## CS771: Introduction to Machine Learning

# Assignment - 1 Team: NEURAL KNIGHTS

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#### Abstract:

This report presents our solution to the Mini Project of CS771, where we investigate the vulnerability of a Companion Arbiter PUF to machine learning attacks. We mathematically derive how a single linear model can predict the responses of the ML-PUF by exploiting delay-based correlations between its component PUFs. We then evaluate the performance of our model, highlighting the impact of hyperparameter tuning on training time and prediction accuracy.



## 1 Mathematical Derivation of Linear Model for Predicting ML-PUF Responses

We will use a straightforward approach to solve this problem. The strategy involves leveraging the known differences in time delays for the upper and lower signals, as well as the sum of their delays. First, we will derive the difference in time delays for 8-bit input in a way similar to as outlined in the lectures, and then proceed to derive the sum of these delays. Also the notations are same as described in lectures.

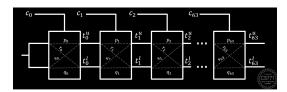


Figure 1: Sample figure caption.

#### 1.1 Deriving the difference of Delays

Here,  $t_i^u$  and  $t_i^l$  represent the times at which the signal departs from the  $i^{th}$  MUX pair. Expressing  $t_i^u$  in terms of  $t_{i-1}^u$ ,  $t_{i-1}^l$  and  $c_i$ , we obtain:

$$t_i^u = (1 - c_i) \cdot (t_{i-1}^u + p_i) + c_i \cdot (t_{i-1}^l + s_i) \tag{1}$$

$$t_i^l = (1 - c_i) \cdot (t_{i-1}^l + q_i) + c_i \cdot (t_{i-1}^u + r_i)$$
(2)

Thus, following the lecture slides we have,  $\Delta_i = t_i^u - t_i^l$ . Subtracting equations (1), (2) we get,  $\Delta_i = \Delta_{i-1} \cdot d_i + \alpha_i \cdot d_i + \beta_i$ , where  $\alpha_i, \beta_i$  depend on constants that are indeterminable from the physical/measurable perspective and thus we call them system constants and are given by:

$$\alpha_i = \frac{(p_i - q_i + r_i - s_i)}{2}, \quad \beta_i = \frac{(p_i - q_i - r_i + s_i)}{2} + a$$

where  $p_i, q_i, r_i, s_i$  are system parameters. Also  $d_i$  is governed by the challenge bits/input  $(c_i)$ :

$$d_i = (1 - 2 \cdot c_i)$$

$$\Delta_{-1} = 0$$

Moreover, observing the recursion unfold carefully we can simplify this relation further:

$$\Delta_{0} = \alpha_{0} \cdot d_{0} + \beta_{0} 
\Delta_{1} = \alpha_{0} \cdot d_{1} \cdot d_{0} + (\alpha_{1} + \beta_{0}) \cdot d_{1} + \beta_{1} 
\Delta_{2} = \alpha_{0} \cdot d_{2} \cdot d_{1} \cdot d_{0} + (\alpha_{1} + \beta_{0}) \cdot d_{2} \cdot d_{1} + (\alpha_{2} + \beta_{1}) \cdot d_{2} + \beta_{2} 
\vdots$$

The only  $\Delta$  we require is  $\Delta_7$ , the last output.

$$\Delta_7 = w_0 \cdot x_0 + w_1 \cdot x_1 + \dots + w_7 \cdot x_7 + \beta_7 = \mathbf{w}^T \cdot \mathbf{x} + b = \mathbf{W}^T \cdot \mathbf{X}$$

where  $\mathbf{w}, \mathbf{x}$  are 8-dimensional vectors and  $\mathbf{W}, \mathbf{X}$  are 9-dimensional, just including the bias term  $W_8 = \beta_7$  and  $X_8 = 1$ . Each term of  $\mathbf{w}, \mathbf{x}$  being:

$$b = \beta_7, \quad w_0 = \alpha_0, \quad w_i = \alpha_i + \beta_{i-1}, \quad x_i = \prod_{i=i}^7 d_i$$

#### 1.2 Deriving the Sum of Delays

We have,

$$t_i^u = (1 - c_i) \cdot (t_{i-1}^u + p_i) + c_i \cdot (t_{i-1}^l + s_i)$$
(1)

$$t_i^l = (1 - c_i) \cdot (t_{i-1}^l + q_i) + c_i \cdot (t_{i-1}^u + r_i)$$
(2)

Adding both the equations,

$$t_i^u + t_i^l = t_{i-1}^u + t_{i-1}^l + (p_i + q_i) + c_i \cdot (s_i + r_i - p_i - q_i)$$

Put

$$(s_i + r_i - p_i - q_i) = r_i'$$

to get,

$$t_i^u + t_i^l = t_{i-1}^u + t_{i-1}^l + (p_i + q_i) + c_i \cdot (r_i')$$

Substituting the value of i = 7, 6, ..., 0 and adding the equations:

$$t_7^u + t_7^l = (c_7 \cdot r_7') + (p_7 + q_7) + (c_6 \cdot r_6') + (p_6 + q_6) + \cdots + (c_0 \cdot r_0') + (p_0 + q_0)$$

We finally get,

$$t_7^u + t_7^l = \sum_{i=0}^7 (c_i \cdot r_i') + \sum_{i=0}^7 (p_i + q_i)$$
 (1)

where

$$r_i' = s_i + r_i - p_i - q_i$$

We also derived the difference in previous sections as:

$$t_7^u - t_7^l = w_0 \cdot x_0 + w_1 \cdot x_1 + \dots + w_7 \cdot x_7 + \beta_7 \tag{2}$$

where

$$w_0 = \alpha_0, \quad w_i = \alpha_i + \beta_{i-1}, \quad x_i = \prod_{j=i}^7 d_j, \quad d_i = (1 - 2 \cdot c_i)$$

and

$$\alpha_i = \frac{p_i - q_i + r_i - s_i}{2}, \quad \beta_i = \frac{p_i - q_i - r_i + s_i}{2}$$

Adding (1) and (2):

$$2 \cdot t_7^u = (c_7 \cdot r_7') + (c_6 \cdot r_6') + \dots + (c_0 \cdot r_0') + w_0 \cdot x_0 + w_1 \cdot x_1 + \dots + w_7 \cdot x_7 + \beta_7$$

Dividing both sides by 2:

$$t_7^u = \frac{1}{2} \left( \sum_{i=0}^7 c_i \cdot r_i' + \sum_{i=0}^7 w_i \cdot x_i + \beta_7 \right)$$

Rewriting  $c_7 = 1 - 2c_7$  and taking  $c_7$  common from  $c_7 \cdot r_7'$  and  $2 \cdot w_7 \cdot c_7$ , we get:

$$t_7^u = \frac{1}{2} \left( c_7 \cdot (r_7' - 2w_7) + \sum_{i=0}^6 c_i \cdot r_i' + \sum_{i=0}^7 w_i \cdot x_i + \beta_7 + w_7 \right)$$

In matrix form, this can be expressed as:

$$t_7^u = \frac{1}{2} \left( \mathbf{W}^T \cdot \phi(c) + b \right)$$

where:

$$\phi(c) = [c_7, c_6, \dots, c_0, x_0, x_1, \dots, x_6]^T$$

$$\mathbf{W} = [r_7' - 2w_7, r_6', \dots, r_0', w_0, w_1, \dots, w_6]^T, \quad b = \beta_7 + w_7$$

In this solution we denote parameters for PUF0 as  $A_{0,i}$ , and parameters for PUF1 as  $A_{1,i}$ .

#### Linear Model for Response0:

$$t_{0,7}^{u} = \frac{1}{2} \left( \left( c_7 \cdot \left( r_{0,7} - 2w_{0,7} \right) \right) + \left( c_6 \cdot r_{0,6} \right) + \dots + \left( c_0 \cdot r_{0,0} \right) + w_{0,0} \cdot x_0 + \dots + w_{0,7} \cdot x_7 + \beta_{0,7} \right) \right)$$

$$t_{1,7}^{u} = \frac{1}{2} \left( \left( c_7 \cdot (r_{1,7} - 2w_{1,7}) \right) + \left( c_6 \cdot r_{1,6} \right) + \dots + \left( c_0 \cdot r_{1,0} \right) + w_{1,0} \cdot x_0 + \dots + w_{1,7} \cdot x_7 + \beta_{1,7} \right)$$

Now

$$t_{0,7}^{u} - t_{1,7}^{u} = \frac{1}{2} \left( c_7 \cdot ((r_{0,7} - 2w_{0,7}) - (r_{1,7} - 2w_{1,7})) + c_6 \cdot (r_{0,6} - r_{1,6}) + \dots + c_0 \cdot (r_{0,0} - r_{1,0}) + (w_{0,0} - w_{1,0}) \cdot x_0 + \dots + (w_{0,6} - w_{1,6}) \cdot x_6 + (\beta_{0,7} + w_{0,7}) - (\beta_{1,7} + w_{1,7}) \right)$$

In matrix form, this can be expressed as:

$$t_{0,7}^u - t_{1,7}^u = \frac{1}{2} \left( \tilde{\boldsymbol{W}}^T \cdot \boldsymbol{\phi}(\boldsymbol{c}) + \tilde{\boldsymbol{b}} \right)$$

Where:

$$\phi(c) = [c_7, c_6, \dots, c_0, x_0, x_1, \dots, x_6]^T$$

$$\tilde{W} = \left[ (r_{0,7} - 2w_{0,7}) - (r_{1,7} - 2w_{1,7}), \ r_{0,6} - r_{1,6}, \dots, r_{0,0} - r_{1,0}, \ w_{0,0} - w_{1,0}, \dots, w_{0,6} - w_{1,6} \right]^T$$

$$\tilde{b} = (\beta_{0,7} + w_{0,7}) - (\beta_{1,7} + w_{1,7})$$

#### Linear Model for Response1:

$$t_{0,7}^{l} = \frac{1}{2} \left( \left( c_7 \cdot \left( r_{0,7} + 2w_{0,7} \right) \right) + \dots + \left( c_0 \cdot r_{0,0} \right) - w_{0,0} \cdot x_0 - \dots - w_{0,7} \cdot x_7 - \left( \beta_{0,7} + w_{0,7} \right) \right) \right)$$

$$t_{1,7}^{l} = \frac{1}{2} \left( \left( c_7 \cdot (r_{1,7} + 2w_{1,7}) \right) + \dots + \left( c_0 \cdot r_{1,0} \right) - w_{1,0} \cdot x_0 - \dots - w_{1,7} \cdot x_7 - \left( \beta_{1,7} + w_{1,7} \right) \right)$$

Now

$$t_{0,7}^{l} - t_{1,7}^{l} = \frac{1}{2} \left( c_7 \cdot ((r_{0,7} + 2w_{0,7}) - (r_{1,7} + 2w_{1,7})) + c_6 \cdot (r_{0,6} - r_{1,6}) + \dots + c_0 \cdot (r_{0,0} - r_{1,0}) - (w_{0,0} - w_{1,0}) \cdot x_0 - \dots - (w_{0,6} - w_{1,6}) \cdot x_6 - ((\beta_{0,7} + w_{0,7}) - (\beta_{1,7} + w_{1,7})) \right)$$

In matrix form, this can be expressed as:

$$t_{0,7}^{l} - t_{1,7}^{l} = \frac{1}{2} \left( \tilde{W}^{T} \cdot \phi(c) + \tilde{b} \right)$$

Where:

$$\phi(c) = [c_7, c_6, \dots, c_0, x_0, x_1, \dots, x_6]^T$$

$$\tilde{W} = \left[ (r_{0,7} + 2w_{0,7}) - (r_{1,7} + 2w_{1,7}), \ r_{0,6} - r_{1,6}, \dots, r_{0,0} - r_{1,0}, \ -(w_{0,0} - w_{1,0}), \dots, -(w_{0,6} - w_{1,6}) \right]^T$$

$$\tilde{b} = (\beta_{1,7} + w_{1,7}) - (\beta_{0,7} + w_{0,7})$$

We now compute the multiplication of the two expressions to model the XOR response of the ML-PUF, as per MP1.

Recall the expressions:

$$t_{0,7}^{u} - t_{1,7}^{u} = \frac{1}{2} \left( c_7 \cdot \left( (r_{0,7} - 2w_{0,7}) - (r_{1,7} - 2w_{1,7}) \right) + c_6 \cdot (r_{0,6} - r_{1,6}) + \dots + c_0 \cdot (r_{0,0} - r_{1,0}) + (w_{0,0} - w_{1,0}) \cdot x_0 + \dots + (w_{0,6} - w_{1,6}) \cdot x_6 + (\beta_{0,7} + w_{0,7}) - (\beta_{1,7} + w_{1,7}) \right)$$

$$t_{0,7}^{l} - t_{1,7}^{l} = \frac{1}{2} \left( c_7 \cdot \left( \left( r_{0,7} + 2w_{0,7} \right) - \left( r_{1,7} + 2w_{1,7} \right) \right) + c_6 \cdot \left( r_{0,6} - r_{1,6} \right) + \dots + c_0 \cdot \left( r_{0,0} - r_{1,0} \right) \right) - \left( w_{0,0} - w_{1,0} \right) \cdot x_0 - \dots - \left( w_{0,6} - w_{1,6} \right) \cdot x_6 - \left( \left( \beta_{0,7} + w_{0,7} \right) - \left( \beta_{1,7} + w_{1,7} \right) \right) \right)$$

Now multiplying:

$$(t_{0,7}^u - t_{1,7}^u) \cdot (t_{0,7}^l - t_{1,7}^l) = \frac{1}{4} \cdot \left( \text{Expression}_u \right) \cdot \left( \text{Expression}_l \right)$$

Writing all terms symbolically:

$$(t_{0,7}^{u} - t_{1,7}^{u}) \cdot (t_{0,7}^{l} - t_{1,7}^{l}) = \frac{1}{4} \left[ \left( \sum_{i=0}^{7} c_{i} \cdot \Delta r_{i}^{(u)} + \sum_{j=0}^{6} \Delta w_{j}^{(u)} \cdot x_{j} + b_{u} \right) \cdot \left( \sum_{i=0}^{7} c_{i} \cdot \Delta r_{i}^{(l)} - \sum_{j=0}^{6} \Delta w_{j}^{(u)} \cdot x_{j} - b_{u} \right) \right]$$

Where:

- 
$$\Delta r_7^{(u)} = (r_{0,7} - 2w_{0,7}) - (r_{1,7} - 2w_{1,7})$$
 -  $\Delta r_7^{(l)} = (r_{0,7} + 2w_{0,7}) - (r_{1,7} + 2w_{1,7})$  -  $\Delta r_i^{(u)} = r_{0,i} - r_{1,i}$ , for  $i = 0$  to 6 -  $\Delta w_j^{(u)} = w_{0,j} - w_{1,j}$  -  $b_u = (\beta_{0,7} + w_{0,7}) - (\beta_{1,7} + w_{1,7})$ 

This final expression models the XOR logic by taking the product of the two linear expressions.

To obtain the predicted response bit, we apply:

Response(c) = 
$$\frac{1 - \text{sign}\left( (t_{0,7}^u - t_{1,7}^u) \cdot (t_{0,7}^l - t_{1,7}^l) \right)}{2}$$

Therefore, the final feature map is:

$$(c_1c_1, c_1c_2, \dots, c_7c_6, c_7c_7, x_1x_1, x_1x_2, \dots, x_6x_5, x_6x_6, c_1x_1, c_1x_2, \dots, c_7x_5, c_7x_6, x_1c_1, x_1c_2, \dots, x_6c_6, x_6c_7, c_1.1, c_2.1, \dots, c_7.1, x_1.1, \dots, x_6.1, 1.c_1, 1.c_2, \dots, 1.c_7, 1.x_1, \dots, 1.x_6, 1)$$

# 2 Dimensionality $\tilde{D}$ Required by the Linear Model for ML-PUF Prediction

#### 2.1 Initial Feature Construction

We begin by identifying the set of base variables involved in forming the feature space. These include:

- 8 challenge bits:  $c_7, c_6, \ldots, c_0$
- 7 intermediate state bits:  $x_0, x_1, \ldots, x_6$
- Constant term: 1

This gives us a total of 8 + 7 + 1 = 16 base variables.

We construct all second-order pairwise product features from these variables. This includes terms of the form:

$$u_i \cdot u_j$$
 where  $u_i, u_j \in \{c_7, \dots, c_0, x_0, \dots, x_6, 1\}$ 

Naively, this yields:

$$16 \times 16 = 256$$
 features

#### 2.2 Removing Duplicate Terms (Due to Commutativity)

Because multiplication is commutative,  $u_iu_j=u_ju_i$ , we remove duplicate terms such as  $c_7c_6$  and  $c_6c_7$ . Hence, we consider unordered pairs (including self-pairs). The number of such combinations is:

$$\binom{16+1}{2} = \binom{17}{2} = 136$$

#### 2.3 Removing Redundant Self-Terms for $x_i$

Each  $x_i$  is defined as:

$$x_i = \prod_{k=i}^{7} d_k$$
, where  $d_k = 1 - 2c_k \in \{-1, +1\}$ 

This implies:

$$x_i^2 = 1$$
 for all  $i$ 

Therefore, all terms of the form  $x_i \cdot x_i$  are constant and provide no useful information for the model. We remove the 7 such terms:

$$x_0x_0, x_1x_1, \ldots, x_6x_6$$

Note: 1 should also be removed

#### Removing Redundant Self-Terms for $c_i$

Since each challenge bit  $c_i \in \{0,1\}$ , we have  $c_i^2 = c_i$  for all i. Therefore, quadratic terms of the form  $c_i \cdot c_i$  do not contribute any new information and can be safely removed from the feature map. We eliminate these 8 redundant terms:

$$c_0c_0, c_1c_1, \ldots, c_7c_7$$

#### Removing Redundant $x_i x_{i+1}$ and $x_i x_{i+2}$ Terms

Each intermediate variable  $x_i$  is defined as:

$$x_i = \prod_{k=-i}^{7} d_k$$
, where  $d_k = 1 - 2c_k \in \{-1, +1\}$ 

This implies that certain pairwise products of  $x_i$  variables can be exactly represented using combinations of  $c_i$  bits:

> $x_i x_{i+1} = \left(\prod_{k=1}^7 d_k\right) \left(\prod_{k=1}^7 d_k\right)$  $=d_i \cdot \left(\prod_{k=i+1}^7 d_k\right)^2$

Since  $x_{i+1} = \pm 1$ , we know that  $(x_{i+1})^2 = 1$  always. Now,  $d_i = 1 - 2c_i$ , which is a linear combination of  $c_i$ , and  $c_i$  is already part of the feature

Therefore, all six  $x_i x_{i+1}$  terms can be removed.

 $x_i x_{i+2} = \left(\prod_{k=i}^7 d_k\right) \left(\prod_{k=i+2}^7 d_k\right)$  $= d_i d_{i+1} \cdot \left( \prod_{k=i+2}^{7} d_k \right)^2$ 

Since  $x_{i+2}=\pm 1$ , we have  $(x_{i+2})^2=1$  always. Now,  $d_id_{i+1}=(1-2c_i)(1-2c_{i+1})$ , which is a linear combination of terms already present in the feature map.

Therefore, all five  $x_i x_{i+2}$  terms can be removed.

Hence, these terms do not contribute new information beyond what is already captured by firstorder or product terms of the challenge bits. Consequently, we remove all such redundant terms of the form  $x_i x_{i+1}$  and  $x_i x_{i+2}$  from the feature set, resulting in a total of 11 terms removed.

#### 2.6 Removing Redundant $c_i x_{i+1}$ Terms

We analyze terms of the form  $c_i x_{i+1}$  in the feature space, where:

$$x_i = \prod_{k=i}^{7} d_k = \prod_{k=i}^{7} (1 - 2c_k)$$

To simplify  $c_i x_{i+1}$ , we start by writing:

$$x_i = d_i x_{i+1} = (1 - 2c_i)x_{i+1} \Rightarrow c_i x_{i+1} = \frac{1}{2}(x_{i+1} - x_i)$$

This identity implies that  $c_i x_{i+1}$  is a linear combination of  $x_i$  and  $x_{i+1}$ , both of which are already included in the feature space.

Therefore, terms of the form  $c_i x_{i+1}$  (6 terms) do not provide new independent information and can be safely removed from the feature set.

#### **2.7** Reducing $x_6$ Term as a Linear Combination

The intermediate state bit  $x_i$  is defined as:

$$x_i = \prod_{k=i}^{7} (1 - 2c_k) = \sum_{S \subseteq \{i, \dots, 7\}} (-2)^{|S|} \prod_{k \in S} c_k$$

For i = 6:

$$x_6 = (1 - 2c_6)(1 - 2c_7) = 1 - 2c_6 - 2c_7 + 4c_6c_7$$

Terms: constant (1),  $c_6$ ,  $c_7$ ,  $c_6c_7$ , all present in the feature map ( $c_i$ ,  $c_ic_j$  for i < j, constant term). Thus:

$$x_6 = 1 - 2c_6 - 2c_7 + 4c_6c_7$$

 $x_6$  can be removed as it is exactly expressed using terms in the feature map.

#### Reducing $c_6x_6$ and $c_7x_6$ Terms

To determine if  $c_6x_6$  and  $c_7x_6$  can be reduced, we check if they can be exactly expressed as linear combinations of the feature map's basis:  $\{c_ic_j \mid 0 \le i < j \le 7\} \cup \{c_i \mid 0 \le i \le 7\}$  (28 + 8 = 36 terms). The intermediate state bit is:

$$x_6 = \prod_{k=6}^{7} d_k = d_6 d_7 = (1 - 2c_6)(1 - 2c_7)$$
$$= 1 - 2c_6 - 2c_7 + 4c_6 c_7$$

For  $c_6x_6$ 

$$c_6x_6 = c_6(1 - 2c_6 - 2c_7 + 4c_6c_7)$$
  
=  $c_6 - 2c_6c_6 - 2c_6c_7 + 4c_6c_6c_7$ 

Since  $c_6^2 = c_6$ ,  $c_6^2 c_7 = c_6 c_7$ :

$$c_6x_6 = c_6 - 2c_6 - 2c_6c_7 + 4c_6c_7$$
$$= -c_6 + 2c_6c_7$$

Terms  $c_6$  and  $c_6c_7$  are in the basis. Thus,  $c_6x_6$  is redundant:

$$c_6x_6 = -1 \cdot c_6 + 2 \cdot c_6c_7$$

For  $c_7x_6$ 

$$c_7x_6 = c_7(1 - 2c_6 - 2c_7 + 4c_6c_7)$$
$$= c_7 - 2c_7c_6 - 2c_7c_7 + 4c_7c_6c_7$$

Since  $c_7^2 = c_7$ ,  $c_7^2 c_6 = c_7 c_6$ :

$$c_7 x_6 = c_7 - 2c_6 c_7 - 2c_7 + 4c_6 c_7$$
$$= -c_7 + 2c_6 c_7$$

Terms  $c_7$  and  $c_6c_7$  are in the basis. Thus,  $c_7x_6$  is redundant:

$$c_7 x_6 = -1 \cdot c_7 + 2 \cdot c_6 c_7$$

Both  $c_6x_6$  and  $c_7x_6$  are redundant and can be removed, as they are exactly expressible using  $c_i$  and  $c_ic_j$ , therefore 2 terms being removed.

$$\tilde{D} = 136-8-8-11-6-1-2=100$$

#### 3 Kernel SVM for ML-PUF Classification

The components of  $\tilde{\phi}(c)$  can be viewed as monomials involving  $d_0, d_1, \ldots, d_{n-1}$ . Given that  $d_i = 1 - 2c_i$ , these expressions can be reformulated entirely in terms of  $c_0, c_1, \ldots, c_{n-1}$ . Therefore, a feature transformation comprising all monomials of these challenge bits is sufficient for our representation.

To compute the inner product in this expanded feature space without explicitly constructing it, we employ the **polynomial kernel**, defined as:

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^{\top} \mathbf{y} + r)^d$$

This kernel function effectively captures a combination of monomials of degrees ranging from 0 up to d, aligning with the structure we aim to represent.

- **Degree:** d = n, to ensure inclusion of all monomials up to degree n.
- Offset: r = 1, to include lower-degree monomials and the constant term.

To achieve perfect classification, the SVM kernel must implicitly generate a feature space equivalent to the 100-dimensional explicit map, capturing all monomials required by the ML-PUF response.

#### Polynomial Kernel Details

Consider a polynomial kernel of degree d:

$$K(c,c') = (\langle c,c'\rangle + r)^d \tag{1}$$

where:

- $c, c' \in \{0, 1\}^8$
- Inner product:  $\langle c,c'\rangle=\sum_{i=0}^7 c_i c_i'$  (note:  $c_i^2=c_i$  in binary)

This induces a feature space that includes all monomials of the challenge bits  $c_i$  up to degree d.

#### Feature Space Size

To capture all required terms including interactions like  $x_j =$  monomials in  $c_i$ , we need a space with up to degree-9 monomials:

This space covers:

- Linear terms:  $c_i$  (degree 1)
- Quadratic terms:  $c_i c_j$
- Higher-order terms:  $c_i x_j, x_i x_j$  up to degree 8 or approximated through combinations

#### **Kernel Parameters**

We choose:

- **Degree:** d = 9, to capture all monomials up to  $x_0$
- Offset: r = 1, to ensure inclusion of constant terms
- Gamma: Default ( $\gamma = 1/9$ ), not critical for polynomial kernels

#### Conclusion

The polynomial kernel:

$$K(c,c') = (c^{\top}c'+1)^9$$

generates a 256-dimensional feature space, sufficient to represent the 100-dimensional explicit map used for ML-PUF classification. It ensures all required polynomial interactions are represented, leading to perfect classification.

Alternative kernels like RBF and Matern are less suitable, as they do not target the specific polynomial structure inherent in the ML-PUF design.

### 4 Delay Recovery by Inverting an Arbiter PUF Model

We aim to recover 256 non-negative stage delays  $x_{\text{delays}} \in \mathbb{R}^{256}_{\geq 0}$  that yield a given 65-dimensional Arbiter PUF linear model  $y = (w_0, w_1, \dots, w_{63}, b)^T \in \mathbb{R}^{65}$ .

#### 4.1 Model Structure

Let:

$$x_{\text{delays}} = (p_0, q_0, r_0, s_0, \dots, p_{63}, q_{63}, r_{63}, s_{63})^{\top} \in \mathbb{R}^{256}$$

We define the following intermediate terms:

$$\alpha_i = \frac{1}{2}(p_i + r_i + s_i), \quad \beta_i = \frac{1}{2}(q_i - r_i + s_i)$$

The output values are formed by:

$$w_0 = \alpha_0, \quad w_i = \alpha_i + \beta_{i-1} \ (1 \le i \le 63), \quad b = \beta_{63}$$

#### 4.2 Step 1: Forward Model

We construct the sparse linear system  $Ax_{\text{delays}} = y$ , where  $A \in \mathbb{R}^{65 \times 256}$ ,  $x_{\text{delays}} = (p_0, q_0, r_0, s_0, \dots, p_{63}, q_{63}, r_{63}, s_{63})^T$ . The model is defined as follows (for N = 64 stages, 0-63):

- 1. Intermediate delays:  $\alpha_i = \frac{1}{2}(p_i q_i + r_i s_i), \ \beta_i = \frac{1}{2}(p_i q_i r_i + s_i) \ \text{for } i = 0, \dots, 63.$
- 2. Model parameters:  $w_0 = \alpha_0$ ,  $w_i = \alpha_i + \beta_{i-1}$  for  $1 \le i \le 63$ , and  $b = \beta_{63}$ .
- 3. Coefficient matrix A: The system  $Ax_{\text{delays}} = y$  encodes these relationships. A is sparse, with at most 8 non-zeros per row. Partitioning columns into 64 blocks of 4 (for  $p_i, q_i, r_i, s_i$ ), the structure is:

$$A = \begin{pmatrix} A^{(0)} & 0 & 0 & \cdots & 0 \\ B^{(1)} & A^{(1)} & 0 & \cdots & 0 \\ 0 & B^{(2)} & A^{(2)} & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & B^{(63)} & A^{(63)} \\ 0 & \cdots & 0 & 0 & B^{(64)} \end{pmatrix} \in \mathbb{R}^{65 \times 256}$$

where the non-zero blocks are:

- Row 0 ( $w_0 = \alpha_0$ ): Block  $A^{(0)} = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right]$  in column block 0.
- Rows  $r = 1 \dots 63$   $(w_r = \alpha_r + \beta_{r-1})$ : Block  $B^{(r)} = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]$  (for  $\beta_{r-1}$ ) in column block r 1, and block  $A^{(r)} = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right]$  (for  $\alpha_r$ ) in column block r.
- Row 64 ( $b = \beta_{63}$ ): Block  $B^{(64)} = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]$  in column block 63.

Sparsity summary: Rows 0 and 64 have 4 non-zeros; rows 1 to 63 have 8 non-zeros.

#### 4.2 Step 2: Inversion under Non-Negativity

To recover a physically valid solution  $(x_{\text{delays}} \ge 0)$ , we solve the Non-negative Least Squares (NNLS) problem:

$$\min_{x\in\mathbb{R}^{256}_{>0}}\|Ax-y\|_2^2\quad\text{subject to }x\geq 0.$$

This can be solved using custom sparse solvers like projected gradient or coordinate descent, adapted for the non-negativity constraint  $x \ge 0$ . This yields a non-negative delay vector  $x_{\rm delays}$  that best reproduces the model y.

### 5 ML-PUF Learning: Linear Model Training Using Sklearn Classifiers Code

Code Submitted

### 6 Arbiter PUF Inversion: Delay Recovery Using Linear Solvers Code

Code Submitted

## 7 Experimental Results: Hyperparameter Analysis of LinearSVC and LogisticRegression for ML-PUF Learning

## 7.1 Modifying the loss Hyperparameter in LinearSVC (Hinge vs. Squared Hinge)

The loss function determines how the model assesses errors in predictions during training. The LinearSVC class from sklearn.svm supports two loss functions: hinge and squared\_hinge.

#### 7.1.1 Setup

• C=100, tolerance =1e-3, penalty =12, max\_iter =5000

Table 1: Impact of Changing Loss Hyperparameters in LinearSVC

Loss	Training Time (s)	Accuracy
Hinge	0.6708	1.000
Squared Hinge	0.9640	1.000

#### 7.2 Tuning the C Hyperparameter in LinearSVC and LogisticRegression

The regularization strength C influences model complexity. Lower C enforces stronger regularization, promoting generalization but potentially underfitting. Higher C allows more complex models, which may fit training data more closely but risk overfitting.

#### Configurations Used

- LinearSVC: tol=1e-3, penalty='12', max\_iter=5000, loss='hinge', dual=True
- LogisticRegression: solver='lbfgs', max\_iter=5000, tol=1e-3, penalty='12'

Table 2: Effect of Varying C in LinearSVC and LogisticRegression

Model	C Value	Training Time (s)	Accuracy
LinearSVC	1	0.2766	0.9962
	10	0.6722	1.000
	100	0.6527	1.000
LogisticRegression	1	0.0808	0.9888
	10	0.0902	1.000
	100	0.1900	1.000

## 7.3 Varying the penalty Hyperparameter in LinearSVC and LogisticRegression (L1 vs. L2)

The penalty parameter determines the type of regularization:

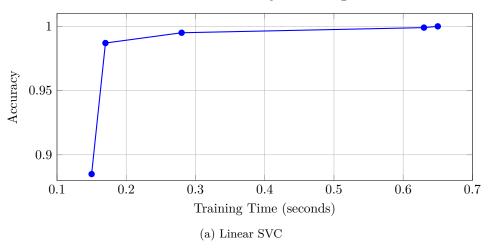
- L2: Encourages smaller coefficients by adding the square of weights to the loss.
- L1: Promotes sparsity by driving some coefficients exactly to zero.

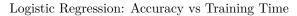
#### Used Configuration

- LinearSVC: C=100, loss='squared\_hinge', tol=1e-3, dual=False, max\_iter=5000
- LogisticRegression: C=100, solver='lbfgs', tol=1e-3, max\_iter=5000

  Note: In LinearSVC, the acceptable combinations of penalty and dual are:
- For penalty='12': dual=True
- For penalty='11': dual=False

#### Linear SVC: Accuracy vs Training Time





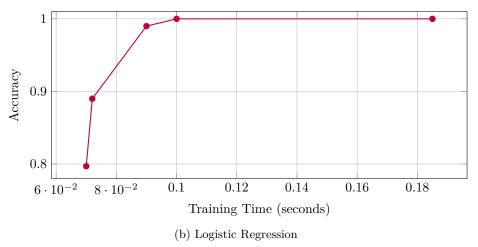


Figure 2: Comparison of Accuracy vs Training Time for Linear SVC and Logistic Regression

Table 3: Effect of Penalty Type on Training Time and Accuracy

Model	Penalty Type	Training Time (s)	Accuracy
LinearSVC	L1	5.3132	1.000
LinearSVC	L2	0.9294	1.000
LogisticRegression	L1	0.8075	1.000
LogisticRegression	L2	0.1900	1.000

