

I develop *machine learning methods for reasoning about real-world events*.

The ability to reason about real-world events is crucial for effective decision-making in various domains, including national security, healthcare, and finance. For example, reasoning about user activities on social media platforms, such as their posts, likes, and shares, can provide insights for predicting and preventing potential social unrest events, as well as identifying fake content and malicious users. In healthcare, reasoning about medical events like diagnosis and treatments can assist in planning future hospital visits and designing personalized exercise routines. Furthermore, despite being ambitious and challenging, reasoning about market events, such as housing price movements and financial institute activities, holds the potential to enable timely prediction and prevention of catastrophic market events like the 2008 global financial crisis.

I envision a future where computers empowered by machine learning possess the capability to reason about real-world events. In pursuit of this vision, my research is dedicated to addressing pivotal problems within the following research areas:

- *Event sequence modeling*. Modeling event sequences can discover how past events influence future events, thus providing valuable insights for predicting the future. For example, by learning from historical financial data, a model may identify useful patterns such as “airline stocks often rise after oil price drops”.

In this area, my research has pioneered in developing *neural and neuro-symbolic* models, which are able to capture complex patterns in real data and thus significantly outperform previous models at making predictions. In addition, my research leverages principles from *classical statistics* to discover opportunities for *accelerating* both the training and inference processes of these neural models. Please see §1.

These innovations have had a profound impact on both academia and industry, receiving significant recognition in subsequent research. They have been integrated into real applications such as Alipay, the world’s largest mobile digital payment platform, which serves more than one billion users.

- *Natural language understanding*. Knowledge about real-world events and their relations is commonly documented by human experts in text forms, such as textbooks and news articles. Natural language technologies can empower computers to acquire such knowledge and apply it to real-world reasoning.

In this area, my research combines *modern large language models*, whose default behavior is like System 1, with *classical logical reasoning methods*, developing *System 2 reasoning* frameworks for challenging tasks. The terms “System 1” and “System 2” are derived from the “dual process” theories of reasoning [21, 22], which propose that human cognition involves an interplay between a fast and intuitive System 1 and a slow but deliberative System 2. Please see §2.

- *World model learning*. Understanding real-world dynamics is a key to intelligent decision-making agents.

In this area, I have planned future research in pursuit of fully automated *language agents*, including projects that embed *modern large language models* into *classical reinforcement learning frameworks*, empowering language models to learn *world dynamics* through real-world interventions. Please see §3.

In addressing research problems, I like to take *probabilistic* approaches, identifying the underlying generative dynamics and formalizing them through principled mathematics. Success hinges on designing effective model architectures, formulating appropriate training objectives, and developing efficient algorithms for training and inference. Alongside emphasizing scientific rigor and elegance, I place a strong emphasis on the practical applicability of my work. I take meticulous care to ensure that my methods are designed in a way that allows them to be seamlessly integrated into large-scale production settings. This emphasis has fostered extensive collaboration with leading tech companies and has attracted research funding from them.

1 Neural Probabilistic Methods for Event Sequence Modeling

The topic of my PhD thesis is event sequence modeling, with a particular emphasis on parameterizing the distribution $p(\text{sequence of events})$. This problem is central in the field because having knowledge of

$p(\text{sequence of events})$ enables various valuable probabilistic inferences. These inferences include predicting future events based on past events by querying $p(\text{future events} \mid \text{past events})$ and filling in missing events based on observed events by referring to $p(\text{unobserved events} \mid \text{observed events})$. For example, by analyzing future hospital visit trajectories drawn from $p(\text{future visits} \mid \text{a patient's past visits})$, we can address a range of questions such as “When will the patient’s next visit occur?” (by averaging the times of the first future visits across all trajectories) and “How likely is the patient to survive the next three months?” (by determining the frequency of death events within the next three months from sampled future trajectories).

Effective neural probabilistic models. We have developed the neural Hawkes process [14], which stands as one of the pioneering neural event sequence models. This model employs a novel *continuous-time* LSTM to capture the complex patterns in which past events may influence the future. It has exhibited strong performance in modeling diverse real-world datasets. Moreover, it has become a standard baseline for comparing new methods and has frequently been integrated as a core component in larger systems [18, 19]. Subsequently, we introduced the neural Datalog through time [11], a neural-symbolic extension of the neural Hawkes process. This model demonstrates superior generalization capabilities in large real-world domains of many types of events. It achieves this by leveraging a temporal deductive database to efficiently and precisely track domain-specific facts, as well as configuring a structurally sparse neural architecture based on the database’s topology. Additionally, we developed Transformer versions of both the neural Hawkes process and neural Datalog through time [10], which enhance performance and efficiency.

Efficient training and inference algorithms. Training a neural event sequence model and performing inference with it present non-trivial challenges. While maximum likelihood estimation serves as a standard training method for generative probabilistic models, estimating the likelihood can be computationally expensive for event sequence models. To tackle this issue, we developed a novel training method [12] based on the principle of noise-contrastive estimation. The parameter estimates obtained from this new method provably maximize the likelihood while bypassing the need for direct likelihood estimation. As a result, it significantly reduces the computational cost compared to maximum likelihood estimation in practice. Utilizing this approach, we developed an energy-based event sequence model [9], for which the likelihood is intractable to compute directly. This model showcases remarkable performance in long-horizon prediction tasks. As for inference, we introduced the first general sequential Monte Carlo method [13] that efficiently approximates $p(\text{unobserved events} \mid \text{observed events})$.

Event-based decision making. An exciting application of event sequence models is their integration into reinforcement learning frameworks to learn intervention policies. For example, in an education technology system, these models can capture user activities, such as lessons and tests taken, as well as performance. By incorporating the model into a policy learning process, the system can effectively assign appropriate new lessons and tests to each user. In such scenarios, all observations and actions are time-stamped events, which means that the agent needs to determine not only what to do (e.g., lesson assignments) but also when to schedule these actions for each user. Timing plays a crucial role: presenting a new lesson too soon may intimidate the user and diminish enjoyment, while delaying it excessively might hinder learning progress. In our research, we have demonstrated the utility of event sequence models in both classical model-based reinforcement learning frameworks [2, 7] and the emerging goal-conditioned framework [5].

2 Logical Reasoning with Large Language Models

Since starting my current research assistant professor position, I have been working on enhancing the logical reasoning capabilities of large language models. This project is driven by the remarkable success of pretrained large language models. Considering that these models acquire knowledge from their training corpora and demonstrate reasoning abilities, it seems plausible to leverage such capabilities for reasoning about real-world events. For example, the Wikipedia article discussing the 2010 Deepwater Horizon oil spill illustrates how this incident adversely impacted wildlife throughout the Gulf of Mexico. By comprehending

this article, a language model may generalize its knowledge and predict the effects of a new old spill event.

Event prediction with language models. Our work [3] first demonstrates that the reasoning capabilities of large language models can indeed be harnessed to improve the prediction accuracy of event sequence models. We designed a modeling and prediction framework in which a large language model performs abductive reasoning to assist an event sequence model. In this framework, the pretrained event sequence model proposes predictions for future events. Instructed by a few expert-annotated demonstrations, the language model learns to suggest possible causes for each proposal. A search module then identifies previous events that match the suggested causes, and a scoring function evaluates whether the retrieved events could plausibly cause the proposal. In extensive experiments, this framework significantly outperform state-of-the-art event sequence models.

System 2 reasoning for language models. Despite the above initial success, I found that large language models behave similar to System 1, generating responses based on patterns in the training data without deep understanding or reasoning. However, there is often a need for them to engage in deliberative System 2 thinking. Thus, my research focuses on developing System 2 reasoning methods for large language models.

One approach is to design new language model architectures. In this regard, we have developed a novel language model called Lookahead Transformer (System 2) [1]. This model estimates the next-token distribution by generating multiple continuations of the past, using an ordinary Transformer model (System 1), and attending to these extended strings. Essentially, our model engages in a form of planning by examining these continuations to consider the potential sentences resulting from different choices of the next token. Our model has demonstrated promising performance across multiple tasks. Furthermore, we have planned various possible extensions to further enhance its performance and efficiency.

Another approach is to develop new frameworks that combine a System 1 language model with a deliberative inference algorithm. In this context, we have devised a novel framework (System 2) [6] that employs language models (System 1) to engage in multi-step logical reasoning, integrating explicit planning into its inference procedure. By incorporating explicit planning, our framework enables informed reasoning decisions at each step, considering the future consequences of the possible choices. Notably, our framework outperforms strong competing methods, including chain-of-thought prompting, across multiple datasets. We are currently generalizing this framework to address more complex problems.

3 Future: Towards Fully Automated Language Agents

An ultimate goal of my research is to enable intelligent agents that assist human users in interacting with real-world environments, anticipating the consequences of specific decisions, and suggesting high-reward actions. The growing success of large language models offers a promising path towards this goal. These models retain valuable knowledge from training data, demonstrate promising reasoning abilities, and possess the capability to communicate with humans and incorporate their feedback. However, significant challenges still remain. Current language models exhibit crucial shortcomings, such as

- their training being constrained to a limited range of real-world interactions,
- limitations in accommodating the ever-growing experiences within their bounded context windows,
- their reliance on task-specific human-crafted demonstrations,
- and their unsatisfactory controllability, occasionally leading to offensive or hallucinatory outputs.

Over the next five years, my plan is to tackle these fundamental challenges.

3.1 Language Agent + X

to leverage richer training signals

By embedding language models within agents operating in domains like robotics, healthcare, law, and finance, there is a potential to leverage richer training signals, enabling the language models to learn from a

broader range of data and interactions. I am particularly interested in the combination of language models with robotics, as it can open up new possibilities for intuitive and efficient human-robot collaboration. In our work [4], we demonstrate that large language models can learn environment dynamics and enhance the long-horizon planning capabilities of robots, surpassing strong baselines like Code-as-Policies [17]. Looking ahead, I plan to explore further improvements in language models, particularly in their capacity to learn world models, by leveraging rich feedback from real-world interactions between robots and environments.

3.2 Experience Summarization *to fit unbounded experiences into bounded context windows*

Humans often condense their concrete experiences into abstract lessons, which then inform their decision-making in similar situations. My plan is to develop methods that enable language models to emulate human-like inductive learning and condense experiences into concise summaries. As the model accumulates more experiences, the repository of summaries will expand, albeit at a slower pace than the accumulation of experiences. Additionally, the repository will be intelligently maintained, allowing for the retrieval of relevant summaries for new experiences. Consulting these retrieved summaries will require much less space within the context window compared to using the actual previous experiences or the entire repository of summaries.

3.3 Meta Learning *to free language models from human-crafted demonstrations of new tasks*

My plan involves developing meta learning methods that empower language agents to autonomously learn how to solve new tasks. Meta learning methods, in general, seek to identify model parameters that allow the model to adapt to new tasks with minimal task-specific training. Within the specific domain of language agents, my aim is to create methods that discover the parameters (for in-house models like LLaMa [16]) or prompts (for blackbox models like GPT-4 [15]) by leveraging human-crafted demonstrations from training tasks. These methods aim to enable large language models to adapt to new tasks with minimal, or even without, human-crafted demonstrations.

3.4 Neural Collapse Analysis *to improve controllability*

Neural collapse [20] is widely observed in various deep neural architectures used for computer vision tasks. It manifests as the formation of linearly separable clusters in the top-layer hidden representations. Our research [8] demonstrates a similar phenomenon in pretrained large language models, where different layers exhibit distinct clusters that prove beneficial for different downstream tasks. Leveraging this phenomenon, we have developed a novel transfer learning method that has significantly reduced computation costs [8]. Moving forward, I am intrigued by the potential of this phenomenon to provide insights for enhancing the controllability of large language models. An idea worth exploring is to identify layers and clusters associated with undesired behaviors and investigate ways to mitigate their impact on other parts of the model.

Funding Plans

I have been fortunate to receive generous support from leading tech companies throughout my research journey. During my PhD, I was awarded a Bloomberg Data Science PhD Fellowship, which provided invaluable support. In recent years, my work has been further bolstered by a series of research gifts from Adobe and Ant Group. Given the continued alignment of my research agenda with the interests of these companies, I am confident in their ongoing interest and potential for future research funding.

I have been actively pursuing the ideas proposed in §3 and have already established collaborations with experts in disciplines outside my primary focus, such as robotics, speech, and finance. Together with my collaborators, we have obtained promising preliminary results. I am now prepared to consolidate these ideas and current findings into funding proposals, targeting suitable programs such as NSF CISE Core Programs. Additionally, I am keen on partnering with other researchers and competing for major funding programs offered by NSF, DARPA, and other agencies like DoD and DoE. I am confident that my expertise in event sequence modeling and natural language processing will bring significant value to the team.

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Part I – My Selected Publications

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