Towards Reliable Machine Learning with Unlabeled Data and Beyond

Overview. In today's rapidly evolving landscape of AI technology, machine learning (ML) models, including the recent foundation models (FMs) have emerged as transformative forces shaping various applications. Despite the immense capabilities, they bring forth challenges related to the model's reliability upon deployment in the real world. For example, classic discriminative neural networks can produce overconfident yet incorrect predictions for unfamiliar out-of-distribution (OOD) classes. Moreover, generative models, such as large language models (LLMs), can generate untruthful or harmful content that contradicts human values, potentially compromising critical decision-making in an ever-changing open world. Addressing these issues is not merely a technical necessity but a fundamental requirement for the responsible deployment of AI technologies.

My research vision, as a crucial part of AI existential safety, is to ***create an AI landscape where algorithmic accuracy and reliability are equally paramount, ultimately broadening the impact and responsible reach of ML technologies***. To achieve this, I focus on developing new algorithmic techniques and providing fundamental, provable understandings that enable safe and reliable decision-making in the open world, where OOD data can naturally emerge. This research direction is increasingly recognized as an important aspect of the AI research roadmap over the next five years and beyond [1]. Additionally, the proposed frameworks can be synergistically integrated with recent FMs (Section 3), making this endeavor both timely and highly relevant.

Reliable ML introduces core challenges in characterizing the reliability of off-the-shelf learning algorithms, which typically minimize errors on in-distribution (ID) data from $\mathbb{P}_{\text{in}}$ without accounting for uncertainties that could arise outside $\mathbb{P}_{\text{in}}$. For instance, the widely used empirical risk minimization (ERM) [2], operates under the closed-world assumption (*i.e.*, no distribution shift between training and inference). Models optimized with ERM are known to produce overconfidence predictions on OOD data [3], since the decision boundary is not conservative. To address this challenge, I develop novel frameworks that jointly optimize for both: **(1)** accurate prediction of samples from $\mathbb{P}_{\text{in}}$, and **(2)** reliable handling of data from outside $\mathbb{P}_{\text{in}}$. Given a weighting factor α, this can be formalized as follows:

$$\text{argmin} \ [\mathcal{R}_{\text{accuracy}} + \ \alpha \cdot \mathcal{R}_{\text{reliability}}]. \tag{1}$$

As an example, $\mathcal{R}_{\text{accuracy}}$ can be the risk that classifies ID samples into known classes while $\mathcal{R}_{\text{reliability}}$ aims to distinguish ID vs. OOD. The introduction of the reliability risk term $\mathcal{R}_{\text{reliability}}$ is crucial to prevent overconfident predictions on unknown data and improve test-time reliability when encountering unknowns. However, incorporating this reliability risk requires large-scale human annotations, e.g., binary ID and OOD labels, which could limit the practical usage of the proposed framework. Therefore, my key research idea is ***developing the foundational dynamics of reliability learning by leveraging unlabeled data***, which spans three key aspects:

1. I develop novel data generation frameworks without explicit knowledge about unknowns. The framework adaptively generates virtual outliers from the low-likelihood region in the feature [4, 5, 6] and input space [7] of ID data, and showed strong efficacy and interpretability for regularizing the model to discriminate the boundaries between known and unknown data.
2. I leverage unlabeled data that is collected from the models' deployment environment for reliability estimation. This in-the-wild data is a mixture of ID and different OOD data (covariate and semantic shift, etc) by an unknown mixing ratio. Methods I designed such as *gradient SVD score* [8, 9] and *constrained optimization* [10] can facilitate detection and generalization on these real-world reliability challenges.
3. I investigate the blind spots of language models, such as untruthful generations [11], malicious prompts [], and noisy alignment data. My work seeks to fundamentally understand the sources of these issues by developing algorithms that leverage unlabeled data to identify and mitigate the unintended information, which ensures safer human-AI interactions.

My research has led to impactful publications in top-tier ML and vision venues and has been recognized by Rising Stars in Data Science and Jane Street Graduate Research Fellowship programs. Many of my works has been integrated into the OpenOOD benchmark [12, 13], and have received considerable follow-ups from major industry labs, such as Google [14], Microsoft [15], Amazon [16], Apple [17], Adobe [18], Air Force Research [19], Toyota [20], LG [21], Alibaba [22] etc. The scientific impact of reliable ML is profound, I am excited to explore interdisciplinary collaborations across computer science, statistics, biology science, and policy to push the boundaries of reliable ML as a professor. I will outline my research in detail next.

(a) Overconfidence on OOD data (b) Outlier Synthesis Framework

Figure 1: (a) An object detection model trained on BDD-100k dataset [24] produces overconfident predictions for OOD objects (e.g., helicopter), highlighting reliability concerns in ML models during deployment. Test images are sampled from MS-COCO [25]. (b) Overview of my proposed outlier synthesis framework for reliability estimation.

1 Estimating Algorithmic Reliability with Virtual Outliers

Motivation. Ensuring safe and trustworthy AI systems requires addressing a critical issue: the overconfident predictions made on out-of-distribution (OOD) test inputs [3]. These inputs arise from unknown categories and should ideally be excluded from model predictions. For example, in self-driving car applications, an object detection model trained on in-distribution (ID) objects (e.g., cars, pedestrians) might confidently misidentify an unusual object, such as a helicopter on a highway, as a known object; see Figure 1 (a). Such failures not only raise concerns about model reliability but also pose serious risks in safety-critical deployments.

The vulnerability to OOD inputs stems from the lack of explicit knowledge of unknowns during training, as neural networks are typically optimized only on ID data. While this approach effectively captures ID tasks, the resulting decision boundaries can be inadequate for OOD detection. Ideally, a model should maintain high confidence for ID data and exhibit high uncertainty for OOD samples, yet achieving this goal is challenging due to the absence of labeled outliers. My research tackles this challenge through an automated outlier generation paradigm, which offers greater feasibility and flexibility than approaches requiring extensive human annotations [23]. I outline three core technical contributions:

Outlier synthesis in the feature space. My project VOS [4] (ICLR'22) introduces a method to model ID features as class-conditional Gaussians, and then samples virtual outliers from low-likelihood regions using rejection sampling. I demonstrated that synthesizing outliers in the feature space is more tractable than generating images directly in high-dimensional pixel space [26]. Additionally, I developed an unknown-aware training objective that contrastively shapes the uncertainty energy surface between ID data and synthesized outliers, while preserving ID task performance. My subsequent work, NPOS [6] (ICLR'23), relaxed the Gaussian assumption through a non-parametric synthesis approach, yielding improved results on language models and larger datasets. The STUD method [5], presented at CVPR'22 as an **oral** presentation, further demonstrated the efficacy of this approach in video object detection, distilling unknown objects in both spatial and temporal dimensions to regularize model decision boundaries.

Understanding synthesized outliers in pixel space. While feature space synthesis is effective, it doesn't allow human-compatible interpretation of outliers. To address this, my NeurIPS'23 paper Dream-OOD [7] developed a framework using diffusion models to generate photo-realistic outliers from ID data. The method learns a text-conditioned visual latent space, enabling sampling from low-likelihood regions and decoding by diffusion models. This approach not only enhances interpretability but also achieves strong results on OOD detection benchmarks. It has garnered interest from the community, prompting follow-up research [21, 27, 28].

Impact of in-distribution accuracy risks. Beyond focusing on reliability risks, it's crucial to address the in-distribution accuracy term $\mathcal{R}_{\text{accuracy}}$ in Equation 1 during training. My work, SIREN [29] (NeurIPS'22) and a subsequent ICML'24 paper [30], fundamentally investigated the influence of *compact representation space* and *ID label supervision* on identifying OOD samples. These insights contribute to designing better training strategies on ID data and enhancing overall model reliability.

2 Leveraging In-the-wild Unlabeled Data for Detection and Generalization

Motivation. Previous research utilizing auxiliary outlier datasets has shown promise in improving OOD detection compared to models trained solely on ID data. These models often regularize confidence scores [23] or energy levels [31] for outlier data. However, this approach faces two significant limitations: (1) auxiliary

Figure 2: Proposed frameworks for hallucination detection in LLMs and malicious prompt detection in VLMs.

data collected offline may not accurately reflect the true distribution of unknown data encountered in real-world settings, potentially undermining OOD detection during deployment; (2) collecting such data is often labor-intensive and requires careful cleaning to avoid overlap with ID data.

My research addresses these challenges by leveraging unlabeled "in-the-wild" data, which can be gathered at minimal cost during the deployment of machine learning models. This type of data has been largely overlooked in OOD learning contexts. Formally, unlabeled data can be represented by a Huber contamination model, $\mathbb{P}_{\text{unlabeled}} := (1-\pi)\mathbb{P}_{\text{in}} + \pi\mathbb{P}_{\text{out}}$, where $\mathbb{P}_{\text{in}}$ and $\mathbb{P}_{\text{out}}$ represent the marginal distributions of ID and OOD data, respectively. Unlabeled data is abundant, does not require human annotation, and often better aligns with true test-time distributions compared to offline-collected data. While this setting is promising for various applications, it introduces unique challenges due to the impure nature of the unlabeled data which comprises both ID and OOD samples.

Provable characterization of the unlabeled wild data. In my ICLR'24 paper, SAL [8], I formally investigate *when and how unlabeled data can enhance OOD detection*, and present three key contributions. (**1**) I propose a novel learning framework that **separates** candidate outliers using singular value decomposition on the model gradient matrix, which facilitates the **learning** of an OOD classifier. (**2**) The framework provides theoretical support for the filtering error and the generalization error of the OOD classifier, proving that these errors can be small under specific conditions. (**3**) Empirically, I demonstrate the generalization bounds of SAL translate into strong empirical performance, establishing state-of-the-art results through extensive evaluations.

Modeling diverse mixtures of unlabeled data for both OOD detection and generalization. Beyond detecting samples with semantic shifts, machine learning models may also encounter covariate shifts—variations in input distributions that do not necessarily affect labels. These shifts can arise from differences in sensor calibration or environmental changes. To effectively address both OOD detection and generalization, my research explores techniques for modeling diverse mixtures of unlabeled data, expressed as $\mathbb{P}_{\text{unlabeled}} := (1-\pi_c-\pi_s)\mathbb{P}_{\text{in}} + \pi_c\mathbb{P}_{\text{out}}^{\text{covariate}} + \pi_s\mathbb{P}_{\text{out}}^{\text{semantic}}$. This framework integrates ID data and various OOD distributions. My ICML'23 paper, SCONE [10], along with a recent preprint [9], employs a *constrained optimization* and *active learning* to effectively leverage these data sources within a unified framework. The formulation and methodologies presented offer strong generality and practicality for real-world applications.

3 Towards Reliable Foundation Models

Motivation. As foundation models become influential in various applications, ensuring their reliability is an urgent research challenge. These models often face reliability risks, such as generating hallucinations, misinterpreting malicious prompts and handling noisy alignment data, raising concerns for safety and trustworthiness when deployed in real-world settings. Given the models' large scale and their training on massive, diverse data, addressing these issues requires innovative strategies beyond the conventional learning methods. My research seeks to address these issues by identifying the origins of reliability risks $\mathcal{R}_{\text{reliability}}$ in FMs and designing innovative mitigation algorithms.

Leveraging unlabeled LLM generations for hallucination detection. In my NeurIPS'24 **spotlight** paper,

HaloScope [11], I introduce a framework for detecting hallucinations in LLM outputs using unlabeled LLM-generated text, which inherently contains a mix of truth and hallucinations (Figure 2 upper). By leveraging the representation space, HaloScope extracts a hallucination subspace to facilitate the training of a binary truthfulness classifier without human labels. This method demonstrates adaptability across various LLM architectures and domains, establishing a foundation for harnessing unlabeled LLM outputs to enhance FM reliability.

Red-teaming VLMs with unlabeled user prompts. My research [] explores the use of naturally occurring, unlabeled user prompts (Figure 2 left) in identifying vulnerabilities in vision language models (VLMs). By analyzing these prompts in the representation space, I develop techniques to detect and counteract malicious inputs, which enhances VLMs' robustness against prompt injection and jailbreak attacks. This work is pioneering in demonstrating how red-teaming can be applied to VLMs to improve their reliability.

Analyzing and denoising preference data for improved AI alignment. While AI alignment research typically assumes human feedback is reliable, my ongoing work reveals that over 25% of feedback data can be inconsistent, highlighting inherent unreliability from biases and labeling errors. To address this, I propose the Source-Aware Cleaning method, which significantly improves data quality. The cleaner data enables training more reliably aligned LLMs, and thus offers a pathway to more reliable LLM alignment research.

4 Future Research

My research has tackled several foundational reliability challenges arising from the ML paradigm shift, yet significant work remains. Moving forward, I am eager to propel the field of reliable ML by exploring several pivotal directions that will strengthen both theoretical foundations and practical applications of ML systems.

Comprehensive investigation of ML reliability challenges. Developing genuinely reliable ML systems necessitates a deep understanding of the limitations and risks across diverse deployment scenarios. I plan to systematically investigate the safety and reliability challenges inherent in current ML models. For instance, foundation models encounter risks from noisy pretraining data, label ambiguity and data fairness in supervised fine-tuning, preference inconsistencies in RLHF for LLMs, and vulnerabilities to adversarial attacks. By rigorously characterizing these challenges, I aim to establish comprehensive benchmarks and devise targeted strategies to enhance model reliability. This work will improve the safety and robustness of ML algorithms across various applications while opening new avenues of research to enrich the reliable ML community.

Development of effective reliable ML techniques beyond leveraging unlabeled data. Building on my work with unlabeled data for OOD detection and foundation model reliability, I intend to expand the development of reliable ML methodologies from three core perspectives: data, representation, and training/inference algorithms. For example, I will investigate (1) the impact of diverse data types, such as human feedback, weak supervision, and semi-supervised data, on model reliability (data perspective); (2) how advancements in representation learning and model architecture can fundamentally enhance reliability (representation perspective); and (3) the design of distributionally robust training methods alongside calibrated, efficient inference algorithms that adapt to varying deployment environments and integrate multiple knowledge sources (algorithm perspective). These principles will serve as a flexible foundation for improving reliability across a wide spectrum of machine learning models and applications.

Reliable ML for boarder scientific discovery. My long-term vision also includes harnessing the power of reliable ML to accelerate scientific discovery across multiple domains, such as reliable biometrics with distribution shifts [32, 33, 34], less human annotations [35, 36], multimodal fusion [37], and reliable protein structural analysis with OOD detection [38], active learning [39], semi-supervised learning [40], and open-set classification [41], where I have expertise in. Moreover, I look forward to collaborating with domain experts in other disciplines, such as chemistry, sociology, and environmental science, to explore how reliable ML can address their unique challenges. By leveraging interdisciplinary knowledge, I aim to develop tailored ML solutions that not only enhance predictive accuracy but also improve the interpretability and trustworthiness of models in complex, data-driven environments. This collaborative effort will ultimately contribute to more robust scientific methodologies and facilitate breakthroughs that are essential for addressing pressing global issues.

Overall, my research approach has been to leverage theories and insights drawn from ML and data analytics to address fundamentally new reliability problems arising from the real world. As a future faculty member, I aspire to maintain this principled approach and advance this compelling research agenda with a vision for impactful contributions to both the academic community and society at large.

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