# Avenger Ensemble: Genetic Algorithm-Driven Ensemble Selection for Deep Learning-based Side-Channel Analysis

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Abstract. Side-Channel Analysis (SCA) exploits physical vulnerabilities in systems to reveal secret keys. With the rise of Internet-of-Things, evaluating SCA attacks has become crucial. Profiling attacks, enhanced by Deep Learning-based Side-Channel Analysis (DLSCA), have shown significant improvements over classical techniques. Recent works demonstrate that ensemble methods outperform single neural networks. However, almost every existing ensemble selection method in SCA only picks the top few best-performing neural networks for the ensemble, which we coined as Greedily-Selected Method (GSM). This method of selecting DNN may not be optimal. In this work, we propose a new genetic algorithm-driven ensemble selection algorithm called Evolutionary Avenger Initiative (EAI) to create effective ensembles for DLSCA. We investigate two fitness functions and evaluate EAI across four datasets, including AES and ASCON implementations. We show that EAI outperforms GSM, recovering secrets with the least number of traces. Notably, EAI successfully recovers secret keys for Ascon datasets where GSM fails, demonstrating its effectiveness.

**Keywords:** Side-channel analysis · Deep learning · Ensemble learning · Genetic algorithm

## 1 Introduction

Side-channel analysis (SCA) exploits the physical vulnerabilities of a system like power consumption [8] and electromagnetic emanation [2] to reveal the secret key. Evaluating such attacks has become crucial, especially with the rise in the usage of Internet-of-Things (IoTs) in recent years [12]. One such side-channel attack is known as the profiling attack. In the profiling attack model, it is assumed that the attacker has access to a clone device that closely resembles the target device. Deep Learning-based Side-Channel Analysis (DLSCA) has been intensively explored in recent years [13, 14, 1, 22], which demonstrated that Deep

Neural Networks (DNNs) can significantly outperform classical SCA techniques like template attacks [13]. Furthermore, DLSCA has garnered significant interest because of its capability to recover the secret key of the protected implementations without needing to resynchronize traces.

Recent studies have demonstrated that ensembling multiple DNNs yields substantial performance gains compared to a single top-performing neural network. [17, 18, 23]. DNNs of varying hyperparameters can extract different information from identical traces, yielding improved performance when combined together as an ensemble. Most of the works in DLSCA create an ensemble by greedily selecting the top few best-performing DNNs [17–19], herein referred to as the Greedily-Selected Method (GSM). However, the GSM may not be optimal as other combinations of DNNs could attain better results. Therefore, a natural question arises:

Can we develop a methodology to efficiently select neural networks for ensembles that outperform the traditional GSM?

To address this question, we focus on ensemble selection, which is defined as the process of selecting pre-trained DNNs to create an effective ensemble.

Our Contributions. Our contributions are stated as follows:

- 1. In this work, we proposed a new genetic algorithm-driven ensemble selection algorithm called Evolutionary Avenger Initiative (EAI) to generate a best-performing ensemble. To the best of our knowledge, this is the first work to investigate ensemble selection within the context of SCA. Furthermore, we investigate two fitness functions for EAI:  $ge_{+ntge}$  and validation loss.
- 2. We assess the efficiency of our methodology across four datasets, comprising three AES datasets (software and hardware implementations) of the widely recognized symmetric-key standard [5], and one ASCON dataset, NIST's lightweight cryptography standard winner, implemented in software [6]
- 3. By integrating EAI, we manage to recover the secret with the least number of traces across all datasets tested, outperforming traditional ensemble selection techniques, i.e., GSM. Furthermore, EAI with  $ge_{+ntge}$  has yielded significant performance gains across all tested settings and datasets. Notably, for the ASCON datasets (i.e., ASCON2 and ASCON4), EAI successfully recovered the secret key within 1000 attack traces, whereas the conventional GSM method failed to do so. This highlights the effectiveness of EAI.

We validate our approach on first-order masking traces, leaving higher-order masking for future work. The source code can be accessed at the following web link.<sup>4</sup>

Paper Organization: The paper is organized as follows. We begin by reviewing some related works in Section 2. We then describe the background necessary for profiled SCA using an ensemble of DNN and a brief outline of Genetic Algorithm

<sup>&</sup>lt;sup>4</sup> https://github.com/Sarahfbb/Avenger-Ensemble

in Section 3. Next, Section 4 presents our proposed ensemble selection algorithm to generate the best-performing ensemble for profiling attacks. Section 5 discusses and analyzes our results on the four datasets tested. Finally, Section 6 concludes with some discussion and provides some future works.

## 2 Related Work

Ensemble within DLSCA The introduction of ensemble methods in DLSCA is attributed to [17]. This pioneering work presented a methodology for computing the maximum log-likelihood of an ensemble for bagging and showcased its efficacy on AES-based datasets. However, they use GSM to build their ensemble, which may be suboptimal. Subsequently, [18] successfully apply GSM to Ascon implementations. Instead of considering GSM, the authors of [23] consider the "diversity" between the optimal DNNs and the non-optimal DNNs. Therefore, they proposed a loss function called Ensemble loss. The Ensemble loss helps to train a diverse ensemble to recover the secret. Nonetheless, the Ensemble loss has a drawback: it cannot scale for more than three classes. Consequently, its application is restricted, and it cannot be applied to block ciphers like AES (with 256 classes). The authors only tested it on an ECC dataset. Unlike [23], we do not take into account the training process but consider the same scenarios as [17]. Perin et al. [17] assume that a set of DNNs with randomly generated hyperparameters have already been trained. We highlight that the above methodologies considered are bagging [4]. In recent years, methods for stacking DNNs [11] and boosting DNNs [20] have been explored in SCA. For this work, we will focus on bagging ensembles. Furthermore, we exploit the capabilities of the genetic algorithm to find the optimal combination of pre-trained DNNs to produce the best-performing ensemble.

Ensemble Construction/Selection The idea of constructing an ensemble is not new, as various works have considered [9, 24]. Prior works use Bayesian optimization to generate well-performing ensembles. For instance, [9] propose using Bayesian optimization to tune the hyperparameters of one neural network while building the ensemble while [15] uses Bayesian optimization to form an ensemble through pre-trained DNNs. Other works like [24] model the ensemble construction as an optimization problem. The authors of [24] propose a method called Neural Ensemble Search to solve this optimization problem in order to attain a well-performing ensemble. For our work, we focus on ensemble selection. Recent advancements in ensemble selection have leveraged genetic algorithms to optimize ensemble composition. Notably, [25] proposed GASEN, which utilizes genetic algorithms to optimize weight coefficients that capture inter-DNN correlations. Specifically, GASEN selects DNNs for the ensemble based on their weight coefficients, including only those exceeding a predefined threshold. Ortiz et al. propose EARN, a multi-objective evolutionary approach that generates efficient DNN ensembles [16] where they consider bagging, boosting, and stacking into the ensemble. Inspired by these, we develop a genetic algorithm for ensemble selection within SCA context.

# 3 Background

## 3.1 Profiling attack using Ensemble

One of the most common side-channel settings is known as the profiling attack. It assumes the worst-case scenario where the adversary has access to a clone device similar to the target device. The profiling attack is executed in two phases: profiling and attack phase.

In the profiling phase, the adversary either knows or can manipulate the key of the clone device. Then, distinguishers can be built from the profiling traces of a known set of random public variables (plaintext or ciphertext). During this phase, the adversary collects a set of traces  $\boldsymbol{t}$  corresponding to known public variables to train distinguishers.

In the attack phase, the adversary performs the attack by collecting several attack traces from another set of known public variables of the target device. Typically, the traces are given to a single trained distinguisher for key recovery.

In [17] consider multiple distinguishers for key recovery. Formally, the traces are given to the trained distinguishers to obtain their output probability scores for each hypothetical sensitive value. These probabilities are combined together via:

$$\operatorname{score}(k) = \sum_{j=1}^{N_{model}} \sum_{i=1}^{N_a} \log(Pr_j(Z = z_{i,k} | \mathbf{t}_i))$$
 (1)

where  $N_a$  represents the number of attack traces used,  $N_{model}$  is the number of models in the ensemble,  $Pr_j(Z = z_{i,k}|\mathbf{t}_i)$  denotes the probability output by the  $j^{th}$  distinguisher in the ensemble, and  $z_{i,k}$  is the hypothetical sensitive value which depends on the key candidate k and the  $i^{th}$  public variable that corresponds to the trace  $\mathbf{t}_i$ .

The score(k) is computed for each key  $k \in \mathcal{K}$ , where  $\mathcal{K}$  is the set of all possible key values. An attacker can sort the scores in descending order to create a guess vector  $[G_0, \ldots, G_{|\mathcal{K}|}]$  where  $G_0$  corresponds to the score for the most likely key candidate while the  $G_{|\mathcal{K}|}$  represents the score for the least likely key candidate. Let the index of the guess vector be the rank of the key. Then, we define the Guessing Entropy (GE) as the rank of the correct key averaging over multiple experiments. In our analysis, we calculate this average over 100 separate experiments. When GE reaches zero, it indicates a completely successful attack - the correct key was consistently ranked first. To quantify attack performance, we denote the least number of traces for GE to reach zero as NTGE, which measures the minimum number of traces needed for key recovery.

## 3.2 Genetic algorithm framework

The genetic algorithm is a population-based optimization method inspired by natural evolution. Let  $\mathcal{X}$  be the search space, and  $f: \mathcal{X} \to \mathbb{R}$  be the fitness function that evaluates potential solutions. The population at generation t is denoted as

$$P^t = \{x_1^t, x_2^t, \dots, x_n^t\},\$$

where each individual chromosome  $x_i^t \in \mathcal{X}$  represents a candidate solution, also referred to as a chromosome.

By evolving the population over successive generations, the genetic algorithm seeks to improve the overall fitness of the population, moving closer to the optimal solution. Each individual chromosome  $x_i^t$  is evaluated using the fitness function f, which assigns a numerical score to indicate its suitability or quality as a solution. The fitness scores guide the selection process, helping to determine which chromosomes will contribute genetic material to the next generation. The evolution process consists of the following phases:

- 1. **Initial Population:** The initial population  $P^0$  is typically generated randomly across the search space  $\mathcal{X}$ .
- 2. **Elitism:** It preserves the best chromosomes from one generation to the next. The basic idea is to ensure that the fittest chromosomes are included in the next generation without any changes.
- 3. **Selection Method:** In genetic algorithms, several distinct selection methods exist for choosing chromosomes to generate subsequent generations. We shall recall the commonly used *Tournament Selection*. The Tournament Selection process in a genetic algorithm involves sampling multiple tournaments of size  $\ell$ , where  $\ell$  chromosomes are randomly chosen from the population. The fittest chromosome in each tournament is selected to generate new chromosomes for the next generation.
- 4. **Generic Operator:** Various genetic operators are proposed to generate new chromosomes; here, we will recall two such operators: Crossover and Mutation.
  - Crossover: The crossover operator is inspired by biological reproduction, where genetic material from two or more parent chromosomes is combined to produce one or more offspring. This process creates new chromosomes by exchanging segments between parents, thus propagating beneficial traits across generations. Crossover is typically applied with a high probability, denoted by  $Pr_{\rm cross}$ , to enhance the convergence rate towards optimal solutions by exploiting existing genetic diversity.
  - Mutation: Mutation introduces variability and maintains diversity within a population. It involves making small, random changes to the values (or "genes") within an individual chromosome. These random tweaks help the algorithm explore new potential solutions, preventing premature convergence to suboptimal solutions. Mutation is typically applied with a low probability, denoted by  $Pr_{\rm mut} = 1 Pr_{\rm cross}$ , to avoid drastic changes while enabling steady exploration of the solution space.

## 4 Evolutionary Avengers Initiative

In this section, we present our algorithm, called the Evolutionary Avengers Initiative (EAI). Each DNN can be viewed as a "superhero" endowed with distinct strengths. Drawing inspiration from the Avengers of the Marvel Studio, EAI

aims to assemble a diverse group of "superheroes" called the Avenger Ensemble to recover the secret key.

The overview of the EAI Framework is described in Algorithm 1. EAI first initializes the population using a set of pre-trained DNNs from set  $\mathcal{M}$ . The population consists of  $N_{ens}$  ensembles, with each ensemble consisting of  $N_{model}$  DNNs. Subsequently, the steps described below are repeated over  $N_{gen}$  generations. Firstly, each ensemble within the population is evaluated using the fitness function (Line 4 of Algorithm 1). Next, the best-performing ensemble is then preserved for the next generation, a process known as elitism (Line 4 of Algorithm 1). Finally, generic operations such as crossover or mutation are applied to the whole previous population, generating a new population of ensembles (Line 5 of Algorithm 1). We shall describe each step in detail.

## Algorithm 1 Evolutionary Avengers Initiative (EAI)

Input:  $\mathcal{M}$ : Set of all trained models,  $N_{ens}$ : Population size,  $N_{model}$ : Number of models per ensemble,  $Pr_{cross}$ : Crossover rate,  $Pr_{mut}$ : Mutation rate, ge\_fitness\_fn: Fitness function,  $N_{gen}$ : Number of generations

```
Output: E_{best}: Best-performing ensemble, s_{best}: Fitness value of E_{best}
```

```
1: Initialize Population of First Generation: P = initialize\_pop(\mathcal{M}, N_{ens}, N_{model})
```

2: 
$$E_{best} = \emptyset, s_{best} = \infty$$

3: for 
$$t \leftarrow 1$$
 to  $N_{qen}$  do

4: Evaluate population and apply Elitism:

$$P_{new}, S, E_{best}, s_{best} = Eval \& Elite(ge_fitness_fn, P, E_{best}, s_{best})$$

5: Apply Crossover or Mutation:

$$P_{new} = GeneticOp(\mathcal{M}, P, P_{new}, S, Pr_{cross}, Pr_{mut})$$

```
6: P = P_{new}
```

7: end for

8: **return**  $E_{best}$ ,  $s_{best}$ 

Initialize Population. Prior to the start of EAI, we train a set of DNNs, denoted as  $\mathcal{M}$ . We label each DNN with  $M_i$  for  $0 \leq i \leq |\mathcal{M}|$ . EAI will first initialize the population (Line 1 in Algorithm 1). Algorithm 2 describes how to initialize the population. The initial population  $P^0$  is generated by picking  $N_{model}$  distinct models from  $\mathcal{M}$  randomly to create a new ensemble E (Line 5 in Algorithm 2). Then, we check if ensemble E is in the initial population  $P^0$  (Line 6 in Algorithm 2). If it is, then E is a duplicate ensemble, so we discarded the ensemble E; if not, the ensemble E is added into the initial population of ensembles (Line 6 to 8 in Algorithm 2). This process is repeated until there are  $N_{ens}$  ensembles within the population  $P^0$ .

## Algorithm 2 Initialize Population

```
1: procedure initialize\_pop(\mathcal{M}, N_{ens}, N_{model})
         P^0 \leftarrow \emptyset
 2:
                                                                  ▶ Population of unique ensembles
 3:
         i = 0
         while i < N_{ens} do
 4:
             E \leftarrow \text{Randomly select } N_{model} \text{ distinct models from } \mathcal{M}.
 5:
             if E is not in P^0 then
 6:
                  P^0 \leftarrow P^0 \cup \{E\}
 7:
                                                                      ▶ Add ensemble to population
                  i = i + 1
 8:
 9:
             end if
10:
         end while
         {\bf return}\ P^0
11:
12: end procedure
```

**Evaluate Population and Apply Elitism.** In this step, all the ensembles' performances are evaluated using a fitness function. Furthermore, the top-performing ensemble is preserved for the next generation. Algorithm 3 provides the algorithm for *Eval\_&\_Elite*. Moreover, when evaluating the ensembles' performance, the best-performing ensemble throughout all the generations is recorded (line 6 to 8 of Algorithm 3).

#### **Algorithm 3** Evaluate Population and Apply Elitism

## Require:

```
1: procedure Eval\_\&\_Elite(ge\_fitness\_fn, P, E_{best}, s_{best})
 2:
        S \leftarrow []
                                                      ▶ Array of scores for current generation
        for each ensemble E \in P do
 3:
 4:
            s = ge\_fitness\_fn(E)
            S \leftarrow S + [s]
                                                                          ▶ Array Concatenation
 5:
            if s < s_{best} then
 6:
 7:
                Set s_{best} = s and E_{best} = E.
 8:
            end if
 9:
        end for
10:
        top\_pop\_ensemble \leftarrow \arg\min_{E \in P} S[E]
         P_{new} \leftarrow \{top\_pop\_ensemble\}
                                                           ▷ Elitism: retain the best ensemble
11:
        return P_{new}, S, E_{best}, s_{best}
12:
13: end procedure
```

• Elitism: Next, when applying elitism to preserve the ensemble(s) for the next generation. EAI only considers the top-performing ensemble within this population to be preserved. It is possible to preserve more than one top-performing ensemble, but it requires sorting the performance of the ensembles, which is time-consuming. Therefore, we only select the top ensemble in the population. Furthermore, this enhances the search capability, allowing

for more exploration of a diverse range of ensembles to identify the optimal combination.

- Fitness Functions: We investigate two fitness functions for EAI in the context of SCA. Namely, we explore  $ge_{+ntge}$  and validation loss (denoted as val\_loss) as the fitness function for ensemble selection.
  - 1.  $ge_{+ntge}$ : The fitness function  $ge_{+ntge}$  is first proposed by [7]. The authors demonstrate that the metric yields consistently better results when combined with multifidelity hyperparameter tuning, called Bayesian Optimization HyperBand, to identify a single best-performing DNN. This composite metric combines GE with NTGE to provide a comprehensive evaluation of side-channel analysis performance. The  $ge_{+ntge}$  function is defined as:

$$ge_{+ntge}(\theta) = \begin{cases} NTGE & \text{if } GE = 0, \\ GE + N_a + c & \text{otherwise} \end{cases}$$

where  $\theta$  represents the model configuration/hyperparameters,  $N_a$  is the fixed number of attack traces for evaluation, and c is a small positive constant (set to 100 in our experiments). This metric considers both the ability to recover the key (GE) and the efficiency of the attack (NTGE). It also penalizes configurations that fail to recover the key within the given number of traces. This provides a single, comprehensive metric for optimizing SCA models.

2. val\_loss: Research has shown that minimizing categorical cross-entropy loss effectively maximizes the mutual information between the leakage model and the trace data, a concept referred to as perceived information in SCA [14]. Here, we investigate whether using the validation loss of attack traces as a fitness function, denoted as val\_loss, can aid in ensemble selection.

**Genetic Operators.** The remaining ensembles in the population are generated using tournament selection, crossover, and mutation, which replace the non-elite ensembles. This configuration supports diversity within the population, which is critical for the effectiveness of subsequent generations.

Algorithm 4 outlines the methodology used to generate new offspring ensembles. To ensure diversity and effectiveness in the evolutionary process, we employ adaptive genetic operators [10], where the mutation and crossover probabilities/rates are dynamically adjusted based on population diversity (i.e., the proportion of unique ensembles in the population). This adaptive approach helps mitigate premature convergence and redundancy, which can arise from fixed probabilities/rates.

Let  $\delta$  represent population diversity, calculated as the ratio of unique ensembles to the total population size. The adaptive mutation rate is defined as:

$$Pr_{\mathrm{mut}}^{\mathrm{adaptive}} = Pr_{\mathrm{mut}} \times (1 + (1 - \delta))$$
.

## Algorithm 4 Genetic Operators with Adaptive Rates

```
1: procedure GeneticOp(\mathcal{M}, P, P_{new}, S, Pr_{cross}, Pr_{mut})
           \delta \leftarrow |set(tuple(ind) \text{ for } ind \text{ in } P)|/|P|
                                                                                 ▷ Calculate population diversity
 2:
           \begin{array}{l} Pr_{\rm cross}^{\rm adaptive} \leftarrow Pr_{\rm cross} \times \delta \\ Pr_{\rm mut}^{\rm adaptive} \leftarrow Pr_{\rm mut} \times (1 + (1 - \delta)) \end{array}
 3:
                                                                                           ▶ Adaptive crossover rate
 4:
                                                                                           ▶ Adaptive mutation rate
           while |P_{new}| < N_{ens} do
 5:
                if random() < Pr_{\text{cross}}^{\text{adaptive}} then
 6:
                                                                                   ▶ Adaptive crossover operation
                     parent_1 \leftarrow TournamentSelection(P, S)
 7:
                     parent_2 \leftarrow TournamentSelection(P, S)
 8:
 9:
                     offspring_1, offspring_2 \leftarrow Crossover(parent_1, parent_2, N_{model})
10:
                     P_{new} \leftarrow P_{new} \cup \{\texttt{offspring}_1, \texttt{offspring}_2\}
11:
                                                                                   ▶ Adaptive mutation operation
12:
                     parent \leftarrow TournamentSelection(P, S)
                     P_{new} \leftarrow P_{new} \cup \{ \text{Mutation}(\texttt{parent}, \mathcal{M}, Pr_{\text{mut}}^{\text{adaptive}}) \}
13:
                end if
14:
15:
           end while
           return P_{new}
16:
17: end procedure
```

When  $\delta$  is low, this formula increases the mutation rate since  $(1 - \delta)$  is larger. A higher mutation rate potentially introduces new models from the set of all the pre-trained DNN,  $\mathcal{M}$ , into the population, encouraging exploration and generating novel ensembles. Conversely, when diversity is high, the mutation rate decreases to avoid disrupting the existing diversity.

Similarly, the adaptive crossover rate is defined as:

$$Pr_{\text{cross}}^{\text{adaptive}} = Pr_{\text{cross}} \times \delta.$$

This rate increases proportionally with  $\delta$ , allowing for more frequent recombination within the population when the population contains a wide variety of ensembles. A high  $\delta$  indicates ample genetic material, making crossover more effective in creating new and potentially superior ensembles. On the other hand, when  $\delta$  is low, the reduced crossover rate prevents the overexploitation of similar ensembles. At the same time, increasing the probability of mutation allows the population to have more unique ensembles.

To implement these adaptive mechanisms, we set the base mutation probability to  $Pr_{\text{mut}} = 0.1$  and the base crossover probability to  $Pr_{\text{cross}} = 0.9$ , following standard practice in genetic algorithms. By maintaining the diversity of ensembles within the population through adaptive mutation and crossover rates, this approach promotes the generation of unique and high-performing ensembles throughout the evolutionary process.

1. **Tournament Selection:** The selection method that EAI uses would be the Tournaments Selection. For each tournament,  $\ell$  ensembles are randomly selected from the population. Using the fitness value computed before, pick the best-performing ensemble out of the  $\ell$  ensemble. This ensemble will be

called a parent ensemble. Figure 1 provides an illustration of a Tournament Selection when  $\ell = 3$ .

Fig. 1: Illustration of a Tournament Selection within EAI when  $\ell = 3$ .

2. Crossover: For Crossover, it uses two tournaments for creating two ensembles (aka offspring) as shown in Figure 2. Assume that the ensembles parent<sub>1</sub> and parent<sub>2</sub> have the best fitness scores for two different tournaments. Then Crossover randomly generates two indexes  $c_1$  and  $c_2$ . The two offspring ensembles are produced via:

$$\mathtt{offspring}_1[j] = \begin{cases} \mathtt{parent}_1[j] & \text{if } j < c_1 \text{ or } j > c_2 \\ \mathtt{parent}_2[j] & \text{if } c_1 \leq j \leq c_2 \end{cases} \tag{2}$$

$$\begin{aligned} & \text{offspring}_1[j] = \begin{cases} \text{parent}_1[j] & \text{if } j < c_1 \text{ or } j > c_2 \\ \text{parent}_2[j] & \text{if } c_1 \leq j \leq c_2 \end{cases} \end{aligned} \end{aligned}$$
 
$$& \text{offspring}_2[j] = \begin{cases} \text{parent}_2[j] & \text{if } j < c_1 \text{ or } j > c_2 \\ \text{parent}_1[j] & \text{if } c_1 \leq j \leq c_2 \end{cases}$$
 
$$& (3)$$

Figure 2 provides an illustration of Crossover when  $c_1 = 3$  and  $c_2 = 6$  are chosen. This indicates that the segments from position 3 to 6 (inclusive) are swapped between the parents. We highlight that if crossover results in duplicate individuals within the population, the process is repeated to ensure uniqueness.

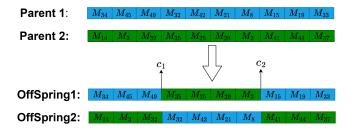


Fig. 2: Illustration of Crossover within EAI when  $c_1 = 3$  and  $c_2 = 6$ .

3. Mutation: As for Mutation, it only uses one tournament. During the Mutation process, one DNN from the selected ensemble is randomly replaced with a different pre-trained DNN from the set  $\mathcal{M}$ . Figure 3 depicts the Mutation process.

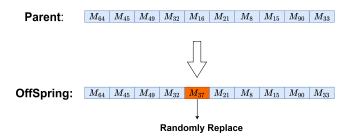


Fig. 3: Illustration of Mutation within EAI when taking a new model  $M_{37}$  from  $\mathcal{M}$ .

If the algorithm chooses Crossover when selecting the last ensemble for the next generation, we pick the first offspring produced.

Time Complexity Analysis: Recall that  $|\mathcal{M}|$  is the total number of pretrained models,  $N_{gen}$  is the number of generations,  $N_{ens}$  is the population size, and  $N_{model}$  is the number of models per ensemble. The time complexity of initialize\_pop is  $O(N_{ens} \times N_{model})$ . For each generation, the time complexity is  $O(N_{model})$  for Eval & Elite while  $O(N_{ens} \times N_{model})$  for GenericOp. Since the time complexity mainly comes from GenericOp, the overall time complexity of the EAI algorithm is given by  $O(N_{gen} \times N_{ens} \times N_{model})$ .

## 5 Experiment Result and Setting

#### 5.1 Datasets and Leakage Models

ASCADf & ASCADr: Both ASCADf and ASCADr are part of the commonly used ASCADv1 dataset [3]. It comprises of traces from first-order masked AES implementation on an 8-bit AVR microcontroller. ASCADf contains traces of the same fixed key for both profiling and attack. On the other hand, ASCADr considers the case where the profiling traces are generated from a random key setting while a fixed key is used to generate the attack traces. Both datasets contain 50000 profiling traces and 10000 attack traces. Each trace contains 700 sample points for ASCADf and 1400 sample points for ASCADr. We target the third byte of the first round sbox output, specifically Sbox<sub>AES</sub>( $pt_3 \oplus k_3^*$ ) where  $pt_3$  represents the third plaintext byte and  $k_3^*$  denotes the third byte of the first round key.

Ascon: We use the publicly available datasets by [21] for Ascon. The Ascon implementation is running on a ChipWhisperer Lite board on top of a STM32F4. The traces are collected using an 8-bit oscilloscope. We will only investigate the first-order protected implementation of Ascon-128. There are 50000 profiling traces from a random key setting and 10000 attack traces collected from a fixed

key setting. We target the first round of permutation proposed by [21] and [18], where the sensitive variable is of the form:

$$y = k_1 \wedge (255 \oplus IV \oplus \mathfrak{n}_0) \oplus \mathfrak{n}_0 \oplus \mathfrak{n}_1,$$

where IV is the constant from the initialization value, while  $\mathfrak{n}_0, \mathfrak{n}_1$  are 8-bits nonces values. Lastly,  $k_1$  is the 8 bits key we are trying to recover. There are a total of 8 different bytes. We shall focus particularly on bytes 2 and 4, which have proven challenging for analysis as shown in [18] even with GSM ensemble. We denote ASCON2 and ASCON4 for byte 2 and byte 4 respectively.

**AES\_HD:** The AES\_HD dataset represents power leakage measurements from an unprotected AES hardware implementation running on an FPGA with a round-based architecture. Our analysis targets the side-channel leakage during the last round, specifically focusing on the Hamming Distance leakage model, i.e.  $\mathrm{Sbox}_{\mathrm{AES}}^{-1}(ct_{15} \oplus k_{15}) \oplus ct_{11}$ , where  $ct_i$  refers to the  $i^{th}$  ciphertext byte and  $k_{15}$  corresponds to the  $15^{th}$  byte of the last round key. The dataset consists of 45000 profiling traces used for training and 3000 attack traces for evaluation.

Throughout this work, we use 1000 attack traces for each dataset.

Leakage Models: In this work, we consider three different leakage models.

- Identity (ID): The Identity leakage model assumes that the sensitive intermediate values, such as the AES S-box output  $Sbox_{AES}(pt \oplus k)$ , leak directly through side-channel emissions.
- Hamming Weight (HW): The HW leakage model corresponds to the Hamming weight of the sensitive variable. For example, for AES S-box output, we have  $HW(\operatorname{Sbox}_{\operatorname{AES}}(pt \oplus k))$  as the leakage model. This model assumes that the amount of leakage is proportional to the number of 1-bits in the binary representation of the sensitive value.
- Hamming Distance (HD): The HD leakage model considers the side channel traces leaks the XOR of two sensitive variables.

For ASCADr and ASCADf datasets, we will investigate with ID and HW leakage models. As for ASCON datasets, we will present results for ID leakage model. On the other hand, we only use HD leakage model for AES\_HD.

## 5.2 Hyperparameters used for DNN and EAI

DNN's Hyperparameter Search Space In this study, we consider the commonly used Multi-Layer Perceptron (MLP) and Convolutional Neural Network (CNN) in our study. We consider three different settings: solely MLPs, solely CNNs, and a Diverse DNN. For Diverse DNN, it consists of 25 MLPs and 25 CNNs. For solely MLPs (resp. solely CNNs), we randomly generate 50 MLPs (resp. CNNs). The 50 neural networks are randomly generated based on the hyperparameter search spaces defined in Tables 1.

Table 1: Hyperparameter Search Space

| Values   |
|--|
| Values   |
| · · · · · · · · · · · · · · · · · · ·                      |
| 1 to 7 (in step of 1)                                      |
| 10, 20, 50, 100, 200, 300, 400, or 500                     |
| ReLU, SELU, ELU, or Tanh                                   |
| 100 - 1000 (in steps of $100$ )                            |
| 1e - 3, 5e - 4, 1e - 4, 5e - 5, or 1e - 5                  |
| RMSprop or Adam  |
| Random uniform, Xavier uniform, or He uniform              |
| CNN  |
| Values   |
| 1-4 (in step of 1)   |
| 4, 8, 12, 16   |
| 26 - 52 (in step of 2)                                     |
| Max pooling, Average pooling                               |
| 2, 4, 6, 8, 10   |
| 0, 4, 8, 12, 16  |
| 1-7  (in step of 1)<br>10, 20, 50, 100, 200, 300, 400, 500 |
| ReLU, SELU, ELU, Tanh                                      |
| 100 - 1000 (in steps of 100)                               |
| 1e - 3, 5e - 4, 1e - 4, 5e - 5, 1e - 5                     |
| RMSprop, Adam  |
| Random uniform, Xavier uniform, He uniform                 |
|  |

**Hyperparameters for EAI** The hyperparameters for EAI are shown in Table 2. All the hyperparameters listed are consistent across all datasets except for the number of generations. This is because both ASCON2 and ASCON4 require more time to run. Hence, we decrease the number of generations.

## 5.3 Experimental Results on Publicly Available Datasets

**ASCADf.** As shown in Table 3 and Figure 4, we analyze the performance of different algorithms on the ASCADf dataset. The results demonstrate that our EAI with the  $ge_{+ntge}$  variant significantly outperforms both EAI with val\_loss

Table 2: Hyperparameters for EAI across all Datasets

| Configuration for Each Datase                 | t and Hvi | perparame | eters of | EAI |        |
|---|-----------|-----------|----------|-----|--------|
|   |           | ASCAD     |          |     | AES_HD |
| Number of Generations, $N_{gen}$              | 50        | 50        | 5        | 5   | 50     |
|   |           |           | 0.9      |     |        |
| Mutation Probability, Pr <sub>mut</sub>       |           |           | 0.1      |     |        |
| Models per Ensemble, $N_{model}$              |           |           | 10       |     |        |
| Number of Ensembles per Generation, $N_{ens}$ |           |           | 30       |     |        |
| Models per Tournament, $\ell$                 |           |           | 3        |     |        |
|   |           |           |          |     |        |

and GSM in terms of number of traces required to recover the key. Across different models, the ID leakage model consistently performs more effectively than the HW leakage model. Notably, the MLP model with ID leakage model achieves the best performance (NTGE=29). We observed significant differences in performance between the use of fitness functions when applying EAI. Our results show that EAI using val\_loss is ineffective in recovering the secret key in certain cases. Conversely, EAI with  $ge_{+ntge}$  consistently recovers the secret key across every scenario, surpassing GSM's performance. In addition, using EAI with  $ge_{+ntge}$  obtain below 100 attack traces (i.e., MLP (ID) has NTGE=29 and Diverse DNN (ID) 58), outperforming the current state-of-the-art hyperparameter tuning techniques for single best-performing DNN (see Table 12 of [7]).

Table 3: NTGE for different algorithms and leakage models in ASCADf Dataset

| Algorithm             | MLP        |     | CN         | N      | Diverse    | DNN    |
|-----------------------|------------|-----|------------|--------|------------|--------|
|                       | $_{ m HW}$ | ID  | $_{ m HW}$ | ID     | $_{ m HW}$ | ID     |
| GSM                   | 785        | 365 | 825        | 385    | 817        | 329    |
| EAI with $ge_{+ntge}$ | 615        | 29  | 727        | 140    | 590        | 58     |
| EAI with val_loss     | (GE = 19)  | 98  | (GE = 3)   | 3) 615 | (GE = 6    | 6) 113 |

However, it requires a longer time when executing EAI compared to GSM, as shown in Figure 5. This is as expected since GSM only needs to select the top few models and execute the attack phase, but EAI will need to compute the fitness function for different ensembles over many different generations.

**ASCADr.** Similar to ASCADf, Table 4 and Figure 6 demonstrates that EAI with  $ge_{+ntge}$  maintains superior performance on the ASCADr dataset, outperforming GSM for all scenarios. In contrast to the ASCADf dataset, the HW leakage model outperforms the ID leakage model. The EAI with val\_loss shows

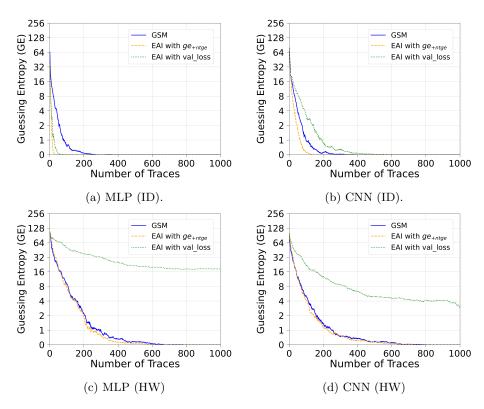


Fig. 4: Guessing entropy for ASCADf.

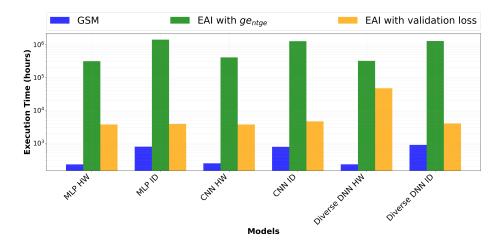


Fig. 5: Execution time comparisons for different algorithms and models in the ASCADf Dataset.

particularly poor performance, failing to recover the encryption key across all model and leakage model combinations.

Table 4: NTGE for different algorithms and leakage models in ASCADr Dataset

| Algorithm             | $\mathbf{N}$ | ILP      | (          | CNN          | Dive       | rse DNN      |
|-----------------------|--------------|----------|------------|--------------|------------|--------------|
|                       | $_{ m HW}$   | ID       | $_{ m HW}$ | ID           | $_{ m HW}$ | ID           |
| GSM                   | 548          | 976      | 810        | (GE = 126)   | 445        | (GE = 14)    |
| EAI with $ge_{+ntge}$ | 296          | 523      | 619        | (GE = 3)     | 257        | 923          |
| EAI with val_loss (   | (GE=1)       | (GE=185) | (GE = 6)   | ) (GE = 178) | (GE = 7)   | ) (GE = 178) |

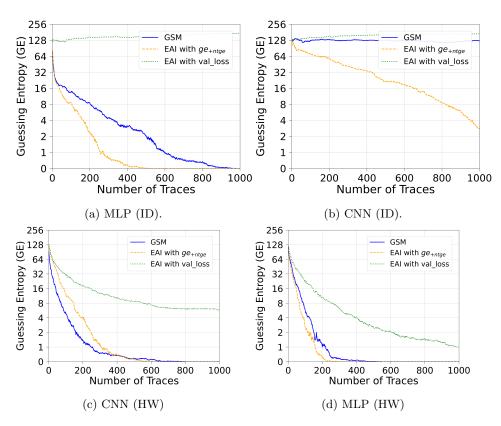


Fig. 6: Guessing entropy for ASCADr.

**Ascon2** Our research investigated both ID and HW leakage models. Due to the unsuccessful recovery of the secret key using the HW leakage model across all tested methods, we will only present findings from the ID leakage model just like in [18]. We see that with GSM and EAI with valloss, we are unable to successfully recover the secret key with  $GE \geq 15$ . However, using EAI with  $ge_{+ntge}$ , we manage to obtain the secret key with NTGE = 977 when building an ensemble of MLPs. Furthermore, we attain  $GE \leq 3$  for having CNN ensembles and under the Diverse DNN setting. This overall shows the effectiveness of EAI with  $ge_{+ntge}$ .

Table 5: NTGE for different algorithms and leakage models in the ASCON2 Dataset

| Algorithm                                  | MLP | CNN | Diverse DNN           |
|--|-----|-----|-----------------------|
| GSM  | '   | '   | (GE = 40)             |
| EAI with $ge_{+ntge}$<br>EAI with val_loss |     |     | (GE = 3) $(GE = 126)$ |

**Ascon4** Our findings show that ASCON4 yields similar results to ASCON2. Both GSM and EAI with valloss attain high GE values, suggesting that these methods are unable to recover the secret key. However, under the Diverse DNN setting, EAI with  $ge_{+ntge}$  recovers the secret key with 914 attack traces. Furthermore, when building a CNN-only ensemble, EAI with  $ge_{+ntge}$  attain GE=1. These instances suggest the effectiveness of EAI with  $ge_{+ntge}$  in obtaining well-performing ensembles for successful key recovery in SCA.

Table 6: NTGE for different algorithms and leakage models in the ASCON4 Dataset.

| Algorithm             | MLP        | CNN        | Diverse DNN |
|-----------------------|------------|------------|-------------|
| GSM                   | (GE = 140) | (GE = 135) | (GE = 136)  |
| EAI with $ge_{+ntge}$ | (GE = 34)  | (GE = 1)   | 914         |
| EAI with val_loss     | (GE = 220) | (GE = 179) | (GE = 138)  |

**AES\_HD** Lastly, we also investigate the effectiveness of our methodology on hardware traces. Here, we only consider the HD leakage model as stated in Section 5.1. EAI with  $ge_{+ntge}$  manages to recover the secret for all the scenarios tested and outperform both GSM and EAI with val\_loss in terms of the NTGE needed for successful key recovery. In fact, the best NTGE is almost half with

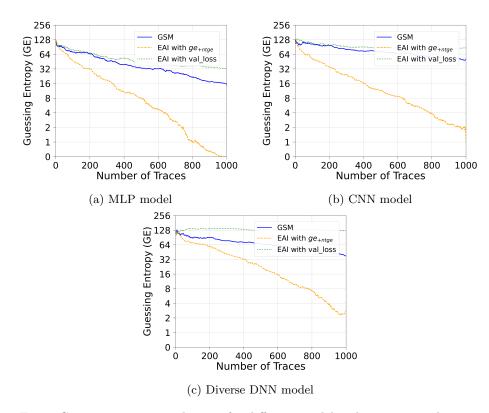


Fig. 7: Guessing entropy evaluation for different model architectures in ASCON2 Dataset.

456 attack traces when using Diverse DNN compared to the traditional GSM, which uses 840 attack traces when using CNN. These highlight once again that EAI with  $ge_{+ntge}$  is effective in finding well-performing neural networks.

Table 7: Number of traces for different algorithms and leakage models in the AES\_HD Dataset

| Algorithm             | MLP | CNN       | Diverse DNN |
|-----------------------|-----|-----------|-------------|
| GSM                   | 925 | 840       | (GE = 3)    |
| EAI with $ge_{+ntge}$ | 569 | 700       | 456         |
| EAI with val_loss     | 998 | (GE = 12) | 662         |

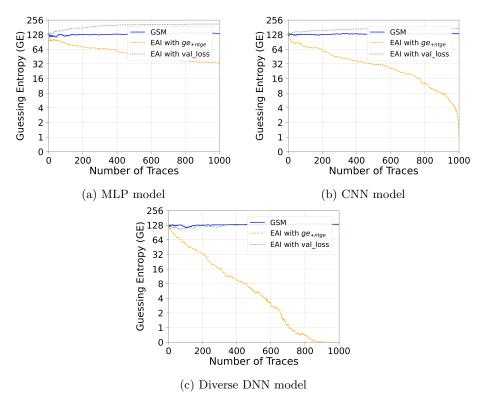


Fig. 8: Guessing entropy evaluation for different model architectures in Ascon4 Dataset.

## 6 Discussion and Future Work

In this work, we propose a novel ensemble selection methodology called EAI for generating well-performing ensembles from pre-trained neural networks. EAI significantly reduces the number of traces required for successful key recovery compared to traditional GSM when paired with an effective fitness function. We investigated two fitness functions,  $ge_{+ntge}$  and valloss. We observe that with  $ge_{+ntge}$  as the fitness function, EAI consistently outperforms other methods across five different datasets. Furthermore, it managed to recover the secret key across all the datasets tested, showing the efficiency of the EAI with  $ge_{+ntge}$  as an ensemble selection algorithm. However, with valloss, it can be observed that it did not find a well-performing ensemble, and in many instances, GSM has much better performances. This suggests that choosing the right fitness function is very important, therefore, we recommend to use  $ge_{+ntge}$  as the primary fitness function when employing EAI. However, EAI demands more computational resources, as evidenced by the longer execution times. Therefore, if resources are limited, GSM remains a preferable alternative.

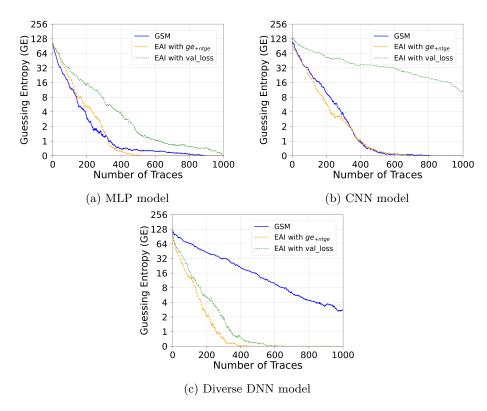


Fig. 9: Guessing entropy evaluation for different model architectures in AES\_HD Dataset.

We hope that this work opens up a new dimension of research into finding the optimal ensemble among pre-trained DNNs. Several directions offer potential for exploration. Firstly, as mentioned above, EAI requires lengthy execution times. One possible direction is to enhance this approach by leveraging multifidelity optimization methods [7]. Furthermore,  $ge_{+ntge}$  fitness function necessitates knowledge of the secret key for deployment. This limitation suggests that its application is restricted to white-box settings during evaluation, specifically for identifying worst-case scenarios. Developing a novel fitness function for EAI that does not require secret key knowledge and achieves comparable performance would be an intriguing area of study.

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