Statement of Purpose

As a Computer Science student, I was initially interested in designing algorithms and solvers to solve real-world problems. However, it wasn't until I discovered the world of Data Science (DS) that I truly found my calling. At the first class of Machine Learning (ML), my professor Shikui Tu exhibited how data boosted *transformers*’ potential to generate textual answers based on the images accurately. I was immediately drawn by the power of data to elicit transformers’ underlying “wisdom” to analyze the problems. In the following few weeks, I read over 20 papers on the frontier of DS and audited Andrew Ng’s Stanford CS229 ML course. I became convinced that DS, especially with ML, was where I belonged to and excited to witness the future developments in DS. I therefore switched my focus to DS and made it my future to become a distinguished DS researcher to explore the potential for real-world applications.

My journey in DS started when I joined the SJTU-ReThinkLab led by Prof. Junchi Yan. I began research on graph matching (GM), which aimed at finding point pairs on the given images. With substantial literature review, I found a gap in works on front-end backbones (e.g. CNNs), as most of the existing works focused on back-end modules while neglected the process of initial image. Inspired by the success of attention mechanism, I decided to design a GM-specific backbone based on ViT. However, the obstacle was that original ViT extracts global information, rather than the local key-point information. To address this limitation, I devoted several days studying the paper and code of ViT, discussing with the professor to understand ViT's capabilities. After reflection, I proposed modifying ViT by introducing patches centered around the key-points and adopting the cross-attention mechanism to leverage the global information as auxiliary for the local information. I also harnessed the attention mechanism to enhance the back-end module's ability to capture the graph's underlying structure. Consequently, my proposed method achieved the state-of-the-art (SOTA) performance on extensively used GM benchmarks and the proposed backbone improved most existing frameworks by over 5%.

The experience for my first research imparted to me the knowledge of how DS research was conducted and further sparked my interest in ML. Therefore, I participated in another group in our lab aiming at designing the guided diffusion model for combinatorial optimization (CO). One of the most challenging problems is the design of guidance. Injecting guidance to the generation required reformulating the Bayesian probability distribution, demanding a strong grasp of mathematical skills. I spent substantial efforts learning the structure of diffusion models and conducting mathematical derivation meticulously. After contemplation, I proposed approximating the cost of solutions as guidance using Taylor’s First Order Expansion and Energy Function to represent to posterior probability. Nevertheless, I found guided diffusion model showed marginal improvement on TSP and MIS (two NP-hard CO problems) compared with existing works. I discussed the phenomenon with my group members and proposed to use Bernoulli distribution instead of Gaussian distribution to model the generation process so as to better represent the discrete distribution of 0 and 1, which was more associated with our tasks. This solution addressed the issue of continuous probabilistic modeling and improved the performance by 10%. Eventually, our proposed guided-diffusion model achieved the SOTA performance on TSP and MIS benchmarks compared with learning-based models and reduced the solving time by one order of magnitude compared with exact solvers (e.g. from 1h to 4 min).

The research in CO honed my programming and mathematical skills and boosted my curiosity to explore DS in more domain-specific problems. Therefore, I joined the ML-PL group led by Prof. Xujie Si affiliated to the University of Toronto and Mila - Quebec AI Institute. I researched on logical puzzles that can be formulated as SAT expressions, such as Sudoku. My work was built on SATNet, a differentiable MaxSAT solver. Nevertheless, while analyzing the paper of SATNet, I found the learned parameters cannot even represent extremely simple rules such as XOR, contradicting paper’s claim. After discussing with group members, we identified a theoretical error in the interpretation. Armed with mathematical knowledge, I intuitively proposed rewriting the SAT conjunctive normal form directly as a parametric matrix. The main challenge in this project was the unfamiliar programming language CUDA, as all my previous projects were written in PyTorch. To implement my idea, I delved into the NVIDIA CUDA tutorial. Although CUDA is a much more obscure programming language compared with PyTorch, I grasped the basic principle and syntax Within three days, and implemented my idea based on SATNet with group members. The proposed idea substantially reduced the number of trainable parameters while remedying theoretical mistakes in the original design. Notably, once the rules are learned, the model can definitely output correct answers, and this representation made the learned rules entirely interpretable, marking a significant breakthrough in the logic reasoning field.

The positive impact of my proposed method on the specific field and the exhilaration once my paper was accepted including at NeurIPS strengthened my determination to be a future prominent researcher in the DS field. Now I dream of employing DS knowledge to design ML frameworks that surpass human experts, well-designed algorithms and solvers in terms of both accuracy and efficiency for scientific scenarios. The DS program at Harvard, with its top-notch faculty and impeccably crafted curriculum, is the perfect incubator for this dream. I can not only gain valuable insights into data science via *Advanced Scientific Computing* but also advance my knowledge of ML with *Topics in Machine Learning*. I am particularly excited to work with the pioneering researcher Prof. *Boris Kozinsky* to combine ML with physics, chemistry and mathematics. I am curious to witness how ML boosts scientific research, drawing on my previous research experience to push the boundaries of this exciting field. I believe my journey at Harvard will equip me with the expertise demanded to make insightful contributions to the DS field and finally contribute back to the community at Harvard.