Towards Probability-based Safety Verification of Systems with Components from Machine Learning

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Abstract. Machine learning (ML) has recently created many new success stories. Hence, there is a strong motivation to use ML technology in software-intensive systems, including safety-critical systems. This raises the issue of safety verification of ML-based systems, which is currently thought to be infeasible or, at least, very hard. We think that it requires taking into account specific properties of ML technology such as: (i) Most ML approaches are inductive, which is both their power and their source of failure. (ii) Neural networks (NN) resulting from deep learning are at the current state of the art not transparent. Consequently, there will always be errors remaining and, at least for deep NNs (DNNs), verification of their internal structure is extremely hard. However, also traditional safety engineering cannot provide full guarantees that no harm will ever occur. That is why probabilities are used, e.g., for specifying a Risk or a Tolerable Hazard Rate (THR). Recent theoretical work has extended the scope of formal verification to probabilistic model-checking, but this requires behavioral models. Hence, we propose verification based on probabilities of errors both estimated for by controlled experiments and output by the inductively learned classifier itself. Generalization error bounds may propagate to the probabilities of a hazard, which must not exceed a THR. As a result, the quantitatively determined bound on the probability of a classification error of an ML component in a safety-critical system contributes in a well-defined way to the latter’s overall safety verification.

Keywords: Software engineering, safety engineering, machine learning, deep neural networks, inductive generalization, probabilistic generalization error bound.
1 Introduction

Software-intensive systems, in particular cyber-physical systems (CPS), need to have essential properties like security and safety. While security especially of deep neural networks (DNN) has already been studied theoretically [Goodfellow et al. 18], there is an urgent need for a new safety framework. Hence, the focus of this paper is on safety verification of systems with components from machine learning (but not on systems that learn while being applied).

In practice, safety is taken very seriously, e.g., for railway systems in certain parts of Europe, at least, and there is a relatively new automotive standard for functional safety (of traditional cars), ISO 26262. It does not address safety assurance of ML-based functions, however. This was a key motivation for ISO/PAS 21448 on safety of the intended functionality (SOTIF), where Annex I (informatively) mentions a few of the issues involved in using ML in safety-critical systems. The Automated Driving Roadmap ERTRAC 17 contains the challenge of applying artificial intelligence, in particular (deep) ML, with regard to safety. There are no hints, however, on how to address it.

A safety risk combines the severity of harm with the probability that it occurs. Also THR and (A)SIL – (Automotive) Safety Integrity Level – are defined based on probabilities. Hence, we approach the difficult issue of safety verification of ML-based software-intensive systems on the basis of probabilities.

In fact, we propose to be even more ambitious than the current approach to verification of conventional automotive software according to the standard ISO 26262, where no explicit estimation of probabilities is included. The safety assurance principle of ISO 26262 assumes that an adequate level of rigor can reduce the residual risk of a hazard due to software failure to an acceptable level.

In this paper, we propose a new theoretical framework for safety verification of software-intensive systems including ML technology. It is based on existing work on safety verification, but has to take into account that especially for DNN only black-box approaches will be applicable, at least in the near future. Including controlled experiments for such a purpose is new for practical use, and the way of managing the data for such experiments will be new as well. In particular, this new framework involves determining a probabilistic generalization error bound.

An essential problem to be solved is that presenting instances for learning requires taking into account the right context in the application and in the final model, such that specific instances or sets of instances become relevant whenever needed. This has to be taken into account in the determination of hazard rates or risks, too.

The remainder of this paper is organized in the following manner. First, we sketch some background material and the state of the art, in order to make this paper self-contained. After that, we lay out the new framework for safety verification. Focusing on one of its key parts, we then sketch how one can take advantage of recent progress with probabilistic generalization error bounds for deep learning for the
purpose of safety engineering. Finally, we draw a tentative conclusion and propose future work.

2 Background and State of the Art

Recently, [Salay and Czarnecki 18] adapted and extended the standard [ISO 26262] to address safety assurance of ML-based functions, making a detailed assessment and adaption of [ISO 26262] for ML, specifically in the context of supervised learning. They carefully analysed and adapted each requirement in this standard and, where gaps were found, they proposed additional requirements. Still, they kept the safety assurance principle of [ISO 26262] that developing software using an adequate level of rigor can reduce the residual risk of hazard due to software failure to an acceptable level. We propose to be more ambitious through experimentally determined probabilities, aiming for higher guarantees of safety assurance for DNN than currently for traditional software. We consider this very important for potential medical applications as well.

Annex I of ISO/PAS 21448 essentially mentions unintended bias or distortion in the collected data as problems, referring to [Koopman and Wagner 17]. In fact, one of the most common assumptions in ML is that the training set and test sets are drawn from the same underlying distribution (i.i.d. – independently drawn from the identical distribution), that is, the training situation resembles the test situation. Without any further precautions or mechanisms, only then and with an increasing number of instances, learning, in the sense of getting measurably better at a task with increasing evidence, can take place.

Verification of DNN models is currently viewed as very hard, due to their high nonlinearity, emerging from a high number of layers and the variety of different architectures and topologies [Wicker et al. 18]. This work and [Huang et al 17] make a claim about safety verification while, in fact, both deal with a kind of robustness, more specifically against adversarial perturbations. It was taken up for confidence claims for analyzing robustness by [Burton et al 19], where more generally confidence arguments are presented for evidence of performance in machine learning for highly automated driving functions (see also the predecessor work in [Burton et al 17] and [Gauerhof et al 18]). We think that such arguments could be much stronger if based on probabilities.

In [Amodei et al. 16], the problem of accidents in machine learning systems is discussed by taking particular properties of ML into account, but not even mentioning induction. Generally, inductive machine learning is a case of inductive generalization, which is by definition not truth-preserving and an unsafe type of inference [Goodman 83]. That is why it is common to study generalization on the basis of learning curves, where the x-axis represents the number of training instances and the y-axis represents a chosen performance measure (for a recent example in the context of software product lines, see [Kaindl et al. 18]).

If probabilistic guarantees for the performance of an ML model are required, one can resort to generalization error bounds [Kääriäinen and Langford 05; Rückert and
Kramer 08]. Considering DNN, it has been observed that their behavior is sometimes unstable, i.e., their output varies largely depending on only small perturbations of the input. First approaches have addressed this problem from a technical point of view [Zheng et al. 16], e.g., by changing the training protocol or by alternative loss functions. From a higher point of view, the problems and variants are not much different than laid out already long time ago [Taylor et al. 03]. Nevertheless, it has been observed that error bounds based on traditional computational learning theory (e.g., based on the VC dimension, PAC-Bayesian approaches, or the Rademacher penalty) do not work for deep learning models, because of their large capacity. This is in contradiction to their often outstanding generalization performance. Recent progress in this area [Kawaguchi et al. 2017; Arora et al., 2018] not only improves this situation, but promises to be applicable in practice, at least in combination with empirical error measurement. For a discussion of the relevant issues and topics, we refer to a recent survey paper [Jakubovitz et al. 2018].

3 The New Framework for Safety Verification

In the new framework, we consider the overall approach as an iterative, systematic and defined process. In particular, we propose to iterate over the following steps:

1. Data preparation and learning (as usual);
2. Estimation of error probabilities through controlled experiments and determination of a probabilistic generalization error bound;
3. If this error bound is insufficient, repeat by going back to 1 with additional data, or otherwise, exit successfully.

As long as the outcome in terms of the generalization error bound is considered insufficient, inductive learning will have to be continued with additional training data, most importantly also including “edge cases” or “near misses”. From a statistical perspective, this poses the problem of the usual assumption that the distribution for testing is identical to the distribution for training. Changing the training procedure in the way proposed above may invalidate this assumption. Hence, some care will have to be taken to ensure it. It should be noted that the proposed procedure makes heuristic use of statistics and statistical learning theory, but due to its theoretical underpinning it is still more reliable than working solely with empirical errors.

Practically useful generalization bounds for deep learning are just about to emerge. A recent paper (and its updates) based on compression [Arora et al., 2018] improves upon previous approaches (e.g., [Kawaguchi et al. 2017]), and shows practical applicability (see Fig. 4 in that paper, with a comparison with existing bounds and between the bound and the measured error). While the scale of the bound still differs by magnitudes, the rankings of the models according to the empirical error and according to the bound are highly correlated. This suggests that the bound could already be used for model selection, i.e., picking a suitable model from a set of differently parameterized candidate models.
For making such an approach sound, also the inclusion of context for the instances involved is relevant. Developing a general scheme for the applicability domain of ML models will contribute to more predictable behavior. The applicability domain has been a concept for machine learning models only in chemical risk assessment so far [Netzeva et al. 05], but could prove valuable in more general settings. The idea is that models should be allowed to interpolate, but not to extrapolate. The applicability domain defines the scope or competence of a classifier. Within the applicability domain, the error rates, in particular the false-positive and false-negative rates, are demanded to remain below specified thresholds. Abstaining classifiers (i.e., classifiers with the reject option) are also likely to play a role, because there will be instances outside the applicability domain. It will be possible to choose machine learning models with desired properties dynamically and systematically according to the current context.

Finally, the probabilistic generalization error bound determined can be propagated to the hazard or risk analysis of the overall safety-critical system, see also below for a sketch.

4 How to Use Probabilistic Generalization Error Bounds

At the current state of the art, usually functional safety engineering is applied to safety-critical systems development. It involves the identification of safety-related functions, where we are interested in cases where a classifier resulting from ML delivers such a function. In such a case, it will also have to be included in probabilistic hazard or risk assessment of this system. Once the causality of some hazard as related to the ML component is understood, the contribution of its error probability to this hazard and related risks of the overall system can be determined. More precisely, we propose to use a probabilistic generalization error bound of the ML component for these analyses, since this will increase safety as compared to directly using error probabilities (see above for the difference).

Actually, a probability of failure will have to be determined, based on both the measured empirical error and a probabilistic generalization error bound of the ML component. While an error just means a wrong answer, a failure means a complete termination of the ability of the ML component to perform its function as required. For example, if an ML component will be deployed on a dedicated computer system based on GPUs (like a DNN), its failure may also be caused by a failure of this computer system, and this has to be taken into account additionally.

For hazard or risk analyses, the envisaged use of the safety-related functions and their possible failure must be analyzed, in order to identify possible hazards in the context of this particular system. For an overview of the key concepts involved, see Figure 1 taken from [Kaindl et al. 16], where we studied these concepts and their relationships qualitatively both for automotive and railway safety standards. First, we created a core ontology of safety risk concepts, since the terminology and even the concepts of the automotive standard [ISO 26262] are not fully aligned with the ones for railway [Hulin et al. 16]. Figure 1 additionally includes the concept of a risk. Since
safety risks involve both the severity and the probability of some harm possibly caused by the failure of a classifier resulting from ML, determining its probabilistic generalization error bound is key.

As shown in Figure 1, the operational situation or circumstance is relevant as well, and this will even reinforce the problem of applicability domains of the classifier resulting from ML. We conjecture that it may be handled analogously to hardware, which has different probabilities of failure at different temperatures.

5 Conclusion and Future Work

For (random) failures of hardware components, assessing their probabilities and using them for hazard or risk analyses is common practice for a long time now. For software failures, in contrast, any practical approach for really determining their probabilities seems to be illusory at the current state of the art. For failures caused by inductively learned classifiers, however, we claim that our approach as outlined here has the potential to do much better in the future than for manually developed software. The prospective benefits of such an approach are high, since there will be even ‘better’ safety cases for ML-based systems in practice than the current ones for traditional software, where usually no probability calculations are done for determining a SIL or ASIL. Hence, the overall scientific relevance for the field of Information and Communication Technology is very high, in order to make ML technology applicable within software-intensive systems, in particular safety-critical systems.

Fig. 1. Conceptual model defining a core ontology of safety risk concepts (diagram taken from [Kaindl et al. 16])
Future work will have to develop a mechanism that recognizes changing distributions, outliers and edge cases and explicitly handles them dynamically in a statistically sound way. Different distributions may be modeled for different contexts, with an additional layer that recognizes the context and picks the right distribution or part of a model [Geilke et al. 15]. An example in the domain of driving would be one distribution or model for driving on a Californian highway, and another one for an old Italian city. Different contexts would require different distributions or parts of models. Generally speaking, presenting hand-picked instances for learning requires taking into account in the application and in the final model, i.e., at testing time, that the right context is picked, such that specific instances or sets of instances become relevant whenever needed.

After the availability of these theoretical results as well as their take-up for engineering practice, both the societal and the economic prospects are great. The safety risks of ML-based systems will be precisely known, and only ‘sufficiently’ safe systems may be used, leading to less harm and greater economic value.

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