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# Enhancing the ECSEER pipeline: Evaluating Large Language Model Classifiers in SE Research

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## Abstract

The various research papers in the field of Software Engineering (SE) that use classification algorithms, LLMs, or other machine learning methods to obtain their results differ in how many and which evaluation metrics are reported, whether or not significance tests are performed, and which steps are taken to aid reproducibility. The ECSEER pipeline was designed to mitigate this issue by providing a step-by-step pipeline that researchers can use to report their results when classification algorithms are used, and the pipeline was empirically shown to be effective in replicating the findings of several studies, as well as producing additional findings and occasionally contradicting the findings of the original papers. However, the ECSEER pipeline is designed for evaluating simple classifiers and gives no specific recommendations for LLM classifiers, despite LLMs being an increasingly popular choice for classification tasks. The goal of this thesis is to expand the ECSEER pipeline for the use of LLMs by adding recommendations from LLM4SE research and related fields. First, an exploratory mapping study will be done of SE studies released in 2024 that use LLM classifiers, summarising which steps are taken and which metrics are (or aren't) reported, in order to get an overview of the current state of LLM4SE research. Subsequently, we design the *ECSEER-LLM* pipeline, an enhanced version of the ECSEER pipeline for the use of LLMs, including recommendations for prompt engineering, evaluating the fairness and robustness of models, and more. Lastly, in order to evaluate the comprehensiveness and ease-of-use of the new pipeline, two replication studies were conducted using the pipeline to test its ability to strengthen or contradict the findings of the original papers.

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The Ethics and Privacy Quick Scan of the Utrecht University Research Institute of Information and Computing Sciences classified this research as low-risk with no fuller ethics review or privacy assessment required.

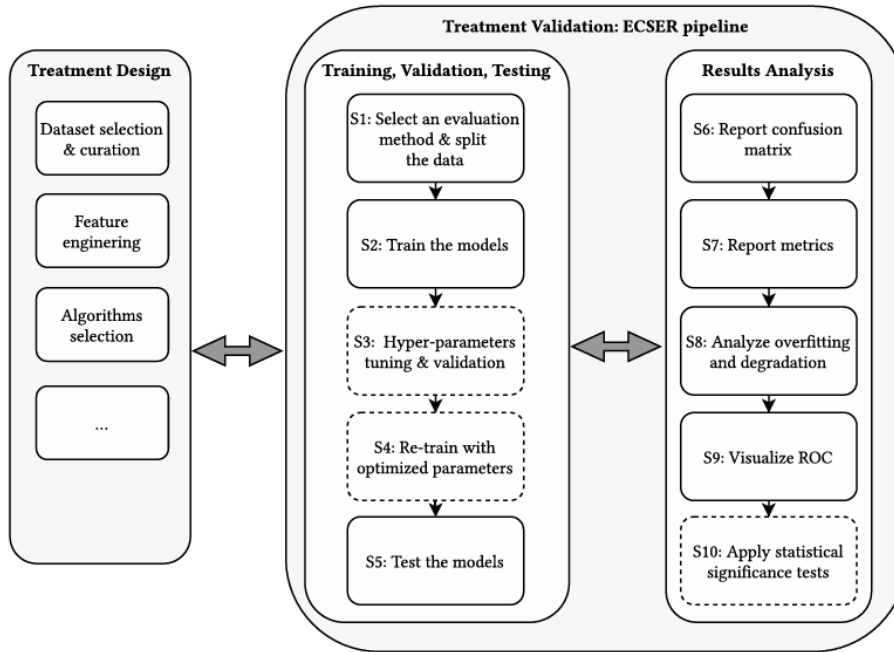
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# 1 Introduction

In recent years, large language models (LLMs) have become an increasingly relevant tool in software engineering (SE), allowing researchers to accomplish complex tasks usually reserved for humans or other machine learning (ML) methods, such as code generation, summarization and classification. However, few guidelines exist for conducting and reporting on LLM research, leaving researchers on their own to decide what choices to make when designing prompts, what evaluation metrics to report in their results and the level of statistical validation needed for their comparisons. Because of these lack of guidelines, researchers using LLMs often omit important details, such as the F1 score or the significance of their results [1]. This problem is not new or unique to LLMs; many researchers have reported that there is a poor standard of empirical software engineering, which inhibits the usefulness of results and impairs reproducibility [2, 3].

To treat the observed poor standard of empirical SE, some researchers have called for a more systematic approach to conducting and evaluating experiments. The ECSER (Evaluating Classifiers in Software Engineering) pipeline, introduced by Dell’Anna et al. [4], provides a systemic pipeline for training, validating and testing ML classifiers and analysing their results. ECSER is based on recommendations from the field of machine learning for software engineering (ML4SE) and is designed to be easy to use for SE researchers, regardless of expertise with machine learning methods. The ECSER pipeline has seen some empirical validation in the form of two replication studies, in requirements engineering and software testing, where Dell’Anna et al. were able to confirm and strengthen some findings, as well as discover additional findings or findings that contradict the original ones. Figure 1 shows the steps of the ECSER pipeline.



**Figure 1** The ECSER pipeline. Reproduced from Dell’Anna et al. [4]. Steps with a dashed border are optional. The  $\leftrightarrow$  arrows indicate feedback loops between phases

However, while ECSER is tailored to traditional ML classifiers (such as logistic regression, SVMs and decision trees), it includes no specific recommendations for LLM-based classifiers, despite LLMs showing

promise for various classification tasks [5, 6]. Thus, the ECSER pipeline is not sufficient for LLM research, since using LLMs for classification comes with unique considerations that are not present for traditional classifiers. For one, it is common to use pre-trained, generalised LLMs and give task-specific instructions to get the desired classification on the input data. This means that designing these instructions, also called prompts, becomes a crucial part to conducting LLM research [7]. There are also unique considerations when it comes to evaluating the fairness and robustness of the results: does the model behave in accordance with human values and are the results resilient to adversarial prompts, such as those containing typos [8, 9]?

The goal of this thesis is to address the lack of LLM-specific guidelines in the ECSER pipeline, by expanding it to include specific recommendations for conducting LLM classifier research. In doing so, we made the following contributions:

- We conducted a mapping study to assess the current state of reporting in LLM4SE classification research.
- We developed the *ECSER-LLM* pipeline, an expanded version of the ECSER pipeline that includes specific recommendations for conducting LLM classifier research, such as prompt engineering and the evaluation of model fairness and robustness.
- We conducted two replication studies of existing LLM classifier papers using the *ECSER-LLM* pipeline, in order to evaluate the pipeline’s applicability and comprehensiveness.

Supplemental materials, including all code that was used, the full intermediary and final results and the source for this document can be found at:

<https://github.com/rubenvdz/Master-Thesis-Enhancing-the-ECSER-pipeline>.

The remainder of this thesis is structured as follows. In Section 2, we provide background information about LLMs. Section 3 describes the research approach and research questions. Lastly, Section 4 discusses related work.

## 2 Background

**Language Models (LMs)** are computational models designed to model the generative likelihood of word sequences [10]. In other words, given a sequence of input text, they predict the next word in the sequence based on what is deemed most likely by the model. One of the oldest examples of language models are N-grams, which model the likelihood of a word given the previous N tokens [11]. Early statistical models like N-gram models suffer from several problems, including limited context and difficulty with unseen words.

**Pre-trained Language Models (PLMs)** are LMs that are designed to take in vast amounts of unannotated text in order to learn knowledge about language and the world [12]. The knowledge that is contained in these models can then be used on new tasks by way of **transfer learning** [13]. PLMs require much more information to be contained within than statistical language models such as N-grams could provide, which has led researchers to design more sophisticated models that rely on neural networks to model language, starting with recurrent neural networks (RNNs) and later Long Short-Term Memory (LSTM) models [14, 15]. The biggest recent breakthrough came with the invention of **transformers**, which performed better than previous models, were easier to train and allowed for the parallel processing of inputs [16]. Transformers typically consist of an **encoder**, which embeds the input sequence into a hidden (latent) space and a **decoder**, which translates the abstract representation of the hidden space to the target text. Both the encoder and decoder use a self-attention mechanism to weigh the contribution of each token to the output [16, 17].

**Large Language Models (LLMs)** were introduced as a way to refer to PLMs with massive parameter sizes,

since it was found that larger parameter sizes lead to better performance and emergent abilities [18, 19]. Almost all LLMs use transformer models with the self-attention mechanism, but not all of them use both the encoder and decoder component [20]:

- **Encoder-decoder LLMs**, such as BART [21] and T5X [22], are good at both understanding and generating language [20]. As such they are useful for tasks like summarization and translation [23, 24].
- **Encoder-only LLMs**, such as BERT and its variants [25–28], are tailored towards language understanding [20]. As such they are good at tasks like classification and inference [29].
- **Decoder-only LLMs**, such as the GPT-series [30–32], are tailored towards language generation [20]. As such they are good at all generation tasks, including code generation [33] and creating conversational agents like ChatGPT [34] and LLama 2 [35].

**Prompt Engineering** is the process of systematically designing natural language instructions (or **prompts**) to guide LLMs towards a desired output [36]. Prompts condition the outputs of the LLM on the given instructions, so that the model generates the next tokens with both the prompt and previously generated tokens in mind [12]. The most common approaches to prompt engineering are:

- **Zero-shot Prompting.** The model is given no examples for a task, forcing it to rely entirely on the prompt [37].
- **Few-shot Prompting.** A limited number of examples for a task are given, which the model can learn from [38].
- **Chain-of-Thought Prompting.** The prompt instructs the model to follow coherent reasoning steps [39].

Another less common approach is automatic prompt engineering, where instructions are automatically generated and selected [40].

### 3 Research Questions

The usage of LLMs in SE research has increased massively over the past few years, but the research of how to best conduct studies and report results in this field remains very limited. In order to approach the problem of LLM4SE reporting standards and design meaningful guidelines, we follow Wieringa’s design cycle of *problem investigation*, *treatment design* and *treatment validation* [41]. This leads us to the following research questions:

#### **RQ1: What is the current state of reporting in LLM4SE classification research?**

RQ1 follows the step of *problem investigation* and is both descriptive and evaluative: what do researchers report in their studies and does this level of reporting contribute or detract from the accuracy and reproducibility of the results. The aim of this question is to provide insights into the potential shortcomings of existing research by conducting a mapping study of the reporting practices of LLM4SE research, in order to provide a basis for additional guidelines that help researchers avoid these shortcomings.

#### **RQ2: What resource can be developed to assist researchers in conducting and reporting on LLM4SE classification research?**

Following the problem investigation of RQ1, RQ2 fulfils the step of *treatment design*. The purpose of RQ2 is to design a tangible artefact that is comprehensive and widely applicable to the field of LLM4SE, with the intent of helping researchers avoid any problems identified in RQ1. This research question was designed to

guide the modification of the existing ECSEER pipeline [4], taking into consideration recommendations from the fields of LLM4SE, ML4SE and Design Science.

### **RQ3: How applicable is the proposed pipeline in assisting LLM4SE classification research?**

The purpose of RQ3 is *treatment validation*: does the designed pipeline in RQ2 achieve its goals of applicability and comprehensiveness. To answer this question we will conduct two replication studies in different subfields of SE that employ LLM classification using the guidelines by Carver [42]. The original studies will be chosen based on the following criteria:

1. The authors provide a ready-to-use replication package.
2. The study is recent (past five years) and represents current practices in LLM4SE well.
3. The study is peer-reviewed and published in a reputable journal.
4. The study does not already follow all the proposed guidelines, so that the added benefit of the pipeline can be evaluated.

By conducting these replication studies, we can evaluate the comprehensiveness of the pipeline and identify potential shortcomings. After the first replication study, the findings from RQ3 were taken into account to make changes to the guidelines from RQ2 where needed, creating a feedback-loop between RQ2 and RQ3. The second replication was conducted using the updated pipeline.

## **4 Related Work**

The main focus of this thesis is to study the usage and evaluation of LLM Classifiers in Software Engineering, but in doing so we touch on several related research fields, including Empirical Software Engineering, Machine Learning for Software Engineering (ML4SE), Large Language Models for Software Engineering (LLM4SE) and Prompt Engineering. Additionally, each of the three research questions has related work that is relevant to their methodologies. Hence, we have split the related work into several sections based on different areas of study to aid readability.

First, we discuss challenges in empirical software engineering which motivated the creation of the ECSEER pipeline and further motivated our mapping study of LLM4SE. Second, we discuss the topic of replication in SE, which is relevant to our replication studies and the field of empirical SE. Third, we discuss how Large Language Models have been used in SE, with a focus on classification tasks. Fourth, we discuss related work in Prompt Engineering, as it has become a vital part to using LLMs and informed our guidelines for prompt engineering in the *ECSEER-LLM* pipeline. Finally, we discuss related work on the evaluation of LLMs and classifiers informed our guidelines for the evaluation of LLM Classifiers.

### **4.1 Challenges in Empirical Software Engineering**

Over the past couple decades, the use of machine learning methods has become ubiquitous in every field of science, among them software engineering. Zhang and Tsai [43] summarized seven main activities that use machine learning in SE: prediction, property/model discovery, transformation, generation, library construction and maintenance, acquisition of specifications and development knowledge management. In addition, they list specific tasks belonging to each activity, such as *predicting* software quality and *generating* test cases. The field of classification research falls almost exclusively in the prediction category.

With the increased popularity of machine learning methods, many software packages have been developed to allow anyone to use these methods without having to write any code or even understand how these methods

work. This leads to many researchers using machine learning without fully understanding the underlying assumptions of the methods they are using and assuming the results are correct without proper (statistical) analysis. This problem is not new: Kitchenham et al. [2] reported at the start of this century that there was a poor standard of empirical software engineering, mostly caused by a lack of statistical expertise from both the authors and reviewers. They go on to provide extensive guidelines for designing and conducting experiments as well as analysing, presenting and interpreting results. In another paper, Kitchenham et al. [44] discuss the benefits of evidence-based software engineering approach by drawing an analogy to evidence-based medicine, but note that the infrastructure needed for widespread adoption of evidence-based SE isn't there yet, which means that SE experiments are vulnerable to subject and experimenter bias.

Methodological problems in SE research can result in problems with the reproducibility of results, which severely reduces the real-world usefulness of said results. Menzies and Shepperd [3] argue that the main goal of science is *conclusion stability*, which means that when you discover an effect, it holds true irrespective of the situation. However, they note that in the software engineering literature there is often as much evidence *for* a given effect, as *against*. This lack of conclusion stability is caused by sources of bias and variance that are introduced at various steps: sampling, pre-processing, training, algorithm selection and the analysis of results. If these sources of bias and variance are accurately analysed and reported, that would make it easier for the authors and other researchers to interpret the conclusions.

Despite being a known issue, the problems of improper analysis and reporting have persisted over the years. In a mapping study of the proceedings of the International Conference of Software Engineering (ICSE) from 2019 to 2021, Dell'Anna et al. [4] analysed 60 SE papers related to classification and found that most papers (36) reported on the precision and recall of their experiment, fewer reported the F-score (27) and accuracy (24), but only 14 papers explicitly justified why they chose the reported metrics. The full confusion matrix was only included in six papers. Other metrics like the receiver operator characteristic (ROC) curve and the area under the curve (AUC) were mostly absent with 3 and 9 respective mentions. Of course, as we know from statistics, it is not enough to report a metric and claim it's better than that of other models, since it could be coincidental, so statistical significance testing is required to make such claims. However, only six papers analysed the statistical significance of their results. Evidently, the situation is dire, which is why Dell'Anna et al. developed the ECSER pipeline to give SE researchers a systematic approach to conducting classification experiments and reporting and analysing the results.

## 4.2 Replications in SE

Replication studies are a vital part of empirical software engineering, allowing researchers to investigate the effects of alternative values for important attributes, vary the strategy with which hypotheses are investigated and make up for certain threats to validity [45]. The importance of replication is not unique to software engineering, after all the so-called "replication crisis" was a massive topic of debate in psychology research in recent years, since it was found that many previous results in the field could not be replicated, even if the original findings were statistically significant [46–48]. Cruz et al. [49] conducted a systematic literature review of replication studies in SE between 2013 and 2018 and found that the number of published replication studies has been steadily increasing, though there are research gaps in certain fields, suggesting that the SE community is taking an increased interest in replicating previous studies.

Shull et al. [50] identify two types of replication studies: *exact replications*, in which the procedures of the original study are strictly followed; and *conceptual replications*, in which the research problem of the original study is evaluated using a different procedure. Additionally, exact replications are subdivided into *dependent* and *independent* replications. Dependent replications keep most of the conditions of the experiment (close to) the same, which allows one to test the effect of specific variables on the results; whereas independent

replications vary the original conditions of the experiment significantly, which allows one to test the robustness of the original results under different conditions. Juristo and Vegas [51] underline the value of non-exact replications, which they define similarly to how Shull et al. define independent exact replications, by conducting a multiple-case replication study using a newly proposed four-phase process, to show that non-identical replications can be used to learn new information about the original results.

While there is a consensus in SE that replication is important, Shepperd et al. [52] show that replication studies often suffer from the same problems as original studies, such as incomplete reporting, low power or potential researcher bias. Notably, many replication studies in their survey did not report any details on the dispersion (e.g., variance) of the response variables. In another paper, Shepperd [53] shows that because of wide prediction intervals, almost all replications are confirmatory, which means the added knowledge is negligible. Because of these problems, they suggest that researchers should focus more on broader meta-analyses instead of replication studies. Other common problems in conducting replication research include difficulty in getting them published, lack of guidelines and the unavailability of replication packages [49, 54].

Communication can also play a factor in successful replication: Vegas et al. [55] investigated the role of communication in successful replication of previous experiments and found that there should be some level of communication, orally or in writing, between the previous authors and authors of the replication study, to avoid unnecessary changes to the experiments.

Given these challenges, guidelines for conducting replications are clearly needed. Despite this, the number of existing guidelines remains low. Guidelines were proposed by Carver [42], which are still commonly used in replications, but these seem to be the only replication guidelines for software engineering and were intended as a starting point for future guidelines. Other artifacts do exist to aid replications: Gómez et al. [56] proposed a classification of replications in SE, differentiating between literal, operational and conceptual replications, that can be used to identify which changes can be made in each type of replication and understand the level or verification needed for that type.

Abualhaija et al. [57] proposed an artifact, referred to as the ID-Card, for summarizing papers in RE research that use NLP techniques. The intention behind the ID-Card is that all the relevant information needed for replication is presented in an easy to read format and can be used for both replication and educational purposes. Lastly, Brandt et al. [58] developed the "Replication Recipe" for psychology research, which lists 36 questions that should be addressed when conducting a replication, most of which are also directly applicable to empirical SE.

### 4.3 Large Language Models for SE

A recent development in SE research is the increased relevance and use of LLMs. Fan et al. [59] looked at all preprints on arXiv categorised under computer science whose title included "LLM", "Large Language Model" or "GPT" and found the number of SE papers that mentioned LLMs grew exponentially from 0 in 2019, 5 in 2020, to 181 in 2023. Naturally, this is only an approximation of the total number of preprints on arXiv that use LLMs, but it undoubtedly signifies a substantial increase. Fan et al. also conducted an extensive survey of how LLMs have been applied to various software development activities (such as code generation and testing) and research domains (such as human-computer interaction and education), but the survey is almost exclusively focused on the generative use of LLMs and does not go into depth on the use of LLMs in classification research. Many other good surveys and analyses of the use of LLMs in Software Engineering have been written, but most of them similarly do not mention any applications to classification tasks and instead exclusively focus on generation [60–62].

Surveys have also been written about specific domains of software engineering: Wang et al. [63] did a com-



prehensive review of 102 studies that use LLMs for software testing and found that LLMs have commonly been applied to various tasks, including test case generation, test input generation, debugging, program repair and more. They also found that while most papers used LLMs to address the entire task, many others combined LLMs with additional techniques to optimize the outputs of the LLM, including mutation testing, differential testing, syntactic checking, program analysis, statistical analysis and other techniques. With these extra techniques, researchers were able to generate more diverse and complex code and overcome some of the limitations of LLMs.

While LLMs are most frequently used to generate text (and code), they have seen considerable success in classification tasks. Guo et al. [5] have shown that LLMs can outperform other methods like SVMs for health-related text classification. Fields et al. [6] present an in-depth survey of text classification using transformers across domains and found that LLMs can perform remarkably well on many (but not all) classification tasks. However, Chen et al. [64] compared the performance of various LLMs to traditional ML methods in clinical prediction and found that LLMs could *not* beat traditional methods in this case. Vajjala and Shimangaud [65] also show that there are large performance disparities between languages in classification tasks. Thus, LLMs might not always be a better choice than traditional ML methods, but they certainly show potential.

Software engineers have also started using LLMs for classification. Hou et al. [20] conducted a systematic literature review of 395 software engineering studies that use LLMs and found that around 21.61% involve classification tasks. The most common classification tasks where LLMs have been used include vulnerability detection, requirements classification, bug prediction and review/commit/code classification, with many other classification tasks having been attempted using LLMs. Zhang et al. [66] conducted a systematic survey of 947 SE studies and summarized 62 unique LLMs of code, including six LLMs specifically fine-tuned for the tasks of code classification, clone detection and defect detection.

Recently, Baltes et al. [67] presented a list of community-driven guidelines for using and reporting on LLMs, providing eight detailed guidelines. These guidelines include: (1) declaring LLM usage and role; (2) reporting model versions, configurations and fine-tuning; (3) documenting tool architectures; (4) disclosing prompts and interaction logs; (5) using human validation; (6) employing an open LLM as baseline; (7) using suitable baselines, benchmarks and metrics; and (8) openly articulating limitations and mitigations. These guidelines were designed to increase the transparency and reproducibility of LLM research and are actively maintained on <https://llm-guidelines.org/>. The guidelines in this thesis serve a similar purpose of helping researchers conduct LLM4SE research; however, their guidelines have a broader focus, since they include all LLM applications, whereas our guidelines are specifically tailored to classification research. Furthermore, unlike their paper, this thesis also includes a mapping study to assess the state of LLM4SE classification reporting and provides a replication study to evaluate the guidelines. Despite the difference in scope, many of their recommendations directly apply to our research and were taken into account for the *ECSE-LLM* pipeline where relevant.

## 4.4 Prompt Engineering

Designing a good prompt for a particular task is vital to ensuring the adequate performance of LLMs, which is why much research has gone into the systematic designing of prompts, or prompt engineering. Marvin et al. [7] provide an overview of prompt engineering principles and techniques and outline the main steps involved in the process of prompt engineering: 1) define the goal of the prompt; 2) understand the model’s capabilities; 3) choose the right prompting format; 4) provide context to the LLM and 5) test and refine the prompt based on the goal. Several resources exist to make it easier to choose the right prompting approach: White et al. [68] introduce prompt patterns, which offer reusable solutions to common prompting challenges, and provide a framework for designing and documenting these patterns in terms of the intent, motivation, structure and

consequences of the patterns. For example, the persona pattern can be used to make the LLM take the point of view of an expert in the field, which is especially useful if the user itself is not an expert. The paper provides a catalogue of this pattern and other successfully applied patterns with example implementations. Further, Ekin [69] provides an accessible (AI-generated) guide to prompt engineering.

Prompt engineering is an important consideration when using LLMs: Sclar et al. [70] show that choices in prompt design, even if minor, can have a very large impact on the performance of several popular LLMs, and this sensitivity is present regardless of the size of the model or the number of examples provided. Because of this, they argue that researchers should forego using only a single prompt and switch to reporting the performance of their models using multiple plausible prompt patterns. They present a novel algorithm, FormatSpread, to evaluate multiple prompts at the same time and measure the sensitivity of the LLM. Mizrahi et al. [71] have found a similar sensitivity of LLMs to prompt design and discuss metrics to evaluate multiple prompts. Lastly, Maia Polo et al. [72] propose PromptEval, an efficient method for evaluating a large number of prompts, and show it can accurately estimate the performance distribution of the prompts.

Prompt engineering research has also been conducted specifically for software engineering: Hou et al. [20] looked at what prompt engineering techniques are commonly applied in SE tasks and found the most common techniques involve few-shot prompting and zero-shot prompting, but the third largest group of studies had no explicit mention of prompting techniques or proposed their own strategies. Other techniques included chain-of-thought, automatic prompt engineering, chain-of-code, automatic chain-of-thought, modular-of-thought and structured chain-of-thought.

Arvidsson and Axell [73] collected prompt engineering recommendations for requirements engineering (RE) in a systematic literature review and classified the guidelines into various themes, after which they interviewed three RE experts to evaluate the guidelines. Ronanki et al. [36] evaluated the effectiveness of 5 prompting patterns (from the catalogue by White et al. [68]) on two RE tasks and proposed a framework for evaluating the effectiveness of prompting patterns for any RE task, providing five steps for conducting a comparison of patterns.

A recent development in prompt engineering is automatic prompt engineering (APE), which has shown good performance compared to baseline models, while avoiding the need for manually designing prompts [40, 74]. Zadenoori et al. [75] investigated the use of automatic prompt engineering in RE and found that, on average, APE outperforms traditional prompt engineering techniques. However, research is still limited.

## 4.5 Evaluating LLM Classifiers

Few papers have been written specifically about the evaluation of LLM-based classifiers, but we can look at the evaluation of classifiers and LLMs separately to get a picture. The ECSER pipeline is the most relevant for evaluating classifiers, since it gives in-depth recommendations about the conducting and reporting of classifier research [4]. Specific recommendations include the reporting of the full confusion matrix, reporting other metrics relevant to the domain such as specificity (true negative rate), analysing overfitting and degradation, visualising the ROC and applying statistical significance tests. Some researchers also recommend reporting the Matthews correlation coefficient (MCC), which combines all four metrics of the confusion matrix and can be more informative than the F1 score [76–78].

Hou et al. [20] looked at whether these metrics were reported in LLM-based classification research and found that out of 147 papers that use LLMs for classification, the most frequently reported metric is precision with 35 papers, followed by recall (34), F1-score (33) and accuracy (23), but the AUC was reported 9 times, the ROC only 4 times and the MCC only twice. Unfortunately, they did not count how many studies did significance testing. These results are very similar to Dell’Anna et al. [4]’s aforementioned mapping study

of classifier research as a whole and suggest that many important metrics are under-reported in LLM-based classification research.

Using and evaluating LLMs comes with more considerations than just the accuracy of the results. Guo et al. [1] categorize the evaluation of LLMs into three types: knowledge and capability evaluation, which assesses the fundamental knowledge and reasoning capabilities of the LLM; alignment evaluation, which refers to evaluating ethical and moral considerations like bias; and safety evaluation, which focuses on the robustness of LLMs and risk evaluation. Liu et al. [79] have created guidelines specifically for evaluating LLM alignment in terms of reliability, safety, fairness, resistance to misuse, explainability and reasoning, adherence to social norms and robustness.

Another consideration is how well the LLM outputs adhere to the format specified in the prompt. For example, it is common to ask an LLM to format its answer as a valid JSON object, allowing for easier processing of the output. Limiting responses to a specified format can be beneficial: Tam et al. [80] compared the performance of several LLMs between free-form response and formatted responses and found that, while reasoning ability was weakened for formatted responses, classification accuracy was increased. However, LLMs do not always follow the format accurately. Long et al. [81] define several measures to analyse the level of adherence to the output format: SysE, which measures the performance of the LLM for answers that *meet the constraint*; TrueE, which measures the performance of all answers *regardless of whether the format is satisfied*; and BiasF, which measures the (mean squared) difference between SysE and TrueE. Li et al. [82] introduce the JScore measure, which measures the similarity between JSON objects and can be used to compare LLM generated JSON objects with the target JSON objects. Lastly, Xia et al. [83] introduce the FoFo benchmark for evaluating LLMs based on their ability to follow complex, domain-specific formats.

Chang et al. [84] conducted another survey of the evaluation of LLMs which focuses on downstream applications, resulting in a classification of four aspects of LLM evaluation: the accuracy, containing measures of correctness such as the F1 score; the calibration, which contains measures for the degree of alignment between the predicted probabilities and actual probabilities, such as the expected calibration error (ECE); the fairness, with measures pertaining to the equal treatment of different groups, such as the equalized odds difference (EOD); and robustness, with measures pertaining to the performance of a model in the face of challenging inputs and noise, such as performance drop rate (PDR). Further, they mention several ways in which human evaluation can be used to evaluate LLMs, such as the degree to which the model outputs align with human values.

Lastly, the model temperature, which regulates the randomness of the model, can also affect its performance. Peeperkorn et al. [85] looked at the effect of model temperature on the level of creativity of the outputs and found that LLMs generate slightly more novel outputs with higher temperature, but the temperature was also correlated with incoherence. No relationship was found between temperature and cohesion or typicality. Model temperature might also affect a model’s susceptibility to security attacks: Yu et al. [86] found that some LLMs became more susceptible to jailbreaking attacks as temperature increased, whereas others had decreased susceptibility to jailbreaking with increased temperature, possibly due to the fact that the former models had a lower susceptibility at 0 temperature and the latter models had a higher susceptibility at 0 temperature.

## **5 RQ1: What is the current state of reporting in LLM4SE classification research?**

In this section, we first discuss the methodology used to conduct a systematic mapping study on the state of reporting of LLM4SE classification research. Subsequently, we discuss the results from the mapping study

and draw conclusions from these results.

## 5.1 Research Approach

To answer the research question, we conducted a mapping study of SE papers published in 2024 that use LLM classifiers using the guidelines by Kitchenham et al. [87, 88] and Petersen et al. [89], consisting of five steps:

1. Define the research question.
2. Conduct a search for primary studies.
3. Screen papers based on inclusion/exclusion criteria.
4. Classify the papers.
5. Extract data.

What follows is a detailed summary of the search strategy (steps 2 and 3) and the information that was obtained from the list of relevant papers (steps 4 and 5).

### Search Strategy

To get a complete image of the state of LLM4SE classifier evaluation, we collected all 528 papers published in 2024 in three of the top SE conferences and journals (Table 1). These venues were narrowed down from the list of venues included in [20] based on their impact and relevance. Using the full list of 528 papers, an automatic keyword search was conducted on the title and abstract of each paper to identify the papers that were potentially relevant to LLM4SE.

The list of keywords was based on previous research ([20, 66]) and designed with the intent of high recall, since it is easier to remove false positives than to retrieve false negatives. Keyword matching was done on the lowercased versions of the title and abstract and allowed for partial matches (e.g., "llm" matches "LLM", "LLMs", "LLM4SE", etc.). The complete list of keywords is as follows:

- *llm, large language model, language model, code generation model, plm, pre-trained, pretrained, pre-training, pretraining, chatgpt, gpt, bert, t5, llama, bart.*

The keyword search resulted in 129 potentially relevant papers. After manually removing false positives, mostly caused by the authors comparing their non-LLM model to previous LLM models, the total number of identified LLM4SE papers was 116, representing 21.97% of total SE papers.

To narrow down the list from all LLM-related papers to those pertaining to SE classification research, the title and abstract of the remaining 116 papers were manually screened for the inclusion and exclusion criteria (Table 2). These criteria were designed to exclude any paper not relevant for answering the research question, such as meta studies and those not related to classification. During the manual search, 18 papers were identified that use LLMs for SE classification research and satisfy all other criteria.

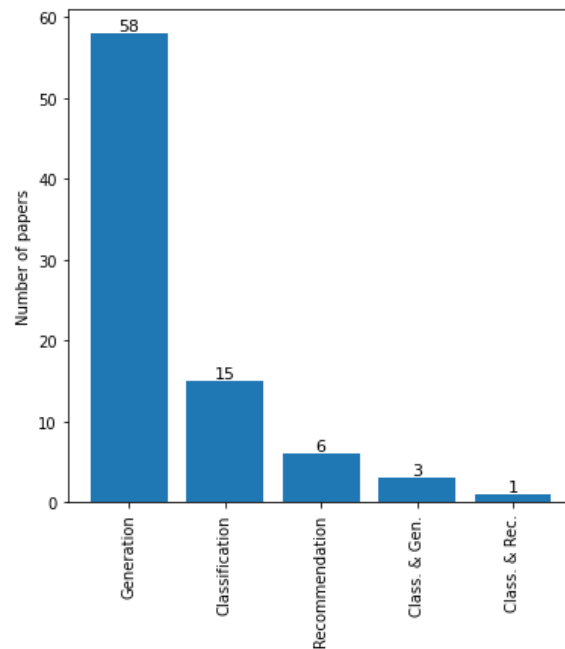
**Table 1** Publication venues included in the mapping study.

| Acronym | Venue                                                               |
|---------|---------------------------------------------------------------------|
| ICSE    | International Conference on Software Engineering                    |
| FSE     | International Conference on the Foundations of Software Engineering |
| TSE     | Transactions on Software Engineering                                |

**Table 2** Inclusion/Exclusion Criteria

|                                                                       |
|-----------------------------------------------------------------------|
| <b>Inclusion Criteria</b>                                             |
| The paper uses an LLM.                                                |
| The paper focuses on a downstream application of the LLM.             |
| The downstream application is a SE classification task.               |
| The full text of the paper is accessible.                             |
| The paper was published in 2024.                                      |
| <b>Exclusion Criteria</b>                                             |
| The paper focuses on LLM architecture with no downstream application. |
| The paper or task is not relevant to SE.                              |
| The full text is inaccessible.                                        |
| The paper is a survey or other meta-analysis.                         |
| The paper focuses on research methodology.                            |
| The paper is a reprint or different version of another paper.         |

While only classification papers were included in the final analysis, all the papers that applied LLMs to SE tasks (a total of 83 papers) were additionally classified based on the type of LLM application (classification, generation or recommendation) to get a view of the relative academic interest in each type (Figure 2). As can be seen, LLMs are most often used for generation, with 73.5% of papers using them in this way, including some that use generation alongside classification. However, classification represents the second largest application of LLMs, with 22.9% in total. Appendix A contains references for Figure 2 and other pie charts contained in this thesis.

**Figure 2** Distribution of LLM application types in collected studies.

### Information Extraction

After completing the manual search and obtaining 18 relevant LLM4SE classification papers, the evaluation

and reporting practices of each paper were manually analysed and recorded. The information that was extracted from the papers was determined based on what is recommended to be included by the ECSEER pipeline [4], metrics that are recommended by other authors (such as the Matthews correlation coefficient [76–78]) and recommendations from the field of LLM4SE. For the latter, we recorded which metrics (if any) were reported for each of Chang et al. [84]’s classification of general metrics: the accuracy, calibration, fairness & robustness. Since the accuracy was already covered by the ECSEER pipeline, this resulted only in the addition of calibration, fairness & robustness to the final list of extracted information.

The calibration of an LLM refers to how well the predicted probabilities of the model align with actual probabilities [92, 93]. Evaluating the fairness of an LLM is done to ensure the alignment of LLM results with human values and prevent a difference in performance across groups of people [79]. The robustness refers to the performance of a model in the face of challenging inputs and can be analysed in several ways, including by making changes in the data distribution, the addition of noise to the data, and adversarial attacks [84].

In total, the following list of evaluation metrics or evaluation metric types were added: *precision*, *recall*, *accuracy*, *F-score*, *Area under curve (AUC)*, *Matthews correlation coefficient (MCC)*, *Confusion matrix*, *Receiver Operation Characteristic (ROC) plot*, *Calibration*, *Fairness* and *Robustness*.

Further, we looked at several factors related to the reproducibility and generalisation of results, particularly whether justification was given for why the chosen evaluation metrics were used, whether results were obtained for multiple datasets, whether the results were compared to external baselines and whether the statistical significance was analysed and the choice of significance test justified.

Lastly, for the papers that used a prompt-based approach for classification, we analysed whether the prompt approach and final prompt text were reported and justified, whether the results were evaluated over multiple prompts and whether the temperatures of the models were reported.

## 5.2 Mapping Study Results



**Figure 3** Distribution of venues in mapping study.



**Figure 4** Distribution of prompt usage in mapping study.

During the search process, 18 papers were identified as relevant for answering the research question. Each venue included in the search strategy is represented in the final selection, with eight ICSE papers, eight TSE

papers and two FSE papers (Figure 3). By including papers from three of the most influential Software Engineering venues, we increase the likelihood that the results are representative of the field.

One of the first things we analysed was whether the papers used a prompt-based approach to LLM classification or another approach such as fine-tuning, since additional information about the prompt engineering approach was extracted from the papers where prompts were used. Figure 4 shows that 44.4% or 8 papers used a prompt-based approach, while 55.6% or 10 papers used a different approach. Note that additional references for the figures and the subsequent tables are included in Appendix A.

**Table 3** Summary of mapping study results.

| Category                                      | Total      |
|-----------------------------------------------|------------|
| Total mapping study papers                    | 18         |
| <b>Evaluation metrics</b>                     |            |
| Precision                                     | 17 (94.4%) |
| Recall                                        | 17 (94.4%) |
| Accuracy                                      | 11 (61.1%) |
| F-Score                                       | 17 (94.4%) |
| AUC                                           | 3 (16.7%)  |
| ROC plots                                     | 0 (0.0%)   |
| MCC                                           | 0 (0.0%)   |
| <b>Calibration</b>                            | 0 (0.0%)   |
| <b>Fairness</b>                               | 0 (0.0%)   |
| <b>Robustness</b>                             |            |
| Data distribution & Adversarial Attacks       | 1 (5.5%)   |
| Noisy data                                    | 1 (5.5%)   |
| <b>Metrics justification</b>                  |            |
| No                                            | 9 (50.0%)  |
| Implicit                                      | 0 (0.0%)   |
| Previous work                                 | 5 (27.8%)  |
| Yes                                           | 4 (22.2%)  |
| Confusion matrix                              | 4 (22.2%)  |
| Evaluation over multiple data sets            | 5 (27.8%)  |
| <b>Type of baseline</b>                       |            |
| None                                          | 2 (11.1%)  |
| Own                                           | 3 (16.7%)  |
| External                                      | 4 (22.2%)  |
| External and Own                              | 9 (50.0%)  |
| Analysis of statistical significance          | 5 (27.8%)  |
| <b>Statistical significance justification</b> |            |
| No                                            | 4 (80.0%)  |
| Implicit                                      | 0 (0.0%)   |
| Previous work                                 | 1 (20.0%)  |
| Yes                                           | 0 (0.0%)   |

Table 3 shows a summary of the information that was extracted from each paper and how many papers reported each piece of information. This includes which evaluation metrics were reported; whether the calibration, fairness and robustness of the models were analysed; whether the confusion matrix was reported; the

level of justification for the reported metrics; whether the models were evaluated over multiple data sets; the type of baseline used; and whether the statistical significance of the results was reported and justified.

Starting with the evaluation metrics that are recommended by the ECSEER pipeline [4], 17 papers reported the precision, recall and F-score of the results, while only 11 papers reported the accuracy and only four papers reported the full confusion matrix. Although less known, some authors also recommend reporting the Matthews Correlation Coefficient (MCC), since it takes the full confusion matrix into account and might therefore give a more balanced representation of the results than the F-score [76], but it was not reported in any of the papers. Further, the AUC, which some researchers consider to be a theoretically and empirically better metric for comparing classification models than the accuracy [90, 91], was reported in only three papers, while none provided a plot of the full ROC curve.

Apart from metrics related to the correctness of the classification results, we extracted three other types of LLM evaluation that are frequently used: the calibration, fairness and robustness [84]. None of the papers reported measures of the calibration or fairness of the LLMs. Only two papers tested the robustness of their models in one or more of these ways; one looked at both altering the data distribution as well as adversarial attacks and the other looked at the effect of noisy data. However, some papers tested something similar to robustness by performing ablation studies, which work by removing parts of the model to see the impact on the performance, which allows one to assess whether the model exhibits graceful degradation [94]. Ablation studies were not initially included in the mapping study but after seeing their successful implementation were added to the *ECSEER-LLM* pipeline as an optional step.

We also looked at whether justifications were provided in the papers for the selection of metrics they chose to include or exclude from the results and whether these justifications went beyond referring to previous research, which runs the risk of bad habits propagating through the field [4]. Only nine papers included a justification for their choice of metrics, with five of those exclusively referring to previous research as a justification, while four provided a more elaborate explanation.

Lastly, we looked at methodological information about the evaluation and comparison of models and found that only five papers evaluated their models over multiple data sets. Further, 13 papers compared their results to external baselines (nine of which compared to both external and their own baselines), though three papers only compared the results to their own baselines and two papers made no comparisons.

Despite almost all papers comparing their results to their own baselines or other research and usually making explicit claims about the superior performance of their models, only five papers did any statistical significance testing on their results. Some papers even claimed their results show a *significant* improvement despite not doing or not reporting on the significance testing. Further, of the five papers that did a statistical analysis of the results, only one justified the statistical test that was chosen, by referring to previous research.



**Table 4** Summary of prompt reporting results in the mapping study.

| Category                                 | Total      |
|------------------------------------------|------------|
| Total prompt-based classification papers | 8          |
| <b>Prompt approach</b>                   |            |
| Chain-of-verification                    | 1 (12.5%)  |
| Few-shot                                 | 2 (25.0%)  |
| Mimic-in-the-background                  | 1 (12.5%)  |
| Not reported                             | 1 (12.5%)  |
| Zero-shot                                | 3 (37.5%)  |
| <b>Final prompt</b>                      |            |
| Not reported                             | 2 (25.0%)  |
| Own                                      | 6 (75.0%)  |
| <b>Prompt approach justification</b>     |            |
| No                                       | 5 (62.5%)  |
| Yes                                      | 3 (37.5%)  |
| <b>Final prompt justification</b>        |            |
| No                                       | 4 (50.0%)  |
| Previous Work                            | 1 (12.5%)  |
| Yes                                      | 3 (37.5%)  |
| <b>Evaluation over multiple prompts</b>  |            |
| No                                       | 8 (100.0%) |
| <b>Temperature</b>                       |            |
| No                                       | 7 (87.5%)  |
| Yes                                      | 1 (12.5%)  |

Eight of the papers used prompting to obtain results from pre-trained LLMs, which comes with additional considerations and challenges, such as what prompt approach to use (few-shot, zero-shot, etc.) and how to effectively write the text of the prompt. Table 4 shows a summary of the reported prompting information of the papers that used prompts in the mapping study.

Firstly, papers used various prompt design approaches; one used chain-of-verification, two used few-shot, one used a novel approach called mimic-in-the-background, three used zero-shot prompting, and one paper failed to report the prompt approach used or didn’t use a systematic approach. However, only three papers provided justification for the chosen prompt approach.

Secondly, the final prompt, which refers to the actual prompt text used with possible placeholder values for data insertion, was only reported in six out of eight papers. Further, the authors of the six papers that provided the prompt wrote the prompts themselves without consulting established patterns, which means there is no prior evidence of the efficacy of the prompt pattern. Only four papers provided a justification for how the prompt was designed, one of which referred to previous work.

The performance of LLMs can be heavily impacted by minor changes in the prompt design, which is why Sclar et al. [70] recommend comparing multiple plausible prompts. However, none of the papers evaluated the performance of their models using multiple prompts, which leaves the vulnerability of the models to prompt variability unknown. Lastly, only one paper reported the temperature used for the LLM, despite this parameter having a potential impact on the performance of LLMs [85].

## Conclusion

Evidently, the results confirm a pattern of incomplete reporting and unsubstantiated claims similar to that

found previously in the fields of ML4SE [4] and LLM4SE [20]. Metrics such as the AUC, ROC plots, the MCC, the full confusion matrix and metrics related to the calibration, fairness and robustness of LLMs go completely or almost completely unreported.

Since none of the included papers seemingly involve human participants or sensitive applications, this could be a valid reason for not evaluating the fairness, but these considerations are not discussed in any of the papers, nor do the papers explain the absence of calibration and robustness metrics.

Even when metrics *are* reported, there is often no explanation as to the why the metrics were chosen for the specific tasks. Further, many papers only use one data set and sometimes make no comparisons to external baselines. Further, many papers make unsubstantiated claims about the relative performance of their models without significant statistical backing and when significance testing is performed, little explanation is given to the choice of test and significance threshold.

For papers that use prompts for LLM classification, there is often little to no explanation for the chosen prompt approach and the design of the final prompt. Further, the prompt texts are generally not based on established patterns with empirical backing, but designed without a systematic approach. Lastly, none of the papers evaluated multiple prompts to avoid the potential sensitivity of LLMs to minor changes in wording, and the temperature of LLMs goes largely unreported as well.

Naturally, although multiple venues were considered and all papers from 2024 were considered from these venues, these results are still based on a limited set of papers. However, the results align with findings from a large base of previous research [1–4, 20], so it is not unexpected to find similar problems here, especially since there are still very few guidelines for conducting LLM research.

In conclusion, there is a clear need for easy to use and comprehensive guidelines to aid researchers in conducting LLM4SE classification research, especially for statistical significance testing and prompt engineering. We designed the *ECSER-LLM* pipeline (section 6) to take into account the mentioned common shortcomings of existing research and provide extra attention to these topics.

## **6 RQ2: What resource can be developed to assist researchers in conducting and reporting on LLM4SE classification research?**

In this section, we first discuss the approach that was used to modify the *ECSER* pipeline with recommendations tailored to the conducting and reporting of LLM4SE classification research. Subsequently, we present the *ECSER-LLM* pipeline, which features a step by step guide to the implementation and results reporting of LLM-based classification research.

### **6.1 Research Approach**

To answer the research question, we developed the *ECSER-LLM* pipeline by enhancing the existing *ECSER* pipeline to include the use of LLMs, taking into consideration recommendations from the fields of LLM4SE and ML4SE, as well as relevant statistical or methodological research in other fields (see section 4).

The *ECSER* pipeline was chosen as the basis for the development of a new LLM-specific resource, since most *ECSER* recommendations apply to all classification research, including LLM-based classification [4]. However, using LLMs comes with additional challenges that weren't considered during the development of the original pipeline, such as the use of prompts to guide pre-trained LLMs or the alignment of LLM behaviour with human values [79].

To enhance the ECSEER pipeline with LLM-specific recommendations, we consulted various existing guidelines and surveys for using and evaluating LLMs, including Hou et al. [20]’s systematic literature review of LLM4SE, Chang et al. [84]’s survey on the evaluation of LLMs, Marvin et al. [7]’s chapter on prompt engineering and Baltes et al. [67]’s guidelines for using LLMs in SE, among many others. These higher level sources lead to more specific sources and recommendations that were included in the pipeline.

Additionally, the results of RQ1 were taken into account to ensure that common issues encountered in the mapping study received additional care in the new pipeline, including issues such as the lack of reporting for common evaluation metrics, the lack of significance testing and the lack of consistent reporting for prompt usage and development. The results of RQ1 also lead to the inclusion of ablation studies as an optional part of the pipeline, which were overlooked during the initial literature review but were shown to be useful in assessing the degradation of the models in the papers that used them [94].

In Table 5, we list each step of the original ECSEER pipeline along with the new version of the step and the major changes that were made in the new *ECSEER-LLM* pipeline, along with the primary source(s) that motivated these changes. Minor changes are not included in the table.

**Table 5** Summary of changes and additions to the ECSEER pipeline.

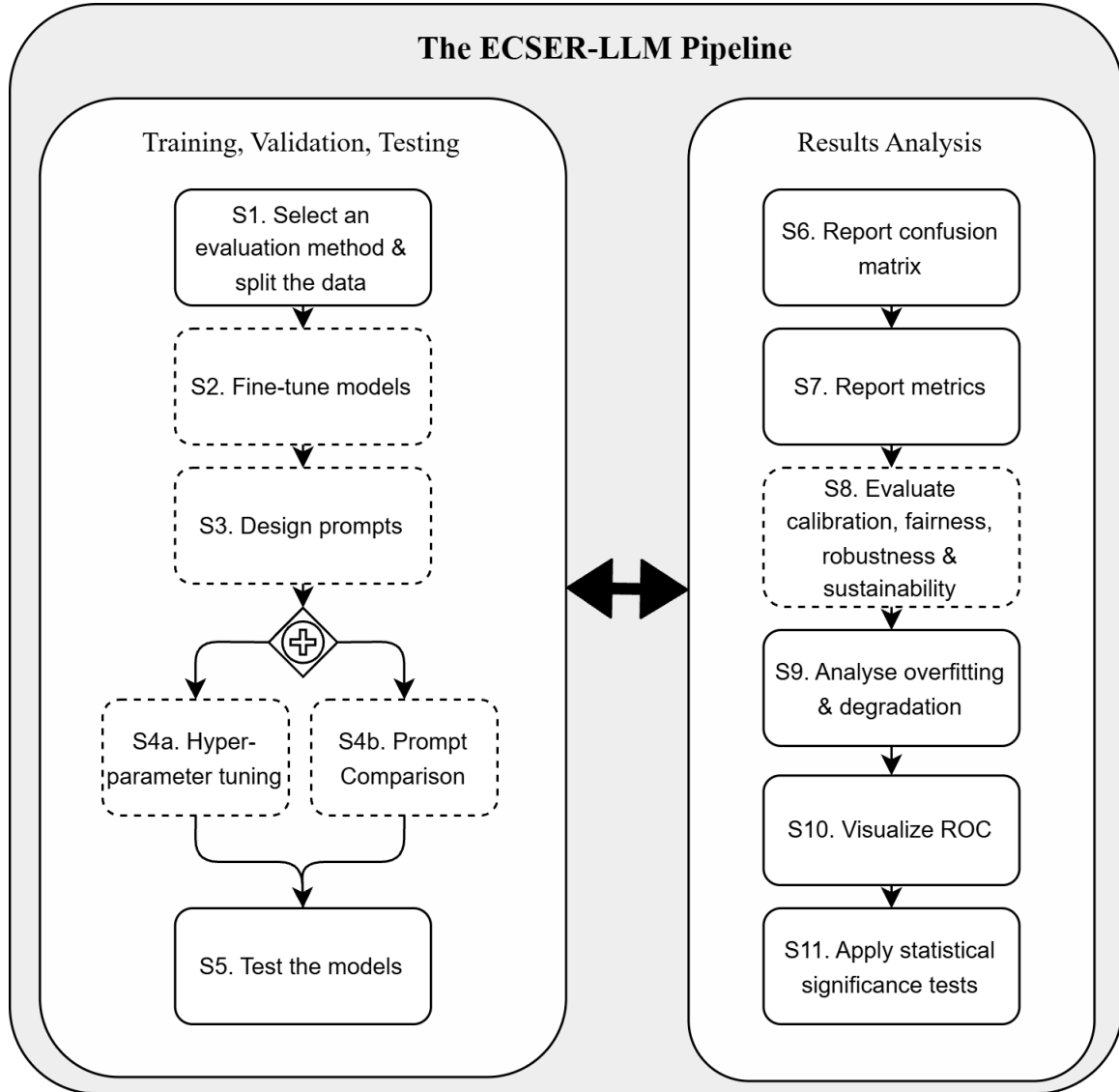
| <b><i>ECSEER</i> Step</b>                           | <b><i>ECSEER-LLM</i> Step</b>                                    | <b>Changes from <i>ECSEER</i> to <i>ECSEER-LLM</i></b>                                                                          |
|-----------------------------------------------------|------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| S1. Select an evaluation method and split the data. | S1. Select an evaluation method and split the data.              | Add specification of desired level of model alignment and safety [1].                                                           |
| S2. Train the model.                                | S2. Fine-tune the model                                          | Change focus to fine-tuning LLMs.<br>Add reporting of LLM configuration and interaction [67].                                   |
| -                                                   | S3. Design Prompts.                                              | Add prompt engineering guidelines [7, 73].<br>Add reporting of LLM configuration and interaction [67].                          |
| S3. Hyper-parameter tuning & validation.            | S4a. Hyper-parameter tuning                                      | Tune LLM model temperature and other hyper-parameters [67, 85].                                                                 |
| -                                                   | S4b. Prompt comparison.                                          | Compare similar prompts [36].<br>Report prompt revisions and LLM interaction logs [67]                                          |
| S4. Re-train with optimized parameters.             | -                                                                | Merged into S4a.                                                                                                                |
| S5. Test the models.                                | S5. Test the models.                                             | -                                                                                                                               |
| S6. Report confusion matrix.                        | S6. Report confusion matrix.                                     | -                                                                                                                               |
| S7. Report Metrics.                                 | S7. Report Metrics.                                              | Report Matthews Correlation Coefficient (MCC) [76–78]                                                                           |
| -                                                   | S8. Evaluate calibration, fairness, robustness & sustainability. | New step that includes guidelines on how to evaluate the calibration, fairness, robustness and sustainability of LLMs [79, 84]. |
| S8. Analyse overfitting and degradation.            | S9. Analyse overfitting and degradation.                         | Conduct ablation studies [94].                                                                                                  |
| S9. Visualize ROC.                                  | S10. Visualize ROC.                                              | -                                                                                                                               |
| S10. Apply statistical significance tests.          | S11. Apply statistical significance tests.                       | Justify the significance test and significance threshold [95, 96].                                                              |

## 6.2 The *ECSEER-LLM* Pipeline

In this section we present the *ECSEER-LLM* pipeline, a step-by-step guideline for SE researchers to conduct classification experiments using LLMs and evaluate the results, which serves to provide an answer to the research question. The pipeline encompasses the *treatment validation* step of Wieringa [41]’s design cycle, which happens after the *treatment design* step. Steps belonging to the *treatment design*, such as feature engineering and algorithms selection, are out of scope of the pipeline.

Figure 5 shows the full pipeline, consisting of 11 steps divided into two macro activities: (1) training, validation and testing and (2) results analysis. The steps are shown consecutively, but it is always possible to return to previous steps. For example, after finding optimal hyper-parameters in S4, one will likely return to S2 to retrain the models with these parameters. Further, there is a possible feedback loop between macro activities, including the *treatment design*. For example, when it is found that the model shows signs of overfitting (S9), one can reconsider the algorithms used (*treatment design*) or increase regularization (S2).

Some steps are marked as optional with a dashed border, since they depend on the *treatment design* or other considerations such as time and space constraints. In particular, when using a pre-trained LLM without fine-tuning, S2 (Fine-tuning) becomes obsolete since no training is performed, and when *not* using prompts to guide LLM outputs, S3 (Design prompts) and S4b (Prompt comparison) become obsolete since they provide guidelines for using prompts. Lastly, S4 is split into two steps: (a) hyper-parameter tuning and (b) prompt comparison. This is done to indicate that these steps can be done in parallel to find the best combination of prompt and/or hyper-parameters, but since both are marked as optional it is possible to do only one of the steps or neither.



**Figure 5** The *ECSER-LLM* pipeline. Dashed borders indicate optional steps. Double arrows show possible feedback loops between macro activities. The steps in S4. can be done in parallel.

### 6.2.1 Training, Validation, Testing

#### S1. Select an evaluation method and split the data.

In experimental software engineering, the treatment that is designed to answer a research question generally consists of a model that must be trained using a data set, but how well the trained model fits the training data is not a good indicator of the performance of the model on unseen data, since the training data is only a sample of the true data distribution. Therefore, some of the available data must be set aside to test whether the trained model generalises well to data that wasn't encountered in the process of training the model; and in the case of hyper-parameter tuning, some of the data must be used to evaluate the performance of models

with different parameters.

When using a pre-trained LLM with no additional training, it is not needed to set aside data for training, but the data should still be split into validation and test sets. The validation set should be used to select hyper-parameters for the LLM, such as the temperature, and during the development and comparison of prompts [97]. The test set should only be used when the final prompt is developed (along with any other part of the model) to ensure the prompt design was not influenced by the test set.

Several methods exist to partition data into training, validation and test sets. The simplest is the *holdout method*, where the data is split into training, validation and test sets. The training set is used for fine-tuning (S2), the validation set is used for prompt development and hyper-parameter tuning (S3 & S4), and the test set is used for evaluating the model (S5). Generally, at least 50-70% of the data is used for training and validation, with the rest being used for testing [98, 99]. The holdout method does have a major issue: since only a portion of the training data is used for validation, the test error rate can be highly variable, leading to unreliable results [100, 101].

A more robust alternative is *resampling*, where models are fitted on multiple samples drawn from the training data. One example is *k-fold cross-validation*, where the training set is split into  $k$  groups (or folds) of equal size, chosen randomly from the data. The model is trained  $k$  times, once for each fold, but each time a different fold is used as the validation set, with the remaining  $k - 1$  folds being used for training. The result of this process is  $k$  estimates of the test error, the average of which can be used for hyper-parameter selection [101]. A special case of  $k$ -fold cross-validation is *leave-one-out cross-validation* (LOOCV), where  $k$  is set to  $N$ , with  $N$  being the number of observations in the training set. This means that the model is trained  $N$  times on  $N - 1$  observations, with a different observation being used as the validation set each time. LOOCV is more computationally expensive than  $k$ -fold cross-validation, although efficient algorithms exist for some applications that don't require training the model  $N$  times [102, 103]. In terms of performance, LOOCV has a lower bias than  $k$ -fold cross-validation, at the cost of a higher variance [102, 104].

It is also possible to use projects to partition the data using *leave-one-project-out cross-validation* (LOPO), where the training data is not split randomly, but grouped with all the data belonging to the same SE project. Each project is set aside in turn to serve as the validation set, while the other projects are used for training [105, 106]. The advantage of LOPO is that a different project is used for validation than what is used for training, which possibly enhances the generalisability of the results [107].

Which of these methods is most appropriate might depend on the available computational power and time, with methods like LOOCV requiring much more training than the holdout method; and whether the data is obtained from distinct projects. In all cases, 10-30% of the data should be set aside for testing and not touched until all parameters are tuned and prompts are finalised.

Finally, when using a pre-trained LLM, if the researcher uses open source data, there is a legitimate concern that the validation and testing sets were also used in training the LLM, leading to data leakage. LLMs have been shown to sometimes repeat training data verbatim [108]. If possible, this can be avoided by using testing data that was released after the creation of the LLM or proprietary data.

## S2. Fine-tune models.

### Optional

This step does not apply when using a pre-trained LLM without fine-tuning or additional training, such as research that only uses prompts to guide the output of the LLM.

After splitting the data and deciding on the evaluation method, the training set is used to fine-tune the LLM or train a classification model on the LLM encodings. Training or fine-tuning a model entails changing the *parameters* of the model to produce outputs that are most similar to the supervised labels in the training data. The training process is usually influenced by *hyper-parameters* that are set before training and don't change during training. For example, when fine-tuning an LLM, the learning rate, batch size and epochs are examples of hyper-parameters that influence the training process, but the weights of the model are the parameters that are actually changed during training.

Since LLMs are often updated after release, the exact LLM version, configuration and experiment dates should be reported to make it easier for other researchers to replicate findings [67]. Additionally, when using fine-tuning, the fine-tuning data and weights should be shared if possible.

### S3. Design prompts.

#### Optional

This step only applies when using prompts to guide LLM outputs, instead of using LLM embeddings with traditional classifiers.

Prompt engineering is an important part of interacting with LLMs, since the prompt design can have a substantial effect on the performance of the LLM. We split the process of designing a prompt into five steps, similar to Marvin et al. [7].

1. Define the goal of the prompt:
2. Choose the right prompt engineering approach:
3. Choose the right prompt template:
4. Provide context:
5. Test and refine:

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# Appendices

## A Supplemental Mapping Study Results

For brevity, sources were excluded for some figures and tables and are included here for further reference. Table 6 shows the distribution of the application types of LLMs of 83 total papers (see Figure 2).

**Table 6** References for the distribution of LLM application types.

| Category                        | Number of studies | References |
|---------------------------------|-------------------|------------|
| Generation                      | 58                | [109–166]  |
| Classification                  | 15                | [167–181]  |
| Recommendation                  | 6                 | [182–187]  |
| Generation & Classification     | 3                 | [188–190]  |
| Classification & Recommendation | 1                 | [191]      |

The following tables apply to the 18 papers included in the mapping study. Table 7 shows the number of studies belonging to each venue. Table 8 shows the number of papers using prompts for classification. See also Figure 3 and 4.

**Table 7** References for distribution of venue in the mapping study.

| Venue | Number of studies | References                    |
|-------|-------------------|-------------------------------|
| TSE   | 8                 | [176–181, 189, 190]           |
| FSE   | 2                 | [174, 175]                    |
| ICSE  | 8                 | [167, 168, 170–173, 188, 191] |

**Table 8** References for the distribution of prompt usage in the mapping study.

| Prompt-based | Number of studies | References                                   |
|--------------|-------------------|----------------------------------------------|
| No           | 10                | [167, 168, 170, 173, 176–178, 188, 190, 191] |
| Yes          | 8                 | [171, 172, 174, 175, 179–181, 189]           |

For the main results of the mapping study, Table 9 shows the full references. Further, Table 10 shows the references for the papers that use a prompt-based approach to classification.



**Table 9** References for the mapping study results.

| Category                                      | Total      | References                                   |
|-----------------------------------------------|------------|----------------------------------------------|
| Total mapping study papers                    | 18         | [167, 168, 170–181, 188–191]                 |
| <b>Evaluation metrics</b>                     |            |                                              |
| Precision                                     | 17 (94.4%) | [167, 168, 170–179, 181, 188–191]            |
| Recall                                        | 17 (94.4%) | [167, 168, 170–179, 181, 188–191]            |
| Accuracy                                      | 11 (61.1%) | [168, 170, 172, 173, 175–178, 180, 181, 189] |
| F-Score                                       | 17 (94.4%) | [167, 168, 170–174, 176–181, 188–191]        |
| AUC                                           | 3 (16.7%)  | [173, 177, 180]                              |
| ROC plots                                     | 0 (0.0%)   |                                              |
| MCC                                           | 0 (0.0%)   |                                              |
| Calibration                                   | 0 (0.0%)   |                                              |
| Fairness                                      | 0 (0.0%)   |                                              |
| <b>Robustness</b>                             |            |                                              |
| Data distribution & Adversarial Attacks       | 1 (5.5%)   | [178]                                        |
| Noisy data                                    | 1 (5.5%)   | [170]                                        |
| <b>Metrics justification</b>                  |            |                                              |
| No                                            | 9 (50.0%)  | [170–176, 178, 189]                          |
| Implicit                                      | 0 (0.0%)   |                                              |
| Previous work                                 | 5 (27.8%)  | [177, 180, 181, 188, 191]                    |
| Yes                                           | 4 (22.2%)  | [167, 168, 179, 190]                         |
| Confusion matrix                              | 4 (22.2%)  | [171, 175, 179, 180]                         |
| Evaluation over multiple data sets            | 5 (27.8%)  | [171, 177, 179, 188, 191]                    |
| <b>Type of baseline</b>                       |            |                                              |
| None                                          | 2 (11.1%)  | [171, 175]                                   |
| Own                                           | 3 (16.7%)  | [172, 174, 190]                              |
| External                                      | 4 (22.2%)  | [168, 177, 189, 191]                         |
| External and Own                              | 9 (50.0%)  | [167, 170, 173, 176, 178–181, 188]           |
| Analysis of statistical significance          | 5 (27.8%)  | [167, 179–181, 190]                          |
| <b>Statistical significance justification</b> |            |                                              |
| No                                            | 4 (80.0%)  | [179–181, 190]                               |
| Implicit                                      | 0 (0.0%)   |                                              |
| Previous work                                 | 1 (20.0%)  | [167]                                        |
| Yes                                           | 0 (0.0%)   |                                              |

**Table 10** References for the mapping study prompting results.

| Category                                 | Total      | References                         |
|------------------------------------------|------------|------------------------------------|
| Total prompt-based classification papers | 8          | [171, 172, 174, 175, 179–181, 189] |
| <b>Prompt approach</b>                   |            |                                    |
| Chain-of-verification                    | 1 (12.5%)  | [172]                              |
| Few-shot                                 | 2 (25.0%)  | [181, 189]                         |
| Mimic-in-the-background                  | 1 (12.5%)  | [171]                              |
| Not reported                             | 1 (12.5%)  | [174]                              |
| Zero-shot                                | 3 (37.5%)  | [175, 179, 180]                    |
| <b>Final prompt</b>                      |            |                                    |
| Not reported                             | 2 (25.0%)  | [174, 181]                         |
| Own                                      | 6 (75.0%)  | [171, 172, 175, 179, 180, 189]     |
| <b>Prompt approach justification</b>     |            |                                    |
| No                                       | 5 (62.5%)  | [174, 175, 179–181]                |
| Yes                                      | 3 (37.5%)  | [171, 172, 189]                    |
| <b>Final prompt justification</b>        |            |                                    |
| No                                       | 4 (50.0%)  | [172, 174, 179, 181]               |
| Previous Work                            | 1 (12.5%)  | [175]                              |
| Yes                                      | 3 (37.5%)  | [171, 180, 189]                    |
| <b>Evaluation over multiple prompts</b>  |            |                                    |
| No                                       | 8 (100.0%) | [171, 172, 174, 175, 179–181, 189] |
| <b>Temperature</b>                       |            |                                    |
| No                                       | 7 (87.5%)  | [172, 174, 175, 179–181, 189]      |
| Yes                                      | 1 (12.5%)  | [171]                              |