

RESEARCH STATEMENT

Chuxu Zhang, czhang11@nd.edu

University of Notre Dame

<https://chuxuzhang.github.io/>

OVERVIEW

In today's information and computational society (see Fig. 1), complex systems (e.g., Amazon, enterprise network, chemical synthesis) are often associated with heterogeneous data (e.g., structural relation, unstructured text/image, temporal context). Can we develop artificial intelligence solutions to extract, represent, fuse knowledge from heterogeneous data so as to solve different problems in complex systems? The heterogeneous data provides researchers and practitioners opportunities to understand complex systems more

comprehensively while poses challenges for knowledge discovery from them. The challenges come from not only the complexity and heterogeneity of the data to be used but also the requirement of the target problem to be solved. Besides the difficulty in extracting useful information from such complex data, it hard to fuse the extracted knowledge from a unified perspective in customized algorithms for different problems.

The goal of my research is to harnesses the power of heterogeneous data, turn them into knowledge, develop artificial intelligence solutions based on the extracted knowledge for a diverse set of real-world applications in complex systems of different disciplines. Successful intelligent solutions should be able to solve two fundamental research questions brought by the above challenges: (1) How to extract and represent useful information from the heterogeneous data of heterogeneous structure (e.g., multi-typed objects interconnected by multi-typed relations), heterogeneous modal/source (e.g., structural data, unstructured data, temporal data), or both? (2) How to fuse the extracted knowledge in customized machine learning models for solving target problems (e.g., recommendation, prediction, classification/clustering, anomaly detection) in different disciplines (e.g., web service, IT network/system, natural science)? I investigate a series of methodologies and algorithms to answer these questions, which have been deployed and validated in several research topics (e.g., personalization, representation learning). **My research has led to over 10 papers in the top conferences of artificial intelligence (e.g., AAAI, IJCAI), data science (e.g., KDD, WSDM), and information systems (e.g., WWW). As of 11/2019, my google scholar citation is more than 400.** In the following sections, I will outline my current research and future agenda.

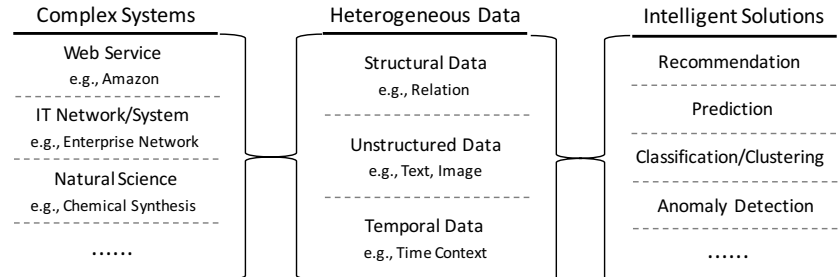


Figure 1: Overview of my research: turning heterogeneous data into knowledge, upon what developing artificial intelligence solutions for a diverse set of applications in complex systems of different disciplines.

CURRENT RESEARCH

During my Ph.D. study, I am fortunate to join Network Science Collaborative Technology Alliance¹ and be supported by U.S. Army Research Lab (ARL). My current research work mainly focuses on heterogeneous networks, which is an important part of ARL Network Sciences Project². Nowadays, people are deeply involved in various online web services such as social media (e.g., Facebook), online shopping (e.g., Amazon), academic search (e.g., Google Scholar), etc. Those complex systems are usually modeled as heterogeneous networks associated with heterogeneous data, representing multi-typed nodes interconnected by multi-typed edges as well as multi-modal/source contents in nodes and edges. For example, the online shopping data is of heterogeneous structure with <shop, item, user, brand, etc.> nodes and <item

¹<http://www.ns-cta.org/ns-cta-blog/>

²<https://www.arl.army.mil/www/default.cfm?page=391>

in shop, user buys item, item of brand, etc.> edges/relations. In addition, nodes (e.g., items) are associated with heterogeneous content (e.g., text description, picture, timestamp). It is hard for individuals to seek personal needs in those systems, especially when the candidate set is large (e.g., millions of items). Thus developing intelligent solutions to automatically filter information for individuals and provide personalized services to them is important. In addition, the abundant heterogeneous information in those systems requires both a domain understanding and large exploratory search space when doing feature engineering activities of customized machine learning models for different purposes. Therefore, developing intelligent solutions to generalize the feature engineering activity through automating the discovery of feature representation for various tasks is crucial. Accordingly, my current research tackles problems from two perspectives: (a) personalization in heterogeneous networks; (b) heterogeneous network representation learning.

A. Personalization in Heterogeneous Networks

The problem of personalization aims at automatically recommending suitable objects (e.g., items) to target objects (e.g., users) in the system. As many online web services (e.g., online shopping) are modeled as heterogeneous networks, extracting and fusing useful information from such complex structure would benefit recommender system designs in those services. I was motivated to do significant work in this area. To address the data sparsity and cold-start issue in recommender systems, I proposed **CUNE** [7], a collaborative user identification model. CUNE leverages user-item bipartite structure to identify top similar users of each user, which are incorporated into standard recommendation models (e.g., matrix factorization, pairwise ranking) and improve performances in both rating prediction and item ranking tasks. I further proposed two models, i.e., **ImWalkMF** [8] for reducing rating prediction error by considering both direct and indirect correlations among users and items, and **WalkRanker** [11] for elevating item ranking quality by incorporating multiple user-item relations into a unified pairwise ranking model. Moreover, to address sequence modeling challenge (i.e., recommending next item), I developed **MARank** [10] to improve sequential recommendation performance by unifying both individual- and union-level item sequential correlations in preference ranking model.

Besides the above general recommender system study, I have also finished some other work for personalization in the online academic service systems, which tackle the data of heterogeneous networks with text content in nodes. I proposed **Camel** [2] for author identification (i.e., predicting potential authors of anonymous papers), which is also useful for other tasks such as reviewer recommendation. The design of Camel (Fig. 2) is briefly illustrated as follows.

- **Information extraction and representation.** Camel uses a deep content encoder (i.e., $f(p)$) and learnable latent feature (i.e., q) to represent paper and author, respectively. Besides, Camel extracts direct author-paper relations and employs meta-path walks [2] to extract multiple indirect correlations between authors and papers in the network.
- **Knowledge fusion.** Camel leverages distance ranking metric to model direct relations between authors and papers (i.e., pulling correlated authors inward while pushing uncorrelated ones outward to the target paper in gradient direction), and further augments the framework through a smoothness regularization term of indirect author-paper correlations extracted from the heterogeneous structure.

By jointly optimizing distance ranking metric and heterogeneous structure regularization, Camel is able to effectively predict correlated/true authors of anonymous papers. Besides Camel, I also developed **TSR** [9], a task-guided and semantic-aware ranking model, to effectively recommend academic papers to researchers, especially for whom with little background knowledge of the discipline.

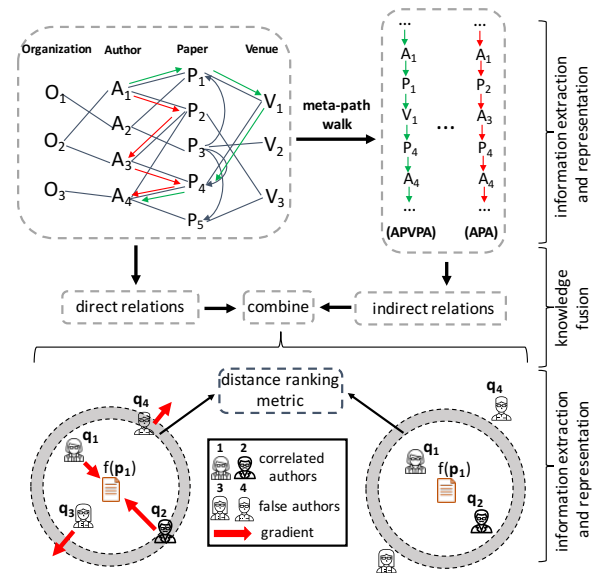


Figure 2: Illustration of Camel [2]: knowledge extraction and fusion for personalization in heterogeneous networks.

B. Heterogeneous Network Representation Learning

The purpose of heterogeneous network representation learning is to automate the discovery of meaningful vector representation for each node in the network so as to reduce labor-consuming feature engineering activity and facilitate various downstream tasks. I have done some work in this area. I proposed **SHNE** [5], i.e., semantic-aware heterogeneous network embedding, to learn node embeddings in heterogeneous networks with text information (e.g., academic network with text content in nodes). SHNE addresses the challenge of extracting and fusing both structural closeness and semantic correlations by integrating node content (i.e., text) as a deep encoding function into the heterogeneous structure embedding framework, and elevates performances in various network mining tasks.

Following the success of SHNE and in order to achieve a bigger scenario goal that learning node representations in heterogeneous networks with heterogeneous content in nodes (e.g., online shopping/reviewing networks with title/description text, review text, image/picture, attribute information in nodes), I further developed **HetGNN** [3], a heterogeneous graph neural network framework. The design of HetGNN (Fig. 3) is briefly illustrated as follows.

- **Information extraction and representation.** HetGNN extracts different types of neighboring nodes of the target node (i.e., node a) by a random walk based approach over heterogeneous structure and selects the most frequently visited nodes as correlated nodes of the target node. Besides, HetGNN employs cross-domain deep learning techniques to obtain feature representations of heterogeneous content in each node (e.g., natural language model for encoding text feature, computer vision model for encoding image feature).
- **Knowledge fusion.** HetGNN aggregates heterogeneous content features of each node and further aggregates representations of heterogeneous correlated node types for the target node by different deep learning modules. Therefore, HetGNN fuses the knowledge extracted from all correlated nodes and obtains the final representation of the target node.

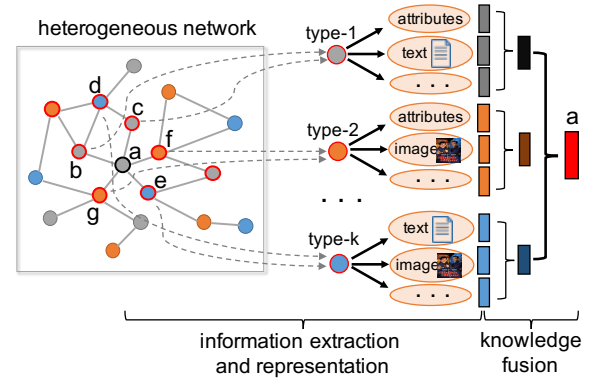


Figure 3: Illustration of HetGNN [3]: knowledge extraction and fusion for representation learning in heterogeneous networks.

HetGNN has been deployed in a number of web service system data and performs very well for various downstream tasks including link prediction, node recommendation, node classification/clustering, and embedding visualization. In addition to SHNE and HetGNN, I also proposed **HRL** [6], a heterogeneous relation learning model in knowledge graphs (a special case of heterogeneous network with abundant node/relation types). HRL considers heterogeneity of both neighboring entities and relations in learning target entity's embedding, which elevates link prediction performance.

FUTURE AGENDA

My future research agenda is directed towards a long-term goal of making artificial intelligence for complex systems with big and complex heterogeneous data impactful research and significant practition. I plan to apply my knowledge and expertise to problems of various disciplines and create intelligent solutions which are effective, efficient, and interpretable, leading to the following research directions.

1. **In-depth analysis and broader applications.** My current research has explored the heterogeneous data associated with heterogeneous structure or heterogeneous content or both. Most of complex systems are also associated with temporal data (e.g., time series, spatial-temporal context) which is useful for investigating system dynamics and improving the predictive analysis. I have done some work for time series and spatial-temporal data analysis [4, 1], and can not wait to leverage those information to further improve the state-of-the-art for different problems in heterogeneous data. In addition, I currently work for the NSF Center for Computer Aided Synthesis³ which aims to

³<https://ccas.nd.edu/>

use quantitative, data-driven approaches to make synthetic chemistry more predictable. Many of chemical synthesis problems can be transformed to machine learning tasks in heterogeneous data. For example, predicting the product of a chemical reaction is to infer edge/relation change (i.e., bond change) in heterogeneous networks (i.e., molecular graphs with multi-typed attributed atoms and bonds). I am excited to use my knowledge to develop intelligent solutions for various problems in different disciplines (e.g., natural science).

2. **Learning with small labeled data.** Missing or lacking ground-truth labels is common in heterogeneous data and it is often expensive to collect such labels. For example, online shopping systems and knowledge graphs face cold-start issue. The product collection of chemical reactivity spends a lot of money for human-laboring and experimental resource. It is practically significant to create efficient machine learning models to solve the challenges of small labeled data. My prior work HRL [6] tackles limited supervisory labels (i.e., few-shot relational entity pairs) in knowledge graphs. Depart from this study, I will try to investigate more techniques (e.g., meta-learning) for developing efficient solutions using small labeled data.
3. **Interpretable learning.** The current machine learning algorithms for heterogeneous data are mostly lack of explainability. For example, the link prediction methods predict potential connection between two nodes yet do not show why such connection is inferred. The recommendation models suggest items to users while do not tell users why such items are recommended. Equipping the machine learning algorithms with explainability will indeed bring benefits in transparency, trustworthiness, and effectiveness. I am interested in leveraging advanced techniques (e.g., reinforce learning) to develop interpretable solutions.

Collaboration and Funding. I am supported by NSF and ARL. In addition, previously I worked at Microsoft Research and NEC Labs America as research intern. I have close collaboration with a good number of researchers in both academia and industry. Moreover, I actively help my advisor in grant proposal writings during Ph.D. study. In the future, I will actively write proposals to apply for research grants from multiple funding agencies (e.g., NSF, ARL, DARPA, NIH) and industry companies.

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