advanced LLMs: Google’s Gemini Pro (Gemini-Team et al., 2023), a multi-modal model for complex reasoning, Mixtral-8x7B (Jiang et al., 2024), which supports long sequences and efficient inference, and Meta’s Llama 3 (Meta-AI, 2024), known for its optimized architecture and versatility across tasks.

GNNs have become a powerful method for homogeneous link prediction. Architectures like GCN (Kipf and Welling, 2016a), GraphSAGE (Hamilton et al., 2017), and GAE (Kipf and Welling, 2016b) encode node features and graph

topology into low-dimensional embeddings for predicting link likelihood between nodes. Variational autoencoders (VAEs) (Ahn and Kim, 2021) further enhance representation learning by encoding data into a latent space for reconstruction. GNNs excel in capturing higher-order relationships and learning expressive node representations, outperforming traditional heuristic methods, especially in large, complex networks. Recent approaches like BUDDY (Chamberlain et al., 2023) and NCN (Wang et al., 2024b) improve link prediction by leveraging pairwise information, including subgraphs and common neighbor data.

DeepWalk (Perozzi et al., 2014), LINE (Tang et al., 2015), and node2vec (Grover and Leskovec, 2016) are network embedding methods. DeepWalk applies Skip-Gram to node sequences generated by random walks, while LINE preserves local and global structures by optimizing first and second-order proximities. Node2vec introduces flexibility with biased random walks, interpolating between BFS and DFS using two parameters. These methods are essential for tasks such as link prediction, node classification, and recommendation systems.

7 Conclusion and Future Work

Our proposed approach offers a promising avenue for enhancing the performance of link prediction models, particularly in scenarios where initial node features are sparse or inadequate. This method not only enriches the feature set available for model training but also improves the model’s ability to capture and represent complex patterns within the data. We applied this method to a quantum computing semantic network constructed from relevant scientific literature, and the models with node feature initialization by LLMs outperformed baseline node embedding methods across various link prediction models. Our approach is easily extendable to other graph datasets in different domains that lack adequate node features.

In this study, we focused exclusively on featurizing nodes within a graph, although edge features are also crucial for training models. Unlike node features, generating edge features via LLMs may not be practical due to the significantly higher number of edges compared to nodes. More effective edge feature generation methods by LLMs, such as clustering edges based on the characteristics of the involved nodes, will be explored in future research. Additionally, our experiments were lim-

ited to static graph settings. Dynamic GNNs and time-dependent graph methods could potentially improve prediction capabilities. Future work will aim to refine this approach further and explore its applicability in other graph-based learning tasks.

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References

- Seong Jin Ahn and MyoungHo Kim. 2021. Variational graph normalized autoencoders. In *Proceedings of the 30th ACM international conference on information & knowledge management*, pages 2827–2831.
- Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C. Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando G. S. L. Brandao, David A. Buell, Brian Burkett, Yu Chen, Zijun Chen, Ben Chiaro, Roberto Collins, William Courtney, Andrew Dunsworth, Edward Farhi, Brooks Foxen, Austin Fowler, Craig Gidney, Marissa Giustina, Rob Graff, Keith Guerin, Steve Habegger, Matthew P. Harrigan, Michael J. Hartmann, Alan Ho, Markus Hoffmann, Trent Huang, Travis S. Humble, Sergei V. Isakov, Evan Jeffrey, Zhang Jiang, Dvir Kafri, Kostyantyn Kechedzhi, Julian Kelly, Paul V. Klimov, Sergey Knysh, Alexander Korotkov, Fedor Kostritsa, David Landhuis, Mike Lindmark, Erik Lucero, Dmitry Lyakh, Salvatore Mandrà, Jarrod R. McClean, Matthew McEwen, Anthony Megrant, Xiao Mi, Kristel Michielsen, Masoud Mohseni, Josh Mutus, Ofer Naaman, Matthew Neeley, Charles Neill, Murphy Yuezhen Niu, Eric Ostby, Andre Petukhov, John C. Platt, Chris Quintana, Eleanor G. Rieffel, Pedram Roushan, Nicholas C. Rubin, Daniel Sank, Kevin J. Satzinger, Vadim Smelyanskiy, Kevin J. Sung, Matthew D. Trevithick, Amit Vainsencher, Benjamin Villalonga, Theodore White, Z. Jamie Yao, Ping Yeh, Adam Zalcman, Hartmut Neven, and John M. Martinis. 2019. [Quantum supremacy using a programmable superconducting processor](#). *Nature*, 574(7779):505–510.
- Kamal Berahmand, Elahe Nasiri, Mehrdad Rostami, and Saman Forouzandeh. 2021. A modified deep-walk method for link prediction in attributed social network. *Computing*, 103:2227–2249.
- Isabella Boverter, Christine Dörflinger, Tim Wolz, Rair Macêdo, Romain Lebrun, Mathias Kläui, and Martin Weides. 2020. [Control of the coupling strength and linewidth of a cavity magnon-polariton](#). *Phys. Rev. Res.*, 2:013154.
- Isabella Boverter, Marco Pfirrmann, Julius Krause, Yannick Schön, Mathias Kläui, and Martin Weides. 2018. [Complex temperature dependence of coupling and dissipation of cavity magnon polaritons from millikelvin to room temperature](#). *Phys. Rev. B*, 97:184420.
- Benjamin Paul Chamberlain, Sergey Shirobokov, Emanuele Rossi, Fabrizio Frasca, Thomas Markovich, Nils Hammerla, Michael M Bronstein, and Max Hansmire. 2023. Graph neural networks for link prediction with subgraph sketching. *ICLR*.
- Zhikai Chen, Haitao Mao, Hongzhi Wen, Haoyu Han, Wei Jin, Haiyang Zhang, Hui Liu, and Jiliang Tang. 2024. [Label-free node classification on graphs with large language models \(LLMs\)](#). In *The Twelfth International Conference on Learning Representations*.
- Hejie Cui, Zijie Lu, Pan Li, and Carl Yang. 2022. On positional and structural node features for graph neural networks on non-attributed graphs. In *Proceedings of the 31st ACM International Conference on Information & Knowledge Management*, pages 3898–3902.
- Chi Thang Duong, Thanh Dat Hoang, Ha The Hien Dang, Quoc Viet Hung Nguyen, and Karl Aberer. 2019. On node features for graph neural networks. *arXiv preprint arXiv:1911.08795*.
- Bahare Fatemi, Jonathan Halcrow, and Bryan Perozzi. 2024. [Talk like a graph: Encoding graphs for large language models](#). In *The Twelfth International Conference on Learning Representations*.
- Gemini-Team, Rohan Anil, Sebastian Borgeaud, Yonghui Wu, Jean-Baptiste Alayrac, Jiahui Yu, Radu Soricut, Johan Schalkwyk, Andrew M Dai, Anja Hauth, et al. 2023. Gemini: a family of highly capable multimodal models. *arXiv preprint arXiv:2312.11805*.
- Google-AI. 2024. Text embeddings api | generative ai on vertex ai. <https://cloud.google.com/vertex-ai/generative-ai/docs/embeddings/get-text-embeddings>.
- Aditya Grover and Jure Leskovec. 2016. node2vec: Scalable feature learning for networks. In *Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 855–864.
- Will Hamilton, Zhitao Ying, and Jure Leskovec. 2017. Inductive representation learning on large graphs. *Advances in neural information processing systems*, 30.
- Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. 2020. Open graph benchmark: Datasets for machine learning on graphs. *Advances in neural information processing systems*, 33:22118–22133.

- Sihao Huang, Benjamin Lienhard, Greg Calusine, Antti Vepsäläinen, Jochen Braumüller, David K. Kim, Alexander J. Melville, Bethany M. Niedzielski, Jonilyn L. Yoder, Bharath Kannan, Terry P. Orlando, Simon Gustavsson, and William D. Oliver. 2021. **Microwave package design for superconducting quantum processors**. *PRX Quantum*, 2:020306.
- Hans Huebl, Christoph W. Zollitsch, Johannes Lotze, Fredrik Hocke, Moritz Greifenstein, Achim Marx, Rudolf Gross, and Sebastian T. B. Goennenwein. 2013. **High cooperativity in coupled microwave resonator ferrimagnetic insulator hybrids**. *Phys. Rev. Lett.*, 111:127003.
- Albert Q Jiang, Alexandre Sablayrolles, Antoine Roux, Arthur Mensch, Blanche Savary, Chris Bamford, Devendra Singh Chaplot, Diego de las Casas, Emma Bou Hanna, Florian Bressand, et al. 2024. **Mixtral of experts**. *arXiv preprint arXiv:2401.04088*.
- Dongfu Jiang, Xiang Ren, and Bill Yuchen Lin. 2023. **Llm-blender: Ensembling large language models with pairwise ranking and generative fusion**. In *The 61st Annual Meeting Of The Association For Computational Linguistics*.
- Ehsan Kamaloo, Nouha Dziri, Charles Clarke, and Davood Rafiei. 2023. **Evaluating open-domain question answering in the era of large language models**. In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 5591–5606.
- Thomas N Kipf and Max Welling. 2016a. **Semi-supervised classification with graph convolutional networks**. *arXiv preprint arXiv:1609.02907*.
- Thomas N Kipf and Max Welling. 2016b. **Variational graph auto-encoders**. *arXiv preprint arXiv:1611.07308*.
- J. M. Kitzman, J. R. Lane, C. Undershute, P. M. Harrington, N. R. Beysengulov, C. A. Mikolas, K. W. Murch, and J. Pollanen. 2023. **Phononic bath engineering of a superconducting qubit**. *Nature Communications*, 14(1):3910.
- Morten Kjaergaard, Mollie E. Schwartz, Jochen Braumüller, Philip Krantz, Joel I.-J. Wang, Simon Gustavsson, and William D. Oliver. 2020. **Superconducting qubits: Current state of play**. *Annual Review of Condensed Matter Physics*, 11(Volume 11, 2020):369–395.
- P. Krantz, M. Kjaergaard, F. Yan, T. P. Orlando, S. Gustavsson, and W. D. Oliver. 2019. **A quantum engineer’s guide to superconducting qubits**. *Applied Physics Reviews*, 6(2):021318.
- Mario Krenn and Anton Zeilinger. 2020. **Predicting research trends with semantic and neural networks with an application in quantum physics**. *Proceedings of the National Academy of Sciences*, 117(4):1910–1916.
- Juanhui Li, Harry Shomer, Haitao Mao, Shenglai Zeng, Yao Ma, Neil Shah, Jiliang Tang, and Dawei Yin. 2023. **Evaluating graph neural networks for link prediction: Current pitfalls and new benchmarking**. In *Advances in Neural Information Processing Systems*, volume 36, pages 3853–3866. Curran Associates, Inc.
- John M. Martinis. 2021. **Saving superconducting quantum processors from decay and correlated errors generated by gamma and cosmic rays**. *npj Quantum Information*, 7(1):90.
- Meta-AI. 2024. **Introducing meta llama 3: The most capable openly available llm to date**. <https://ai.meta.com/blog/llama3>. Accessed: 2024-04-19.
- Ashley Montanaro. 2016. **Quantum algorithms: an overview**. *npj Quantum Information*, 2(1):15023–15030.
- Luis Müller, Mikhail Galkin, Christopher Morris, and Ladislav Rampásek. 2024. **Attending to graph transformers**. *Transactions on Machine Learning Research*.
- Conal E. Murray. 2021. **Material matters in superconducting qubits**. *Materials Science and Engineering: R: Reports*, 146:100646.
- Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. 2014. **Deepwalk: Online learning of social representations**. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 701–710.
- Alexander P. M. Place, Lila V. H. Rodgers, Pranav Mundada, Basil M. Smitham, Mattias Fitzpatrick, Zhaoqi Leng, Anjali Premkumar, Jacob Bryon, Andrei Vrajitoarea, Sara Sussman, Guangming Cheng, Trisha Madhavan, Harshvardhan K. Babla, Xuan Hoang Le, Youqi Gang, Berthold Jäck, András Gyenis, Nan Yao, Robert J. Cava, Nathalie P. de Leon, and Andrew A. Houck. 2021. **New material platform for superconducting transmon qubits with coherence times exceeding 0.3 milliseconds**. *Nature Communications*, 12(1):1779.
- Andrey Rzhetsky, Jacob G Foster, Ian T Foster, and James A Evans. 2015. **Choosing experiments to accelerate collective discovery**. *Proceedings of the National Academy of Sciences*, 112(47):14569–14574.
- Suvash Sedhain, Scott Sanner, Darius Braziunas, Lexing Xie, and Jordan Christensen. 2014. **Social collaborative filtering for cold-start recommendations**. In *Proceedings of the 8th ACM Conference on Recommender systems*, pages 345–348.
- Peter W. Shor. 1997. **Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer**. *SIAM Journal on Computing*, 26(5):1484–1509.

Yutaka Tabuchi, Seiichiro Ishino, Atsushi Noguchi, Toyofumi Ishikawa, Rekishu Yamazaki, Koji Usami, and Yasunobu Nakamura. 2015. [Coherent coupling between a ferromagnetic magnon and a superconducting qubit](#). *Science*, 349(6246):405–408.

Jian Tang, Meng Qu, Mingzhe Wang, Ming Zhang, Jun Yan, and Qiaozhu Mei. 2015. [Line: Large-scale information network embedding](#). In *Proceedings of the 24th international conference on world wide web*, pages 1067–1077.

Minghu Tang and Wenjun Wang. 2022. [Cold-start link prediction integrating community information via multi-nonnegative matrix factorization](#). *Chaos, Solitons & Fractals*, 162:112421.

Heng Wang, Shangbin Feng, Tianxing He, Zhaoxuan Tan, Xiaochuang Han, and Yulia Tsvetkov. 2024a. [Can language models solve graph problems in natural language?](#) *Advances in Neural Information Processing Systems*, 36.

Liang Wang, Nan Yang, Xiaolong Huang, Linjun Yang, Rangan Majumder, and Furu Wei. 2023. [Improving text embeddings with large language models](#). *arXiv preprint arXiv:2401.00368*.

Xiyuan Wang, Haotong Yang, and Muhan Zhang. 2024b. [Neural common neighbor with completion for link prediction](#). In *The Twelfth International Conference on Learning Representations*.

C. D. Wilen, S. Abdullah, N. A. Kurinsky, C. Stanford, L. Cardani, G. D’Imperio, C. Tomei, L. Faoro, L. B. Ioffe, C. H. Liu, A. Opremcak, B. G. Christensen, J. L. DuBois, and R. McDermott. 2021. [Correlated charge noise and relaxation errors in superconducting qubits](#). *Nature*, 594(7863):369–373.

Da Xu, Xu-Ke Gu, He-Kang Li, Yuan-Chao Weng, Yi-Pu Wang, Jie Li, H. Wang, Shi-Yao Zhu, and J. Q. You. 2023. [Quantum control of a single magnon in a macroscopic spin system](#). *Phys. Rev. Lett.*, 130:193603.

Yang Yang, Ryan N Lichtenwalter, and Nitesh V Chawla. 2015. [Evaluating link prediction methods](#). *Knowledge and Information Systems*, 45:751–782.

E. Yelton, C. P. Larson, V. Iaia, K. Dodge, G. La Magna, P. G. Baity, I. V. Pechenezhskiy, R. McDermott, N. A. Kurinsky, G. Catelani, and B. L. T. Plourde. 2024. [Modeling phonon-mediated quasiparticle poisoning in superconducting qubit arrays](#). *Phys. Rev. B*, 110:024519.

Damiano Zanardini and Emilio Serrano. 2024. [Introducing new node prediction in graph mining: Predicting all links from isolated nodes with graph neural networks](#). *CoRR*.

Muhan Zhang and Yixin Chen. 2018. [Link prediction based on graph neural networks](#). *Advances in neural information processing systems*, 31.

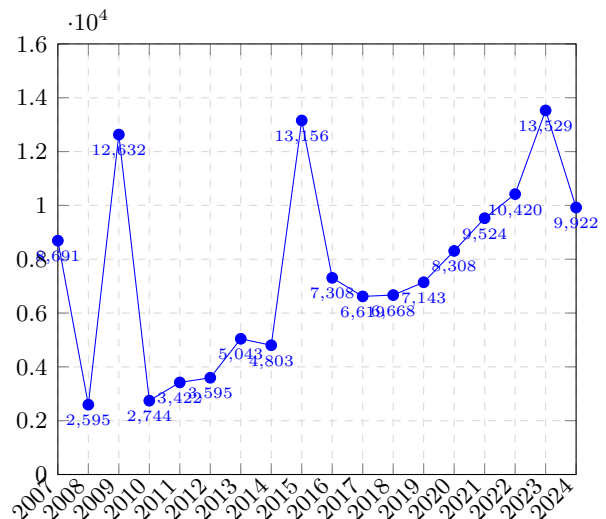


Figure 2: The number of quantum computing related papers in arXiv from 2007 to 2024 (as of June 15, 2024)

Wei Zhang and Jianyong Wang. 2015. [A collective bayesian poisson factorization model for cold-start local event recommendation](#). In *Proceedings of the 21th ACM SIGKDD international conference on knowledge discovery and data mining*, pages 1455–1464.

He Zhao, Lan Du, and Wray Buntine. 2017. [Leveraging node attributes for incomplete relational data](#). In *International conference on machine learning*, pages 4072–4081. PMLR.

Yutao Zhu, Huaying Yuan, Shuting Wang, Jiongnan Liu, Wenhan Liu, Chenlong Deng, Haonan Chen, Zhicheng Dou, and Ji-Rong Wen. 2023. [Large language models for information retrieval: A survey](#). *CoRR*, abs/2308.07107.

Zhaocheng Zhu, Zuobai Zhang, Louis-Pascal Xhonneux, and Jian Tang. 2021. [Neural bellman-ford networks: A general graph neural network framework for link prediction](#). *Advances in Neural Information Processing Systems*, 34:29476–29490.

A Quantum Computing related Papers in arXiv

Figure 2 illustrates the number of quantum computing papers published on arXiv over time.

B Evaluation on Isolated Nodes

Table 4 presents the model evaluation on the 1,368 connections to the isolated nodes.

C Time Decay Embedding Generation

Time-decayed information is essential for analyzing time series data and predicting future trends due to several reasons: First, it ensures the relevance of

Node Embedding	MLP		GCN		GraphSAGE	
	AUROC	AP	AUROC	AP	AUROC	AP
DeepWalk	71.57 ± 1.33	49.80 ± 1.96	49.18 ± 2.16	19.95 ± 1.60	53.26 ± 1.84	22.18 ± 1.85
LINE	69.53 ± 5.64	50.06 ± 6.79	87.01 ± 0.10	68.21 ± 0.72	65.91 ± 11.62	39.25 ± 15.08
node2vec	53.28 ± 3.40	23.40 ± 4.72	51.80 ± 0.71	21.34 ± 0.91	49.67 ± 0.22	19.31 ± 0.01
Gemini-1.0-pro	81.37 ± 1.16	62.91 ± 1.10	58.40 ± 9.04	28.42 ± 8.27	70.70 ± 4.63	40.85 ± 7.63
LLaMA3 (70B)	84.79 ± 1.09	65.09 ± 2.78	56.06 ± 12.38	27.67 ± 10.48	72.54 ± 3.49	42.58 ± 4.42
Mixtral-8x7B (46B)	85.55 ± 1.43	69.02 ± 1.91	51.28 ± 13.48	23.88 ± 10.68	75.92 ± 4.01	45.25 ± 5.38

Node Embedding	GAE		NCN		BUDDY	
	AUROC	AP	AUROC	AP	AUROC	AP
DeepWalk	68.82 ± 3.50	42.41 ± 4.90	29.81 ± 18.98	17.45 ± 15.45	76.56 ± 3.50	48.86 ± 4.84
LINE	86.95 ± 0.09	68.48 ± 0.74	60.85 ± 1.60	38.64 ± 1.04	80.09 ± 3.44	52.26 ± 3.01
node2vec	36.34 ± 8.40	15.16 ± 2.82	42.40 ± 11.97	17.23 ± 5.38	79.59 ± 1.16	52.99 ± 3.47
Gemini-1.0-pro	89.23 ± 0.24	70.99 ± 0.72	69.96 ± 13.01	39.05 ± 15.39	85.17 ± 2.40	58.19 ± 2.80
LLaMA3 (70B)	88.95 ± 0.37	70.01 ± 1.22	69.23 ± 16.72	40.42 ± 17.79	85.68 ± 2.26	57.57 ± 2.44
Mixtral-8x7B (46B)	88.67 ± 0.38	70.64 ± 0.81	67.11 ± 15.40	38.10 ± 17.71	83.68 ± 4.50	55.82 ± 5.11

Table 4: Comparison of LLM-generated node embeddings with other node embeddings in link prediction methods on 1,382 edges to 30 isolated nodes in the quantum computing concept graph.

recent data, which is often more indicative of future behavior than older data. This is crucial in scenarios like stock market analysis where recent trends are more predictive. Second, it allows models to adapt quickly to changes by emphasizing recent data, which reflects current underlying processes more accurately. Third, time decay reduces noise by minimizing the influence of older, potentially irrelevant data, thus focusing on meaningful patterns. Fourth, it enhances computational efficiency by potentially discarding less important older data. Finally, time-decayed information aids in anomaly detection by highlighting recent unusual behaviors. In summary, time-decayed information enables models to focus on the most pertinent data, adapt to changes, reduce noise, improve efficiency, and identify anomalies, thus providing a robust tool for time series analysis and trend prediction.

We utilized time decay information of pairs of concepts over time to represent node embeddings. To this end, we created co-occurrence matrices by each year. We then converted the co-occurrence matrices to PPMI (Positive Point-wise Mutual Information) matrices that are useful in word-word co-occurrence matrices as it addresses issues of normalization, sparsity, and noise reduction, thereby enhancing the quality and utility of semantic representations derived from such matrices. We adopted an exponential time decay function that assigns decreasing weights or importance to past events or observations based on their age or distance from

the present. In the context of time series data or decay processes, an exponential decay function is commonly expressed as: $N(t) = N_0 e^{-\lambda t}$ where: t is the time elapsed since the event or observation. λ is a decay constant that determines how quickly the weight decreases over time. After applying the time decay function, the matrices were aggregated and then the dimension of the aggregated matrix was reduced to the same embedding size to the LLM feature embedding by the SVD (Singular Value Decomposition). This time decayed embeddings were concatenated with the LLM feature embeddings. Algorithm 1 illustrates the node embedding generation procedure.

Algorithm 1 Time-Decayed Node Embedding Generation Procedure

Require: Co-occurrence matrices for each year

Ensure: Node embeddings

- 1: Convert co-occurrence matrices to PPMI matrices
 - 2: **for** each year **do**
 - 3: Apply exponential time decay function:

$$N(t) = N_0 e^{-\lambda t}$$
 - 4: **end for**
 - 5: Aggregate the matrices
 - 6: Reduce the dimension of the aggregated matrix to the same embedding size as the LLM feature embedding using SVD
 - 7: Concatenate the time decayed embeddings with the LLM feature embeddings
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