# Uncertainty Estimation in Neural Network-enabled Side-channel Analysis and Links to Explainability

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**Abstract.** Side-channel analysis (SCA) has emerged as a critical field in securing hardware implementations against potential vulnerabilities. With the advent of artificial intelligence(AI), neural network-based approaches have proven to be among the most useful techniques for profiled SCA. Despite the success of NN-assisted SCA, a critical challenge remains, namely understanding predictive uncertainty. NNs are often uncertain in their predictions, leading to incorrect key guesses with high probabilities, corresponding to a higher rank associated with the correct key. This uncertainty stems from multiple factors, including measurement errors, randomness in physical quantities, and variability in NN training. Understanding whether this uncertainty arises from inherent data characteristics or can be mitigated through better training is crucial. Additionally, if data uncertainty dominates, identifying specific trace features responsible for misclassification becomes essential.

We propose a novel approach to estimating uncertainty in NN-based SCA by leveraging Rényi entropy, which offers a generalized framework for capturing various forms of uncertainty. This metric allows us to quantify uncertainty in NN predictions and explain its impact on key recovery. We decompose uncertainty into epistemic (modelrelated) and aleatoric (data-related) components. Given the challenge of estimating probability distributions in high-dimensional spaces, we use matrix-based Rényi  $\alpha$ -entropy and  $\alpha$ -divergence to better approximate leakage distributions, addressing the limitations of KL divergence in SCA. We also explore the sources of uncertainty, e.g., resynchronization, randomized keys, as well as hyperparameters related to NN training. To identify which time instances (features in traces) contribute most to uncertainty, we also integrate SHAP explanations with our framework, overcoming the limitations of conventional sensitivity analysis. Lastly, we show that predictive uncertainty strongly correlates with standard SCA metrics like rank, offering a complementary measure for evaluating attack complexity. Our theoretical findings are backed by extensive experiments on available datasets and NN models.

Keywords: NN-assisted SCA. · Uncertainty. · Metrics.

# 1 Introduction

Assessing the security of an implementation against side-channel analysis (SCA) is a complex task. Since their introduction in the 1990s [Koc96, KJJ99], extensive research has been dedicated to analyzing physical leakage in the form of time, power, electromagnetic emanation, etc. This line of research focuses on evaluating mechanisms based on a solid theoretical foundation. A key advancement toward establishing rigorous, information-theoretic security has been the introduction of profiled SCA, which uses an open sample to estimate the device's leakage model [CRR02]. Profiled SCA represents the worst-case security scenario for an implementation, as there is no universal attack strategy capable of

extracting secret information from physical observables without prior knowledge of the device's leakage distribution [SMY09, WOS14, MCHS23]. [HRG14] has established that an optimal attack strategy from an information-theoretic perspective relies on distinguishing the correct key with regard to the probability distribution of leakage conditioned on the targeted secret. Establishing such an optimal distinguisher is known to be highly non-trivial due to the unknown true leakage distribution of a device that is complex to even estimate, especially in the presence of countermeasures like masking [CJRR99]. In fact, if one can perfectly learn the probability density function (pdf) of the leakage conditioned on the targeted secret, it can be further involved in a maximum likelihood distinguisher to obtain the optimal solution cf. [MDP20]. In the absence of knowledge about this pdf, supervised classification using deep neural networks (NNs) has emerged as a sub-optimal solution.

Despite major breakthroughs and increases in the effectiveness of NN-enabled attacks, obstacles should be faced to link NNs' concepts widely adopted in machine learning and SCA. One of the already known missing links in this regard is the link between performance metrics in both domains. While key rank, guessing entropy, and key discrimination success rate [SMY09] have been used as metrics in SCA, accuracy serves as the primary metric in machine learning. The lack of a direct equivalent for accuracy in SCA severely limits not only the evaluation of SCA effectiveness cf. [BPS<sup>+</sup>18, PHJ<sup>+</sup>19, MDP20], but also our ability to *explain* why an NN makes a correct/wrong key guess.

In fact, regardless of their applications, NN classifiers often assign a high prediction probability to an incorrect label, i.e., NNs are overconfident in their predictions [TB24, GTA<sup>+</sup>23]. This means that an NN model can be *uncertain* in its predictions even with a high predictive probability obtained at the end of the pipeline (the softmax output, for instance). In the context of SCA, the uncertainty can be translated to wrong guesses with high probabilities delivered by the NN (i.e., the correct key has a high rank instead of being ranked first). SCA-specific metrics, unfortunately, fail to provide a clear assessment of the model's predictive uncertainty.

The root cause of uncertainty in NN-enabled SCA can be measurement errors, randomness in physical quantities, and errors in the NN's architecture specification or its training. Calibration issues, limitations in precision, as well as human errors during measurement account for measurement errors. Randomness in physical quantities encompasses thermal noise, manufacturing, or environmental variations and can influence the consistency of patterns in traces, making the traces less exploitable [DCEM18, MHK<sup>+</sup>24, GOKT16]. On the other hand, the training process of an NN involves numerous parameters, e.g., batch size, optimizer, learning rate, stopping criteria, and regularization. Other stochastic elements like batch generation and weight initialization introduce more randomness during training [LBH15]. These directly lead to a strong factor for uncertainties in NNs' predictions.

The key question to address here is whether it is possible to *explain* why an NN's key guess is incorrect. In other words, one seeks to understand whether the uncertainty stems from the inherent characteristics of the data or if it can be mitigated through improved NN training. The second question that arises is: if data characteristics are determined as the primary contributor to predictive uncertainty in an NN employed in SCA, can one identify which trace features led to ambiguity in guessing the correct key?

**Contribution.** Our paper positively answers these questions by making the following contributions. We stress that we do not treat the concepts borrowed from the machine learning field as simple, "plug-and-play" solutions; instead, we adapt and tailor them to meet the specific needs of SCA. Through extensive experimentation, we validate our proposed uncertainty estimation framework and its implications for NN-based SCA, as detailed below.

1. We introduced the predictive uncertainty metric quantified by looking at the entropy of

the classification output conditioned on the input traces. In the context of SCA with high dimensional data, the precise probability density function pdf estimation required to approximate the entropy is infeasible. Therefore, we employ the matrix-based Rényi  $\alpha$ -entropy. Moreover, as the side-channel leakage can follow a multimodal and/or multivariate distribution [LPMS18, LM18, RBAF24, MMOS16, BGH<sup>+</sup>17, GLRP06, RBFA21, DCGRP19, Riv08, SMY09], conventional measures for approximating probability distributions cannot be employed. After discussing why one of the most popular measures, i.e., Kullback-Leibler divergence, fails to approximate the leakage distribution, we propose using  $\alpha$ -divergence [Ama12, ZR95] to approximate the pdfs and then compute the predictive uncertainty. In doing so, we also examine the relationship between uncertainty and standard SCA evaluation metrics, such as rank. Our findings reveal a strong relationship between uncertainty levels and rank. As opposed to an ideal case, our work demonstrates that higher predictive uncertainty often corresponds to lower-rank key guesses in existing NN-assisted SCA.

- 2. The second contribution of our paper is related to how explainability links to predictive uncertainty in SCA. Our approach explains whether the uncertainty arises from data uncertainty and/or model uncertainty. As a prime example, we evaluate the impact of desynchronization and key randomization on model uncertainty. Using datasets that introduced such characteristics, we show that they not only reduce attack performance, but also increase uncertainty in model predictions. We further take into account hyperparameters closely related to the NN training, including the number of epochs, the number of training/evaluation traces, and the network configuration. In this regard, we highlight the fact that the uncertainty can explain whether better hyperparameters could improve the attack. Such an explanation helps the evaluators understand whether the uncertainty is reducible, i.e., can be resolved by, e.g., feeding more traces to the NN. Hence, the uncertainty metric directly connects the NN performance to the attack cost and effectiveness.
- 3. Our third contribution deals with which time instance(s) in a trace causes uncertainty. The existing method in machine learning for this is uncertainty sensitivity analysis, which is improper in the context of SCA. The reason is that if a leakage trace is segmented into multiple sub-traces corresponding to successive operations, these sub-traces are likely to exhibit some degree of dependency. In other words, a correlation exists between successive leakage points, making multivariate statistical methods particularly suitable for SCA [CRR02]. Therefore, we conduct an in-depth analysis of time sample contributions using SHapley Additive exPlanations (SHAP) [LL17] to identify the most critical time features influencing model uncertainty. Clearly, given that side-channel traces contain thousands of time features, not all contribute equally to classification tasks. By integrating SHAP values with uncertainty estimations, we determine which time samples are most responsible for the uncertainty in model predictions, providing valuable insights for optimizing SCA models and improving attack efficacy.

#### 1.1 Organization of the Paper

The remainder of this paper is organized as follows. Section 2 provides a detailed background on profiled SCA and its evaluation metrics. In this section we also introduce uncertainty quantification techniques, SHAP values and the datasets that we used for our experiments. Section 3 details our methodology for uncertainty analysis in NN-enabled SCA. Section 4 presents extensive experimental results on benchmark datasets, focusing on uncertainty analysis under various conditions, such as desynchronization, calibration or different training setups. Section 5 concludes the paper by summarizing our findings, discussing their implications for SCA, and suggesting directions for future research.

# 2 Background

#### 2.1 Notations

In this paper, we adopt calligraphic letters such as  $\mathcal{X}$  to represent sets. Correspondingly, uppercase letters, such as X, denote random variables (random vectors are represented as  $\mathbf{X}$ ), while lowercase letters like x (or  $\mathbf{x}$  for vectors) indicate specific realizations of these random variables. Matrices are distinguished using bold capital letters. The *i*-th component of a vector  $\mathbf{x}$  is expressed as  $\mathbf{x}[i]$ , whereas the *i*-th observation of a random variable X is written as  $x_i$ . The pdf of a continuous random variable X is denoted as  $f_X$ , where  $f_X(x) = p(X = x)$ . The expected value is represented by  $\mathbb{E}[\cdot]$ , which may be sub-scripted by a random variable, as in  $\mathbb{E}_X[\cdot]$ , or by a probability distribution, written as  $\mathbb{E}_{f_X}[\cdot]$ , to specify the context in which the expectation is computed. Formulation of Shannon's conditional entropy is  $H(y \mid x) = H(y, x) - H(x)$ , whereas mutual information (MI) and conditional mutual information (CMI) is I(x; y) = H(x) + H(y) - H(x, y) and I(x; y|x') = H(x, x') + H(y, x') - H(x, y, x') - H(x'). Here, H denotes entropy or joint entropy:  $H = -\sum_{x \in X} p(x) \log p(x)$  and p(x) denotes the probability of random variable X taking value x.

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#### 2.2 Profiled Side-Channel Analysis

SCA exploits the observations **L** obtained during the operation of an algorithm to extract its secret [BPS<sup>+</sup>18]. When an SCA adversary gains control over an open device (i.e., a device where she can manipulate at least some inputs, including the secret), they can execute a specific class of attacks known as profiling attacks. A profiling SCA consists of two primary phases: a profiling phase and an attack phase [BPS<sup>+</sup>18]. For each possible key  $k \in \mathcal{K}$ , the attacker computes an estimated probability distribution function  $\hat{g}_k$  as follows:

$$g_k : (\ell, p) \mapsto p(\mathbf{L} = \ell \mid (P, K) = (p, k)).$$

$$\tag{1}$$

The estimated function  $\hat{g}_k$  is obtained from a profiling set  $\mathcal{D}_{\text{profiling}} \doteq \{(\ell_i, p_i, k_i)\}_{i=1}^{N_p}$ , where  $N_p$  represents the number of traces  $\ell_i$ . These traces are collected under known plaintext chunks  $p_i$  and key values  $k_i$ . Throughout this paper, the trace set is denoted by  $\mathcal{L}$ , while the corresponding set of inputs is referred to as  $\mathcal{X}$ .

In the attack phase, the attacker collects an attack set from a closed device, denoted as  $\mathcal{D}_{\text{attack}} \doteq \{(\ell_i, p_i)\}_{i=1}^{N_a}$ , where the unknown secret, say  $k^*$ , remains fixed but undisclosed. The attacker's goal is to recover this key. For traces in  $\mathcal{D}_{\text{attack}}$ , a score based on the maximum-likelihood of each hypothetical key can be obtained as

$$\mathbf{d}_{Na}[k] = \prod_{i=1}^{N_a} \Pr((P,K) = (p_i,k) \mid \mathbf{L} = \ell_i) = \prod_{i=1}^{N_a} \frac{\Pr(\mathbf{L} = \ell_i \mid (P,K) = (p_i,k)) f_{\mathbf{L}}(\ell_i)}{f_{P,K}(p_i,k)}.$$
 (2)

where Bayes' theorem has been applied to derive the equation. The posterior probabilities  $p(\mathbf{L} = \ell_i \mid (P, K) = (p_i, k))$  are obtained from the generative model built during the profiling phase.

Metrics for SCA. In the realm of SCA, model performance is often assessed using the rank function. Let  $k^* \in \mathcal{K}$  denote the true key used during  $\mathcal{D}_{\text{profiling}}$  acquisition. The rank function of a model  $\hat{g}$  trained on  $\mathcal{D}_{\text{profiling}}$  and tested on  $\mathcal{D}_{\text{attack}}$  is:

$$\operatorname{rank}(\hat{g}, \mathcal{D}_{\operatorname{profiling}}, \mathcal{D}_{\operatorname{attack}}, n) = |\{k \in \mathcal{K} \mid \mathbf{d}_{Na}[k] > \mathbf{d}_{Na}[k^*]\}|,$$
(3)

where  $\mathbf{d}_{Na}[k]$  represents the score for candidate k, as defined in Equation 2. The score is derived from the conditional probability model built on  $\mathcal{D}_{\text{profiling}}$  and evaluated on the

first *n* traces in  $\mathcal{D}_{\text{attack}}$ . If  $k^*$  achieves the highest score, the rank is 0; if it has the lowest, the rank is  $|\mathcal{K}| - 1$ . Since the rank varies based on the traces used, it is common practice to calculate it across different dataset chunks and determine the average rank, also known as guessing entropy [MPP16].

#### 2.3 Matrix-based Estimation of Rényi Entropy

When using a generalized version of Shannon entropy—specifically Rényi entropy—informationtheoretic measures can be computed through functionals applied to normalized positive definite matrices. These matrices are constructed by evaluating a positive definite kernel on all pairs of data points [GRP14, YWJP20], which implicitly maps the data into a reproducing kernel Hilbert space (RKHS) of functions. This approach enables the analysis of information quantities without requiring explicit estimation of the underlying probability distribution of the data.

**Definition 1.** (cf. [YP19]) Consider n samples  $\{x_1^i, x_2^i, \dots, x_k^i\}_{i=1}^n$ , where each sample contains k ( $k \ge 2$ ) measurements, we define the kernels  $\kappa_1 : \mathcal{X}_1 \times \mathcal{X}_1 \mapsto \mathbb{R}, \dots, \kappa_k : \mathcal{X}_k \times \mathcal{X}_k \mapsto \mathbb{R}$  ( $X_z = x_z^1, \dots, x_z^n$  with  $1 \le z \le k$ ). The kernels are real-valued positive definite and infinitely divisible [Bha06, YP19]. The Rényi's  $\alpha$ -order joint-entropy for k variables is

$$\mathbf{J}_{\alpha}(\mathbf{X}_{1},\cdots,\mathbf{X}_{k}) = \mathbf{S}_{\alpha}\left(\frac{\mathbf{A}_{1}\odot\cdots\odot\mathbf{A}_{k}}{tr(\mathbf{A}_{1}\odot\cdots\odot\mathbf{A}_{k})}\right),\tag{4}$$

where  $(\mathbf{A}_1)ij = \kappa_1(x_1^i, x_1^j), \dots, (\mathbf{A}_k)ij = \kappa_k(x_k^i, x_k^j)$ . Here,  $tr(\cdot)$  and  $\odot$  denote the transpose and Hadamard product operators, respectively. Furthermore, the function  $\mathbf{S}_{\alpha}(\cdot)$  is defined as follows.

$$\mathbf{S}_{\alpha}(\mathbf{A}) = \frac{1}{1-\alpha} \log_2(tr(\mathbf{A}^{\alpha})) = \frac{1}{1-\alpha} \log_2 \sum_{i=1}^n \lambda_i(\mathbf{A}^{\alpha}), \tag{5}$$

where  $\lambda_i(\mathbf{A})$  denotes the *i*<sup>th</sup> eigenvalue of  $\mathbf{A}$ .

The relationship between the matrix **A** in Equation (5) and the Gram matrix **K** can be formulated as  $\mathbf{A}_{ij} = \frac{\mathbf{K}_{ij}}{n\sqrt{\mathbf{K}_{ii}\mathbf{K}_{jj}}}$ . In order to approximate Shannon entropy, the information quantities are computed by setting  $\alpha = 1.01$  in the matrix-based Rényi entropy formula [GP13, GRP14].

#### 2.4 SHAP Values

SHAP (SHapley Additive exPlanations) values provide an interpretable method to understand the contributions of individual features in a machine learning model. Based on cooperative game theory, SHAP fairly attributes the prediction of a model to its input features by considering their marginal contributions across all possible feature subsets [SREG<sup>+</sup>25].

**Definition 2.** For a model  $f : \mathcal{X} \to \mathbb{R}$  and a set of input features  $\mathcal{N}$ , the SHAP value  $\phi_i$  for feature  $i \in \mathcal{N}$  is defined as:

$$\phi_i = \sum_{S \subseteq \mathcal{N} \setminus \{i\}} \frac{|S|! \cdot (|\mathcal{N}| - |S| - 1)!}{|\mathcal{N}|!} \left[ f(S \cup \{i\}) - f(S) \right],\tag{6}$$

where S represents a subset of features, and f(S) is the model output when only the features in S are included. SHAP ensures *additivity* and *fairness*: the sum of contributions from all features equals the model's output. This property makes SHAP particularly suitable for analyzing time sample contributions in side-channel traces. By applying SHAP to profiled SCA, we can identify which time samples have the greatest impact on model predictions and key recovery performance.

#### 2.5 Datasets

This paper uses two versions of the ASCAD dataset, which serve as benchmarks for evaluating the performance of NN-based SCA models.

**ASCAD Fixed (ASCAD-f).** The ASCAD fixed dataset targets an 8-bit AVR microcontroller running a masked AES-128 implementation. Electromagnetic (EM) emanations are recorded as side-channel traces. The dataset consists of a profiling set with 50,000 traces and an attack set with 10,000 traces. Each trace contains 700 features extracted from a fixed time window, and the profiling and attack sets use the same encryption key. The attack focuses on recovering the third key byte, which corresponds to the first masked intermediate value. This dataset also has traces with parametrized desynchronization to check the efficiency of the algorithm against jitter, here we also use traces with 50 and 100 desynchronization [BPS<sup>+</sup>20].

**ASCAD Random (ASCAD-r).** The ASCAD random dataset is an extension of the ASCAD family, featuring random encryption keys for the profiling phase. This dataset contains a profiling set with 200,000 traces recorded with random keys and an attack set with 100,000 traces using a fixed key. The attack still focuses on the third key byte, but the traces contain a larger window of 1,400 features to account for increased variability due to random keys. ASCAD-r is more challenging than ASCAD-f due to the presence of key randomness, which increases noise and reduces the effectiveness of simple leakage models.

Both ASCAD-f and ASCAD-r provide a controlled environment for evaluating NN-based profiled attacks. The use of masked AES-128 ensures that these datasets are representative of real-world cryptographic implementations [BPS<sup>+</sup>20].

**CHES CTF 2018.** The database refers to the CHES Capture-the-flag (CTF) AES-128 trace set, which was released in 2018 for the Conference on Cryptographic Hardware and Embedded Systems (CHES) [Ris18]. The traces are derived from masked AES-128 encryption executed on a 32-bit STM microcontroller. In our experiments, we utilize 45,000 traces for the training set, which incorporates a fixed key. The test set comprises 5,000 traces, with the key used in the training set being different from the key configured for the test set. Additionally, every trace contains 2,200 features.

# 3 Uncertainty Analysis in SCA

Our main objective in this section is to study the uncertainty associated with the predictions of NNs in SCA. To achieve this, we start with formulation of NN-enabled SCA to understand sources of uncertainty.

#### 3.1 NN-enabled Profiled SCA

As explained in Section 2.2, the attacker aims to disclose the secret  $k^*$ , where she must determine which of the estimated probability distributions  $\hat{g}_k$  (for each  $k \in \mathcal{K}$ ) best fits the attack set. Given reasonable assumptions about the distributions, the most efficient way to determine this is through a maximum likelihood strategy. This strategy involves computing the following likelihood function  $\mathbf{d}_{Na}[k]$  for each key candidate  $k \in \mathcal{K}$  and selecting the most probable candidate; see Equation 2. Estimating  $\Pr(\mathbf{L} \mid (P, K) = (p, k))$ for a given pair  $(p, k) \in \mathcal{Y}$  with  $\mathcal{Y} \doteq \mathcal{P} \times \mathcal{K}$  is recognized as a prediction problem (also referred to as a generation problem). Conversely, estimating  $p((P, K) = (p, k) | \mathbf{L})$  is known as a classification problem. Bayes' theorem provides a means to relate the latter more complex pdf to the simpler former one, making two problems closely interconnected [BPS<sup>+</sup>18, LTR17].

NNs have found application in SCA since they provide tools for handling classification problems, enabling a discriminative approach [LTR17]. This means that the classification problem is directly addressed by estimating  $Pr((P, K) = (p, k) | \mathbf{L})$  without relying on Bayes' inversion [BN06]. This methodology aims at constructing an approximation  $\hat{f}_{\mathbf{L},P}$ of the function  $f_{\mathbf{L},P} : (\ell, p) \mapsto Pr((P, K) = (p, k) | \mathbf{L} = \ell)_{k \in \mathcal{K}}$ . The classification of a new trace  $\ell$  observed for an input p is carried out by computing  $\mathbf{y} = \hat{g}_{\mathbf{L},P}(\ell, p)$  and selecting the key candidate  $\hat{k}$  (or equivalently, the corresponding label in ML terminology) as:  $\hat{k} = \arg \max_{k \in \mathcal{K}} \mathbf{y}[k]$ . When key discrimination is conducted over  $N_a$  pairs  $(\ell_i, p_i)$ , the maximum likelihood approach is applied as follows:

$$\mathbf{d}_{N_a}[k] = \prod_{i=1}^{N_a} \mathbf{y}_i[k],\tag{7}$$

where  $\mathbf{y}_i$  represents the output of the function  $\hat{f}_{\mathbf{L},P}$  when evaluated with the pair  $(\ell_i, p_i)$ . Using the same notation, accuracy is defined as:

$$\operatorname{acc}(\hat{g}, \mathcal{D}_{\operatorname{train}}, \mathcal{D}_{\operatorname{test}}) = \frac{|\{(\ell_i, p_i, k^*) \in \mathcal{D}_{\operatorname{test}} \mid k^* = \arg \max_{k \in \mathcal{K}} \mathbf{y}_i[k]\}|}{|\mathcal{D}_{\operatorname{test}}|},$$
(8)

where  $\mathbf{y}_i$  is the output vector from  $\hat{g}(\ell_i, p_i)$ .

Notably, Equation 7 is a straightforward reformulation of Equation 2, where the conditional probability  $Pr((P, K) = (p_i, k) | \mathbf{L} = \ell_i)$  is replaced by its approximation  $\mathbf{y}_i[k] = \hat{f}_{\mathbf{L},P}(\ell_i, p_i)[k]$  cf. [BPS<sup>+</sup>18]. This approximation of  $\hat{g}_{\mathbf{L},P}$  can be performed by NNs from a family of functions (often referred to as models in ML terminology) whose types are usually specified a priori by the data analyst to suit the problem's specific characteristics. Selecting the appropriate type of NNs in SCA is the first step, where the first attempts have been devoted to combining convolutional NNs (CNNs) with data augmentation in order to enhance attack performance, even against protected designs [BPS<sup>+</sup>18, PYW<sup>+</sup>17, WAGP20, ZBHV20]. Later, studies have shown similar performance, and sometimes even superiority, when using multi-layer perceptrons (MLPs) [WPP22, AGF23]. Regardless of NN types, the approximated function  $\hat{g}_{\mathbf{L},P}$  is selected from a predefined class of parameterized hypotheses established by the evaluator (i.e., the adversary). This class can be thought of as a collection of models  $G_{\theta} = \{g_{\theta}(x) | g_{\theta} : x \mapsto g_{\theta}(x, \theta)\}$  with  $\theta \in \Theta \subseteq \mathbb{R}^{q}$ , where q is the dimension of the vector gathering all the parameters cf. [MDP20].

Within the ML community, various evaluation frameworks are utilized to measure model performance and select optimal parameters within a given family of models. According to Bayes error in supervised classification, accuracy maximization is the optimal strategy for setting model parameters  $\theta$ . Maximizing the accuracy is equivalent to only finding the model that maximizes the probability that the right key is ranked first [BPS<sup>+</sup>18, MDP20].

#### 3.2 Uncertainty in NNs' Predictions

The prediction process constitutes three principal steps. First, the data acquisition phase is devoted to capturing observations, whereas during the NN building phase, the NN is designed and trained to learn patterns from the measurements. The trained model is then deployed in the applied inference phase, where it is utilized to make predictions. The predictive uncertainty deals with the uncertainty sources within the NN and the data to quantify whether the model's outputs should (not) be trusted [GTA<sup>+</sup>23]. (see Section 1 for sources of uncertainty in SCA). Model uncertainty accounts for the uncertainty arising from limitations in the model itself, which may result from errors in the training process, an inadequate model architecture, or insufficient knowledge due to the presence of unknown samples or an incomplete representation of the training data, see Figure 1. In contrast, data uncertainty is linked to uncertainties inherent in the data itself. It arises from the loss of information when capturing real-world phenomena within a dataset. While model uncertainty can, in principle, be mitigated by refining the model architecture, training process, or dataset quality, data uncertainty is intrinsic to the data and cannot be eliminated [KG17].

The Bayesian framework provides an elegant approach for modeling uncertainty in deep learning [GG16, TB24]. The underlying principle of this framework is that to estimate  $y^*$ , one commonly employs the maximum a posteriori (MAP) approach, which determines the most probable outcome as  $y^* = \arg \max_y p(y|x^*, \theta)$ . Since the underlying model relies on an unknown latent variable  $\theta$ , an approximation is constructed using a sampled training dataset  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ , which contains N training samples. In the Bayesian framework, model uncertainty is expressed as a probability distribution over the model parameters  $\theta$ , whereas data uncertainty is represented as a probability distribution over predictions  $y^*$ , given a parameterized model  $f_{\theta}$ . When predicting  $y^*$  for a new sample  $x^*$ , the distribution of prediction is given by:

$$p(y^*|x^*, \mathcal{D}) = \int p(y^*|x^*, \theta) p(\theta|\mathcal{D}) d\theta.$$
(9)

In a classification problem, predictive uncertainty is measured by the entropy of the softmax output distribution as  $H(y^*|x^*, \mathcal{D})$  [G<sup>+</sup>16, GG16, GIG17, HHGL11].

Moreover, in Equation 9, the term  $p(\theta|\mathcal{D})$ , known as the posterior distribution, corresponds to the uncertainty in the model parameters given the training dataset  $\mathcal{D}$ . However, this posterior

distribution is often intractable. Applying the Bayes theorem to reformulate the posterior distribution yields  $p(\theta|\mathcal{D}) = p(\mathcal{D}|\theta)p(\theta)/p(\mathcal{D})$ , with  $p(\theta)$  represents the prior distribution over model parameters, incorporating general knowledge about  $\theta$  without specific observations [BN06]. The likelihood term  $p(\mathcal{D}|\theta)$  measures the probability that the dataset  $\mathcal{D}$  aligns with the distribution defined by a model parameterized by  $\theta$ . Many standard loss functions, such as cross-entropy and mean squared error, are derived from or directly related to this likelihood function [GTA<sup>+</sup>23].

Despite this reformulation, the predictive uncertainty remains intractable. To approximate that, various methods have been proposed, offering different trade-offs in accuracy and computational complexity. Next, we discuss how we can use Bayesian methods to estimate uncertainty in the context of SCA. For that, we use the matrix-based estimation of Rényi Entropy introduced next.

#### 3.3 Uncertainty Analysis through Bayesian Modeling

In this work, we develop tools to derive practical uncertainty estimates in NNs by employing Bayesian models—without altering the NN models themselves or the optimization process. Bayesian modeling offers a principled way to estimate uncertainty by treating model parameters as probability distributions rather than fixed values [GG16, G<sup>+</sup>16, Cha18, JLB<sup>+</sup>22, SG05, JLB<sup>+</sup>22]<sup>1</sup>. This modeling does not aim to enhance NN's performance,

Figure 1: Uncertainty decomposition in a binary classification task.



 $<sup>^1\</sup>mathrm{Note}$  that we do not train Bayesian NNs, but employ principles of Bayesian modeling to compute the uncertainty.

but to explain why a prediction is made by the NN [TB24]. Our approach captures both *epistemic* (model-related) and *aleatoric* (data-dependant) uncertainties more effectively. As shown in Equation 9, estimating the posterior distribution of the weights is essential to computing the predictive uncertainty. Therefore, given an already-trained NN, the following steps should be taken cf. [VdSDK<sup>+</sup>21]: (1) representing existing knowledge about the NN's parameters in a statistical model through a prior distribution  $p(\theta)$ —usually defined before data is collected; (2) defining the likelihood function based on information about the parameters contained in the observed data ( $p(\mathcal{D}|\theta)$ ); and (3) combining the prior and likelihood using Bayes' theorem to obtain the posterior distribution  $p(\theta|\mathcal{D})$ .

#### 3.3.1 Defining the Prior Distribution

To implement this, we first need to determine the appropriate distribution for the model's parameters. A reasonable assumption is that the weights follow a normal (Gaussian) distribution. This assumption is supported by the central limit theorem, which states that the sum of many independent variables tends to be normally distributed [Ros14]. More importantly, it is known that NNs with random Gaussian weights can create a stable embedding of the data, serving as a universal classifier [GSB16]. Additionally, common training techniques, such as stochastic gradient descent (SGD), introduce randomness that can contribute to a normal-like distribution of the trained weights. Another reason to assume normality is the weight initialization method used in SCA-related literature, e.g., [WAGP20, AGF23], which follows He initialization [HZRS15]. This initialization method relies on sampling weights from a normal distribution, confirming our assumption. Toy example. Among multiple NNs trained on ASCAD-f dataset (see Section 2.5), we select the model used in [WAGP20] due to its simple and compact structure (code is available in [KUL20]), which achieves a great deal of attack performance in terms of the number of attack traces needed to reach rank = 0. The network consists of two convolutional and 3 dense layers, trained on 90% of the profiling traces. To examine whether the trained model's weights indeed follow a normal distribution, we use quantilequantile (Q-Q) plots [WG68]. These plots visually compare the quantiles of our sample distribution (the model's weights) with those of an ideal normal distribution. If the points align along the diagonal, the weight distribution is approximately normal. Deviations from this diagonal indicate skewness, heavy tails, or other irregularities in the distribution.

In our scenario, once we confirm the normality assumption for our model's weights, the next step is to determine the mean and variance of the distribution. By fitting a Gaussian distribution, we experiment with different values of mean and variance to find a distribution that closely matches the actual weight distribution. The blue curve in Figure 3 illustrates the weight distribution for the second layer of the trained model. The orange curves represent distributions close to the original distribution, and we observe that the one on the right provides a closer match to the actual distribution, yielding a higher similarity score (see Section 3.3.3).

#### 3.3.2 Defining the Likelihood Function

In order to determine the likelihood function, one specifies a data-generating model and includes observed data [VdSDK<sup>+</sup>21]. The likelihood  $p(\mathcal{D}|\theta)$  is a function of  $\theta$  for a given dataset  $\mathcal{D}$ ; hence, the likelihood function summarizes a model that stochastically generates all the traces and a range of possible values for  $\theta$  explaining the observations. This specified model, represented by the likelihood function, is the foundation for the uncertainty analysis, as the posterior distribution is the result of the prior distribution determined in this step. **Background knowledge offered by SCA.** In various fields, specifying a likelihood function can be nontrivial; however, SCA provides insight into this problem. In the context of SCA, it is assumed that each trace is measured independently from others. Hence,



Figure 2: Q-Q plots of the layers in [WAGP20]. The model consists of six layers and achieves high performance on the ASCAD-fixed dataset with fewer than 150 traces. Notably, this model does not include convolutional layers to capture repetitive patterns.

the likelihood function can be written as  $p(\mathcal{D}|\theta) = \prod_{i=1}^{N} p(\mathbf{y}_i \mid \theta, p_i)$  for a given key. The likelihood  $p(\mathbf{y}_i \mid \theta, x_i)$  can be thought of as the output of the output layer in the NN, where logits are translated to probabilities.

The choice of the output layer is closely tied to the selection of the loss function. In line with deep learning principles, classification neural networks that employ a softmax output layer tend to learn more efficiently and robustly when trained with the negative loglikelihood (NLL) loss function [GBC16]. Interestingly, it has been shown that minimizing the negative log-likelihood (NLL) function (similarly, the cross-entropy loss) during training is asymptotically equivalent to maximizing the estimated mutual information between the side-channel traces and the leakage profiling model (i.e., the machine learning model trained on the traces) [MDP20]. Hence, for networks employing the softmax function and trained on side-channel traces, predictions of the NN can be directly used as the likelihood  $p(\mathbf{y}_i \mid \theta, p_i)$ .

#### 3.3.3 Bayesian Inference

Defining the likelihood function is followed by *Bayesian Inference*<sup>2</sup>. Bayesian inference requires evaluating the true posterior  $p(\theta \mid D)$ , which cannot be evaluated analytically, as explained before. To address this, we use variational inference [Cha18], a powerful technique in Bayesian modeling that allows us to approximate the complex, intractable posterior distributions of the network's parameters. During the profiling phase, this

<sup>&</sup>lt;sup>2</sup>It is important to note that the term "inference" means differently in Bayesian modeling and deep learning. In Bayesian modeling, "inference" refers to the process of integrating over model parameters  $\theta$ , which often involves approximation techniques. In contrast, in deep learning, inference typically refers to evaluating the model on test data after training is complete.



Figure 3: Weight distribution for the second layer of the trained model [WAGP20]. Two different parameter settings are used for sampling (orange curves). The right distribution, which has a closer mean and variance to the actual weights, produces more accurate results.

distribution is learned by the model  $\hat{g}$  given the profiling traces. Intuitively, variational inference approximates the intractable posterior distribution  $p(\theta|\mathcal{D})$  with a tractable distribution over the model weights,  $q_{\nu}(\theta)$ , with variational parameters  $\nu$ . In other words, variational inference makes it feasible to use Bayesian methods to transform the problem into an optimization task. The approximated distribution should be as close as possible to the posterior distribution obtained from the original model. Hence, the approximated distribution is usually minimized by calculating the Kullback-Leibler (KL) divergence with regard to  $\theta$ :

$$\operatorname{KL}(q_{\nu}(\theta) \parallel p(\theta|X)) := \int q_{\nu}(\theta) \log \frac{q_{\nu}(\theta)}{p(\theta|X)} d\theta.$$
(10)

To solve Equation 10, an approximating variational distribution  $q_{\nu}(\theta)$  should be defined first, and then the KL divergence can be minimized to determine the variational parameter  $\nu$ . A common choice is a mean-field approximation, where the variational distribution factorizes into independent Gaussian distributions over the weights [HVC93]:

$$q_{\nu}(\theta) = \prod_{l=1}^{L} \prod_{i=1}^{V_{l-1}} \prod_{j=1}^{V_l} \mathcal{N}\left(\theta_{ijl}; \mu^{\theta}_{ijl}, (\sigma^{\theta}_{ijl})^2\right), \qquad (11)$$

where L is the number of layers, and  $V_{\ell}$  is the number of parameters per layer. The parameters  $\mu_{ijl}^{\theta}$  and  $\sigma_{ijl}^{\theta}$  define the mean and standard deviation of the weight distributions. This approximation assumes the independence of each weight scalar in each layer from all other weights to simplify the Bayesian inference. It is clear that if this assumption does not hold true in practice, the approximation loses important information about weight correlations. To resolve the issue, Monte Carlo sampling [Gra11] and using a mixture of Gaussians prior to each weight [BCKW15] have been introduced.

Why SCA does not comply well with KL divergence. KL divergence-based variational inference suffers from issues known to the machine learning community, including scalability and computational complexity [G<sup>+</sup>16]. Besides, when it comes to SCA, leakage can follow a multimodal and/or multivariant distribution [LPMS18, LM18, RBAF24, MMOS16, BGH<sup>+</sup>17, GLRP06, RBFA21, DCGRP19, Riv08, SMY09]. In SCA-related literature, it has been theoretically verified that the estimated leakage function  $\hat{g}_{L,P}$  is always composed of some Gaussian PDFs (i.e., following a Gaussian mixture model–GMM), where the key hypothesis k determines how the Gaussian PDFs are mixed cf. [PR09, PR10, BGP<sup>+</sup>11]. In such scenarios,  $q_{\nu}(\theta)$  fitted with the KL divergence criterion fails to capture the global behavior of the posterior as it fits a local mode of that. In other words, KL divergence neither exhibits "mass-covering property", nor offer the ability to adjust the



Figure 4: Solutions for minimizing the  $\alpha$ -divergence between the complicated posterior distribution p (shown in blue) and the tractable, unnormalized Gaussian approximation q (shown in red) [DHLDVU16, M<sup>+</sup>05].  $\alpha \rightarrow 0$  corresponds to KL.

impact of likelihood ratios as in GMMs [HLLR<sup>+</sup>16, LG17]. These lacks can result in less accurate approximations—particularly in the case of complex models.

 $\alpha$ -divergence. The KL-divergence is one of the options for measuring the distance between the posterior and the tractable distribution  $q_{\nu}$ . A more general alternative is the  $\alpha$ -divergence, defined as:

$$D_{\alpha}(p(x) \parallel q(x)) := \frac{1}{\alpha(1-\alpha)} \left( 1 - \int p(x)^{\alpha} q(x)^{1-\alpha} dx \right).$$
(12)

 $\alpha$ -divergence measures the "similarity" between two distributions. To explore how the choice of  $\alpha$  influences the outcome of inference, we consider the task of approximating a complex distribution p with a more manageable Gaussian distribution q by minimizing the divergence between the two; see Figure 4. When  $\alpha$  is large and positive, the approximation q tends to cover all the modes of p, whereas for  $\alpha \to -\infty$  (assuming the divergence remains finite), q is drawn toward the mode with the highest probability mass cf. [HLLR<sup>+</sup>16]. If the true posterior is multimodal, a global approximation using  $\alpha \geq 1$  will capture multiple modes; however, it also assigns large enough probability to regions where the true posterior has low density.

#### 3.4 Uncertainty Decomposition in SCA

Understanding what a model does not know is a critical part of NN-enable NNs. If one is able to assign a high level of uncertainty to the NN's erroneous predictions, then poor attack performance can be explained and, to some extent, improved by taking the right measures into account. The ultimate goal of decomposing the uncertainty in SCA is to link the high rank of the correct key (as one of the possible metrics) to inherent noise in traces and/or uncertainty in the model parameters. While the former cannot be reduced even if more data were to be collected, the latter can be resolved by considering different means, e.g., better hyperparameter tuning, regulation, etc. In this regard, as in the machine learning field, uncertainty can be decomposed into *epistemic* and *aleatoric* uncertainties [DKD09, KG17]. As described in Section 3.2, the predictive uncertainty of an attack trace  $x^*$  and its output  $y^*$ , denoted as  $H(y^*|x^*, D)$ , is expressed as [DHLDVU18, KG17]:

$$H(y^*|x^*, \mathcal{D}) = I(y^*, \theta | x^*, \mathcal{D}) + \mathbb{E}_{\theta \sim p(\theta | \mathcal{D})}(H(y^*|x^*, \theta)).$$
(13)

The terms in Equation 13 are explained below.

#### 3.4.1 Predictive uncertainty estimation for SCA.

The core idea of employing the variational distribution  $q_{\nu}(\theta)$  is that, after minimizing the divergence to select  $\nu$ , it closely approximates the posterior weight distribution while remaining simple to sample from. To this end, because the exact posterior  $p(\theta|\mathcal{D})$  is intractable, we substitute it with an approximate variational distribution  $q(\theta)$ , once the variational parameters  $\nu$  have been optimized. This yields  $p(y^*|x^*, \mathcal{D}) \approx \int p(y^*|x^*, \theta)q(\theta)d\theta$  (see Equation 9). Instead of performing direct integration over the weight space, a common approach is to use Monte Carlo sampling. In this method, m samples are drawn from the weight distribution  $\theta_m \sim q(\theta)$ , and each sample is used to compute the likelihood  $p(y^*|x^*, \theta_m)$ . With this approximation, the output distribution can be written as:  $p(y^* \mid x^*, \mathcal{D}) \approx (\sum_{m=1}^M p(y^* \mid x^*, \theta_m))/M$  with each  $\theta_k$  is a sample drawn from the approximate weight distribution  $q(\theta)$ .

In the context of SCA, to calculate the predictive uncertainty  $H(y^*|x^*, \theta_m)$ , we use matrix-based Rényi entropy [YWJP20]. The reason for our choice is twofold. First, large datasets with high dimensions in SCA can be analyzed more straightforwardly when employing matrix computations, which effectively reduce computational complexity. The second reason is more delicate. Information-theoretic quantities, e.g., entropy, heavily depend on the underlying probability distribution of the data. When these probability distributions are unknown, and only a finite set of samples is available, such quantities must be estimated. A common method is the "plug-in" approach, which first fits a model to the available data and then uses this model to compute the desired quantity [GRP14]. While intuitive and (sometimes) easy to compute, this method relies on accurately estimating the data distribution, which can be intractable when, for instance, dealing with noisy data. On the other hand, parametric statistical models require selecting an appropriate model and balancing complexity and tractability, while non-parametric statistical approaches often involve tuning an extra hyperparameter. Moreover, non-parametric statistical models may suffer from overfitting, where smoothing and regularization techniques must be employed to control statistical model capacity.

Interestingly enough, if a generalized form of Shannon entropy, namely Rényi entropy, is considered, the information-theoretic measures can be quantified using functionals on normalized positive definite matrices. To put it simply, the matrices are obtained by evaluating a positive definite kernel on all pairs of data points [GRP14, YWJP20]. This implicitly maps the data to a reproducing kernel Hilbert space (RKHS) of functions.

To calculate  $H(y^* | x^*, \theta_m)$  for a given model with parameters  $\theta_m$  using matrix-based Rényi entropy as in Definition 1, we have

$$H(y^* \mid x^*, \theta_m) = \mathbf{S}_{\alpha}(\mathbf{A}) = \mathbf{S}_{\alpha}\left(\frac{\mathbf{A}_1 \odot \cdots \odot \mathbf{A}_k}{\operatorname{tr}(\mathbf{A}_1 \odot \cdots \odot \mathbf{A}_k)}\right).$$
(14)

In Equation 14,  $\mathbf{A}_1, \cdots, \mathbf{A}_{k_t}$  denote the Gram matrices evaluated over the output of the softmax function in the NN.

#### 3.4.2 Estimating aleatoric uncertainty.

Aleatoric uncertainty is defined as the expected entropy of the model's predictions over the sets of weights. To estimate that, we perform

$$\mathbb{E}_{\theta \sim p(\theta|\mathcal{D})} \left[ H(y^* | x^*, \theta) \right] = -\int p(\theta \mid \mathcal{D}) H(y^* | x^*, \theta) d\theta \tag{15}$$

Since the true posterior  $p(\theta \mid D)$  is intractable, we approximate it with the variational distribution  $q(\theta)$ , and use Monte Carlo sampling with M samples:  $\mathbb{E}_{\theta \sim p(\theta \mid D)} [H(y^* \mid x^*, \theta)] \approx -(\sum_{m=1}^{M} \sum_{c} H(y^* = c \mid x \cdot \theta_m))/M$ , where  $\theta_m \sim q(\theta)$  are samples from the approximate posterior. This estimates the aleatoric uncertainty by averaging over the model's predictive distributions conditioned on sampled weights.

#### 3.4.3 Estimating epistemic uncertainty.

Epistemic uncertainty  $I(y^*, \theta | x^*, D)$  is computed as the difference between predictive entropy and aleatoric entropy. This captures the uncertainty due to model limitations, highlighting areas where the model requires more information for improved predictions.

#### 3.5 Sensitivity Analysis in SCA

After understanding how much the model contributes to the predictive uncertainty, one can be interested in explaining which measurement in time (i.e., a feature in the side-channel trace) can account for the uncertainty. Determining the contribution of the time features  $x_j$   $(1 \le j \le k)$  to predictive uncertainty allows us to pinpoint areas where profiling data is sparse [ABA<sup>+</sup>20]. A feature exhibiting high aleatoric sensitivity suggests a strong relationship with unobserved or latent variables, e.g., noise in side-channel traces. In such cases, collecting more traces could be helpful. On the other hand, a feature with high epistemic sensitivity indicates that the model's confidence heavily depends on it, and thus, careful feature selection can reduce the attack cost and complexity. Hence, sensitivity analysis helps establish the relationship between leakage points and attack cost.

In the machine learning domain, sensitivity analysis is a straightforward technique that offers insights into how variations in the input influence the network's predictions. The importance score  $S_i$  for the measurement  $x_i^*$  quantifies this influence. This score measures the overall significance of an input dimension with respect to a selected uncertainty metric through summing linear approximations centered around each test data point as formulated below cf. [DHLUR17].

$$S_{i} = \frac{1}{|\mathcal{D}_{\text{test}}|} \sum_{n=1}^{|\mathcal{D}_{\text{test}}|} \left| \frac{\partial H(y|x)}{\partial x_{n,i}} \right|; \ 1 \le i \le k.$$
(16)

One can leverage the chain rule to compute these derivatives.

However, the derivative-based approach assumes that other time features remain constant, thereby failing to account for interactions between features. Given that side-channel traces can be inherently multivariate, the contributions of time samples to uncertainty are interdependent, necessitating a method that captures their interconnections.

To address this limitation, we use SHAP values, as discussed in Section 2.4. SHAP values assess the contribution of a time feature by considering all possible subsets of other features [LC23]. More precisely, SHAP aims to allocate credit for a model's output among its input features, based on principles from cooperative game theory. The algorithm associates input features with players in a game and aligns the model function with the game's rules. In game theory, players can choose to participate or not, which translates in machine learning to whether a feature "influences" the uncertainty. Specifically, for each feature, we track changes in uncertainty when that feature is included or excluded from all possible subsets of features. To evaluate the influence of a feature on the uncertainty, the influence of the remaining features is integrated out using a conditional expectation approach as  $\mathbb{E}_{x^* \in \mathcal{D}_{test}}[H(y \mid x_i^*)]$ .

## 4 Results and Discussion

#### 4.1 Experimental Setup

The experiments were conducted on a high-performance computing system running Ubuntu 22.04.3 LTS with a 6.5.0-44-generic Linux kernel. The system was equipped with dual Intel(R) Xeon(R) Silver 4216 CPUs, each with 16 cores and 32 threads, providing a total of 64 logical processors. The system had 256 GB of RAM. For GPU-accelerated computations, an NVIDIA RTX A4000 GPU with 16 GB of dedicated memory was utilized. In all experiments presented in this section, the parameter  $\alpha$  associated with  $\alpha$ -divergence is set to 1. Moreover, for Rényi entropy,  $\alpha = 1.01$  to approximate Shannon's entropy definition.

Table 1: The architecture of the models used in our case studies. Here, C(filters, kernel size, strides) and P(size, stride) show the hyperparameters for a convolutional layer and average pooling. FLAT denotes a flatten layer, whereas FC(#neurons) denotes a fully connected layer with the number of neurons given in parentheses. SM(#classes) shows the number of classes at the softmax layer.

Data set	Leakage model	Architecture	
ASCAD-f [WAGP20]	ID	P(350,1),FLAT, FC(10), FC(10), SM(256)	
ASCAD-r [WPP22]	ID	$\begin{array}{c} C(120,3,1), \ P(32,2), \ C(8,1,1), \\ P(32,2), \ FLAT, \ FC(30), \\ FC(5), \ FC(5), \ SM(256) \end{array}$	
CHES CTF [WPP22]	HW	P(1100,1), FLAT, FC(512), FC(256), FC(128), FC(64), FC(9), SM(9)	



Figure 5: Average rank (so-called guessing entropy–GE) plots of the datasets used in this paper.

Architecture of the models. The architectures of the models that we used are described in Table 1. In the models considered in our study, negative-log-likelihood (NLL) has been used as the loss function. We emphasize that minimizing the NLL loss function (similarly, cross-entropy) during NN training is asymptotically equivalent to maximizing the perceived information as proved in [MDP20]. Furthermore, none of the models used in our study has gone under hyperparameter tuning by us. We aim to understand how previously proposed models work and how their attack performance is related to undersecretaries. **GE curves.** Figure 5 plots the average rank (so-called guessing entropy–GE) vs. the number of attack traces for the models that we use in our experiments. The model trained on CHES CTF reaches to the rank 0 with 514 attack traces while in the ASDAC-r this number is 475 and for the ASCAD-f is 153.

## 4.2 Toy Example: Uncertainty Decomposition for CIFAR10

Before we proceed to the results of the SCA datasets, we show the results obtained for the **CIFAR** dataset [Kri09] to illustrate the uncertainty decomposition in a well-known dataset cf. [Cha18]. Analysis of the CIFAR10 test images was performed by decomposing the predictive uncertainty into its aleatoric and epistemic components, as described in Section 3.3. The predictive softmax output  $p(y^* = c \mid x^*)$  was computed by averaging weight samples. When the maximum probability delivered by softmax reaches 1, a full probability assignment to a single class is observed. This results in zero uncertainty with regard to both epistemic and aleatoric uncertainties. A low softmax output (around 0.2, as shown in Fig. 6) indicates that predictive uncertainty is influenced by epistemic contributions, e.g., differences between the test examples and training examples. The aleatoric uncertainty reflects the inherent difficulty in categorizing an image based on the available features.



Figure 6: Uncertainty decomposition in **CIFAR** [Kri09, Cha18]. Each point represents a single image in the test dataset. A reduction in the probability delivered by the softmax in the NN results in an increase in epistemic and aleatoric uncertainties (downward trend observable in all three sub-figures).

## 4.3 What Can Be Explained in SCA through Uncertainties?

In this section, we show our results for different case studies. These case studies are designed to explain the behavior of the models trained on SCA datasets. Considering ASCAD-f, as we can see in Figure 5, it takes more than 100 traces for the models to reach rank zero. This can be associated with giving higher probabilities to the wrong keys in the attack phase. Now, we try to find the root cause of this behavior by decomposing the uncertainty based on Equation 13. In our first scenario, we use the model trained on the ASACAD-f dataset with no desynchronization as proposed in [WAGP20]<sup>3</sup> We find the variational distribution  $q(\theta)$  of the model as we discussed in 3.2 and decompose the uncertainty for this model.

Figure 7 illustrates the results for 5,000 attack traces. We decompose the overall predictive uncertainty into two primary components, aleatoric and epistemic uncertainties, which were found to contribute equally in this case. The relatively high value of aleatoric uncertainty indicates that the available traces do not contain enough information to reliably predict the key, implying that intrinsic noise and variability within the traces limit classification performance. To reduce this type of uncertainty, we need more informative traces, for example, by employing better probes to minimize noise. On the other hand, the significant amount of epistemic uncertainty suggests that the trained model cannot generalize well to the attack traces. This implies that the model's predictions are less reliable in regions where no data has been seen.

In Figure 7, we also illustrate the link between uncertainty and the attack performance, specifically the rank of the correct key. To achieve this, we calculate the rank of the correct key based on the output probabilities (see Equation 3). Subsequently, we summed up the uncertainty values associated with the traces with the same rank. The results reveal a clear trend: traces with lower ranks exhibit higher uncertainty. This observation shows that the model is unsure about its prediction, although the rank is low.

Is there any link between the labels and uncertainties? Specifically, the objective is to observe whether there is any relationship between the model's uncertainty and the labels of the traces (one-hot encoding of the respective output of the SBOX). The sub-figures in the first row of Figure 8 present the uncertainty of the traces labeled with the correct key. We summed up the uncertainty values of traces sharing the same label, i.e.,

 $<sup>^{3}</sup>$ We emphasize that none of the models in our study underwent hyperparameter tuning. Our goal is to evaluate how existing models perform and how their attack effectiveness relates to uncertainty.



Figure 7: Uncertainty decomposition and rank comparison for the model proposed in [WAGP20] and trained on ASACAD-f dataset with no desynchronization. The first row shows the relationship between the softmax output and uncertainty, where each point corresponds to one trace. The sub-figures in the second row depict how the rank relates to maximum uncertainty for all traces with a given rank. Here, each point represents the summation of uncertainty for all traces with a given rank.

the correct key. As depicted in Figure 8, the results do not indicate a clear relationship between these two parameters, suggesting that trace labels do not significantly influence the uncertainty associated with model performance.

In Figure 8, we also analyze the relationship between the NN predicted key and the uncertainty for 5000 traces (see the second row). An interesting observation about this is that some of the key candidates never achieve rank 0, resulting in an assigned uncertainty of "1" (or "0" on a log scale) for those classes. Apart from this, the results once again reveal no strong relationship between the predicted key and uncertainty.

What is the impact of randomized keys on the uncertainties? In the ASCAD-f dataset, the same key is used for collecting both profiling and testing traces, while in ASCAD-r, random keys are used during the profiling stage, and a fixed key is used for the attack stage [BPS<sup>+</sup>17a, BPS<sup>+</sup>17b]. We employed the model trained on ASCAD-r [WPP22] to evaluate the feasibility of our approach under more challenging conditions. Specifically, we use 5000 attack traces from the ASCAD-r dataset. This setup further shifts the distribution of the test set from the profiling set compared to the results presented in this section so far. Consequently, the model faces greater difficulty in generalizing its learned patterns from the profiling phase to the attack phase. Therefore, intuitively, we expected to observe a higher degree of epistemic entropy than ASCAD-f. The use of different keys for the profiling and attack phases effectively reduces the model's prior knowledge of the unseen data and, consequently, the model's ability to recover the correct key. Figure 9 gives us a good insight: epistemic uncertainty dominates the overall uncertainty in this scenario. This indicates that the uncertainty stems largely from the model's lack of knowledge about the relationship between the profiling and attack phases. This observation underscores



Figure 8: Uncertainty decomposition for the model from [WAGP20], trained on the ASACAD-f dataset without desynchronization. The first row shows the relationship between the softmax output of the correct class, where each point corresponds to the summation of uncertainty values when the given class was the correct class. The sub-figures in the second row depict the summation of uncertainty values when the given class was the predicted class.

the importance of system-specific knowledge in SCA and suggests that the task becomes increasingly tedious when such knowledge is limited.

Now, if we set Figures 9.c and 7.c side by side, the reduction in the aleatoric uncertainty is clearly observable, corresponding to the reduced noise in the dataset. We highlight that the ASCAD-f and ASCAD-r differ in their measurement settings cf. [EST+22]. The ASCAD-f dataset contains 100,000 time instance recorded at a sampling rate of 200MS/s (not 2GS/s as reported in [BPS+18]), while the ASCAD-r dataset includes 250,000 samples captured at 500MS/s. Both datasets include traces from the first round of an AES software implementation running on an ATmega8515 microcontroller clocked at 4MHz, resulting in 50 and 125 samples per clock cycle, respectively. Increasing the sampling rate can help better capture signal details as one can track rapid transitions in the signal more accurately, potentially separating the signal from some types of noise. Better time resolution can also be achieved, i.e., side-channel leakage can be isolated from other overlapping operations in time. Such differences in the two campaigns can result in reduced aleatoric uncertainty for ASCAD-r.

What is the impact of countermeasures like desynchronization on the uncertainty? The objective of this case study is to understand the influence of jitter on the model's uncertainty. To investigate this, we evaluated the model trained on ASCAD-f with no desynchronization as in [WAGP20] when applied against 5000 attack traces from the ASCAD-fixed dataset subjected to 100 desynchronization. This setup introduces temporal shifts, enabling the analysis of their impact on the model's performance and uncertainty levels. Although the model was trained on a dataset without desynchronization, where a



Figure 9: Uncertainty decomposition and rank comparison for the model proposed in [WPP22] and trained on ASACAD-r dataset with no desynchronization. The first row shows the relationship between the softmax output and uncertainty, where each point corresponds to one trace. The sub-figures in the second row depict how the rank relates to maximum uncertainty for all traces with a given rank. Here, each point represents the summation of uncertainty for all traces with a given rank.

small jitter should not significantly affect performance, our results reveal that the model fails to recover the correct key under desynchronized conditions.

Figure 10 illustrates how a substantial shift of the test set distribution introduced by desynchronization causes the increase in epistemic uncertainty. Even minor desynchronization increases the model's uncertainty, disrupting the patterns typically observed in synchronized traces; see Figure 7. Additionally, Figure 10 highlights that although the probability vs. uncertainty plots may seem similar, a small change in their skewness indicates a significant shift in the trend of uncertainty vs. rank plots (see Figure 7). The NN's uncertainty leads to incorrect predictions, and as a result, all guessed keys exhibit high uncertainty regardless of their rank. In a noisy setting like this, such behavior strongly suggests that the model is not functioning effectively.

#### 4.4 What Model Changes Benefit SCA?

This section aims to look at some hyperparameters thought to be useful in the context of SCA through the lens of uncertainty. Given the large space of possible hyperparameters, we focus on some existing methods proposed in SCA-related literature.

Can convolutional filters help the model reduce its uncertainty when dealing with desynchronization? We have already studied how uncertainties can indicate reduced attack effectiveness when an MLP model is trained on a dataset and tested against a dataset containing desynchronized traces. It can be interesting to make a similar observation for convolutional neural networks (CNNs). For this, our model incorporates a convolutional layer and has been proposed in [WPP22]. CNNs are powerful tools for



Figure 10: Uncertainty decomposition and rank comparison for the MLP model proposed in [WAGP20] and trained on ASACAD dataset with no desynchronization and tested against 5000 attack traces of ASCAD dataset with 100 desynchronization. The first row shows the relationship between the softmax output and uncertainty, where each point corresponds to one trace. The sub-figures in the second row depict how the rank relates to maximum uncertainty for all traces with a given rank. Here, each point represents the summation of uncertainty for all traces with a given rank.

handling sequential or spatial data, as they are designed to identify and capture local patterns through convolutional filters [HTFF09]. Can these filters help the model reduce its uncertainty? The answer is negative. The epistemic uncertainty remains high, although we can observe a clear reduction in the aleatoric uncertainty (as explained before, this is due to the ASCAD-r capturing setting). In this case, the epistemic uncertainty values are relatively high, showcasing the inefficacy of the model. As shown in Figure 11 for 5000 attack traces, again, there is no clear relationship between the rank and uncertainty as the model performs poorly, confirmed by the high epistemic uncertainty.

Can an increase in the number of training/validation traces be helpful? Our goal is to showcase the influence of the number of traces in the training process on the uncertainty values. In other words, can uncertainties indicate that more training traces are needed? In doing so, we used different numbers of the training and validation traces to see the impact on the uncertainty decomposition. In this setup, the number of attack traces is 5000 for all models. As shown in figure 12, changing the number of the training and validation traces does not affect the predictive uncertainty significantly. Nevertheless, its impact on both aleatoric and epistemic uncertainties is clear. An increase in the number of validation traces reduces the variance of these uncertainties, suggesting a more stable setting. Comparing the results for Model 1 and Model 3, where the training set is divided into 45K/5K and 49K/1K training/validation traces, the average epistemic uncertainty is much reduced for Model 3 as expected. Nonetheless, the average aleatoric uncertainty is increased as the model has not undergone extensive validation in contrast to Model 1. A better balance between the number of traces in the validation and training datasets



Figure 11: Uncertainty decomposition and rank comparison for the CNN model proposed in [WPP22] and trained on the ASACAD-r dataset with no desynchronization but tested against the ASACAD-r dataset with 100 desynchronization. The first row shows the relationship between the softmax output and uncertainty, where each point corresponds to one trace. The sub-figures in the second row depict how the rank relates to maximum uncertainty for all traces with a given rank. Here, each point represents the summation of uncertainty for all traces with a given rank.

can be observed in Model 2. However, if there could be an option to reduce the epistemic uncertainty, Model 3 (49K/1K training/validation traces) could be a viable option.

Can we calibrate the softmax outputs to reduce uncertainty? Recently, [NG24] has introduced temperature calibration [GPSW17] in the context of SCA. That study has demonstrated that temperature calibration enhances the performance of the attack [NG24], but how can we see that in terms of uncertainty? In the context of model calibration, let  $\hat{q}_i$  denote the calibrated probabilities for class i, and  $\mathbf{z}_i$  represent the logits (pre-softmax outputs) of the model. Temperature calibration introduces a scalar parameter T > 0 to rescale the logits, modifying the softmax function as follows:

$$\hat{q}_i = \sigma_{SM} (\mathbf{z}_i/T)_i = \frac{\exp(z_i/T)}{\sum_i \exp(z_j/T)}.$$

When T > 1, the output probabilities are distributed more evenly across all classes, effectively increasing the entropy of the predictions. This process is commonly referred to as "softening" the softmax [GPSW17]. Conversely, when T < 1, the probabilities become skewed, concentrating on the most likely classes. For T = 1, no scaling is applied, and the original softmax probabilities are retained. For the MLP model trained on ASCAD-f and used in our paper, namely [WPP22], the temperature has been calculated as 4.11 [NG24].

As depicted in Figure 13, compared to the results in Figure 7, our observation for 5,000 attack traces is the change in the shape of the uncertainty patterns. The softmax probabilities are reduced, and the aleatoric uncertainty is much reduced. This shows that the M sampled model could approximate the true posterior  $p(\theta \mid D)$  well. Nevertheless,



Figure 12: Models trained different validation and training set sizes. Model 1 is trained with 45,000 training traces and 5,000 validation traces; for Model 2, we use 47,500 training and 2,500 validation traces, and these numbers were 49,000 and 1,000 for the third model. Here, the gray box is for predicted entropy, the green box is for the epistemic entropy, and the red box is for aleatoric entropy.

the epistemic uncertainties are increased, more specifically, the shape is now skewed toward right indicating a higher epistemic uncertainty in the prediction. This means that although the output of the model is calibrated, the model lacks the knowledge to be certain about its predictions. The same phenomenon can be observed in sub-Figure 13.f, where regardless of the rank, the aleatoric uncertainty remains (more or less) the same. In other words, the main contributor to the predictive uncertainty is the epistemic one, which is related to the dataset.

Can an increase in the number of epochs be beneficial to reduce the uncertainty? In this case study, we train three different models with varying numbers of epochs, leading to differences in their attack performance. Model 1, trained for 50 epochs, demonstrated the best performance, while Model 2, trained for 35 epochs, ranked second. Model 3, trained for only 20 epochs, performed the worst among the three. As shown in the figure 14, the guessing entropy of these models varies significantly, reflecting the impact of training duration on the models' ability to recover the correct key.

Increasing the number of training epochs typically enhances model accuracy by enabling it to learn more complex patterns in the data. However, this comes with a trade-off that an excessive number of epochs can lead to overfitting, where the model becomes too tailored to the training data and fails to generalize well to unseen inputs. Before conducting this analysis, we examined whether the model overfit, which was the case for none of the three models. To further explore the relationship between rank and uncertainty, we categorize model predictions into four groups: accurate and certain (AC), accurate and uncertain (AU), inaccurate and certain (IC), and inaccurate and uncertain (IU). Predictions are labeled as "accurate" if the rank is below a predefined threshold, set to 128 in this paper. Being "certain" or "uncertain" depends on whether the uncertainty lies below or above the average uncertainty. This approach allows us to evaluate the trade-offs between rank and uncertainty across different models.

Table 2 presents the results of this analysis for the three models. From the table, we can see that Model 1, the best-performing model, achieved the highest number of accurate and certain predictions (#AC = 59) and accurate and uncertain predictions (#AC = 45) and accurate and uncertain predictions (#AC = 45) and accurate and uncertain predictions (#AC = 45) and accurate and uncertain predictions (#AU = 2480). Model 3, with the poorest performance, showed only 27 accurate and certain predictions (#AC = 27) and a slightly higher count of accurate and uncertain predictions (#AU = 3003).



Figure 13: Uncertainty decomposition and rank comparison for the model proposed in [WAGP20] trained on ASACAD-f dataset with no desynchronization. Temperature scaling proposed in [NG24] has been applied. The first row shows the relationship between the calibrated softmax output and uncertainty, where each point corresponds to one trace. The sub-figures in the second row depict how the rank relates to maximum uncertainty for all traces with a given rank. Here, each point represents the summation of uncertainty for all traces with a given rank.



Figure 14: A model trained for different numbers of epochs against ASCAD-f.

Model	#AC	#AU	#IC	#IU
1	59	3566	2	1373
2	45	2480	31	2444
3	27	3003	2	1968

Table 2: Rank vs. uncertainty: AC: accurate and certain, AU: accurate and uncertain, IC: inaccurate and certain, IU: inaccurate and uncertain for 5000 attack traces.

### 4.5 Interesting Case of CHES-CTF Dataset

Next, we move to the CHES CTF dataset [Ris18]. In this dataset, three key differences impact the results compared to the ASCAD datasets. First, the leakage model is hamming weight [GJS19]. This means the output of the model has 9 possible values; as a result, the maximum value of the uncertainty is decreased. Secondly, the sub-key used during the profiling phase differs from the one employed in the attack phase, which induces a distribution shift between the training traces and the test samples. Figure 15 illustrates the uncertainty decomposition for 5,000 attack traces of this dataset, where the change in



Figure 15: Uncertainty decomposition and rank comparison for the model proposed in [WPP22] and trained on CHES CTF dataset. The first row shows the relationship between the softmax output and uncertainty, where each point corresponds to one trace. The sub-figures in the second row depict how the rank relates to maximum uncertainty for all traces with a given rank. Here, each point represents the summation of uncertainty for all traces with a given rank.

key leads to an increased contribution of epistemic uncertainty. By looking at this figure, we can see a much different pattern in the probabilities delivered by softmax. Compared to other results in this section, the probability varies between 0 and one.

More interestingly, epistemic uncertainty is equal to zero for some of the points, indicating that the model successfully approximates the probability density related to  $Pr((P, K) = (p, k) | \mathbf{L})$  through  $\hat{g}_{\mathbf{L},P,\theta}$ . It is known that  $\mathbf{y} = \hat{g}_{\mathbf{L},P,\theta}$  is composed of Gaussian pdfs [PR09, PR10]. Hence, the predictive uncertainty  $H(y^*|x^*, \mathcal{D})$  for a given trace  $x^* = \ell^*$  can be approximated by the entropy of t-dimensional Gaussian random variable cf. [PR09, PR10]. This gives  $H(y^*|x^*, \mathcal{D}) = 1/2(\log((2\pi e)^t | \Sigma |)))$ , with  $\Sigma$  being the covariance matrix of X. To confirm that, we fit an exponential curve to the predictive uncertainty. Curve fitting yields that a single Gaussian distribution can approximate the pdf of  $\mathbf{y}$ , where the mean and variance are 0.2293 and 0.1218, respectively. This result is in line with what has been observed in [GJS19]. The uncertainty vs. rank curves also show piece-wise upward trends, meaning that the model is more certain about lower-ranked guessed keys compared to previous cases in this section.

#### 4.6 Sensitivity Analysis with SHAP Values

The question that we aim to answer here is that, given the predictive uncertainty  $H(y^*|x^*, \mathcal{D})$ , we can determine which time instances in a trace have an influence on the uncertainty. Figure 17 demonstrates the contribution of time instance to the uncertainty of the model trained on the ASCAD dataset [WAGP20] using SHAP values for 1000 attack traces. To create SHAP plots, we use a function that maps the time instance to uncertainty, i.e., the trained model that maps the time instance to output distributions. We integrate the Rényi entropy estimation alongside the trained model, using them in



Figure 16: SNR in ASCAD dataset: there are 700 time instances in ASCAD-fixed dataset [BPS<sup>+</sup>20] that based on the SNR we can divide them into four groups: 1. MO (masked SBOX output) 2.CM (common SBOX output mask) 3.MOL (masked SBOX output in linear parts) 4. OML (SBOX output mask in linear parts).



Figure 17: SHAP values of time instances. 1000 attack traces in ASCAD-f are given to the trained model as in [WAGP20]. The x-axis shows the feature indices (time instance), whereas we have 4 groups corresponding to SNR categories in Figure 16. Here, the intensity of the time instances shows more contribution, and the color shows the negative/positive contribution. Positive SHAP values (colored in red) indicate that the time instance increases the uncertainty, while the negative values reduce that.

series to construct a comprehensive function for uncertainty estimation. This setup enables us to analyze the contribution of individual time instances to the uncertainty of the model outputs effectively.

The results reveal that, unlike trace labels, which did not show a significant relationship with uncertainty, time instances play a substantial role in determining uncertainty. Moreover, SHAP values show that the time instance that has a higher SNR contributes the most to the uncertainty; see Figure 16. As illustrated in Figure 17, the feature sets do not play the same role for all instances. Negative SHAP values indicate that these time instances reduce the uncertainty of the model output (depicted in blue), demonstrating their stabilizing influence. Conversely, the positive SHAP values (depicted in red) indicate that these time instances increase the uncertainty, highlighting their destabilizing impact. This differentiation underscores the varying contributions of time instances to the model's predictions, emphasizing the importance of feature-specific analysis in understanding model behavior.

## 5 Conclusion and Future Work

In this paper, we provide a framework to estimate and decompose the uncertainties associated with the outputs of the NN models used in SCA. The main goal of this study is to explain why these models tend to assign high probabilities to the wrong key candidates. Our analysis helps find the root cause of this problem. To this end, we use matrix-based Rényi entropy to estimate the entropy as a measure of uncertainty. Through decomposition, it is possible to explain whether uncertainty comes from the lack of information in the traces due to, e.g., the intrinsic noise. This part of the uncertainty can be reduced by employing a better capturing setup, for instance, using better probes while collecting the traces. The other component of the uncertainty is the epistemic uncertainty, which suggests that the model has limits when classifying unseen traces. Multiple case studies have been carried out in this paper to highlight the power of uncertainty as a metric to explain the outcome of an NN-enable SCA. Specifically, the impact of desynchronization and randomized keys have been considered. Furthermore, changing some hyperparameters in the model has been studied to investigate the impact of convolutional filters, the number of training/validation traces, and the number of training epochs.

Moreover, we utilize SHAP values as an explainable AI tool to find the time sample that contributes the most to the predictive uncertainty. We have demonstrated that the points with high SNR contribute the most to the uncertainty value, which is reasonable since these points have more information regarding the key.

Analyzing the characteristics of the traces with high impact in rank curves and their influence on the uncertainty remains an open problem that we leave to future work.

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