A Software Engineering Perspective on Engineering Machine Learning Systems: State of the Art and Challenges

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Abstract:

Context: Advancements in machine learning (ML) lead to a shift from the traditional view of software development, where algorithms are hard-coded by humans, to ML systems materialized through learning from data. Therefore, we need to revisit our ways of developing software systems and consider the particularities required by these new types of systems.

Objective: The purpose of this study is to systematically identify, analyze, summarize, and synthesize the current state of software engineering (SE) research for engineering ML systems.

Method: I performed a systematic literature review (SLR). I systematically selected a pool of 65 studies from SE venues and then conducted a quantitative and qualitative analysis using the data extracted from these studies.

Results: The non-deterministic nature of ML systems complicates all SE aspects of engineering ML systems. Despite increasing interest from 2018 onwards, the results reveal that none of the SE aspects have a mature set of tools and techniques. Testing is by far the most popular area among researchers. Even for testing ML systems, engineers have only some tool prototypes and solution proposals with weak experimental proof. Many of the challenges of ML systems engineering were identified through surveys and interviews. Researchers should conduct experiments and case studies, ideally in industrial environments, to further understand these challenges and propose solutions.

Conclusion: The results may benefit (1) practitioners in foreseeing the challenges of ML systems engineering; (2) researchers and academicians in identifying potential research questions; and (3) educators in designing or updating SE courses to cover ML systems engineering.

Keywords:
Machine learning; deep learning; software engineering; software development; software process; challenges; concerns; systematic literature review
1 INTRODUCTION

“Software has been eating the world” [16], and with machine learning (ML) capabilities, software has become even more voracious. With the wide availability of digitized data and computational power, ML algorithms, which have been around for many decades, empowered software-intensive systems for providing additional beneficial functionalities. Some of the remarkable tasks that are successfully tackled by ML algorithms include autonomous driving [108], social network analysis [109], natural language processing [110], image recognition [111], and recommendation [112]. Compelling examples of ML systems can be seen in various sectors, including finance [106][107], healthcare [8], and manufacturing [113], etc. Despite several promising examples, 47% of AI projects remain prototypes due to the lack of the tools to develop and maintain a production-grade AI system, according to Gartner Research [189].

ML systems engineering in real-world settings is challenging since it adds additional complexity to engineering “traditional” software. We have separate bodies of knowledge for engineering ML capabilities [2][9][62] and engineering traditional software [17]. On the other hand, ML capabilities are generally served as parts of larger software-intensive
systems (besides embedded software in robots or vehicles). Therefore, we need a holistic view of engineering software-intensive systems with ML capabilities (ML systems) in real-world settings. Many researchers from software engineering (SE) [18], [23] and ML [20], [21], as well as industry practitioners [19], [22], [54], have stated the requirement of such a holistic view.

Another trend we can recently observe is the events organized to discuss how to engineer ML systems. The Software Engineering for Machine Learning Applications (SEMLA) international symposium [P27] has been arranged to bring together researchers and practitioners in SE and ML to explore the challenges and implications of engineering ML systems. In 2018, two main topics were addressed intensively in SEMLA [P27]: (1) How can software development teams incorporate ML related activities into existing software processes? (2) What new roles, artifacts, and activities would be required to develop ML systems? In addition to applying ML techniques to SE tasks (such as defect prediction), researchers started to explore engineering ML systems within the scope of the International Workshop on Realizing Artificial Intelligence Synergies in Software Engineering (RAISE). Another event is the International Workshop on Artificial Intelligence for Requirements Engineering (AIRE) that welcomes submissions addressing requirements engineering and AI, such as [118]. Christian Kästner at Carnegie Mellon University started to deliver a course called “Software Engineering for AI-Enabled Systems (SE4AI)”, which takes an SE perspective on building software systems with a significant ML component [24].

Industrial events are being held to discuss the implications of engineering ML systems on the current SE practices. One of such events is QCon.ai, which aims to bring SE and ML practitioners together to exchange experiences and thoughts on all aspects of SE for ML. In such circumstances, speakers started to address the SE viewpoint of ML systems. For instance, Kishau Rogers suggested a roadmap for adopting enterprise architecture to AI capabilities at O’Reilly Software Architecture Conference. Srim Srinivasan from IBM presented SE practices for data science and ML lifecycle in DataWorks Summit 2018. Peter Norvig from Google delivered talks on the intersection of SE and ML. Recently, Ivica Crnkovic addressed the new challenges in architecting and managing the lifecycle for AI-based systems at the European Conference on Software Architecture (ECSA) 2020.

This study aims to present a repository of researchers and organizations working on SE aspects of ML systems and a repository of SE challenges of ML systems presented in SE venues. The distinction between SE and AI/ML has been blurred by as many disciplines and research areas. Researchers and practitioners from both fields need to understand the other side’s concerns and have a holistic view of engineering ML systems. This paper can serve as a starting point to obtain such a holistic view and a repository of papers, researchers, and organizations to explore this topic.

The goal of this paper is to summarize the state-of-the-art and identify challenges when engineering ML systems. Section 2 sets out the context and the vocabulary to be used in this paper. Section 3 presents the related work. Section 4 details the research objectives and method. Section 5 involves the results of detailed analysis and synthesis. Section 6 explains the findings by discussing potential research directions and threats to validity. Section 7 shall conclude the paper.

2 BACKGROUND

This section introduces the foundational concepts and describes the vocabulary by defining the essential concepts used in this paper.

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1 “The Applied AI Software Conference for Developers”, https://qcon.ai/
2 “Enterprise architecture for artificial intelligence”, https://conferences.oreilly.com/software-architecture/sa-eu-2018/public/schedule/detail/71390
3 “Software engineering practices for the data science and machine learning lifecycle” at “DataWorks Summit” in 2018, https://www.youtube.com/watch?v=IA3UX7XBXw
4 For instance, “SE with/and/for/by ML”, https://www.youtube.com/watch?v=MP-wAc-XNUU
5 “AI engineering - new challenges in system and software architecting and managing lifecycle for AI-based systems”, at ECSA 2020, https://ecsa2020.disim.univaq.it/details/ecsa-2020-keynotes/1/AI-engineering-new-challenges-in-system-and-software-architecting-and-managing-lif
2.1 Artificial Intelligence, Machine Learning, and Deep Learning

Artificial intelligence (AI) is the name of the field involving the efforts for building intelligent agents [134]. Intelligent agents perceive their environment and try to achieve their goals by acting autonomously [134]. Machine learning (ML) is a subfield of AI, which tries to acquire knowledge by extracting patterns from raw data [6][132] and solve some problems using this knowledge. Deep Learning (DL) is a subfield of ML that focuses on creating large neural network models capable of making accurate data-driven decisions [133]. DL has emerged from research in AI and ML and is particularly suited to contexts where large datasets are available and the data is complex [133].

Based on the dataset representation and the approach to defining the candidate models and final model (or function), three different categories of ML are identified: supervised, unsupervised, and reinforcement learning [133]. In supervised learning, an ML model (or a function mapping inputs to outputs) is constructed using a training dataset with labels. Classification and regression problems are typical examples of supervised learning. In unsupervised learning, a function to describe a hidden structure is inferred from unlabeled data. Common problems for unsupervised learning are clustering and association rule learning. In reinforcement learning, an agent learns from a series of reinforcements, i.e., rewards and punishments [134]. Reinforcement learning finds lots of uses in video games.

2.2 Traditional Software and Machine Learning Systems

Engineering traditional software (or conventional software [136]) is about the implementation of programs (arithmetic & logic operations, a sequence of if-then-else rules, etc.) explicitly by engineers in the form of source code, which can be decomposed into units (e.g., classes, methods, functions, etc.) [136]. As the left side of Figure 1 shows, the input and hand-designed program are provided to the computer, and an output is generated. On the contrary, in ML systems, ML algorithms search through a large space of candidate programs, driven by training experience, to find a program that optimizes the performance metric [135] (i.e., fulfills the requirements). As the right side of Figure 1 shows, the computer extracts patterns using input and output data; in other words, learn a function that maps from inputs to outputs.

![Figure 1. Traditional software development (on the left) vs. ML system development (on the right)](image)

One of the success factors for ML system development is the identification of a subset of input data (the process of feature selection) that is informative for a given task. Traditional ML algorithms entail a manual feature selection process, which may require domain expertise, statistical analysis of input data, and experiments for building models with different feature sets [133]. As the left side of Figure 2 shows, engineers provide hand-designed features to computers to have a function (or program) that maps inputs to outputs. Since the design of features often involves a significant amount of human effort in traditional ML, DL takes a different approach to feature selection by automatically learning features that are most useful for a given task from the input data [133]. As the right side of Figure 2 shows, features are learned by computer using DL algorithms. DL systems development is generally possible when large enough datasets are available and is particularly useful for the tasks in complex high-dimensional domains, such as face recognition and machine translation [133].

![Figure 2. ML system development (on the left) vs. DL system development (on the right) – adapted from [171] and [132](image)

Practitioners and academicians do not use a standard term to name systems that incorporate AI/ML/DL capabilities. Software that applies AI techniques can be referred to “AI software” [137] or “AI-based software” [136]. In Cyber-Physical systems, a component whose behavior is driven by an ML/DL model obtained via training and updated through a learning process is called a “learning-enabled component” [138]. Recently, in parallel with the success of ML, such systems are referred to as ML systems [141]/applications [140]/solutions [139]. In this paper, I use the term “ML system” as either a
software framework, tool, library, or component that provides ML (including DL) functionalities or software systems that include ML components [P56].

2.3 SE FOR ML AND ML FOR SE
Researchers have been addressing the interplay between SE and ML (as well as AI more broadly and DL more narrowly) for many years [143][144][145]. On the other hand, some researchers point out the rift between SE and ML communities. One of the reasons for this rift may be these communities’ focus: the ML community focuses on algorithms and their performance, whereas the SE community focuses on implementing and deploying software-intensive systems [P27]. Bringing together the knowledge and experience of these two communities uncovers two areas of synergy:

1. **SE for ML** refers to addressing various SE tasks for engineering ML systems, i.e., designing, developing, and maintaining ML-enabled software systems. Researchers are trying to identify the different aspects of engineering ML systems compared to traditional software and develop new techniques and tools to cope with these differences.

2. **ML for SE** refers to applying or adapting AI technologies to address various SE tasks [65], such as software fault prediction [146], code smell detection [147], reusability metrics prediction, and cost estimation [148], etc. Researchers utilize ML models obtained from SE data (source code, requirement specifications, test cases, etc.) to engineer software more efficiently and effectively.

This paper focuses on SE for ML by systematically reviewing the SE literature on engineering ML systems.

3 RELATED WORK
According to my literature search, whose summary is presented in Table 2, researchers started to allocate effort in identifying SE aspects of engineering ML systems. Masuda et al. aimed to discover the techniques for evaluating and improving the quality of ML systems [3]. Ashmore et al. [6] and Liu et al. [149] focused on ML systems’ safety and security aspects, respectively. Sherin et al. [5] and Felderer et al. [152] conducted a systematic mapping study (SMS) to identify, analyze, and classify the literature on ML testing. Zhang et al. worked a more comprehensive SLR on various aspects of testing ML systems, including testing properties (correctness, robustness), testing components (data, ML framework), and testing workflow (generation and evaluation) [125]. Watanabe et al. published an SLR involving seven papers to understand the current practices for developing ML systems [4]. Washizaki et al. collected good and bad SE design patterns for ML systems from the academic and gray literature [117].

To the best of my knowledge, Kumeno et al. published the first SLR addressing the challenges of engineering ML systems [142]. Unlike [142], I was able to identify more SE papers (65 vs. 47) and provided a taxonomy of challenges and proposed solutions classified under SE’s main knowledge areas. Lwakatare et al. have recently published an SLR to identify the challenges of developing and maintaining large-scale ML-based systems in industrial settings [97]. The primary study pool of [97] includes papers mainly from journals and conferences on ML/DL, data engineering, big data, knowledge discovery, and data mining. Around five primary studies of [97] were published in SE journals and conference proceedings. On the contrary, based on my research objective, I am identifying the challenges of engineering ML systems from an SE perspective.

| Ref | Year | Objective | Research Method & Source of Information | Knowledge Area Focus |
|-----|------|-----------|----------------------------------------|----------------------|
| [3] | 2018 | discover techniques to evaluate and improve the software quality of ML systems | SLR using DB search on a limited scope of venues 78 papers from 16 academic conferences & 5 academic magazines on AI & SE | Quality |
| [6] | 2019 | identify assurance desiderata for ML for each stage of ML lifecycle, review existing methods that contribute to achieving these desiderata, and identify open challenges | Non-systematic review 40+ papers | Quality (Safety) |
In addition to the academic literature, practitioners and researchers in the industry have also begun to address the SE aspects of developing and maintaining ML systems. Lorica and Loukides [153] stated that “Machine learning is poised to change the nature of software development in fundamental ways, perhaps for the first time since the invention of FORTRAN and LISP.” Heck identified “engineering ML systems” as a new discipline, which needs further work on methods, tools, frameworks, and tutorials [154]. Sato et al. argued that the process for developing, deploying, and continuously improving ML systems is more complex than traditional software, such as a web service or a mobile application [67]. As these examples show, the industry is calling for action to resolve the challenges of engineering ML systems and to propose new techniques to cope with the additional complexity of ML systems.

### 4 Research Objectives and Method

This section describes the research objectives and the method used in this study. An SLR approach was adopted to synthesize the knowledge of engineering ML systems from an SE perspective. The research method was based on established guidelines [98][99], some previous good examples [100][116], and my previous experience in conducting SLR.
Table 2. Protocol summary

| Research questions | RQ1. When were the primary studies published? |
|--------------------|---------------------------------------------|
|                    | RQ2. Where were the primary studies published? |
|                    | RQ3. Who is conducting the research? |
|                    | RQ4. What are the types of researchers’ affiliations? |
|                    | RQ5. What research methods are used? |
|                    | RQ6. What ML problem types and datasets are used for in experiments and case studies? |
|                    | RQ7. Which challenges and solutions for engineering ML systems have been raised by SE researchers? |
| Search string | Population: “software engineering” |
| Intervention | “machine learning” OR “deep learning” |
| Search strategy | - DB search: ACM, Google Scholar, IEEE, ScienceDirect, Springer, Wiley |
|                | - Backward and forward snowballing using Google Scholar |
|                | - Manual search: |
|                | o International Workshop on Artificial Intelligence for Requirements Engineering (AIRE): 2014 – 2019 |
|                | o International Workshop on Realizing Artificial Intelligence Synergies in Software Engineering (RAISE): 2012 – 2019 |
|                | o IEEE/ACM International Conference on Software Engineering: 2017 – 2019 |
|                | o ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering: 2017 – 2019 |
| Inclusion and Exclusion criteria | Inclusion: |
|                | - The paper is written in English. |
|                | - The paper is published in a scholarly SE journal or conference/workshop/symposium proceedings. |
|                | - The paper explicitly involves at least one SE challenge of engineering ML systems. |
|                | Exclusion: |
|                | - The paper is published in a scholarly AI/ML/Data Science journal or conference/workshop/symposium proceedings. |
|                | - The paper focuses only on an ML-specific aspect are (such as proposing a new ML algorithm, hyperparameter optimization, etc.). |
|                | - The paper is an editorial, issue introduction or secondary study (literature review, SMS, SLR). |
| Study type | Primary studies |

4.1 Goal and review questions

The scope and goal of this study were formulated using the Goal-Question-Metric approach [114] as follows.

**Analyze the state-of-the-art in engineering machine learning systems**

for the purpose of exploration and analysis

with respect to the reported challenges; proposed solutions; the intensity of the research in the area; the most active venues, researchers, and organizations in the area; the research methods

from the point of view of software engineering researchers

in the context of software engineering.

As Kitchenham et al. [115] pointed out, research questions (RQs) must embody secondary studies’ goals. Accordingly, the purpose of this study can be broken down into the following seven main RQs.

RQ1. When were the primary studies published?
RQ2. Where were the primary studies published?
RQ3. Who is conducting the research?
RQ4. What are the types of researchers’ affiliations?

RQ5. What research methods are used?

RQ6. What ML problem types and datasets are used for in experiments and case studies?

RQ7. Which challenges and solutions for engineering ML systems have been raised by SE researchers?

### 4.2 PRIMARY STUDY SELECTION

Figure 3 displays the primary study selection process used in this study.

![Diagram of study selection process]

**Figure 3. The primary study selection process**

### 4.2.1 Database search

I started by applying the database (DB) search method to identify relevant primary studies. I used five widely used online databases, i.e., ACM, IEEE Xplore, ScienceDirect, Springer, and Wiley. Besides, I used Google Scholar to enrich the pool of candidate primary studies. I used two search strings to query online databases: Query 1: “software engineering” AND “machine learning”; Query 2: “software engineering” AND “deep learning.” I used general terms for the search to have high recall and relatively lower precision. Although this required more effort for screening, I obtained a broader initial set of papers and substantially decreased the possibility of missing some relevant studies.
I searched each of the six online databases using the defined search strings in January 2020. I applied a filter for publication date and included the studies that have been published until the end of 2019. Table 3 shows the number of results obtained via two search strings.

| Database       | Query 1 | Query 2 |
|----------------|---------|---------|
| ACM            | 6,889   | 782     |
| IEEE Xplore    | 1,817   | 485     |
| ScienceDirect  | 40      | 5       |
| Springer       | 22,931  | 3,178   |
| Wiley          | 165     | 176     |
| Google Scholar | ~148,000 | ~19,800 |

Due to the general search terms used, the number of results was high for manual primary study selection for ACM, IEEE Xplore, Springer, and Google Scholar databases. Therefore, as others have done [126][127][128][129], I had to restrict the search space by assuming a “search saturation effect.” Thus, I checked the first 200 results of each query in each database. I only continued further when the results between 190 and 200 still looked relevant.

To identify the relevant primary studies, I defined the inclusion and exclusion criteria listed in Table 4. To present a SE perspective and keep the size of the final primary study pool manageable, I only considered papers published in the SE journals and conference/workshop/symposium proceedings, as others have done [7].

| Inclusion criteria                                                                 | Exclusion criteria                                                                 |
|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
| The paper is written in English.                                                   | The paper is published in a scholarly AI/ML/Data Science journal or conference/workshop/symposium proceedings. |
| The paper is published in a scholarly SE journal or conference/workshop/symposium proceedings. |                                                                                     |
| The paper explicitly involves at least one SE challenge of engineering ML systems. | The paper focuses only on an ML-specific aspect are (such as proposing a new ML algorithm, hyperparameter optimization, etc.). |
|                                                                                   | The paper is an editorial, issue introduction, or secondary study (literature review, SMS, SLR). |

4.2.2 Backward and forward snowballing

To ensure the inclusion of relevant primary studies as much as possible, I conducted backward and forward snowballing, as recommended by systematic review guidelines [99]. For backward snowballing, I applied the inclusion and exclusion criteria to each primary study’s reference list found via database search. For forward snowballing, I checked the citations listed on Google Scholar to each primary study against the inclusion and exclusion criteria. Snowballing provided 54 primary studies.

4.2.3 Manual search

To enrich the primary study pool, I conducted a manual search in two top SE conference proceedings (ICSE and ESEC/FSE) for the years 2017, 2018, and 2019. Also, I investigated all papers published in AIRE and RAISE, since these workshops directly target the intersection of AI and SE. The manual search yielded 22 primary studies.
4.2.4 De-duplication

I manually entered the metadata of primary studies (e.g., title, abstract, keywords, publication year, venue, etc.) into a spreadsheet. I identified and removed 41 duplicate studies from the list.

4.2.5 Quality assessment

To assess the quality of primary studies, I used the quality assessment criteria (Table 5) proposed by Mohanani et al. [100]. I divided the included studies into empirical (56) and non-empirical (10), as suggested by [100]. Empirical studies are the ones that analyze primary data; non-empirical studies include both opinion papers and conceptual research [100].

For each criterion, I scored the primary studies using a 2-point Likert scale (yes = 1, no = 0). To maintain a high-quality input of primary studies for this SLR, I decided to exclude the papers with a score lower than six points out of 12 for empirical studies and three points out of six for non-empirical studies. I excluded one study with a score under the threshold.

| Quality criteria                                      | Empirical | Non-empirical |
|-------------------------------------------------------|-----------|---------------|
| Was a motivation for the study provided?              | X         | X             |
| Was the aim (e.g., objectives, research goal, focus)  | X         | X             |
| Was the study’s context (i.e., knowledge areas)       | X         | X             |
| Does the paper position itself within the existing    | X         | X             |
| literature?                                           |           |               |
| Is relevance (to industry or academia) discussed?     | X         | X             |
| Were the findings or conclusions reported?            | X         | X             |
| Was the research design or method described?          | X         |               |
| Was the sample or sampling strategy described?        | X         |               |
| Was the data collection method(s) reported?           | X         |               |
| Was the data analysis method(s) reported?             | X         |               |
| Were limitations or threats to validity described?    | X         |               |
| Was the relationship between researchers and          | X         |               |
| participants mentioned?                               |           |               |

4.2.6 Finalization of primary study pool

After excluding one study (found via DB search), the final primary study pool included 65 individual results. As shown in Figure 4, the DB search yielded 30 results, snowballing 54, and manual search 22. There were 33 studies found via one search method (DB search: 6, Snowballing: 25, Manual search: 2) and 32 studies via more than search method.

Figure 4. Number of primary studies per search method
I recorded all the metadata of the primary studies into the spreadsheet and checked its completeness. The primary study pool has been finalized with this step and became ready for data extraction.

4.3 DATA EXTRACTION

After selecting the primary studies, I started with the data extraction phase. I formed an initial data extraction form (Table 6) based on my RQs. The first eight columns (from paper title to authors) constitute the metadata of the papers. I derived affiliation type simply from affiliation data. I used the list of research methods proposed in [130] to identify the primary studies’ methods. I used the knowledge areas presented in [P56] (derived from SWEBOK [17]) to classify the challenges and solutions. I recorded the challenges and solutions to the spreadsheet without making any changes as written in the primary studies.

| Field                          | Categories                        | Relevant RQ |
|--------------------------------|-----------------------------------|-------------|
| Paper title                    | Free text                         | -           |
| Abstract                       | Free text                         | -           |
| Keywords                       | Free text                         | -           |
| Publication year               | Number                            | RQ1         |
| Venue (Journal/Conference)     | Free text                         | RQ2         |
| Affiliation(s) (University/Research Institution/Company) | Free text | RQ3         |
| Country(s)                     | Free text                         | RQ3         |
| Author(s)                      | Free text                         | RQ3         |
| Affiliation types of study authors | University, Industry, Collaboration | RQ4         |
| SE knowledge area              | Requirements Engineering, Design, Software Development and Tools, Testing and Quality, Maintenance and Configuration Management, Software Engineering Process and Management, Organizational Aspects | RQ5, RQ6, RQ7 |
| Research method                | Experiment, Interview, Survey, Thematic Analysis, Case Study, Statistical Analysis, Opinion/No Research Method | RQ5         |
| ML problem type                | Classification, Regression, Clustering, Structured output, Ranking | RQ6         |
| Traditional ML/DL Algorithm(s) | Traditional ML, DL, Traditional ML & DL, Not mentioned | RQ6         |
| Dataset(s)                     | Free text                         | RQ6         |
| Challenge(s)                   | Free text                         | RQ7         |
| Solution(s)                    | Free text                         | RQ7         |

4.4 DATA SYNTHESIS AND REPORTING

Since I managed to categorize the extracted data for most of the RQs, the data extraction phase yielded a set of quantitative data to be synthesized. I reported the frequencies and percentages of each identified category to answer the RQs.
The only RQ that required qualitative analysis is RQ6, that is, the challenges and proposed solutions. I conducted open coding [131] to analyze the challenges and solutions. A code symbolically assigns a summative or evocative attribute for a portion of qualitative data [131]. I conducted open coding in cycles. In the first cycle, I tried to identify any emerging patterns of similarity or contradiction. In the second cycle, I collapsed and expanded codes to understand any patterns. After I extracted the main themes and codes, I revised the codes assigned to each challenge/solution and reported the results.

5 RESULTS

In order to obtain an overall impression on the paper pool’s content and display which areas the studies concentrate on, I created a bar chart of the most frequently used 50 terms in the primary studies’ abstracts (Figure 5). I used unigrams, bigrams, and trigrams when calculating frequencies. Besides, I used lemmatization and removed stopwords when constructing the list of unigrams. Not surprisingly, “system,” “software,” “DL system,” and “program” are among the most frequently used terms to refer to traditional software or ML systems. We can observe many terms that represent the population of this study, i.e., “software engineering,” “development,” “developer,” “testing,” “test,” “bug,” “quality,” “coverage,” “criterion,” “requirement,” “fairness,” “safety.” “Testing” term is the second most frequently used term showing researchers’ high interest in testing ML systems, as addressed in RQ4-RQ7. There are also many terms representing the intervention of this study, i.e., “machine learning” OR “deep learning”: “DL,” “ML,” “AI,” “model,” “machine learning,” “deep learning,” “training,” “DNN,” “neural network.”

![Figure 5. The most frequently used 50 terms in abstracts](image)

In the rest of this section, I address each research question from RQ1 to RQ7.

5.1 WHEN WERE THE PRIMARY STUDIES PUBLISHED?

Figure 6 shows the number of primary studies published each year. The earliest paper [P39] was published at the International Conference on Software Engineering & Knowledge Engineering in 2007. There was no paper or one paper per year until 2017. Three papers were published in 2017, after which we see a sharp increase starting from 2018. Since I conducted the search and primary study selection in January 2020, I did not include the papers that have been published in 2020 to see the trend over the years.
5.2 \textbf{WHERE WERE THE PRIMARY STUDIES PUBLISHED?}

Table 7 displays the software engineering venues in which the primary studies were presented and published. 91\% of the studies were presented in conferences and workshops (59 papers in conferences/workshops and six papers in journals). The conference with the most papers (11) is the International Conference on Software Engineering (ICSE). The journal with the most papers (three out of six papers) is IEEE Transactions on Software Engineering.

\begin{table}[h]
\centering
\begin{tabular}{|l|c|c|}
\hline
\textbf{Venue} & \textbf{Number of Primary Studies} & \textbf{Reference(s)} \\
\hline
IEEE/ACM International Conference on Software Engineering (ICSE) & 11 & [P4][P28][P30][P31][P42][P45][P46][P49][P50][P53][P65] \\
ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering (ESEC/FSE) & 10 & [P1][P7][P13][P16][P19][P25][P32][P37][P38][P63] \\
ACM/IEEE International Conference on Automated Software Engineering & 5 & [P20][P35][P51][P54][P61] \\
ACM SIGSOFT International Symposium on Software Testing and Analysis & 3 & [P14][P59][P64] \\
IEEE International Conference on Software Testing, Verification and Validation (ICST) & 3 & [P10][P41][P47] \\
IEEE Transactions on Software Engineering & 3 & [P18][P29][P56] \\
ACM/IEEE International Symposium on Empirical Software Engineering and Measurement (ESEM) & 2 & [P2][P12] \\
IEEE International Conference on Software Quality, Reliability and Security (QRS) & 2 & [P11][P43] \\
International Conference on Fundamental Approaches to Software Engineering & 2 & [P9][P15] \\
International Symposium on Software Reliability Engineering (ISSRE) & 2 & [P36][P62] \\
Australasian Software Engineering Conference (ASWEC) & 1 & [P48] \\
Euromicro Conference on Software Engineering and Advanced Applications (SEAA) & 1 & [P5] \\
European Conference on Information Systems (ECIS) & 1 & [P6] \\
IEEE Access & 1 & [P52] \\
\hline
\end{tabular}
\caption{Distribution of the primary studies per venue}
\end{table}
5.3 Who is conducting the research?

To investigate the most prolific universities and organizations (companies and research institutions), I ranked all 67 universities and 20 organizations by the number of primary studies. Of these, 48 universities and 15 organizations had a single paper. Table 8 lists the universities with more than one paper. Nanjing University in China is the most prolific university, followed by Kyushu University in Japan.

Table 8. Universities having more than one primary study

| University                                | Country  | Number of Primary Studies | References                                      |
|-------------------------------------------|----------|---------------------------|-------------------------------------------------|
| Nanjing University                        | China    | 9                         | [P10][P11][P31][P32][P37][P43][P52][P58][P63]   |
| Kyushu University                         | Japan    | 8                         | [P13][P20][P34][P35][P36][P57][P59][P62]        |
| Nanyang Technological University          | China    | 6                         | [P13][P20][P34][P35][P36][P56]                  |
| University of Illinois at Urbana-Champaign | USA      | 5                         | [P34][P35][P36][P59][P65]                       |
| Carnegie Mellon University                | USA      | 4                         | [P34][P35][P36][P59]                            |
| Chalmers University of Technology         | Sweden   | 4                         | [P22][P28][P30][P33]                            |
| Monash University                         | Australia| 4                         | [P34][P35][P36][P56]                            |
Table 9 lists the research institutions and companies that have contributed to more than one paper. IBM Research Centers in India, Japan, and Israel contributed to five studies.

### Table 9. Research institutions/companies having more than one primary study

| Research Institution / Company | Country          | Number of Primary Studies | References          |
|-------------------------------|------------------|---------------------------|---------------------|
| IBM Research                 | India, Japan, Israel | 4                         | [P1][P7][P41][P45]  |
| Defense Science and Technology Laboratory | UK             | 2                         | [P49][P50]          |
| Microsoft Research            | USA              | 2                         | [P4][P29]           |
| National Institute of Informatics | Japan        | 2                         | [P24][P40]          |
| RISE Research Institutes of Sweden AB | Sweden     | 2                         | [P30][P55]          |

To investigate the researchers who contributed to this research topic the most, we ranked all 238 authors by the number of papers in our paper pool. Of these, 197 authors had one paper, 27 authors had two papers, and 14 authors had three or more papers. Table 10 shows the top 14 researchers who published three or more papers in SE venues. Lei Ma is the most prolific author working on this research topic, followed by Jianjun Zhao and Yang Liu. As can be seen in Table 10, the most prolific authors are generally collaborating.

### Table 10. Top 14 researchers

| Researcher        | Number of Primary Studies | References                      |
|-------------------|---------------------------|---------------------------------|
| Lei Ma            | 8                         | [P13][P20][P34][P35][P36][P57][P59][P62] |
| Jianjun Zhao      | 7                         | [P13][P20][P34][P35][P36][P57][P59] |
| Yang Liu          | 6                         | [P13][P20][P34][P35][P36][P57][P59] |
| Bo Li             | 4                         | [P34][P35][P36][P59]            |
| Chang Xu          | 4                         | [P11][P31][P32][P43]            |
| Felix Juefei-Xu   | 4                         | [P34][P35][P36][P59]            |
| Minhui Xue        | 4                         | [P34][P35][P36][P59]            |
| Xiaoxing Ma       | 4                         | [P11][P31][P32][P43]            |
To conduct a geographical analysis, I extracted the countries of author affiliations. If a paper had several authors from several countries, one credit was given to each country. Figure 7 shows the host countries of the organizations working on this research topic. The American researchers authored or co-authored 37% (24 out of the 65) papers in the pool. Researchers from China and Japan are ranked second and third with 21 and 14 papers, respectively. Only 16 countries around the world have contributed to this research topic in SE venues.

Figure 7. Countries of affiliations on the world map

5.4 What are the types of researchers’ affiliations?

I have classified the papers based on the researchers’ affiliations: university, industry (research organizations and companies), and collaboration (for papers whose authors are from both university and industry). Forty-four papers (68%) were authored solely by academic researchers, eight papers (12%) by researchers from research organizations or companies, and 13 papers (20%) were written jointly by universities and other organizations.

Figure 8 shows the affiliation types per knowledge area. Since a paper can address more than one knowledge area, a paper may have been classified under more than one area. Testing & Quality is the most focused knowledge area by academia and industry. Also, researchers collaborated the most within the scope of testing and quality. Requirements engineering and development & tools areas the second and third areas in which researchers collaborated.
5.5 WHAT RESEARCH METHODS ARE USED?

Figure 9 summarizes the research methods used to investigate SE challenges of engineering ML systems. Most of the empirical studies employed experiments. Besides experiments, the researchers interviewed and surveyed experts to learn about the challenges they face in engineering ML systems. Thematic analysis, case study, and statistical analysis are the other approaches used by the researchers. Ten papers either provide the author’s opinions or did not report enough details about the research method. Two studies [P4][P56] combined interview and survey, and one paper [P2] used thematic and statistical analysis together. Due to these three primary studies using multiple research methods, the total number of primary studies equals 68 in Figure 9.

Figure 10 displays the research methods used in the primary studies split across the SE knowledge areas addressed in the papers. The dominant research method, i.e., experiment, is primarily used in studies addressing testing and quality. A small part of these deals with development & tools and maintenance & configuration management knowledge areas. As expected, experts mentioned many challenges covering all aspects of engineering ML systems in interviews and surveys. As a result
of thematic and statistical analysis, the researchers have identified several difficulties in development & tools, test & quality, and organizational topics.

![Diagram showing research methods used per SE knowledge area](image)

**Figure 10. Research methods used per SE knowledge area**

### 5.6 WHAT ML PROBLEM TYPES AND DATASETS ARE USED FOR IN EXPERIMENTS AND CASE STUDIES?

The studies that used an experiment or case study as a research method involved one or more ML problems to observe SE challenges and validate a solution. There are several subclasses of ML problems based on what the output looks like [157]. I used the types listed in Table 11 [157] to categorize the ML problems used in the primary studies.

| Type of ML Problem | Description | Example |
|--------------------|-------------|---------|
| **Classification** | assign one of the predefined classes to an input | - assign a post a label of positive or negative  
- assign an email a label of spam or ham  
- predict the multiple known objects in a photo |
| **Regression**     | predict a numerical value for an observation | - predict the price of a house  
- predict the number of bugs in a source code |
| **Clustering**     | group similar examples (unsupervised) | - find the most relevant documents  
- group customers into segments |
| **Structured output** | create complex output | - parse a sentence and produce a parse tree  
- translate text  
- recognize the boundaries of an object in a photo |
Figure 11 shows the distribution of ML problem types used in 42 of the primary studies, the research method of which is either an experiment or a case study. Since one study may involve more than one research method and may cover more than one SE knowledge area, the total of the numbers presented in Figure 11 exceeds 42.

The most popular ML problem type is classification, followed by regression problems. Some studies were concerned with the problem of generating a complex output [156], e.g., recognizing object boundaries in images. There was only one study involving a ranking problem. Surprisingly, no study used a clustering problem, which is a prevalent unsupervised learning problem.

As mentioned in the previous RQ, most studies involve experimentation as a research method and address testing and quality aspect of engineering ML systems. Thirty-two studies conducted experiments using a classification problem. Twenty-one of these involve an image classification problem. Three of them included a text classification problem like sentiment analysis. The remainder of the studies worked with an artificial dataset and did not involve a real-world ML problem. Out of five studies addressing the development and tools knowledge area, four studies use an image classification problem. The rest of the studies dealing with maintenance & configuration management, process and management, and organization aspects also involve image classification problems except for one study.

Regression problems are the second most common category of ML problems. A characteristic problem used in the studies is the prediction of the steering wheel angle for autonomous driving.

The structured output type of problems includes recognizing objects for autonomous driving and complex natural language processing tasks, like machine translation.

Only one study [P39] is concerned with a ranking problem. Murphy et al. aim at ranking the probabilities of observing a failure in a device [P39].

![Figure 11. ML problem types per SE knowledge area](image)

I also classified the algorithms used in the experiments and case studies into two groups: traditional ML and DL algorithms. Among 42 papers, 25 papers (60%) used only DL algorithms. Eleven papers used traditional ML algorithms, and three papers used both DL and traditional ML algorithms. Three papers did not report the algorithms used.
Figure 12. Distribution of traditional ML and DL algorithms used in the experiments and case studies

Table 12 shows some details of the experiments’ datasets and case studies of 42 primary studies. Since most of the studies are focused on image classification problems, most of the datasets in Table 12 are the datasets for image classification, such as MNIST [158], CIFAR-10 [159], ImageNet [160], Fashion-MNIST [162], DSRC Vehicle Communications Data [164], Handwritten Letters, IRIS Flower Data, IRIS Waveform Data, and SVHN [170]. Eleven studies include custom datasets constructed by researchers (including synthetic datasets) or privately owned by a company. Some datasets are related to natural language processing, like Enron Email Dataset [165], Newsgroups [166], and Reuters-21578 Text Categorization Collection Dataset [167]. Three studies [P28][P32][P53] aim at predicting steering wheel angle and used Udacity self-driving car challenge dataset for experiments.

Sixty-four datasets were reported in 42 studies, which means most of the studies used 1-2 datasets on average. One reason may be the cost of conducting experiments using various datasets [125].
# Table 12. Datasets used in experiments and case studies

| Dataset                        | Description                                                                 | Web Site                                                                 | # of Primary Studies |
|--------------------------------|------------------------------------------------------------------------------|-------------------------------------------------------------------------|----------------------|
| MNIST [158]                    | Images of handwritten digits                                                 | http://yann.lecun.com/exdb/mnist/                                       | 21                   |
| CIFAR-10 [159]                 | Various color images in 10 classes                                           | https://www.cs.toronto.edu/~kriz/cifar.html                              | 11                   |
| Custom                         | Private dataset constructed by researchers or private dataset of a company   | -                                                                        | 11                   |
| ImageNet [160]                 | Visual recognition challenge dataset                                        | http://www.image-net.org/                                                | 7                    |
| UCI machine learning repository [161] | Collection of databases, domain theories, and data generators that are used by the ML community for the empirical analysis of ML algorithms | https://archive.ics.uci.edu/ml/index.php                                | 4                    |
| Udacity self-driving car challenge | Udacity Self-Driving Car Challenge images                                   | https://github.com/udacity/self-driving-car                              | 4                    |
| Fashion-MNIST [162]            | MNIST-like dataset of fashion images                                         | https://www.kaggle.com/zalando-research/fashionmnist                      | 2                    |
| Bank marketing [163]           | Bank client subscription term deposit data                                  | https://archive.ics.uci.edu/ml/datasets/Bank+Marketing                    | 1                    |
| DSRC Vehicle Communications Data [164] | Dataset regarding wireless communications between vehicles and roadside units | http://archive.ics.uci.edu/ml/datasets/DSRC+Vehicle+Communications       | 1                    |
| Enron Email Dataset [165]      | A corpus containing about 500 emails from about 150 users                   | http://www.cs.cmu.edu/~enron/                                            | 1                    |
| Fraud Detection                | Fraudulent claims in the car damage insurance domain                        | https://www.kaggle.com/c/frauddetection/data                              | 1                    |
| Fruits 360                     | A dataset with 90483 images of 131 fruits and vegetables                    | https://www.kaggle.com/moltean/fruits/data                               | 1                    |
| Handwritten Letters | Color images with 33 letters and labels | https://www.kaggle.com/olgabelitskaya/handwritten-letters-keras-applications-2/data | 1 |
|---------------------|----------------------------------------|--------------------------------------------------------------------------------|---|
| IRIS Flower Data    | The Iris flowers                       | http://archive.ics.uci.edu/ml/datasets/iris                                 | 1 |
| IRIS Waveform Data  | Waveform (time-series) data from stations around the world | https://ds.iris.edu/ds/nodes/dmc/data/types/waveform-data/                  | 1 |
| MovieLens [168]     | 25 million ratings and one million tag applications applied to 62,000 movies by 162,000 users | https://grouplens.org/datasets/movielens/                                      | 1 |
| Newsgroups [166]    | A collection of approximately 20,000 newsgroup document | https://huggingface.co/datasets/newsgroup                                      | 1 |
| IMDB WIKI Dataset   | Human faces with gender, name, and age information | https://github.com/imdeepmind/processed-imdb-wiki-dataset                        | 1 |
| Reuters-21578 Text Categorization Collection Dataset [167] | A collection of documents that appeared on Reuters newswire in 1987 | https://archive.ics.uci.edu/ml/datasets/reuters-21578+text+categorization+collection | 1 |
| Stanford Large Network Dataset Collection [169] | Datasets with information about entities and relationships between entities | http://snap.stanford.edu/data/                                                | 1 |
| SVHN [170]          | A real-world image dataset of house numbers | http://ufldl.stanford.edu/housenumbers/                                       | 1 |
| US Executions       | Records of every execution performed in the United States | https://deathpenaltyinfo.org/executions.execution-database                    | 1 |
5.7 Which challenges and solutions for engineering ML systems have been raised by SE researchers?

This subsection presents the main SE challenges of engineering ML systems identified from the primary studies. The identified SE challenges are classified based on the main SE knowledge areas presented in [P56]. The proposed solutions are also presented in this subsection. Table 13 provides a consolidated list of the challenges with proposed solutions.

5.7.1 Requirements Engineering:

Requirements engineering involves eliciting, analyzing, specifying, and validating requirements that represent a software system’s intended purpose. Many stakeholders may play a role in the RE process with various backgrounds and possibly conflicting objectives. Although a satisfactory RE phase is not sufficient for project success, it is a necessary condition. RE process has numerous potential obstacles, such as incomplete, hidden, inconsistent, underspecified requirements, communication flaws [10], even for traditional software development. The development of ML systems makes the RE process even more challenging [90][91].

Managing expectations of customers: A potential gap between customers’ expectations and the delivered system has been reported as a potential problem in software projects [28]. Frequent customer engagement is an effective way of reducing this “expectation gap” [28]. Adding ML capabilities to a software system brings an extra complexity that can increase this gap. Customers generally do not understand the difference between traditional software and ML system [P6][P55]. While it is always possible to develop traditional software that always meets customers’ expectations (despite its challenges), this is not always possible for ML systems.

Nevertheless, customers may ask for “perfect ML systems” and have unrealistic expectations [P24][P29]. It is important to inform customers about the benefits of ML systems even without being imperfect [P24] and explain the possibility of change in the level of success of ML systems on production in time [P56]. Customers should be guided to think about possible alternative scenarios in which ML systems are not acting as expected and providing input on how to detect such scenarios on production and how the system should behave in such circumstances.

Eliciting and analyzing requirements: Requirements of ML systems are heavily dependent on available data; different data sets may lead to different needs [P44][P56]. Requirements are much more uncertain [P24][P44][P56][90][118], and hence they are more difficult to elicit and analyze. Some requirements should be stated as hypotheses to be tested via experiments [P56] to understand what is possible to deliver. Conducting such experiments requires additional skills to deal with data [P4] while eliciting and analyzing requirements. Besides, new techniques are necessary for analyzing requirements regarding ML capabilities [P44].

Specifying requirements: Requirements to be fulfilled by ML components are generally specified using quantitative measures (such as accuracy, precision, recall, F measure) [P29][P55][P56] that are new for many stakeholders. It may also be difficult to map these measures to business objectives [P6][P12]. While it is relatively easy to measure a metric such as accuracy, if that metric decouples from business objectives, customers think that the ML system does not deliver what it should provide [12]. Besides specifying each requirement correctly, all specified requirements should exhibit qualities such as completeness and consistency [25]. Some researchers present recommendations and examples for specifying requirements correctly [27][38][39]. In parallel with the rise of ML systems, new quality metrics to ensure completeness, consistency, etc. should be defined [P3] and contemporary techniques for specifying types of requirements, such as performance [P26], robustness [P26], and fairness [P22][P26], should be developed.

Dealing with new types of quality attributes: Quality attributes (also named as non-functional requirements) have been defined and well understood for traditional software [25][26]. Stakeholders need to elicit requirements on new types of quality attributes, such as explainability, fairness [P22][92][95], and freshness [78].

Explainability of an ML system measures how a human observer can understand the reasons behind a decision (such as a prediction) made by that ML system [15]. Explainability is quite essential in building trust between an ML system and its users [30]. Therefore, requirements on explainability should be elicited. Users may need to have explanations on a failure [P6][P24], a single decision [P55], or a model used in an ML system [P55]. In some domains, such as software analytics, making models explainable to users is as important as making accurate decisions [15]. Defense Advanced Research Projects Agency (DARPA) has started a program named “Explainable AI (XAI),” which aimed at developing more explainable models [29][31].

As ML systems are increasingly being used in domains sensitive to discrimination (such as education, employment, healthcare) due to protected characteristics (such as gender and race), it becomes crucial to avoid making decisions biased
by protected characteristics. Various definitions of this new type of quality attribute, fairness, have been presented [13]. It is essential to elicit requirements on fairness and identify protected characteristics [P55]. If protected characteristics are directly identifiable, excluding them from the training data can fulfill the fairness requirement. On the other hand, some characteristics, which do not seem to be protected, may highly correlate with a protected characteristic [14]. For instance, address data, which may be correlated with race, may be used to train a model for credit scoring. It is crucial to find out such red-lining effects [33] or indirect discrimination [34].

Freshness requirement [78] refers to the conditions for updating ML models. ML models’ performance may change over time due to some reasons, such as changing patterns in input data (data drift). It is crucial to determine the tolerance to performance degradation and the conditions that will trigger ML model updates. Freshness requirements can be defined as a period (daily, weekly, monthly update of ML models). A set of rules can also be defined for ML model updates. In such a case, the performance of ML models should be monitored, and required actions should be taken. Analyzing freshness requirements is essential to get prepared for ensuring a certain level of satisfaction for users continuously.

There are also efforts to identify possible risks and negative impacts of ML systems [96]. For instance, “Ethics guidelines for trustworthy AI” define the ethical principles that an ML system should adhere to [94]. These principles should be continuously considered while engineering ML systems to ensure Trustworthy AI [94].

**Dealing with new types of conflicts between requirements:** It is crucial to find the right balance of quality attributes for delivering successful software systems [35]. To be able to do this, conflicts among desired quality attributes should be identified [35]. Possible conflicts for traditional software have been identified and documented a long time ago [25][35][36][37]. ML systems pose new challenges for conflict resolution [P22]. Recently, researchers started to explore conflicts between specific quality attributes, such as the trade-off between fairness and performance or accuracy [14].

**Dealing with changing emphasis on different requirements:** Stakeholders often focus on functional and non-functional requirements during the RE process. On the other hand, data requirements analysis is an integral part of RE and focuses on information needs, providing a set of procedures for identifying, analyzing, and validating data requirements [40]. Stakeholders aim at understanding data entities to be used in traditional software. Description, data type, length, and value range of data elements are analyzed to understand the data entities’ structure [25]. To develop ML components, stakeholders also have to analyze what data instances of these data entities are present and what they can get out of these [P55].

Business rules include government regulations, corporate policies, and industry standards and form the rules that a software system must comply with [25]. Business rules are not software requirements themselves, but they sometimes originate new requirements or apply constraints on requirements. With the digitalization of high-volume data, especially personal data, data privacy regulations have been put in place. For instance, the EU’s new data privacy rules, the General Data Protection Regulation (GDPR), significantly impact the development and use of ML systems in Europe. Besides, companies also form their data privacy policies [57]. For instance, Google’s data privacy policy only allows working with anonymized and aggregated summary statistics, making exploratory analysis extremely difficult [57]. Data privacy rules should be considered carefully while analyzing requirements [P6][P55][118]. Although this should also be done for traditional software, data privacy rules can significantly affect what an ML system can perform. A team can allocate some effort to anonymize data [42][43] by assessing its cost and benefit [41]. New approaches are being developed to provide a better understanding of various privacy-related requirements for improving privacy policy enforcement when developing systems integrated with social networks [58].

### 5.7.2 Design

Design activities aim at producing logical descriptions of how a system will work [44]. These descriptions can be at a high-level, i.e., architectural design and lower levels. Many best practices for designing traditional software have been presented in the literature. Design patterns for low-level design [49], architectural patterns and styles [51][52] for high-level design, and some other design principles, such as GRASP [49] and SOLID [50], are already in place to be used by software engineers. While all of these are valid for engineering many software systems components, developing ML capabilities requires some changes and additions to these best practices [45][117].

There is some literature on designing the internals of ML components, such as design patterns for convolutional neural networks [55] and architecture for computer vision [56]. As I pointed out before (in Section 4.1), I focus on design from a SE perspective.
Designing for monitoring performance degradation on production: A degradation in how well an ML system meets users’ expectations should be expected on production in time [P56]. Known as “concept drift,” underlying training data distribution may change, and these changes make the model built on old data inconsistent with the new data [102]. This change poses two crucial challenges: detecting when concept drift occurs and keeping the models up-to-date [103].

Yokoyama [P60] proposes an architectural pattern for locating performance problems and rolling back in case of a failure on production. Defense Advanced Research Projects Agency (DARPA) started a program named “Assured Autonomy” [53], who’s one of the aims is developing design toolchains to achieve continual assurance. Continual assurance is defined as an assurance of the safety and functional correctness of a system provided provisionally at design time and continually monitored, updated, and evaluated on production as the system and its environment evolves.

Using new solution patterns for solving problems: Engineers do not have a mature set of solution patterns for solving the issues posed by ML. Sculley et al. reflected upon their own experiences in a position paper recounting their views on the difficulties of developing ML systems [46]. They reported one of the complexities posed by ML systems as the “change anything, changes everything” principle, which refers to the dependencies among all the parts of an ML system, i.e., application code, “glue code,” ML libraries, and external data [46]. This principle prevents the use of standard techniques (such as abstraction and information hiding) for reducing coupling [P56], which is a fundamental design principle for traditional software [46]. Not being able to isolate the impact of a specific change anywhere in the system of dependencies could be why our practitioners so often resorted to ad hoc practices like trial and error and rules of thumb.

Researchers started to publish the lessons learned from failures as anti-patterns [46]. Belani et al. [118] state avoiding anti-patterns as a design challenge and warns engineers for staying away from producing glue code, pipeline jungles, dead experimental code paths, and configuration debt [118]. Washizaki et al. [117] state that ad-hoc solutions are being used for solving everyday problems in developing ML systems. Washizaki et al. [117] list some of the patterns and anti-patterns for designing ML systems by stating that these patterns do not cover all the common problems. There is a need for a catalog of patterns dedicated to ML-specific problems [117]. A recent study [47] has surveyed architectural and design (anti-)patterns for ML systems to bridge the gap between traditional and ML systems concerning design.

Dealing with high-volume data: Distributed architectural patterns are widely used in designing ML systems to cope with high-volume data [P56], which leads to additional complexity in architectural and detailed design [P56]. While Anderson [48] emphasizes the paramount significance of data modeling in engineering data-intensive systems that are scalable, robust, and efficient, de Souza Nascimento et al. [P12] state the difficulty of succeeding in doing this. Benton [54] proposes an architecture for an ML system that deals with high-volume data. This architecture includes a component for data federation to deal with structured, unstructured, and streaming data.

5.7.3 Software Development and Tools

While developers code the solution in traditional software components, they infer the solution using data and ML algorithms in ML components [84]. Therefore, developing ML systems necessitates rethinking current development practices, tools, and infrastructures [84]. ML model development practice differs from traditional software development due to its data dependency, uncertainty, and experimentation requirements. Organizations, which continuously develop and deploy ML systems, must have a proper process to support the highly iterative development, testing, and deployment of ML models [83]. Based on the final paper pool, most challenges in developing ML systems manifest in issues related to data; models; dependencies; infrastructure and tools; ML algorithms, techniques, and libraries; and reuse.

Dealing with data: Data preparation is a vital and inevitable group of activities for developing ML systems [83]. Discovering, accessing, collecting, cleaning, and transforming data is challenging and time-consuming [P4][P6][P21][P29][P33][P45]. There may be various types of data sources, such as transactional systems, data warehouses, data lakes, data meshes, and real-time data streams [67]. Developers may build data pipelines to have data ready for model development. Developing data pipelines may involve dealing with structured and unstructured data [P2]. In addition, combining data is not always straightforward [P29][P33] since different systems can have other objectives for storing data, hence leading to data semantics heterogeneity and data integration problems. Data pipelines are essential artifacts, which should be version-controlled, tested, deployed, and maintained [67]. A frequently seen type of bug in ML systems is a “data bug” [P25]. Data verification tools may help engineers catch data bugs, such as improper format or encoding, missing data, etc. [P25].

Understanding ML algorithms, techniques, and libraries: Once data is ready, developers use algorithms, techniques, and libraries to produce models [67]. They face challenges in understanding these [P62][P2], especially the ones related to DL
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[P2], and identify a proper model [P25]. Use of automated model and parameter recommendation tools [P25], better documentation [P2], or having ML engineers in a team may help in overcoming this challenge.

**Dealing with models:** After having requirements and data ready, the team develops models. This development endeavor involves some sub-activities, such as feature engineering, model training, model evaluation, and model deployment [P4]. Developing models may require many iterations and experimentation, including many feedback loops between sub-activities [P4]. Even the model requirements may not be apparent before starting with model development and may be clarified after many experiment iterations. Developers work on extracting informative features for models [P4][P21][P29]. They may need to optimize a possible tradeoff between the best features and model complexity [83]. For some models (convolutional neural networks), feature engineering is performed implicitly during model training [P4].

Developers usually reported that analyzing and understanding the structure and behavior of ML models (mainly neural networks) is very difficult [P63][P57][P5][P4][P21]. This difficulty may lead to problems in evaluating and debugging models. Researchers attempt to provide a solution for this challenge via visualization. DeepVisual is a visual programming tool for designing and developing DL systems [P57]. DARVIZ tool supports a visual model-driven development environment [P45].

Model deployment involves some challenges. In some cases, a lot of manual work may be needed for deployment [P6]. If deployments are widespread, some automated deployment mechanism may be considered [P4]. Moreover, developers may have to scale up models to deployment architectures using code parallelization [P6][48].

**Dealing with dependencies:** Building highly cohesive and loosely coupled components is a powerful way of managing complexity in traditional software development [44]. It is possible to encapsulate behavior and associated data in modular components. On the other hand, ML components generally depend on external data [66]. Although there are some tools for exploring such data dependencies [85], these are not as capable and common as the static analysis tools for traditional software. Another type of dependency is named “undeclared consumers” [66]. The outputs of an ML model may be used by many other components implicitly. In such cases, the changes in the ML model may negatively affect the dependent components [P21][P33][118]. Therefore, it is vital to consider the potential negative impacts of such dependencies during development.

**Reusing models:** Reuse in traditional software development is vital to increase productivity and quality and decrease development time and cost [86]. While reusing ML libraries is very common, effective, and efficient, reusing ML models in different domains or systems is not straightforward [P3][P4][P6][P20][P45]. Adapting the implementation of a neural network for a different task [P62] or transferring a built solution to another domain [P6] remains a challenge. Using training data from other domains is another reuse strategy in ML. Transfer learning refers to using training data from another domain to develop an ML model in a domain of interest [87][88]. Transfer learning is mostly preferred when it is not possible or too costly to obtain training data. Although transfer learning is an attractive topic in ML, it has not been addressed by the studies in the final paper pool.

**Dealing with the development environment, tools, and infrastructure:** The presence of diverse and incompatible programming and data tools is a severe concern for engineering ML systems [P29]. A heterogeneous tool set challenges engineers in many tasks, such as data processing, environment setup, and model deployment [P2]. Therefore, researchers recognized the importance of having a proper ML system development infrastructure [P6], preferably by integrating ML development support into traditional software development infrastructure [P3][P4]. On the other hand, such integration may be challenging due to the different characteristics of ML and traditional software components [P4]. There are some attempts to bring ML system development capabilities to existing Integrated Development Environments, such as Azure ML for Visual Studio Code [P4]. Due to the highly iterative nature of ML model development, the infrastructure should enable experiment management [P5][P17][P33]. ModelKB is a tool prototype to manage experiments involving DL models [P17].

Tripakis [P45] and Menzies [P20] points out the heterogeneity of DL platforms that leads to interoperability problems. The model-driven development approach may increase the level of abstraction and facilitate the intuitive development of DL models in a platform-agnostic fashion [P45].

Working with a large volume of data that requires a distributed system brings additional complexity to development [P5]. Distributed systems require further knowledge and experience and additional cost and management of associated hardware and software [P5].
5.7.4 Testing and Quality

Testing ML systems poses challenges that arise from the fundamentally different nature and development of ML systems (as briefly explained in Section 2.2), compared to relatively more deterministic traditional software systems [125]. In 2007, Murphy et al. mentioned the idea of testing ML systems and classified such systems as “non-testable” [P39]. Although non-testability is attributed to a lack of reliable test oracle [185], there are several challenges in testing ML systems. I classified these challenges into eight categories.

**Designing test cases**: Test case design refers to identifying test inputs and outputs that allow tests to be executed. Chechik et al. [P9] and Wan et al. [P56] mentioned the difficulty of test case generation for ML systems. As early as in 2007, Murphy et al. proposed creating test cases to test ML systems, particularly those that implement ranking algorithms [P39]. Groce et al. proposed a method for effective test case selection [P18]. Ma et al. proposed a test generation technique based on combinatorial testing for DL systems [P34].

The Discovery of adversarial examples is a fundamental problem in engineering ML systems [P51]. As a result of this, Sun et al. [P49] presented DeepConcolic, a tool for testing deep neural networks. DeepConcolic adopted concolic analysis approach and generates test cases guided by neuron coverage and MC/DC variants for deep neural networks [P49]. Braiek and Khomh proposed DeepEvolution, a search-based approach for testing DL models that relies on metaheuristics to ensure the maximum diversity in generated test cases [P8].

Some researchers focused on generating test inputs as naturally as possible for testing autonomous cars, such as DeepTest [P53], DeepHunter [P59], and DeepRoad [P61]. On the other hand, some of the generated images (test inputs) were still unnatural and could not be recognized by humans [125]. Gambi et al. followed a different approach and proposed an approach to generate test cases from police reports of car crashes to cope with the scarcity of sensory data collected during real car crashes [P16].

Fairness can be an essential quality attribute of ML systems [13], as pointed out in Section 5.7.1. Udeshi et al. proposed an approach to systematically generate discriminatory test inputs and reveal fairness violations in ML models [P54]. They first performed random sampling on the input space and then derived further test cases based on these random samples [P54]. Aggarwal et al. performed systematic searching to generate test cases for detecting problems in fairness and aimed at eliminating the redundancies produced by random sampling [P1]. Sharma and Wehrheim proposed a metamorphic testing framework for testing balancedness (which complements fairness) of an ML classifier [P47]. They mutated training datasets in various ways to generate new datasets [P47].

**Evaluating test cases**: Test case evaluation is a complex task since it is hard to formalize and measure test cases’ characteristics influence quality [122]. Coverage of a test suite is used for test case evaluation when precise quality measures are not present [122]. The higher coverage a test suite achieves, the more defects hidden in code are expected to be detected [125]. Unlike traditional software, code coverage cannot be used for ML components since the decision logic of ML capability is obtained via training an ML model, not via explicit coding [P24] [P27] [P28] [P36] [P46] [P51] [125]. The size of test case sets is enormous, and missing test cases is a more challenging problem for ML systems [P27]. [P28] and [P46] state that existing coverage criteria are not sufficiently fine-grained to capture subtle behaviors exhibited by ML systems. Ma et al. designed a set of coverage criteria for deep neural networks to assess the testing adequacy [P35]. Sun et al. formalized the coverage criteria for deep neural networks studied in the literature and used it to increase the coverage [P51]. In their more recent study, Sun et al. proposed four coverage criteria tailored to deep neural networks’ structural features and semantics [P50]. Du et al. proposed new coverage criteria for DL systems based on recurrent neural networks and utilized these criteria to generate more adversarial samples and reveal more failures [P13]. Although researchers try to develop new coverage criteria appropriate for DL models, Li et al. could not find a strong correlation between the number of misclassified inputs in a test set and its structural coverage [P31]. Ma et al. focused on test data quality and proposed a mutation testing framework specialized for DL systems for data quality assessment [P36].

**Preparing test data**: Test data preparation has been identified as a challenge for traditional software development decades ago [32]. Access to high quality test data is a concern for developing ML systems [P5] [P19] [P30] [P32] [P35] [P36] [P56]. In some cases, collecting testing datasets may require manual labeling, which is labor-intensive [P32] [P56]. DLFuzz, proposed by Guo et al., aims to generate adversarial examples without manual labeling effort [P19]. By finding new and especially rare inputs that improve neuron coverage in DL models, DLFuzz tries to ensure the reliability and robustness of DL systems [P19]. Besides, since ML systems are expected to cope with the external world’s dynamic nature to some degree, datasets should be updated [P5]. Therefore, an infrastructure for automated data collection and labeling may be developed [P30].
**Executing tests**: Test execution refers to running the code (including an ML model) and comparing the expected and observed results. One needs a test environment involving trained ML models to execute the tests [P17]. ModelKB tool allows a tester to test a specific experiment model via a user interface [P17]. On the other hand, ModelKB tool prototype does not support all kinds of ML algorithms and ML problems [P17].

Cross-framework and cross-platform support become more critical as ML models are deployed on various hardware types, such as cloud platforms, mobile devices, and edge computing devices [P62]. To this respect, Zhang et al. proposed a differential testing framework to test ML models against potential inconsistent behavior in different settings [P62].

**Evaluating test results**: Test evaluation refers to assessing the testing results using test oracles and giving pass or fail decisions for test scenarios [126]. Identifying test oracle (“oracle problem” [183]) is one of the challenges in ML systems testing [P39]. Dwarakanath et al. applied metamorphic relations to image classifications with SVM and DL systems to tackle the oracle problem [P14]. Similarly, Xie et al. proposed an approach based on metamorphic testing to alleviate the oracle problem in testing ML classification algorithms [P58]. Nakajima proposed a behavioral oracle that monitors changes in certain statistical indicators during the training process and forms a basis for metamorphic relations to be checked [P40]. Based on these metamorphic relations, Nakajima generated test inputs for testing neural network models [P40]. Cheng et al. conducted some experiments and found out that metamorphic relations are not effective [P11]. Qin et al. proposed a program synthesis technique to systematically construct oracle-alike mirror programs to alleviate the oracle problem [P43]. Chen et al. applied the variable strength combinatorial testing technique to measure the adequacy of deep neural network testing [P10]. Barash et al. proposed generating test cases using the modeling process of combinatorial testing [P7]. They tried to utilize business requirements and detect weak sides of an ML system from a business perspective [P7].

Zheng et al. proposed a method for identifying translation failures in neural machine translation systems without reference translations, i.e., test oracle [P65]. Sun and Zhou used a metamorphic testing technique to test machine translation services without a human assessor or reference translation [P48].

The non-deterministic nature of ML systems makes test evaluation more challenging [P5][P23][P24][P41][P52]. Unlike testing traditional software, finding one or a few incorrect results does not necessarily indicate the presence of a bug [P14]. Since ML systems are validated via probabilistic ML performance metrics (like accuracy, F-measure), observing an unexpected output resulting from a single test case execution does not necessarily mean a bug [P64]. Moreover, good performance during testing cannot guarantee the satisfactory performance of ML systems on production [P56]. Barash et al. introduced a method to bridge the gap between business requirements and ML performance metrics [P7]. By doing so, they were able to evaluate test results against business requirements [P7].

**Debugging and fixing**: It is very critical to detect and remove bugs as much as possible before launching an ML system. Different from traditional software, data bugs are also very vital for ML systems besides bugs in code. The difficulties of debugging ML systems were pointed out by several studies [P27][P56][P62][P64]. One reason for this is the prevalence of non-determinism in the training process, which leads to hard-to-reproduce bugs [P56][P64]. Zhang et al. pointed out the importance of debugging and profiling for ML systems [P62]. To this end, some approaches and tools have been developed for finding bugs in training data, ML/DL models, and code, such as DeepFault [P15], LAMP [P37], MODE [P38], and DARVIZ [P45]. DeepFault is a whitebox deep neural network testing approach to identify suspicious neurons that may lead to inadequate performance [P15]. Ma et al. proposed LAMP technique and developed a prototype tool for finding bugs in input data, graph models, and graph-based ML algorithm implementations [P37]. MODE identifies faulty neurons in neural networks [P38]. DARVIZ tool helps in debugging the training process of DL models [P45]. ML systems heavily depend on ML libraries, frameworks, and platforms. The bugs in these components impair ML systems [P20]. With this, Pham et al. proposed an approach, named CRADLE, to find and localize bugs in DL libraries [P42].

**Managing tests**: Test management refers to planning, controlling, and monitoring testing activities [126]. [P3] states the need for certification and qualification activities to manage tests, especially for safety-critical software systems.

**Automating tests**: Software test automation has already moved beyond a luxury to become a necessity to cope with large complex systems [123] and decrease testing costs [124]. The cost and required resources to test ML components, especially for autonomous driving, is steadily increasing [P30]. Therefore, new tools and techniques are required to automate testing for ML systems for providing more robust systems, especially in safety-sensitive domains [P30]. Tian et al. automated test case generation for safety-critical DL-based systems like autonomous cars [P53].
### 5.7.5 Maintenance and Configuration Management

With the emergence of many general-purpose ML libraries, services, platforms combined with the accumulation of ML experience, developing ML systems has become relatively easy and cheap, whereas maintaining them over time is difficult and expensive [66]. Maintaining ML systems involves keeping track of additional configuration items, models, and data, besides code [67]. Moreover, ML systems should be monitored continuously since their performance is subject to change due to their non-deterministic nature. The papers in my pool mainly identify three groups of challenges, which are interrelated:

**Dealing with configuration management of data and ML models:** ML systems enlarged the scope of tracking and controlling change. Data and ML models are essential configuration items besides code [67][118]. While versioning data is a vital need [P3][P4][P56][P60][118], the methods and tools to support this is not mature yet [P4]. Versioning data does not only involve keeping track of datasets but also keeping track of metadata of datasets [69] and their relationships to ML models [P4]. Another requirement can be comparing datasets and exploring differences between datasets [70]. All of these aspects make configuration management of the data component complicated [68]. ML models derived from data constitute the other type of essential configuration item [P3][P17][P56][P60][118]. Models are mainly made up of algorithms, hyperparameters, and their dependencies on datasets [P4][P60]. Model management, which refers to tracking, storing, query, comparing, reproducing, and sharing models [P17], has been identified as one of the most challenging and time-consuming activities [71][75]. There are some attempts to address the challenges in model management, such as ModelHub [72], ModelDB [73], and MLflow [61]. Open source tools, such as DVC (dvc.org), were launched for version control of ML components. These methods and tools should be integrated with the overall engineering process and the other tools used to develop and maintain ML systems.

**Dealing with the history of experiments:** While it is necessary to keep track of changes in data and ML models, some large-scale ML systems involve configuration management at a higher level, i.e., keeping track of experiments. Each experiment may have many components that affect the outcome, i.e., the ML model. These components can include hardware (GPU models primarily), platform (operating system and installed packages), source code (model training and pre-processing), configuration (model configuration and pre-processing settings), training data (input signals and target values), and model state (versions of trained models) [P5][P56][P60]. The development of ML components is an iterative and experimental process [76], and hence, it is prevalent to perform a vast number of experiments to identify the optimal ML model [P5]. Also, it is also possible to use automated meta-optimization methods and conduct lots of experiments without human intervention. Whether done automatically or manually, experimentation activities generate many artifacts (datasets, hyperparameters, models, libraries, etc.), which should be versioned [77]. Therefore, experiment management is a recent and complicated challenge in engineering ML systems [61][74]. Teams may require to compare, reproduce, and share experiments [P33][P17]. Improper experiment management may result in some problems: (1) experiments may not be reproduced when needed [P21][61]; (2) some experiments may be repeated unintentionally [P21]; (3) experiments and their results may not be analyzed, reported, and shared appropriately.

**Dealing with re-training and re-deployment:** One of the hardest parts of maintaining ML systems is to keep the performance (such as accuracy) at a certain level or improve it if needed. Unforeseen changes in the external world may cause changes in input data patterns and negatively affect the performance of ML components (known as “concept drift” [102], see Section 5.7.2). The type of concept drift, i.e., sudden or gradual [102], and its impact should be considered when dealing with re-training and re-deployment. In some cases, concept drifts in data streams should be detected promptly [104]. Žliobaitė provides a framework for thinking about decision points when addressing concept drift [105].

Therefore, it is critical to monitor the performance and take the necessary actions, if required, [P6][P56][89]. Automatic maintenance mechanisms can be built to keep the performance at a certain level [P56]. Such mechanisms can detect performance degradation and take the required actions by re-training ML models with new data. On the other hand, it is questionable to what extent this can be achieved in all domains without human intervention, especially in risky domains, such as health. In risky domains, automated checks can be used to trigger notifications if predefined thresholds are violated [P6].

In some cases, it may be required to deploy an updated ML model to the production environment to get users’ feedback. Canary release approach may limit the possible negative impact of the new ML model and help to cope with the risk of deploying an updated ML model [P60]. Canary release refers to deploying a new ML model (or any other component) for a restricted number of users and rollback the deployment if a negative impact is observed [155].
5.7.6 Software Engineering Process and Management

There are some process models, phases, activities that document steps to develop and maintain ML models. For instance, Hulten [62] breaks down the ML process into five stages: (1) getting data to model, (2) feature engineering, (3) modeling, (4) deployment, (4) maintenance. Shams [64] shows the typical steps involved in the model development lifecycle: (1) define the problem, (2) collect, cleanse, and prepare data, (3) build and train model, (4) tune hyperparameters and validate model, (5) deploy to production. The steps are not executed as a waterfall process; there is feedback from deployment to problem definition and an iteration from building a model to deployment [64]. Rao [63] demonstrates a three-phase ML product development process to shorten the delivery time from idea generation to deployment. On the other hand, processes that guide teams in engineering ML systems with ML and traditional software components are needed.

Harmonizing the activities for developing ML components with software process: Adding ML components to a software system involves additional actions to be performed. Teams developing ML systems need more guidance in the form of a software process that can be tailored according to specific project needs [P3][P12][118]. Data lifecycle activities form a critical and compelling subgroup of activities, which profoundly affect ML projects’ success [P56][79]. Therefore, SE process standards should be enriched to handle data lifecycle activities [81]. Besides, new agile approaches, such as DataOps [80][187], are needed to meet increasingly demanding and evolving business requirements via ML systems. ML model lifecycle activities are another vital subgroup of activities integrated with the SE process [P3][12]. Besides data and ML model lifecycles, teams need guidance on various aspects, such as engineering requirements [P3][118], handling data [P12], testing [P3], and maintenance [P6].

Assessing the ML process: Teams may need to evaluate their ML process to understand and improve their capabilities. There are some early attempts to determine the ML process’ maturity [P4] and how ML components are used in larger software systems [P33]. A mature process assessment is required to identify possible smells regarding the ML process, especially in large-scale ML systems [66].

Estimating effort: Due to the uncertainties in the ML process, it is hard to estimate effort and do planning [P56]. In some cases, the team cannot know whether the quantitative targets are achievable until final ML models are obtained [P56]. As a result of not being able to estimate effort, business owners act impatiently and cancel ML component development despite promising intermediate results [P5].

5.7.7 Organizational Aspects

Engineering complex systems, such as ML systems, is a complicated endeavor with organizational and technical aspects [59]. Part of the organizational challenges involves identifying skill sets and roles required to engineer ML systems [82]. Seven papers in the final pool address the challenges in two main categories from an organizational perspective: Having the required skill sets and having a team working harmoniously.

Dealing with various skill sets: Engineering an ML system involves skill sets from multiple fields, i.e., machine learning, deep learning, data science, mathematics, algorithms, software engineering, and statistics [P2][P3][P56][60][118]. A proliferation of roles, including specialists, in particular, SE phases, such as design [18] or specific types of algorithms such as natural language processing [12]. Practitioners and academicians already started to identify emerging roles to classify skill sets and have proper people in teams to engineer ML systems [P29][60]. While there are generic roles such as data scientist, ML engineer, data analyst, ML software engineer, ML researcher, and software engineer, there are more specific roles, such as data evangelist, data preparer, data shaper, data analyzer [P29].

Building harmony among isolated roles: Having the required people with proper skill sets is necessary but not sufficient to engineer ML systems. People having different backgrounds have cultural [P5] and language differences. Therefore, it is challenging to get all these people working together towards achieving a common objective [P4]. It is even challenging to have all these people on the same page [P29].

6 DISCUSSION

This section presents some potential research directions from the SE perspective (Section 6.1), other implications independent from SE aspects (Section 6.2), the possible benefits of this review (Section 6.3), and then limitations and potential threats to validity of this review (Section 6.4).
6.1 Potential research directions from the SE perspective

In this subsection, I summarize the main research directions from an SE perspective. Researchers may refer to Table 13 to form more detailed research questions.

Requirements engineering for ML systems: Specifying ML components’ requirements requires a different perspective than traditional software components. It is difficult and mostly impossible to characterize all of the behaviors of ML components under all circumstances [178]. Rather than specifying precise requirements, hypothesizing what outcomes can be obtained from data should be the starting point [P56], and requirements shall be refined via experimentation [P24]. Besides, ML systems include traditional software components as well. Therefore, integrating proper practices to specify ML and traditional software components’ requirements is a research problem [P55]. Specification of new types of quality attributes, such as explainability [180], fairness [P22][92][95], and freshness [78], for ML components, may initiate new research questions.

Designing ML systems: Components with ML capabilities are becoming an architectural part of software systems, sharing cross-cutting functional and non-functional concerns [179]. Monitoring for potential performance degradation on production [P56][P60] and high-volume data processing [P12][P56] are two important design considerations for ML systems. New architectural styles and patterns for ML systems are required for robust systems to address these concerns [P56][22].

SE tooling for developing ML systems: ML systems’ development involves a diverse set of frameworks, tools, libraries, and programming languages [172]. The popularity of ML has brought a lot of tools, mostly open-source [173]. However, this diverse set of tools have emerged with challenges, such as compatibility [172], integration of various components [172], required knowledge and experience, etc. Lack of developer support tools for data-intensive systems is a challenge for developing ML systems [48]. Some tools emerged from academia, such as DARVIZ [P45], DeepVisual [P57], NeuralVis [P63], ModelKB [P17], to solve specific problems in developing ML systems. There are some efforts to bring various tools together to support the effective development of ML systems [174]. There are some platforms, such as MLflow [61], focusing only on the ML lifecycle. To support other SE aspects, such as generating Python components ready for deployment, version control conflict handling, and continuous integration, some tools, such as nbdev, have been released [175]. On the other hand, compared to tool support for traditional software development, there is room for improvement to have SE tooling for developing ML systems.

Testing ML systems: SE researchers focused mostly on testing ML systems. Despite many studies, we do not have mature testing techniques and tools to develop ML systems in industrial settings. Designing and evaluating test cases, preparing test data, executing tests, and assessing test results contain many research problems. To name a few of the research problems, generating test inputs, ensuring adequate test coverage, coping with oracle problem, and ensuring test data quality.

Debugging tool support: Debugging and profiling tool support is an essential deficiency for engineering ML systems [P62]. Although there are some approaches and prototype tools, such as DeepFault [P15], LAMP [P37], MODE [P38], and DARVIZ [P45], more mature debugging tools integrated with ML system development environments are required.

Test management: Planning, controlling, and monitoring of testing activities for ML systems have not been addressed by researchers. Some domains involving safety-critical ML systems, such as healthcare and autonomous driving, may be in urgent need of certification to reduce harmful risks.

Test automation: Automating tests has become a necessity to cope with large-scale complex systems [123]. More testing can be conducted via test automation to reduce the risks of ML systems. Therefore, new tools and techniques are required to automate testing for ML systems.

Maintaining ML systems: Data, ML models, and experiments have become essential configuration items in maintaining ML systems. Keeping versions of data and ML models require tools integrated with the development environment. Keeping track of experiments, reproducing, and comparing them on demand are open research areas for software engineers and tool developers.

Tailoring and assessing SE process: While there are many processes for ML lifecycle [62][63][64] and traditional software development [186], a set of harmonized practices for developing ML systems is required [P3][P12][118]. Blending the knowledge and experience in ML and SE areas and applying harmonized practices in industrial case studies seem to be a research direction. Researchers should develop DevOps practices for data and ML model components (like DataOps
[80][187] and ModelOps [188]) to keep ML systems up-to-date against rapidly changing external factors. Moreover, frameworks for process assessment can be another open area for research [66].

**Managing ML systems development projects:** While there are some examples of using ML algorithms for project management (two examples in ML for SE [176][177]), our primary study pool does not include any practices for managing ML systems development projects. Wan et al. only mentioned the difficulty of effort estimation in ML projects [P56]. Planning, controlling, and monitoring ML projects involve open research questions, such as effort estimation (an early work from 1993 is [137]).

**Forming coherent teams:** Engineering an ML system involves skill sets from various fields, i.e., machine learning, deep learning, data science, mathematics, algorithms, software engineering, and statistics [P2][P3][P56][60][118]. Organizations need to determine the roles and responsibilities and associated required skillsets for engineering ML systems. Forming a coherent team from people with different backgrounds may bring new problems to tackle.
### Table 13. Challenges and proposed solutions identified by researchers classified by knowledge area

| Knowledge Area                  | Challenge                                         | Primary Study ID | Proposed Solution(s)                                                                 |
|---------------------------------|---------------------------------------------------|------------------|--------------------------------------------------------------------------------------|
| **Requirements Engineering**    | Managing expectations of customers                 | [P6][P24][P29][P55][P56] | • inform customers about the benefits of ML systems even without being imperfect [P24]  
• explain the possibility of change in the level of success of ML systems on production in time [P56] |
|                                 | Eliciting and analyzing requirements               | [P4][P24][P44][P56] | • state some requirements as hypotheses to be tested via experiments [P56]            
• refine requirements by means of experiments [P24] |
|                                 | Specifying requirements                            | [P3][P6][P12][P22][P26][P29][P55][P56] | • use a checklist to identify business metrics [P12]  
• use logical formulas to express classification performance, robustness, and fairness of ML classifiers [P26] |
|                                 | Dealing with new types of quality attributes       | [P6][P22][P24][P55] | -                                                                                   |
|                                 | Dealing with new types of conflicts between       | [P22]             | -                                                                                   |
|                                 | requirements                                       |                  |                                                                                     |
|                                 | Dealing with changing emphasis on                 | [P6][P55]        | -                                                                                   |
|                                 | different types of requirements                   |                  |                                                                                     |
| **Design**                      | Designing for monitoring performance degradation on | [P56][P60]       | • use a specific software architectural pattern to deal with operational problems such as problem localization and rollback at failure [P60] |
|                                 | production                                         |                  |                                                                                     |
|                                 | Using new solution patterns for solving problems   | [P56]            | • design effective solutions via experiments [P56]                                  |
|                                 | Dealing with high-volume data                      | [P12][P56]       | • use a checklist to validate a design model against high-volume data [P12]         |
| **Software Development and Tools** | Dealing with data                                  | [P2][P4][P6][P21][P25][P29][P33][P45] | • use data verification tools [P25]                                                |
|                                 | Understanding ML algorithms, techniques, and       | [P2][P25][P62]   | • produce better documentation for ML libraries (better explanations for methods and parameters, more tutorials covering various use cases, FAQ sections) [P2]  
• use automated model and parameter recommendation tools [P25] |
|                                 | libraries                                          |                  |                                                                                     |
|                                 | Dealing with models                                | [P4][P5][P6][P21][P29][P45][P57][P63] | • use a model-driven development based and platform agnostic framework to generate DL library specific (for TensorFlow, CAFFE, Theano, Torch, etc.) code (such as DARVIZ) [P45]  
• use a visual tool to develop DL models (such as DeepVisual) [P57] |

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| **Testing and Quality** | **Dealing with dependencies** |  
| | [P21][P33] | • use a visual tool for supporting engineers in the understanding structure of neural network models (such as NeuralVis) [P63]  
| Reusing models | [P3][P4][P6][P20][P45][P62] | -  
| **Dealing with the development environment, tools, and infrastructure** | [P2][P3][P4][P5][P6][P17][P20][P29][P33][P45] | • develop and use extensions on current IDEs for ML system development, such as Azure ML for Visual Studio Code [P4]  
| | | • use a tool (such as DARVIZ) for model abstraction to provide interoperability across platforms [P45]  
| | | • use a tool to visualize and compare experiments (such as ModelKB) [P17]  
| **Designing test cases** | [P1][P7][P8][P9][P16][P18][P34][P39][P47][P49][P51][P53][P54][P56][P59][P61] | • use a method/tool for testing DL models [P18][P34][P39], such as DeepEvolution [P8], DeepCT [P34], DeepConcolic [P49]  
| | | • use a method/tool for generating test inputs for autonomous cars [P16][P53][P59][P61]  
| | | • use an approach to generate discriminatory test inputs to reveal fairness violations [P1][P47][P54]  
| **Evaluating test cases** | [P13][P24][P27][P28][P31][P35][P36][P46][P50][P51] | • use a coverage criterion appropriate for ML/DL models [P13][P28][P35][P46][P50][P51]  
| | | • use an approach to execute tests (such as ModelKB) [P17]  
| **Preparing test data** | [P5][P19][P30][P32][P35][P36][P56] | • use a tool (such as DLFuzz) to generate adversarial examples without manual labeling effort [P19]  
| | | • develop an infrastructure for automated data collection and labeling [P30]  
| **Executing tests** | [P17][P62] | • use a tool to execute tests (such as ModelKB) [P17]  
| | | • use a differential testing framework to detect potential inconsistent behavior of ML models on different settings [P62]  
| **Evaluating test results** | [P5][P7][P10][P11][P14][P23][P24][P39][P40][P41][P43][P48][P52][P56][P58][P64][P65] | • use metamorphic relations to tackle with oracle problem [P14][P40][P48][P58]; counter-evidence to use metamorphic relations [P11]  
| | | • use combinatorial testing to tackle with oracle problem [P7][P10]  
| | | • use a program synthesis technique to tackle with oracle problem [P43]  
| **Debugging and fixing** | [P15][P20][P27][P37][P38][P42][P45][P56][P62][P64] | • use an approach/tool to debug and fix DL models, such as DeepFault [P15], LAMP [P37], MODE [P38], DARVIZ [P45]  
| | | • use an approach to find and localize bugs in DL libraries, such as CRADLE [P42]  
| | | • compare the ML model with a model produced by a simple ML algorithm as a baseline and use the result as an indication for possible bugs in code and data [P56]  

| **DRAFT – Under review** |
|--------------------------|
| **Managing tests**       | [P3] | - |
| **Automating tests**     | [P30][P53] | - |
|                         |     | • use a systematic technique to automate test case generation, such as DeepTest [P53] |
| **Maintenance and Configuration Management** |     | - |
| Dealing with configuration management of data and ML models | [P3][P4][P17][P56][P60] | - |
|                         |     | • use a tool for data and ML model configuration management (such as ModelKB) [P17] |
| Dealing with the history of experiments | [P5][P21][P33][P56][P60] | - |
|                         |     | • use a proper software architecture suitable for troubleshooting [P60] |
| Dealing with re-training and re-deployment | [P6][P56][P60] | - |
|                         |     | • apply Canary release [155] approach for risky ML model re-deployments [P60] |
| **Software Engineering Process and Management** |     | - |
| Harmonizing the activities for developing ML components with software process | [P3][P6][P12][P56] | - |
|                         |     | • use checklists to perform ML-related activities in a standard way [P12] |
| Assessing the ML process | [P4][P33] | - |
| Estimating effort       | [P5][P56] | - |
| **Organizational Aspects** |     | - |
| Dealing with various skillsets | [P2][P3][P29][P56] | - |
| Building harmony among isolated roles | [P4][P5][P29] | - |
6.2 OTHER IMPLICATIONS

**Industry-academia collaboration:** As we can see from the answer of RQ4, this research topic is mostly dominated by academicians, although engineering ML systems is a highly practical area. Encouraging researchers from the industry to collaborate with academia and share their experience in SE venues may empower structured information on this research topic.

**Formation of research groups:** The answer to RQ3 reveals that the most prolific authors are generally collaborating. This observation may not be surprising because ML systems engineering brings together two challenging research areas, i.e., SE and ML. The formation of research groups could lead to better and more relevant results.

**Use of various research methods for all SE aspects:** As pointed out under RQ5, experiments are mostly used for testing and quality aspects. There are a few studies targeting development and maintenance. The paper pool does not include any study that uses experiment and case study to address requirements- and design-related challenges. Experiments and case studies should be undertaken to examine requirements- and design-related challenges identified via interviews and surveys. Process, management, and organizational aspects should also be addressed using various research methods.

**Use of various ML problems:** The answer to RQ6 indicates that researchers have mainly used classification problems for their experiments and case studies. It may be useful to use different ML problems, such as clustering, to find further challenges. Some of the concerns, such as some non-functional requirements, may be domain-specific [179] and can be discovered by exploring various ML problems.

6.3 POTENTIAL BENEFITS OF THIS REVIEW

Next, I will explore the potential benefits of this SLR for practitioners, researchers and academicians, and educators.

**For practitioners:** More and more software systems are involving ML capabilities. Practitioners should be aware of the new challenges that emerged with ML components since ML’s influences on software systems are expected to affect their role significantly [182]. This study provides an overview of these challenges and some suggestions for solutions (mostly not directly applicable but providing guidance).

**For researchers and academicians:** This SLR can be a valuable resource for future research on engineering ML systems’ challenges. As Table 13 reveals, many challenges have not been addressed. Moreover, even for the difficulties addressed, the proposed solutions are mostly conceptual or implemented as a prototype tool without industrial use. Researchers and academicians can use the challenges reported in this study for initiating research projects. In addition, I believe that the bibliography provides a good base for understanding the current situation. The answers for RQ2 and RQ3 give a starting point for deciding which venues and researchers to follow.

**For educators:** The 2020 version of the Future of Jobs Survey reveals that the top increasingly strategic job roles are data analysts and scientists, AI and ML specialists, robotics engineers, software and application developers, and digital transformation specialists [181]. The adaptation of university curricula based on this industrial need is therefore essential. Educators may use this study to either design new courses or adapt existing SE courses. One of the pioneer courses is the “Software Engineering for AI-Enabled Systems” course offered at Carnegie Mellon University [24]. The course takes a SE perspective on building software systems with a significant AI/ML component. It discusses how to take an idea and an ML model developed by data scientists and deploy it as part of a scalable and maintainable system.

6.4 LIMITATIONS AND POTENTIAL THREATS TO VALIDITY

The scope of this study is limited to the following parameters:

- **Date:** This study covers primary studies published until the end of 2021, i.e., 31 December 2019.
- **Type of Literature:** This study comprises studies published in peer-reviewed academic venues. Gray literature, e.g., papers only published in arxiv.org, blogs, videos, etc., have been excluded.
- **Perspective:** The primary studies have been selected from SE venues to reflect an SE perspective on ML systems engineering. Therefore, papers published in AI, ML, DL, Data Science, Data Management venues have been excluded.

Validity considerations are applicable for SMS and SLR studies, similar to empirical studies [150][151]. The threats to this SLR’s validity are mainly related to the specification of the candidate pool of papers, primary study selection bias, data extraction, and data synthesis.
The candidate pool of papers was specified by searching online databases using keywords. I used broad terms to form search keywords to reduce the risk of excluding potentially relevant studies. With this approach, I decreased precision and increased recall found more candidate papers to be assessed for specifying the final set of primary studies. I also searched for five widely used online databases in SMS and SLR studies in computer science and software engineering. Besides these five databases, I also searched Google Scholar to enrich the paper pool. In order to mitigate the risk of missing some relevant studies, I also carried out both backward and forward snowballing along with a manual search. I believe that an adequate pool of candidate papers has been formed for this study, and if there is any missing journal paper, the rate will be negligible.

Personal bias might have been introduced during the application of inclusion and exclusion criteria. To minimize this type of bias and errors whenever I could not decide on inclusion/exclusion by reading the abstract, I scanned the full text for the final decision.

The validity of data extraction is another essential aspect that directly affects this study’s results. In order to ensure the accuracy of the extracted data, I used existing categories in the literature where possible (RQ5, RQ6, and SE knowledge areas in RQ7). I aimed to decrease the risk of researcher bias by mapping the relevant data in primary studies to the specified groups. I applied the open coding technique iteratively and incrementally to identify the challenges and solutions (RQ7). This coding process potentially entails some researcher bias.

In general, primary study selection, data extraction, and synthesis are subject to researcher bias, and this bias may be higher than those SLRs with multiple authors. On the other hand, we can also find SLRs with single authors in SE [146] and other research areas [184].

7 CONCLUSIONS AND FUTURE WORK
Advances in machine learning lead to a transition from the conventional view of software development, where algorithms are hard-coded by humans, to ML systems that are materialized through learning from data. Therefore, we need to rethink our ways of developing software systems and consider the particularities required by these new types of applications.

This study aims to systematically identify, analyze, summarize, and synthesize SE research’s current state for engineering ML systems. Researchers have been showing an increasing interest in this research area since 2018 (RQ1). Although there are a lot of primary studies (Section 8.1) and secondary studies (Section 3) on this topic, many research questions remain unanswered (Section 6.1 and Table 13). More cooperation between industry and academia and conducting more experiments using real-world problems would help to extend the SE body of knowledge for engineering ML systems. Moreover, reporting on lessons learned from action research in the industry can provide valuable insights for answering research questions.

I plan to conduct a multi-vocal literature review to identify more challenges and solution proposals reported by the industry in future work.

8 REFERENCES
This section is divided into two parts: (1) Citations to the primary studies reviewed in the SLR; and (2) Other (regular) references cited throughout the paper.

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