Password Guessing Using Random Forest

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Abstract

Passwords are the most widely used authentication method, and guessing attacks are the most effective method for password strength evaluation. However, existing password guessing models are generally built on traditional statistics or deep learning, and there has been no research on password guessing that employs classical machine learning.

To fill this gap, this paper provides *a brand new technical route* for password guessing. More specifically, we re-encode the password characters and make it possible for a series of classical machine learning techniques that tackle multi-class classification problems (such as random forest, boosting algorithms and their variants) to be used for password guessing. Further, we propose RFGuess, a random-forest based framework that characterizes the three most representative password guessing scenarios (i.e., trawling guessing, targeted guessing based on personally identifiable information (PII) and on users' password reuse behaviors).

Besides its theoretical significance, this work is also of practical value. Experiments using 13 large real-world password datasets demonstrate that our random-forest based guessing models are effective: (1) RFGuess for trawling guessing scenarios, whose guessing success rates are comparable to its foremost counterparts; (2) RFGuess-PII for targeted guessing based on PII, which guesses 20%∼28% of common users within 100 guesses, outperforming its foremost counterpart by 7%∼13%; (3) RFGuess-Reuse for targeted guessing based on users' password reuse/modification behaviors, which performs the best or 2nd best among related models. We believe this work makes a substantial step toward introducing classical machine learning techniques into password guessing.

1 Introduction

Passwords are likely to remain the dominant method in the foreseeable future due to its simplicity to use, easiness to change and low cost to deploy [12, 13, 20, 27]. However, users tend choose popular strings, employ personally identifiable information (PII), and reuse an existing password. Such behaviors make passwords vulnerable to guessing attacks (including trawling guessing [11, 43] and targeted guessing [40, 57]).

To address this issue, service providers often employ a password strength meter (PSM) [15, 60] to detect weak passwords, and research shows that well-designed PSMs do help users improve their password strength [48]. In practice, guess number is found to be a good metric to evaluate password strength [15, 35], and those easily guessed by an attacker are considered weak passwords. Thus, it is imperative to study password strength from the attacker's perspective. While unending password data breaches [3, 6, 8] provide favorable material for attackers, there are still realistic attack scenarios (e.g., for e-banking sites, and for passwords from sites beyond USA, China, and Russia) where training data is scarce (e.g., size$\leq 10^6$), and/or when little is known about the target. Therefore, it is equally imperative to understand guessing threats when the available training data is not abundant.

In 1979, Morris and Thompson [36] designed several heuristic transformation rules to generate variants of dictionary words, and exploited them to perform password guessing. Since then, a series of trawling password guessing approaches that employ users' behavior of choosing popular passwords have been proposed, major ones are probabilistic context-free grammar (PCFG [59]), and Markov-based models [34,37]. Besides, frequent large-scale PII leaks (e.g., 240 million Deezer leak [47], 553 million Facebook leak [9] and 77 million Nitro PDF leak [23]) make targeted password guessing (e.g., Targeted-Markov [55] and TarGuess-I [57] that employ users' PII, and TarGuess-II [57] that employ users' sister passwords) more and more realistic. All these password guessing algorithms are *statistics-based* models that crack passwords by counting the frequency of elements in the training set (such as the letter segments in PCFG and the *n*-gram strings in Markov). These "simply counting" models have the inherent limitations of data sparseness and overfitting [34].

To address these limitations, *deep learning based* guessing models (e.g., RNN [35], PassGAN [28], Adams [42] and CPG/DPG [43]) have been proposed. They mainly use complex neural networks to process the short length and small feature dimension texts (i.e., passwords). While the model training only happens once for these models, they usually require extremely large training set (e.g., $>10^8$ for dynamic dictionaries [42]), but have no significant success-rate advantages over statistics-based guessing models (e.g., PCFG [59] and Markov [34]) within 10^{10} guesses [51].

Since Melicher et al. [35] first modeled password guessability using long short-term memory (LSTM) in 2016, sustained attention has been attached to applying deep learning to password guessing research [28,42,43]. It turns out that *password guessing research has bypassed classical machine learning and entered into the era of deep learning directly from the statistics-based period*, leaving a huge gap. In reality, as the development of statistical learning and also the foundation of deep learning, classical machine learning[1] techniques (e.g., support vector machine [38] and random forest [14]) have shown extensive applications in various fields like natural language processing (NLP), speech recognition and computer vision [30]. Compared with traditional statistical methods, classical machine learning algorithms usually have stronger fitting and predictive abilities; Compared with deep learning techniques, classical machine learning techniques usually have more concise models, entail easier parameter tuning, and require less training data to achieve satisfactory results.

However, to the best of our knowledge, no attention has been given to designing password guessing models based on classical machine learning techniques. Particularly, there has been no satisfactory answer to the following key questions: (1) Can classical machine learning techniques be used to design password guessing models? (2) If it is possible, how can these techniques be used for typical guessing scenarios? (3) Whether password guessing models based on classical machine learning techniques can improve the attacking success rate while reducing the computational overhead? In this paper, we aim to provide concrete answers to these key questions. Though applying classical machine learning techniques to password guessing looks deceptively simple, it is actually rather challenging. Now we explain why.

Firstly, passwords are essentially short texts and have the following characteristics that differ significantly from traditional NLP tasks: (1) A password is usually composed of 6$\sim$30 characters [34, 53], which is much shorter than standard NLP texts; (2) A password is a piece of artificially constructed sensitive text, which may contain rich semantics, but it is not limited by (and often deliberately deviated from) the syntactic structure of the ordinary text, such as the password `loveu4ever` (with the semantic love you forever); (3) For password guessing, it is required that the generated passwords can *precisely* match the target. This means any inconsistency will lead to the failure of password cracking. For example, we take `P@ssword123` as the target and generate a series of guesses that are very close to it but different, such as `password123`, `p@sswrod123`, `Password123`, etc. Though they are all similar to the targeted password, none of them constitutes a correct guess. This is particularly concerned in guessing scenarios where the number of guesses allowed is limited, e.g., online guessing [57], while online guessing is the primary security threat that normal users need to devote efforts to mitigate (see [12,22,57]). In contrast, some amount of ambiguity is allowed in traditional NLP tasks, as long as the ambiguity does not significantly impair understanding. Hence, classical machine learning techniques originally designed for NLP tasks (or computer vision) cannot be directly or easily used for password guessing.

Secondly, password guessing models based on deep learning ([28, 35, 43]) usually use one-hot encoding for password characters, and use neural networks to learn the internal connections of these characters automatically. However, classical machine learning techniques usually require manually extracting and constructing features (i.e., feature engineering). Thus, it is a considerable challenge to tackle the question of how to accurately characterize passwords, so that we can not only reflect the inherent properties of the characters, but also ensure the effectiveness of the machine learning algorithm.

We summarize our contributions as follows:

- **A new technical route**. We represent each password character in an n-order (e.g., n=4, 5, 6) string in four dimensions: $\langle$character type, the rank of the character (e.g., letter `a` is the first lower letter in `a`$\sim$`z`), keyboard row number, keyboard column number$\rangle$, and represent the entire n-order string in two additional dimensions: $\langle$position of the character in a password, position of the character in the current segment$\rangle$. These representations are *generic* and make the classic machine learning techniques (e.g., Random Forest and Boosting), for the first time, be successfully applied to password guessing.
- **A new PII matching algorithm**. To overcome the limitations of existing PII matching algorithms (i.e., using heuristic tags to represent PII usages in passwords [57]), we propose a new approximately optimal PII matching algorithm that more accurately captures users' PII usages, and can improve the success rates of leading guessing models by 7%$\sim$13%. We show the effectiveness of our algorithm through both theory and experiments.
- **Extensive evaluation**. We perform a series of experiments to demonstrate the effectiveness and general applicability of our models. Results show that the guessing success rate of our RFGuess is comparable to its foremost counterparts in trawling guessing scenarios, and is 7.03%$\sim$27.54% higher than its counterparts in targeted guessing scenarios based on PII.
- **Some insights**. When predicting the next character after the n-order strings in a password, RFGuess can clearly show the importance of each character in different dimensions (e.g., type/continuity/position-information). Such knowledge can help us optimize the model training and

[1]For simplicity of presentation, the term "machine learning" that appears in this work stands for the "classical machine learning".

password generation time by making easier the detection (and elimination) of password features with low importance, and also sheds light on the design of new machine learning based guessing models.

2 Background and related work

2.1 Three guessing scenarios

Trawling guessing. Trawling guessing means that the attacker does not care who the specific target is, and its only goal is to guess more passwords under the guess number allowed. In 2009, Weir et al. [59] proposed a fully automated password guessing algorithm based on a rigorous probabilistic context-free grammar (PCFG). First, the algorithm divides a password string into three categories: letter segment L, digit segment D, and special character segment S. Then, the password is transformed into a template structure (e.g., `Password123!` $\rightarrow$ $L_8D_3S_1$) and the corresponding terminals that fit into the structure (e.g., $L_8 \rightarrow$Password). Finally, the probability of a generated password is calculated according to the probability of its structure multiplied by those of its terminals. In this context, researchers have proposed a series of improved techniques, such as performing further semantic mining in passwords [50], adding keyboard and multiword patterns [29] and adaptive improvement for long passwords [25].

Unlike PCFG [59], which divides passwords into different segments according to the character type, the Markov model proposed by Narayanan and Shmatikov [37] trains the whole characters in a password, and calculates the probability of passwords through the connection between the characters from left to right. Particularly, the n-gram Markov needs to record the frequency of a character followed by a string of length n-1. Like PCFG, many researchers have conducted follow-up research on the Markov model. For example, Ma et al. [34] smoothed and normalized the Markov model to alleviate the problem of data sparseness and overfitting; Markus et al. [19] enumerated the passwords in descending probability order to improve the guessing speed.

At USENIX'16, Melicher et al. [35] first introduced deep learning techniques to password guessing. More specifically, they build a neural network composed of LSTMs (which are denoted as FLA, i.e., Fast, Lean, and Accurate). Compared with the traditional statistical password guessing models (e.g., PCFG [59] and Markov [34]), FLA has better cracking rate under relatively large guesses (i.e., $>10^{10}$). In 2019, Hitaj et al. [28] introduced generative adversarial networks (GAN) to password guessing, and proposed the PassGAN, which shows the potential of GAN's application in this field. After that, Pasquini et al. [43] alleviated the mode collapse problem of GAN during training, so that the cracking rate of GAN-based approaches under large guesses has been significantly improved. On this basis, they constructed two password guessing frameworks, that is, conditional password guessing (CPG) and dynamic password guessing (DPG). However, compared with statistics-based models (e.g., PCFG [59] and Markov [34]), CPG/DPG [43] generally requires extremely large training data (e.g., size$>10^7$), consumes longer training time, and suffers cumbersome parameter tuning.

Targeted guessing based on PII. The goal of a targeted password guessing is to crack the password of a given user in a given service (e.g., an online banking account, and personal mobile phone) as quickly as possible [57]. Thus, the attacker would use PII related to the target victim to enhance the pertinence of cracking. Overall, the current research on targeted password guessing is still in its infancy, mainly focusing on how to use demographic information (such as name, birthday and mobile phone number). In 2015, Wang and Wang [55] first proposed a targeted guessing model based on Markov [37] (namely Targeted Markov). Their basic idea is that the frequency of names in the training sets reveals the likehood of the targeted user choosing a name-based password. In 2016, Li et al. [32] proposed a targeted guessing model based on PCFG [59]. The difference with trawling PCFG is that some PII segments representing different lengths have been added to the original LDS segments. At CCS'16, Wang et al. [57] revealed the inherent limitation of length-based PII matching method, and proposed a new targeted guessing model with a *type-based* PII matching method, namely TarGuess-I.

Targeted guessing based on password reuse. At NDSS'14, Das et al. [17] proposed the first cross-site password-guessing algorithm based on transformation rules. This algorithm performs several artificially defined transformations (e.g., delete, insert, and leet) on users' existing passwords, and then generates guesses in a pre-defined order. However, users would hardly reuse/modify passwords in such a pre-defined unified approach, hence limiting its performance in the real world.

At CCS'16, Wang et al. [57] proposed a PCFG-based model for password reuse, namely TarGuess-II. The core idea is to characterize users' password reuse behaviors in two levels of modification operations (i.e., structure- and segment-level). During training, it first learns the probability of the two-level transformation path of sister password pairs to build a PCFG. Second, the guess with the highest probability in the PCFG is output each time through the priority queue, and then they are transformed and inserted into the priority queue again. In this way, the guesses sorted by probability can be obtained.

At IEEE S&P'19, Pal et al. [40] proposed Pass2Path, a targeted guessing model for password reuse based on deep learning. More specifically, it employs a sequence-to-sequence (seq2seq) model [46] to predict the path of modifications needed to transform one password into its sister password. Its guessing success rate is better than that where the input and output of the model are directly the user's original password and the new password, respectively. In other words, this way of training focuses the model better on learning common transformations found in password datasets.

2.2 Password guessing modeling

The Markov n-gram model was originally introduced at CCS'05 [37] and improved at IEEE S&P'14 [34]. Generally, n is recommended to be 3, 4, or 5 [34,56]. Its core assumption is that: Each character is only related to the first d characters in front of it and has nothing to do with other characters, where $d(=n+1)$ is the order of the Markov model. The conditional probability for character c_i following the string $c_1c_2\dots c_{i-1}$ is

$$\begin{aligned}\Pr(c_i|c_1c_2\cdots c_{i-2}c_{i-1}) &= \Pr(c_i|c_{i-d}\cdots c_{i-1}) \\ &= \frac{\texttt{Count}(c_{i-d}\cdots c_{i-1}c_i)}{\texttt{Count}(c_{i-d}\cdots c_{i-1}\cdot)},\end{aligned} \tag{1}$$

where $\texttt{Count}(c_{i-d}\cdots c_{i-1}c_i)$ denotes the number of occurrences of the string $c_{i-d}\cdots c_{i-1}c_i$, and $\texttt{Count}(c_{i-d}\cdots c_{i-1}\cdot)$ denotes the number of occurrences of the string $c_{i-d}\cdots c_{i-1}$ where it is followed by an undetermined character (i.e., where it is not at the end of a string). Then the probability of the string $s=c_1c_2\cdots c_n$ is given by:

$$\begin{aligned}\Pr(s) &= \Pr(c_1)\Pr(c_2|c_1)\cdots\Pr(c_n|c_{n-1}c_{n-2}\cdots c_1) \\ &= \prod_{i=1}^{n}\Pr(c_i|c_{i-d}\cdots c_{i-1}).\end{aligned} \tag{2}$$

In reality, while each character in a password may have varying degrees of security impact on other characters [41], this paper assumes that the order in which users create passwords is from left to right (i.e., the same order with how they type passwords), and each character is only related to a few characters before it (This means our model makes the same assumption with the well-known Markov model [34,37]). Under this assumption, the password generation process can be regarded as a *multi-class classification problem*.

More specifically, given a password, the n-order string in the front of each of its character can be seen as the target to be classified (and features can be extracted from this n-order string), and the character itself can be seen as the classification label corresponding to the string to be classified. From this perspective, all supervised learning algorithms that tackle multi-classification problems can be applied to password guessing. Considering that when the data dimension is low and the task accuracy required is high (which are exactly the characteristics of password guessing tasks), ensemble learning methods generally performs well (see the potential applicability of some representative classification algorithms in Appendix A of the full paper at `https://bit.ly/41w5M0b`). Without loss of generality, in what follows, we take Random Forest as a typical case study to show how to employ classical machine learning techniques for password guessing.

Assume that $\mathbf{T}=\{(x_1,y_1),(x_2,y_2),...,(x_n,y_n)\}$ is the training set, then we can build a mapping f from the input space $\mathbf{X}$ to the output space $\mathbf{Y}$ by learning $\mathbf{T}$. Here $\mathbf{X}=\{n\text{-order strings of a password set}\}$, $\mathbf{Y}=\{95 \text{ printable ASCII codes}\}\cup\{E_s\}$, i.e., 96 different categories, where E_s denotes the end symbol.

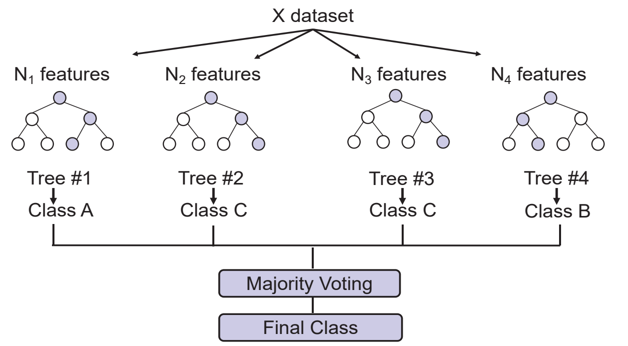


Figure 1: A high-level example of random forest [14]. Here, $\mathbf{X}$ is all the n-order strings of a training dataset, $N=\{N_1,N_2,...,\}$ is a randomly extracted feature subset, and class {A, B,...} represents the category (95 printable ASCII codes and the end-symbol) to which each n-order string belongs.

2.3 Introduction of random forest

Random forest [14] is a an ensemble learning method for classification (and regression) that consists of multiple decision trees [44]. When predicting the category of a sample, the algorithm counts the prediction results of each tree in the forest, and then selects the final result by voting (see Fig. 1). "Randomness" lies in two aspects: the random selection of features and the random selection of samples. Hence, each tree in the forest has both similarities and differences.

Formally, we denote the decision tree model as $\{h_k(\mathbf{X}), k=1,2,3,...\}$. Given an independent variable x in $\mathbf{X}$ dataset, each decision tree has one vote to select the optimal classification result. The final classification decision is:

$$\mathrm{H}(x) = \arg\max_{y\in\mathrm{Y}} \sum_{i=1}^{k} \mathrm{I}(h_i(x)=y), \tag{3}$$

where $\mathrm{H}(x)$ represents the combined classification model (i.e., the random forest), h_i is a single decision tree, $y\in\mathrm{Y}$ is the output, and $\mathrm{I}(\cdot)$ is the characteristic function.

The decision tree [44] has three mainstream node splitting algorithms: ID3, C4.5 and CART. These algorithms use different feature selection criteria, namely, information gain, gain ratio and Gini impurity. Among them, the Gini impurity represents the probability that two samples are randomly selected from the dataset and their categories are different. It has a relatively small calculation cost and is easy to understand. Therefore, this paper uses the CART decision tree (see Fig. 2). For a dataset D (composed of n-order strings), the calculation formula of the Gini impurity is as follows:

$$\mathrm{Gini}(D) = \sum_{k=1}^{|y|}\sum_{k'\neq k} p_k p_{k'} = 1-\sum_{k=1}^{|y|} p_k^2, \tag{4}$$

where $|y|$ represents 96 classification categories (i.e., 95 printable characters and the end-symbol E_s), and p_k represents the proportion of the category k in D. When dividing features, the Gini impurity of feature a (the detailed feature construction method of n-order strings can be seen in Sec. 3.1) is:

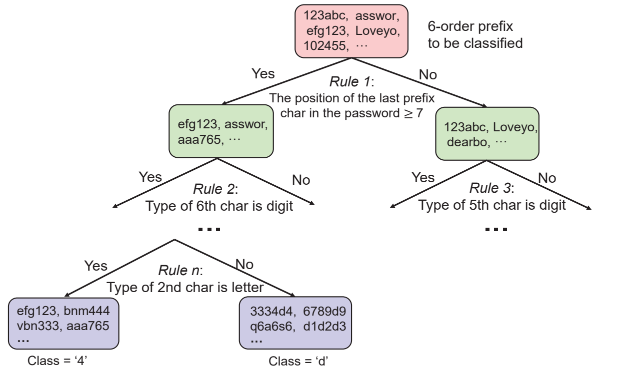


Figure 2: A high-level example of a decision tree for password prefix classification. The node division is determined according to the corresponding rules through the if-else logic, and finally, each prefix is divided into the character category to which it belongs. For example, class=`4` means that all prefixes in this leaf node are followed by the character `4` like `efg1234`.

$$\mathrm{Gini}(D|a) = \sum_{v=1}^{V} \frac{|D^v|}{|D|} \mathrm{Gini}(D^v), \tag{5}$$

where v represents each value of feature a, and D^v represents the subset of D divided according to the value v. Formula 5 indicates that when selecting features, the weighted average method is used to calculate the total Gini impurity, and finally, the feature that minimizes the Gini impurity after division is selected as the optimal division feature.

2.4 Analysis of random forest

Now we explain why the random forest model [14] can solve the shortcomings of the Markov n-gram model [37] when applying to password guessing from three aspects.

The fitting principle. Fig. 3 shows that the Markov n-gram model [37] can essentially be seen as a decision tree [44] divided by prefix string of height one. It divides all strings with the same prefix into the same leaf node, resulting in that when the prefix string appears very rarely in the training set (i.e., data sparseness issue), it can only be classified according to the few samples that appear in the training set. In comparison, the decision tree divides its node according to the *impurity* (representing how well the trees split the data, and there are several impurity measures like the Gini impurity as defined in Sec. 2.3.) of each feature (i.e., division rules) in the prefix. It selects the feature with the least impurity as the rule of feature division, which makes the final sample meeting the same division rule fall to the same leaf node. These samples can be regarded as similar samples with the same classification results (see Fig. 2 for a high-level example). Thus, the prefixes that appear less frequently or do not appear in the training set can also be divided into leaf nodes composed of similar samples.

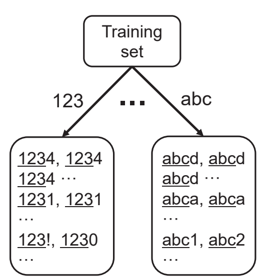


Figure 3: Tree diagram of the Markov model [37]. Here we take 3-order as an example.

Automatic feature screening. The most critical parameter in the Markov model [37] is the order d, which is the length of the prefix that needs to be considered. When the order is too high, the model is easy to overfit [34]. However, this is not a problem for the random forest [14]. Specifically, the decision tree [44] selects the feature with the smallest impurity (after splitting) as the division rule. That is, it will select features with a higher degree of importance for division, and will not be affected by those with poor division effects. For example, the string `1234` followed by the character `5` is a natural law and should not be changed due to the training set, so the substring `1234` is more important than the whole string `#1234` when predicting the next character, while the 5-order Markov model only considers the frequency of `#1234`.

Minimum number of samples in each leaf node. For samples that appear less frequently or have never appeared before, the decision tree [44] will divide the samples into a specific leaf node according to the training rules. Since the samples that meet the same set of rules have the same classifications, the probability of each category will be obtained according to the distribution of the sample categories in the leaf nodes. When the number of samples in the leaf node is large, the decision tree [44] can smooth the samples well; when the number of leaf nodes is small, or even if there is only one sample in a leaf node, this situation degenerates to the Markov model with the low-frequency prefix problem. Fortunately, the decision tree can reasonably solve this problem by limiting the minimum number of samples in leaf nodes.

3 RFGuess: A new trawling guessing model based on random forest

3.1 Password character feature construction

To construct a password guessing model based on classical machine learning techniques, feature engineering is an essential step. A password is usually composed of characters and has two important characteristics: the type of characters and the continuity of characters. Particularly, there are three types of characters used in passwords: digits, letters, and special characters. Each type of character has a certain internal continuity, such as 0∼9 and a∼z. Therefore, to well represent these two characteristics of characters in a password, we need to *re-encode* the password characters.

We first represent the password characters in two dimensions. One is the character type. Here we use 0, 1, 2, and 3 to represent special characters, digits, uppercase letters, and lowercase letters, respectively; the second is the serial number of the characters in each type. For example, letters `a`∼`z` are represented by 1∼26, digits `1`∼`9` represented by number 1∼9, and digit `0` represented by 10 (since 0 stands for the beginning symbol). In this way, the type and continuous characteristics of password characters can be displayed explicitly.

Secondly, keyboard pattern is a popular way to create passwords [57, 62], so the characteristics of keyboard pattern are also considered in the feature construction. The keyboard pattern usually means creating passwords through adjacent keyboard positions, such as `1qa2ws` and `123qwe`. Thus, we also use two-dimensional features to represent the keyboard characteristics of password characters: the row and column position of the keyboard in the form of coordinates. For example, 1 is represented as $(1,1)$, q is represented as $(2,1)$, s is represented as $(3,2)$. Thus, the position coordinate representation can clearly show the continuous characteristics of the characters and improve the model fitting ability.

The last consideration is the length characteristic of the string. More specifically, we construct two length features: position of the character relative to the entire password (i.e., trained length) and position of the character relative to the current segment (i.e., trained length in the current L/D/S segment). Considering that the password length of most users is at least six [34, 53], we set the order of our model to six. That is, we use a 6-order prefix to predict the next character.

As a result, every 6-order prefix can be represented by a 26-dimensional feature vector (26=4×6+2), because there are 6 prefix characters, 4 feature dimensions for each character and 2 additional feature dimensions for the length information of the entire prefix. We take the 6-order prefix `wer654` of password `qwer654321` as an example. First, each character in `wer654` can be *uniquely* represented as a 4-dimensional feature vector. For instance, character `r` is represented as (3, 18, 2, 4), where 3 represents the character type of lowercase letter, 18 is the rank of `r` in the lower letter sequence `a`∼`z`, 2 and 4 are the keyboard row and column positions of `r`, respectively. Now, `wer654` can be represented by a 24-dimensional feature vector (24=4×6). Then, we add 2-dimensional length feature (7, 3) of prefix `wer654`, where 7 represents the position information relative to the entire password (i.e., digit `4` in `wer654` is the 7th character of `qwer654321`), and 3 represents the position information relative to the current digit segment (i.e., digit `4` in `wer654` is the 3th character of segment `654321`).

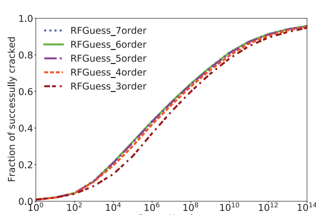


Figure 4: Impacts of varied orders (1M Rockyou→Rockyou_rest).

Note that, we have tested a number of different order values (i.e., n=3, 4, 5, 6, 7) of our RFGuess, and found that when $n \geq 4$, RFGuess can achieve similar cracking success rates (as shown in Fig. 4). Generally, when the order decreases (e.g., n=3), the number of features (i.e., $4n+2$) decreases accordingly, which may make RFGuess underfit. While when the order is too large (e.g., $\geq$7), passwords whose length is smaller than this value cannot be well modeled. Since the cracking success rate is slightly better when n=6, we set n=6 in the following experiments.

3.2 Feature importance analysis

To verify the effectiveness of the constructed features, the feature importance scores are calculated by random forest in different training datasets. According to the results shown in Figs. 10 and 11 of Appendix E (and Fig. 11 in the full version of this paper), we find that the trained length feature (i.e., position of the last prefix character in the password) has the highest score, indicating its significant impact on fitting RFGuess. Other top-ranked features are mainly characters that are closer to the target character. Among the four different dimensional features of the same character, the serial number feature (e.g., `a` is the first in alphabetic types `a`∼`z`, 0 is the first of digits 0∼9) and the keyboard column number feature are more effective, while the type of character (letter/digit/special character) and the trained length of current segment features (position of the character in the L/D/S segment) are relatively unimportant, and keyboard row number offers little gain on the model fitting. A plausible reason is that when building passwords, users create more horizontal keyboard modes (e.g., `qwerty`) than vertical modes (e.g., `1qaz`) [62]. Particularly, we have counted the Top-10 most frequency keyboard patterns of CSDN, Dodonew, Taobao, and Rockyou, and found that the Top-10 patterns are either horizontal keyboard modes or just the repetition of a single character (e.g., `aaaaaa`).

3.3 Model training and password generation

At a high level, our RFGuess is similar to the Markov 7-gram model [37]. More specifically, it first processes the password into the form of 6-order character prefixes and their corresponding characters (e.g., the resulting 6-order set of password `abc123` is $\{(B_sB_sB_sB_sB_sB_s,a),(B_sB_sB_sB_sB_sa,b),...,(abc123,E_s)\}$, where B_s and E_s stand for the beginning and ending symbol respectively). Then, it represents the 6-order prefix as a 26-dimensional vector (each character is represented by 4 dimensions, plus two additional length features for the entire prefix), the single character following this prefix in an ASCII value, and the beginning and ending symbol are represented by 0 and -1, respectively. When training the model, RFGuess traverses the 6-order set of each password in the training set, takes the 26-dimensional prefix feature vectors as training input, and takes the numerical label of the corresponding characters as training output. Fig. 2 shows a high-level example of the decision tree classification process.

The process of guess generation is quite similar to the Markov n-gram model [34]. The key difference is that we do not use the Bayes formula when calculating the conditional probability, but use the trained random forest to get this value. More specifically, each decision tree will vote on which category (one of the 95 characters and end-symbol) the input sample (i.e., the 6-order string prefix) belongs to, and its probability is the proportion of the number of votes obtained by this category to the total number of trees. For example, suppose there are 10 decision trees in the random

Table 1: Basic information about our 13 password datasets.†

Dataset	Web service	Language	When leaked	Total PWs	Length>30	Removed %	Unique PWs	With PII
Taobao	E-commerce	Chinese	Feb., 2016	15,072,418	88	0.01%	11,633,759	
126	Email	Chinese	Oct., 2015	6,392,568	621	0.23%	3,764,740	
Dodonew	E-commerce	Chinese	Dec., 2011	16,283,140	13,4758	0.15%	10,135,260	
CSDN	Programmer	Chinese	Dec., 2011	6,428,632	0	0.01%	4,037,605	
Wishbone	Social	English	Jan., 2020	10,092,037	250	0.01%	5,933,902	
Mate1	Dating website	English	Mar., 2016	27,401,505	12,430	0.06%	11,916,080	
000Webhost	Web hosting	English	Oct., 2015	15,299,907	4,159	0.76%	10,526,769	
Yahoo	Web portal	English	July, 2012	453,491	0	2.35%	342,510	
LinkedIn	Job hunting	English	Jan., 2012	54,656,615	17,162	0.22%	34,282,741	
Rockyou	Social forum	English	Dec., 2009	32,603,387	3,140	0.07%	14,326,970	
12306	Train ticketing	Chinese	Dec., 2014	129,303	129,303	0	117,808	✓
ClixSense	Paid task platform	English	Sep., 2016	2,222,045	0	0	1,628,018	✓
Rootkit	Hacker forum	English	Feb., 2011	69,330	5	0.01%	56,835	✓

†PW stands for password, and PII for personally identifiable information. We clean up passwords longer than 30 or containing non-ASCII characters.

forest voting on the string prefix "123456". Among them, 6 votes are cast for the character "7", 3 votes for the character "a", and 1 vote for the character "6". Then the probabilities of the entire string (6-order prefix plus a single character) are {"1234567": 0.6; "123456a": 0.3; "1234566": 0.1}.

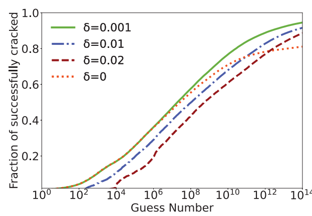


Figure 5: Impacts of varied values of δ (0.1M Rockyou→Rockyou_rest).

Our exploratory experiment shows that in the process of generating 1.8 million (M) guesses (training with 6M CSDN passwords using 30 decision trees), an average of 70% of the characters do not get a vote in one-step prediction, constituting the majority of the alphabet. This indicates that RFGuess may not be good at generating previously unseen characters.To address this issue, we employ the add-δ smoothing technique [34] to smooth characters that do not get a vote. For example, $\Pr(\#|123456) = \frac{\Pr_{\text{RFGuess}}(\#|123456)+\delta}{1+\delta\cdot|\Sigma|}$ (where $\Pr_{\text{RFGuess}}(\#|123456)$ means the probability of # calculated by RFGuess when the input string is 123456, and Σ is the character table of the training set). We have tested a number of values of δ (e.g., 0, 0.01, 0.02, 0.001), and found δ=0.001 is the best among all (see Fig. 5).

3.4 Experimental setups and results

Datasets. We evaluate the existing password guessing approaches and our RFGuess model based on 13 large real-world password datasets (see Table 1), a total of 241.27 million(M) passwords. Eight of our password datasets are from English sites and five from Chinese sites. As Table 1 shows, three datasets (i.e., 12306, ClixSense and Rootkit) are originally associated with various kinds of PII (e.g., name, birthday, email). To enable extensive targeted guessing evaluation, we match the *non*-PII-associated password datasets with these three PII-associated ones through email, and this produces a total of six PII-associated password datasets (see Table 2). For targeted guessing based on password reuse, we obtain eight password pair datasets by matching email (see Table 4).

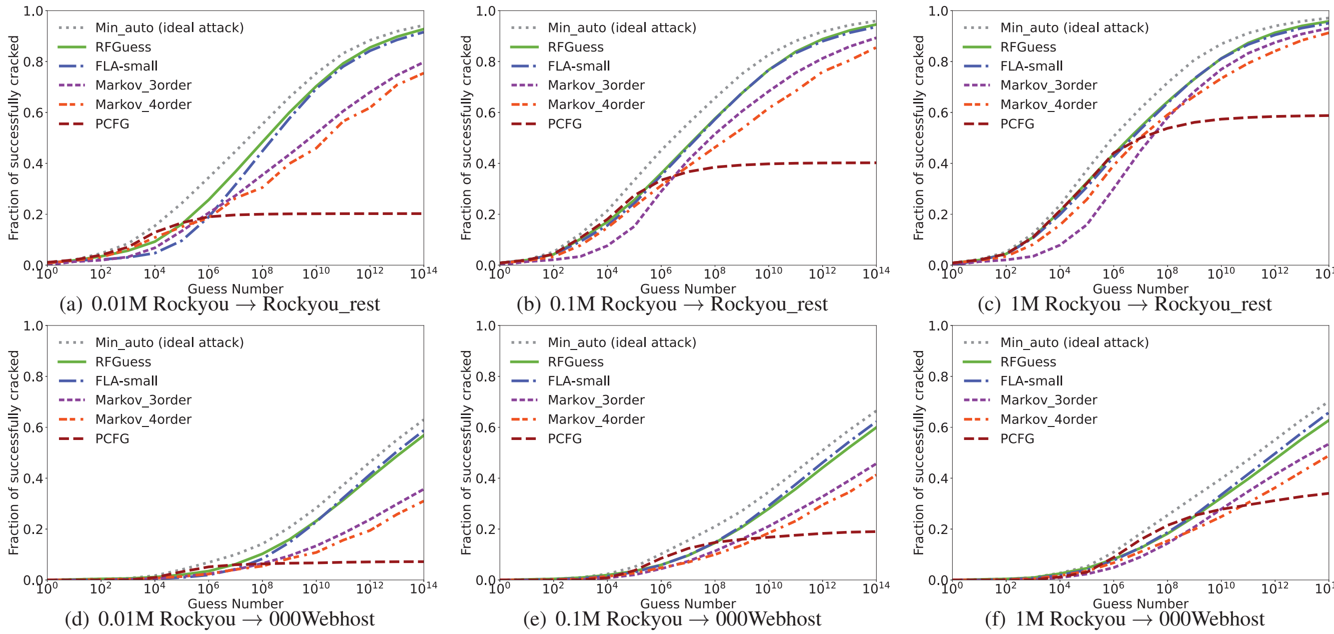
Ethical considerations. Though ever publicly available on the Internet and widely utilized in existing studies [17, 40, 42, 43, 57], these datasets are private data. Hence, we only illustrate the aggregated statistical information and keep each individual account as confidential in order to avoid bringing additional risks to the corresponding victim. While these datasets may be misused by attackers for cracking, our use is both beneficial for the academic community to understand the strength of users' password choices and for security administrators to prevent creating weak passwords. As our datasets are widely used and publicly downloadable on the Internet, this facilitates fair comparison and good reproducibility.

Experimental setup. To well establish the generality and effectiveness of our RFGuess, we evaluate it on both one-site (intra-site) and cross-site guessing scenarios. For intra-site scenarios, we randomly select 0.01M, 0.1M, and 1M (M=million) passwords from Rockyou as the training set, respectively, and randomly select 100,000 passwords from the remaining dataset as the test set. Since the attacker is smart and will constantly improve her training set to make it as close as possible to the test set (to improve her success-rates), our intra-site experimental methodology just reflects this situation (this methodology is quite routine in password research [54, 57, 59]). Particularly, many sites (e.g., Yahoo [39], Flipboard [4], Twitter [26] and Anthem [21]) have leaked their user passwords more than once, and thus it's practical/realistic to conduct/consider the intra-site guessing scenarios. For cross-site scenarios, we apply the trained model (on an older leaked dataset) to crack a newer leaked dataset (i.e., Rockyou→000Webhost and 000Webhost→Wishbone). Note that we do not remove the identical password pairs (i.e., direct reuse) that occur in the training sets from the test sets, because the attacker has no prior knowledge of which passwords are used by the target account, and excluding duplicate passwords from the test set hinders the evaluation of a guessing model's fitting ability. We discuss this point in detail in Sec. 6.

We compare RFGuess with three leading guessers (i.e., PCFG [59], Markov [34], and FLA [35]). Also, we introduce the Min_auto approach [49] to avoid the bias of a single approach. The setups of each approach are as follows.

PCFG. The PCFG we use is consistent with [34], that is, the probability of the L segment comes from the training set, which is better than the original version in [59].

Markov. For the Markov model, due to the great influence of order, this paper carries out the 3-order and 4-order experiments at the same time, and adopts the Laplace smoothing



(a) 0.01M Rockyou → Rockyou_rest (b) 0.1M Rockyou → Rockyou_rest (c) 1M Rockyou → Rockyou_rest

(d) 0.01M Rockyou → 000Webhost (e) 0.1M Rockyou → 000Webhost (f) 1M Rockyou → 000Webhost

Figure 6: Guessing performance of our RFGuess in comparison with other approaches (i.e., PCFG [59], 3/4-order Markov [34], FLA [35] and Min_auto [49]) in the intra-site and cross-site trawling guessing scenarios. Note that Min_auto [49] represents an *idealized* strategy: A password is considered cracked as long as any of these five real-world password models cracks it. Rockyou_rest means the original Rockyou dataset excluding the corresponding training set.

and end symbol regularization as used in [34].

FLA. We use the source code of FLA [35], and follow its recommended parameters in our experiments. More specifically, we train a model consisting of three LSTM layers with 200 cells (namely the "small" model in [35]) in each layer and two fully connected layers, a total of 20 epochs.

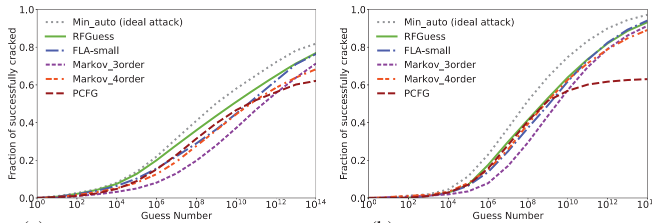
RFGuess. As detailed in Appendix A, we train a random forest with 30 decision trees. Its minimum number of leaf nodes is 10, the maximum ratio of features is 80%, and the rest are in default of the scikit-learn framework [2].

Min_auto. It represents an idealized guessing approach [49], in which a password is considered cracked as long as any of these real-world guessing models cracks it.

Experimental results. Since explicitly enumerating large guesses is computationally intensive, we use the Monte-Carlo algorithm [18] to reliably estimate a password's guess number. That is, how many guesses it would take for an attacker to arrive at that password when password guesses are attempted in descending order of likelihood. Fig. 6 shows the results. To accurately show the attack success rates of different approaches, we give the concrete result values at some specific guess numbers (i.e., 10^7 and 10^{14}; see Table 10 at `https://bit.ly/41w5M0b`). In intra-site guessing scenarios, RFGuess performs slightly better than FLA [35], and beats PCFG [59] and Markov [34] beginning at around 10^7 guesses. In cross-site scenarios, the guessing success rates of RFGuess are slightly worse than FLA [35] within 10^{14} guesses, but are significantly higher than PCFG [59] and Markov [34].

To demonstrate the generality of RFGuess, we evaluate it with larger training datasets (i.e., 75% 000Webhost of size 11,474,930). Fig. 7 shows that, when using a ten million-sized training set, RFGuess outperforms all its counterparts in intra-site guessing scenarios, and is slightly better than (or comparable to) its counterparts in cross-site guessing scenarios. This suggests that RFGuess is better at modeling the guessability of passwords from the same (or similar) distribution. By employing the same training and test set (i.e., 75% of 000Webhost→25% of 000Webhost), we also compare RFGuess with dynamic dictionaries [42]. However, the success rate of dynamic password guessing (DPG) [42] is only 0.13% within 5×10^9 guesses (which are the maximum number of guesses that can be reached using 75% of 000Webhost). A plausible reason is that DPG is more suitable for extremely large training sets, and this partially explains why the original paper [42] uses the 1.4 billion-sized 4iQ as its training set. Our RFGuess is just on the opposite: It is particularly suitable for guessing scenarios where the training data is not abundant (e.g., passwords from sites beyond USA, China, and Russia).

We further make an apples-to-apples performance comparison of these approaches in three key criteria (i.e., training time, model size, and time to generate guesses), and summarize the comparison results in Table 6 (see Appendix B for details). In all, RFGuess has relatively high training efficiency (it only takes 0.3 hours to train five million data), but it has relatively large model size (i.e., 4.5G when the compress parameter in the joblib tool is set to three), and its guess generation is relatively slow (about 130∼677 passwords/s). This makes RFGuess particularly suitable for online password guessing attacks where the number of guesses allowed is small. In practice, online password guessing is the



(a) 75% 000Webhost→25% 000Webhost (b) 75% 000Webhost→Wishbone

Figure 7: Evaluate our RFGuess using 75% 000Webhost of size 11,474,930.

most concerning (and unmatured) scenario regarding password security [7, 40, 57], because offline guessing can be well eliminated by slow/memory-hard hashes (e.g., Bcrypt and Argon2), but online guessing is unavoidable and its success-rate is rather high (see Tables 3 and 5) even if there are rate-limiting/blocking mechanisms. This is because the guess number allowed for an attacker cannot be too small, otherwise the system will suffer from DoS attacks, which explains why 100 in one month is recommended by NIST-SP800-63B [24].

If one wants to improve the password generation efficiency of RFGuess, she can set the number of trees to one (i.e., use the decision tree model). At this time, the password generation speed can be increased to 1,520 passwords/s, while the attack success rate is reduced by about 0.4%∼2% (see Fig. 9).

Insights. To understand the impacts of features, we remove the relatively unimportant 5-, 10-, and 15-dimensional features according to the feature importance ranking, and remove 4-, 8-, and 12-dimensional features according to the character position information (e.g., the 4-dimensional features of character `123` in prefix `123456` are removed in turn). Results show that the training time and password generation speed of our RFGuess are improved by up to 35%, while the success rates remain stable (see Fig. 8).

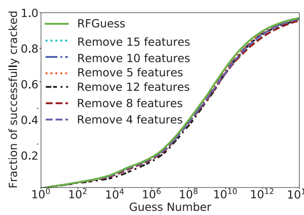


Figure 8: Impacts of varied features on RFGuess (Taobao→Taobao_rest).

Thus, when designing new password guessing models based on classical machine learning techniques, one can create as many new features as possible (e.g., the number of character types contained in the prefix, the Shannon entropy of the prefix, etc.) to explore more effective password representation. Then, the most effective features can be figured out by measuring the feature importance score and/or success rates. This improves the training efficiency while maintaining the success rates, which makes our RFGuess highly scalable.

4 RFGuess-PII: A targeted password guessing model based on PII

We now use random forest [14] to design a targeted password guessing model based on PII, called RFGuess-PII. We first analyze the limitations of the PII matching strategy used in current targeted guessing models, and then propose a more effective PII matching algorithm. Based on this algorithm and the RFGuess model in Sec. 3, we propose RFGuess-PII and demonstrate its effectiveness through large-scale experiments.

4.1 Problems in mainstream methods

Previous PII matching methods. Li et al. [32] first proposed a PII matching method similar to PCFG [59] (for example, N_4 represents name information with a length of four like `Wang`). At CCS'16, Wang et al. [57] pointed out that this method has severe limitations. Instead, they introduced a series of *type-based* PII tags and achieved drastically better results. More specifically, they use N standing for name usages, while N_1 for the usage of full name, N_2 for the abbr. of full name,$\cdots$; U stands for username usages, U_1 for full username, U_2 for the letter segment of the user name,$\cdots$. We summarize these notations in Table 6 of our full version paper.

In the process of training, the leftmost and longest matching strategy is adopted for disambiguation when matching the PII contained in the passwords. For example, if a user's username is `Alice0102`, name is `Alicexxx`, birthday is `19930102`, and password is `Alice01021993`, then according to the leftmost and longest matching strategy used in [57], it should be represented as $\mathsf{U}_1\mathsf{B}_5$ instead of $\mathsf{N}_3\mathsf{B}_2$ (where B_5 represents the birthday year, N_3 represents the full name of the surname, and B_2 represents the birthday in the MY format), because the username `Alice0102` will be matched first.

This matching strategy uses a greedy strategy to first match the longest PII at the leftmost position, and it is not optimal. "Optimal" here refers to the *global* optimum for the entire training password set rather than the local optimal for a single password. To explain the concept of global optima more clearly, we introduce information entropy for analysis. Shannon Entropy [45] metric is proposed in 1948 to measure the uncertainty of a distribution. The greater the information entropy, the more random the password distribution, and the more secure the password set. Thus, for the same password set, the feature extraction and representation method that makes the password set's information entropy lower can better make use of the characteristics of the training set.

4.2 New PII matching algorithm

The current strategy for PII matching is not optimal because there will be ambiguities (multiple representations for the same password) when matching, and as in the above example, using the leftmost and longest matching strategy would result in heuristically selecting one option for PII tagging. This cannot minimize the information entropy. In other words, it cannot entirely and accurately extract the PII usage behavior of the entire user group. To address this issue, we propose an approximately optimal PII matching algorithm.

The first step of our proposed algorithm is similar to the type-based PII matching method [57], which subdivides the various possible transformations of PII and use different tags

Table 2: Basic information about our PII datasets.

Dataset	Language	Items num	Types of PII useful for this work
12306	Chinese	129,303	Email, User name, Name, Birthday, Phone
CSDN	Chinese	77,216	Email, User name, Name, Birthday, Phone
Dodonew	Chinese	161,517	Email, User name, Name, Birthday, Phone
ClixSense	English	2,222,045	Email, User name, Name, Birthday
000Webhost	English	79,580	Email, User name, Name, Birthday
Rootkit	English	69,418	Email, User name, Name, Birthday

to represent them. Notably, we use digital tags instead of letter tags (e.g., $\mathsf{N}_1\sim\mathsf{N}_7, \mathsf{B}_1\sim\mathsf{B}_{10}$ in TarGuess-I [57]), and summarize these notations in Table 6 at `https://bit.ly/41w5M0b`. Thus, they can be conveniently used as input to the machine learning model for training. For example, starting from 1,000 to stand for name usages, where 1,000 for the usage of full name, 1,001 for the lowercase letter of last name,$\cdots$.

The second step is to list all the possible representations with PII tags for each of the passwords in the training set (e.g., three representations {4000, 2001}, {4001, 2003, 2004, 2001} and {1002, 2003, 2004, 2001} for `Alice01021993`). After that, we sort the representations by frequency from high to low. Specifically, the most frequent representation (e.g., {4000, 2001}) is denoted as R_1, the second is denoted as R_2 (e.g., {4001, 2003, 2004, 2001}),$\cdots$. Then, we use R_1 to represent all passwords that can be represented as R_1, and the frequency of each of their remaining representations (e.g., {4001, 2003, 2004, 2001} and {1002, 2003, 2004, 2001}) subtracts one. Next, the remaining passwords (remove those already represented by R_1) that can be represented as R_2 are all represented by R_2, and their frequency of the remaining representations continues to subtract one. The process repeats until the frequency of all remaining representations is less than or equal to one. Finally, the password whose representation has not been determined is represented by the shortest structure, and the algorithm ends. We formalize this process in Algorithm 1, and demonstrate its generality and effectiveness both theoretically and experimentally (see Appendix C for details).

4.3 New targeted guessing model based on PII

Based on RFGuess proposed in Sec. 3 and the approximately optimal PII matching algorithm, we now propose a new targeted password guessing model RFGuess-PII. The password training and generating process is similar to the trawling guessing scenario. The difference is that the PII string in the password is replaced with the corresponding digital tag through PII matching, and then the password set containing PII tags is used for training. Also, the generated guesses may have PII tags, and they need to be replaced with the corresponding PII string of the target user to obtain a final guess.

Similar to the construction of character features in trawling guessing scenarios, we also use four-dimensional features to represent PII tags in targeted guessing scenarios. Specifically, we have used ⟨character type, the rank of this character in its type, keyboard row number, and keyboard column number⟩ to represent an ordinary character. For PII tags, they are similar to ordinary characters except for the lack of keyboard features. Therefore, we use ⟨PII type, PII serial number, 0, 0⟩ to represent PII tags. The last two 0s are to align with the four-dimensional features of ordinary characters.

4.4 Experimental setups and results

Datasets. In Table 1, only 12306, ClixSense and Rootkit datasets are with PII (name, email, birthday, etc.). To enable extensive targeted guessing evaluation, we match the non-PII-associated datasets with these PII-associated ones through *email*, and this produces six PII-associated password datasets (i.e., PII-12306, PII-CSDN and PII-Dodonew, PII-ClixSense, PII-000Webhost and PII-Rootkit; See Table 2). Among them, Rootkit is a hacker forum, and 000Webhost is a free web hosting site and is mainly used by web administrators. Therefore, the users of both sites are likely to be more security-savvy than normal users, and this has been observed in [57]. We use these six PII-associated datasets to conduct six comparative experiments. In each experiment, half of each dataset is used as the training set, and the other half is used as the test set as recommended in [15, 54, 57] (see Table 3).

Approaches for comparison. The current mainstream targeted guessing models employing PII mainly include the TarGuess-I [57] based on PCFG [59] and the Targeted-Markov [55] based on the Markov model [34]. Note that the original Targeted-Markov proposed by Wang et al. [55] exploits only name information, but it can be easily extended to incorporate user name, birthday, email, etc. For a more comprehensive comparison, we apply our proposed PII matching algorithm to FLA [35], leading to FLA-PII. To our knowledge, this is the first time that FLA can capture PII semantics.

More specifically, we first identify the PII in a password, and encode it to a one-dimensional array based on the dictionary order (e.g., `wang666`→[1001, 6, 6, 6], where 1001 and 6 are the numerical labels corresponding to the surname and the digit 6 in the dictionary, respectively.). Here, we use *an embedding layer* rather than the canonical one-hot encoding layer to reduce the sparsity of the embedding vector due to the large size of PII tags. Then, the embedded vector is fed into LSTM neural networks. Finally, the dense layer converts the hidden layers into the output size. The output is the possible subsequent labels with probabilities, and FLA-PII chooses the next label with the highest probability. Here we set the embedding size to 128, and the remaining parameters are completely consistent with trawling FLA [35] in Sec. 3.4.

Note that, theoretically, an online guessing attacker can only perform very limited guessing attempts if the protection measures (e.g., lockout, rate-limiting [20]) are deployed on the server. For instance, NIST requires that "the verifier (server) *shall* limit consecutive failed authentication attempts on a single account to no more than 100" [24]. However, in reality, as revealed in [33], 72% of the top 182 websites "allow frequent, unsuccessful login attempts without account lockout or login throttling". Overall, the system has to balance

Table 3: Comparison of four PII-based models.†

Experimental setup: Guessing scenario	Guess #	RFGuess-PII	4-order Tar-Markov [55]	Tar-Guess-I [57]	FLA [35]-PII
50% PII-12306 ↓ 50% PII-12306	10	**11.19%**	11.00%	10.60%	8.41%
	10^2	**21.37%**	20.91%	20.30%	17.47%
	10^3	**28.89%**	28.20%	26.30%	24.01%
	10^7	**52.75%**	42.00%	44.79%	50.51%
	10^{14}	**98.42%**	87.68%	48.12%	97.50%
50% PII-CSDN ↓ 50% PII-CSDN	10	**21.24%**	20.13%	21.20%	15.94%
	10^2	**28.23%**	27.01%	27.90%	21.96%
	10^3	**33.30%**	32.96%	33.00%	26.97%
	10^7	**53.14%**	46.94%	42.23%	52.85%
	10^{14}	**94.68%**	80.74%	44.00%	94.51%
50% PII-Dodonew ↓ 50% PII-Dodonew	10	**9.54%**	9.52%	9.40%	6.07%
	10^2	**20.45%**	20.33%	19.10%	16.00%
	10^3	30.21%	**30.29%**	26.50%	24.93%
	10^7	**61.21%**	59.62%	59.45%	60.72%
	10^{14}	**99.12%**	92.61%	64.86%	93.80%
50% PII-Clixsense ↓ 50% PII-Clixsense	10	**5.99%**	5.87%	4.90%	4.12%
	10^2	**9.51%**	9.05%	7.70%	7.67%
	10^3	**13.48%**	12.06%	11.70%	11.15%
	10^7	**48.30%**	41.01%	43.48%	33.75%
	10^{14}	**92.38%**	85.33%	56.38%	82.60%
50% PII-Rootkit ↓ 50% PII-Rootkit	10	**6.96%**	6.77%	6.77%	3.97%
	10^2	**11.40%**	11.07%	10.46%	8.21%
	10^3	14.88%	**15.17%**	14.59%	12.45%
	10^7	**39.45%**	35.73%	27.73%	38.70%
	10^{14}	**89.81%**	76.01%	33.24%	86.91%
50% PII-000Webhost ↓ 50% PII-000Webhost	10	**3.86%**	3.75%	0.90%	1.76%
	10^2	**7.31%**	6.89%	6.10%	4.64%
	10^3	**10.88%**	10.52%	9.54%	7.71%
	10^7	25.56%	22.26%	**26.17%**	25.73%
	10^{14}	**77.10%**	60.45%	36.43%	70.60%

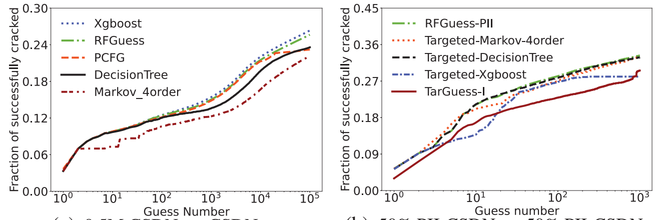
†A **bold** value (attack success rate) means that it is the highest one in each row.

online guessing attacks and denial-of-service (DoS) attacks. Without loss of generality, we set $T = 10^3$ as with mainstream online-guessing literature [40, 57] in our experiments.

In reality, there also exist offline attack scenarios that target specific users. For example, after obtaining a leaked password file, attackers will focus on some specific, most valuable accounts (such as celebrities, politicians, or specific common users deemed valuable/profitable), and devote more effort to them. In this case, the number of guesses will be limited only by the cost the attacker is willing to pay, which can be extremely large (e.g., $>10^{10}$). Thus, as recommended by [18], we also evaluate all the PII-models under larger guesses (i.e., 10^{14}) through the Monte-Carlo algorithm.

Experimental results. We design six targeted guessing scenarios, and the results are summarized in Table 3. For a more comprehensive comparison, we further use the guess-number-graph to evaluate the effectiveness of our RFGuess-PII with its counterparts, and put the results in Appendix C of our full version paper. For a fair comparison, all three counterpart targeted models (i.e., TarGuess-I [57], Targeted-Markov [55] and FLA [35]-PII) employ our improved PII matching algorithm. Results show that RFGuess-PII achieves a slightly better attack success rate in most cases within $10 \sim 10^3$ guesses. As the number of guesses increases, the superiorities of RFGuess-PII over its counterparts are enhanced. More specifically, RFGuess-PII outperforms its foremost counterpart (i.e., FLA-PII [35]) by 5.20%∼8.36% within $10^7 \sim 10^{14}$ guesses.

Further exploration. We now show that our representation of passwords can be easily transferred to other machine learning algorithms. More specifically, we replace the random forest with Xgboost [16]/DecisionTree (We simply replace the `RandomForestClassifier` class in our script with `Xgboost` and `DecisionTreeClassifier` with all the remaining processing flows unchanged), and perform two exploratory experiments in both trawling and targeted guessing scenarios. Fig. 9 show that attack success rates of Xgboost and DecisionTree (and also Targeted-Xgboost and Targeted-DecisionTree) are comparable to state-of-the-art models. Notably, their parameters can be better tuned for potential optimization, and we leave further exploration as future work.



(a) 0.5M CSDN → CSDN_rest (b) 50% PII-CSDN → 50% PII-CSDN

Figure 9: Using Xgboost [16] and decision tree for password guessing: (a) trawling guessing; (b) targeted guessing based on PII.

5 RFGuess-Reuse: A new targeted guessing model based on reuse

We now focus on modeling users' password reuse behavior. Based on our RFGuess in Sec. 3, we first design a targeted guessing model called RFGuess-Reuse, and then conduct large-scale experiments to demonstrate its effectiveness.

5.1 New targeted password guessing model based on reuse

We now describe how the random forest model can be used for password reuse-based scenarios. Inspired by TarGuess-II [57], we also consider both structure-level and segment-level transformations. First, we count structure-level transformations like $L_8S_2 \rightarrow L_7D_3$) by calculating the editing matrix for each password pair in the training set. Then we train a segment-level transformation (i.e., a transformation within a string of the same type, e.g., `password`→`passwor` in letter segment) model based on random forest. The formula for calculating the probability of generating a new password is

$$\Pr(pw_1 \rightarrow pw_2) = \left(\prod_{i=1}^{n} \Pr(Pt^i_{pw_1 \rightarrow pw_2})\right) * p_n, \qquad (6)$$

where $Pt^i_{pw_1 \rightarrow pw_2}$ stands for a specific transformation operation (e.g., inserting the digital structure `123`) from pw_1 to pw_2, and p_n represents the probability of ending after n operations. For example, given a password `password!!`, Pr(`password!!`→`p@sswor123`)=Pr(`password!!`→`password`)∗Pr(`password`→`passwor`)∗Pr(`passwor`→`passwor123`)∗Pr(`passwor123`→`p@sswor123`)∗p_4, where Pr(`password!!`→`password`) (i.e., $L_8S_2 \rightarrow L_8$) and Pr(`passwor`→`passwor123`) (i.e., $L_7 \rightarrow L_7D_3$) are the probability of structure-level transformation, and can be obtained by statistics of password pairs in the training set; Pr(`password`→`passwor`) (i.e., delete a single character `d`) and Pr(`passwor123`→`p@sswor123`) (i.e., `a`→`@`) are the probability of segment-level transformation, and can be obtained by the trained random forest model; p_4 is the probability of ending after four transformations, and can also be obtained by statistics of the training set.

For structure-level transformation, we take the insertion of the structure `123` (i.e., D_3) at the tail of `passwor` as an example. Its probability is Pr(`passwor`→`passwor123`)= $\Pr(T_1) * \Pr(T_2) * \Pr(\texttt{123}|\mathsf{D}_3)$, where T_1 denotes the event "Insert structures at the tail of `passwor`", and $\Pr(T_1)$ can be obtained by counting the reuse behaviors in the training set according to the length distribution of the training set (see Table 11 in Appendix D); T_2 denotes the event "Insert the specific structure D_3", and both $\Pr(T_2)$ and $\Pr(\texttt{123}|\mathsf{D}_3)$ can be obtained by training a PCFG model [34].

For segment-level transformation, we consider four atomic transformations based on [57]: head insertion, head deletion, tail insertion, and tail deletion. For three types of segments (i.e., letters, digits, and special character), we train random forests in positive order and reverse order, respectively, and this generates 3×2 models in total. For example, when determining the probability of performing the tail insertion operation of `passwor`, we input `passwor` into the positive order letter random forest to obtain this conditional probability; when determining the probability of performing the head insertion operation, we input `rowssap` into the reverse order letter random forest to obtain this conditional probability.

We take the *positive order letter* random forest as an example, and consider the operations related to the last character. When training the password `password!!`, three behavioral characteristics need to be trained for the letter string `password`: inserting characters, unchanged, and deleting characters. For inserting characters, our model uses `assword` as the training input, and uses `d` as the training output; for unchanged, our model uses `ssword` as the training input, and uses the end character E_s as the training output; for deleting characters, our model uses `ssword` plus any letter as the training input and uses `-1` as the training output (i.e., the input is `sword*` and the output `-1`, where `*` can be any letter).

Here we give a toy example of how to calculate the probability of a segment-level transformation. Given a password `password!!`, it can be divided into two segments L_8 and S_2 (denoted as p_1,p_2), and we calculate the probability of deleting `d` at the tail of the first segment p_1 (denoted as event P_1^t) as $\Pr(P_1^t) = \Pr(S_1) * \Pr(S_2) * \Pr(S_3) * \Pr(S_4)$, where S_1 denotes the event "Perform segment-level transformation" , and $\Pr(S_1)$ can be obtained by counting the reuse behavior of the training set; S_3 and S_4 denote the event "Perform tail deletion operation on p_1" and the event "Delete character `d` at the end of p_1", respectively, and both $\Pr(S_3)$ and $\Pr(S_4)$ are calculated by the trained random forest model; S_2 denotes the event "Perform operation on p_1", and $\Pr(S_2)$ is calculated by $\frac{1-\Pr(E_s|p_1)+1-\Pr(E_s|\overline{p_1})}{\sum_{i=1}^{2}(1-\Pr(E_s|p_i)+1-\Pr(E_s|\overline{p_i}))}$, where $\overline{p_1}$ represents the inversion of p_1 (i.e., `password`→`drowssap`), and $\Pr(E_s|p_1)$/$\Pr(E_s|\overline{p_1})$ is obtained by the positive/reverse order random forest model; "$1-\Pr(E_s|p_1)$" represents the probability of performing the *tail* operation (because $\Pr(E_s|p_1)$ represents the probability of unchanged operation), and "$1-\Pr(E_s|\overline{p_1})$" represents the probability of performing the *head* operation.

The formula of calculating $\Pr(S_2)$ is used to solve the problem of unequal operation probability of each segment. For instance, the structure of `password!!` is $\mathsf{L}_8\mathsf{S}_2$, and the operation probability (e.g., insertions or deletions) on different segments (i.e., L and S) is not equal in practice, while TarGuess-II [57] regards it as equal in the structure-level. To address this issue, we treat the probability of each segment (take L segment as an example) be expressed by the ratio of "the sum of the operation probabilities of L segment (i.e., `password`) to that of all the segments (L and S segments)".

In the guess-generation phase as with [57], after each operation performed on the original password, the corresponding probability is calculated and inserted into a priority queue, and the guess with the highest probability is output. Then we repeat this process until the number of generated guesses reaches the predefined threshold (e.g., 10^3).

Table 4: Basic information about password reuse datasets.

Dataset	Language	Items	# Same password pair	# Similar password pair†
CSDN→126	Chinese	195,832	62,686	47,690
CSDN→12306	Chinese	12,635	7,079	2,815
12306→Dodonew	Chinese	49,775	35,395	9,386
CSDN→Dodonew	Chinese	5,997	2,040	1,597
000Webhost→Clixsense	English	150,273	35,470	41,731
000Webhost→LinkedIn	English	231,452	50,875	52,731
000Webhost→Yahoo	English	36,936	5,960	6,303
000Webhost→Mate1	English	51,942	7,613	25,504

† Similar means that the similarity score s is within [0.5, 1.0], and it is calculated as $s = 1 - \text{EditDistance}(pw1, pw2)/\max(|pw1|, |pw2|)$.

5.2 Experimental setups and results

Datasets. We select four English and four Chinese datasets to conduct experiments on password-reuse guessing scenarios (see Table 4). Among them, 000Webhost→ClixSense and CSDN→126 are selected as the training set for English and Chinese guessing scenarios. We take the dataset "000Webhost→ClixSense" as an example. It is obtained by matching two datasets (000Webhost and ClixSense) through *email* and consists of password pairs like $(email_{U_i}, pw_{i1}, pw_{i2})$ for user U_i. In the training phase, U_i's password pw_{i1} comes from the 1st dataset (000Webhost), and the attacker $\mathcal{A}$ learns/trains how it can be used to guess pw_{i2} from the 2nd dataset (ClixSense). Then, suppose the dataset "000Webhost→Yahoo" is used for testing. $\mathcal{A}$ exploits pw_{j1} from 000Webhost as victim j's leaked password, and uses the trained password model to generate guesses until pw_{j2} from Yahoo is generated.

We compare our proposed model with TarGuess-II [57] and Pass2Path [40]. TarGuess-II and our RFGuess-Reuse require additional PCFG structure dictionaries (see Sec. 5.1) and popular password dictionaries (see Sec 4.2 in [57]), and we maintain the same datasets for these two models. For

Table 5: Comparison of three password reuse models.†

Experimental setup		RFGuess-Reuse	Pass2-Path [40]	TarGuess-II [57]
Guessing scenario	Guess number			
CSDN → 12306	10	68.41%	68.80%	68.13%
	100	73.09%	70.72%	73.19%
	1,000	75.86%	72.16%	75.57%
CSDN → Dodonew	10	48.59%	48.82%	48.44%
	100	53.86%	51.79%	54.56%
	1,000	57.71%	53.84%	57.58%
12306 → Dodonew	10	84.14%	83.44%	84.11%
	100	86.00%	85.69%	86.34%
	1,000	87.65%	86.78%	87.58%
000webhost → Mate1	10	27.70%	25.11%	30.17%
	100	31.29%	26.42%	32.14%
	1,000	33.77%	27.73%	34.37%
000webhost → LinkedIn	10	35.67%	32.65%	36.17%
	100	37.77%	34.06%	38.16%
	1,000	39.52%	35.69%	39.72%
000webhost → Yahoo	10	26.53%	24.84%	27.12%
	100	28.59%	25.87%	28.69%
	1,000	30.13%	26.99%	30.19%

†A value with dark gray (resp. light gray) represents the highest one (resp. 2nd one).

Pass2Path, we use the recommended parameters in [5] to train the model. Similar to the targeted guessing scenarios based on PII, we also generate 10^3 guesses for each model.

Table 5 shows that RFGuess-Reuse achieves the best or 2nd best results among three models. In particular, within 10^3 guesses, the attack success rates of TarGuess-II [57] and our RFGuess-Reuse are about 1%∼7% higher than that of Pass2Path [40]. For English datasets, although the attack success rate of RFGuess-Reuse is slightly lower than that of TarGuess-II, it is still 7%∼22% higher than Pass2Path.

6 Discussion

We now discuss the security implications of this work and our insights on online/offline password guessing.

Honeywords. At CCS'13, Juels and Rivest [31] proposed a decoy password mechanism to timely detect password file compromises, called honeywords. This mechanism can generate $k-1$ (e.g., k=20 in [31]) honeywords for each account, and both the real password and its corresponding honeywords are stored together. In addition, the index of each real password is stored in another server named honeychecker. When an attacker tries to log in with a honeyword, the system signals a possible leak. As a leading password model, RFGuess can be potentially employed to generate honeywords to timely detect password leakage. In this application scenario, the model size and password generation speed are not particularly important since the server only needs to generate 20∼40 honeywords (as recommended by [58]) for each account, and such generation is conducted only once for an account. For example, the Markov/TarMarkov model employed by the hybrid method proposed in [58] can simply be replaced by our RFGuess/RFGuess-PII to generate flatter honeywords (that are harder to be differentiated from real passwords).

Feature importance score. As shown in Sec. 3.2, RFGuess can efficiently identify the dominant factors of password security through the feature importance score to resist against data-driven guessing. For example, we only need to set the number of character classes as a password prefix feature, and RFGuess can automatically show if it is one of the dominant factors impacting password security through the feature importance score. This can help administrators enforce more effective password policies. For example, more character classes contribute marginally improvement in password security due to the imbalanced use of symbol strings, while more segments (i.e. a continuous string whose characters have a strong correlation) can significantly help resist against guessing [52]. Also, the feature importance score allows users to understand which dimensions of a character (e.g., type, continuity, and position-information) impact the password security to what extent, thus helping them create more secure passwords.

Online/Offline password guessing. Before cracking, the offline guessing attacker has the salted-password accounts, but generally has no prior knowledge of which passwords are used by the target accounts, and thus it is more realistic/reasonable to do *not* exclude duplicate passwords in the training set from the test set when evaluating a guessing algorithm, as done in Sec. 3.4 (and [34,35,51]) and opposed to [28,59,61]. Besides, excluding duplicate passwords can only evaluate/simulate the generalization ability, but overlooks the evaluation of fitting ability. In practice, the *generalization* ability corresponds to offline guessing scenarios with relatively large guess numbers (e.g., $>10^7$). Although previous work [22] suggested that 10^{14} could be a lower boundary for offline guessing, the size of guessing dictionaries explicitly generated by existing password guessing literature (e.g., [34,35,43,59]) generally does not exceed 10^{11} (due to the limitation of generation speed and computing resources). This implies that the practical significance of guessing algorithms' generalization ability is mainly highlighted in 10^7∼10^{10} guesses. In contrast, the *fitting* ability mainly corresponds to online guessing scenarios with relatively small guess numbers (e.g., $<10^7$), while online guessing is the most concerning threat that normal users need to devote efforts to mitigate [7,22,57]. Thus, when evaluating a guessing model/algorithm, it is of practical significance to consider both the fitting ability and generalization ability.

In all, it is more realistic to do *not* exclude duplicate passwords in the training set from the test set. Actually, this practice has been preferred in password research (see [34,35,51]), but we *for the first time* explain why it is acceptable.

7 Conclusion

This paper, for the first time, introduces classical machine learning techniques for password guessing, and designs three new guessing models for the three most representative guessing scenarios: trawling guessing, targeted guessing based on PII and on reuse. Extensive experiments with 13 real-world datasets demonstrate the effectiveness and scalability of our models. This work provides a brand new technical route for modeling users' password guessability and opens up new directions for designing effective password guessing models.

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A Parameter selection

As far as we know, there are few scientific methods to find the best hyperparameters. However, a task-oriented analysis along with a number of empirical experiments provide a promising way: Since the password length of most users is at least six [34, 53], the order of our model is set to six. In this way, the total number of prefixes (6-order strings) is about 8.9∼10.4 times the number of passwords, so the minimum number of samples in each leaf node is set to 10. For the number of trees, we take the CSDN dataset as an example, and set this value to 10, 30, 50, and 70, respectively. We find that when the number of trees is >30, the increase in the attack success rate is very limited (<0.5%). Also, the greater the value, the larger the RAM consumed during training (e.g., with 30 trees and five million training sets, it occupies about 40GB of RAM), and the slower the password training and generating will be. Therefore, we set this value to 30. In addition, the maximum ratio of features is determined by the importance score of each feature after our preliminary exploratory experiment (see Sec. 3.4). Compared with the complex parameters (e.g., number and type of layers, number of neurons per layer, activation function, etc.) of deep learning based models, the hyperparameter tuning of random forest are more concise and straightforward.

Table 6: Performance of different trawling guessing models.†

Model	RFGuess	PCFG [59]	3-order Markov [34]	FLA [35]
Training time	0.3h	24s	102s	16h
Model size	4.5G	93.2M	1.4G	5.8M
Generated PW/s	130	82,372	13,303	2,500

† CPU: Xeon silver 4210R 2.4GHz; GPU: GeForce RTX 3080 (5M dataset).

Table 7: Model size of different PII-based models.†

Model	RFGuess-PII	TarGuess-I [57]	3-order Tar-Markov [55]	FLA [35]-PII
Model size	101M	893K	12.2M	5.8M

†CPU: Xeon silver 4210R 2.4GHz; GPU: GeForce RTX 3080 (50% CSDN-PII).

B Supplementary experiment results

We compare different approaches in terms of training time, generation speed as well as trained model size. Table 6 reveals that statistics-based models (i.e., PCFG [59] and 3-order Markov [34]) require the shortest training time, followed by our RFGuess, and FLA [35] is the longest. Our RFGuess has the largest model size even after the compress (we set the compress parameter in the joblib tool to three and the number of trees to 30), but its fast training speed enables it to be trained *on site* without the need to save/maintain model files, and this property is quite desirable. While computational complexity is not particularly important for online guessing, we give the detailed model size of all tested models in targeted guessing scenarios, and the results are shown in Tables 7 and 8.

As for the guess-generation speed, RFGuess is first built on the scikit-learn framework [2], which does not support GPU acceleration. As a result, the generation speed is low: 130 passwords/s. We further migrate our RFGuess to the cuML framework (which supports GPU acceleration) [1], and the generation speeds increase by 5.2 times to 677 passwords/s in our preliminary experiments with 1,000 training data. Be-

Table 8: Model size of different reuse-based models.†

Model	RFGuess-Reuse	Pass2Path [40]	TarGuess-II [57]
Model size	121M	40.1M	1.04G

†CPU: Xeon silver 4210R 2.4GHz; GPU: GeForce RTX 3080 (CSDN→12306).

sides, if we use the decision tree model (i.e., set the number of trees to one), the password generation speed will be further increased to 1,520 passwords/s. In general, for online password guessing, an account should have been blocked quickly after a predefined number of failed login attempts (e.g., 100 and 1,000 are typical values considered by the main-stream standard [24] and academic literature [40, 57]); For offline guessing, memory hard hash algorithms such as SCRYPT or Argon2 are recommended [24], and they might move offline attackers closer to $10^6 \sim 10^7$ guesses [10]. Thus, the guess-generation speed of RFGuess is practically acceptable.

C Evaluation of PII matching algorithm

Experimental evaluation. Considering that the Chinese dataset contains complete PII (which can better reflect the advantages of our PII matching algorithm), we take three Chinese datasets as examples, and compare the attack success rate of TarGuess-I [57] and Targeted-Markov model [55] (4-order) after using the two PII matching methods, respectively (the results can be seen in Table 9). We find that, within 100 guesses, our proposed PII matching algorithm can improve the guessing success rate of TarGuess-I [57] by 7%, and can improve Targeted-Markov [55] by 13%. For three English datasets, our PII matching algorithm has not much optimization effect. This is because: 1) Many PII attributes in English datasets are missing; 2) The three English PII-associated passwords are from more security-savvy users (i.e., hackers/administrators/tech-savvyers) [57]. Specifically, Rootkit is a hacker forum, and 000webhost is a free web hosting site and is mainly used by web administrators. Therefore, the users of both sites are likely to be more security-savvy than normal users, and this has been observed in Fig.13 of [57].

Theoretical proof. We now prove the effectiveness of our proposed PII matching algorithm (in Sec. 4.2) in theory. Assume that there are N passwords in the password set D. For any two PII representations R_p and R_q, passwords that can be represented as R_p is denoted as S_p, and passwords that can be represented as R_q is denoted as S_q, where $|R_p| > |R_q|$. Then D can be divided into the following four sets.

$$\begin{aligned} A_{pq} = S_p \bigcap S_q,\ \ A_p = S_p - S_q, \\ A_q = S_q - S_p,\ \ A_o = D - S_p - S_q. \end{aligned} \tag{7}$$

The calculation of information entropy is given by: $H = \sum_{i=1}^{n} -p_i \cdot \log(p_i)$, so let

$$f(x) = -\frac{x}{D} \cdot \log(\frac{x}{D}), \tag{8}$$

Algorithm 1: PII matching algorithm.

Input: Passwords set $\mathcal{X} = \{pw_1, pw_2, ..., pw_n\}$.
Output: Passwords with corresponding PII matching structures ($\mathcal{P}$).

$match\_set = matchOrder(\mathcal{X})$;/* Get all PII structure representations and their corresponding frequency of set $\mathcal{X}$ in descending order. *match_set* is a priority queue.*/
$item = match\_set.pop()$; /* *item* contains the PII structure representation and its frequency i.e., (structure,frequency). */
while $!match\_set.empty()$ **and** $item.frequency > 1$ **do**
  for pw_i **in** $\mathcal{X}$ **do**
    $match\_pw_i = pwMatch(pw_i)$/* All PII structure representations of pw_i. */
    if $item.structure$ **in** $match\_pw_i$ **then**
      $\mathcal{P}.push((pw_i, item.structure))$;
      $\mathcal{X}.remove(pw_i)$;
    for $remain\_item.structure$ **in** $match\_pw_i$ **do**
      $remain\_item.frequency$-=1;
while $!\mathcal{X}.empty()$ **do**
  $pw = \mathcal{X}.pop()$;
  $structure = shortMatch(pw)$;/* The shortest PII matching structure of *pw*. */
  $\mathcal{P}.push((pw, structure))$
return $\mathcal{P}$

Table 9: The effect of PII matching algorithm (100 guesses).†

Targeted guessing model	TarGuess-I [57]		Targeted-Markov [55]	
Attack scenarios	Optimal	Original	Optimal	Original
50% PII-CSDN→50% PII-CSDN	27.90%	22.90%	27.01%	25.55%
50% PII-Dodo→50% PII-Dodo	19.10%	19.00%	20.33%	17.48%
50% PII-12306→50% PII-12306	20.30%	20.20%	20.91%	17.86%

†Optimal means using our new proposed PII matching algorithm, and original means using the leftmost&longest PII matching algorithm; Dodo=Dodonew.

where $f(x)$ is an upward convex function. Then the information entropy is expressed as H=$\sum_{i=1}^{m} f(c_i)$, where m is the number of representation tags, and c_i is the frequency of representation tags R_i. We now prove that when only two representations are considered, the information entropy is lower when the password is first represented as R_p with higher frequency than as R_q. Here, only the influence of R_p and R_q on the information entropy is considered, so the passwords that cannot be represented in these two ways (i.e., the set A_o) is not considered. For the set A_{pq}, A_p and A_q, if the password is first represented as R_p, and then represented as R_q, the information entropy is H_p=$f(|A_{pq}| + |A_p|) + f(|A_q|)$. If the password is first represented as R_q, the information entropy is $H_q = f(|A_{pq}| + |A_q|) + f(|A_p|)$. Considering $|A_{pq}| + |A_p| = |R_p| > |R_q| = |A_{pq}| + |A_q|$, we get $|A_p| > |A_q|$.

Let $g(x) = f(x) - f(x + |A_{pq}|)$, where $x > 0$, and take the derivative of $g(x)$, we get

$$\begin{aligned} g'(x) &= f'(x) - f'(x + |A_{pq}|) \\ &= \frac{\frac{-1-ln(\frac{x}{|D|})}{|D|} - \frac{-1-ln(\frac{x+|A_{pq}|}{|D|})}{|D|}}{ln2} \\ &= \frac{ln(\frac{x+|A_{pq}|}{|D|}) - ln(\frac{x}{|D|})}{|D| \cdot ln2} > 0. \end{aligned} \tag{9}$$

Since the derivative of $g(x)$ is greater than 0, $g(x)$ is a monotonically increasing function. And $|A_p| > |A_q|$, we have $g(|A_p|) > g(|A_q|)$, namely

$$\begin{aligned} g(|A_p|) &= f(|A_p|) - f(|A_p| + |A_{pq}|) > g(|A_q|) \\ &= f(|A_q|) - f(|A_q| + |A_{pq}|). \end{aligned} \tag{10}$$

By shifting the term, we get

$$f(|A_q|)+f(|A_p|+|A_{pq}|)<f(|A_p|)+f(|A_q|+|A_{pq}|), \tag{11}$$

that is, $|H_p| < |H_q|$. Therefore, when only two representations are considered, the information entropy is lower when the password is first expressed as R_p with higher frequency than as R_q. It can be seen from this conclusion that preferential representation as R_1 can make the information entropy the lowest. According to the algorithm proposed in Sec. 4.2, the highest frequency representation taken out for the first time is R_1. Then the current highest frequency representation is taken out in each round. That is, the representation taken out each time can be used as a priority representation. As a result, each round of selection is the current optimal choice, and the representation obtained at the end of the algorithm can be regarded as an approximately optimal solution.

Overhead. Although computational complexity is not particularly important for online guessing, we have tested the time consumption of our optimal PII matching algorithm. More specifically, it takes about 440s on a common server (CPU: Xeon Silver 4200R; System: Ubuntu 20.04) to complete PII matching on 50% of the Dodonew-PII dataset (about 80,000 pieces of data), which is acceptable.

D Structure-level transformation behavior statistics

Through the analysis of the problems in TarGuess-II [57], we find that the focus is whether the behavior of inserting and deleting structures is related to the password itself. Taking the CSDN→126 dataset as an example (which is a dataset composed of password pairs matched through email), we count the similar but different password pairs among them (“similar" here means the similarity score s is greater than 0 and less than 0.5, and it is calculated as $s = 1 - \text{EditDistance}(pw1, pw2)/\max(|pw1|, |pw2|).$). More specifically, there are a total of 25,917 items, accounting for 26.47% of the entire dataset. We have made statistics on the insertion and deletion of structural behaviors of them, and the top-ten frequent ones are shown in Table 10.

Table 10 shows that the tenth-ranked reuse behavior (i.e., insert or delete the string “11”) only occurs 49 times, which makes it challenging to learn the behavior of inserting and deleting password structures based only on the number of occurrences in the dataset. To address this issue, we divide the probability of structure-level transformation into two parts in RFGuess-Reuse: the probability of the structure-level transformation, and the probability of which specific structure is performing on structure-level transformation.

Table 10: Structure-level insertion/deletion statistics.

Insertions/Deletions	Position	Frequency	Example
`a`	Prefix	264	`a3221041 →3221041`
`123`	Suffix	196	`cwhwan123→cwhwan`
`a`	Suffix	154	`4231294a →4231294`
`1`	Suffix	93	`wuchunlei→wuchunlei1`
`qq`	Suffix	87	`qq849210 →849210`
`aa`	Suffix	79	`5631842aa→5631842`
`aa`	Prefix	71	`aa123321 →123321`
`.`	Prefix	56	`3232334. →3232334`
`abc`	Suffix	53	`81983064 →81983064abc`
`11`	Suffix	49	`resing11 →resing`

Table 11: Structure-level transformation in each length.

Password length	Tail insertion	Tail deletion	Head insertion	Head deletion
3	0	0	0	0
4	3	0	11	0
5	14	0	128	0
6	1757	0	2274	0
7	1853	3	2339	2
8	396	1010	380	1223
9	178	1141	96	1667
10	95	1061	42	1169
11	37	429	37	556
12	23	358	2	373
13	5	159	1	166
14	3	131	1	115
15	2	39	0	19
16	0	30	0	20

For the first part, we consider the correlation between password length and structure-level transformation behaviors. We still take the CSDN→126 dataset as an example, and the statistics are summarized in Table 11. We find that the behavior of structure-level transformation has a great relationship with the password length. More specifically, passwords with lengths of 6 and 7 are more likely to be inserted into new structures, while passwords with lengths of 8∼10 are more tend to delete existing structures. Therefore, the probability of structure-level transformation can be obtained by statistics of corresponding transformation behaviors of passwords with different lengths in the training set. As for the transformation probability of a specific structure, it can be learned in a relatively large password set through PCFG [59].

E Feature importance

Although there is a slight difference in feature importance between the Chinese and English datasets (see Fig. 10), they are still very similar overall (the value of the cosine similarity between Chinese and English datasets is 0.98). Furthermore, there is almost no difference in the feature importance of the same language datasets (the cosine similarity within the Chinese and English datasets are both 0.99). Therefore, we calculate the average of the feature importance scores of the four datasets for observation (see Fig. 11).

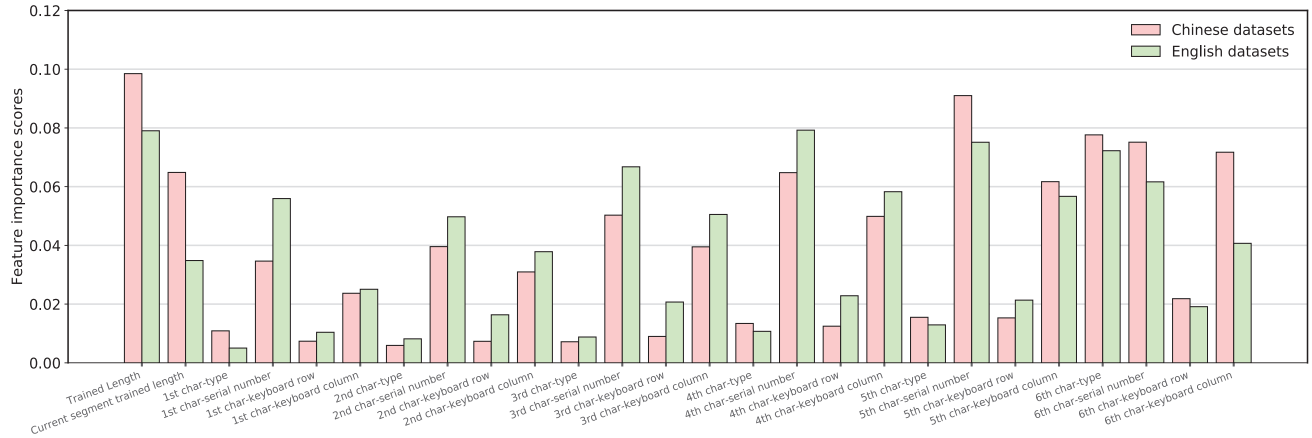

Figure 10: Feature importance obtained by our trained RFGuess. The Y-axis represents the proportion of the feature as the model classification rule: It reflects the importance of the feature. Thus, the larger the value, the higher the importance, and the sum of all feature importance scores for one dataset is one. The green bar is the average of the feature importance scores of the 000Webhost and Rockyou datasets (English datasets); the red bar is the average of the Taobao and CSDN datasets (Chinese datasets). Overall, the length of the trained characters (position of the character in a password) and the characters close to the predicted target character are more important in the Chinese datasets. While in English datasets, characters near the middle position (relative to the order) are more important (third and fourth character). We calculate the cosine similarity of feature importance scores between the two language and find this value to be 0.98. Besides, the cosine similarity of scores in the same language datasets is greater than 0.99. This shows that these two scores are very similar, indicating that language has little effect on feature importance scores, so we further calculate the average feature importance scores of the four datasets in Fig. 11.

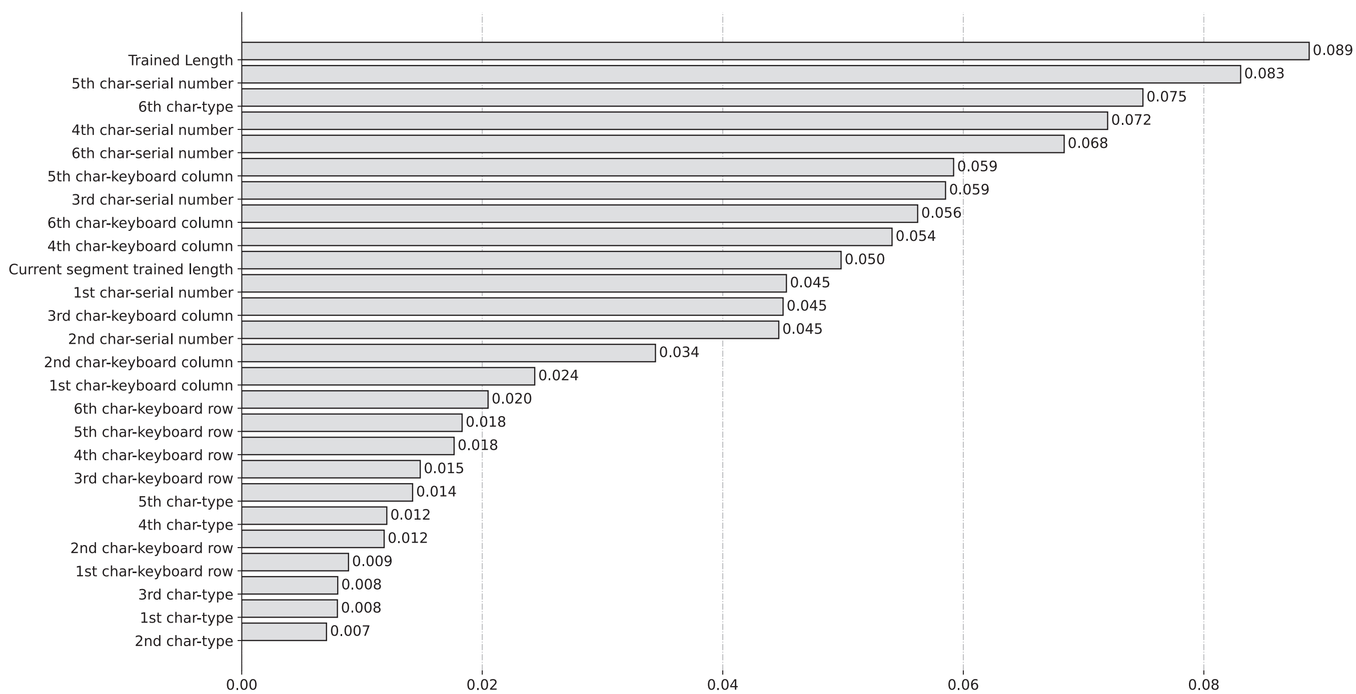

Figure 11: Feature importance (average). We sort the average of feature importance scores of two Chinese and two English datasets. Among these features, the serial number feature (e.g., `a` is the first in alphabetic types `a`∼`z`, 0 is the first of digits 0∼9) and the keyboard column number feature (e.g., `d` is located in the third column of the keyboard) are more effective, while the type of character (whether this character is a letter, digit or special character) and the current segment trained length (position of the character in the segment) are relatively unimportant, and the feature of keyboard row number has little effect on the model fitting. Since random forest can filter features, existing of some unimportant features will not affect the fitting ability of the model. In particular, relatively unimportant features can be selectively removed before training. For example, our experiments show that if the relatively unimportant 10-dimensional features are removed, the model training speed is improved by 30%. However, the maximum decrease in success rates is no more than 0.4% compared with the original.