A Framework for Identifying Underspecification in Image Classification Pipeline Using Post-Hoc Analyzer

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Abstract: Underspecification — a failure mode where multiple models perform well during development but fail to generalize to new, unseen data due to reliance on insufficient or spurious features — remains critical challenge in machine learning (ML) and deep learning (DL). In this paper, we focus on a specific aspect of underspecification: the inconsistency in feature learning. We hypothesize that models with similar performance should exhibit consistent behavior in terms of feature reliance. However, in practice — especially in deep learning — this consistency is often lacking due to various factors influencing the learning process. To uncover where this inconsistency occurs, we propose a framework leveraging XAI techniques (specifically LIME and SHAP) to identify underspecification by analyzing inconsistencies across ML pipeline components, including feature extractors, optimizers, and weight initialization. Experiments on MNIST, Imagenette, and Cats_vs_Dogs reveal significant variability in feature reliance, particularly due to the choice of feature extractor. This variability highlights how different factors contribute to the learning of varied features, ultimately leading to potential underspecification. While this study focuses on the impact of specific pipeline components, our framework can be extended to analyze other factors contributing to underspecification in machine learning systems.

1 INTRODUCTION

Despite the remarkable advancements of Machine learning (ML) and Deep Learning (DL) algorithms, concerns about their reliability, interpretability, and trustworthiness remain significant (Kamath and Liu, 2021; Li et al., 2023; Molnar, 2020). One significant threat undermining these crucial properties from the modeling pipeline of ML is *underspecification* — where the modeling pipelines perform strongly well in the development settings but fail to generalize to the real-world settings. It is well studied that factors such as the limitations of empirical risk minimization (ERM), which prioritize error minimization over robust feature learning (Teney et al., 2022), along with distribution shifts (Ovadia et al., 2019; Quiñonero-Candela et al., 2022), inadequate data quality and representation (D'Amour et al., 2022; Hinns et al., 2021), and model complexity, can often exacerbate this problem. **From the literature, underspecification occurs when the modeling pipeline — ranging from data curation to learning algorithms — fails to sufficiently constrain the predictor for a target problem, leading to multiple valid but divergent solutions.**

Roughly, this issue can be viewed from two perspectives. First, from the **predictive perspective**, an ML pipeline is considered *underspecified* if it can yield multiple plausible outcomes for the same input, indicating ambiguity in its predictions (Madras et al., 2019). That is, the model has not learned a definitive way to represent the input. Second, from the **training perspective**, insufficient specificity across various components of the pipeline — including data preprocessing (Bouthillier et al., 2021), model architecture, weight initialization (Alahmari et al., 2020; D'Amour et al., 2022), hyperparameter settings (Arnold et al., 2024; Bischl et al., 2023; Müller et al., 2023), and others — can lead the model to learn different, potentially inconsistent behaviors during training. These inconsistencies arise because the model's inherent inductive biases, shaped by the pipeline's design choices, can influence how the model prioritizes features during learning. As a result, the model may emphasize different features, some of which may be irrelevant, leading to divergent learned representations (Mehrer et al., 2020). In this paper, we particularly focus on the later perspective.

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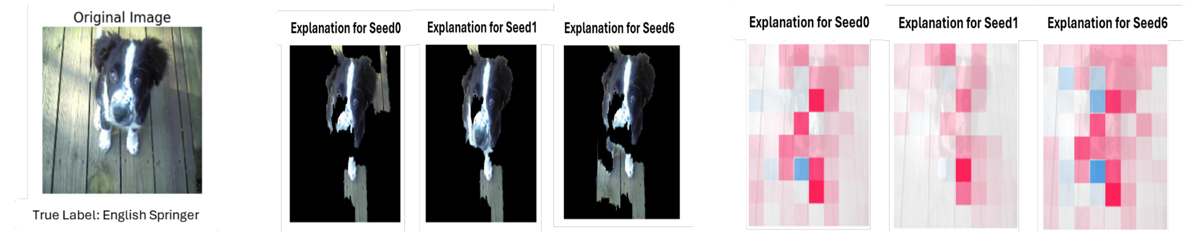


(a) Selected Test image (b) LIME explanations (c) SHAP explanations

Figure 1: **An example of underspecification in model explanations for an "English Springer" input from the Imagenette testset.** DenseNet121 models trained with identical pipelines but different random seeds yield varying feature-importance explanations. **(a)** An image of interest. **(b)** LIME explanations for seeds 0, 1, and 6, highlighting positive features. **(c)** SHAP explanations for the same models; red is positive, and blue is negative. These variations highlight initialization effects.

This phenomenon is closely analogous to the well-known "Rashomon Effect" (Breiman, 2001), where models with varying structures (called the Rashomon set) can fit with the training data equally well but rely on different features. In deep learning, such effects are amplified by the aforementioned design choices made during training, which collectively shape the model's learning trajectory. Thus, models with different architectures may achieve similar performance on the same dataset yet rely on entirely or partially distinct features. While some models may capture robust, generalizable patterns, others might exploit noise or spurious correlations, raising concerns about their reliability on unseen data.

Under ideal conditions — where the pipeline components influencing the learning process (e.g., data quality, optimization methods, model complexity, etc.) are properly controlled — it is reasonable to expect that any well-specified pipeline will exhibit more consistent behavior and rely on similar feature representations across models. However, even in such conditions, subtle differences in optimization dynamics or model architecture can introduce some variability. In underspecified systems, this variability is amplified, causing models that perform well during development to rely on differing feature representations, leading to significant differences in behavior during deployment, highlighting the issue of underspecification. Figure 1 illustrates this phenomenon — varying only the initial weights with different random seeds (see Subsection 4.1) while keeping all other pipeline components identical reveals, through LIME and SHAP explanations, that random initializations influence the model's feature learning mechanisms.

In this paper, we aim to identify underspecification within ML pipelines by pinpointing the components that contribute most to divergent learning processes. We propose a framework using posthoc analysis techniques, namely Local Interpretable Model-Agnostic Explanations (LIME) (Ribeiro et al., 2016) and SHapley Additive exPlanation (SHAP) (Lundberg and Lee, 2017), to analyze variations in feature-learning behavior. Our framework posits that models with similar development performance should exhibit consistent feature reliance, and any variability in explanation features signals a certain degree of underspecification. We validate this framework through experiments on MNIST (LeCun et al., 1998), Imagenette (Howard, 2019), and Cats_vs_Dogs (Kaggle, 2013) datasets. Our findings indicate that feature extractor architecture plays a more significant role in underspecification than other pipeline components.

2 RELATED WORKS

Underspecification in machine learning (ML) occurs when models perform well on in-distribution data but fail to generalize to out-of-distribution (OOD) or unseen data. A study (D'Amour et al., 2022) revealed that models trained with different random initializations can exhibit significant variations in their OOD performance despite similar in-distribution accuracy, underscoring that high development accuracy does not necessarily indicate a reliable model, especially in complex or dynamic environments.

Ensemble methods, for example, have been used to quantify uncertainties, distinguishing between epistemic and aleatoric types (Lakshminarayanan et al., 2017; Ovadia et al., 2019). These studies demonstrate that underspecification contributes to epistemic uncertainty — uncertainty due to model parameters — which can be undermine model reliability, particularly in high-stakes applications where predictability is key. Moreover, several works have focused on OOD generalization, proposing techniques like domain adaptation (Teney et al., 2022) and evaluating models on local geometric loss properties (Madras et al., 2019). These methods aim to identify and mitigate performance degradation when models are exposed to new, unseen distributions. Additionally, (Hinns et al., 2021) explored the role of dataset quality and representativeness in underspecification, highlighting how the training data itself introduce biases and inconsistencies that affect model robustness.

While these studies offer valuable insights into various aspects of underspecification, they generally do not investigate "how specific components of the ML pipeline, contribute to the variability in feature reliance and decision-making". Early-stage pipeline choices have significant implications for model behavior but remain underexplored in the context of underspecification.

In contrast, our study systematically measures variability in feature learning across different ML pipeline configurations. By varying pipeline components and using post-hoc tools like LIME and SHAP, we quantify their impact on model decision-making. This work advances understanding of underspecification by identifying key contributing components and emphasizing the need for more interpretable models.

3 PROPOSED FRAMEWORK

Our framework is designed to quantify the degree of underspecification in the context of supervised learning settings by allowing practitioners to systematically vary individual components of their machine learning pipeline. We also demonstrate their applications on the image classification task. We formalize the pipeline as an n-tuple representation and describe a generalized approach to measure the impact of varying any single component on the underspecification[1].

3.1 Pipeline Representation

Any machine learning pipeline P_i can be represented as a n-tuple $P_i := (p_1, p_2, \ldots, p_n)$, where $n \in \mathbb{Z}^+$ and each p denotes a distinct component of the pipeline, such as, data preprocessing, feature extraction, classifiers, or optimization methods. In our framework, the index i is used to enumerate multiple pipelines by varying specific components, enabling controlled comparisons across different configurations. When it is clear from the context, i might be omitted.

Our objective is to analyze the degree of underspecification by varying individual components p_j of the pipeline P while fixing other components, enabling to study the effect of a specific component of the learned representations and predictive behavior of the ML pipeline.

[1]Our implementation source code is available online at: https://github.com/realearn-jaist/underspecification-in-computer-vision

3.2 Framework Overview

Our framework is composed of the following steps:

3.2.1 Component Selection and Variation

We select a specific component p_j of the ML pipeline for underspecification analysis. For instance, it could be the feature extractor, optimizer, etc. For any selected p_j, a finite set of k-variations $\{p_j^k \mid k \in \mathbb{Z}^+, 1 \leq k \leq m\}$ is computed, where m represents the total number of variations considered. This choice of p_j generates a set of ML pipelines $\{P_i \mid 1 \leq i \leq k\}$ to test the underspecification, where each pipeline P_i is constructed as $P_i := (p_1, \ldots, p_j^i, \ldots, p_n)$, differing solely in the specified component p_j. For instance, if we choose to vary the feature extractor component p_j, the variations might correspond to different network architectures, e.g., CNN, ResNet, or VGG.

3.2.2 Pipeline Modeling and Training

Next, each pipeline P_i is complete by attaching with a predictor (or classifier) g_i for training with a training set D_{tr}, drawn from a dataset D; we divide D into subsets of training (D_{tr}), validation (D_{val}), and test (D_{test}) while reserving D_{test} for later use, i.e., generating explanations and analyzing underspecification.

In our procedure, any completed pipeline P_i takes in D_{train} to produce a function m_i, which maps from any input x into label y. Explicitly, each pipeline P_i can be thought of as a composite function $m_i(x) := g_i(f_i(x))$, where f_i and g_i represent a feature extractor and classifier, respectively. Thus, we use the term "model" from now onward, which essentially represents an individual pipeline. To illustrate this process, Algorithm 1 provides the procedure to generate a set M of models by varying specific component p_j across its predefined values. It takes as input the dataset D and the variation set $\mathcal{P}_j$, iteratively creates a set P_i of pipeline candidates with each variation $p_j \in \mathcal{P}_j$, and stores the trained models m_i in the set M. This set of models is then used in subsequent steps for explanation generation and underspecification measurement.

Furthermore, in order to ascertain that any interpretability differences observed across the models are not attributed to performance disparities, we ensure that each model achieves a predefined performance threshold t on both D_{val} and D_{test}.

3.2.3 Explanation Generation and Underspecification Measurement

For each test sample $x \in D_{test}$ and model m_i given by a pipeline P_i, the next step is to generate expla-

Algorithm 1: Model Generation with Pipeline Variations.

Input : dataset: D, set of variations for a chosen component p_j: $\mathcal{P}_j$, predefined threshold: t
Output: Set of trained models: M

Function `train_and_validate`$(P_i, D_{\text{tr}}, D_{\text{val}}, D_{\text{test}})$:
  train(m_i, D_{tr});
  if $eval(m_i, D_{\text{val}}) \geq t$ ***and*** $eval(m_i, D_{\text{test}}) \geq t$ **then**
    return m_i;
  return None;

Function `create_models`$(D, \mathcal{P}_j)$:
  split$(D, D_{\text{tr}}, D_{\text{val}}, D_{\text{test}})$;
  $M \leftarrow []$;
  foreach $v \in \mathcal{P}_j$ **do**
    $P_i \leftarrow$ construct_pipeline$(\ldots, v, \ldots)$;
    $m_i \leftarrow$ `train_and_validate`$(P_i, D_{\text{tr}}, D_{\text{val}}, D_{\text{test}})$;
    if $m_i \neq None$ **then**
      M.append(m_i);
  return M;

nations $\xi_x^{m_i}$ using LIME and SHAP. These explanations highlight the features reliance that contribute to the model's predictions, allowing for a comparison of predictive behavior across models given by the pipelines. Consequently, we quantify the degree of underspecification by measuring the variation in explanations across models:

$$UnderspecificationDegree := Variation\left(\xi^{m_i}_{(x)}{}_{i=1}^{k}\right),$$

where $\xi_x^{m_i}$ is the explanation given by model m_i for input x, and $Variation(\cdot)$ is a metric such as cosine distance or any other metric that quantifies differences between explanations.

Using LIME and SHAP for model-agnostic interpretability, we explore underspecification from both instance and class perspectives.

3.3 Instance-Level Underspecification

The instance-level underspecification refers to a situation extended for analyzing any individual in the dataset. This view is necessary to analyze which instance the ML pipeline fails to generalize. Intuitively, we compare the explanations between the models in M and inspect the input x from D_{test} assessing the consistency or variability of their local behavior.

Formally, let x be a test instance in D_{test}. For any model $m_i \in M$, the predicted label is $y := m_i(x)$. To provide an explanation of the features of x that contribute to this prediction, we apply both LIME and SHAP independently (one at a time). Let $\xi_x^{m_i}$ denote the explanation generated by the chosen method (either LIME or SHAP). We gather explanations from all models for x as: $\Xi := \{\xi_x^{m_1}, \xi_x^{m_2}, \ldots, \xi_x^{m_k}\}$

The instance-level comparison can thus be defined as follows: The cosine similarity metric, which allows us measure angular differences between explanation vectors, focuses on orientation rather than magnitude. Specifically, we compute the pairwise cosine distance (denoted by d) for all possible pairs of explanations $\left(\xi_x^{m_i}, \xi_x^{m_j}\right)$, where $i \neq j$ as:

$$d\left(\xi_x^{m_i}, \xi_x^{m_j}\right) := 1 - \frac{\xi_x^{m_i} \cdot \xi_x^{m_j}}{\|\xi_x^{m_i}\| \|\xi_x^{m_j}\|} \tag{1}$$

As the explanations are binarized for the calculation process (see details in Subsection 4.2), the cosine distance $d\left(\xi_x^{m_i}, \xi_x^{m_j}\right)$ ranges from 0 to 1. A value of 0 indicates perfect similarity (maximum consistency) between explanations, while a value of 1 represents no similarity at all (maximum variability).

Figure 2 depicts the general workflow for instance-level underspecification analysis procedure at test time, where we vary only weight initialization with different seeds during training and analyze the variations in explanations at test time.

3.4 Class-Level Underspecification

The instance-level underspecification gives one perspective to quantify this problem in the ML pipeline. It still does not capture the overall predictive behavior of the model pipeline. To gain more comprehensive understanding and quantify overall behavior, we select a set of instances associated with class c_i. Selecting instances can be somewhat subjective, as these instances should ideally represent the overall class's feature distribution. To mitigate this concern, we first select a diverse set of instances from D_{test} that capture a range of feature variations within the class. We then filter out incorrectly predicted instances, retaining only those that are correctly predicted by all models in M. The resulting set X, ensures that the remaining instances reflect the class's feature distribution and provide reliable, consistent predictions across all models. Using LIME or SHAP, each model m_i can be provided an explanation $\xi_{x_l}^{m_i}$ for any instance $x_l \in X$. We then compute *ClassLevelScore* (denoted by $\hat{d}$) by averaging the instance-level underspecification of explanation pairs $(\xi_{x_l}^{m_i}, \xi_{x_l}^{m_j})$ across all instances in X:

$$\hat{d}(m_i, m_j) := \frac{1}{|X|} \sum_{l=1}^{|X|} d(\xi_{x_l}^{m_i}, \xi_{x_l}^{m_j}) \tag{2}$$

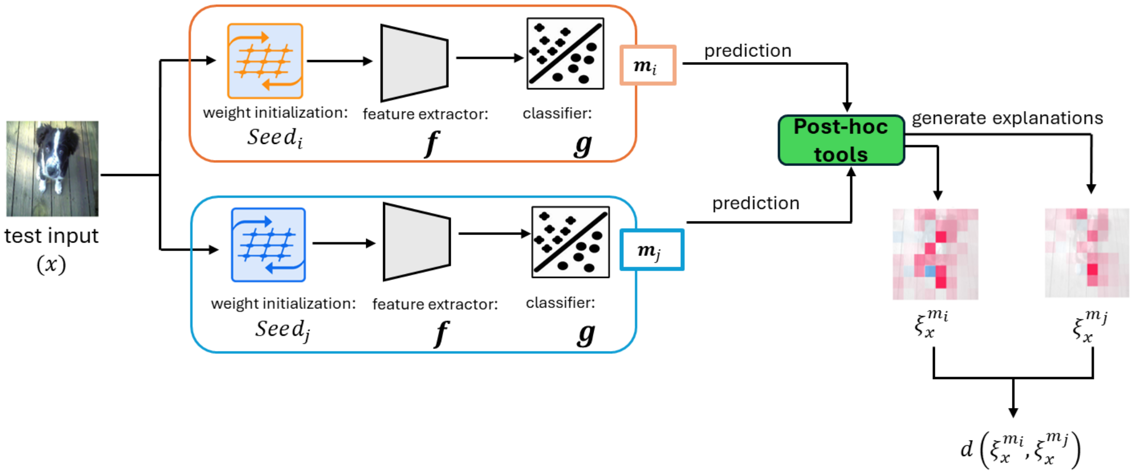


Figure 2: **An example workflow for instance-level underspecification analysis at test time.** Here, a test input x is drawn from D_{test}, and passed through two models, $m_i : g(f(x))_{\text{seed}_i}$ and $m_j : g(f(x))_{\text{seed}_j}$, each shaped by different weight initialization: $Seed_i$ and $Seed_j$, while keeping all other components, such as, D_{tr}, feature extractor f, classifier-head g, etc., fixed during training. Post-hoc explanation tools (e.g., SHAP in this case) are then used to analyze and compare the generated explanations, revealing the influence of weight initialization on model predictions and their interpretability.

where $|\cdot|$ represents the set cardinality and $\hat{d}$ ranges from 0 to 1. The lower $\hat{d}$ indicate higher consistency and lower degrees of underspecification for the class c_i, while the higher scores imply greater variability and higher degrees of underspecification.

4 EXPERIMENTS AND ANALYSIS

In this work, we investigate the roles of various components within the ML pipeline to identify which component contributes most to underspecification problem. To achieve this, we systematically vary specific components of the ML pipeline while keeping all other components constant and then analyze the resulting feature reliance using LIME and SHAP. Our focus in this work is mainly on three components of the pipeline — feature extractor, optimizer, and initial weight — as these are potential sources of variation in model behavior under underspecified conditions.

4.1 Experimental Setup

The ML pipelines in this study are designed to isolate the impact of specific components by changing one component at a time, enabling us to observe the relative contribution of each component to variation in feature reliance, reflecting underspecification problem. That is, for each experiment (each dataset), we vary one component at a time across three primary phases: feature extractors, optimizers, and initial weights. The remaining components are held constant to ensure any observed differences in feature reliance are due to the varied component. The following pipeline's configurations are used:

1. **Dataset:** Each experiment is conducted on three datasets with different levels of complexity:
   MNIST: It is a relatively small, clean dataset of 28×28 handwritten digits, ideal for testing the impact of complex models over simple tasks. We resize them to 32×32 using bilinear interpolation, making it suitable for implementing different pretrained architectures. It includes 60,000 training images and 10,000 validation images, from which we create a test set of 2,000 images.
   Imagenette[2]: A subset of the ImageNet dataset with 10 classes that contains large-scale, detailed backgrounds, introducing additional complexity. We employ a "320 px" version of it containing approximately 9,500 training images and about 3,920 validation images, from which we create a test set by taking 20% of it. Again, the bilinear interpolation method is used to resize the images to 224×224.
   Cats_vs._Dogs: It is a binary classification dataset from a past Kaggle competition, consisting of detailed images with higher intra-class variation, offering another layer of complexity. We employ the dataset from the Tensorflow Dataset[3] library, where the dataset was preprocessed and corrupted data were excluded, consisting approximately 25,000 images. Here, the images are re-

[2] https://github.com/fastai/imagenette
[3] https://www.tensorflow.org/datasets/catalog/Cats_vs_Dogs

Table 1: Training, validation (Val), and test accuracy (Acc) of models with different feature extractors and optimizers across datasets.

Dataset	Configuration	Model	Train Acc (%)	Val Acc (%)	Test Acc (%)
MNIST	Feature Extractor	CNN	98.92	99.00	99.35
		MobileNet	99.61	98.84	99.20
		DenseNet121	99.88	99.25	99.45
		EfficientNetB0	98.79	98.33	98.95
	Optimizer	CNN-Adam	99.57	99.00	99.45
		CNN-SGD	98.92	99.00	99.35
		CNN-RMSprop	99.60	99.14	99.40
		CNN-Nadam	99.55	99.14	99.20
Imagenette	Feature Extractor	Xception	99.69	98.45	98.31
		InceptionV3	99.43	97.91	97.26
		DenseNet121	98.64	98.40	97.79
		ResNet50V2	99.25	98.10	97.66
	Optimizer	DenseNet-Adam	98.92	98.35	98.30
		DenseNet-SGD	97.63	98.43	97.27
		DenseNet-RMSprop	98.60	98.45	97.79
		DenseNet-Nadam	98.91	98.23	97.65
Cats_vs_Dogs	Feature Extractor	Xception	98.88	98.64	98.72
		InceptionV3	98.90	98.74	99.22
		DenseNet121	98.56	98.08	98.77
		ResNet50V2	98.98	98.50	98.44
	Optimizer	DenseNet-Adam	98.52	97.97	98.83
		DenseNet-SGD	97.92	98.11	98.94
		DenseNet-RMSprop	98.41	98.71	99.22
		DenseNet-Nadam	98.68	98.60	99.16

sized to 224×224 using bilinear interpolation and created a validation set by splitting 80:20, then reserving 20% of the validation set for testing.

2. **Varying Feature Extractors:** For those pipelines where we vary the feature extractor component while keeping all others fixed, we use different architectures. The development performances are summarized in Table 1.

   For MNIST: Four different architectures — a custom CNN and three pretrained architectures: MobileNet (Howard et al., 2017), DenseNet121 (Huang et al., 2017), and EfficientNetB0 (Tan and Le, 2019) were tested. Given MNIST's simplicity, overly complex models would be excessive; thus, these architectures were selected carefully to balance model parameters and complexity. For instance, the custom CNN is relatively shallow, capturing basic spatial hierarchies in the MNIST digits, while others are deeper networks typically applied to more complex datasets. Although each architecture differs in its approach to feature learning, we consider them ideal candidates as long as they perform equally well during training time. For the pretrained architectures, we retained only the architectural structure without any pre-initialized weights, i.e., we trained them from scratch. For training, we found that the Stochastic Gradient Descent (SGD) optimizer was effective and smooth across all models. To ensure a fair comparison, we set the training duration to 15 epochs for each architecture. To prevent overfitting, we incorporated dropout layers and $L2$ regularization of strength 0.01, especially for deeper networks like DenseNet121 and EfficientNetB0.

   For Imagenette and Cats_vs_Dogs: We leveraged transfer learning (as both datasets align with the ImageNet domain) and utilized four pretrained architectures — Xception (Chollet, 2017), DenseNet121 (Huang et al., 2017), InceptionV3 (Szegedy et al., 2016), and ResNet50V2 (He et al., 2016). These deeper, complex architectures were chosen for their suitability to larger, more complex datasets compared to MNIST.

   For consistency, we applied the same classifier head structure (g) as in the MNIST experiments. The Adam optimizer, with its adaptive learning rate, proved most effective for these architectures, ensuring smooth convergence. Training over 10 epochs was sufficient to achieve stable performance on both datasets.

3. **Varying Optimizers:** In the second phase of our experiments, we explored the effects of vary-

ing the optimizer while keeping all other pipeline components fixed, including the dataset, feature extractor, classifier structure (deep layers, regularizers, etc.), and initialization weights. Upon testing, four optimizers — Adam (Kingma, 2014), SGD (Ruder, 2016), RMSprop (Hinton, 2012), and Nadam (Dozat, 2016) — demonstrated similar performance during training. As for the feature extractor, we used a simple CNN for MNIST and DenseNet121 for the other two, chosen for their relative complexity (least complex in terms of parameters than others used in the earlier phase). Training configurations were adapted based on dataset complexity and optimizer performance. For instance, on MNIST, all optimizers achieved similarly high accuracy within 15 epochs, though some optimizers required additional tuning on the other two datasets. The development accuracies are summarized in Table 1.

4. **Varying Initial Weights:** To investigate the impact of initial weight variations on feature learning, we introduced different random seeds for initialization while keeping all other pipeline components constant. This setup isolates the effects of initialization on underspecification. Following a similar configuration as in the "Varying Optimizers" experiment, we used Adam as the sole optimizer and applied a CNN for MNIST and DenseNet121 for both Imagenette and Cats_vs_Dogs. Each model was trained ten times with different random seeds — resulting in ten CNN and ten DenseNet121 models — to measure the consistency of feature reliance across different initializations. Training epochs varied based on dataset complexity and model convergence's requirements to achieve comparable accuracy. The development accuracy scores closely align with the baseline scores from the "Varying Optimizers" experiment (specifically, the configurations for CNN-Adam for MNIST and DenseNet121-Adam for the other two datasets). Given that the accuracy results for all ten CNN and ten DenseNet models are similar to these baselines in Table 1 , we would like to omit them for clarity and conciseness.

4.2 Underspecification Analysis

Observing the development accuracy scores in Table 1 alone does not clarify whether these scores arise from reliance on spurious or irrelevant features, which could indicate an underspecification issue. This ambiguity underscores the need for further analysis to understand feature reliance. To this end, we employed two widely-used explanation techniques — LIME and SHAP — to probe the models' decision-making processes. By analyzing which features are most influential across different configurations of the ML pipeline, we can assess the extent to which each component contributes to variability in feature reliance and, thereby, to underspecification.

4.2.1 LIME and SHAP Configuration

For LIME, we used the ImageExplainer module with 1,000 perturbed samples per instance, focusing on the top-3 features for multiclass problems and top-2 for binary classification. The kernel width was set to 3 for MNIST (with the default slic segmentation) and left at default for the other two datasets, with output restricted to positive features for interpretability.

For SHAP, the SHAP Explainer module with the default partition explainer for image data was used. Explanations were generated using 1,000 model evaluations with the inpaint_telea masker technique. To improve efficiency, we focused only on the top-1 feature for the probable class.

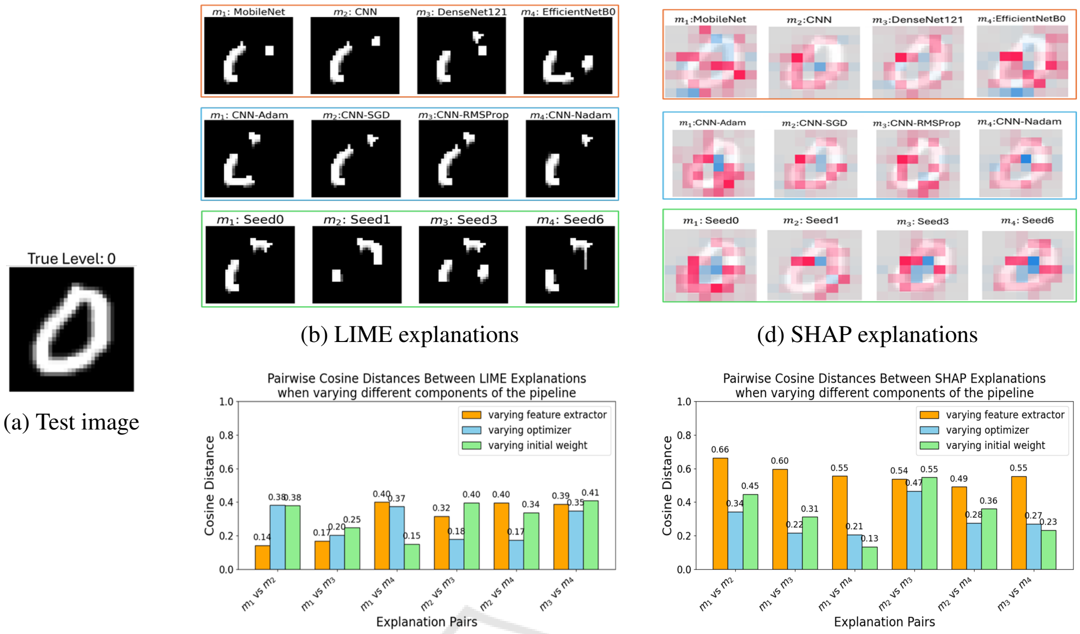
Both methods assessed the impact of feature extractor, optimizer, and initial weights on feature reliance. To manage computational load, we analyzed 100 instances per MNIST class and 50 per class for Imagenette and Cats_vs_Dogs datasets.

To compare feature explanations across configurations, we used the proposed *ClassLevelScore* metric (Section 3). Explanations were standardized to binary masks: for LIME, binary masks of superpixels were used directly; for SHAP, pixels exceeding 20% of the maximum positive SHAP value were set to 1, while the rest were set to 0. These binary representations facilitated consistent pairwise comparisons using cosine distance.

4.2.2 Interpretating Explanations

Our analysis using LIME and SHAP reveals the extent to which different components of the ML pipeline contribute to feature reliance underspecification. Our instance-level underspecification examines the variability in feature importance explanations for a single test instance when specific pipeline components are varied. Our analysis, conducted on a random test sample from MNIST D_{test} (Figure 3), highlights the sensitivity of instance-level explanations to changes in the feature extractor, optimizer, and initial weights.

When varying the "feature extractor," the explanations and pairwise cosine distance scores in Figure 3 revealed contrasting behaviors between LIME and SHAP. LIME explanations appeared relatively consistent, whereas SHAP explanations exhibited the high-



(a) Test image

(b) LIME explanations

(d) SHAP explanations

(c) Variation on LIME explanations

(e) Variation on SHAP explanations

Figure 3: **Instance-level experiments with varying pipeline components for a test input (a)**. (b) and (d) show LIME and SHAP explanations clustered by component: top (orange border), middle (skyblue border), and bottom (green border) rows represent the feature extractor, optimizer, and weight initialization, respectively. (c) and (e) summarize statistical variations using color-coded bar plots matching the rows in (b) and (d).

est variability for this component. Since these results are based on a single instance, they may not fully capture the broader variation in model behavior. Therefore, class-level quantification is necessary to assess the true impact of feature extractor variations. In contrast, variations in the "optimizer" and "initial weights" (Figure 3) resulted in less pronounced, though still observable differences in the highlighted regions. These variations suggest that even subtle changes, such as optimization strategies or initialization seeds, can influence how the model interprets and assigns importance to features for a specific instance.[4]

Class-level underspecification analyzes the consistency of feature importance explanations across classes. Our analysis across all three datasets and explanation methods, supports our instance-level analysis and reveals that varying the feature extractor leads to the highest average *ClassLevelScore* across classes, indicating the greatest variability in feature reliance (Figure 4, orange bars). This inconsistency suggests that the choice of feature extractor is a primary factor in underspecification, as differences in architecture result in distinct feature representations and significant shifts in feature importance and reliance.

In contrast, variations in the optimizer and initial weights produced lower average *ClassLevelScore* (the blue and green bars in Figure 4), reflecting reduced variability in explanations. Although these variations were smaller, they suggest that optimizers and initialization seeds do play pivotal roles in underspecification.

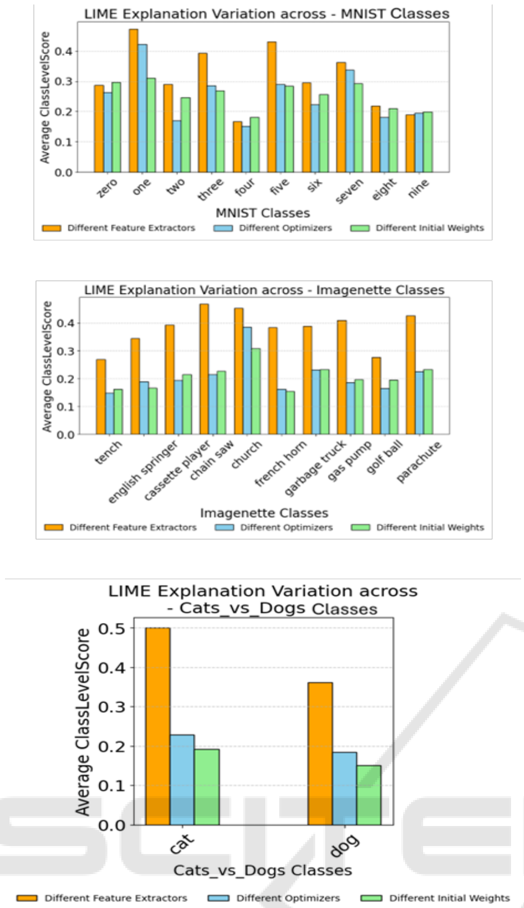
Overall, these findings highlight that while feature extractors are a dominant factor in the occurrence of underspecification in ML pipelines, each component has the potential to introduce some degree of underspecification. This underscores the importance of carefully considering all components in the model pipeline to reduce underspecification and improve model interpretability and robustness.

4.2.3 Time Complexity Analysis

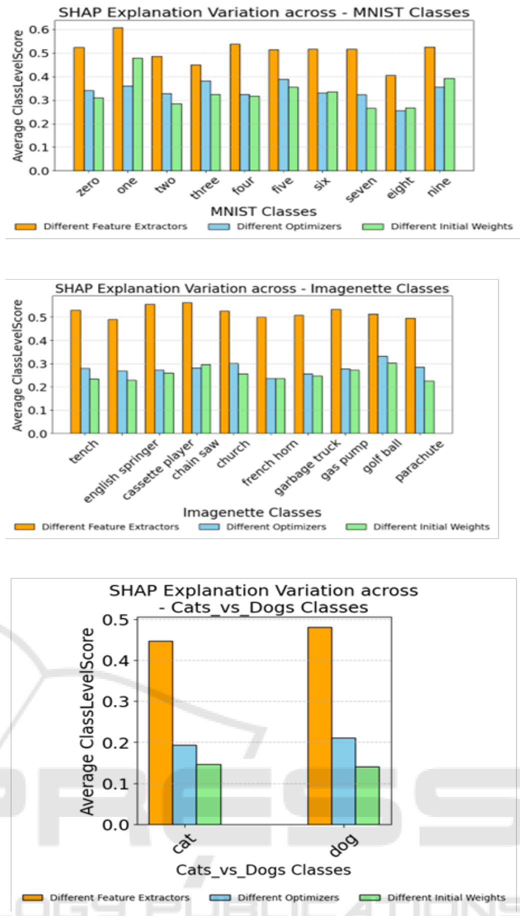
Our proposed framework involves three main steps, each contributing to the overall time complexity:

- **Pipeline Modeling and Training:** Let m be the number of variations for a selected component, and let $\mathcal{T}$ denote the average training time for each model. The complexity for training all m models is: $O(m \cdot \mathcal{T})$.

[4] We focus on presenting instance-level analysis only for MNIST due to space constraints and its limited informativeness compared to class-level analysis. Extending to other datasets would add redundancy without significant additional value.



(a) LIME explanation variations across different datasets



(b) SHAP explanation variations across different datasets

Figure 4: **Class-Level Explanation Inconsistency across Pipeline Components for all Three Datasets.** (a) LIME explanation variations (left column) for MNIST (top), Imagenette (middle), and Cats_vs_Dogs (bottom). (b) SHAP explanation variations (right column) for the same datasets. Bars indicate the impact of varying key pipeline components: feature extractor (orange), optimizer (sky blue), and initial weights (light green).

- **Explanation Generation:** We employ LIME and SHAP on each of the k models to explain N test instances. Let e represent the number of perturbations or evaluations needed per instance. Consequently, the complexity of generating explanations is:
$$O(k \cdot N \cdot e)$$
- **Underspecification Measurement:** To compare explanations across different models, we compute pairwise distances. Since there are $\binom{k}{2} = \frac{k(k-1)}{2}$ pairs among k models, and we perform these comparisons for N instances, the overall complexity is on the order of:
$$O(k^2 \cdot N)$$

Putting it all together, the total time complexity of the framework can be expressed as:

$$O\Big(\underbrace{m \cdot \mathcal{T}}_{\text{model training}} + \underbrace{k \cdot N \cdot e}_{\text{explanation generation}} + \underbrace{k^2 \cdot N}_{\text{calculation}}\Big)$$

In practical settings, the explanation generation step $(O(k \cdot N \cdot e))$ often dominates, especially if e (the number of perturbations or evaluations) is large, if the black-box models are expensive to query.

5 CONCLUSION

We introduce a framework to systematically examine how different ML pipeline components contribute to underspecification by evaluating feature reliance through post-hoc explanation tools, specifically LIME and SHAP. Our experiments reveal that models with similar and high accuracy can rely on different features — potentially spurious and irrelevant ones — in the decision-making process, emphasizing that high accuracy alone does not guarantee model reliability. Among the components tested, varying the feature extractor introduced the highest variability in feature reliance, identifying it as the primary factor in underspecification. However, optimizers and initial weights can also contribute to underspecification. While this study primarily focuses on these three components, our proposed framework can be extended to investigate additional elements within ML pipelines.

While this study effectively highlights the prevalence of underspecification in various ML pipeline components and identifies where it potentially occurs, it is important to note that it does not directly address how to reduce it. Additionally, we observe slight inconsistencies in LIME explanations due to its inherent randomness, which suggests that relying solely on LIME may limit the robustness of underspecification analysis. Additionally, our cosine distance-based *ClassLevelScore* metric, despite its effectiveness, displays sensitivity on simpler datasets like MNIST, potentially amplifying variability and underspecification in these cases. Furthermore, while dataset quality and representation are known to significantly impact underspecification, these aspects are not directly explored in this work, as they are extensively studied in the literature. Lastly, although post-hoc explanation tools such as LIME and SHAP provide valuable insights, their computational intensiveness may limit their applicability to datasets with large numbers of classes or instances, posing a challenge for scalability in more complex settings.

Future work will focus on addressing these limitations by exploring strategies to mitigate underspecification. This may involve identifying which feature extractors or optimizers contribute most consistently to stable feature reliance, testing alternative initialization methods, and developing a framework to guide pipeline configurations toward reduced variability.

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