Practical Machine Learning Safety: A Survey and Primer

SINA MOHSENI, ZHIDING YU, CHAOWEI XIAO, and JAY YADAWA, NVIDIA, USA
HAOTAO WANG and ZHANGYANG WANG, The University of Texas at Austin, USA

The open-world deployment of Machine Learning (ML) algorithms in safety-critical applications such as autonomous vehicles needs to address a variety of ML vulnerabilities such as interpretability, verifiability, and performance limitations. Research explores different approaches to improve ML dependability by proposing new models and training techniques to reduce generalization error, achieve domain adaptation, and detect outlier examples and adversarial attacks. In this paper, we review and organize practical ML techniques that can improve the safety and dependability of ML algorithms and therefore ML-based software. Our organization maps state-of-the-art ML techniques to safety strategies in order to enhance the dependability of the ML algorithm from different aspects, and discuss research gaps as well as promising solutions.

CCS Concepts:
- Computer systems organization → Embedded systems; Redundancy; Robotics;
- Networks → Network reliability.

Additional Key Words and Phrases: neural networks, robustness, safety, verification uncertainty quantification

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1 INTRODUCTION

Advances in machine learning (ML) have been one of the most significant innovations of the last decade. Among different ML models, Deep Neural Networks (DNNs) [130] are well-known and widely used for their powerful representation learning from high-dimensional data such as images, texts, and speech. However, as ML algorithms enter sensitive real-world domains with trustworthiness, safety, and fairness prerequisites, the need for corresponding techniques and metrics for high-stake domains is more noticeable than before. Hence, researchers in different fields propose guidelines for Trustworthy AI [208], Safe AI [5], and Explainable AI [155] as stepping stones for next generation Responsible AI [6, 247]. Furthermore, government reports and regulations on AI accountability [75], trustworthiness [216], and safety [31] are gradually creating mandating laws to protect citizens’ data privacy, fair data processing, and upholding safety for AI-based products.

The development and deployment of ML algorithms for open-world tasks come with reliability and dependability limitations rooting from model performance, robustness, and uncertainty limitations [156]. Unlike traditional code-based software, ML models have fundamental safety drawbacks, including performance limitations on their training set and run-time robustness in their operational domain. For example, ML models are fragile to unprecedented domain shift [65] that could easily...
occur in open-world scenarios. Data corruptions and natural perturbations [90] are other factors affecting ML models. Moreover, from the security perspective, it has been shown that DNNs are susceptible to adversarial attacks that make small perturbations to the input sample (indistinguishable by the human eye) but can fool a DNN [74]. Due to the lack of verification techniques for DNNs, validation of ML models is often bounded to performance measures on standardized test sets and end-to-end simulations on the operation design domain. Realizing that dependable ML models are required to achieve safety, there is a need to investigate gaps and opportunities between conventional engineering safety standards and a set of ML safety-related techniques.

1.1 Objectives and Contributions
In this paper, we review challenges and opportunities to achieve ML safety for open-world tasks and applications. We first review the dependability limitations of ML algorithms in uncontrolled open-world scenarios and compare them with conventional safety standard requirements. We decompose our ML dependability objective by categorizing ML techniques into three safety strategy categories of (1) achieve safe design, (2) improve model performance and robustness, and (3) run-time error detection. We review over 250 papers from a broad spectrum of state-of-the-art ML papers and organize them in our safety strategy categorization. Our review is summarized in a representative reference table (Table 1), which serves ML researchers and designers as a collection of best practices. Our organization allows to checkup the coverage and diversity of safety strategies employed in any given ML system. In the end, we identify several open problems in each category and propose potential directions for future work, including the role of Human-AI Interactions in building user trust and understanding for safe end-user control over ML systems.

1.2 Paper Scope and Organization
ML safety includes diverse hardware and software techniques for the safe execution of algorithms in open-world applications [120]. In this paper, we limit our scope to software techniques and specifically to only ML techniques and not the execution of those algorithms in platforms. With that being said, we also mainly focus on “in situ” techniques to improve run-time dependability and not on further techniques for network or training efficiency.

The organization of this paper is as follows: in Section 2 we first review safety terminologies and situate ML safety limitations with reference to conventional software engineering safety requirements to better understand the problem space. In Section 3 we discuss a unified “big picture” of different ML error types for real-world applications and common benchmark datasets to evaluate these errors. Next, we propose our ML safety strategies in Section 4 and categorization of ML techniques into these strategies, with Table 1 as a hierarchical summary of reviewed papers. Sections 5, 6, and 7 present the main body of the reviewed papers organized into ML topics and techniques for each safety strategy. Finally, Section 8 presents a discussion of open problems and research directions for ML safety.

2 BACKGROUND
In order to introduce and categorize ML safety techniques, we start with reviewing background on ML dependability, engineering safety strategies, and the relation between these two. In the following, we start by decomposing and clarifying common terminologies in this space and emphasize the differences between Algorithmic Dependability and Software Safety for ML-based systems. Then, we review ML dependability concerns from different perspectives across domains. At last, we review safety limitations for ML algorithms in terms of key engineering safety requirements that do not stand for the design and implementation of ML-based software. Note that we identify and introduce model dependability limitations as a subgroup of safety limitations.
2.1 Safety Terminologies

We start the background review by introducing common terminologies on the topic of ML safety that are referenced in the rest of this paper. Similar surveys also introduce ML safety-related terms to connect the relation between ML safety and code-based software safety [101, 107, 156, 233]. We aim to decompose and clarify the relationship between ML Safety, Security, and Dependability that are often interchangeably used in the literature. Safety is a System-Level concept as a set of processes and strategies to minimize the risk of hazards due to malfunctioning of system components. Safety standards such as IEC 61508 and ISO 26262 mandate complete analysis of hazards and risks, documentation for system architecture and design, detailed development process, and thorough verification strategies for each component, integration of components, and final system-level testing. Dependability is a Unit-Level concept to ensure performance and robustness of the software in its operational domain. We define ML dependability as the model’s ability to minimize test-time prediction error and therefore software unit failure. Therefore, a highly dependable ML algorithm is expected to be robust to natural distribution shifts within their intended operation design domain. Security is both a System-Level and a Unit-Level concept to protect from harm or other non-desirable (e.g., data theft, privacy violation) outcomes caused by adversaries. Note that engineering guidelines distinguish safety hazards (e.g., due to natural perturbations) from security hazards (e.g., due to adversarial perturbations) as the latter intentionally exploits system vulnerabilities to cause harm. However, the term safety is often loosely used in ML literature to refer to the dependability of algorithms against adversaries [107].

In this paper, we use the term safety as a set of unit-level strategies to maintain the dependability of ML algorithms in an intelligent system. We also cover adversarial training and detection techniques regardless of the role of the adversary in generating the attack.

2.2 Safety Limitations in ML

Engineering safety broadly refers to the management of operations and events in a system in order to protect its users by minimizing hazards, risks, and accidents. Given the importance of dependability of the system’s internal components (hardware and software), various engineering safety standards have been developed to ensure the system’s functional safety based on two fundamental principles of safety life cycle and failure analysis. Built on collection of best practices, engineering safety processes discover and eliminate design errors followed by probabilistic analysis of safety impact of possible system failures (i.e., failure analysis). Several efforts attempted to extend engineering safety standards to ML algorithms [31, 190]. For example, European Union Aviation Safety Agency released a report on concepts of design assurance for neural networks [31] that introduces safety assurance and assessment for learning algorithms in safety-critical applications. In another work, Siebert et al. [211] present a guideline to assess ML system quality from different aspects specific to ML algorithms including data, model, environment, system, and infrastructure in an industrial use case. However, the main body of engineering standards do not account for the statistical nature of ML algorithms and errors occurring due to the inability of the components to comprehend the environment. In a
recent review of automotive functional safety for ML-based software, Salay et al. [190] present an analysis that shows about 40% of software safety methods do not apply to ML models.

Given the dependability limitations of ML algorithms and lack of adaptability for traditional software development standards, in the following, we identify 5 open safety challenges for ML and briefly review active research topics for closing these safety gaps presented in Figure 1. We will extensively review the techniques for each challenge in Sections 5, 6, and 7.

2.2.1 Design Specification. Documenting and reviewing the software specification is a crucial step in engineering safety; however, formal design specification of ML models is generally not feasible, as the models learn patterns from large training sets to discriminate (or generate) their distributions for new unseen input. Therefore, ML algorithms learn the target classes through their training data (and regularization constraints) rather than formal specification. The lack of specifiability could cause mismatch between “designer objectives” and “what the model actually learned”, which could result in unintended functionality of the system. The data-driven optimization of model variables in ML training makes it challenging to define and pose specific safety constraints. Seshia et al. [203] surveyed the landscape of formal specification for DNNs to lay an initial foundation for formalizing and reasoning about properties of DNNs. To fill this gap, a common practice is to achieve partial design specification through training data specification and coverage. Another practical way to overcome the design specification problem is to break ML components into smaller algorithms (with smaller tasks) to work in a hierarchical structure. In the case of intelligent agents, safety-enforcing regularization terms [5], and simulation environments [20] are suggested to specify and verify training goals for the agent.

2.2.2 Implementation Transparency. Implementation transparency is an important requirement in engineering safety which gives the ability to trace back design requirements from the implementations. However, advanced ML models trained on high-dimensional data are not transparent. The very large number of variables in the models makes them incomprehensible or so-called black-box for design review and inspection. In order to achieve traceability, significant research has been performed on interpretability methods for DNN to provide instance explanations of model prediction and DNN intermediate feature layers [277]. In autonomous vehicles application, Bojarski et al. [18] propose VisualBackProp technique and show that a DNN algorithm trained to control a steering wheel would in fact learn patterns of lanes, road edges, and parked vehicles to execute the targeted task. However, the completeness of interpretability methods to grant traceability is not proven yet [2], and in practice, interpretability techniques are mainly used by designers to improve network structure and training process rather than support a safety assessment.

2.2.3 Testing and Verification. Design and implementation verification is another demanding requirement for unit testing to meet engineering safety standards. For example, coding guidelines for software safety enforce the elimination of dead or unreachable functions. Depending upon the safety integrity level, complete statement, branch coverage, or modified condition and decision coverage are required to confirm the adequacy of the unit tests. Coming to DNNs, formally verifying their correctness is challenging and in fact provably an NP-hard [202] problem due to the high dimensionality of the data. Therefore, reaching complete testing and verification of the operational design domain is not feasible for domains like image and video. As a result, researchers proposed new techniques such as searching for unknown-unknowns [10] and predictor-verifier training [54], and simulation-based toolkits [49] guided by formal models and specifications. Other techniques, including neuron coverage and fuzz testing [244] in neural networks incorporate these aspects. Note that formal verification of shallow and linear models for low dimensional sensor data does not carry verification challenges of the image domain.
2.2.4 Performance and Robustness. Engineering safety standards treat the ML models as a black box and suggest using methods to improve model performance and robustness. However, improving model performance and robustness is still an open problem and a vast research topic. Unlike code-based algorithms, statistical learning algorithms typically contain a residual error rate (due to false positive and false negative predictions) on the test set. In addition to the error rate on the test set, operational error is referred to as the model’s error rate that commonly occurs in open-world deployment. Section 6 reviews various approaches like introducing larger networks, training regularization, active learning and data collection, and domain generalization techniques to increase the model’s ability to learn generalizable representations for open-world applications.

2.2.5 Run-time Monitoring Function. Engineering safety standards suggest run-time monitoring functions as preventive solutions for various system errors, including less frequent transient errors. Monitoring functions in code-based algorithms are based on a rule-set to detect hardware errors and software crashes in the target operational domain. However, designing monitoring functions to predict ML error (e.g., false positive and false negative errors) is different in nature. ML models generate prediction probability that could be used to predict uncertainty for run-time validation of predictions. However, research shows that prediction probability in complex models like DNN does not fully represent uncertainty and hence can not guarantee failure prediction [89]. Section 7 reviews different approaches for run-time estimation of ML uncertainty and detection of outlier samples and adversarial attacks.

2.3 Engineering Standards

Software engineering safety standards mandate a meticulous analysis of hazards and risks, followed by a detailed development process focusing on system requirements, documented architecture and design, well-structured code, and thorough verification strategies for the unit, integration, and system-level testing. Autonomous systems are one of the major safety-critical applications of ML. This section briefly introduces two well-established safety standards and their shortcomings for ML-based software.

Functional safety standards define safety as the absence of unreasonable risk due to malfunctioning of system components (e.g., automotive ISO 26262 standard). This type of standards suggest multi-step procedures to identify safety needs, define safety requirements, and finally verify the design accordingly. Specifically, functional safety requires hazard analysis and risk assessment to determine system-level hazards that guide safety engineers towards identifying safety goals that are then used to create safety requirements. These safety requirements guide the system development process which is also decomposed into all aspects of development processes. A safety pipeline (V-Model) is used to ensure that safety needs are sufficiently fulfilled in different levels of architectural design, unit design, and unit testing and verification.

As data collection, model training, and evaluation are core pieces in ML software development process, the integrity of these offline activities is an important part of safety requirements. However, functional safety standards do not account for errors occurring due to the inability of the components to comprehend the environment (e.g., due to performance and robustness limitations) or foreseeable user misuse of the system. In a recent review of automotive functional safety for ML-based software, Salay et al. [190] presented an analysis of ISO-26262 part-6 methods with respect to the safety of ML models. Their assessment of software safety methods’ applicability on ML algorithms (as software unit design) shows that about 40% of software safety methods do not apply to ML models.

More tailored for ML-based software, new safety standards are proposed (e.g., ISO/PAS 21448 or Safety Of The Intended Functionality) that recognize ML performance limitations and expect
inputs or scenarios that belong to unsafe-unknown (e.g., out of distribution samples) and unsafe-known (e.g., out of operational design domain samples) situations. The hazard and risk analysis in these standards acknowledge ML limitations and therefore identifies hazards due to inadequate performance functionality, insufficient situational awareness, reasonably foreseeable misuse, and shortcomings of the Human-AI interface. Nevertheless, these standards are only limited to suggesting functional modifications are performed to reduce failure risks if the risk is estimated (during validation steps) to be higher than acceptable.

2.4 AI Safety
Considering ML being a subset of AI, studying ML safety limitation could be done through the more general topic of AI Safety for a variety of intelligent algorithms. Amodei et al. [5] present five open research problems regarding safe AI behavior in real-world systems. They characterize and review AI safety problems into defining and evaluating the agent’s objective function that could result in unintended and unsafe behavior. In another work, Hernandez-Orallo et al. [101] present a list of safety-related AI characteristics that could be considered for AI-based system design. Authors suggest a broad range of AI system characteristics that require future research, such as types of AI interactions and integration with the environment, and computation of inputs (e.g., Turing-complete vs. non Turing-complete).

Leike et al. [134] introduced a suite of reinforcement learning environments to measure the agent’s compliance with the intended safe behavior. Their work categorizes AI safety problems into two areas of specification and robustness, which cover various problems, including avoiding side effects and safe exploration, and robustness to self-modification and distributional shift. Later, Ortega et al. [166] suggests agent’s assurance as an addition to monitoring (for human and automated inspection) and controlling (to enforce and restricting the behavior) on the agent in run-time.

2.5 ML Trustworthiness
ML trustworthiness is another related topic to safety that explores limitations of ML algorithms when used in domains and tasks with high social and health impacts. Examples include fairness [51] and rationale decision-making [185] of ML models in domains like law [46] and ethics [100], and healthcare [60, 247] which model errors could cause damage. The relationship between ML trustworthiness and safety is tied in domains and applications in which the failure of the intelligent system could cause hazardous scenarios for the users. Here we review common tasks and domains in which the model trustworthiness is particularly important.

Recently, the ethical and privacy aspects of intelligent systems resulted in new regulations such as General Data Protection Regulation (GDPR) to data-driven software such as ML algorithms [237]. Data privacy is a crucial aspect of ML trustworthiness which may cause discrimination [51] or private information disclosure [1]. Additionally, various design guidelines and requirements can improve building trustworthy ML systems at different stages, including the training data creation and performance evaluations [3].

Model fairness is another aspect of trustworthiness in automated decision-making. Du et al. [51] categorizes roots of discrimination in ML and reviews common evaluation metrics for model fairness. They review different techniques to process the training data, regularize the training, and calibrate trained models as solutions to mitigate modeling bias. In another work, Huang et al. [107] focus on verification, testing, adversarial defense, and interpretability as the main pillars to achieve model trustworthiness. However, their review and analysis of trustworthiness consider model explanation and verification as necessary proofs of trustworthiness. In the importance of interpretability for trustworthiness, Zhang et al. [284] present a case of using ML explanations to find representation learning flaws caused by potential biases in the training dataset. Their...
technique mines the relationships between pairs of attributes according to their inference patterns. Interpretability results can then be used to regularize the training for trustworthy and rationale feature learning [185].

2.6 ML Best Practices

Nowadays, ML algorithms are applied in various domains and applications. However, ML solutions’ reliability depends on the best workflow practices from development teams in model design, data collection, and training. For example, in a recent paper, Amershi et al. [4] reviewed best practices in ML software engineering such as end-to-end development pipelines, data management, and automated evaluations. They proposed a ML process maturity model based on concepts like capability maturity model [170] to assess and improve the maturity of ML software projects. Additionally, Sculley et al. [197] reviewed hidden technical debt in ML systems that are less explored by the research community. They reviewed a range of limitations in the current state of designing, testing, and maintaining ML systems. From a more practical view, Breck et al. [19] present a list of 28 specific tests, and monitoring needs to quantify ML system reliability. They propose a road map with a testing rubric to improve ML production reliability using a set of best model training and maintenance practice metrics.

3 ML DEPENDABILITY

ML dependability is the model’s ability to minimize prediction risk. Unlike code-based algorithms, the dependability of ML algorithms is bounded to the model’s learning capacity and statistical assumptions under which the model is trained. Examples of these assumptions include the Independent and Identically Distribution (i.i.d) relation of source and target domains and the assumption for uniform distribution of data across all classes (i.e., class balance) [43, 146]. However, maintaining data distribution assumptions when deployed in the open-world is challenging and results in different types of prediction errors.

We envision the following categorization of model prediction error types into (i) Generalization Error, (ii) Distributional Error, and (iii) Adversarial Error as a unified “big picture” to achieve dependable and robust ML models in open-world. Additionally, we review relevant benchmarks commonly used for sound and fair evaluation of each ML error type.

3.1 Generalization Error

The first and foremost goal in representation learning is in-distribution generalization. Consider a model learned by empirical risk minimization (ERM) on training set $S = \{(x_i, y_i)\}_{i=1}^N$ i.i.d sampled from the underlying distribution $D$. The model should not only fit $S$ by minimizing the empirical error $L_S(f) = \frac{1}{N} \sum_{x \in S} L(x)$, but also have low generalization error on unseen data $L_D(f) = \mathbb{E}_{x \in D} L(x)$. The generalization gap is defined as the difference between the model performance on training data and unseen data sampled from the same distribution, is a commonly used metric to evaluate model generalization ability [102]. The de facto method nowadays of probing generalization is to split the available dataset into two (or three) subsets: one for training, (one for validation), and the other for testing. To facilitate fair comparison, the splitting is typically fixed. The goodness of fit on the test set provides an approximation of generalization beyond training. Recent years have witnessed the successful application of this holdout evaluation methodology to monitoring the progress of many ML fields, especially where large-scale labeled datasets are readily available.

Multiple factors such as weak representation learning affect the model’s generalization error which is common in open-world setups [109]. On the importance of generalizable representation learning, Zhang et al. [278] point out the capacity of large DNNs is sufficient enough to memorize a small training set even in the case of random labels without any correlation between training labels
and test labels. On the other hand, the training set quality can greatly affect model generalization error as many assumptions such as uniform distribution of training data may not be easy to achieve in open and uncontrolled environments.

**Benchmark Datasets:** Model generalization is commonly evaluated on a separate test set provided for the dataset, which is often found to be inherently limited. For example, Wang et al. [241] show that the fixed ImageNet [38] test set is not sufficient to reliably evaluate the generalization ability of state-of-the-art image classifiers, due to the insufficiency in representing the rich visual open-world. Other efforts have been made to collect new samples to improve test sets for image classification tasks. For instance, ImageNet-V2 was collected in [180] with the same data source and collection pipeline to reproduce the original ImageNet test set. This new benchmark leads to the observation that the prediction accuracy of even the best image classifiers is still highly sensitive to minutiae of the test set distribution and extensive hyperparameter tuning. In another work, Tsipras et al. [231] focus on the effects of noisy data collection pipeline on a systematic misalignment between the training sets and the real-world tasks.

### 3.2 Distributional Error

Domain shift (also known as distribution shift and dataset shift) describes variations in the target data distribution ($D_{target}$) in comparison to the source training distribution ($D_{train}$). Distributional error is the misprediction of target samples due to inconsistency between source and target distributions and hence reduces the Operational Performance compared to the test set ($D_{test}$) performance. In this regard, domain generalization techniques are necessary elements in training ML models for open-world applications in which target samples are captured from uncontrolled and constantly changing environments. Common examples of domain shift include non-semantic distribution changes due to input perturbations (e.g., natural perturbations due to weather and lighting changes), data changes over time (e.g., seasonal variations of data), and even more substantial texture and breed variations. On studies to measure distributional error, different work show that using a fixed test set are insufficiently representative of the whole target distribution. For instance, Recht et al. [179, 180] found that a minute natural distribution shift leads to a large drop in accuracy for a broad range of image classifiers on both CIFAR-10 [121] and ImageNet. Taori et al. [225] presented a series of experiments to measure model robustness to natural distribution shifts. The authors evaluated 204 ImageNet models in 213 different test conditions, only to find little to no transfer of robustness from current synthetic to natural distribution shift.

Beyond generalization to reasonably foreseeable domain shifts, Out-of-Distribution (OOD) or outlier samples are referred to undesirable test-time samples with disjoint label space and high semantic discrepancy. OOD samples commonly occur in open environments and may belong to any unknown $D_{out}$ distribution outside the source training set. OOD detection is an approach to detect OOD samples and abstain those predictions to reduce distributional error from undesirable OOD samples (please see Section 7.2 for details).

**Benchmark Datasets:** Several variants of the ImageNet dataset have been introduced for reliable benchmarking of distributional error in ML. Hendrycks and Dietterich [90] pioneered to show that ML models exhibit unexpected prediction errors on simple naturally occurring perturbations. The authors introduced two variants of the original ImageNet validation set: ImageNet-C benchmark for input corruption robustness and the ImageNet-P dataset for input perturbation robustness. Later, the authors present ImageNet-A and ImageNet-O [98] real-world unmodified samples to test classification performance under distribution shifts and out-of-distribution detection performance under label distribution shifts, respectively. For evaluating model robustness on subdomain shifts, Santurkar et al. present Breeds [193], a suite of subdomain shift benchmarks of varying granularity.
They define data subdomains as a way to evaluate how well models can generalize beyond the limited diversity of source training datasets. In another work, Hendrycks et al. [99] present a series of benchmarks for measuring model robustness to variations on image renditions (ImageNet-R benchmark), imaging time and geographic location (StreetView benchmark), and objects size, occlusion, camera viewpoint, and zoom (DeepFashion Remixed benchmark). In the video domain, [207] utilized temporal consistency in video frames to construct image-level robustness benchmarks: they assembled sets of contiguous video frames that appear perceptually similar to humans, but produce inconsistent predictions for classifiers. Lastly, regarding benchmarking out-of-distribution detection performance in semantic segmentation task, Hendrycks et al. [94] present a benchmark for natural OOD samples with multi-class, multi-label in large-scale images.

### 3.3 Adversarial Error

In comparison to distributional error, an adversarial error could be viewed as an augmented distribution shift for a given model by intentionally manipulating the pristine input data to mislead the model without fooling the human [74]. We called the manipulated input data as adversarial examples. Therefore, adversarial errors are the worst-case model performance evaluated by the carefully crafted adversarial examples. The core problem to get the adversarial error is to generate adversarial examples. One important criterion for adversarial examples is the visual perceptual property so that the adversarial example could not fool a human viewer. To maintain this criterion, common threat models of adversarial examples, including the $l_p$ constrained perturbation, spatial perturbation [256] and semantically meaningful perturbation [177] are proposed. Beyond studies on generating adversarial examples in the digital domain, there has been significant progress on generating physically possible adversarial examples by altering physical surfaces, i.e., applying adversarial printable 2D patches [21] or by altering the shape of 3D surfaces [258].

**Benchmarks Datasets:** Most adversarial defense works benchmark their results on standard test sets (such as CIFAR and ImageNet) perturbed by popular adversarial attack algorithms leading to adversarial robustness measurements. However, the main challenges here are (1) how to fairly compare different defense methods as they often leverage different attack algorithms and (2) how to fairly assess the defense generalizability to diverse unseen attacks. To this end, [112]
created standardized evaluation frameworks of ImageNet-UA and CIFAR-10-UA to measure model generalization to a diverse set of distortions not seen during defense creation by introducing diverse attack suites, including four novel adversarial attacks. RobustBench [34] is another standardized benchmark of adversarial robustness, which as accurately as possible reflects the robustness of the considered models within a reasonable computational budget. The authors evaluate model robustness against AutoAttack [33] and also analyzed general trends in adversarial robustness and its impact on other tasks such as robustness to various distribution shifts and out-of-distribution detection.

4 ML SAFETY STRATEGIES

Looking at fundamental limitations of code-based software safety for machine learning on one hand and research debt in AI safety on the other hand, we review and organize practical solutions to improve ML dependability and safety. Our organization decomposes the ML dependability objective into multiple safety strategies for improving dependability of ML-based systems for their safe execution in open-world scenarios. In order to do so, we connect ML safety-related techniques with appropriate engineering safety strategies to find common ground in safety needs for ML.

Our categorization is similar to Varshney’s [233] review of four main engineering safety strategies gathered from different industries. We review a broad spectrum of state-of-the-art ML techniques to achieve reasonable coverage and diversity of research papers. Our safety strategies followed by ML solutions and detailed techniques serve as a way to checkup the safety strategies employed in any given ML system. As illustrated in Figure 2, we propose categorizing ML techniques in three following safety strategies:

• (1) Inherently Safe Model: refers to techniques to design ML models that are intrinsically error-free or verifiable to be error-free in their intended target domain. We review model transparency and formal methods such as model specification, verification, and formal testing as main pillars to achieve the inherently safe design. However, there are many open challenges for these solutions to guarantee ML safety.

• (2) Enhancing Performance and Robustness: refers to techniques to increase model performance (on the source domain) and robustness against distributional shifts. Perhaps the most commonly used in practice, these techniques contribute to safety by improving the operational performance of ML algorithms. We review key approaches and techniques such as training regularization, domain generalization, adversarial training, etc.

• (3) Run-time Error Detection refers to strategies to detect model mispredictions at the run-time (or test-time) to prevent model errors from becoming system failures. This strategy can help mitigating hazards related to ML performance limitations in the operational domain. We review key approaches and techniques for model uncertainty estimation, out-of-distribution detection, and adversarial attack detection.

Additionally, we will briefly discuss the importance of (4) Human-AI Interactions for user awareness, user trust, and misuse prevention in Section 8.6. However, we do not include those in our main categorization and review since the human factors related to Human-AI interfaces and interactions are out of scope for this paper. Also, we differentiate ML safety from Security because the external factors (i.e., attacker) which intentionally exploit system vulnerabilities are the security threats rather than a design limitation. Table 1 presents a summary of reviewed techniques and papers for each safety strategy. Reviewed papers are organized into different solutions (middle column) to group papers into individual research approaches. We go through details and describe complement each other in the following sections.
Table 1. We organize and review key research papers in the field of practical machine learning techniques to improve the safety of ML algorithms. Left column presents engineering safety strategies and right column maps machine learning techniques with representative research papers.

| Safety Strategy                    | ML Solutions                      | ML Techniques                                      |
|------------------------------------|-----------------------------------|---------------------------------------------------|
| Inherently Safe Design             | Model Transparency                | Visualizations ([103, 111, 148, 220, 251])         |
|                                    | Design Specification              | Model Specification ([11, 50, 172, 189, 202, 203]) |
|                                    |                                   | Environment Specification ([188])                  |
|                                    | Model Verification and Testing     | Formal Verification ([53, 106, 113, 163, 244])     |
|                                    |                                   | Semi-Formal Verification ([24, 48, 49, 54])       |
|                                    |                                   | Formal Testing ([10, 123, 171, 221, 283])         |
|                                    |                                   | End-to-End Testing ([47, 59, 117, 266])           |
|                                    | Robust Network Architecture       | Model Capacity ([42, 80, 105, 141, 149, 162, 198, 240, 267]) |
|                                    |                                   | Model Structure and Operations ([26, 44, 84, 164, 226, 234, 263, 285]) |
|                                    |                                   | Training Regularization ([108, 161, 168, 238, 239, 273, 286, 290]) |
|                                    | Robust Training                   | Transfer Learning and Pretraining ([27–29, 95, 110, 205, 269, 271, 274]) |
|                                    |                                   | Adversarial Training ([41, 74, 76, 204, 249, 279–281]) |
|                                    |                                   | Domain Randomization ([133, 228, 229, 265, 291])  |
|                                    |                                   | Robust Representation Learning ([108, 238, 239, 242]) |
|                                    |                                   | Multi-source Training ([9, 72, 129, 137, 224, 254]) |
|                                    | Data Sampling and Augmentation    | Active Learning ([12, 64, 87, 210])               |
|                                    |                                   | Hardness Weighted Sampling ([58, 282])            |
|                                    |                                   | Data Cleansing ([15, 86, 276])                    |
|                                    |                                   | Data Augmentation ([35, 69, 97, 99, 235, 275, 289, 292]) |
| Uncertainty Estimation and Error Detection | Uncertainty Calibration | Uncertainty Calibration ([82, 122, 159, 222, 288]) |
|                                    | Out-of-distribution Detection     | Uncertainty Estimation ([125, 39, 62, 128, 142, 152, 160, 167, 232]) |
|                                    |                                   | Distance-based Detection ([13, 132, 186, 197, 217, 223, 227, 256]) |
|                                    | Adversarial Detection and Guard   | Classification-based Detection ([71, 77, 93, 96, 104, 131, 157, 272]) |
|                                    |                                   | Density-based Detection ([30, 52, 78, 143, 195, 201, 245, 294]) |
|                                    |                                   | Adversarial Detection ([157, 73, 79, 92, 138, 147, 155, 264]) |
|                                    |                                   | Adversarial Guard ([387, 83, 191, 206, 261])      |

5 INHERENTLY SAFE DESIGN

The inherently safe design represents the goal of building ML systems that are provably error-less w.r.t. specified operational domain and requirements. Although trivial for code-based algorithms, safety by design is an open problem (NP-hard in high-dimensional domains) for ML algorithms. In this section, we review the three main requirements to achieve safe ML algorithms as being (1) model transparency, (2) formal specification, and (3) formal verification and testing. These three requirements aim to formulate high-level system design specifications into low-level task specifications, leading to transparent system design, and formal verification or testing for model specifications.

5.1 Model Transparency

Transparency and interpretability of the ML model is an essential requirement for trustworthy, fair, and safe ML-based systems in real-world applications [155]. However, advanced ML models with high performance on high dimensional domains usually have very large parameter space, making them hard to interpret for humans. In fact, the interpretability of a ML model is inversely proportional to its size and complexity. For example, a shallow interpretable model like a decision tree becomes uninterpretable when a large number of trees are ensemble to create a random forest model. The inevitable trade-off between model interpretability and performance limits the transparency for deep models to “explaining the black-box” in a human understandable way w.r.t. explanations complexity and length [45]. Regularizing the training for model interpretability is a way to improve model transparency for low-dimensional domains. For example, Lage et al. [123] present a regularization to improve human interpretability by incorporate user feedback in model
training by measuring users’ mean response time to predict the label assigned to each data point at inference time. Lakkaraju et al. [124] build predictive models with sets of independent interpretable if-then rules. In the following, we review techniques for model transparency in three parts: model explanations (or global explanations), prediction explanations (or instance explanations), and evaluating the truthfulness of explanations.

5.1.1 Model Explanations. Model Explanations are techniques to estimate ML models for explaining the representation space or what the model has learned.

Model Estimations. One way to explain ML models is through estimation and approximation of deep models to generate simple and human understandable representations. The descriptive decision rule set is a common way to generate interpretable model explanations. For example, Guidotti et al. [81] present a technique to train local decision tree (i.e., interpretable estimate) to explain any given black-box model. Their explanation consists of a decision rule for the prediction and a set of counterfactual rules for the reversed decision. Lakkaraju et al. [126] propose to explain deep models with a small number of compact decision sets through subspace explanations with user-selected features of interest. Ribeiro et al. [183] introduce Anchors, a model-agnostic estimator that can explain the behavior of deep models with high-precision rules applicable for different domains and tasks. To address this issue, Lakkaraju et al. [127] present a framework to optimize a minimax objective for constructing high-fidelity explanations in the presence of adversarial perturbations. In a different direction, Wu et al. [253] present a tree regularization technique to estimate a complex model by learning tree-like decision boundaries. Their implementations on time-series deep models show that users could understand and trust decision trees trained to mimic deep model predictions.

Visual Concepts. Exploring a trained network by its learned semantic concepts is another way to inspect model rationale and efficiency in recognizing patterns. Kim et al. [116] introduce concept activation vectors as a solution to translate model representation vectors to human understanding of concepts. They create high-level user-defined concepts (e.g., texture patterns) by training auxiliary linear “concept classifiers” with samples from the training set to draw concepts that are important in model prediction. Ghorbani et al. [70] take another direction by clustering the super-pixel segmentation of image saliency maps to discover visual concepts. Their post-training explanation method provides meaningful concepts to create coherent and important examples for model prediction. Along the same line, Zhou et al. [293] propose a framework for generating visual concepts by decomposing the neural activations of the input image into semantically interpretable components pretrained from a large concept corpus. Their technique is able to disentangle the features encoded in the activation feature vectors and quantify the contribution of different features to the final prediction. In another work, Yeh et al. [268] study the completeness of visual concepts with a completeness score to quantify the sufficiency of a particular set of concepts in explaining the model’s prediction.

Visualization Tools. ML visualization tools enable various dependability assurance techniques such as monitoring and inspection of training data [246], the data flow graphs [251], training process [220] and inspecting a trained model [103]. For example, Kahng et al. [111] designed an interactive visualization system to interpret models and results for large-scale deep learning implementations. Their visualization tool integrates multiple coordinated views, such as a computation graph overview of the model architecture, neuron activation view for pattern discovery and comparison. Additionally, model analytic tools allow for exploring complex networks with example inquiries such as counterfactual and neighbor subsets. The explanation by example is referred to model-agnostic techniques to explain model behavior by picking samples from the training or test set that are similar to the target sample in the model representation space [103]. Although it is a very
popular approach for model and data inspection, the example-based explanations could generate misleading examples in cases with small training sets (w.r.t. model size and input dimensionality) or non-uniform distribution of the training set [115].

5.1.2 Instance Explanations. Instance or local explanations explain the model prediction for specific input instances regardless of overall model behavior. This type of explanation carries less holistic information about the model but informs about model behavior near the examples input, which is suitable for investigating the edge cases for model debugging.

Local Approximations. Training shallow interpretable models to locally approximate the deep model’s behavior can provide model explanations. A significant benefit of local approximation techniques is their model agnostic application and clarity of the saliency feature map. However, the faithfulness of explanations is greatly limited to factors like the heuristic technique, input example, and training set quality. For instance, Ribeiro et al. [182] proposed LIME which trains a linear model to locally mimic the deep model’s prediction. The linear model is trained on a small binary perturbed training set located near the input sample which the labels are generated by the deep model. Lundberg and Lee [145] present a model agnostic prediction explanation technique that uses the Shapley values of a conditional expectation function from the deep model as the measure of feature importance. DeepLIFT [209] is another local approximation technique that decomposes the output prediction for the input by backpropagating the neuron contributions of the network w.r.t each input feature. They compare activations for the specific input to its “reference activation” to assign feature contribution scores.

Saliency Map for DNNs. Various heuristic gradient-based, deconvolution-based, and perturbation-based techniques have been proposed to generate saliency maps for DNNs. Gradient-based methods use backpropagation to compute the partial derivative of the class prediction score w.r.t. the input image [212]. Later, Smilkov et al. [215] proposed to improve the noisy visualization of saliency map by introducing noise to the input. Grad-CAM [200] technique combines feature maps from DNN’s intermediate layers to generate saliency maps for the target class. Zeiler and Fergus [277] propose a deconvolution-based saliency map by adding a deconvnet on each layer which provides a continuous path from the prediction back to the image. Similarly, Springenberg et al. [218] propose a guided backpropagation technique that modifies ReLu function gradients and uses class-dependent constraints in the backpropagation process. For real-time applications, Bojarski et al. [18] presents a variant of layer-wise relevance propagation for fast execution of saliency maps. Perturbation-based or sensitivity-based techniques measure the sensitivity of the model output w.r.t. the input features. For example, Zeiler and Fergus [277] calculate the saliency map by sliding fixed size patches to occlude the input image and measure prediction probability.

5.1.3 Explanation Truthfulness. Since model explanations are always incomplete estimation of the black-box models, there need to be mechanisms to evaluate for both correctness and completeness of model explanations w.r.t. the main model. Particularly, the fidelity of the ad-hoc explanation technique should be evaluated against the black-box model itself. Aside from the qualitative review of model explanations and their consistency compared to similar techniques [145, 165, 200], we look into sanity check tests and human-grounded evaluations in the following.

Sanity Checks and Proxy Tasks. Examining model explanations with different heuristic tests is shown to be an effective way to evaluate explanation truthfulness for specific scenarios. For example, Samek et al. [192] proposed a framework for evaluating saliency explanations by their correlation between saliency map quality and network performance under input perturbation. In a similar work, Kindermans et al. [119] present the inconsistencies in saliency maps due to simple image transformations. Adebayo et al. [2] propose three tests to measure the fidelity of any
interpretability technique in tasks that are either data sensitive or model sensitive. Ribeiro et al. [182] evaluates explanations generated by LIME against gold standard explanations directly from a sparse logistic regression model. A drawback of this approach is the limitation of shallow models on learning complex data. On the other hand, presenting the usefulness of explanations as a proxy task has been used in some literature. For instance, Zeiler and Fergus [277] propose using visualization of features in different layers to improve network architecture and training by adjusting network layers. In another example, with model trustworthiness evaluation as a proxy-task, Zhang et al. [284] present cases of evaluating explanations’ usefulness to find representation learning flaws caused by biases in the training dataset as a proxy task.

**Human Evaluation and Ground-truth.** Evaluating model explanations with user input is based on the assumption that good model explanations should be consistent with human reasoning and understanding of data. Multiple works [145, 182, 183] made use of end-user evaluation for explanations and tested a hypothesis on how users would identify and prefer better models and explanations by only looking at explanations. However, there are multiple human factors in user feedback on ML explanations such as average user understanding, the task dependency and usefulness of explanations, and user trust in explanations. Therefore, more concise evaluation metrics [135] have been introduced to reveal model behavior to human users, justifying the predictions, and helping humans investigate uncertain predictions. Another challenge in human study evaluations is the time and cost to run human subject studies and collect user feedback. To eliminate the need for repeated user studies, Mohseni et al. [158] implemented an evaluation benchmark for model explanations with multi-layer user annotation of important features w.r.t. the target class. Another similar work introduced a human-attention benchmark [36] for visual question answering task.

### 5.2 Formal Methods

Formal methods require rigorous mathematical specification and verification of a system to obtain “guarantees” on system behavior. A design cycle in formal methods involves two main steps of (1) listing design specifications to meet the system requirements and then (2) verify the system to prove the delivery of requirements in the target environment. Specifically, formal verification certifies that the system $S$ exhibits the specified property $P$ when operating in the environment $E$. Therefore, system specification and verification are two complementary components in formal methods. Unlike the common practice in data-driven algorithms which rely on available data samples to model the environment, formal methods require exact specification of the algorithm properties. In contrary to model validation in ML, formal methods require verification of the system given the environment space. Related to ML specification and verification, Huang et al. [107] reviews ML verification methods by the type of guarantees they can provide such as deterministic guarantees, approximate bounds, and converging bounds. However, due to challenges in model specification and verification in high-dimensional domains, many works such as Sheshia et al. [202] and Yamaguchi et al. [266] suggest end-to-end simulation-based validation of AI-based systems as a semi-formal verification of complex systems in which a realistic simulation of the environment and events is used to find counterexamples for system failures. In the following, we review different research on formal methods for ML algorithms.

#### 5.2.1 Formal Specification.

The specification is a necessary step prior to the software development and the basis for the system verification. Examples of common formal specification methods in software design are temporal logic and regular expressions. However, in the training of ML algorithms, the training set specifies the model task in the target distribution rather than a list of
rules and requirements. Here we review techniques and experiments in model and environment specifications.

**Model Specification:** Specifying the desired model behavior is a design requirement prior to any system development. However, formal specification of ML algorithms is very challenging for real-world tasks involving high-dimensional data like images. Sheshia et al. [202, 203] review open challenges for ML specifications and survey the landscape of formal specification approaches. For example, ML for semantic feature learning can be specified on multiple levels (e.g., system-level, input distribution level, etc.) to simplify overall specifications. Bartocci et al. [11] review tools for specifying ML systems in complex dynamic environments. They propose specification-based monitoring algorithms that provide qualitative and quantitative satisfaction score for the model using either simulated (online) or existing (offline) inputs. Additionally, as ML algorithms carry uncertainty in their outputs, the benefits of including prediction uncertainty in the overall system specification is an open and under investigation topic [151]. Focusing on invariance specifications, Pei et al. [172] decompose safety properties for common real-world image distortions into 12 transformation invariance properties that a ML algorithm should maintain. Based on these specifications, they verify safety properties of the trained model using samples from the target domain. In the domain of adversarial perturbations, Dreossi et al. [50] propose a unifying formalization to specify adversarial perturbations from formal methods perspective.

**Environment Modeling:** Modeling the operational or target environment is a requirement in formal system specification. Robust data collection techniques are needed for full coverage of the problem space environment. Several techniques such as active learning, semi-supervised learning, and knowledge transfer are proposed to improve the training data by following design specifications and encourage the model to learn more generalizable features in the target environment. As a result, a training set with enough coverage can better close the generalization gap between the source training and target operational domains. Similarly, in AI-based systems with multiple ML components, a robust specification of the dynamic environment with its active components (e.g., humans actions) enables for better system design [188].

5.2.2 **Model Verification.** Formal verification in software development is an assurance process for design and implementation validity. There are several approaches in software engineering such as constraint solving and exhaustive search to perform formal verification. For instance, a constraint solver like Boolean Satisfiability (SAT) provides deterministic guarantee on different verification constraints. However, verification of ML algorithms with conventional methods is challenging for high-dimensional data domains. In this section, we review different approaches for system-level and algorithm-level verification on ML systems.

**Formal Verification.** A line of research adapts conventional verification methods for ML algorithms. For example, Narodytska et al. [163] present a SAT solver for Boolean encoded neural networks in which all weights and activations are binary functions. Their solution verifies various properties of binary networks such as robustness to adversarial examples; however, these solvers often perform well when problems are represented as a Boolean combination of constraints. Recent SMT solvers for neural networks present use cases of efficient solvers for DNN verification on airborne collision avoidance and vehicle collision prediction applications [113]. However, the proposed line of solutions is limited to small models with limited number of parameters commonly used on low dimensional data. Additionally, given the complexity of DNNs, the efficiency and truthfulness of these verification techniques require sanity checks and comparisons against similar techniques [53].

Huang et al. [106] present an automated verification framework based on SMT theory which applies image manipulations and perturbations such as changing camera angle and lighting conditions.
Their technique employs region-based exhaustive search and benefits from layer-wise analysis of perturbation propagation. Wang et al. [244] combine symbolic interval and linear relaxation that scales to larger networks up to 10000 nodes. Their experiments on small image datasets verify trained networks for perturbations such as brightness and contrast.

**Quantitative and Semi-formal Verification.** Given the complexity of ML algorithms, quantitative verification assigns quality values to the ML system rather than a Boolean output. For example, Dvijotham et al. [54] present a jointly predictor-verifier training framework that simultaneously trains and verifies certain properties of the network. Specifically, the predictor and verifier networks are jointly trained on a combination of the main task loss and the upper bound on the worst-case violation of the specification from the verifier. Another work presents random sample generators within the model and environment specification constraints for quantitative verification [24].

Further, system-level simulation tools provide the environment to generate new scenarios to illustrate various safety properties of the intelligent system. For example, Leike et al. [134] present a simulation environment that can decompose safety problems into robustness and specification limitations. In more complex AI-based systems, Dreossi et al. [48] presents a framework to analyze and identify misclassifications leading to system-level property violations. Their framework creates an approximation of the model and feature space to provide sets of misclassified feature vectors that can falsify the system. Another example is VerifAI [49], a simulation-based verification and synthesis toolkit guided by formal models and specifications. VerifAI consists of four main modules to model the environment to abstract feature space, search the feature space to find scenarios that violate specifications, monitor the properties and objective functions, and analyze the counterexamples found during simulations.

### 5.2.3 Formal Testing.

Testing is the process of evaluating the model or system against an unseen set of samples or scenarios. Unlike model verification, testing does not require formal specification of the system or environment but instead focuses only on the set of test samples. The need for a new and unseen test set is because often model errors happen due to systematic biases in the training data resulting in learning incorrect or incomplete representations of the environment and task. Structural coverage metrics such as statement and modified condition/decision coverage (MC/DC) have been used in code-based algorithms to measure and ensure the adequacy of testing of safety-critical applications. However, testing in high-dimensional space is expensive as it requires very large number of test scenarios to ensure adequate coverage and an oracle to identify failures [283]. We review these two aspects in the following.

**Test Coverage.** The coverage of test scenarios or samples is a particularly important factor to satisfy the testing quality. Inspired by the MC/DC test coverage criterion, Sun et al. [221] propose a DNN specific test coverage criteria to balance between the computation cost and finding erroneous samples. They developed a search algorithm based on gradient descent which looks for satisfiable test cases in an adaptive manner. Pei et al. [171] introduce the neuron coverage metric as the number of unique activated neurons (for the entire test set) over the total number of neurons in the DNN. They present DeepXplore framework to systematically test DNN by its neuron coverage and cross-referencing oracles. Similar to adversarial training setups, their experiments demonstrate that searching for samples that both trigger diverse outputs and achieving high neuron coverage in a joint optimization fashion can improve model prediction accuracy.

In guided search for testing, Lakkaraju et al. [125] present an explore-exploit strategy for discovering unknown-unknown false positive samples in the unseen $D_{test}$. Later, Bansal and Weld [10] present a search algorithm which is formulated as an optimization problem that aims to select samples from $D_{test}$ maximize the utility model subject to a budget of maximum number of oracle
calls. Differential testing techniques use multiple trained copies of the target algorithm to serve as a correctness oracle for cross-referencing [175].

*End-to-end Simulations.* End-to-end simulation tools enable testing for complex AI-based systems by generating diverse test samples and evaluating system components together. For instance, Yamaguchi et al. [266] present a series of simulations to combine requirement mining and model checking in simulation-based testing for end-to-end systems. Fremont et al. [59] present a scenario-based testing tool which generates test cases by combining specification of possible scenarios and safety properties. In many cases, samples and scenarios from the simulation tests are used to improve the training set. For example, Dreossi et al. [47] propose a framework for generating counterexamples or edge-cases for ML to improve both the training set and test coverage. Their experiment results for simulation-based augmentation show edge-cases have important properties for retraining and improving the model. In the application of object detection, Kim et al. [117] present a framework to identify and characterize misprediction scenarios using high-level semantic representation of the environment. Their framework consists of an environment simulator and rule extractor that generates compact rules that help the scene generator to debug and improve the training set.

### 6 Enhancing Model Performance and Robustness

Enhancing model performance and robustness is the most common strategy to improve product quality and reduce the safety risk of ML models in the open world. Specifically, techniques to enhance model performance and robustness reduce different model error types to gain dependability w.r.t criteria reviewed in Section 3. In the following, we organize and review ML solutions to improve performance and robustness into three parts focusing on (1) robust network architecture, (2) robust training, and (3) data sampling and manipulation.

#### 6.1 Robust Network Architecture

Here we review how network size and architecture impact model performance and robustness.

*Model Capacity.* Djolonga et al. [42] studied the impacts of model capacity and training set size on distributional shift robustness. The results show that with enough training data, increasing model capacity (both width and depth) consistently helps model robustness against out-of-distribution generalization errors. Madry et al. [149] showed that increasing model capacity (width) alone can increase model robustness against adversarial attacks. Xie et al. [260] observed that increasing network depth for adversarial training can largely boost adversarial robustness, while the corresponding clean accuracy quickly saturates as the network goes deeper. The above empirical findings that larger models lead to better robustness are also consistent with theoretical results [66, 162]. In contrast, Wu et al. [252] conducted a thorough study on the impact of model width on adversarial robustness and concluded that wider neural networks may suffer from worst perturbation stability and thus worst overall model robustness. To accommodate for computational resources while maintaining model robustness, a surge of works have studies robustness-aware model compression [80, 105, 141, 198, 240, 267]. For instance, Lin et al. [141] observe a non-monotonic relationship between model size and robustness in deep network quantization. In studying how sparsity affects DNN robustness, Guo et al. [85] empirically discovered that an appropriately higher deep model sparsity led to better robustness, whereas over-sparsification could in turn cause fragility.

*Network Structure and Operators.* Besides the model’s total size or capacity, the network structure, including the topology and operators, also explicitly impact the network’s generalization and robustness. Guo et al. [84] first took an architectural perspective and investigate the patterns of network architectures that are resilient to adversarial attacks. The authors leveraged Neural Architecture Search (NAS) to discover a family of robust architectures (RobNets). They empirically...
observed that densely connected patterns result in improved robustness and adding convolution operations to direct connection edge is effective. Following that, Dong et al. [44] explored the relationship among adversarial robustness, Lipschitz constant, and architecture parameters and show that an appropriate constraint on architecture parameters could reduce the Lipschitz constant which can further improve the model robustness. The research trend of NAS for adversarially robust architectures continues to develop [26, 164], although they still lack a clear comprehension of how an architectural inductive bias could be represented and translated to the robustness analysis. Recent research suggests activation functions may also play an important role in model robustness. Xie et al. [263] proposed to use asymmetric activation functions for forward and backward passes in neural network training. Specifically, the authors observe that the smoother activation function in the backward pass can generate better gradients, which has been shown to empirically help both accuracy and robustness. Tavakoli et al. [226] proposed a set of learnable activation functions, termed SPLASH, which can be used to simultaneously improve model accuracy and robustness. Zhang et al. [285] first pointed out the use of down-sampling methods (e.g., pooling, strided convolutions) in modern deep neural networks ignores the sampling theorem and limits the models to be invariant to domain-shifts. The authors proposed to use traditional anti-aliasing methods by adding low-pass filters after sampling operations to increase model shift invariance. Following that, [234] modified the ResNet [88] model structure by adding blur filters and using smooth activation functions at key locations. The improved ResNet structure achieves better robustness on multiple out-of-distribution generalization tasks. The recent success of Visual Transformer (ViT) has also extracted attention from the robustness community. Some recent works [16, 150] benchmarked model robustness of ViT and observed it to have better general robustness than traditional CNNs.

6.2 Robust Training

Training of ML models has a direct impact on their operational performance and robustness. Various techniques have been proposed to efficiently learn generalizable representations.

6.2.1 Training Regularization. Regularization techniques have been widely used to improve model generalization ability and robustness. For instance, conventionally $L_1$ and $L_2$ penalties have been used to avoid over-fitting. Stability training [290] stabilizes deep networks against small input distortions by regularizing the feature distance between the original image and its corrupted version constructed by adding random Gaussian noises. With a different approach, Zhang and LeCun [286] explored using unlabeled free data to regularize model training for robustness and uncertainty. Yuan et al. [273] showed that model distillation can be taken as a learned label smoothing [161] regularization which helps in-distribution generalization. Hendrycks et al. [97] use the JSD divergence among the original image and its augmented versions as a consistency regularizer to improve model robustness against common corruptions. Virtual Adversarial Training (VAT) [154] proposed a new regularizer based on measuring local smoothness of the conditional label distribution given input. Unlike classical adversarial training (see Section 6.2.3), VAT needs no label information and is hence more suitable for semi-supervised learning. Lipschitz continuity is a well studied regularization to enforce both empirical and certified model robustness (see Section 6.2.3). For example, Huster et al. [174] propose a methodology of controlling Lipschitz constants to maximize model robustness by regularizing the model to learn a class of well-conditioned neural networks in which a unit amount of change in the inputs spaces only causes at most the same unit amount of change in the outputs. Singla and Feizi [213] proposed a differential upper bound on Lipschitz constant of convolutional layers, which can be directly optimized to improve model generalization ability and robustness.

6.2.2 Transfer Learning and Pretraining. Several research show using pre-trained models from similar domains helps to improve the quality of learned representations, and therefore, model
performance and robustness [269]. Hendrycks et al. [95] show pre-training can improve model robustness and out-of-distribution awareness by transferring universal representations from a pre-trained model to the new domain. That direction continues to be explored by [270]. Shafahi et al. [205] demonstrated the feasibility to transfer not only performance but also robustness from a source model to a target domain. The authors of [27] first introduced adversarial training into self-supervised pre-training to provide general-purpose robust pre-trained models for the first time. They found these robust pre-trained models can benefit the subsequent fine-tuning to boost final model robustness and reduce the computation cost. More recently, [28, 29] show that pre-trained ImageNet knowledge can be leveraged through distillation to significantly improve zero-shot synthetic-to-real generalization. Further, [110] leverages pre-training from a contrastive learning framework to train feature invariances under differently augmented views to achieve adversarial robustness. As a closely related approach, simultaneous training for multiple tasks encourages the model to learn diverse features to improve robustness.

6.2.3 Adversarial Training. Adversarial training (AT) incorporates adversarial examples into training data to increase model robustness against adversarial attacks at test-time. State-of-the-art AT methods are arguably top-performers [149, 281] to enhance deep network robustness against adversarial attacks. AT algorithms optimize a hybrid loss consisting of a standard classification loss \( L_c \) and a adversarial robustness loss term \( L_a \):

\[
\min_{\theta} \mathbb{E}_{(x, y) \sim D} \left[ (1 - \lambda) L_c + \lambda L_a \right], \quad L_c = L(f(x; \theta), y), \quad L_a = \max_{\delta \in B(\epsilon)} L(f(x + \delta; \theta), y) \tag{1}
\]

where \( B(\epsilon) = \{ \delta \mid \| \delta \|_{\infty} \leq \epsilon \} \) is the allowed perturbation set to keep samples are visually unchanged, and \( \lambda \) is a fixed training weight hyper-parameter. For example common AT methods, both Fast Gradient Sign Method (FGSM-AT) [74] and Projected Gradient Descent (PGD-AT) [149] uses an \( \epsilon \) for the allowed perturbation set that formalizes the manipulative power of the adversary. Examples of variations of PGD include, TRADES [281] which uses the same clean loss as PGD-AT, but replace \( L_a \) from cross-entropy to a soft logits-pairing term. In MMA training [41], the adversarial \( L_a \) loss is to maximize the margins between correctly classified images. Additionally, despite the possible trade-off between adversarial robustness and prediction accuracy, some works [230] show that both the model accuracy and adversarial robustness may benefit from sufficiently large model capacity, as well as more training data.

Fast Adversarial Training. Despite the effectiveness of AT methods against attacks, they suffer from very high computation cost due to multiple extra backward propagations to generate adversarial examples. The high training cost would make AT impractical in certain domains and large-scale datasets [262]. Therefore, a line of work tries to accelerate AT. Zhang et al. [279] restricted most adversarial updates in the first layer to effectively reduce the total number of the forward and backward passes to improve the training efficiency. Shafahi et al. [204] used a “free” AT algorithm by updating the network parameters and adversarial perturbation simultaneously on a single backward pass. Wong et al. [250] showed that, with proper random initialization, single-step PGD-AT can be as effective as multiple-step ones but much more efficient.

Semi-supervised and self-supervised for Adversarial Training. Schmidt et al. [196] show that sample complexity in adversarial learning can be significantly larger than that of “standard” learning and hence requires more samples to achieve non-trivial adversarial robust classifier. However, conventional adversarial training needs class labels and can not be easily applied to unlabeled data. Adversarial training under semi-supervised and self-supervised environments can boost the adversarial robustness [23] to use unlabeled data. To benefit from self-supervised learning, Hendrycks et al. [95] used the self-supervision to improve the robustness by simply adding a rotation loss into the training pipeline. After it, Chen et al. [27] study different combinations between...
pre-train and fine-tune on self-supervised settings and showed that fine-tuning the pre-trained self-supervised learning could contribute to the dominant portion of robustness improvement. Adversarial Self-Supervised Contrastive Learning Different from the above methods which still require the labeled data to perform adversarial training, [118] proposed a contrastive self-supervised learning framework to train an adversarially robust model without any class labels.

Certified Adversarial Training. Certified AT aims to obtain networks with provable guarantees on robustness under certain assumptions and conditions. Certified AT uses a verification method to find an upper bound of the inner max, and then update the parameters based on this upper bound of robust loss. Minimizing an upper bound of the inner max guarantees to minimize the robust loss. Linear relaxations of neural networks [249] use the dual of linear programming (or other similar approaches [243]) to provide a linear relaxation of the network (referred to as a “convex adversarial polytope”) and the resulting bounds are tractable for robust optimization. However, these methods are both computationally and memory intensive which can increase model training time by a factor of hundreds. Interval Bound Propagation (IBP) [76] is a simple and efficient method for training verifiable neural networks which achieved state-of-the-art verified error on many datasets. However, the training procedure of IBP is unstable and sensitive to hyperparameters. Similarly, Zhang et al. proposed CROWN-IBP [280] to combine the efficiency of IBP and the tightness of a linear relaxation based verification bound. Other certified adversarial training techniques include ReLU stability regularization [259], distributionally robust optimization [214], semi-definite relaxations [55, 178] and random smoothing [32].

6.2.4 Domain Generalization. Cross-domain generalization presents an important indicator of “in-the-wild” model robustness for open-world applications such as autonomous vehicles and robotics where deployment in different domains is common.

Domain Randomization. Utilizing randomized variations of the source training set can improve generalization to the unseen target domain. Domain randomization with random data augmentation has been a popular baseline in both reinforcement learning [228] and general scene understanding [229], where the goal is to introduce randomized variations to the input to improve sim-to-real generalization. Yue et al. [274] use category-specific ImageNet images to randomly stylize the synthetic training images. YOLOv4 [17] benefits from a new random data augmentation method that diversifies training samples by mixing images for detection of objects outside their normal context. Data augmentation can also be achieved through network randomization [133, 265], which introduces randomized convolutional neural networks for more robust representation. Data augmentation for general visual recognition tasks is discussed in Section 6.3.

Robust Representation Learning. The ability to generalize across domains also hinges greatly on the quality of learned representations. As a result, introducing inductive bias and regularizations are crucial tools to promote robust representation. For instance, Pan et al. [168] show that better designed normalization leads to improved generalization. In addition, neural networks are prone to overfitting to superficial (domain-specific) representations such as textures and high-frequency components. Therefore, preventing overfitting by better capturing the global image gestalt can considerably improve the generalization to unseen domains [108, 238, 239, 242]. For example, Wang et al. [238] prevents the early layers from learning low-level features, such as color and texture, but instead focus on the global structure of the image. Representation Self-Challenging (RSC) [108] iteratively discards the dominant features during training and forces the network to utilize remaining features that correlate with labels.

Multi-Source Training. Another stream of methods assume multiple source domains during training and target the generalization on the held-out test domains. They use multiple domain
information during training to learn domain agnostic biases and common knowledge that also apply to unseen target domains. A representative work is the PACS Dataset [136], which has inspired many follow-up work [9, 137]. Sharing a similar root, Gong et al. [72] aim to bridge multiple source domains by introducing a continuous sequence of intermediate domains and thus be able to capture any test domain that lies between the source domains. More recently, Lambert et al. [129] propose to construct a composite semantic segmentation dataset from multiple sources to improve the zero-shot generalization ability to unseen domains of semantic segmentation models. Multi-source training has also been shown to benefit open-world applications. For instance, Tang et al. [224] present a pose-aware multi-task vehicle re-identification technique to overcome viewpoint dependency of the objects. In another recent work, Wu et al. [254] propose a new technique for improving model robustness to domain shift in unmanned aerial vehicle (UAV), by casting a cross-domain object detection problem with multiple fine-grained domains.

6.3 Data Sampling and Augmentation
The quality of training data is an important factor for machine learning with big data [146]. In this section, we review a collection of algorithmic techniques for data sampling, cleansing, and augmentation for improved and robust training.

Active Learning. Active learning is a framework solution to improve training set quality and minimize data labeling costs by selectively labeling valuable samples (i.e., “edge cases”) from an unlabeled pool. The sample acquisition function in active learning frameworks often relies on prediction uncertainty such as Bayesian estimation [64] and ensemble-based [12] uncertainties. Differently, ViewAL [210] actively samples hard-cases by measuring prediction inconsistency across different viewpoints for multi-view semantic segmentation tasks. Haussmann et al. [87] presents a scalable active learning framework for open-world applications in which both the target and environment can greatly affect model predictions.

Hardness Weighted Sampling. Another data sampling strategy to improve model performance and robustness is assigning larger training weights (in the loss function) to hard training samples [58, 282]. For instance, Zhang et al. [282] achieve this by estimating sample hardness with their distance to the classification boundary and assigning larger weights to hard samples. Fidon et al. [58] perform weight sampling by modeling sample uncertainty through minimizing the worst-case expected loss over an uncertainty set of training data distributions.

Data Cleansing. Label errors on large-scale annotated training sets induce noisy or even incorrect supervision during model training and evaluation [15, 241]. For example, Yun et al. [276] emphasize on the effect of label noise in training and present a re-labeled ImageNet training set with localized multi-label training samples. Bey er et al. [15] develop a data cleansing and multi-labeling framework for collecting human annotations of the ImageNet validation set. In another work, Han et al. [86] proposed an end-to-end label correction framework to reduce label noise from a noisy dataset for improved model performance. Their results show that training on the new cleansed annotations improved both classification accuracy and robustness against distributional shifts [86, 276].

Data Augmentation. Data augmentation is commonly used to gain prediction invariance to simple image variations like rotation and scaling. More advanced techniques such as adaptive augmentation transformations [56], random patch erasing [292], or automatically composing augmentation chains [35] also shown to be effective for both robustness and representation learning. Recently, style transfer augmentations [69] have been shown to improve model robustness to texture bias. AugMix [97] utilizes stochasticity and diverse augmentations by mixing multiple augmented images. This augmentation is shown to significantly improve robustness and uncertainty measures on challenging benchmarks, including ImageNet-C and ImageNet-P [90]. CutMix [275] proposed
to remove image patches and replace the removed regions with a patch from another image, where the new ground truth labels are also mixed proportionally to the number of pixels of combined images. CutMix is shown to improve the model robustness against input corruptions and its out-of-distribution detection performance. Lately, Hendrycks et al. [99] propose DeepAugment to increase robustness to cross-domain shifts by employing image-to-image translation networks for data augmentation rather than conventional data-independent pixel-domain augmentation. Besides, adversarial data augmentation [235, 289] has also shown promise for training robust deep neural networks against unforeseen data shifts or corruptions, where fictitious target distributions are generated adversarially to resemble “worst-case” unforeseen data shifts throughout training. Zhang et al. [287] implemented learning-based approaches to synthesize foreground objects and background contexts for new training samples in extremely low data regimes.

7 RUN-TIME ERROR DETECTION

Our third strategy for ML safety leverages from the range of techniques for detecting ML misclassification errors at run-time (or test time). Although in recent years, advanced neural networks, regularization techniques, and large training datasets significantly improved model representation learning and hence their performance and robustness. However, prediction uncertainty is an inseparable characteristic of ML algorithms and run-time monitoring of the model is necessary from the safety standpoint. Run-time error detection techniques could be used to improve the dependability of ML at the time of model misclassification due to the existence of unknown-unknown samples and adversarial attacks (see Section 3). Selective classification (or classification with reject option) is the main approach to incorporate these techniques in decision-making and ultimately triggering appropriate warnings to trigger Safe Fail plans at the time of system failure. In selective classification, the model cautiously provides predictions for high-confidence samples and abstain when in doubt. For instance, in the multi-class image classification problem with \( X \) being the space of all “natural” images consist of both target \( D_{in} \) (normal distribution) and undesirable \( D_{out} \) (unknown outlier distribution). Given the run-time input \( S \subseteq X \), we aim to have an outlier detector that \( h_S(x) : X \rightarrow \{0, 1\} \), where \( h_S(x) = 1 \iff x \in D_{out} \) and \( h_S(x) = 0 \iff x \in D_{in} \). Threshold \( \lambda \) controls the detection rate based on the detection signal \( n_S(x) : X \rightarrow \mathbb{R} \). Therefore a gate function is constructed as follows:

\[
    h^\lambda_S(x) = \begin{cases} 
        1 & n_S(x) \geq \lambda \\
        0 & n_S(x) < \lambda
    \end{cases}
\]  

(2)

Selective classification of high-confident predictions can significantly improve model performance at the cost of test coverage. Recent examples [67, 68] present simple and effective implementations which guarantee control over the true risk when running on in-domain test samples.

In the rest of this section, we review model uncertainty estimation, out-of-distribution detection, and adversarial attack detection techniques as run-time error detection strategies for ML safety. Note that although these techniques have overlapping contributions, we separate them by their targeted error types and discuss their relationships and limitations.

7.1 Uncertainty Calibration and Quantification

Uncertainty in probabilistic learners is an important factor in maintaining the fail-safety of the system. Even well-trained and calibrated predictors that are robust to noise, corruption, and perturbations can benefit from uncertainty estimation to detect domain shift and out-of-distribution samples at run-time. Characterizing and estimating uncertainty can explain what a model does not know in terms of model confidence on its prediction which provides useful information to planners for subsequent decision making [151]. In addition, active learning is an important offline application of uncertainty estimation to improve training sets quality by measuring by identifying ambiguous data points [210].
However, obtaining reliable uncertainty estimation is difficult for several reasons. First, unlike semantic categories or objective measurements such as depth, uncertainty by nature is subjective and difficult to define. Second, the ground truth for uncertainty is also difficult to obtain because of the subjectiveness. Third, current deep neural networks are known to be overconfident, especially on unseen data [139]. As a result, leveraging network output (such as softmax) as a proxy to interpret uncertainty can result in ridiculously wrong estimations.

To overcome the network overconfidence issue, researchers have widely resorted to uncertainty calibration which aims to predict probability estimates that represent true correctness likelihood [82]. In this regard, advances in uncertainty estimation have studied the sources of uncertainties and broadly divided them into two categories: (1) Aleatoric uncertainty which captures noise inherent in the observations; (2) Epistemic uncertainty which accounts for uncertainty in the model due to limited data [39]. These studies have led to better understandings of the network behaviors and allow one to differentiate the predictions on different samples for better safety guarantees in open-world applications.

7.1.1 Uncertainty Calibration: It is known that deep neural networks tend to be miscalibrated. Accordingly, a wide range of previous work have been proposed to solve this problem. Label smoothing [222] has been a popular technique that promotes more uniform output distribution through regularization. It was shown that label regularization not only gives more calibrated output but also leads to improved network generalization. Guo et al. [82] proposed to measure the calibration quality primarily based on expected calibration error (ECE), defined as the difference in expectation between confidence and accuracy. Other measures such as maximum calibration error (MCE) and negative log-likelihood (NLL) are also considered. The authors found that temperature scaling is the most effective among all evaluated methods, even though it is a simple variant of Platt scaling by dividing the logit scores of a classifier with a scalar $T$ (termed temperature). This technique was later found to be also very effective on alleviating overconfidence for unfamiliar samples [139]. Considering that temperature scaling may undesirably clamp down legitimate high confidence predictions, Kumar et al. [122] proposed maximum mean calibration error (MMCE) which is a trainable calibration measure based on a reproducible kernel Hilbert space (RKHS), and is minimized alongside the NLL loss during training. In another direction, Zhang et al. [288] used structured dropout to promote model diversity and improve confidence calibration.

7.1.2 Uncertainty Quantification: There have been rich studies of uncertainty quantification in many fields, ranging from science and engineering to many real-world applications. Der Kiureghian and Ditlevsen [39] presents one of the early works by identifying and categorizing the sources of uncertainty into two types: aleatoric uncertainty and epistemic uncertainty. Such categorization and definitions are also inherited in deep learning [61], where Bayesian learning has been a classical tool to quantify uncertainties. Specifically, Gal [61] considered modeling aleatoric uncertainties in deep neural networks following a Bayesian modeling framework where one assumes some prior distribution over the space of parameters. The author described an instantiation of this Bayesian modeling framework using Bayesian Neural Networks (BNNs) as well as approximate inference techniques with variational inference. The author derived a practical approximate inference method for BNNs which essentially leads to model ensembling with statistical regularization techniques such as dropout [219] and other more advanced variants [62, 63]. Kendall and Gal [114] further proposed a Bayesian framework that jointly models both aleatoric and epistemic uncertainties and demonstrated its successful applications in computer vision tasks such as semantic segmentation and depth estimation. Indeed, Bayesian methods and deep ensembling [128, 167] have been popular approaches to achieve uncertainty quantification with the disadvantage of additional computation cost. To overcome high computation cost in uncertainty quantification, uncertainty
quantification approaches with single deterministic models have been proposed. For instance, Chen et al. [25] propose an Angular Visual Hardness (AVH) distance-based measure which shows good correlation to human perception of visual hardness. AVH shows the underlying connection to aleatoric uncertainty and significantly improves tasks such as self-training. The fact that AVH can be computed using regular training with softmax cross-entropy loss makes it convenient to obtain and a drop-in uncertainty measure for most existing neural networks. Several other works also improve uncertainty estimation and its computation cost by using only a single model and employing RBF networks [142], distance training [232], and inductive biases [160].

7.2 Out-of-distribution Detectors

Model prediction errors on OOD inputs can be reduced by detecting OOD samples and then rejecting their predictions. In the following, we categorize and review OOD detection techniques into three groups.

7.2.1 Distance-Based Detection. Distance-based methods measure the distance between the input sample and source training set in the representation space. These techniques involve pre-processing or test-time sampling of the source domain distribution and measure their averaged distance to the test sample. Various distance measures including Mahalanobis distance [132], cosine similarity [227], and Euclidean distance [77] have been employed. For example, Ruff et al. [186] present a deep learning one-class classification approach to minimize the representation hypersphere for normal distribution and calculating the detection score by the distance of the outlier sample to the center of the hypersphere. They later [187] extended this work using samples labeled as OOD in a semi-supervised manner. Bergman and Hoshen [13] presented a technique that learns a feature space such that inter-class distance is larger than the intra-class distance. Sohn et al. [217] presented a two-stage one-class classification framework that leverages self-supervision and a shallow one-class classifier. The OOD detection performance of distance-based methods can be improved by ensembling measurements over multiple input augmentations [223] and network layers [132, 194]. Sastry and Oore [194] used gram matrices to compute pairwise feature correlations between channels of each layer and identify anomalies by comparing inputs values with its respective range observed over the training data. Tack et al. [223] applied contrastive learning for OOD detection by ensembling over random augmentations to improve OOD detection performance.

7.2.2 Classification-Based Detection. Classification-based detection techniques seek effective representation learning to encode normality together with OOD detection scores. Various OOD detection scores have been proposed including maximum softmax probability [91], prediction entropy [93], KL-divergence and Jensen-Shannon divergence [96] from uniform distribution as detection score. For example, a simple baseline approach for classification-based OOD detection is to use class probabilities as a measure for OOD detection [91]. Further, to improve the detection performance, Lee et al. [131] and Hsu et al. [104] proposed a combination of temperature scaling and adversarial input perturbations to calibrate the model to increase the gap between softmax confidence for the inlier and outlier samples. Another line of research proposes using disjoint unlabeled OOD training set to learn normality and hence improve OOD detection. Hendrycs et al. [93] present a case for joint training of natural outlier set (from any auxiliary disjoint training set) with the normal training set resulting in fast and memory efficient OOD detection with minimal architectural changes. Yu and Aizawa [272] present a two-head network to maximize prediction disagreements for outlier samples.

Recent work show that self-supervised learning can further improve OOD detection and surpass prior techniques [71, 96, 159, 199, 248]. Tack et al. [223] propose using geometric transformations like rotation to shift different samples further away to improve OOD detection performance. Other classification-based techniques including revising network architecture for learning better
prediction confidence during the training [40]. Vyas et al. [236] present a framework for employing an ensemble of classifiers that each leave out a subset of the training set as OOD examples and the rest as the normal in-distribution training set.

7.2.3 Density-based Detection. Using density estimates from Deep Generative Models (DGM) is another line of work to detect OOD samples by creating a probability density function from the source distribution. Recent work on Variational Autoencoders (VAE) and Generative Adversarial Networks (GAN) [195] shows these models often assign higher likelihoods to samples with high similarity to the training set and low likelihood to outliers with significantly different semantics. Different scores based on likelihood are proposed for OOD detection [181] using GANs and based on reconstruction error [294] using VAEs. However, some recent studies present counterintuitive results that challenge the validity of VAEs and DGMs likelihood ratios for semantic OOD detection [245] in high-dimensional data and propose ways to improve likelihood-based score such as using natural perturbation [30] For instance, Serrà et al. [201] connect the limitations of generative models’ likelihood score for OOD detection with the input complexity and use an estimate of input complexity to derive a new efficient detection score.

Energy-based models (EBMs) are another family of DGMs that has shown higher performance in OOD detection. Du and Mordatch [52] present EBMs for OOD detection on high-dimensional data and investigate limitations of reconstruction error on VAEs compared to their proposed energy score. A recent line of work reinterprets standard discriminative classifiers of \( p(y|x) \) as an energy-based model for the joint distribution \( p(x,y) \). For instance, Grathwohl et al. [78] present a joint energy-based model (JEM), an architecture that uses logits of a supervised classifier to define the joint density of training points. Liu et al. [143] propose another energy-based framework for model training with a new OOD detection score based on discriminative models.

7.3 Adversarial Detection and Guards

Adversarial detection and adversarial guards are test-time methods to mitigate the risk of adversarial attacks. Adversarial detection refers to designing a separate detector before the ML model to identify adversarial perturbations. Adversarial guarding refers to leveraging different methods to remove the effects of adversarial perturbations from a given image sample. Note that neither of these approaches manipulates model parameters or model training process; therefore, these solutions are complementary to adversarial training solutions reviewed in Section 6.2.3.

7.3.1 Adversarial Attack Detection. The most straightforward way to detect adversarial examples is to train a Secondary Model as the attack detector. To achieve this, Grosse et al. [79] and Gong et al. [73] propose adding adversarial examples directly to the training set and train the secondary model to detect them. Adversarial and clean examples have different intrinsic properties which can be used as low dimensional features to detect adversarial examples. For instance, Hendrycks and Gimpel [92] apply Principal Component Analysis (PCA) to the natural and adversarial images directly. They find that the adversarial images have consistently greater variances for low-ranked principal components than clean images. In another work, Ma et al. [147] show that Local Intrinsic Dimensionality (LID) which assesses the space-filling capability of the region surrounding a reference example, is significantly larger for adversarial examples than normal images. MagNet [153] uses the distance between the test-time inputs and training data manifold for detecting adversarial examples.

Statistical Testing utilizes the difference in distribution of adversarial examples and natural clean examples for adversarial detection. For example, Grosse et al. [79] use the Maximum Mean Discrepancy (MMD) test to evaluate whether the clean images and adversarial examples are from the same distribution. They observe that adversarial examples are located in the different output surface regions compared to clean inputs. Similarly, Feinman et al. [57] leverage the kernel density
estimations from the last layer and Bayesian uncertainty estimations from the dropout layer to measure the statistical difference between adversarial examples and normal ones.

Applying Transformation and Randomness is another approach to detect adversarial examples based on the observation that natural images could be resistant to the transformation or random perturbations while the adversarial ones are not. Therefore, one can detect adversarial examples with high accuracy based on the model prediction discrepancy due to applying simple transformations and randomness. For instance, Li and Li [138] apply a small mean blur filter to the input image before feeding it into the network. They show that natural images are resistant to such transformations while adversarial images are not. Similarly, Xu et al. [264] apply the feature squeezing methods such as reducing the color bit and spatial smoothing to inputs.

7.3.2 Test-Time Adversarial Guard. Test-Time adversarial guard aims to accurately classify both adversarial and natural inputs without changing the model parameters. Various test-time transformations have been proposed to diminish the adversarial effect of the adversarial perturbations by pre-processing inputs before feeding to the model. The research investigates the efficiency of applying different basis transformations to input images, including the JPEG compression [37, 83, 206], bit-depth reduction, image quilting, total variance minimization [83], low-pass filters, PCA, low-resolution wavelet approximations, and soft-thresholding [206]. Pixel Deflection [173] randomly selects pixels from the test image and replaces their values with other randomly selected pixels within their neighborhood. It has been shown that the adversarial effect could be canceled out with these transformations without hurting the benign performance.

Different from the above transformation-based methods, a separate denoising network or operation can be used on adversarial images to remove the adversarial effects. For instance, Liang et al. [140] use a noise reduction method to mitigate the adversarial effects and Samangouei et al. [191] use a generative adversarial network trained on clean training samples to “denoise” adversarial examples. Additionally, randomness has also been used to map the adversarial examples back to the natural image manifold. For example, Xie et al. [261] propose to apply randomization operations including random resizing and random padding to input images to remove adversarial effects.

7.3.3 Gradient Masking and Defense Evaluation. Although a wide range of test-time adversarial detection and guard methods have been proposed, Carlini and Wagner [22] and Athalye et al. [7] emphasize on the importance of evaluation pipelines to measure defense robustness against diverse attacks. In other words, the evaluation must include the setting that the attackers tried their best to break the defense. For example, Papernot et al. [169] introduce gradient masking as a category of failed defense methods that work by trying to deny the attacker access to a useful gradient. On the importance of defense evaluation, Carlini and Wagner [22] propose three stronger threat models which can break the fake robustness achieved by gradient masking. Athalye et al. [7] propose the techniques including the Backward Pass Differentiable Approximation, Expectation Over Transformation, and reparameterization techniques to overcome the gradient masking problems.

8 OPEN PROBLEMS AND RESEARCH DIRECTIONS

In our survey, we presented a review and categorization of classical software safety methods with fundamental limitations in ML algorithms. The impetus of this work was to leverage from both engineering safety strategies and state-of-the-art ML techniques to enhance the dependability and safety of ML components in autonomous systems. However, maintaining the safety of autonomous systems requires a multidisciplinary effort across multiple fields including machine learning, software engineering, and hardware engineering [120]. In the following, we briefly review and discuss other dimensions of safety and security of ML-based systems that could benefit research communities’ attention.
8.1 Inherently Safe and Transparent Design
The first main challenge of designing inherently safe ML models lies in the computation complexity and scalability [107, 283]. As ML models are becoming exponentially more complex, it will become extremely difficult to design specification and verification mechanisms that are well-adapted to large ML models. For example, Dreossi et al. [48] pointed out that a modular approach is central to scaling up formal methods to large systems, even when some components (such as perception) do not themselves have precise formal specifications.

On the other hand, recent advancements in 3D rendering and simulation have introduced promising solutions for end-to-end testing and semi-formal verification in simulated environments. However, it is challenging to mitigate the gap between simulation and real-world situations, causing questionable transfer of simulated verification and testing results. Recent work starts exploring how simulated formal simulation aid in designing real-world tests [59]. Additionally, thorough and scenario-based simulations enable system verification in broader terms such as monitoring interactions between ML modules in a complex system, e.g., how would an attack on the perception module affect the control module.

8.2 Robust and Dependable Machine Learning
Despite advances in studying natural corruptions, distributional shift and adversarial robustness, respectively, there lacks systematic efforts to tackle robustness limitations in a unified framework to cover the "in-between" cases within this spectrum. Historically, the study of one robustness type does not always translate to benefiting other types. The recent paper [50] formalized various types of robustness that the research communities have considered in the literature, yielding a unifying quantitative-Boolean formulation of robustness. To date, most robustness work has focused on model invariances to small perturbations. However, alternate specifications for properties directly relevant in real-world can offer more favorable research opportunities. One example of practical relevance is to perturb in the semantic feature spaces: modeling the underlying semantic context in which ML systems operate can be crucial to scale up analysis and also provide more meaningful task-oriented results [184].

Another less explored direction for ML robustness is to benefit from multi-domain and multi-source training data for improved representation learning. The rich contexts captured from sensor sets with diverse orientations and data modality can significantly improve prediction robustness compared to a single input source (e.g., single camera). Self-checking based on temporal and semantic coherence of data could also be exploited to enhancing robustness and performance in practical applications such as autonomous vehicles.

8.3 Uncertainty Awareness and Self-Assessment
There are profound demands to research and develop new ML techniques for system self-assessment of task confidence or skill proficiency in a dynamic environment where the input distribution or the task goal may vary. Although current efforts mostly arise from Bayesian statistics and data-driven calibration, domain knowledge is a crucial component to benefit from in open-world applications. For example, incorporating prior knowledge from physical phenomena like sensor noise and lighting conditions can be cast into information theoretical forms for robust uncertainty estimation [144]. Another practical and understudy uncertainty-aware design proposed in [151] is to use prediction uncertainty together with the prediction itself to impact downstream decision-making and planning tasks in the system.

Another direction to support objective self-assessment is to identify, develop, and validate suitable metrics. Note that although well-defined metrics exist for different machine learning tasks, such as classification accuracy or task completion time, the system confidence, uncertainty or skill
proficiency is often not easily quantifiable and leaves a large open room. To operationalize and quantify self-awareness in the context of autonomous and intelligent systems, one may use a specific cognitive model of self-awareness derived from experimental studies of pre-linguistic infants and non-linguistic animals [14]. In outline, the intelligent system identifies five dimensions of self-awareness that are relevant to autonomous and intelligent systems, namely: spatial self-awareness, bodily self-awareness, goal self-awareness, agential self-awareness, and cognitive self-awareness. Research could develop concrete evaluation metrics along those five dimensions for different applications.

8.4 Adversarial Robustness and Detection
Detecting adversarial examples will remain an open research as new attacks are introduced to challenge and defeat detection methods. A potential future direction is by leveraging domain knowledge and data properties to improve attack detection. For example, Xiao et al. [255] study the spatial consistency property in the semantic segmentation task by randomly selecting image patches and cross-checking model predictions among the overlap area. Based on this property, they propose a consistency check-based method to detect adversarial examples. In video domain, Xiao et al. [257] study the temporal property of data in time by applying optical flow estimation to the target and previous frames and introducing a random noise to the estimated optical flow to generate pseudo frames. Then, they evaluate the consistency of the learner output between pseudo and target frames in different video tasks.

Utilizing new network architectures is another research direction to improve adversarial robustness and detection. Recently, Qin et al. [176] show adversarial detection by leveraging class-conditional reconstruction networks (CapsNets). Their experiments indicate that CapsNets use features that are in fact more aligned with human perception and could be used effectively to detect adversarial examples.

8.5 Safety-Aware Training Data
The quality of training data has a direct impact on representation learning and hence model performance and robustness. Unlike training datasets and evaluation benchmarks commonly used in research, a safety-aware training set is a dynamic repository of samples belonging to target distributions (specified in the operational design domain). A dynamic safety-aware training set repository requires regular data capturing, cleaning, and labeling to improve dataset quality on different factors. Such regular training dataset self-assessments will result in the identification of noisy labels and possible imbalance sub-distributions in the dataset. Active learning and self-labeling techniques allow for efficient and targeted data collection by individual ML algorithms to performance improvement. Ultimately, the safety-aware training dataset seeks to increase the coverage of edge cases by collecting them directly from the open-world.

8.6 Human-AI Considerations for ML Safety
Beyond functional safety of the intelligent system, Human-AI interaction research aims to prevent end-users (e.g., driver in the autonomous vehicle) from unintentional misuse of the system due to lack of instructions, over-trusting, and unawareness [156]. Algorithmic transparency and user interface design are two main approaches to improve the safety of the operations by the user in autonomous systems [155]. In this approach, users can benefit from explainable interface design which provides useful and comprehensible information about model reasoning and prediction uncertainty. For example, user interface design could leverage real-time visualization of ML predictions, uncertainties in perception and system planning to help calibrate users’ understanding of the system’s limitations during operation. A further ambition is for ML systems to communicate prediction uncertainty with users and potentially to incorporate user feedback at run time.
9 CONCLUSION

We proposed a categorization for broad range of ML techniques that support algorithmic safety for open-world deployment of ML based software. Our organization of ML techniques is supported by a thorough reviewing of key papers in each branch. At the end, we identified open problems and research directions that can benefit from research community. We hope our categorization and review helps in building new ML safety guidelines and development frameworks for safety-critical applications.

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