TestifAI: A Comprehensive Testing Framework For Safe AI

By

Arooj Arif

aa3506phd

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ABSTRACT

Deep neural networks (DNNs) models are critical in high-stake domains such as autonomous driving, medical diagnostics, and security systems, where their deployment in real-world scenarios requires rigorous robustness testing due to diverse environmental conditions. Traditional metrics like neuron coverage, while essential, do not fully capture all corner cases, which can lead to unexpected model failures. To address this gap, this research introduces a comprehensive testing framework that enhances the correctness evaluation of models through a structured five-stage process. The first stage is specification, defines essential system properties to guide the entire testing process and ensure comprehensive coverage. The second sampling stage, gathering relevant samples for exhaustive model testing. In the test case generation stage, the defined properties are applied to create targeted test scenarios. The testing and probabilistic graph stage validates the effectiveness of these test cases and conducts robustness assessments both locally (within individual category) and globally (across multiple scenarios), employing a Problog for detailed probabilistic and quantitative analysis of performance. The final stage is error summarisation, compiles and analyzes recorded errors to generate actionable graphical error reports and recommendations, thus guiding the refinement of models. This framework not only fills existing gaps in DNNs testing but also supports the development of models that are correct across varied environmental conditions.

TABLE OF CONTENTS

List of Figures

List of Tables

List of Algorithms

How to read this document

This thesis uses terms such AI system, deep learning models, model, system or DNNs, interchangeably in this document. Terms related to class in dataset (supervised learning case) such as component or class, are also used interchangeably.

Important reading notes:

Terms that are used but not defined/explained in the text are listed and defined in the **Appendix A**. They are displayed in SMALL CAPS in the text. Clicking on a word shown in SMALL CAPS (e.g., LOCAL COVERAGE) takes the reader directly to the definition of that term in the Glossary. From there, one may click on the page number shown at the end of the definition to return.

Chapter 1

Introduction

1.1 Background and Motivation

Deep Neural Networks (DNNs) are increasingly being used in diverse applications due to their ability to match or exceed human-level performance. With the broader deployment of DNNs in various safety-critical systems like autonomous vehicles, healthcare, and avionics, concerns over their safety and trustworthiness have been raised [1]. The availability of large datasets, fast computing methods, and their high performance has enabled the use of DNNs in safety-critical applications [2]. The critical nature of such applications makes it essential to thoroughly evaluate these DNNs before deployment to guarentee their reliability and safety.

In recent years, there has been significant amount of publications focused on tackling this concern. Figure. 5.1 visualizes the significant growth in the number of published papers related to DNNs safety from 2008 to 2023[1].

An important requirement for DNNs is that they are robust against input perturbations [3]. DNNs have shown a lack of robustness due to their vulnerability to adversarial examples, where even minor modifications to an input, sometimes imperceptible to humans, can destabilize the neural network [4, 5]. Unlike traditional software, DNNs do not have a clear control-flow structure. They learn their decision policy through training on large datasets, adjusting parameters gradually using various methods to achieve the desired accuracy. Consequently, traditional software testing methods like functional coverage and branch coverage cannot be applied to DNNs, thus challenging

[1]The data is gathered using a comprehensive set of relevant keywords. The keywords used for data extraction include: 'deep neural network safety,' 'DNN verification,' 'DNN testing,' 'deep learning robustness,' 'neural network adversarial attacks,' 'DNN defense mechanisms,' 'DNN interpretability,' 'deep learning certification,' 'neural network validation,' and 'machine learning security.'

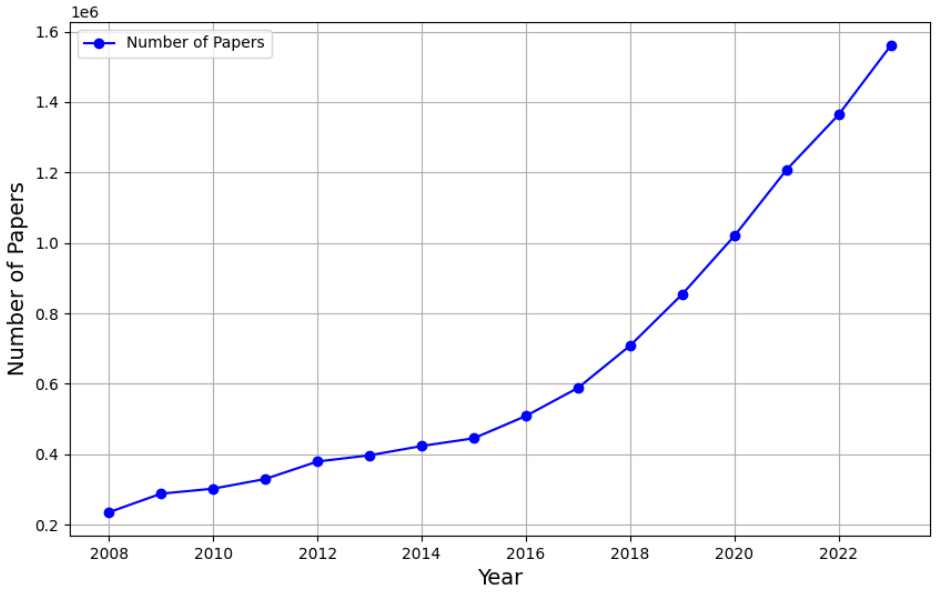


FIGURE 1.1: Number of Published Papers on DNN Safety

their use in safety-critical applications. This is because DNNs lack explicit paths and branches that can be directly tested; their behavior emerges from complex interactions within their learned parameters, making it difficult to apply traditional coverage metrics that rely on predefined control flows [6].

In the past, researchers have extensively discussed both verification and testing techniques, which are useful for evaluating the DNNs. Verification involves proving the property (e.g. adversarial examples (noise, rotation, brightness, etc.)) of a system through mathematical proof. This approach ensures that certain property is met by the system based on a formal analysis. However,DNN verification techniques are promising, they suffer from a scalability problem, due to the high computational complexity and the large size of DNNs. Up to now, DNN verification techniques either work with small scale DNNs or with approximate methods with convergence guarantees on the bounds [3]. This limitation impacts the ability to achieve high coverage, which means to cover all input scenarios and conditions to ensure that all potential issues are identified.

On the other hand, testing focuses on identifying defects (i.e, counter example to a property) or provide assurance cases [7], by evaluating the behavior of system through empirical methods. As a result, they can achieve high coverage, which suggests that more of a DNN's behavior has been tested and therefore the DNN has a lower chance of containing undetected bugs [3]. While these coverage metrics are useful, they often fall short in providing COMPREHENSIVE evaluations. This is because they primarily focus on the internal structure of the deep models, such as neuron activation patterns,

rather than evaluating the DNNs behavior on a diverse set of inputs. This internal focus can miss identifying specific inputs that cause failures or unexpected behavior.

10th Month Report Goal

The primary aim of my work in the first year is to review existing testing methods for assessing the robustness of DNNs, identify opportunities for improvement, and highlight the need for a fast, scalable, and generalizable end-to-end testing method. This report also aims to outline key research questions and objectives based on these findings and present initial contributions to the field.

1.2 Research Goal

The primary goal of this research is to enhance the robustness of DNNs used in safety-critical systems by designing and implementing a comprehensive testing framework. This framework will formalize specifications related to model architecture, environmental properties and input data characteristics, including the type of data (e.g., images, text), size (e.g., number of samples), size for each class, and the number of classes involved.

The framework will adapt these specifications based on the **type of testing** being conducted. In **white-box testing**, full access to the model's internal details (e.g., number of neurons, layers, weights, gradients, and types of architectures like CNN, ResNet) is utilized to create precise adversarial examples using methods like FGSM. In **grey-box testing**, partial access allows the use of input-output pairs and basic model structures (e.g., general architecture without detailed parameters) to train surrogate models that approximate the target model's behavior, enabling the generation of effective test cases without need full internal details. In **black-box testing**, the framework relies on input-output behavior and environmental properties (e.g., expected input ranges, conditions like rain, dust, brightness, and noise) to iteratively probe and test the model's robustness without internal access. Defining these properties is crucial as it specifies the expected conditions the model should handle.

User requirements, such as specific modules to test and critical scenarios, as well as evaluation metrics (e.g., accuracy, precision, recall), will also be incorporated. If no specific requirements are provided, default parameters will ensure thorough assessment.However, it can also be customized for specific cases or multiple cases based on user specifications. For instance, a user might require the framework to focus on a particular class or scenario that is critical. This flexible and detailed approach aims to provide a robust method for testing DNNs in safety-critical environments.

To accurately identify weaknesses and areas for improvement, the framework will calculate both local coverage and global coverage using probabilistic programming language that allows you to define bayesian probability models and solve them automatically. This approach allows for a detailed analysis of the model's behavior under different conditions, providing insights into how the model performs in specific scenarios and overall. By examining local-level coverage, the framework can detect vulnerabilities that may arise in specific parts of the model or under particular conditions. Global-level coverage assessment, on the other hand, evaluates the model's overall stability across a wide range of scenarios. Together, these analyses help pinpoint specific vulnerabilities and highlight areas where the model can be improved, ultimately leading to more robust systems.

Additionally, the framework will generate a comprehensive error summary, providing insights into the types and frequencies of errors encountered. This summary will highlight critical failure points and suggest targeted improvements, enabling developers to enhance the system robustness. Through continuous evaluation and iterative refinement, the framework aims to significantly enhance the safety and dependability of DNN models across different operational levels. This ongoing process ensures that the models remain robust and effective in a wide variety of real-world applications, ultimately contributing to their reliability in safety-critical systems.

Thesis Goal

An end-to-end automated framework that thoroughly integrates data, test cases, and test coverage according to given specifications and provides a detailed error summary.

1.3 Research Questions and Objectives

This section outlines the research questions and their corresponding objectives.

1. **How can we design a comprehensive framework to test system robustness?** Create a framework that test the DNN under a variety of conditions, ensuring it meets performance standards even in edge cases and adverse scenarios **(Obj1)**.

2. **How can we clearly define and specify the properties of the system?** Formalize specifications by developing templates and a specification language that enable users to clearly define and specify the properties of the system and its associated data for testing purposes **(Obj2)**.

3. **How can we sample inputs efficiently?**Develop a sampling approach that effectively identifies and prioritizes corner cases. It can be used to guide best selection of inputs for test case generation**(Obj3)**.

4. **Can interpretability analysis aid in effective test case generation?** Implement interpretability analysis to identify and prioritize key influential features in the DNN testing process, exploring the use of high influential features for effective test case generation**(Obj4)**.

5. **How can we generate highly effective test cases that ensure complete coverage?** Generate highly effective test cases by first developing a sampling approach to collect efficient samples, and then using these samples to identify critical pixels. The identified critical pixels will form the basis for creating test cases that ensure complete coverage and thoroughly assess model vulnerabilities**(Obj5)**.

6. **How can we ensure comprehensive test coverage for deep learning models?** Integrate advanced probabilistic methods to evaluate both LOCAL COVERAGE and GLOBAL COVERAGE **(Obj6)**.

7. **How can error summarization be employed to quantify the impacts on model robustness?** Develop method for error summarization that analyze the results of DNNs testing to identify weaknesses. This method will help quantify the impacts of errors on model robustness and provide insights into areas requiring improvement**(Obj7)**.

1.4 Contribution of this Report

This research makes the following key contributions to the field of deep learning correctness evaluation:

- An *end-to-end pipeline* is designed for evaluating the robustness of the system Chapter 3.
- A *hybrid sampling* technique is proposed to identify and prioritize the corner cases Chapter 3.
- A *conceptual framework* is proposed that quantifies both local and global robustness. This framework uses Problog, a probabilistic logic programming language, to verify system global robustness Chapter 3.
- An *interpretability-driven test case generation* approach is employed to pinpoint critical input features, which are then used to create test cases with a higher

probability of inducing mispredictions, thus effectively evaluating and enhancing model robustness Chapter 3.

- All *experiments* are conducted using publicly available datasets, including DAWN, CIFAR, and MNIST Chapter 3.

Note: The contributions of this report do not include methods for defining system properties and error summarization technique. Additionally, adversarial examples used in the experiments are taken from existing literature.

1.5 Organization of the Thesis

The remainder of the thesis is organized as follows: related studies are presented in Chapter 2. The system model and proposed methodology are demonstrated in Chapter 3. Chapter 4 describes the simulation results of our proposed schemes. Finally, the findings of this work along with future directions are presented in Chapter 5.

Chapter 2

Literature Review

2.1 Deep Neural Networks and AI Systems

Deep neural networks (DNNs) mimic the structure of the human brain, consisting of millions of interconnected neurons. They extract high-level features from raw input using labeled training data without human interference.

Formally, a DNN is a function $f\colon \mathbb{R}^{s_0} \mapsto \mathbb{R}^{s_k}$ that takes as input a vector of size s_0 and produces a vector of size s_k. The function f is computed by composing k layers $L_1\colon \mathbb{R}^{s_0} \mapsto \mathbb{R}^{s_1}, \ldots, L_k\colon \mathbb{R}^{s_{k-1}} \mapsto \mathbb{R}^{s_k}$ as $f(x) = L_k(\cdots L_2(L_1(x))\cdots)$.

Each layer L_i typically implements a non-linear function. For instance, a *fully-connected* layer linearly transforms its input x_{i-1} as $Wx_{i-1} + b$, where $W \in \mathbb{R}^{s_i \times s_{i-1}}$ is the matrix of weights and $b \in \mathbb{R}^{s_i}$ is the bias vector. Then, it applies a non-linear activation function (e.g., sigmoid or Rectified Linear Unit (ReLU)) component-wise, generating the output vector x_i. The weights specify how its input neurons are connected to its output neurons and are known as *DNN parameters*. For more information about DNNs, we refer the reader to [11, 12, 13].

The objective of DNN training is to learn parameters during training to make accurate predictions on unseen data during real-world deployment.

When the prediction task is classification, then s_k represents the number of classes. Assuming that $f(x) = (y_1, \ldots, y_{s_k})$, the *classification result* is $\underset{i=1}{\overset{s_k}{\operatorname{argmax}}}\, y_i$, which is the index of the component with the highest probability y_i. By abuse of notation, sometimes we write $f(x) = c$ to denote the fact that x was classified as c. We also write $f(x)_c$ to refer to y_c which represents the probability of x being in class c.

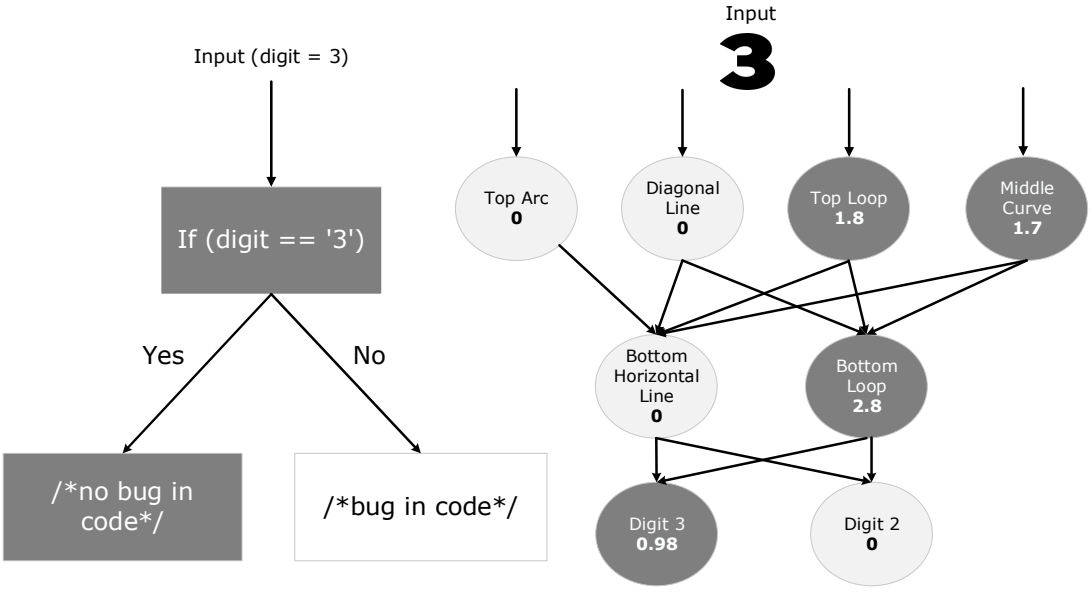


FIGURE 2.1: Comparison between program flows of a traditional program (left) and a neural network (right). The nodes in gray denote the corresponding basic blocks or neurons that participated while processing an input.

By an *AI system*, we refer to any software system capable of performing complex tasks through the use of data, algorithms, and high computational power, which typically require human intelligence. These tasks include problem-solving, reasoning, decision-making, and natural language understanding.

Deep learning is a subset of AI that utilizes deep neural networks (DNNs) for complex pattern recognition. Some AI systems are solely based on DNN components, whereas *hybrid* AI systems combine DNNs with traditional software to produce the final output.

2.2 Robustness of Deep Neural Networks

Deep neural networks (DNNs) are known for their lack of robustness. Research has shown DNNs to be vulnerable to two main categories of adversaries [8]: *adversarial examples* [9] and *semantic adversarial examples* [10].

Let $\mathcal{A}$ denote an adversary. Each category can be described formally as follows:

Adversarial Examples $\mathcal{A}_{\text{adv}}$

(ADV) This involves the generation of perturbations δ such that $x' = x + \delta$ misleads the DNN f into making incorrect predictions, where x is the original input and x' is the perturbed input. Various methods under this category include:

- *Fast Gradient Sign Method (FGSM)*: For an input x and its true label y, FGSM generates $x' = x + \epsilon \cdot \text{sign}(\nabla_x J(x, y))$, where J is the loss function and ϵ is a small perturbation factor.
- *Basic Iterative Method (BIM)*: This extends FGSM by iteratively applying small perturbations: $x'^{(i+1)} = x'^{(i)} + \alpha \cdot \text{sign}(\nabla_x J(x'^{(i)}, y))$.
- *Carlini and Wagner (C&W) Attack*: Utilizes optimization to find δ that minimizes the L_p-norm while ensuring $f(x + \delta) \neq y$.
- *DeepFool*: Iteratively perturbs x by δ to move it across decision boundaries.
- *Jacobian-based Saliency Map Attack (JSMA)*: Manipulates specific features of x to achieve targeted misclassifications.

Semantic Adversarial Examples $\mathcal{A}_{\text{trans}}$

This involves modifying the input images in a manner that exploits the model's sensitivity to variations, potentially causing misclassifications. Various methods under this category include:

- *Noise Addition*: Introducing noise η such that $x' = x + \eta$. We consider *Gaussian* noise and *salt-and-pepper* noise.
- *Translation*: Shifting the image x by a vector t to obtain $x' = \text{translate}(x, t)$.
- *Scaling*: Resizing the image x by a factor s to get $x' = \text{scale}(x, s)$.
- *Shearing*: Applying a shear transformation to x resulting in $x' = \text{shear}(x, \theta)$.
- *Rotation*: Rotating the image x by an angle θ to produce $x' = \text{rotate}(x, \theta)$.
- *Contrast Adjustment*: Modifying the contrast of x, represented as $x' = \text{adjust\_contrast}(x, \alpha)$.
- *Brightness Change*: Altering the brightness of x, yielding $x' = \text{change\_brightness}(x, \beta)$.
- *Blurring*: Applying a blur effect to x, giving $x' = \text{blur}(x, k)$, where k is the kernel size.
- *Occlusion*: Partially hiding regions of x, leading to $x' = \text{occlude}(x, m)$, where m denotes the mask.

By analyzing various types of adversaries, our proposed comprehensive testing framework evaluates model robustness, providing probabilities of model effectiveness against each adversary and assessing accuracy under adversarial conditions across different classes within any dataset.

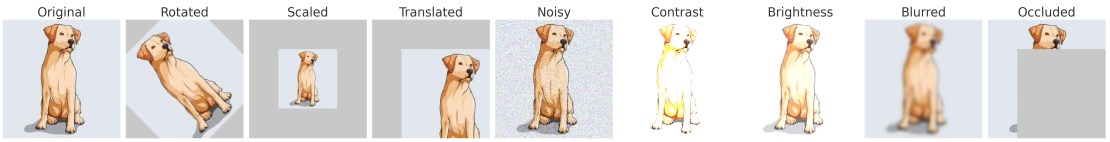


FIGURE 2.2: Image transformations for ...

2.3 Sampling Techniques

Sampling is a crucial step in the testing of DNNs, as it involves selecting a representative subset of inputs from a potentially vast input space. Various sampling techniques are employed to ensure comprehensive testing. Random sampling, which involves randomly selecting inputs, is simple to implement and provides broad coverage, but it might miss critical edge cases [14]. Stratified sampling, which divides the input space into strata and samples from each, ensures representation of all strata but requires prior knowledge of the strata [15]. Random over-sampling balances class distribution by duplicating examples in the minority class, though it can lead to overfitting [16]. SMOTE (Synthetic Minority Over-sampling Technique) generates synthetic examples in the minority class to reduce overfitting compared to random over-sampling, but it can introduce noise [16]. ADASYN (Adaptive Synthetic Sampling Approach for Imbalanced Learning) adjusts the number of synthetic samples generated for each minority class example according to its difficulty level, thereby focusing more on difficult-to-learn examples and enhancing model performance on challenging cases [17]. NearMiss focuses on selecting examples close to the decision boundary, emphasizing difficult examples, but may discard useful information [18]. Borderline-SMOTE generates synthetic examples near the class borders, targeting challenging areas, though it may still introduce noise [19]. Adaptive sampling dynamically adjusts the strategy based on intermediate results, efficiently focusing on areas with higher uncertainty or potential errors, but it is complex to implement [20]. These techniques enhance the robustness of DNN testing by ensuring diverse and representative input coverage, each with specific advantages and limitations that need to be considered in the context of the testing objectives.

Currently, I am employing a hybrid sampling approach that combines Borderline-SMOTE and ADASYN. Borderline-SMOTE generates synthetic examples near decision boundaries to enhance class balance and model robustness, focusing on areas prone to misclassification. ADASYN adjusts the number of synthetic samples for each minority class example based on its difficulty level, targeting hard-to-learn examples. This combined approach ensures balanced classes and effectively addresses corner cases, thereby significantly improving overall model performance.

Challenge: Synthetic sampling can introduce noise. While Borderline-SMOTE might add noise, ADASYN mitigates this by focusing on challenging examples, reducing the risk of overfitting. The hybrid technique leverages the strengths of both methods, resulting in a robust and accurate model.

2.4 Testing and Formal Verification

Testing (t) and formal verification (v) are two distinct approaches used to ensure the reliability and correctness of DNNs. Testing is an empirical process that involves executing a system with a variety of inputs to identify defects or bugs. For example, to verify the detection of stop signs in an autonomous vehicle's neural network, testing would involve generating a set of images with variations in brightness, rotation, and noise. These images are then fed into the neural network, and the outputs are analyzed to check if the stop sign is correctly detected. Specific test cases might include images taken in different lighting conditions (daylight, twilight, night), with stop signs at various angles (0°, 15°, 30°, 45°), and with added Gaussian noise. The main advantage of testing is its practicality, providing immediate feedback on the neural network's performance under these conditions [28].

In contrast, formal verification uses mathematical and logical reasoning to prove that a system meets its specifications under all possible conditions. This involves formalizing the properties of the system and using formal methods such as model checking or theorem proving to verify these properties. For instance, the property that the neural network must detect stop signs correctly under different brightness levels, rotations, and noise can be formalized as follows: for any input image containing a stop sign, regardless of these variations, the network should output a correct detection. Tools like SMT solvers are then used to verify this property. Unlike testing, formal verification aims to provide rigorous guarantees of correctness, ensuring that the system adheres to its specifications in all cases [29, 28].

A key difference between the two approaches is the scope of their validation. Testing is limited to the specific cases generated, which may not cover all possible scenarios. Formal verification, however, aims to cover all possible scenarios within the defined properties, offering stronger guarantees. For example, while testing might reveal that the neural network fails to detect a stop sign under very dim lighting, formal verification would mathematically prove whether such failures can occur under any possible input within the specified range. This makes formal verification particularly valuable in safety-critical applications where ensuring the absence of errors is crucial [30].

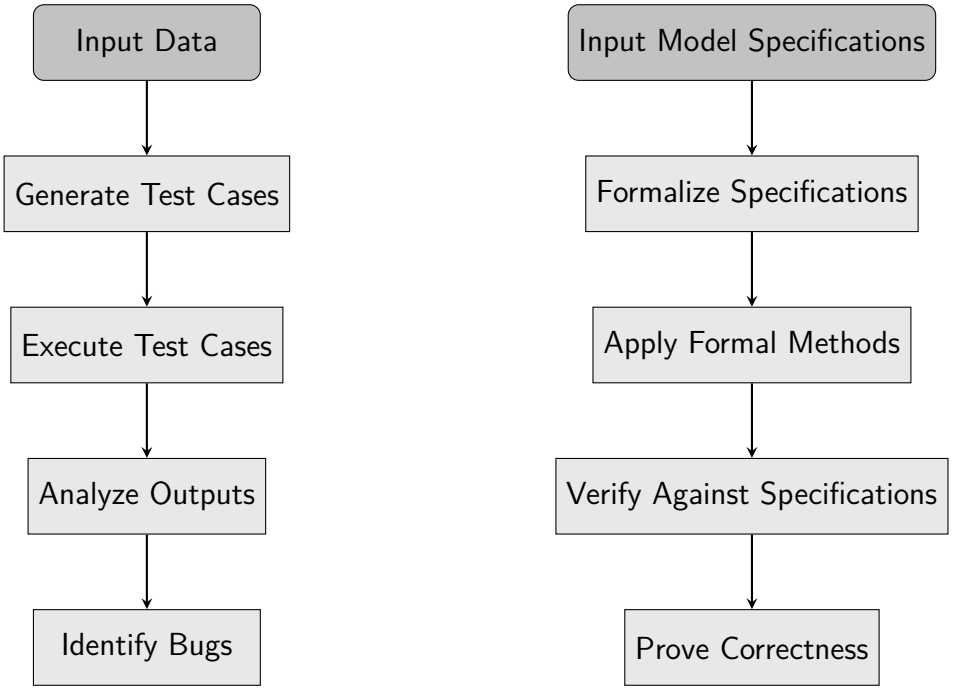


FIGURE 2.3: Comparison of Testing and Verification Processes

2.5 DNN Testing Techniques

The development of DNNs is significantly different from traditional software. While developers explicitly define logic in traditional software, DNNs learn logic rules from raw data. Developers shape these rules by modifying the training data, selecting features, and designing the DNN architecture, such as the number of neurons and layers.

Since the logic of a DNN is non-transparent [21], identifying the reasons behind its erroneous behavior is challenging. Therefore, testing and correcting its errors are crucial, particularly in safety-critical systems. Next, we briefly introduce two major DNN testing techniques: coverage criteria and test-case generation.

Coverage Criteria

In traditional software testing, coverage criteria measure how thoroughly software is tested. In DNNs, coverage might not directly apply to lines of code but rather to the input space or the variety of data the model can effectively handle or provide predictions for.

Neuron coverage (NC) [21] is the first coverage metric proposed in the literature to test DNNs. It is defined as the ratio of neurons activated by a test input to the total number of neurons in the model, where a neuron is activated when its activation value exceeds a predefined threshold.

Ma et al. [22] proposed a variety of coverage metrics, including K-multisection neuron coverage (KMNC), Neuron boundary coverage (NBC), and Strong neuron activation coverage (SNAC). KMNC calculates coverage by dividing the interval between lower and upper bounds into k-bins and measuring the number of bins activated by the test inputs. NBC measures the ratio of corner case regions covered by test inputs, with corner cases defined as activation values below or above those observed during training. SNAC similarly measures how many upper corner cases, defined as activation values above the training range, are covered by test inputs.

Modified Condition/Decision Coverage (MC/DC) [23] captures causal changes in test inputs based on the sign and value change of a neuron's activation.

Likelihood-based Surprise Adequacy (LSA) uses Kernel Density Estimation (KDE) to estimate the likelihood of a test input during the training phase, prioritizing inputs with higher LSA scores as they are closer to classification boundaries. Distance-based Surprise Adequacy (DSA) is an alternative to LSA that uses the distance between activation traces of new test inputs and those observed during training [24].

DNN Test-case Generation

Test-case generation methods are influenced by traditional software testing methods like fuzz testing, metamorphic testing, and symbolic execution. In the following sections, we will explore the current state of the art in DNN test generation.

DeepXplore [21] is a whitebox test-case generation method that checks how different DNNs behave using domain-specific rules on inputs. It uses multiple models trained on the same data to find differences in their prediction. It aims to jointly optimize neuron coverage and different predictions between models, using gradient ascent for test generation.

DeepTest [10] focuses on generating test inputs for autonomous cars by applying domain-specific rules on seed inputs. It uses a greedy search method based on the NC metric to create effective test cases.

Adapting traditional fuzzing techniques for DNN test-case generation includes methods like DLFuzz [25] and TensorFuzz [26]. DLFuzz generates adversarial inputs based on NC, akin to DeepXplore, but does not require multiple models and uses constraints to keep new inputs similar to originals. TensorFuzz employs coverage-guided testing to uncover numerical issues and discrepancies in DNNs and their quantized versions.

DeepConcolic [27] employs a concolic testing approach to generate adversarial inputs for DNN testing. It combines symbolic execution with concrete execution path information to meet coverage criteria, supporting both NC and MC/DC criteria.

Traditional techniques are simple, failing to capture the full complexity and precision of model behaviors. Exploring all possible behaviors of a model is nearly impossible due to the vast number of paths to consider. These metrics also often overlook the detailed interactions within and between layers of the model. Defining and testing all necessary decision boundaries, especially in complex models, is a daunting task. Many existing metrics do not provide clear directions for improving the model, leaving you without actionable insights. Scalability and adaptability are other major issues. Many criteria are not scalable or adaptable across diverse model architectures.

In this thesis, we address these issues and design a systematic testing framework for DNNs.

2.6 Probabilistic Logic Programming (PLP)

Probabilistic Logic Programming (PLP) integrates probabilistic reasoning with the flexibility and expressiveness of logic programming. Traditional logic programming paradigms are deterministic, where each statement is either true or false. However, real-world scenarios often involve inherent uncertainties which deterministic logic cannot adequately handle. PLP addresses this limitation by allowing the representation of uncertainties directly within the logic framework, thereby enabling more nuanced and accurate modeling of complex domains [46, 47].

PLP has been explored extensively in various domains, including artificial intelligence, bioinformatics, and robotics. Sato and Kameya's introduction of PRISM [40] was a significant milestone, combining statistical modeling with logic programming. Subsequent work by Koller and Friedman [41] on probabilistic graphical models further influenced

PLP frameworks. Various approaches to PLP, such as Logic Programs with Annotated Disjunctions (LPADs) [42], ProbLog [43], Probabilistic Horn Abduction (PHA) [44], Independent Choice Logic (ICL) [45], and PRISM [46], have been developed, each leveraging the distribution semantics introduced by Sato [46].

Among these, ProbLog has gained prominence due to its simplicity and expressive power, making it a preferred choice for many applications [47]. ProbLog extends a logic program with probabilistic facts, defining a probability distribution over possible worlds (sets of facts). The probability of a query is computed by marginalizing over the probabilities of the worlds where the query is true.

The need for explainable AI (XAI) has become increasingly important, particularly in domains where decisions must be transparent and interpretable, such as medical diagnosis and finance. Various approaches to XAI emphasize model interpretability and the generation of comprehensible explanations for model predictions [49]. PLP, with its ability to generate explanations as part of its reasoning process, fits well within the XAI paradigm. Vidal [48] proposes a novel approach where explanations in PLP are represented as programs generated from a given query through unfolding-like transformations. This approach preserves the causal structure of inferences and ensures minimality by excluding irrelevant information. Such explanations can be parameterized to hide uninteresting details, making them comprehensible to non-expert users.

Despite the extensive research in PLP and its applications, its use in testing DNNs is still very new. DNNs are powerful but often act like "black boxes," making it hard to understand and trust their predictions. This thesis presents a new way to use PLP for testing DNNs, an area that has not been explored before.

By using PLP, we can turn the probabilistic outputs of DNNs into probabilistic facts and rules. This helps in reasoning about uncertainties in the model's predictions and generating clear explanations for each prediction. This approach makes it easier to understand why a model made a certain prediction, giving insights into the model's decision-making process. PLP can also help in debugging DNNs by identifying and fixing inconsistencies or unexpected behaviors in the predictions. By examining the probabilistic rules and their explanations, we can find areas for improvement more effectively. Additionally, PLP allows us to simulate different scenarios by changing probabilistic facts, which is useful for testing how robust the DNNs are under various conditions. This innovative method opens up new opportunities for research and practical applications, making deep learning systems more transparent, reliable, and trustworthy.

Chapter 3

Proposed Framework

3.1 Proposed Approach

This section introduces our comprehensive approach to evaluating AI system performance, summarized in Figure 3.1. It takes as input the description of an AI system and a set of relevant specifications against which the AI system should be checked. The framework itself has four main components:

(i) *Sampling*: Choosing the original inputs for the AI system.

(ii) *Testcase Generation*: Generating specific test cases from the sampled inputs according to the specifications.

(iii) *Validation*: Checking the behavior of the AI system on the generated test cases, which can be fully-fledged *verification* or more lightweight *testing*.

(iv) *Error Summarization*: Quantifying the performance of the AI system in terms of its global/local robustness/correctness.

We focus on AI systems with DNN components performing classification tasks. We assume that an AI system $\mathcal{S}$ is a pair $(\mathcal{F}, \mathcal{D})$ where:

- $\mathcal{F}$ is the functional unit consisting of n DNN *classifiers* $f_1, \ldots, f_n$ and a symbolic (software) component ω such that given an input $\boldsymbol{x} = (x_1, \ldots, x_n)$, the *output* $\mathcal{F}(\boldsymbol{x})$ is defined as $\omega(f_1(x_1), \ldots, f_n(x_n))$.
- $\mathcal{D}$ (for dataset) is a structure that describes valid inputs and the corresponding correct outputs (i.e., labels). In particular, $\mathcal{D}.next(c)$ returns a valid input $\boldsymbol{x}$,

given the parameter c, which represents the number of classes in the dataset. Moreover, $\mathcal{D}.N$ is the total number of distinct class labels.

To ensure clarity in cases where multiple functional units are present, it is essential to specify which dataset belongs to which functional unit. Formally, let $\mathcal{F} = \{f_1, \ldots, f_n\}$ represent the set of functional units and $\mathcal{D} = \{\mathcal{D}_1, \ldots, \mathcal{D}_m\}$ represent the set of datasets. Each dataset $\mathcal{D}_j$ is associated with one or more functional units $\{f_{i_1}, \ldots, f_{i_k}\} \subseteq \mathcal{F}$. This means that each $\mathcal{D}_j$ provides valid inputs and corresponding correct outputs specifically for the classifiers $f_{i_1}, \ldots, f_{i_k}$. In this framework, each dataset $\mathcal{D}_j$ must clearly define its scope of association with the functional units. For instance, if $\mathcal{D}_1$ is associated with f_1 and f_3, then $\mathcal{D}_1$ provides valid inputs and correct outputs for both f_1 and f_3. This explicit association ensures that datasets are correctly utilized for their respective functional units, avoiding any ambiguity in the evaluation process.

To handle user-defined specifications and provide default behaviors when specifications are not explicitly defined, we assume that *specifications* Σ is a pair (P, V), where P is a set of perturbations against which we are characterizing the behavior of $\mathcal{S}$. Each perturbation comes with parameters to instantiate the set of all possible perturbations. V is a validation flag, where if $V = t$, then we do testing, and if $V = v$, we do verification.

If the user does not specify which classes to test or which properties to evaluate, our framework defaults to testing all classes in the dataset and evaluating all possible properties. Formally, let $\mathcal{C}$ be the set of all classes in the dataset $\mathcal{D}$ and $\mathcal{P}$ be the set of all possible properties. If the user does not define a subset $\mathcal{C}_u \subseteq \mathcal{C}$ or $\mathcal{P}_u \subseteq \mathcal{P}$, then $\mathcal{C}_u = \mathcal{C}$ and $\mathcal{P}_u = \mathcal{P}$, respectively.

FIGURE 3.1: Overview of the Proposed Framework

Example 3.1. *An instance of a simple AI system is an* MNIST Digit Adder $\mathcal{S}_{CNN} = (\mathcal{F}, \mathcal{D})$, *where* $\mathcal{F} = (\{f_{CNN}\}, +)$, f_{CNN} *is an MNIST Digit classifier and* $\mathcal{F}$ *takes as input two MNIST Digit images, recognizes the digits in the images, and computes their sum, i.e.,* $\mathcal{F}(x_1, x_2) = f_{CNN}(x_1) + f_{CNN}(x_2)$. $\mathcal{D} = \{\mathcal{D}_{mnist}\}$ *is the testing dataset for digits consisting of 10,000 labeled images (0-9), where* $\mathcal{D}_{mnist}$ *is associated with the classifier* f_{CNN}.

We assume that *specifications* Σ is a pair (P, V), where P is a set of perturbations against which we are characterizing the behavior of $\mathcal{S}$. Each perturbation comes with

parameters to instantiate the set of all possible perturbations. V is a validation flag, where if $V = t$, then we do testing, and if $V = v$, we do verification.

Example 3.2. *To evaluate the correctness of the $\mathcal{S}_{MNIST}$, we define the specifications $\Sigma = (P, V)$ as follows: $P = \{\text{GAU}(0, 0.1), \text{SAP}(200 : 255, 0 : 5, 0.2), \text{ROT}(3, 30, 3)\}$ and $V = t$. Here, $\text{GAU}(0, 0.1)$ specifies Gaussian noise with a mean of 0 and standard deviation of 0.1, $\text{SAP}(200 : 255, 0 : 5, 0.2)$ specifies salt and pepper noise, where 10% of pixels are bleached up to values 200 to 255 and 10% of pixels are darkened to values between 0 and 5, and $\text{ROT}(3, 30, 3)$ specifies the set of rotations with the minimum rotation angle of 3, maximum of 30, and the step size of 3.*

3.2 Sampling

The sampling process is designed to identify efficient and corner cases by employing a hybrid approach that combines Borderline-SMOTE and ADASYN. This combined method generates synthetic examples, enhancing class balance and model robustness. Borderline-SMOTE focuses on creating samples near decision boundaries, while ADASYN targets hard-to-learn examples, ensuring that both typical and challenging cases are effectively covered. It is important to note that this sampling process is used solely for testing purposes, not for training the model.

To ensure a balanced and representative dataset for testing, we perform the following steps for each classifier f_i independently:

- Apply Borderline-SMOTE to generate synthetic samples near decision boundaries to enhance class balance.
- Use ADASYN to adjust the number of synthetic samples for each minority class example based on its difficulty level.

The full sample S_i for classifier f_i, $i = 1, \ldots, n$, is computed as:

$$S_i = \bigcup_{c=1}^{\mathcal{D}.N_i} S_i^c \tag{3.1}$$

where S_i^c is a subset of the correctly classified samples for a class c consisting of M_i (the number of samples for each class specific to f_i) elements:

$$S_i^c = \Big\{ x = \mathcal{D}.next_i(class = c) \mid f_i(x) = c \Big\}|_{M_i}$$

After the initial sampling, we enhance S_i^c by applying Borderline-SMOTE and ADASYN as follows:

$$S_i^c = S_i^c \cup \text{Borderline-SMOTE}(S_i^c) \cup \text{ADASYN}(S_i^c)$$

Note that each sample is obtained by a call to the method $\mathcal{D}.next_i$.

Challenges in Sampling

- **Synthetic Sample Quality:** Ensuring generated samples represent true corner cases, not noise.
- **Computational Overhead:** Managing the intensive computation required for hybrid sampling.

3.3 Test Case Generation

The test case generation process aims to create test cases based on the given specifications to evaluate the correctness/robustness of the AI system.

Let S_i^c be the set of samples produced in the sampling step for the classifier f_i and a class c. For each perturbation $p \in P$, we generate a set $\mathcal{T}_p^c$ of test cases. Specifically, for each sample $x \in S$ we produce $testcases(p, c, x)$ according to p. Then $\mathcal{T}_p^c = \bigcup_{x \in S} testcases(p, c, x)$.

Example 3.3. *To generate test cases for the MNIST Digit Adder $\mathcal{S}_{MNIST}$, we use the specifications defined in Example 2, which include noise and rotation perturbations. Let S be the set of sampled images obtained in Example 3. For each pair of images $(x_1, x_2) \in S$, we define the following test cases:*

- ***Rotation**: For a given angle θ, generate the perturbed images $x_1' = rotate(x_1, \theta)$ and $x_2' = rotate(x_2, \theta)$. The test case is then: $\mathcal{T}_{rotation} = \{(x_1', x_2') \mid x_1', x_2' \in rotate(S, \theta)\}$*
- ***Noise**: For a given mean μ and standard deviation σ, generate the perturbed images $x_1'' = noise(x_1, \mu, \sigma)$ and $x_2'' = noise(x_2, \mu, \sigma)$. The test case is then: $\mathcal{T}_{noise} = \{(x_1'', x_2'') \mid x_1'', x_2'' \in noise(S, \mu, \sigma)\}$*

The overall set of test cases $\mathcal{T}$ is the union of the individual test cases: $\mathcal{T} = \mathcal{T}_{rotation} \cup \mathcal{T}_{noise}$

3.4 Validation

The validation process aims to evaluate the correctness and robustness of the AI system under various perturbations.

Fix a perturbation $p \in P$ and a class c. For every test case in $\mathcal{T}_p^c$, we store the results in the form:

$$\text{Raw}_{p,c} = \left\{ \left(\text{query}(f_i, x, c), f_i(x)_c \right) \mid x \in \mathcal{T}_p^c \right\}$$

After generating test cases, measure the AI subsystem's confidence for each class under each type of property.

3.4.1 Local Robustness

Local robustness involves evaluating the AI subsystem's performance on individual images subjected to various transformations. For each image x from a set of samples S_i^c, the AI subsystem produces a confidence score $f_i(x)$ representing its certainty in recognizing the class c. The local robustness for a transformation T applied to an image x is defined as:

$$\text{Local Robustness}(x, T) = f_i(T(x))$$

where T can be any transformation such as noise addition, rotation, brightness adjustment, occlusion, or scaling. Each transformation is evaluated to determine its impact on the confidence score.

To quantify local robustness, we compute the accuracy for each transformation applied to the images of a specific class:

$$\text{Local Robustness}(c, T) = \frac{1}{|S_i^c|} \sum_{x \in S_i^c} \mathbb{I}[f_i(T(x)) = c]$$

where: - Local Robustness(c, T) is the accuracy of the classifier f_i for class c under transformation T. - $\mathbb{I}[f_i(T(x)) = c]$ is an indicator function that is 1 if the classifier correctly predicts the class c for the transformed image $T(x)$, and 0 otherwise. - $|S_i^c|$ is the number of correctly classified images in class c.

Example 3.4. *Consider the class $c = 3$ and the transformation T being a rotation by 25 degrees. If we have three images x_1, x_2, x_3 from class c, and the model correctly classifies x_1 and x_2 but misclassifies x_3, the local robustness is computed as follows:*

$$\textit{Local Robustness}(3, \textit{rotation}) = \frac{1}{3}(\mathbb{I}[f_i(\textit{rotate}(x_1, 25)) = 3] +$$
$$\mathbb{I}[f_i(\textit{rotate}(x_2, 25)) = 3] + \mathbb{I}[f_i(\textit{rotate}(x_3, 25)) = 3])$$

If the indicator values are 1, 1, and 0 respectively, the local robustness would be:

$$\textit{Local Robustness}(3, \textit{rotation}) = \frac{1}{3}(1 + 1 + 0) = \frac{2}{3} \approx 0.67$$

3.4.2 Global Robustness

Global robustness evaluates the AI subsystem's performance across multiple images and transformations. It is an aggregate measure of how well the AI system performs under various properties on a set of images S_i^c.

For a given transformation T and a set of images S_i^c, the global robustness is defined as:

$$\text{Global Robustness}(S_i^c, T) = \frac{1}{|S_i^c|} \sum_{x \in S_i^c} \mathbb{I}[f_i(T(x)) = c]$$

This measures the average confidence score for the AI subsystem over the entire dataset when subjected to a particular transformation.

To quantify global robustness, we compute the expected confidence score over all transformations and images. Depending on whether the relationship is AND or OR, the formulas vary:

AND Relationship:

For an AND relationship between transformations, the global robustness is calculated as:

$$P(\text{Property 1} \cap \text{Property 2}) = P(\text{Property 1}) \times P(\text{Property 2})$$

OR Relationship:

For an OR relationship between transformations, the global robustness is calculated as:

$$P(\text{Property 1} \cup \text{Property 2}) = P(\text{Property 1}) + P(\text{Property 2}) - P(\text{Property 1} \cap \text{Property 2})$$

Example 3.5. *Consider a pair of images (x_1, x_2) representing the digits '3' and '5'. Let the transformation T be rotation. If the model's confidence scores for these transformations are as follows:*

$$f_i(\textit{rotation}(x_1)) = 0.78,$$
$$f_i(\textit{rotation}(x_2)) = 0.85,$$

For the AND relationship, the global correctness for the pair is computed as follows:

$$P(\textit{Global Robustness}_{\textit{AND}}) = 0.78 \times 0.85$$

For the OR relationship, the global correctness for the pair is computed as follows:

$$P(\textit{Global Robustness}_{\textit{OR}}) = 0.78 + 0.85 - (0.78 \times 0.85)$$

(Note: The complete OR relationship formula requires including all images and transformations as per the OR formula.)

3.4.3 Use Cases and Examples

To illustrate the application of ProbLog for global robustness in real-world scenarios, we present the following use cases:

3.4.3.1 Use Case 1: Handwritten Digit Recognition

Scenario: Consider an AI system designed to recognize handwritten digits, such as the MNIST dataset. The system is evaluated under various transformations, including noise addition, rotation, and brightness adjustment. The goal is to determine the global robustness of the system in recognizing digit pairs correctly under these properties.

The tables below provide the probabilities for correctly recognizing digit pairs under different conditions (AND and OR relationships) for an MNIST 2-digit addition system. Each world represents a different combination of transformations applied to the digits.

Explanation: The table shows the global correctness probabilities for pairs of digits under various transformation conditions. Each row represents a different combination of transformations applied to the two digits in the pair: - AND Probability: The probability that both digits are correctly recognized under the specified transformations. - OR

TABLE 3.1: Specification Probabilities for MNIST 2-Digit Addition Under Different Transformations

World	Conditions	Probability Expression (AND)	Probability (AND)	Probability Expression (OR)	Probability (OR)
w_1	{noise(0), noise(1)}	$0.85 \cdot 0.8$	0.68	$0.85 + 0.8 - (0.85 \cdot 0.8)$	0.97
w_2	{noise(0), correct(1)}	$0.85 \cdot 0.9$	0.765	$0.85 + 0.9 - (0.85 \cdot 0.9)$	0.985
w_3	{correct(0), noise(1)}	$0.9 \cdot 0.8$	0.72	$0.9 + 0.8 - (0.9 \cdot 0.8)$	0.98
w_4	{rotation(0), correct(1)}	$0.88 \cdot 0.9$	0.792	$0.88 + 0.9 - (0.88 \cdot 0.9)$	0.992
w_5	{correct(0), rotation(1)}	$0.9 \cdot 0.77$	0.693	$0.9 + 0.77 - (0.9 \cdot 0.77)$	0.977
w_6	{rotation(0), rotation(1)}	$0.88 \cdot 0.77$	0.6776	$0.88 + 0.77 - (0.88 \cdot 0.77)$	0.9696
w_7	{noise(0), rotation(1)}	$0.85 \cdot 0.77$	0.6545	$0.85 + 0.77 - (0.85 \cdot 0.77)$	0.9655
w_8	{rotation(0), noise(1)}	$0.88 \cdot 0.8$	0.704	$0.88 + 0.8 - (0.88 \cdot 0.8)$	0.976
w_9	{correct(0), correct(1)}	$0.9 \cdot 0.9$	0.81	$0.9 + 0.9 - (0.9 \cdot 0.9)$	0.99

Probability: The probability that at least one of the digits is correctly recognized under the specified transformations.

For example, in world w_1, both digits are subjected to noise, leading to an AND probability of 0.68 and an OR probability of 0.97.

Problog Code:

```
% Define probabilities for digit 0 under different transformations
0.9::noise_0. % Digit 0 correctly predicted with 90% probability under noise
0.85::brightness_0. % Digit 0 correctly predicted with 85% probability under brightness
0.88::rotation_0. % Digit 0 correctly predicted with 88% probability under rotation

% Define probabilities for digit 1 under different transformations
0.8::noise_1. % Digit 1 correctly predicted with 80% probability under noise
0.75::brightness_1. % Digit 1 correctly predicted with 75% probability under brightness
0.77::rotation_1. % Digit 1 correctly predicted with 77% probability under rotation

% Define rules for correct prediction under each transformation for digit 0
correct_noise_0 :- noise_0.
correct_brightness_0 :- brightness_0.
correct_rotation_0 :- rotation_0.

% Define rules for correct prediction under each transformation for digit 1
correct_noise_1 :- noise_1.
correct_brightness_1 :- brightness_1.
correct_rotation_1 :- rotation_1.

% Define rules for incorrect prediction under each transformation for digit 0
wrong_noise_0 :- +correct_noise_0.
wrong_brightness_0 :- +correct_brightness_0.
wrong_rotation_0 :- +correct_rotation_0.

% Define rules for incorrect prediction under each transformation for digit 1
wrong_noise_1 :- +correct_noise_1.
wrong_brightness_1 :- +correct_brightness_1.
wrong_rotation_1 :- +correct_rotation_1.

% Define rules for correct prediction of both digits under noise
pair_correct_noise_0_1 :- correct_noise_0, correct_noise_1.
% Define rules for incorrect prediction of both digits under noise
pair_wrong_noise_0_1 :- wrong_noise_0, wrong_noise_1.
```

```
% Define global correctness based on either both correct or both incorrect under noise
global_correct_noise_0_1 :- pair_correct_noise_0_1; pair_wrong_noise_0_1.

% Query the global correctness under noise
query(global_correct_noise_0_1).
```

FIGURE 3.2: Problog code snippet for evaluating handwritten digit recognition under noise, brightness, and rotation transformations.

Explanation: In this scenario, we are interested in the global correctness of recognizing pairs of digits (0 and 1) under different transformations. The ProbLog code models the local robustness probabilities for each transformation and combines them to evaluate the global correctness.

3.4.3.2 Use Case 2: Autonomous Vehicle Perception

Scenario: An AI system used in autonomous vehicles must reliably detect objects such as vehicles under various weather conditions (rain, sand, fog, and snow). The goal is to evaluate the system's robustness in identifying these objects correctly under these weather conditions.

```
% Probabilities for Vehicle Detection under Different Weather Conditions
0.75::rain_vehicle. % Vehicle correctly detected with 75% probability under rain
0.55::fog_vehicle. % Vehicle correctly detected with 55% probability under fog
0.7::snow_vehicle. % Vehicle correctly detected with 70% probability under snow

% Correct Detection Rules for Vehicle
correct_rain_vehicle :- rain_vehicle.
correct_fog_vehicle :- fog_vehicle.
correct_snow_vehicle :- snow_vehicle.

% Incorrect Detection Rules for Vehicle
wrong_rain_vehicle :- +correct_rain_vehicle.
wrong_fog_vehicle :- +correct_fog_vehicle.
wrong_snow_vehicle :- +correct_snow_vehicle.

% AND conditions for Vehicle Detection under all weather conditions
global_correct_vehicle_and :- correct_rain_vehicle, correct_fog_vehicle, correct_snow_vehicle.

% OR conditions for Vehicle Detection under any weather condition
global_correct_vehicle_or :- correct_rain_vehicle; correct_fog_vehicle; correct_snow_vehicle.

% Mixed conditions (AND & OR) for Vehicle Detection
global_correct_mixed_vehicle :- correct_rain_vehicle, (correct_fog_vehicle; correct_snow_vehicle).

% Queries for Global Correctness
query(global_correct_vehicle_and).
query(global_correct_vehicle_or).
query(global_correct_mixed_vehicle).
```

FIGURE 3.3: Problog code snippet for evaluating vehicle detection under different weather conditions.

Explanation: The ProbLog code assesses the global robustness of the AI system in detecting objects (vehicles) under individual and combined weather conditions. This ensures that the system can reliably perform in diverse environmental scenarios.

TABLE 3.2: Specification Probabilities (AND) for Vehicle Detection Under Different Weather Conditions

$$P(A \cap B \cap C) = P(A) \times P(B) \times P(C)$$

World	Conditions	Probability Expression (AND)	Probability (AND)
w_1	{rain, fog}	0.75×0.55	0.4125
w_2	{rain, snow}	0.75×0.7	0.525
w_3	{rain, sand}	0.75×0.6	0.45
w_4	{fog, snow}	0.55×0.7	0.385
w_5	{fog, sand}	0.55×0.6	0.33
w_6	{snow, sand}	0.7×0.6	0.42
w_7	{rain, fog, snow}	$0.75 \times 0.55 \times 0.7$	0.28875
w_8	{rain, fog, sand}	$0.75 \times 0.55 \times 0.6$	0.2475
w_9	{rain, snow, sand}	$0.75 \times 0.7 \times 0.6$	0.315
w_{10}	{fog, snow, sand}	$0.55 \times 0.7 \times 0.6$	0.231

Explanation: This table shows the global correctness probabilities for detecting vehicles under different combinations of weather conditions using AND relationships. Each row represents a different combination of weather conditions applied to the detection scenario: - AND Probability: The probability that the vehicle is correctly detected under all specified weather conditions.
For example, in world w_1, the vehicle detection system is subjected to rain and fog, leading to an AND probability of 0.4125.

TABLE 3.3: Specification Probabilities (OR) for Vehicle Detection Under Different Weather Conditions

$$P(A \cup B \cup C) = P(A) + P(B) + P(C) - P(A \cap B) - P(A \cap C) - P(B \cap C) + P(A \cap B \cap C)$$

World	Conditions	Probability Expression (OR)	Probability (OR)
w_1	{rain; fog}	$0.75 + 0.55 - (0.75 \times 0.55)$	0.8875
w_2	{rain; snow}	$0.75 + 0.7 - (0.75 \times 0.7)$	0.925
w_3	{rain; sand}	$0.75 + 0.6 - (0.75 \times 0.6)$	0.9
w_4	{fog; snow}	$0.55 + 0.7 - (0.55 \times 0.7)$	0.835
w_5	{fog; sand}	$0.55 + 0.6 - (0.55 \times 0.6)$	0.82
w_6	{snow; sand}	$0.7 + 0.6 - (0.7 \times 0.6)$	0.88
w_7	{rain; fog; snow}	$0.75 + 0.55 + 0.7 - (0.75 \times 0.55) - (0.75 \times 0.7) - (0.55 \times 0.7) + (0.75 \times 0.55 \times 0.7)$	0.966625
w_8	{rain; fog; sand}	$0.75 + 0.55 + 0.6 - (0.75 \times 0.55) - (0.75 \times 0.6) - (0.55 \times 0.6) + (0.75 \times 0.55 \times 0.6)$	0.95125
w_9	{rain; snow; sand}	$0.75 + 0.7 + 0.6 - (0.75 \times 0.7) - (0.75 \times 0.6) - (0.7 \times 0.6) + (0.75 \times 0.7 \times 0.6)$	0.967
w_{10}	{fog; snow; sand}	$0.55 + 0.7 + 0.6 - (0.55 \times 0.7) - (0.55 \times 0.6) - (0.7 \times 0.6) + (0.55 \times 0.7 \times 0.6)$	0.938

Explanation: This table shows the global correctness probabilities for detecting vehicles under different combinations of weather conditions using OR relationships. Each row represents a different combination of weather conditions applied to the detection scenario: - OR Probability: The probability that the vehicle is correctly detected under at least one of the specified weather conditions.

For example, in world w_1, the vehicle detection system is subjected to rain and fog, leading to an OR probability of 0.8875.

3.5 Error Summarization

Error summarization involves evaluating the performance of the AI system by identifying and quantifying errors. We use Bayesian Network-based Coverage Metrics to assess both local and global coverage. Two testing coverage metrics are defined in Figure **??**: local coverage (LC) and global coverage (GC).

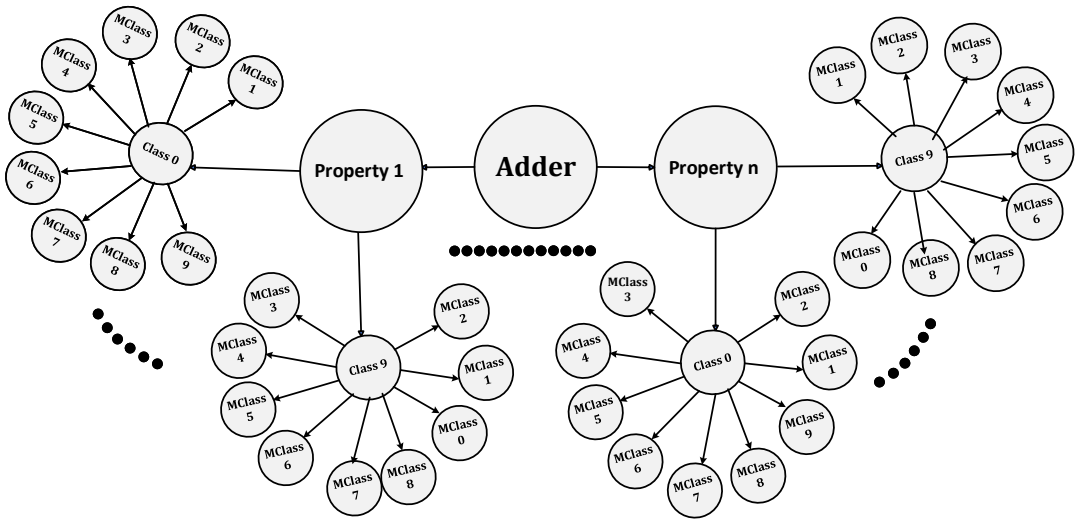


FIGURE 3.4: Error Summarization

3.6 Algorithm for Evaluating Model Robustness Using ProbLog

Algorithm 1 Evaluating Model Robustness Using ProbLog

Require: M: Pre-trained model
Require: D: Dataset
Require: N: Number of samples per class
Require: P: Set of properties
Ensure: G: Global correctness values for each specification

Load and Preprocess Data
$(X_{\text{train}}, y_{\text{train}}), (X_{\text{test}}, y_{\text{test}}) \leftarrow$ load_data(D)
$X_{\text{test}} \leftarrow$ preprocess_data(X_{test})
$\hat{Y} \leftarrow M$.predict(X_{test})
$\hat{y} \leftarrow$ extract_predictions$(\hat{Y})$
Determine Number of Classes
$C \leftarrow$ num_classes(y_{test}) {Number of unique classes in the dataset}
Select Correctly Classified Samples
correct_samples $\leftarrow \{\}$
for $c = 0$ **to** $C - 1$ **do**
    correct_samples$[c] \leftarrow$ select_correct_samples$(X_{\text{test}}, y_{\text{test}}, \hat{y}, c, N)$
end for
Define Transformation Functions
define_transformations()
Generate Test Cases
for $c = 0$ **to** $C - 1$ **do**
    for all $x \in$ correct_samples$[c]$ **do**
        for all $T \in P$ **do**
            generate_test_cases(x, T)
        end for
    end for
end for
Evaluate Model on Transformations
for $c = 0$ **to** $C - 1$ **do**
    for all property $\in P$ **do**
        $L_{c,\text{property}} \leftarrow$ compute_accuracy$(M, \text{property}, c)$
    end for
end for
Specification Definitions:
Specification1: $P(\text{Property1} \cap \text{Property2}) = P(\text{Property1}) \times P(\text{Property2})$ {AND relationship}
Specification2: $P(\text{Property1} \cup \text{Property2}) = P(\text{Property1}) + P(\text{Property2}) - P(\text{Property1} \cap \text{Property2})$ {OR relationship}
Specification3: Custom definitions
...
Generate and Evaluate ProbLog Code for Each Specification
Initialize G as an empty list
for spec $= 1$ **to** num_specs **do**
    ProbLog Code$_{\text{spec}} \leftarrow$ generate_problog_code$(L_{c,\text{property}}, \text{spec})$
    $G_{\text{spec}} \leftarrow$ evaluate_problog(ProbLog Code$_{\text{spec}}$)
    Append G_{spec} to G
end for
return G

Chapter 4

Simulations and Results

4.1 Datasets

4.1.1 MNIST Dataset

The MNIST dataset is a widely recognized benchmark in the field of deep neural networks (DNNs), comprising 70,000 grayscale images of handwritten digits. These images are split into 60,000 training samples and 10,000 testing samples, each of size 28x28 pixels. The dataset includes labels for each digit from 0 to 9, making it a total of 10 classes. This dataset is extensively used for evaluating the performance of various DNN algorithms due to its simplicity and the well-established baseline results it offers. To ensure the correctness our model, we selected 100 correctly classified samples from each class. This selection process involved comparing the model's predictions with the actual labels and choosing only those samples where the predictions were correct. This resulted in a balanced subset of 1,000 samples, with 100 samples from each of the 10 classes.

4.1.2 DAWN Dataset

The DAWN (Vehicle Detection in Adverse Weather Nature Dataset) dataset focuses on vehicle detection under adverse weather conditions, providing a diverse set of real-traffic images categorized into four weather conditions: fog, snow, rain, and sandstorms. Initially, the class distribution in the training set was imbalanced, with the following counts: 258 for label 1, 240 for label 0, 163 for label 3, and 160 for label 2.
To address this imbalance, we resampled the training set to ensure an equal number of samples for each class. This resulted in a balanced training set with 258 samples for each label. This balancing step was crucial for fair training and evaluation of the model, ensuring that no class was overrepresented or underrepresented.

For the testing set, we selected 100 samples from each class, ensuring a balanced evaluation dataset. This selection process was critical to accurately assess the model's performance across different classes and adverse weather conditions.

4.2 Use Case 1: Handwritten Digit Recognition

4.2.1 Local Correctness Evaluation

In this section, we evaluate the local correctness of the model under different transformations, namely rotation, noise, and brightness. Each transformation is applied with specific parameters to simulate real-world variations. Images are rotated by 25 degrees to evaluate the model's performance under rotation. Gaussian noise with a noise factor of 0.2 is added to the images to test the model's robustness to noisy conditions. The brightness of the images is increased by a factor of 0.3 to simulate different lighting conditions.

The local correctness graphs provide insights into the model's robustness under these transformations for each digit class. The model exhibited high performance under rotation (0.99) and brightness (1.00) for Class 0, with slightly reduced accuracy under noise (0.81). For Class 1, the model maintained consistently high accuracy across all transformations: rotation (0.99), noise (0.99), and brightness (1.00). However, the model struggled more with rotations (0.76) and noise (0.79) for Class 2 compared to brightness (1.00). Similarly, for Class 3, the model showed lower accuracy for rotations (0.82) and noise (0.78), but performed perfectly under brightness (1.00).

Class 4 demonstrated high accuracy across all properties, with rotation (0.91), noise (0.86), and brightness (1.00). Class 5 maintained high performance under all transformations: rotation (0.89), noise (0.99), and brightness (1.00). The model showed noticeable difficulty with noise (0.64) for Class 6, while maintaining high accuracy for rotation (0.87) and brightness (0.99). For Class 7, high accuracy was observed under brightness (1.00), with reduced performance under rotation (0.75) and noise (0.86). The model faced significant challenges under noise (0.02) for Class 8, but maintained good performance for rotation (0.68) and brightness (0.99). Finally, for Class 9, the model showed moderate performance under noise (0.51), and high accuracy under rotation (0.93) and brightness (0.99).

Overall, the model demonstrates strong robustness to brightness changes across all classes, frequently achieving perfect accuracy. However, performance under noise is highly variable, with some classes, such as Class 8, experiencing a dramatic drop in accuracy. While the model generally handles rotations well, there remains room for improvement, particularly in addressing noise-induced challenges. This analysis highlights

the necessity for targeted training to enhance the model's robustness, especially under noisy conditions for specific classes.

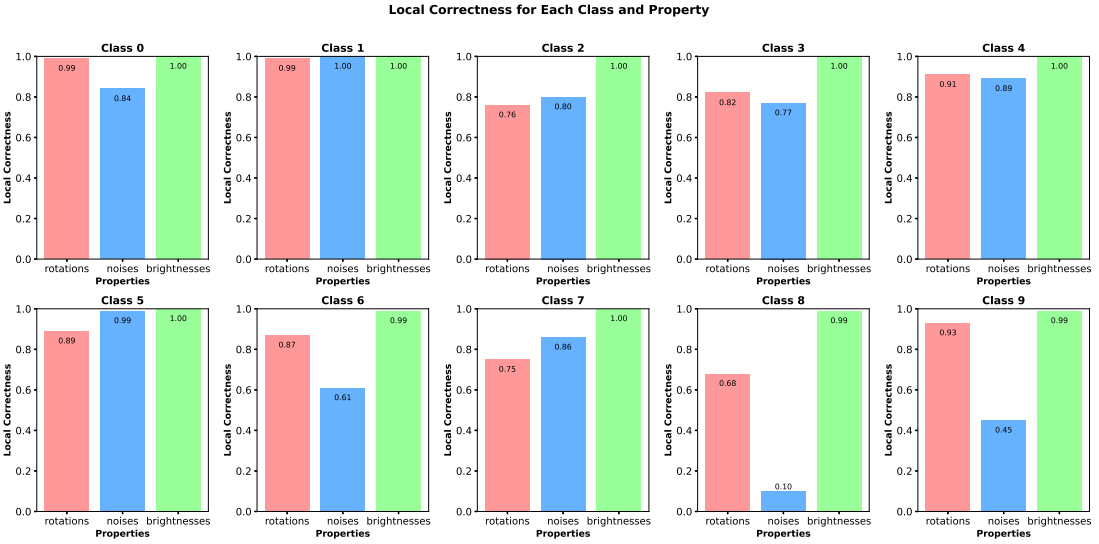


FIGURE 4.1: Local Correctness for each Class and Property

4.2.2 SHAP Analysis and Pixel Modification

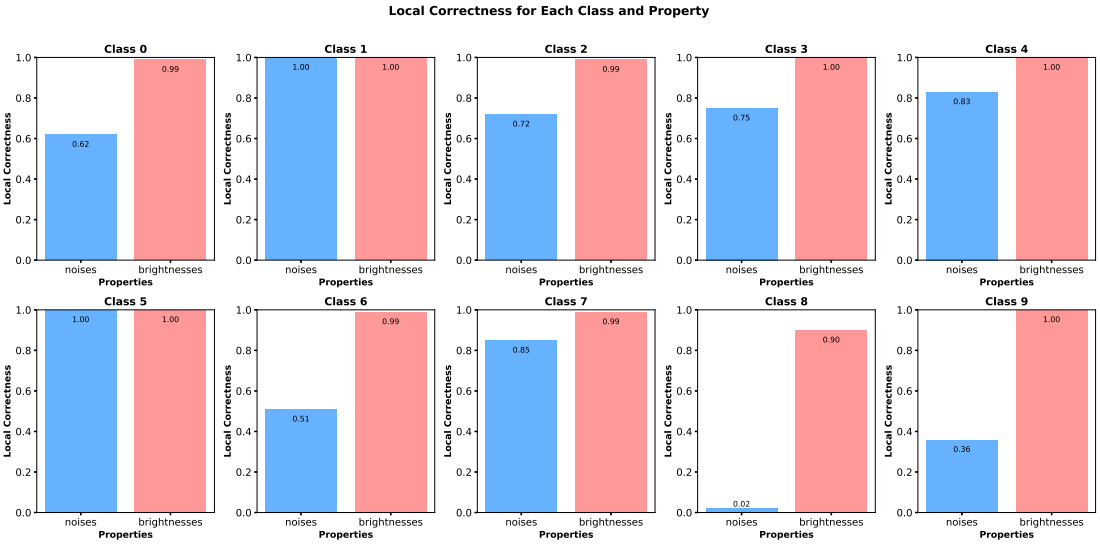


FIGURE 4.2: Local Correctness for each Class and Property based on SHAP Analysis. The bars represent the accuracy of correctly classified samples after applying noise and brightness transformations, highlighting the influence of these properties on model predictions.

The analysis presented in Figure 4.2 provides a detailed examination of the model's performance across different classes in response to noise and brightness perturbations.

This evaluation was conducted following the application of SHAP (SHapley Additive exPlanations) analysis, which identified the top 30% most influential pixels. These critical regions were then modified to simulate realistic scenarios, testing the model's robustness. The results reveal varying degrees of resilience across classes. For instance, Class 0 shows moderate robustness to noise with a correctness of 0.62, while demonstrating high robustness to brightness changes with a correctness of 0.99. Class 1, on the other hand, exhibits perfect robustness to both noise and brightness with correctness values of 1.0. Classes such as 2 and 3 maintain high robustness to brightness (0.99 and 1.0, respectively) but show a moderate decline in performance under noise. Notably, Class 8 is highly sensitive to noise, with a correctness of only 0.02, highlighting its vulnerability. Overall, brightness changes have a relatively lower impact on the model's performance compared to noise, as evidenced by consistently higher correctness values. This analysis underscores the need for targeted improvements to enhance noise robustness, particularly for classes like 6, 8, and 9, which show significant sensitivity. Addressing these weaknesses through techniques such as noise-augmented data training or more robust architectural designs will lead to a more resilient and reliable model, better suited for real-world applications where such perturbations are common.

4.2.3 Global Correctness Evaluation

The following figures illustrate the global correctness of various pairs of digits under different transformations: noise, brightness adjustment, and rotation. The final global correctness for each transformation is also depicted.
In my experiment, I checked the following specifications:

$$global\_noise \leftrightarrow (noise\_0\_0 \wedge noise\_0\_1 \wedge noise\_0\_2 \wedge \ldots \wedge noise\_9\_9)$$
$$global\_brightness \leftrightarrow (brightness\_0\_0 \wedge brightness\_0\_1 \wedge brightness\_0\_2 \wedge \ldots \wedge brightness\_9\_9)$$
$$global\_rotation \leftrightarrow (rotation\_0\_0 \wedge rotation\_0\_1 \wedge rotation\_0\_2 \wedge \ldots \wedge rotation\_9\_9)$$
$$global\_system \leftrightarrow (global\_noise \vee global\_brightness \vee global\_rotation)$$

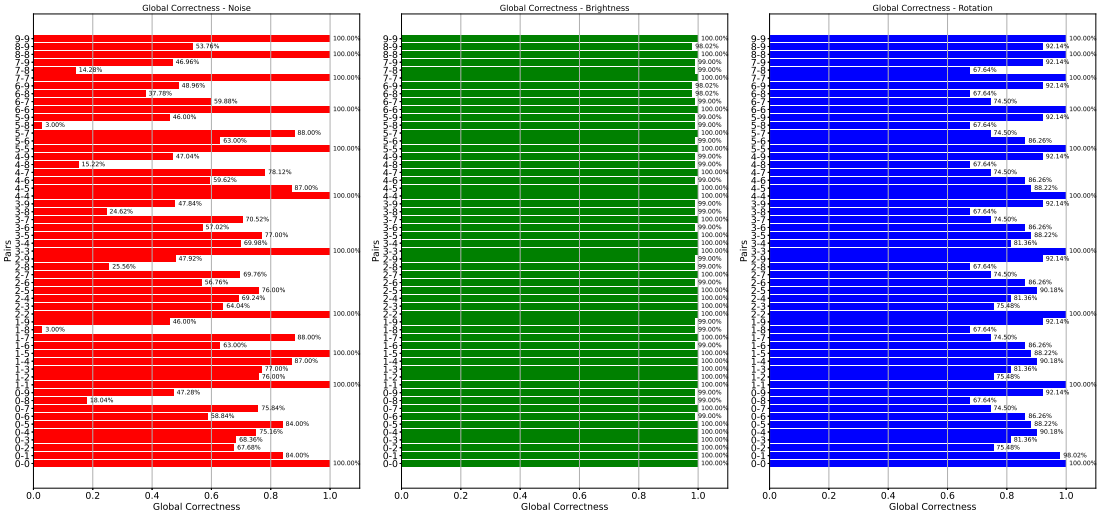


FIGURE 4.3: Global Correctness for Noise, Brightness, and Rotation Transformations

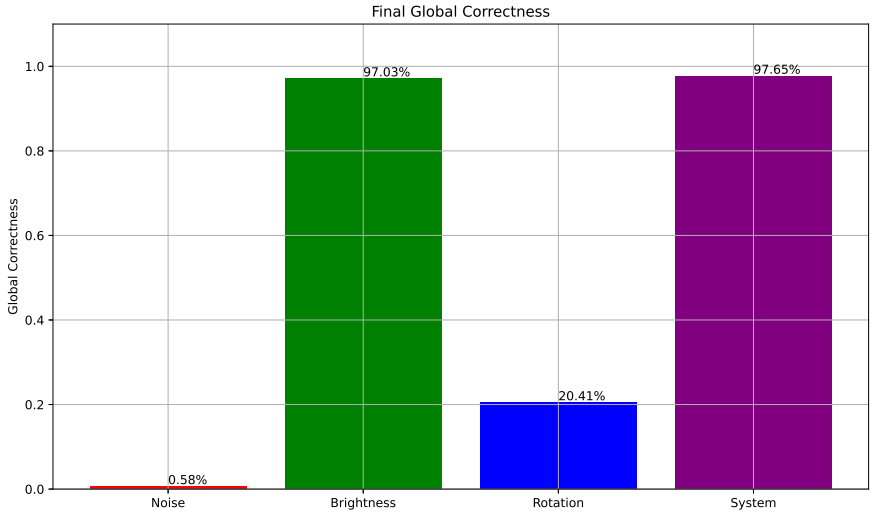


FIGURE 4.4: Final Global Correctness

The global correctness values for pairs of digits under the noise transformation vary significantly. Some pairs such as (0,0), (1,1), (2,2), etc., achieve perfect correctness (100%), while others like (0,5) and (1,8) exhibit very low correctness (3.00% and 18.04%, respectively). This indicates that the model's performance is highly inconsistent under noise, likely due to the distortion introduced affecting digit recognition. The model performs exceptionally well under brightness adjustments, with most pairs achieving near-perfect correctness. This suggests that the model is robust to changes in brightness, maintaining high confidence scores despite variations in image illumination. Performance under rotation is moderate, with significant variations across different pairs. Some pairs like (0,0), (1,1), (3,3), etc., achieve high correctness, while others such as (2,5) and (5,8) have lower correctness values. This variation suggests that

while the model can handle certain rotations well, it struggles with others, potentially due to the angles and the inherent difficulty in recognizing rotated digits.
Combining the global correctness across all transformations, we observe an overall high performance with a final global correctness of 97.65%. **Brightness** contributes the most to this high score (97.03%), while Noise contributes the least (0.58%). Rotation has a moderate impact (20.41%), reflecting its varied performance across different pairs. These observations highlight the strengths and weaknesses of the AI subsystem under different transformations. The high performance under brightness adjustments indicates robustness to illumination changes, while the challenges with noise and rotation suggest areas for improvement in handling these perturbations.

4.2.4 Analysis of Global Correctness After SHAP Analysis

The analysis of the global correctness graphs for noise transformations, both with and without SHAP analysis, clearly shows the importance of using SHAP to find key areas in the data.
In the first graph, which looks at individual noise pairs, supports this finding by consistently showing lower correctness for each pair when SHAP analysis is used. The pattern of reduced performance across different pairs indicates that SHAP is effective at identifying critical parts of the data that, when altered, reveal the model's weaknesses.
The second graph, we see that the global correctness for noise transformations drops dramatically from 58% without SHAP to just 0.25% with SHAP. This significant drop suggests that when the most important pixels identified by SHAP are changed, the model's performance suffers greatly. This is important because it helps us find areas where the model is weakest against noise.
These results demonstrate that using SHAP to create test cases by focusing on important pixels is a powerful method for discovering counterexamples. By systematically changing these key areas, we can stress-test the model and uncover its limitations under noisy conditions. This approach not only highlights where the model currently struggles but also points to ways we can improve its robustness. By addressing these weaknesses, we can build more reliable models that perform well even when there is noise in the data.

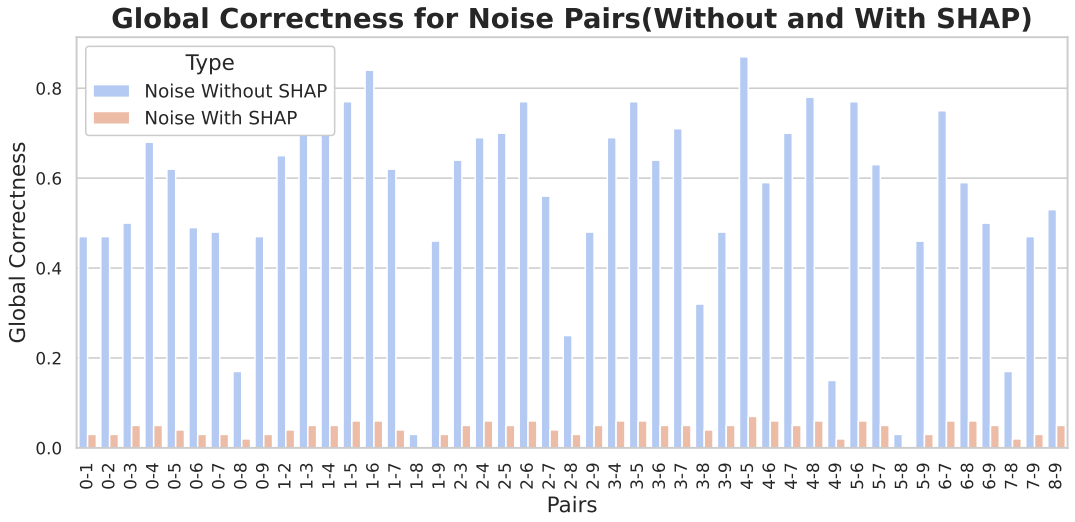


FIGURE 4.5: Global Correctness for Noise pairs

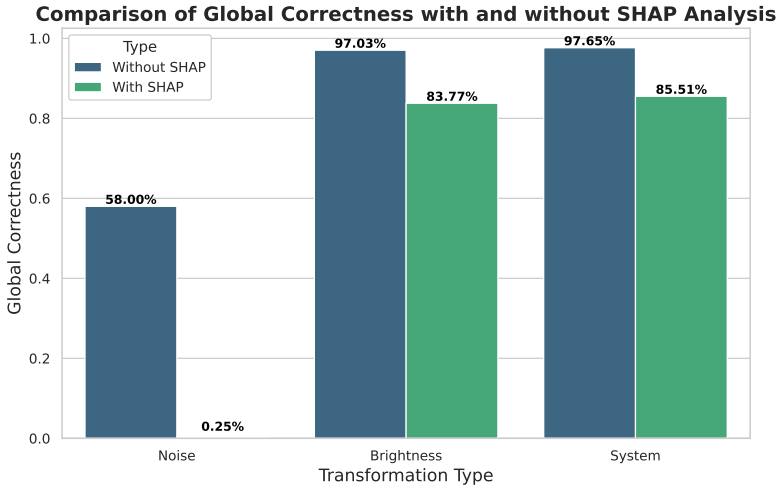


FIGURE 4.6: Combine Global Correctness

4.3 Use Case 2: Autonomous Vehicle Perception

In this use case, we investigate the robustness of an AI system for autonomous vehicles in detecting objects, particularly vehicles, under various weather conditions including fog, rain, snow, and sand. The goal is to assess the system's performance across these challenging environments to ensure reliable operation.

The dataset was split into training and validation sets, with class balancing performed through oversampling to address any class imbalances. Data augmentation techniques such as rotation, width and height shifts, shear transformation, zoom, and horizontal flips were applied to the training set to enhance the model's generalizability.

The trained model's performance was evaluated on a balanced validation set resampled to ensure uniform class distribution.

4.3.1 Local Correctness Analysis

The local correctness of the model for each weather condition is depicted in the first graph. The AI system exhibits the following correctness values: - **Fog:** The detection correctness is 51%, indicating moderate performance. Fog conditions likely introduce significant visual obstructions that challenge the model's ability to correctly identify vehicles. - **Rain:** Achieving a correctness of 75%, the model performs relatively well in rainy conditions, suggesting robustness to moderate visual disturbances caused by rain. - **Snow:** Similar to rain, the system shows a correctness of 75%, demonstrating its capability to handle snowy environments, where the visual contrast might be reduced. - **Sand:** With the highest correctness of 88%, the model excels in sandy conditions, possibly due to clearer visibility compared to other adverse weather scenarios.

4.3.2 Global Correctness Analysis

The second graph illustrates the global correctness for vehicle detection under different combination methods of weather conditions:

$$global\_weather \leftrightarrow (fog \wedge rain \wedge snow \wedge sand)$$
$$global\_weather \leftrightarrow (fog \vee rain \vee snow \vee sand)$$
$$global\_weather \leftrightarrow (fog \wedge (rain \vee snow \vee sand))$$

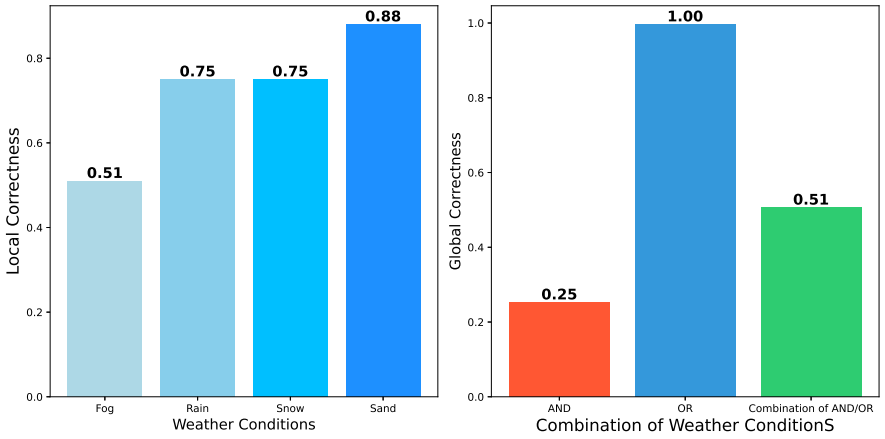


FIGURE 4.7: Local and Global Correctness of Vehicle Detection Under Various Weather Conditions

- **AND (Intersection):** The model's correctness is 25%. This low value reflects the stringent requirement for the system to correctly detect vehicles under all

specified conditions simultaneously, highlighting potential vulnerabilities when multiple weather challenges are present.

- **OR (Union):** Achieving a perfect correctness of 100%, the model successfully detects vehicles under at least one of the conditions. This high performance underscores the system's reliability when at least one favorable condition is present.
- **Combination of AND/OR:** The correctness stands at 51%, representing a balanced approach where the model must correctly detect vehicles under fog and any one of the other conditions (rain, snow, or sand). This mixed strategy provides a realistic measure of the system's robustness in practical scenarios with varying weather conditions.

Chapter 5

PhD Two-Year Plan

5.1 Research Modules

I have categorized my research into seven modules as depicted in Figure 5.1: Module 1 (DNN Testing Framework), Module 2 (Specification), Module 3 (Sampling), Module 4 (Interpretability), Module 5 (Testcase Generation), Module 6 (Coverage Criteria), and Module 7 (Error Summarization).

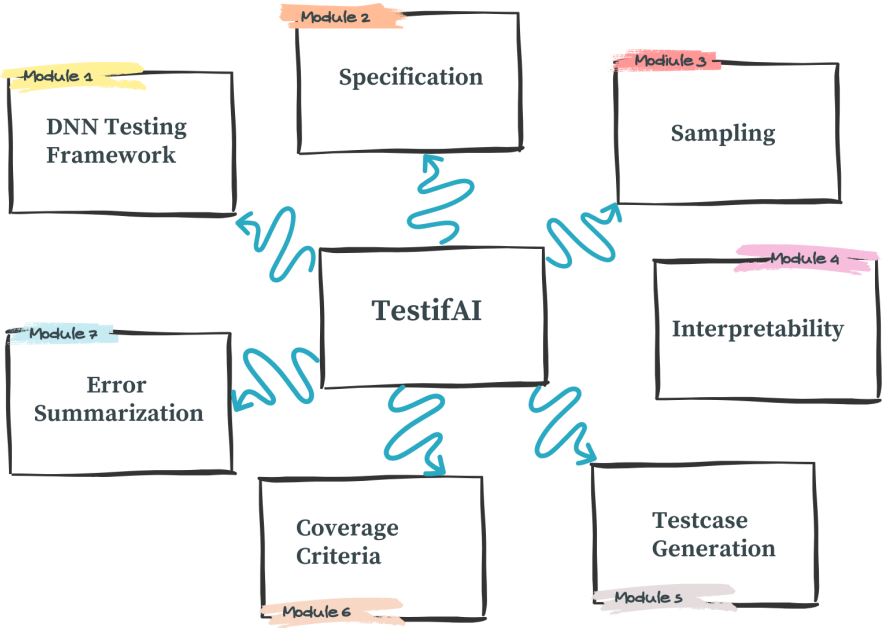


FIGURE 5.1: Research Modules

5.2 Mapping of Research Modules to Objectives

The research is structured into seven distinct modules, each addressing a specific objective. Table 5.1 outlines the mapping of these research modules to their corresponding

objectives discussed in Section **??**.

Research Modules	Research Objectives
DNN Testing Framework	Obj1
Specification	Obj2
Sampling	Obj3
Interpretability	Obj4
Testcase Generation	Obj5
Coverage Criteria	Obj6
Error Summarization	Obj7

TABLE 5.1: Mapping of Research Modules to Objectives

These modules are further divided into specific tasks to streamline the research process:

5.2.1 DNN Testing Framework (Module 1, 43% completion)

5.2.1.1 Literature review (M_1 - M_5, 60% completion)

Outline comprehensive testing requirements.

5.2.1.2 Designing a conceptual framework (M_8 - M_{12}, 100% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.3 Design local and global coverage flow (M_8 - M_{10}, 70% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.4 Implementing the Simple real life Example to cauclate local to global robustness(M_8 - M_{10}, 100% completion)

Implement Adder for this

5.2.1.5 Implementing ProbLog for calculating global robustness with one example (M_9 - M_{11}, 100% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.6 Integrate ProbLog code with python code (M_9 - M_{11}, 100% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.7 Integrate interpratability analysis to identify critical features (M_{Oct24} - M_{Dec24}, 0% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.8 Integrate efficient sampling approach (M_{Jan25} - M_{Feb25}, 0% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.9 Integrate error summarzation modules($M_{March25}$ - M_{May25}, 0% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.10 Integrate all developed techniques (M_{Sep25} - M_{Oct25}, 0% completion)

Set clear criteria for evaluating test outcomes.

5.2.1.11 Generate results on different datasets and make scenarios to validate this framework (M_{Sep25} - M_{Oct25}, 0% completion)

Set clear criteria for evaluating test outcomes.

5.2.2 Specification (Module 2, 0% completion)

5.2.2.1 Find a way to define specification, how to formalize it (M_{20} - M_{23}, 0% completion)

Outline comprehensive testing requirements.

5.2.2.2 How to pass specifications to ProbLog (M_{20} - M_{23}, 0% completion)

Set clear criteria for evaluating test outcomes.

5.2.2.3 How to automatically change specifications into desired format of framework(M_{20} - M_{23}, 0% completion)

Set clear criteria for evaluating test outcomes.

5.2.3 Sampling (Module 3, 45% completion)

5.2.3.1 Reading Papers Related to Sampling Techniques and Identify Gaps (M_9 - M_{10}, 50% completion)

M_9 - M_{10}, 50% completion.

5.2.3.2 Develop Efficient Sampling Technique (M_{10} - M_{12}, 0% completion))

Develop a technique that will cover all inputs or corner cases (M_{10} - M_{12}, 0% completion).

5.2.3.3 Implement Existing Sampling Techniques (M_9 - M_{10}, 30% completion)

Identify corner cases and prioritize those corner cases (M_9 - M_{10}, 30% completion).

5.2.3.4 Automate sample generation according to specification(M_9 - M_{10}, 0% completion)

M_9 - M_{10}, 0% completion.

5.2.4 Interpretability (Module 4, 42% completion)

5.2.4.1 Literature Review (M_4 - M_{24}, 30% completion)

M_4 - M_{24}, 30% completion.

5.2.4.2 Implementation of SHAP Tool (M_4 - M_6, 80% completion)

M_4 - M_6, 80% completion.

5.2.4.3 Applying SHAP to Identify Important Pixels (M_4 - M_5, 80% completion)

M_4 - M_5, 80% completion.

5.2.4.4 Explore Other Interpretability Analysis Techniques (M_{15} - M_{17}, 0% completion)

Explore techniques such as LIME to identify key features that can guide the generation of optimal test cases for evaluating model robustness (M_{15} - M_{17}, 0% completion).

5.2.4.5 Automate Interpretability Approach in Test Case Generation Module (M_{16} - M_{17}, 0% completion)

M_{16} - M_{17}, 0% completion.

5.2.5 Testcase Generation (Module 5, 50% completion)

5.2.5.1 Literature Review (M_1 - M_{18}, 50% completion)

M_1 - M_{18}, 50% completion.

5.2.5.2 Exploring Libraries for Test Case Generation (M_1 - M_2, 80% completion)

M_1 - M_2, 80% completion.

5.2.5.3 Implementing Adversarial Attacks and Semantic Adversarial Test Cases (M_3 - M_4, 80% completion)

M_3 - M_4, 80% completion.

5.2.5.4 Apply Existing Test Case Generation Methods to Benchmark Datasets (Analyze the results (M_{13} - M_{14}, 0% completion))

Analyze the results (M_{13} - M_{14}, 0% completion).

5.2.5.5 Automate Proposed Test Generation Module (M_{15} - M_{16}, 0% completion)

M_{15} - M_{16}, 0% completion.

5.2.6 Coverage Criteria (Module 6, 35% completion)

5.2.6.1 Reading Papers and Identifying Gaps (M_6 - M_9, 50% completion)

M_6 - M_9, 50% completion.

5.2.6.2 Apply Existing Coverage Criteria to Benchmark Datasets ((M_{13} - M_{14}, 0% completion))

Analyze the results (M_{13} - M_{14}, 0% completion).

5.2.6.3 Reading Literature on ProbLog to Understand its Application in Calculating DNN Global Coverage(M_6 - M_8, 50% completion)

M_6 - M_8, 50% completion.

5.2.6.4 Understand the Problog Language and Editor (M_9 - M_{10}, 80% completion)

M_9 - M_{10}, 80% completion.

5.2.6.5 Implementing and Automating ProbLog for DNN Coverage Calculations(M_9 - M_{10}, 70% completion)

M_9 - M_{10}, 70% completion.

5.2.7 Error Summarization (Module 7, 0% completion)

5.2.7.1 Find Ways to Properly Summarize the Counter Examples (M_{17} - M_{18}, 0% completions)

M_{17} - M_{18}, 0% completion.

5.2.7.2 Best Visuals to Represent Errors Report (M_{18} - M_{20}, 0% completion)

M_{18} - M_{20}, 0% completion.

5.2.7.3 Integrate Error Summarization Module in Framework (M_{20} - M_{21}, 0% completion)

M_{20} - M_{21}, 0% completion.

5.3 Mapping of Research Milestones to Objectives

5.3.1 Milestone 1: Conference 1 (MS1)

5.3.2 Milestone 2: Conference 2 (MS2)

5.3.3 Milestone 3: Journal 1 (MS3)

5.3.4 Milestone 4: Conference 3 (MS4)

5.3.5 Milestone 5: Conference 4 (MS5)

5.3.6 Milestone 6: Journal 2 (MS6)

5.3.7 Milestone 7: Thesis writing (MS7)

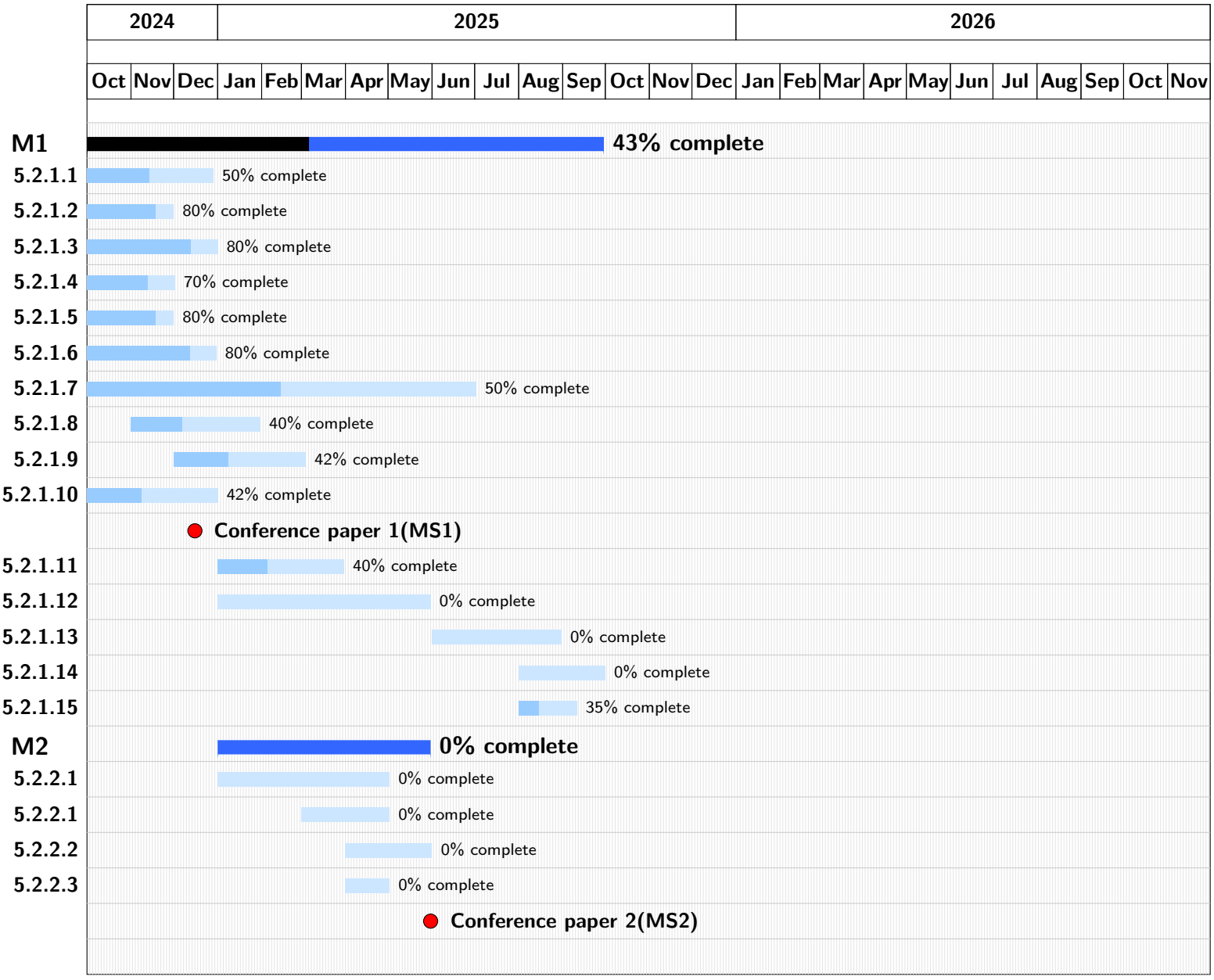
5.3.8 Milestone 8: Thesis submission (MS8)

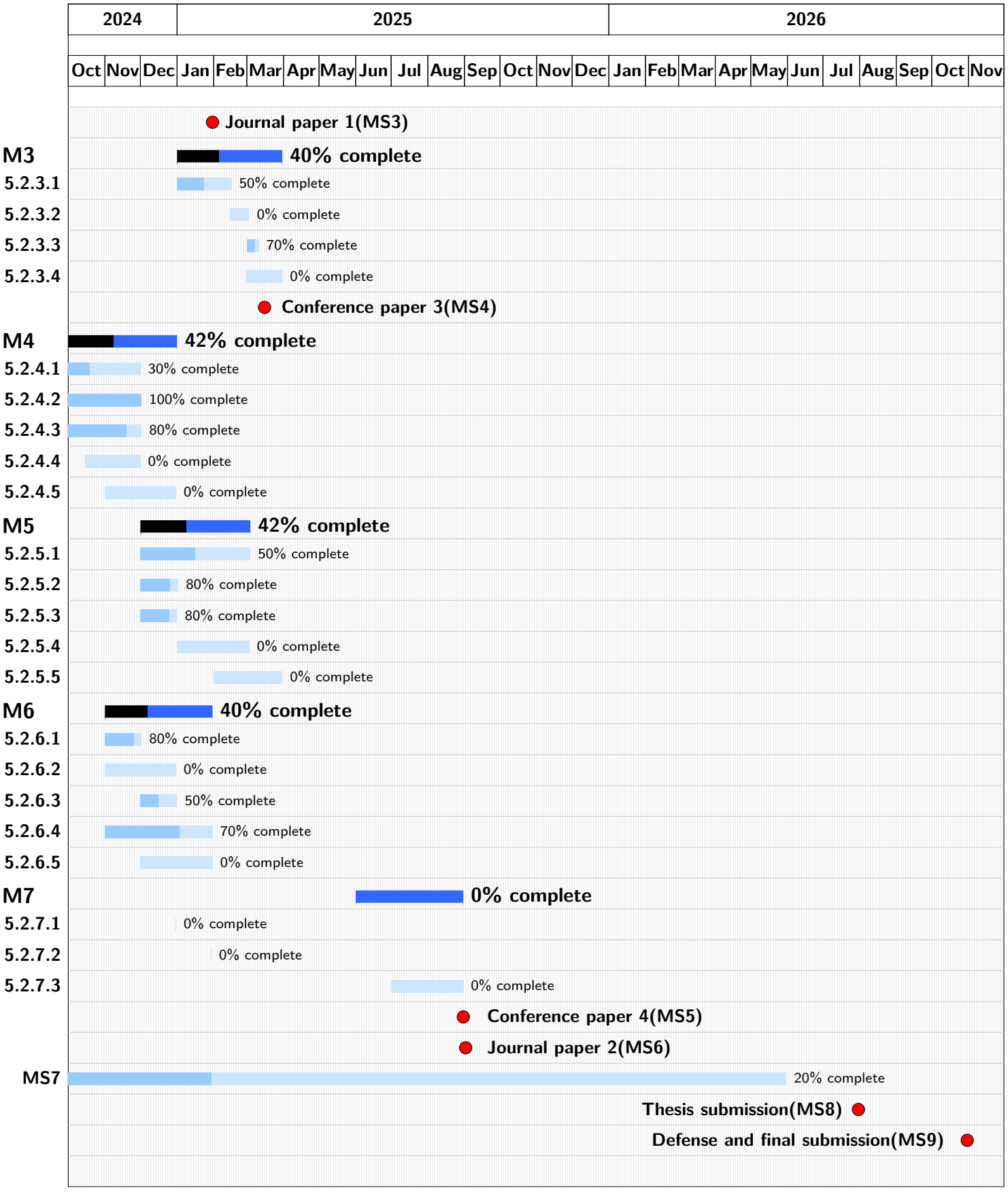
5.3.9 Milestone 9: Defense and final submission

Milestones	Research Objectives
Conference 1 (EuroML Conf 2025)	Obj1, 4, 6
Conference 2 (ICSE 2025)	Obj2
Conference 3 (ASE 2026)	Obj3
Conference 4 (ICST 2026)	Obj7
Journal paper 1 (Neural Networks)	Obj1, 3, 4, 5
Journal paper 2 (IEEE Transaction on Software Engineering)	Obj1, 2, 6, 7
Thesis writing	compile and synthesize research findings
Thesis submission	finalize and submit the complete thesis
Defense and final submission	present research, address feedback, and submit final version

TABLE 5.2: Mapping of Research Milestones to Objectives

5.4 Gantt Chart for Task-Wise Completion




2024
2025
2026
Oct Nov Dec Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov
Journal paper 1(MS3)
M3
40% complete
5.2.3.1
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5.2.3.2
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5.2.3.3
70% complete
5.2.3.4
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Conference paper 3(MS4)
M4
42% complete
5.2.4.1
30% complete
5.2.4.2
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80% complete
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5.2.4.5
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M5
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5.2.5.5
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M7
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0% complete
5.2.7.2
0% complete
5.2.7.3
0% complete
Conference paper 4(MS5)
Journal paper 2(MS6)
MS7
20% complete
Thesis submission(MS8)
Defense and final submission(MS9)

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Appendix A

LOCAL COVERAGE refers to evaluating the DNN performance and robustness for each individual class in a dataset separately. This includes assessing correctness and robustness under various transformations or test cases for each class independently. Section 6 of Chapter 1.

GLOBAL COVERAGE involves assessing the AI system performance and robustness in real-world scenarios where multiple classes interact together. This ensures the model correctness and robustness in dynamic environments with complex class combinations. Section 6 of Chapter 1.

COMPREHENSIVE refers to a structured and complete approach designed to cover all necessary aspects and components of a particular system or process. It ensures that every critical element is included and addressed, leaving no gaps. Section 1.1 of Chapter 1.

SYSTEMATIC refer to an organized approach, often characterized by step-by-step procedures. Section **??** of Chapter 1.