Can machine learning identify interesting mathematics? An exploration using empirically observed laws

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Abstract

We explore the possibility of using machine learning to identify interesting mathematical structures by using certain quantities that serve as fingerprints. In particular, we extract features from integer sequences using two empirical laws: Benford's law and Taylor's law and experiment with various classifiers to identify whether a sequence is nice, important, multiplicative, easy to compute or related to primes or palindromes.

1 Introduction

Machine learning has made significant strides in solving classification problems in several domains that humans excel at, for instance in image processing and speech recognition. There have been some effort to classify scientific knowledge as well [1] by analyzing the text of scientific articles. So far, there have been much less progress in terms of classification using only the mathematical equations and quantities in scientific knowledge. Part of the difficulty is that there is less leeway in the interpretation of mathematics; similar numbers, symbols and equations can have completely different meaning based on the way these objects are composed on the page. On the other hand, classical logic-based AI and symbolic computer algebra systems have been more successful in this regard [2].

The purpose of this paper is to investigate the following perhaps simpler problem: can machine learning identify qualitative attributes of scientific knowledge, i.e. can we tell whether a scientific result is elegant, simple or interesting? We will start our investigation by restricting the domain to mathematical sequences of numbers.

2 Online Encyclopedia of Integer Sequences

The object of study in this paper are sequences of integers. One reason of choosing them to study is that many fundamental mathematical ideas are captured in these structures. Another reason is that there exists an extensive database of integer sequences that has been edited and curated for over 50 years: the Online Encyclopedia of Integer Sequences (OEIS) [3]. The OEIS was created by Neil Sloane in 1964 and has grown to over 300,000 sequences as of this writing with thousands of volunteers from the OEIS community editing and adding metadata and references to these sequences. To each sequence are associated keywords assigned by the community members. Some examples of keywords are: 'nice', 'core', 'base', 'hard', etc. A complete set of keywords and their definitions can be found at `http://oeis.org/wiki/Keywords`. Many classical sequences are in the database,

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such as the sequence of primes, the binomial coefficients, the Fibonacci numbers, etc. There is a range of complexity, ranging from sequences that are very easy to compute (such as the sequence of odd numbers A005408), hard to compute (such as the number of nonsingular $n \times n$ 0-1 matrices A055165) to sequences for which it is not known whether it is finite or not (such as the list of Mersenne primes A000668).

3 Empirical laws

To classify such sequences, we would like to have a fixed number of features that can be computed on sequences of any finite length. In this paper we look at 2 empirically observed laws that has appeared in the literature. Empirical laws are not mathematical theorems per se, but are empirical observations of relationships that seem to apply to many natural and man-made data sets (e.g. Moore's law in electrical engineering [4] or the 80/20 Pareto principle in economics), but why these occur so frequently are typically still not completely understood. As these empirical laws are discovered because many data sets of interest seem to abide by them, they are a good starting point for finding features for classification.

3.1 Benford's law

Benford's law [5] states that in a set of numerical data, terms with small leading digit tend to occur more frequency. More precisely, in base b, terms with leading digit d occurs with probability equal to $\log_b(\frac{d+1}{d})$. In particular we will denote the discrete distribution $\{d_i\}$ where $d_i = \log_{10}(\frac{i+1}{i})$ and $i = 1, \cdots 9$ as the *Benford* distribution $b(i)$.[1]

This empirical law was first observed by Simon Newcomb [6] who noted that in logarithms tables there were more numbers starting with 1 than with any other digit. This was noted later by Frank Benford who analyzed it for other data sets. Recently, Benford's law has been shown to apply to several integer sequences [7].

3.2 Taylor's law

Another empirical law is discovered by Lionel Taylor in 1961 [8] who noted that in ecology, the mean μ and the variance v in species data appear to satisfy a power law:

$$v = T_a \mu^{T_b} \tag{1}$$

where T_a and T_b are positive constants.

Taylor's law has been observed in many naturally observed data sets [9, 10] and in integer sequences such as the list of primes [11] and binomial coefficients [12].

4 The data set

For the data set, we selected 40,000 sequences randomly from OEIS each with at least 990 terms accessible in the database.[2] On average, approximately 1 in 4 sequences in the OEIS has over 990 terms. Although most sequences in OEIS are infinite sequences, it is not always easy to compute many terms. For each sequence, we collect all the terms that are available in OEIS and compute several quantities for each sequence.

4.1 Checking for Benford's law

To check for Benford's law, we compute the following features for each sequence: $b_d(i)$ is the proportion of terms with leading digit i for $i = 1, \cdots 9$.

[1] This is the base 10 version of Benford's law which has been verified for many experimental data sets, and it appears to hold in other bases as well.

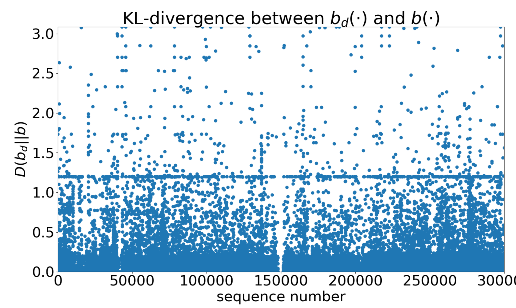
[2] The reason for this odd number (990) is because the terms in the OEIS database are (for the most part) limited to 1000 digits, and some sequences such as "smallest prime containing at least n consecutive identical digits" (OEIS sequence A034388) will have slightly less than 1000 terms in the database.

For each sequence $\{a(n)\}$,[3] we compared the proportion of terms $b_d(i)$ with the Benford distribution $b(i)$ by using 4 different statistical distances: (1) the Kullback-Leibler (KL) divergence $D_{KL}(b_d||b) = \sum_i b_d(i) \log \frac{b_d(i)}{b(i)}$, (2) the Kolmogorov-Smirnov (KS) statistic $KL(b_d, d)$, (3) the Wasserstein distance (or earth mover's distance) $WD(b_d, b)$ and (4) the total variation distance $TV(b_d, d)$.

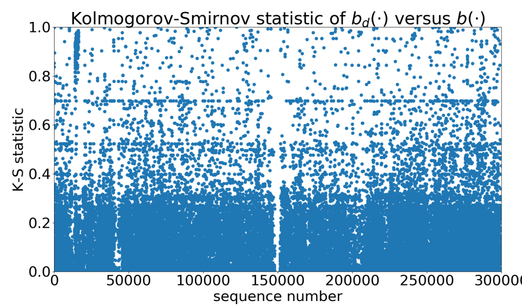
Fig. 1a shows the KL divergence of the various sequences. We see that for many of the sequences, the KL-divergence is small and in the range [0,0.2]. The KL-divergence between the uniform distribution and $b(i)$ is 0.191, indicating that for most sequences $b_d(i)$ is a decreasing function. There is a cluster of sequences with KL-divergence about 1.2. These are due to sequences whose terms all start with the digit 1, such as sequences that expresses the terms in binary notation (e.g. OEIS sequence A035526) for which $b_d(i) = 1$ if $i = 1$ and 0 otherwise (a distribution we will denote as δ_9) as the corresponding KL-divergence is $\log\left(\frac{1}{\log_{10}(2)}\right) = \log(\log_2(10)) \approx 1.2005$. Fig. 1b shows the KS statistic which shows similar behavior as Fig. 1a.

We also computed the Wasserstein distance $WD(b_d, b)$ between b_d and b for these sequences. As the Wasserstein distance take into account a permutation of the digits (i.e. the Wasserstein distance does not change if the values of b_d or b are permuted), $WD(b_d, b) \le WD(\delta_9, b) = \frac{2(1-\log_{10}(2))}{9} \approx 0.1553$, the plot in Fig. 1c shows relatively smaller values.

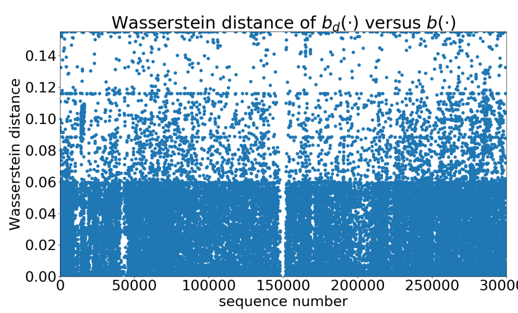
Finally, in Fig. 1d we show the total variation distance of b_d and b which is similar to Fig. 1b. There are some sequences (i.e. A000038) which is all zero except for a single term which has a total variation distance close to 1.



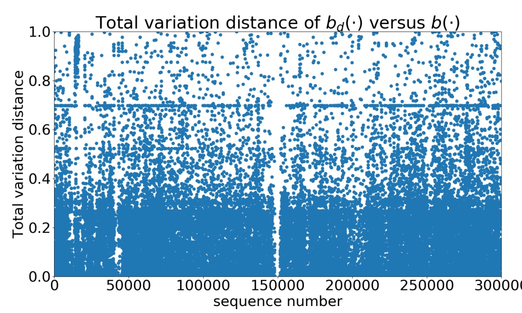
(a) Kullback-Leibler divergence of b_d versus b.



(b) Kolmogorov-Smirnov statistic of b_d versus b.



(c) Wasserstein distance of b_d versus b.



(d) Total variation distance of b_d versus b.

Figure 1: 4 statistical distances between b_d and the benford distribution b.

These figures show that b_d is relatively close to b for many sequences which implies that they adhere to Benford's law.

[3] As mentioned before, since the sequences are generally infinite, we mean here all the terms of the sequence that are available in the OEIS database.

4.2 Checking for Taylor's law

To check for Taylor's law, we compute the following quantities for each sequence $\{a(n)\}$: $\mu(n) = \frac{1}{n}\sum_{i=1}^{n} a(i)$ and $v(n) = \frac{1}{n-1}\sum_{i=1}^{n}(a(i)-\mu(i))^2$ with $v(1) = 0$.

Note that we use the sample variance as we interpret the sequence as samples from an experimental process. Using the population variance instead ($\frac{1}{n}\sum_{i=1}^{n}(a(i)-\mu(i))^2 = (n-1)v(n)/n$) gives very similar results as the total number of terms for each sequence is relatively large.

We fitted $\log v$ against $\log \mu$ with a linear regressor to obtain the following features: slope s, intercept b and correlation coefficient r. When r is close to 1, Taylor's law (Eq. 1) is closely satisfied with slope $s = T_b$ and the intercept $b = \log(T_a)$.

Figure 2 shows the correlation coefficient r against the sequences number. We see that for many (but not all) sequences the correlation coefficient r is close to 1. We also notice sequences where r is negative, indicating a negative correlation. In this case s is negative, corresponding to a negative exponent T_b in Taylor's law. This is quite different from the original form of Taylor's law where $T_b > 0$ and observed in general data sets [9–12].

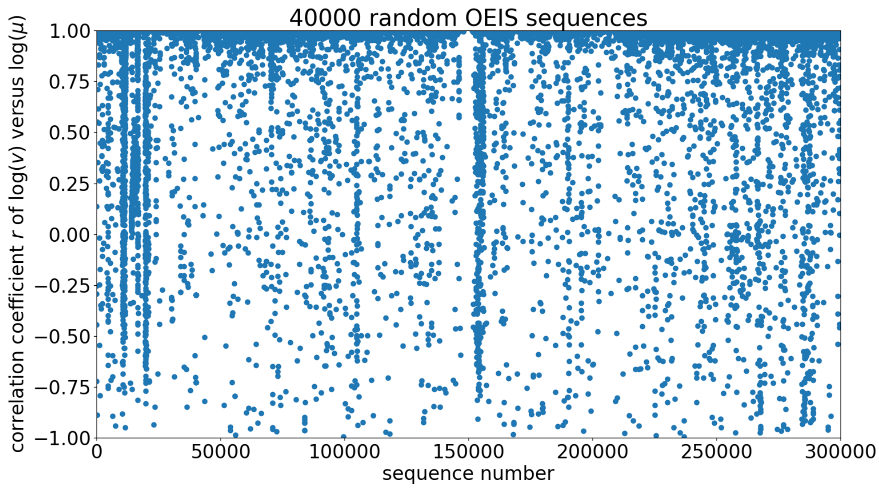


Figure 2: Correlation coefficient r of $\log(v)$ versus $\log(\mu)$.

Figure 3 shows r plotted against s, along with a regressor derived from the RANSAC algorithm [13] with a slope of approximately 2. Since $\frac{s}{r} = \frac{Sl_v}{Sl_\mu}$, where Sl_v and Sl_μ are the standard deviation of $\log(v)$ and $\log(\mu)$ respectively, this implies that for many sequences $Sl_v \approx 2Sl_\mu$. This is further accentuated by the inliers in Fig. 3, which represents about 50% of the sequences considered, which matches the regressor line with slope 2 with a very high correlation coefficient of 0.999.

For each sequence, we also compute p_z which is the proportion of terms that are positive resulting in a total of 14 features: s, b, r and p_z, and $b_d(i)$ for $i = 0, \cdots 9$. The feature $b_d(0)$ denotes the proportion of zero terms in the sequence.

5 Classifiers for identifying OEIS sequences

The above results show that many, but not all sequences satisfy to some degree Benford's law (BL) and Taylor's law (TL), suggesting that BL and TL could be used to identify whether a sequence would be of interest to OEIS. For instance, if $s \approx 2r$, then the sequence is a candidate for inclusion in OEIS. To test this idea we generated approximately 40,000 sequences of 2000 random integers and calculated the 14 features for these random sequences as well. We add these to the OEIS sequences to obtain a dataset of features from 80,000 sequences and randomly choose 70,000 for training and 10,000 for testing. We implemented a random forest classifier [14] with 665 trees and other parameters obtained via hyperparameter optimization. Preprocessing the data with a Principal

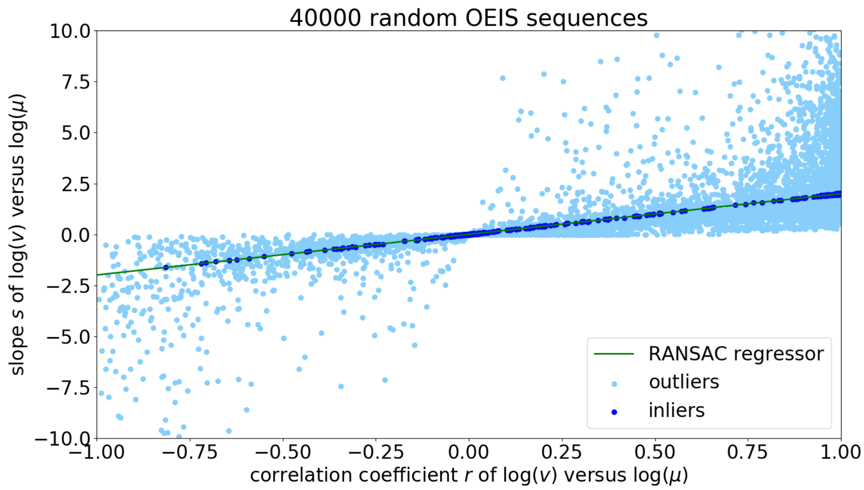


Figure 3: Slope s vs correlation coefficient r. The inliers (about half of the sequences) matches the regressor line with slope 2.001, intercept = 0.003 with a correlation coefficient equal to 0.999.

Component Analysis, we were able to obtain the following performance metrics in distinguishing OEIS sequences from random sequences: accuracy: 0.999, precision: 0.9984, recall: 0.9996, F_1 score: 0.9990.

On the other hand, even though it appears relatively easy to distinguish OEIS sequences from random sequences, the complement of OEIS is hard to define precisely. In fact, almost any integer sequence can be submitted to the OEIS and included if the editors deemed it interesting mathematically. But given the sequences in the database so far we could draw the conclusion that such interesting sequences tend to satisfy BL and TL (or at least distinguishable by the features derived from BL and TL). The purpose of the next sections is to see if the parameters derived from the sequences to test for adherence to BL and TL can be used to further categorize sequences within OEIS.

6 Classifiers for identifying keywords in OEIS sequences

We first identify the following labels for each sequence.

6.1 Sequence labels

We note for each sequence the absence or presence of the following OEIS keywords: ‘nice’, ‘core’, ‘easy’, ‘mult’. They describe sequences that are “nice”, important, easy to compute and multiplicative (in the number theory sense) respectively. In addition we added the keywords ‘prime’, ‘binomial’, ‘palindrome’[4] if these words appear in the title or in the comments section of the sequence in the OEIS database. We also added a keyword ’other’ to denote the absence of any of the above keywords. Thus we have total of 8 labels for each sequence. Each sequence can have more than one label.

We train different types of classifiers to analyze the dataset. A total of 35000 sequences will be use for training and validation. The test set consists of 5000 sequences. Preprocessing based on statistics of the training set are applied to normalize the training and test set.

6.2 Neural network

The neural network has 6 dense layers with 933 neurons and about 140,000 trainable parameters, and using ReLu activation functions, except the output layer which uses a sigmoid activation function. A dropout layer with probability 0.25 is inserted after each input and hidden layer. We train this neural

[4] A number is called a *palindrome* if it is the same when read left to right or right to left. Examples include the numbers 1348431 and 9889. When the base is not specified, the number is assumed to be written in base 10.

network for 40000 epochs with a batch size of 32. We use 31500 sequences for training in each epoch and 3500 sequences for validation.

6.3 Random forest ensemble classifier

We will consider 2 types of ensemble classifiers: The random forest classifier and the extra trees ensemble classifier. For both these classifiers, the hyperopt-sklearn module is used to tune the hyperparameters. A standard scaling normalizes the data based on the variance and mean of the training set. The random forest consists of 744 trees, and all features have similar Gini importance.

6.4 Extra trees ensemble classifier

The extra trees (extremely randomized trees) classifier [15] is a generalization and an improvement of the random forest classifier. The number of trees is 1059 and again all features have similar Gini importance.

6.5 Baseline classifier

As a baseline, we also construct a random classifier, where each predicted label is chosen with a probability derived from the training set.

Since some labels occur much more frequently than other labels, the (subset) accuracy for such a unbalanced problem is generally not the best metric [16], and therefore as in Section 5 we will also compute the precision, recall and F_1-score for each classifier.

7 Experimental results

The performance of these various models in predicting each label class is shown in Figure 4, where we plotted the (subset) accuracy, precision, recall and F_1-score of each model[5]. Since each sequence can have multiple labels, these quantities are computed for each label and are averaged among the labels weighted by their support. In Figure 5 we plot these quantities for each of the classes for each of the models. We find that the extra trees ensemble classifier performs the best, followed by a random forest classifier, and then a deep neural network. All of them performed better than the baseline classifier. Furthermore, they all had problems classifying labels that are not well supported: ‘nice’, ‘core’, ‘palindrome’, ‘binomial’ and ‘mult’, a well known problem of multilabel data sets that are not balanced. Note that for the class "palindrome" the extra trees classifier has a nontrivial recall and precision unlike the other classifiers for which these quantities are either 0 or undefined. The neural network classifier has perfect precision (no false positives and at least one true positive) for ‘nice’ sequences and the extra trees classifier has perfect precision of ‘palindrome’ sequences. Note also that the scores for the ‘mult’ labels are significantly higher for the 3 classifiers versus the baseline classifier, suggesting that multiplicative sequences can be detected using these empirical laws. Can this conclusion be a consequence of the definition of multiplicative?

The performance of the models are not stellar, but it is better than the baseline classifier. As the OEIS database consists of sequences that people have submitted and the editors approved, it is biased towards sequences which people have found to be interesting or useful mathematically. This means that the ability to predict sequences with the "prime" label does not mean it was able to classify all prime-related sequences, but merely that it was able to classify prime sequences that are interesting or relevant. Furthermore, labels such as ‘nice’ and ‘easy’ are subjective and can vary depending on the person who assigned the label, and such issues are common in classification tasks such as sentiment analysis [17].

In some cases the models were able to find related sequences. For instance sequence A059260 was in the training set which included the labels ‘nice’ and ‘binomial’. The sequence A059259 which was in the test set is a related sequence which enumerated the triangle of terms in a different order and the extra trees classifier also predicted the labels ‘nice’ and ‘binomial’ even though these labels were not assigned to A059259. The extra trees classifier predicted the label ‘binomial’ for sequence A080575 which is appropriate since it list the triangle of multinomial coefficients. Similarly, sequence A182009

[5]Precision, recall and F_1 score is set to 0 when it is undefined (i.e. the denominator is 0).

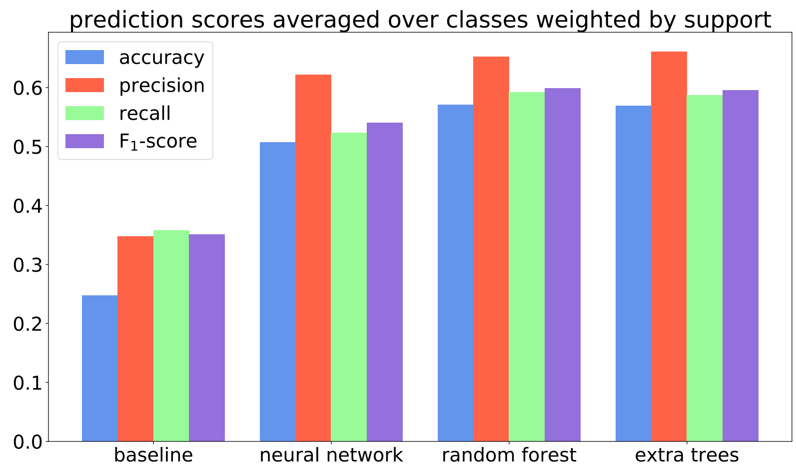
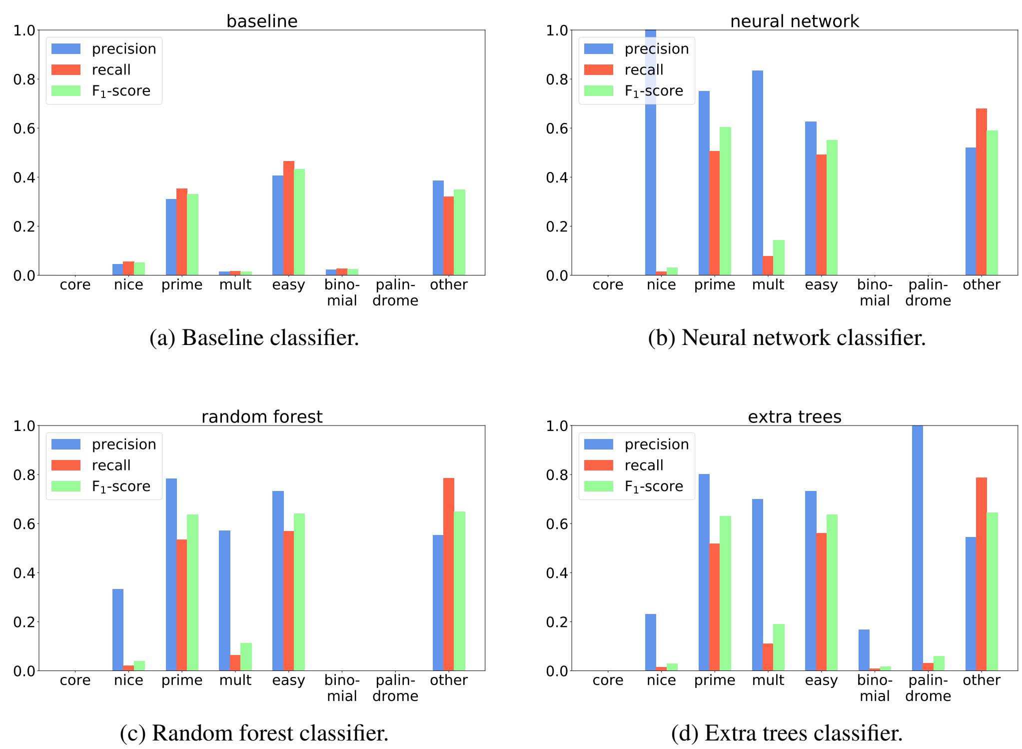


Figure 4: Accuracy, precision, recall and F_1 score of 3 classifiers compared with the random classifier.



(a) Baseline classifier.
(b) Neural network classifier.
(c) Random forest classifier.
(d) Extra trees classifier.

Figure 5: Performance (precision, recall and F_1 score) of various classifiers on each label class.

which is an approximation (and is almost identical to) of sequence A033810 (which is in the training set), the extra trees classifier also predicted the labels of A033810 for sequence A182009.

8 Conclusions

The experimental results point to the possibility of classifying interesting or relevant integer sequences using derived parameters based on empirical laws. We believe that this is due to empirical laws capturing inherent salient properties of numerical data that are interesting or important to study. Future work include training a deeper network, and adding other features perhaps from other empirical laws (such as Zipf's law [18][6] which is a general form of Benford's law) to see if the performance improves. Some other ideas to consider include looking at the mean and variance of n-th order differences and how well a sequence fits a polynomial equation or a linear recurrence relationship.

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