Deep Learning Model Generalization in Side-Channel Analysis

Analysing class probabilities, metrics and ensembles

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Abstract. The adoption of deep neural networks for profiled side-channel attacks provides different capabilities for leakage detection of secure products. Research papers provide a variety of arguments with respect to model interpretability and the selection of adequate hyper-parameters for each target under evaluation. When training a neural network for side-channel leakage classification, it is expected that the trained model is able to implement an approximation function that can detect leaking side-channel samples and, at the same time, be insensible to noisy (or non-leaking) samples. This is basically a generalization situation where the model can identify main representations learned from the training set in a separate test set. Very few understanding has been achieved in order to demonstrate if a trained model is actually generalizing for the current side-channel problem. In this paper, we provide guidelines for a correct interpretation of model's generalization in side-channel analysis. We detail how class probabilities provided by the output layer are very informative for the understanding of generalization and how they can be used as an important validation metric. Moreover, we demonstrate that *ensemble learning* based on averaged class probabilities improves the generalization of neural networks in side-channel attacks.

Keywords: Side-Channel Analysis · Neural Networks · Model Generalization · Ensemble Learning

1 Introduction

Implementation of secure products considers the threat imposed by side-channel attacks. The growing markets of embedded computing, and specially internet-of-things, require even more confidential data to be processed on electronic devices. Cryptographic algorithms are usually implemented as part of those systems and, if not properly protected, are vulnerable to side-channel analysis. Depending on the level of access and control of the target device, side-channel analysis can be categorized as profiled (e.g., template attacks[1], linear regression[2], machine learning[3][4]) or non-profiled attacks (e.g., DPA[5], CPA[6], MIA[7], clustering[8]). Profiled side-channel attacks consider a scenario where the adversary has fully or sufficient control over a device that is identical to the target device. The adversary then learns the statistics from the device under control and tries to match them on other target devices.

In the last three years, deep learning, in its supervised learning setting, has been intensively considered as an important method for profiled side-channel analysis [9][10][11]. With the adoption of deep neural networks, and specially the availability of open-source frameworks, their applications to side-channel analysis have improved the comprehension of what are the main capabilities of this type of non-invasive attacks. Different publications have proposed different approaches to solve a variety of questions. Part of the research topics explore the strengths of deep learning against crypto implementations specially due to the limitations of other profiled side-channel attacks. Other topics investigate the relationship between trained models and the leakage detection [12][13][14][15]. However, there is still a lack of explanations about model generalization and how to improve it in side-channel attacks.

This paper proposes an analysis about the *generalization* of deep neural networks in side-channel analysis, specially against protected cryptographic implementation. The motivation comes from the risk of overestimating the security of a device due to the misinterpretations of deep learning metrics and its results. As emphasized in [16], for some data sets, the classification accuracy obtained from the test set usually does not translate the corresponding side-channel metric, as guessing entropy or success rate. As our experiments demonstrate, key recovery is successful on a masked implementation of AES even when the test accuracy is close to a random guessing. If this accuracy would be used to determine the level of generalization of the trained model, we would assume that this model is underfitting or overfitting, which can be checked by looking at training and validation metrics. Therefore, there is still a lack of explanations about model metrics and their corresponding side-channel results. This scenario leads us to the conclusion that the model is only providing a *good enough* generalization for the side-channel analysis case.

In this work, we demonstrate that the observation of output class probabilities from validation or test sets can explain the generalization of the model. To provide more details about model metrics and how they are related to the side-channel analysis metrics, we decided to interpret the output probabilities obtained either in the validation or in the test phases. The output layer of a neural network contains an amount of neurons (or units) that is equivalent to the amount of classes (or the range of labels) defined for the data sets. The amount of classes is directly derived from the selected leakage model. For every tested trace, this output layer provides class probabilities if the activation function is *softmax*. By ranking these output class probabilities by order of magnitude for each trace and for each key candidate, we observe that these ranked class probabilities can be seen as a valid distinguisher or metric for side-channel analysis. We show that key rank from a fixed-key validation set is the best metric to validate a trained model.

Having the analysis of output class probabilities as a reference, we propose the usage of *ensemble learning* to relax the difficult selection of hyper-parameters for the neural network and also to improve model's generalization. The selection of correct hyper-parameters for each trace set is a challenging task. The publication from [17] proposes some experiments in order to verify what are the most promising hyper-parameters for specific trace sets. Even if this publication provide valuable information for side-channel analysis, it is still difficult to port the same conclusions for different trace sets measured from different devices and with different equipment. Therefore, we conclude that a interesting approach would be to usage ensemble learning or ensemble models. This is a technique that combines the decisions from multiple models to improve the overall performance. Among different techniques proposed in the machine learning literature, we select the *bagging* technique that (among other variations) averages output class probabilities from several single trained models.

This paper is structured as follows. Section 2 review the publications that are related to our proposed analysis and also lists our main contributions. An overview of metrics, generalization, data sets in side-channel analysis is presented in Section 3. Section 4 provides a detailed investigation of output class probabilities and their importance as a metric for *good enough* generalization in side-channel analysis. In Section 5, we provide practical results demonstrating how validation key rank is a good validation metric for deep learning-based SCA. Section 6 provides practical experiment results from ensemble learning for side-channel analysis. Finally, conclusion and discussions are given in Section 7.

2 Related works and contributions

As this paper tackles the problem of generalization of neural network models and metrics in side-channel analysis, we would like to provide an overview of what has been published recently that is related to this problem. Basically, we identify main trends of research within this field:

- **Deep learning as a profiled side-channel attack**: Bypassing misalignment and masking countermeasures on AES [9][10] and public-key [11][18] implementations with the application of deep convolutional neural networks. Different techniques for regularization, like data augmentation through random shifts [10][17][19] or noise addition [20] have been tested. The authors of [21] investigate the efficiency of deep learning with respect to misalignment in side-channel traces. In [22], it is shown results of convolutional neural networks on time-frequency representations of traces. The work of [23] proposes the usage of crypto information (plaintext and ciphertext) as additional inputs to the first dense layer in a convolutional neural network in order to improve key enumeration.

- **Trained neural networks as a side-channel distinguisher:** the work proposed by [24] considers a DPA-like deep learning attack where models are trained for each key byte candidate in an AES implementation. Training and validation metrics are then considered for reference to distinguish between correct and incorrect key byte candidates.

- **Model interpretability** and *leakage assessment*. In this group, several works propose different techniques to verify what a neural network learns from side-channel traces. Different works proposed the evaluation of input activation gradient [12], occlusion techniques [13] and layer-wise back propagation [14] as a metric to assess which input features (or points of interest) the neural network selects as the most important for its decisions. By doing so, it is possible to verify what are the points of interests or features that a trained model considers in order to make its classification decision. Moreover, also related to interpretability, the work of [25] investigates the performance of neural networks through information theory.

- **Relationship of deep learning and side-channel metrics**. The work proposed in [16] concludes that there is an inconsistency between accuracy, recall and precision when compared to conventional side-channel metrics like success rate and guessing entropy. To the best of our knowledge, the work of [16] is the only one that evaluates the meaning of deep learning metrics for side-channel analysis.

- **Deep learning for leakage assessment**. The authors of [15] provide a methodology for leakage assessment with deep neural networks in order to leverage the benefits of deep learning in terms of location, alignment and statistical order of the leakage.

By looking to the above list of publications on this topic, we concluded that there is still some lack of technical explanations to justify why a trained model is able to provide successful key recovery even when deep learning accuracy is close or below a random guessing. The work of [16] provide valuable information through practical experiments on several data sets in order to prove the existence of such inconsistencies with several deep learning metrics. In order to look more close to this problem, and also to colaborate to the improvement of trained model generalization in side-channel analysis, the main contributions of this paper are:

1. **A didactic analysis of output class probabilities and their relation to successful key recovery:** Motivated by the idea of exploring metrics discrepancy, in Section 4 we explore the information contained in the output probabilities from the output neural network layer as a valid information for verifying the performance of a trained neural network for side-channel analysis.

2. **How to select a reference metric for selecting a neural network model:** in cases where the adversary possess an additional validation set with a fixed key, we demonstrate how generalization gap is not a good reference metric to judge the performance of a trained model. Our experiments confirm the arguments of [16] and we extend the analysis by showing that key rank computed from a fixed-key validation set is the most promising validation metric for side-channel analysis against protected AES implementations.

3. **How to improve generalization through ensemble learning:** this analysis demonstrates that the usage of ensembles provides higher success rate if compared to electing a best trained model among several models with different hyper-parameters configurations.

First, we start by reviewing the concepts of deep learning metrics and data sets as well a recapitulation about the meaning of underfitting, generalization and overfitting for side-channel analysis.

3 Data Sets, Metrics, Generalization in SCA

As a profiled side-channel attack, the application of deep learning requires a training set for the learning or profiling phase. Considering X_i as a vector representing a side-channel trace, where $x_{i,j}$ would be an observation from X_i, each trace is then labelled according to a selection function $l_i = f(p_i, k_i)$ that represents the side-channel leakage model. Thus, the leakage model defines the amount of classes in the training set. The assumption of a profiled attack is that the adversary has a device that is identical to the target one and this adversary has (in the best case scenario) fully control of the device. Ideally, the training set should be composed by side-channel traces where each trace is measured with random input data (ciphertext or plaintext) p_i and random key k_i.

In addition to the training set, the adversary also collects a validation set from the device under control. The keys k_i and in input p_i are also known for the validation set. After training the neural network with training set, the validation set is evaluated in order to check the generalization capacity of this trained model. If validation metrics indicate good level of generalization, the adversary has a trained model to apply to test traces collected from other identical devices having an unknown private key. It is assumed that test traces are drawn from same underlying distributions defining training and validation sets.

The conventional deep learning metrics (at least the ones taken into account in this work) are accuracy, recall and loss (or error). *Accuracy* indicates the ratio between correctly predicted data and total number of predictions. *Recall* returns the ratio between true positives and the sum of true positives and false negatives. For multi-class classification, here we consider recall as an average of the recall per class. *Loss* indicates the overall error for the evaluated set. The metrics obtained during the training step of a neural network may indicate the presence of different phases that can occur when the parameters (weights and biases) are being learned from the training data set. Here, we assume the presence of three main phases (that does not occur necessarily in this order, even if usually it happens in this order):

1. Underfitting: it occurs when the approximation function defined by the neural network model is unable to fit both the training and validation sets. The error is significantly high for the training set.

2. Generalization: during this phase, the neural network achieves an approximation function that can fit the training and validation sets with acceptable error. The metric results are sufficient to solve the classification problem under question. The is the ideal scenario in a machine learning problem. In side-channel analysis, a *good enough* generalization is what we look for. The concept of *good enough* will be understood when we discuss output class probabilities in the next section.

3. Overfitting: this phase happens when the neural network is able to fit the training set with very high accuracy and very low error, however it cannot fit the validation set. The metrics obtained when the validation set is evaluated are insufficient to solve the machine learning (or classification) problem. Typically, it is relatively easy to overfit the model for a training set in side-channel analysis. The number of traces is typically limited in size (up to few millions) and an over-parameterized neural network has conditions to overfit this training set. Usually what happens is a big *generalization gap*, i.e., difference between a model's performance on training data and its performance on unseen data drawn from the same underlying distribution.

Ideally, we should always train a neural network until it achieves the maximum quality in terms of generalization with respect to the validation set. Obviously, if this happens, we should be able to assess whether the model is in the generalization phase or not. This seems to be an easy task, however there are quite some difficulties in the interpretation of metrics in order to identify which phase the model actually belongs to while the training evolves. An interesting observation would be the detection of the boundaries between two of the aforementioned phases. These boundaries may be detected with the observation of conventional metrics (loss, accuracy, recall or precision). By detecting these boundaries, it is possible to conclude, for example:

- the moment when the training must stop (boundary between the end of *generalization* and the beginning of *overfitting*);

- the minimum amount of epochs (boundary between the end of *underfitting* the beginning of *generalization*). For clarification, an epoch is the process of the entire training set which is divided in batches;

- the level of agressiviness of, e.g., the learning rate (boundary between the end of *underfitting* and the beginning of *overfitting* without passing by the *generalization*).

By clearing detecting these three phases during the neural network training, we may draw strong conclusions about the selected hyper-parameters for the side-channel traces under analysis. As expected, different trace sets will require different hyper-parameters for the achievement of a good generalization. However, as practically demonstrated in [16], conventional deep learning metrics are not very consistent in the context of side-channel analysis. To verify if a model is actually generalizing to the validation or even to a separate test set requires a different understanding of training and validation metrics. Usually, side-channel traces collected from modern cryptographic implementations provide limited leakage due to state-of-art countermeasures. In this paper, we attack a masked AES implementation and the successful results cannot be represented by deep learning metrics. For example, the trained model presents test accuracy close to a random guessing and still the target key can be recovered from the side-channel test set. The trained model clearly indicates a level of generalization that is limited however sufficient for the considered case. We define this limited level of generalization as *good enough*.

Therefore, at this point in time, it is very opportunistic to discuss what this *good enough* generalization actually means for side-channel analysis. To fill up this gap, the next section provides some guidelines on how to interpret output class probabilities from the last neural layer, obtained after the *softmax* activation function.

4 Output class probabilities as an indication for "good enough" generalization

To deal with this poor generalization of trained models in side-channel attacks, there are four main alternatives:

- **Data generation**: it includes the acquisition of more training data from a device under control, where the key is known and the inputs and/or outputs can be controlled by the attacker.
- **Data augmentation**: to deal with misalignment and noise, one can modify the training data in order to produce artificial traces by implementing the effects that are expected in the test data. The works from [10] and [20] focus on data augmentation to improve generalization.
- **Regularization**: these are techniques that prevent the model to ovefit the training data. Dropout, L1, L2 and noisy layers are some of the examples of regularizers that can be used for side-channel analysis.
- **Ensembling**: this is a technique the combines the results from multiple models in order to improve the test accuracy. Stacking, averaging, boosting and bagging are examples of techniques adopted for ensemble learning.

There are many fields where the application of a trained neural network would require a very high test accuracy in order to solve the problem. As a consequence, the generalization phase will start only after a sufficiently high accuracy is achieved for the test set. In side-channel analysis, the generalization phase is directly related to key recovery and it may start very soon in the evolution of training because a considerable low accuracy can already represent the turning point from underfitting to generalization. Moreover, as we mentioned in the last section, accuracy or recall may not be reliable metrics for the identification of this turning point. Usually, key ranking, success rate or guessing entropy appear to be more indicative metrics of success in the usage of neural network in side-channel analysis.

When a neural network is trained to classify side-channel traces according to a chosen leakage model (e.g., the Hamming weight of an intermediate byte in the target crypto algorithm), the output layer of the network is able to provide the probability for each class that the side-channel trace is labelled with. For that, the *softmax* activation function is defined for the output layer. These probabilities indicate the likelihood that a specific test trace contains an intermediate value translated into a class by the selection function or the leakage model.

Therefore, a key ranking can be calculated and this process is similar to a differential power analysis where all possible key byte values are tested for the same trace set. By selecting the output probability value given by the neuron in the last layer corresponding to the predicted class of each trace, we can compute a cumulative probability for each key byte hypothesis. The assumption is that if the trained model achieves a *good enough* generalization, and if the number of test traces is sufficiently large, the correct key byte candidate provides cumulative probability that is higher than the cumulative probability obtained from incorrect key hypothesis.

Now, why a low accuracy (sometimes close to a random guessing or flip coin statistics) can still be associated to this *good enough* generalization phase? Here, the assumption is that the accuracy may not represent this generalization, which can only be represented by the output class probabilities. The accuracy is a metric that takes into account the predicted class for each test trace. However, as we will detail in this section, not only the output probability from the predicted class are taken into account for the key ranking calculation and, in addition, if the trained model already provides good enough generalization. Classes that are not predicted as the first for not containing the highest probability also contain valuable information and are taken into account.

The cumulative probabilities for each key byte candidate is a valid distinguisher for the side-channel analysis and it is given by:

$$P(g) = \sum_{i=1}^{N_T} log(p_i(c)^g) \tag{1}$$

For clarification, N_T is the number of test traces. The term $p_i(c)^g$ indicates the output class probability associated to the class c ($c = 0, ..., N_C$, where N_C is the number of classes) for trace i and c is obtained from the leakage model associated to the key byte candidate g. In case of side-channel analysis of AES, the value c can be represented by an intermediate value in a inner AES state (e.g., Hamming weight of S_{box} output in the first round).

Note that the equation (1) would only select the highest output class probabilities for the correct key candidate and for all test traces in case the test accuracy is 100%. In cases when accuracy is very low, and insufficient to indicate the generalization, the values of $p(c)^g$, for the correct g, would be one of the output class probabilities that are not the highest in the output layer. If key ranking still indicates a successful key recovery, we can conclude that not only the highest output class probability provides valuable classification information and the trained model is still in a good enough generalization phase.

Next, we provide practical experiments to prove the aspects described in this section.

4.1 Output class probabilities from a leaky target: unprotected software AES

As a proof-of-concept, we consider a trace set measured from an unprotected software AES-128 implementation. In this case, the leakage of information is quite significant. For this simple example, the training set contains 6,000 traces and the validation and test sets contain 1,000 traces each. The leakage model is based on the Hamming weight of a byte in the S_{box} output from the first encryption round. This defines a maximum of 9 classes in all the trace sets (Hamming weights ranging from 0 to 8). As we target one round key byte at a time, it is necessary to train 16 models to recover the 16 round key bytes. To make it simple, we provide the results for a single round key byte.

As the training set is relatively small, we define a very simple multiple layer perceptron as well. For all the experiments from this paper, we considered *Keras* Python package for neural networks. To attack this unprotected AES, the configured model is a multiple layer perceptron with three hidden layers containing 40 units or neurons each. The activation function for the hidden layers is *Relu* and the output layer, containing 9 neurons (equivalent to the amount of classes) has *softmax as activation function.* The learning rate is set to 0.001 with *Adam* as the optimizer for the back propagation algorithm. The loss function is computed from *categorical crossentropy*, which returns the cross-entropy between an approximation distribution a (predictions) and a true distribution b (true values): $-\sum_x a(x)log(b(x))$.

The model is trained for 20 epochs and the achieved training and validation accuracy are 83% and 52%, respectively. For side-channel analysis, this validation accuracy already indicates a good level of generalization and the key recovery will be successful if a reasonable

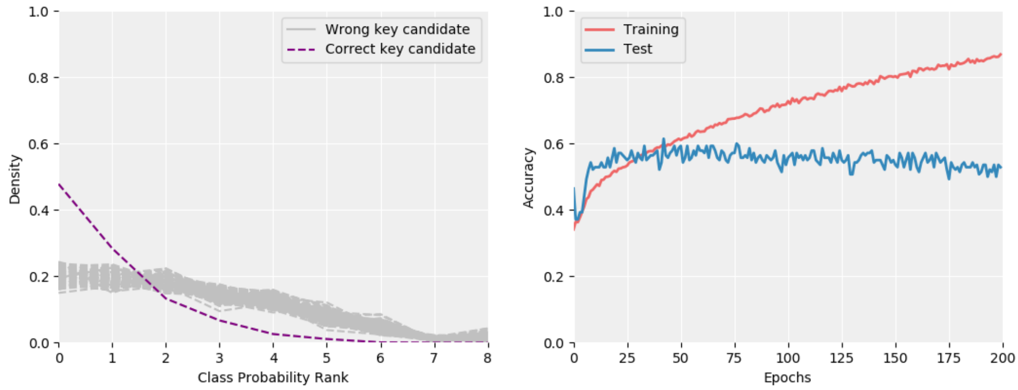


Figure 1: Rank of output class probabilities for the test set by considering correct and incorrect key candidates.

amount of test traces is considered. In this case, the target key byte is recovered after the processing of approximately 20 traces. The evaluated test accuracy is close to 48%.

Now, let us analyse the information contained in the output class probabilities for the current test set. As stated before, the key ranking is the procedure to evaluate what key byte value the known-key side-channel test phase returns. Once again, if the test accuracy would be 100%, for each test trace the value of $p(c)^g$, that represent the output probability associated to class c for the key guess g, would always return the highest output value in the output network layer (i.e., the expected class is always equal to the predicted class). However, as our test accuracy is 48%, only 48% of the tested traces will contribute to cumulative probability $P(g)$ with the highest class probability. The rest of the traces will contribute with output class probabilities that are not ranked as the first in the output layer.

Figure (1) shows the density distribution for the rank of output class probability for correct (red) and incorrect (grey) key byte candidates. By ranking the output probabilities from the last network layer from 0 (highest probability) to 8 (lowest probability), this figure indicates the rate (from 0 to 1) that test traces are predicted (due to key guess g) for each rank if output class probabilities are listed by order of magnitude. For example, for the correct key candidate, the expected class is ranked as the second most important probability for approximately 16% of the test traces. As we can see, the expected classes obtained from the correct key byte candidate tends to be significantly ranked as the most important (or first) classes in the output layer. On the other hand, for the incorrect key candidates, the level of importance (or rank) of output probabilities for the expected classes is mostly distributed equally for all key candidates.

This analysis basically proves that output class probabilities contain valuable information and that they can be considered as an important metric for side-channel analysis and generalization.

4.2 Output class probabilities from a masked AES (ASCAD)

The ASCAD database (github link) was released in 2017 [17] to be a used as a reference trace set for side-channel experiments with deep learning. The traces refer to a 8-bit microcontroller software implementation of AES-128, where boolean masking is implemented as a countermeasure to side-channel attacks. The provided trace set contains 200,000 traces with **random keys** and an additional trace set with 1,000 traces with **fixed key**. The latter is used as a test set.

The randomly generated masks for every AES encryption are also provided with the

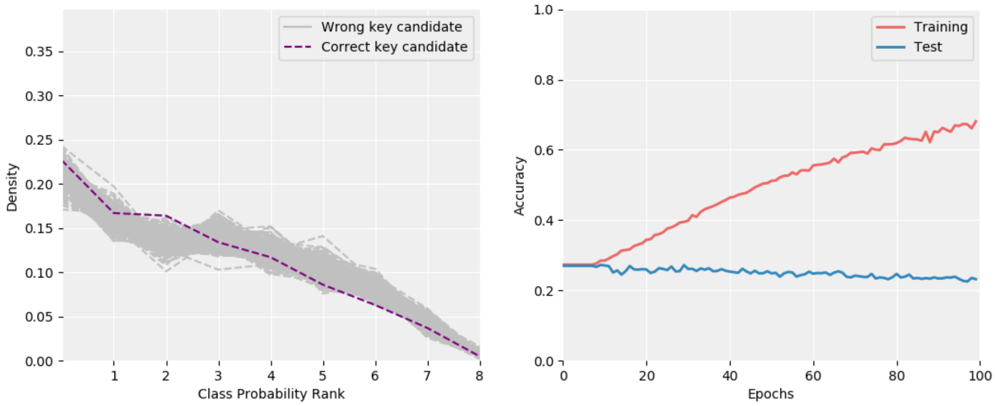


Figure 2: Rank of output class probabilities for the test set by considering correct and incorrect key candidates for ASCAD database.

database metadata. From these mask values, we could confirm that in the first encryption round the intermediates associated to key bytes 0 and 1 are unprotected because the mask values that would generate a masked S_{box} output byte value is set to zero for all traces. For the rest of key bytes, the remaining 14 mask bytes are random. Therefore, and to keep it simple, we decided to apply our analysis on the processing of key byte 2. For training, validation and test phases, the selected leakage model is Hamming weight of S_{box} output *without the consideration of mask values and the knowledge of countermeasures* (black-box scenario).

The implemented neural network model is more complex if compared to the previous example (Section 4.1). This time, we define a multiple layer perceptron with five hidden layers, where each layer contains 200 neurons and activation function *Relu*. The rest of the hyper-parameters are the same as the ones considered for the leaky AES in the previous subsection.

Figure (2) shows the ranks for the output class probabilities for correct and incorrect key candidates. Due to countermeasures, we can see that these probabilities are ranked similarly for all key candidates. However, it is slightly more concentrated as the most important predicted classes for the correct key candidate (specially rank 2 which appears more for this correct key candidate). Our conclusion is that the model is being able to generalize to the test data under the stipulated conditions for the side-channel analysis.

By simply observing the main metrics like accuracy in Figure 2, we are unable to identify the generalization phase. In the current experiment, the test accuracy decreases with the processing of epochs. If we would have to identify the main training phases (underfitting, generalization or overfitting) from the accuracy metrics, we would assume that the neural network model starts in a underfitting scenario (up to 25 epochs) and next it starts to fit the training set until the overfitting scenario would be achieved if more epochs would be processed. From the test accuracy, we assume that the generalization phase never happened. Nevertheless, this is not what the rank of output class probabilities indicates and for the side-channel problem the trained model provides good enough generalization. The correct key byte can actually be recovered from this test and it can be distinguished from output class probabilities. The cumulative probability therefore is a valid distinguisher for side-channel analysis with neural networks.

5 The meaning of generalization gap and validation metrics in SCA

Generalization gap is well-known in the deep learning community because it explains the difference between model's performance on training data and unseen or test data. As explained in the previous section, output class probabilities, when ranked by order of magnitude according to key candidates, represents the generalization of a trained model expressed in terms of successful key recovery. In other words, if the model is generalizing, the output class probabilities for the correct key candidate will be concentrated as the first ones by order of magnitude, explaining the reason why a very low accuracy (sometimes slightly above the random guessing value) can be associated to a trained model that is able to recover the correct key candidate.

In [26], the authors propose a measure for predicting generalization gap, which is based on the concept of margin distribution, i.e., distance of the training points to the decision boundary, which is a concept used in support vector machines. In short, the authors question how to predict the generalization gap based on training data and the network parameters. Moreover, they propose a predictor with a high correlation between the predicted and the real generalization gap. The motivation behind the work of [26] comes from the importance of predicting the gap between training and validation metrics in order to find ways of minimizing this gap and also to identify the main reasons for the occurrence of this gap. In side-channel analysis, predicting the generalization gap is important for the understanding of how the trained model would be able to generalize to any test data and not only to the validation set that it is available during the known-key analysis scenario.

The original concept of generalization gap is restricted to the analysis on training and validation sets. In side-channel analysis, the generalization might be significantly low and indeed deep learning metrics sometimes cannot be used to represent the side-channel attack performance (this is explained in more details in [16]). *If the model is optimized for the validation set, there is still a big risk of misleading generalization for a separate test set.* Therefore, to validate a model based on generalization gap may lead to inconsistent results in side-channel analysis. To sustain this last argument, in this section we conduct some experiments to verify if the minimum gap between training and validation metrics leads to good levels of generalization.

In our methodology, several hyper-parameters configurations are defined for neural networks (multiple layer perceptrons and convolutional neural networks) and the best model is selected based on a metric. We start by checking the test performance (key rank and success rate) when the reference metrics are generalization gap based on accuracy, recall and loss values. The success rate represents the probability of recovering the key byte for the processing of specific amount of traces.

5.1 Metrics for a leaky AES

Initially, a leaky AES implementation is evaluated in order to compare the test performance if generalization gap is a reference metric to select the best model. We train 10 different neural networks with the same training data consisting of 2,000 traces. The validation set and test sets consist of 100 traces each. The process of training 10 different models is called a *campaign* and therefore the number of campaigns is 20. For each campaign, the best trained model is selected from generalization gap metrics, which are: (1) different of training and validation accuracy, (2) difference of training and validation recall and (3) difference of training and validation loss. Figure 3 shows the averaged key rank computed from the key ranks from the best model of each campaign. Figure 4 shows the averaged key rank from the 20 campaigns when only the validation metrics (accuracy, recall and loss) are used as a reference.

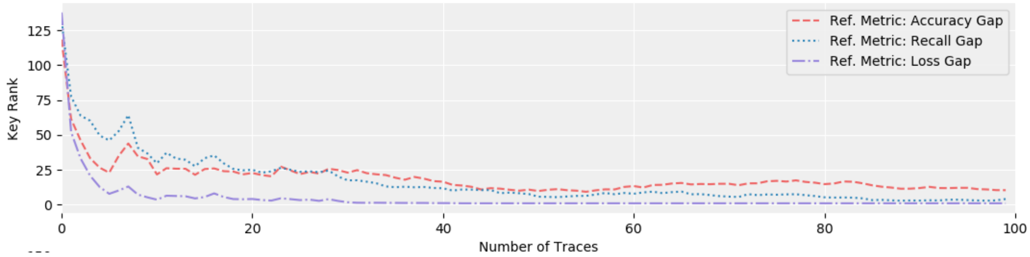


Figure 3: Key rank for test set of leaky AES: trained model selected from generalization gap of metrics.

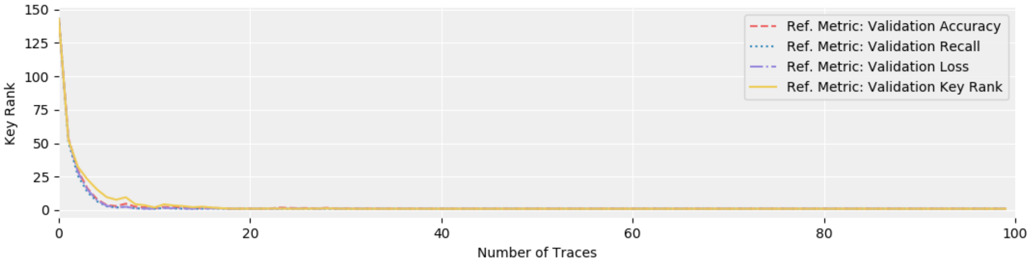


Figure 4: Key rank for test set of leaky AES: trained model selected from validation metrics only.

Comparing Figures 3 and 4, we can conclude that validation metrics are a better alternative than generalization gap for the validation of a trained model. As we can see in Figure 3, not all reference gap metrics lead to the selection of a best model from each campaign. Moreover, Figure 4 also provide the averaged key rank when the *best models are selected when validation key rank is used as a reference validation metric*. It is important to mention that this is a very leaky target, and, for most of trained models, validation metrics indicate a good level of generalization for side-channel analysis. This explains why, in Figure 4 all reference metrics result in a good test performance. Figures 5 and 6 show the success rate for the 10 evaluated campaigns. Again, test results achieved from validation metrics are slightly superior than the ones obtained from generalization gap metrics. For the latter, the success rate achieves 100% with more test traces if compared to the validation metrics case.

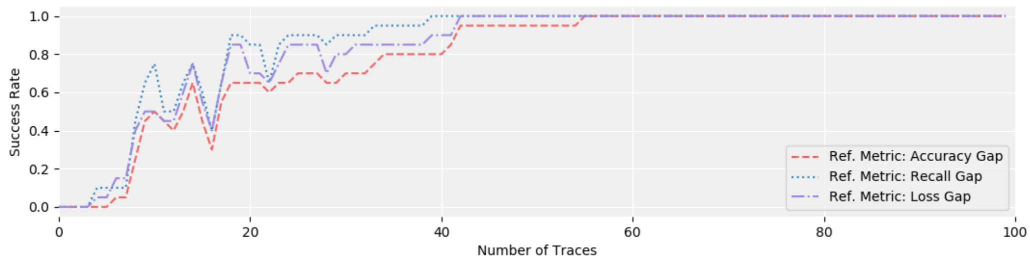


Figure 5: Success rate for test set of leaky AES: trained model selected from generalization gap of metrics.

Now, the analysis of Figure 7 gives a graphical indication of how metrics obtained from differences between training and validation (gap) and test metrics are related to each

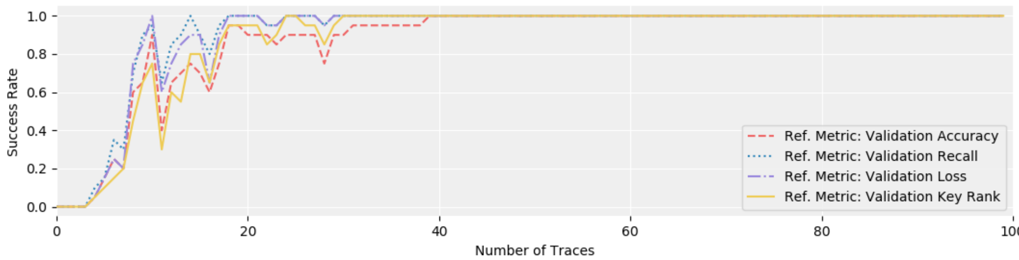


Figure 6: Success rate for test set of leaky AES: trained model selected from validation metrics only.

other. In this case, one would expect a negative correlation (i.e., lower the gap metric, higher the test metric). On the other hand, the results provided in 8 indicates a high correlation between validation and test metrics, which enforces why validation metrics are more relevant for conclusions about a trained model and, indeed, the prediction of generalization in side-channel analysis.

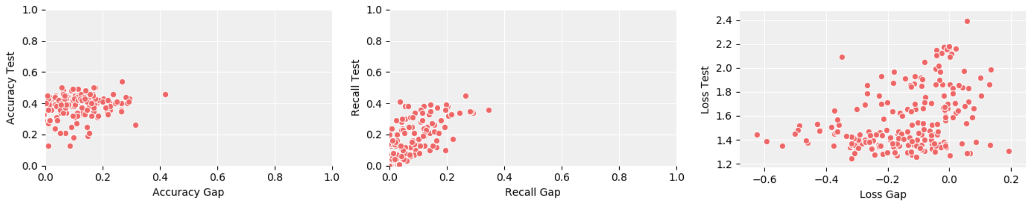


Figure 7: Correlation between gap and validation metrics for leaky AES traces (200 trained models = 20 campaigns × 10 models).

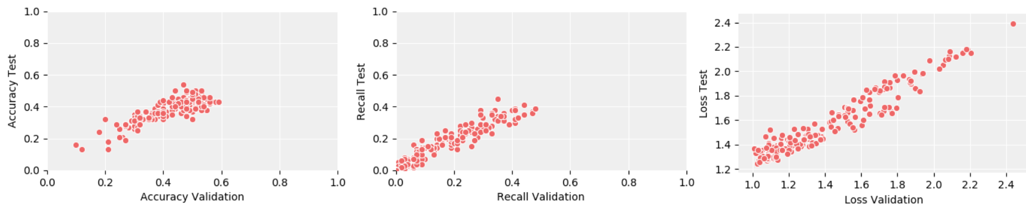


Figure 8: Correlation between test and validation metrics for leaky AES traces (200 trained models = 20 campaigns × 10 models).

5.2 Metrics for masked AES

The key rank and success rate results obtained from a leaky AES indicate that any validation metric is a good choice to define a neural network model among several models with different hyper-parameters. However, validation metrics (e.g. accuracy or recall) obtained from a model trained with side-channel traces measured from protected AES implementations usually are close to a random guess. As a consequence, the generalization gap (either based on accuracy or recall) might provide meaningless metrics. The same procedure applied to the leaky AES traces are now repeated for the masked AES traces from ASCAD database, which is described in the previous section. Again, 10 different models (with different hyper-parameters) are trained and this campaign is repeated 20 times. The training set is composed of 50,000 traces. Figure 9 shows the final key ranks averaged over the best models selected for each one of the 20 campaigns. In this case, the models are selected by having the generalization gap as a reference. Figure 10 provides the averaged key rank results when best models are selected from validation metrics only. Additionally, this last figure also contains the averaged key rank when the best model in each campaign is selected from the best final key rank result obtained from the validation set. The validation key rank calculation assumes a known-key scenario, i.e., validation traces are collected from a device where the key is known or can be set by the adversary.

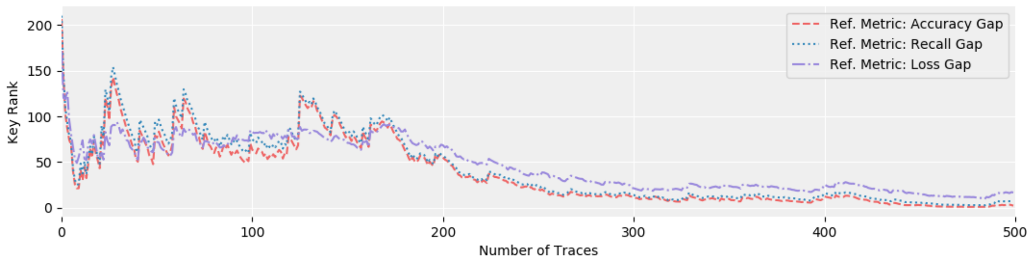


Figure 9: Key rank for test set of masked AES: trained model selected from generalization gap of metrics.

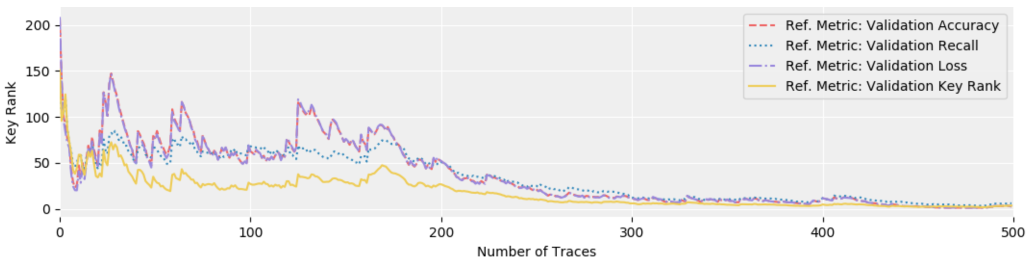


Figure 10: Key rank for test set of masked AES: trained model selected from validation metrics only.

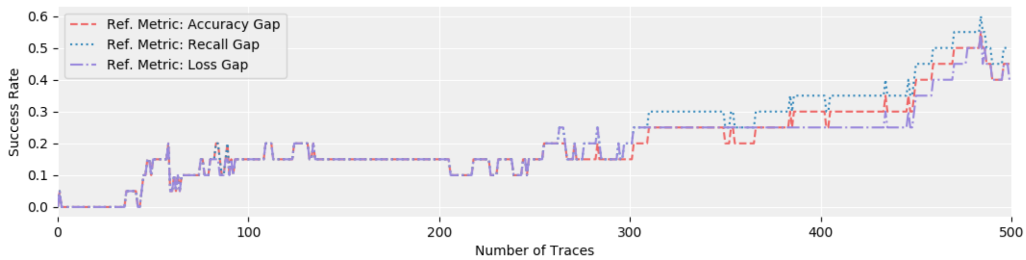


Figure 11: Success rate for test set of masked AES: trained model selected from generalization gap of metrics.

Not surprisingly, as illustrated by Figure 12, selecting the best model based on best validation key rank per campaign as a validation metric leads to the best success rate as well as the best averaged key rank in the test set, as shown in Figure 10. The key rank is computed from output class probabilities and due to the cumulative probability procedure, key rank appears to be a promising metric for validating a model. We reinforce that this is the typical case where generalization (large generalization gap) is very limited due to noise and countermeasures.

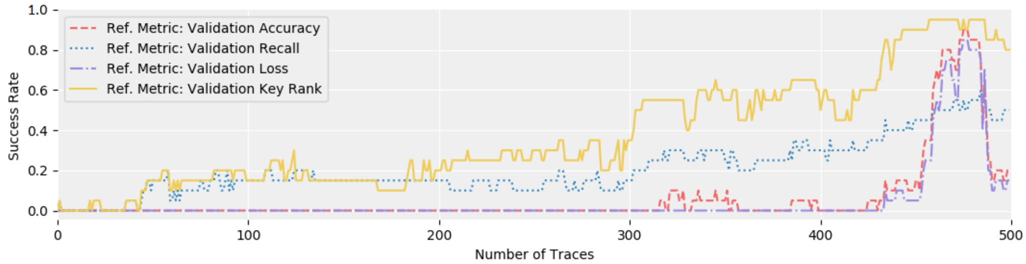


Figure 12: Success rate for test set of masked AES: trained model selected from validation metrics only.

Figure 13 shows the correlation between gap and validation metrics for the experiments on the masked AES traces. The statistical relation between these two groups of metrics shows that test metrics (specially accuracy and recall) are not varying as the gap between training and validation metrics vary. In other words, in a ideal scenario, one would expect that the gap should be small and the test metrics should correspondent by growing proportionally. However, as mentioned before, the generalization of neural networks against protected targets is very limited and therefore the gap between training and validation metrics is not a good reference for the validation of a model. On the other hand, validation metrics only are highly correlated to the test metrics, even against protected AES. This can be confirmed by observing the success rates in Figure 12. Despite the result with accuracy, recall and loss metrics from validation set only, the validation key rank resulted in the best reference metric for selecting the best trained model for each one of the campaigns.

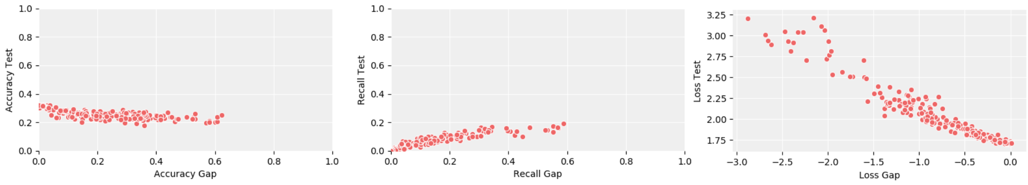


Figure 13: Correlation between gap and validation metrics for masked AES traces (200 trained models = 20 campaigns $\times$ 10 models).

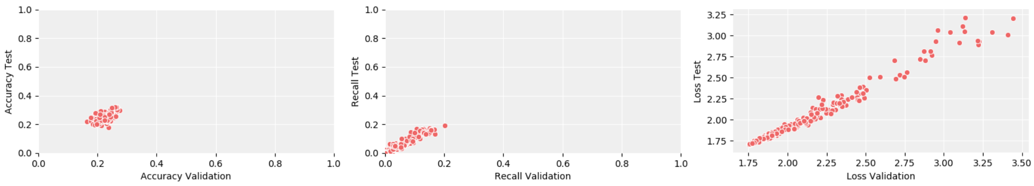


Figure 14: Correlation between test and validation metrics for masked AES traces (200 trained models = 20 campaigns $\times$ 10 models).

6 Model ensembles for side-channel analysis

Ensemble learning is a technique that combines the predictions from several models in order to reduce the generalization error. The expected result is that the prediction obtained from ensemble models is superior if compared to a single model. This is motivated by the statistical intuition that averaging measurements (or predictions) can lead to a more stable and reliable estimate because we reduce the influence of random fluctuations in single measurements.

Ideally, the hyper-parameters for each model should vary in order to learn different features from the same training set. If the models have equal configurations, it is very likely that the neural network will learn similar representations from the training set and provide similar classification results for the same test set. Another option, which we follow in this paper, is to randomly split the training set into smaller sets and train a separate model for each one of them. In this case, the single models can have same structure. On the other hand, we can build an ensemble of slightly different models from the same training data, which can reduce the influence of random fluctuations in single models.

Here, the main goal of the ensemble learning application is to improve the distinguishability of the cumulative probability (or output class probability ranks) in the key recovery or test phase. When a deep learning-based side-channel attack is successful, the main reason for that comes from the cumulative probability (Equation 1) being larger for the correct key candidate in the lower ranks (see for example Figure 1 where the lower ranks are more concentrated for the correct key candidate). As a result, successful ensembles should increase the cumulative probability for the correct key candidate while averages out the variations for the incorrect candidates.

Note, however, that we are not assuming that ensemble learning is *always* better if compared to a single learning model. The main goal of this analysis is to demonstrate that the chances of success in terms of key recovery are higher for ensembles when compared to single models. For a very large training set, one expects that a complex deep neural network needs to be defined. This actually requires a careful selection of hyper-parameters and to try each new configuration may takes a significant amount of time and computation power. Ensemble learning makes use of smaller training sets, which reduces the complexity for defining appropriate hyper-parameters. Moreover, because several models are combined into one, if few of the models contain hyper-parameters that does not provide good learnability from training sets, the fluctuations introduced by these models will be removed by having models that are actually generalizing. The experiments provided in this section demonstrate that ensembles are more likely to succeed if compared to single learning models for a specific amount of trained models.

Ensemble learning methods do not exclude the importance of a correct hyper-parameters selection for each single model. The selection of these hyper-parameters can vary for each model (*heterogeneous*) or remain the same (*homogeneous*). The idea of using heterogeneous models is the possible removal of errors imposed by the wrong selection of hyper-parameters if a sufficient amount of models is trained and if most of the neural networks are configured with reasonable hyper-parameters (i.e., hyper-parameters that provide a minimum level of generalization). Hyper-parameters search methods, like random search, grid search, Bayesian optimization or genetic algorithms, also provide solutions to define the best configuration for a neural network. However, these types of search would consider a large training set and several iterations (e.g., the generations in the genetic algorithm search). This could render the analysis impractical due to computational or time contraints. Ensembles can work on smaller training sets and they require a limited amount of models, which reduces the complexity.

Main methods for ensemble learning include *boosting*, *bagging* and *stacking*. In this work, the implemented ensembles are more similar to *bagging* methodology. We decided to use **ensembles with averaged probabilities**. The boosting and stacking methods will be reserved for future works. Here, the applied method computes the new likelihood for each key candidate by averaging the probabilities from all the single models. The cumulative probabilities from ensemble learning $P_e(g)$ are then computed for each key byte candidate g as follows:

$$P_e(g) = \sum_{m=1}^{N_M} \sum_{i=1}^{N_T} log(p_{m,i}(c)^g) \tag{2}$$

In Eq. (2), the term N_M refers to the number of single models. The term $p_{m,i}(c)^g$ refers to the output class probability c for model m and trace i according to key guess g. After building the ensembles, we expect an improvement in the key ranking convergence which, in the end, comes from the ensemble cumulative probabilities. The main goals of this analysis are:

- To verify the benefits of ensemble learning in side-channel analysis when ensembles are built from all trained single models;
- To verify the benefits of ensemble learning in side-channel analysis when ensembles are built from N_b best trained single models. The best models are selected based on key rank for validation set, as this metric provided better results in the previous section;

In the following, we conduct the analysis on leaky and masked AES traces.

6.1 Ensembles on a leaky AES

As an initial proof-of-concept, we firstly provide results for the unprotected AES case. We train 10 models with a very small training set of 2,000 traces. The validation and test sets contain 200 traces each. The data sets are labelled according to the Hamming weight of S_{box} output byte in the first AES round. The analysis and success rate are conducted for the first key byte.

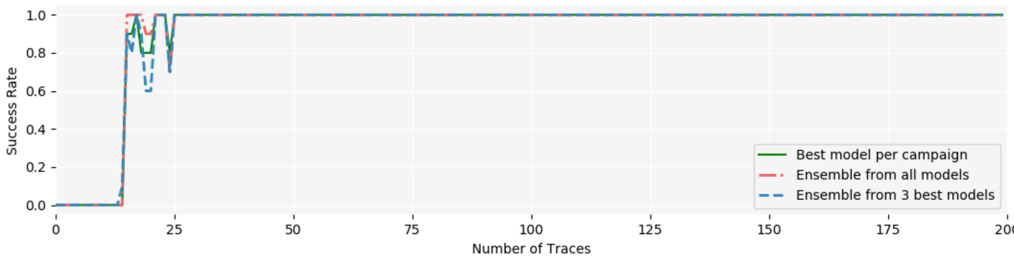
To compute the success rates, 40 campaigns with 10 single models each are executed. Ensembles are built from homogeneous and heterogeneous single models. For both cases, we set a weight initialization with *random uniform* method from *Keras* library, which in the end will provide different trained models even if the same model is trained with the same training data. The neural network topologies are multiple layer perceptron and the varied hyper-parameters for heterogeneous models are: number of layers, units per layer, activation functions and learning rate.

Figure 15 shows the success rate for each single trained model and also for the resulting ensemble models. As we can see, the ensemble models are at least good as electing a best model per campaign. For the heterogeneous case, the ensemble are slightly (but not much) superior than the best model. The fact that ensembles are not providing meaningful improvement is actually expected, mainly due to the presence of significant leakages that can be easily learned from different models.

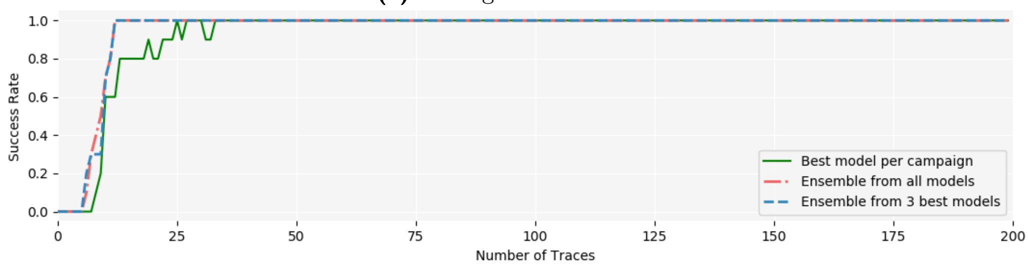
6.2 Ensembles on a masked AES

Side-channel traces from ASCAD database are again considered here in order to verify the benefit of ensembles against masked AES implementations. For all the experiments of this section, the training set contains random keys (as detailed in Section 4.2) and validation and test sets contain 500 traces each. The amount of training traces varies for each experiment, as detailed in this section. Traces are labelled according to Hamming weight of S_{box} output byte in the first AES round. Again, we consider the attack on only one key byte. We conduct the following tests with ensemble learning:

- **Homogeneous case:** Train 10 equal single models for different training set sizes. For each model, the training set is randomly selected out of 200,000 available training traces. All single models are convolutional neural networks containing identical hyper-parameters configuration.



(a) Homogeneous models.



(b) Heterogeneous models.

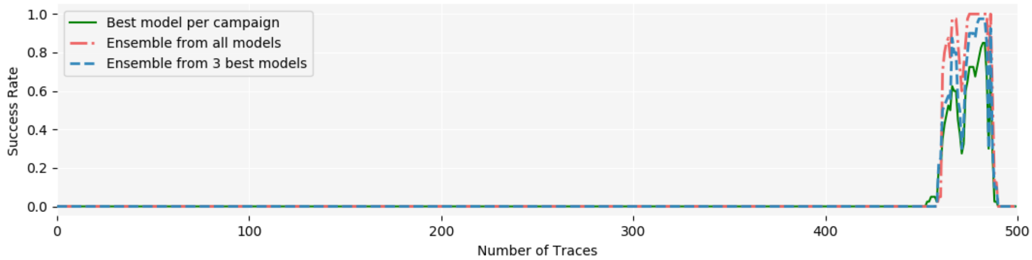
Figure 15: Success rates from averaged ensemble learning on a leaky AES. This experiment considers the ensemble of 10 single (a) homogeneous and (b) heterogeneous models and trained over a small set of 2,000 traces

- **Heterogeneous case:** Train 10 different single models for different training set sizes. The hyper-parameters are different for each of the 10 models. A model can be either multiple layer perceptron or convolutional neural network. For each model, we randomly select an activation function (for dense and convolution layers), number of convolution filters, number of convolution or dense layers, number of units per dense layer and learning rate.

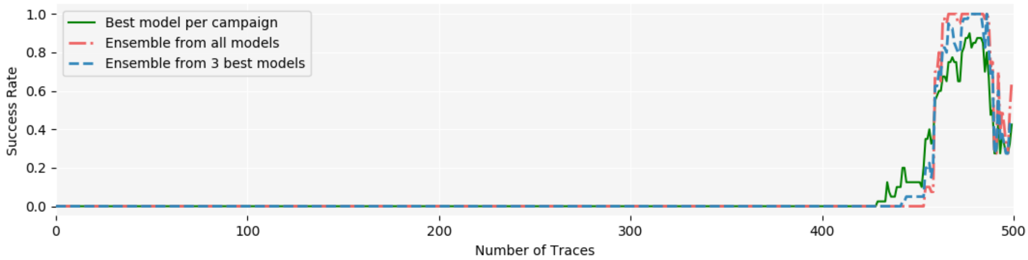
The main idea is to verify if the option for ensembles is more promising than simply electing a best model or $N_b = 3$ best models based on a reference metric that, in this case, is the validation key rank.

For each case, we conduct 40 campaigns. Each group of 40 campaigns is repeated for different amounts of training sets: 10000, 25000, 50000 and 75000. The results showed in Figure 16 demonstrate the benefit of ensembles when the same model trained several times (in our case, 10). Because the network parameters are randomly initialized and also because the training set is randomly selected from a larger set, each single model is not always successful. This fluctuations are therefore corrected with ensembles. For all different training set sizes, ensembles provided better results than simply electing the best model based on a validation reference.

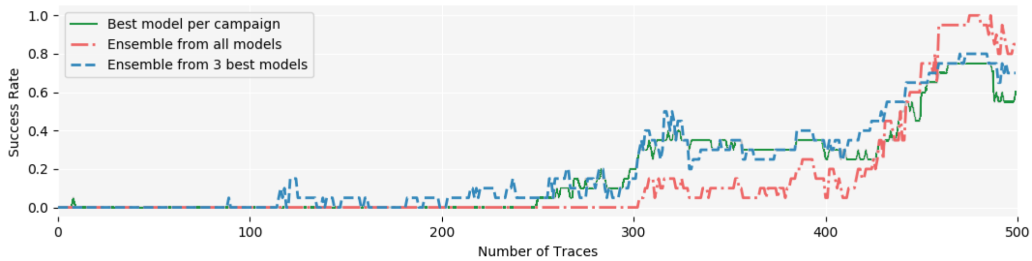
The building of ensembles with heterogeneous models demonstrate that selecting the ensemble as the final model for the key recovery is more reliable than defining a best and unique model for different training set sizes. As shown in Figure 17, for single models with 10,000 and 25,000 traces, the success rate after combining 10 models is clearly better than simply electing a best model based on the key rank for the validation set. Nevertheless, creating an ensemble with 3 best models is also not as good as the ensemble with all models for these two amount of training sets. On the other hand, for 50,000 and 75,000 training traces per model, the best model and the ensembles provide similar success rate results. Even so, the final success rate for 500 test traces for the ensemble was 100% while the best model (or the ensemble with 3 best models) achieved 97,5% (as shown in Figures 17c and



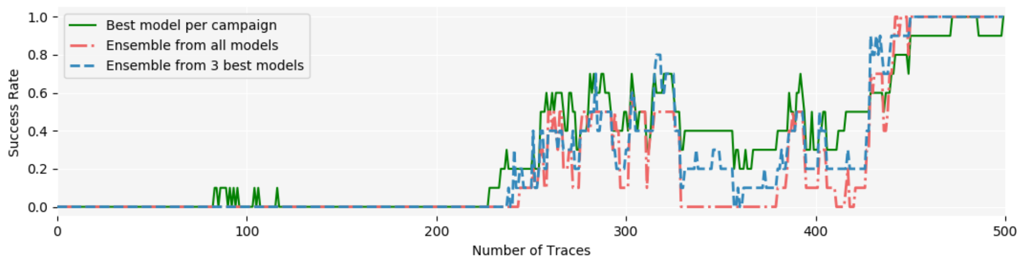
(a) 10,000 training traces per single model.



(b) 25,000 training traces per single model.

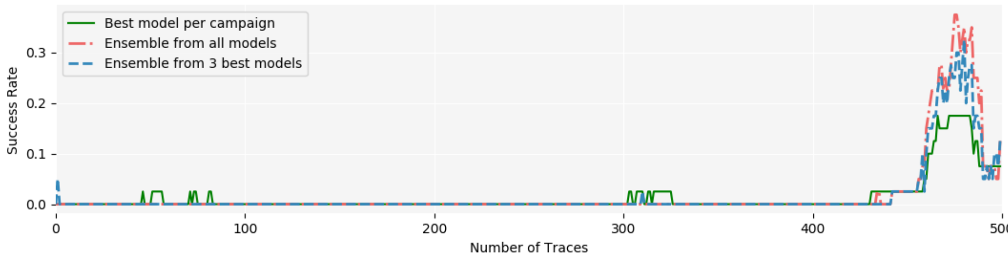


(c) 50,000 training traces per single model.

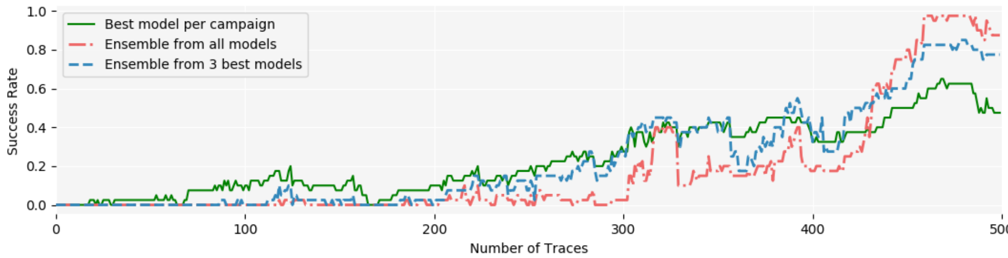


(d) 75,000 training traces per single model.

Figure 16: Success rates from averaged ensemble learning on masked AES traces (ASCAD database). This experiment considers the ensemble of 10 single homogeneous models.



(a) 10,000 training traces per single model.



(b) 25,000 training traces per single model.

(c) 50,000 training traces per single model.

(d) 75,000 training traces per single model.

Figure 17: Success rates from averaged ensemble learning on masked AES traces (ASCAD database). This experiment considers the ensemble of 10 single heterogeneous models.

17d). This confirms that defining an ensemble from all models is as good as selecting a best model from, e.g., hyper-parameters search. However, ensembles are not a replacement for hyper-parameters search based on optimization algorithms. The usage of ensembles ensures more reliable results by eliminating the variance of different model results.

7 Conclusions and Future Works

This paper proposed an analsyis of deep learning model generalization in side-channel analysis. We provided an analysis of the output class probabilities from the test phase of a deep learning-based side-channel analysis. After reviewing the recent literature, we verified that deep learning metrics are actually not completely aligned with side-channel metrics. We checked this argument with respect to test accuracy when the model is trained from traces measured from a masked AES implementation (ASCAD database). The results confirmed that indeed test accuracy (and other deep learning metrics as recall or loss) usually does not translate the generalization of the trained model. The key ranking, in its turn, is computed from output class probabilities. We graphically demonstrated how the cumulative probabilities in the key ranking calculation actually benefits not only from the highest output class probability for each tested trace. With these results, we verified the reason why a relatively poor test accuracy, that would indicate underfitting or overfitting (which depends on the training metrics), can still result in a successful key recovery. To fill up the gap for a reference metric in order to define a best model for side-channel analysis, we verified that key rank for a fixed-key validation set leads to higher success rate results.

From the fact that output class probabilities are directly linked to the success of a side-channel analysis, we proposed the usage of ensemble learning by averaging the output class probabilities from several single models that may be trained with smaller training sets. The main conclusions from the use of ensembles in deep learning-based side-channel analysis are:

- The ensembles are more likely to succeed in a side-channel test. After retraining the same model with the hyper-parameters, we observed different key recovery results. The ensembles showed more stables results for different training set sizes;

- Ensembles are good alternatives for speeding up the training phase because it may be successful on smaller training sets, as we could see in the previous section for the case of deveral models trained with 25,000 traces. A single model was not successful after training on 25,000 traces.

- The use of ensembles relax the need of a careful selection of a strong group of hyper-parameters in neural networks. However, we *do not* conclude that ensembles replace hyper-parameter search algorithms. When a deep neural network is able to recover the key from masked AES implementations (as is the case of ASCAD dataset), not always a selected group of hyper-parameters will be successful for smaller training sets. The ensembles demonstrated the ability of removing fluctuations from some of the models;

- We *do not* assume or conclude that ensembles improve the correct learnability of neural networks from side-channel traces. If the model is configured and trained in a way that the generalization is very poor, it is very likely that ensembles will not improve the generalization.

- The ensembles tend to provide a success rate that is at least good as the best single model among several hyper-parameters configuration options. In our experiments, the ensembles always provided superior results.

As mentioned in Section 6, ensembles are built with different methodologies. In this paper, we considered the bagging methodology by averaging all and the best models. As future works, we propose to investigate other ensemble methodologies as boosting and stacking. Moreover, there is room to investigate the benefits of ensemble learning in combination with regularization techniques such as data augmentation and classical regularizers (l1, l2 and dropout).

Acknowledgements

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