AUTOMATIC CLASSIFICATION OF KEPLER PLANETARY TRANSIT CANDIDATES

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ABSTRACT

In the first three years of operation, the Kepler mission found 3697 planet candidates (PCs) from a set of 18,406 transit-like features detected on more than 200,000 distinct stars. Vetting candidate signals manually by inspecting light curves and other diagnostic information is a labor intensive effort. Additionally, this classification methodology does not yield any information about the quality of PCs; all candidates are as credible as any other. The torrent of exoplanet discoveries will continue after Kepler, because a number of exoplanet surveys will have an even broader search area. This paper presents the application of machine-learning techniques to the classification of the exoplanet transit-like signals present in the Kepler light curve data. Transit-like detections are transformed into a uniform set of real-numbered attributes, the most important of which are described in this paper. Each of the known transit-like detections is assigned a class of PC; astrophysical false positive; or systematic, instrumental noise. We use a random forest algorithm to learn the mapping from attributes to classes on this training set. The random forest algorithm has been used previously to classify variable stars; this is the first time it has been used for exoplanet classification. We are able to achieve an overall error rate of 5.85% and an error rate for classifying exoplanets candidates of 2.81%.

Key words: astronomical databases: miscellaneous – binaries: eclipsing – catalogs – methods: statistical – planets and satellites: detection – techniques: photometric

1. INTRODUCTION

Kepler is a single instrument spacecraft that maintains its pointing at the designated field almost constantly in order to collect the most contiguous and long-running, photometric time series possible. The primary mission of Kepler was to detect large numbers of transiting exoplanets. The ultimate goal of the primary mission was to characterize the frequency of exoplanets with respect to diameter, orbital period, and host star. Manual classification of the findings of Kepler has proven very time consuming and only provides a coarse ranking of unclassified data. New, space-based, transit photometry missions such as K2 (Howell et al. 2014), TESS (Ricker et al. 2014), and PLATO 2.0 (Rauer et al. 2014) will also be plagued with the same embarrassment of riches that Kepler has faced, and will require some level of automation.

Using a machine-learning approach, we can speed this process and provide a more continuous ranking of PCs. The technique presented in this paper has already been used to assist in finding new, habitable-zone planets (Torres et al. 2015).

A threshold crossing event (TCE) is a sequence of significant, periodic, planet transit-like features in the light curve of a target star. TCEs are subjected to a vetting process performed by the Kepler TCE Review Team (TCERT). An initial stage of vetting, known as triage, partitions the set of TCEs into problematic light curves that have instrumental noise and Kepler objects of interest (KOIs). A KOI is a TCE that contains convincing transit-like features that do not present any obvious evidence that the TCE was generated from non-transiting phenomena (NTP; e.g., instrumental noise). These potential objects are further scrutinized with Kepler data in later stages of vetting, which seek to find evidence that the signal results from an eclipsing binary star or more subtle forms of instrumental noise. TCEs that do not present such evidence are disposed as PC. This process is performed by individuals manually inspecting light curves and detection statistics. The vetting process is described in greater detail in the KOI catalog papers Batalha et al. (2013), Burke et al. (2014), Rowe et al. (2015), and Mullally et al. (2015).

We automate this process of classifying TCEs into one of three classes: PC, astrophysical false positives (AFP), and NTP. PCs are confirmed as planets, statistically validated as planets, or determined to be a PC by the TCERT. AFPs are those TCEs that have been shown to be eclipsing binary stars or have shown evidence that the transiting object being detected is not located around the target star. The class NTP are those TCEs that failed triage.

We use a machine-learning algorithm known as the random forest (Breiman 2001) to find a function that maps attributes produced by the Kepler pipeline for each TCE to a classification of PC, AFP, or NTP. This classification function is purely based on the statistical distributions of the attributes for each TCE (e.g., signal-to-noise ratio, S/N, of the transit model fit) with respect to TCEs classified in the manual vetting process. These algorithms do not attempt to physically model the process of planet transits beyond what is already present in the TCE attributes. Random forests have been applied to a variety of classification problems; perhaps closest to this problem is that of classifying variable stars (Dubath et al. 2011; Richards et al. 2011).

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² While operating, Kepler can simultaneously observe approximately 170,000 stars. Data gaps on the order of days result from a monthly data down link and a quarterly 90° roll used to maintain the orientation of the solar panels. This roll causes the vast majority of stars to be observed by a different CCD every three months with a one year cycle.
This paper is organized as follows. In Section 2 we give an overview of the relevant portions of the Kepler pipeline that generate the inputs to the random forest. Section 3 introduces notation and describes the rationale behind the random forest algorithm. In Section 4 we discuss the provenance of our data and the source of our known class labels. Section 5 talks about how we pruned our set of attributes and which attributes turned out to be the most important. Section 6 contains an analysis of the classification performance and a comparison to reference classification algorithms on the training data set. Section 7 discusses issues involving how the automated classification would be applied to an exoplanet transit survey. A survey for transiting planets will initially discover larger, shorter-period planets before discovering smaller, longer-period planets, so that the training set will lag in period behind the unknown data. Section 7.1 shows what happens to classification performance when this happens. Sections 7.2 and 7.3 deal with testing and adjusting priors. Finally, Section 8 talks about future work we may perform to assist in discovering additional transiting exoplanets as well as improving the performance of the classifier.

2. KEPLER PIPELINE

2.1. Kepler Light Curves

A single sample of photometric data is composed of a set of co-added 6 s integrations with a readout time of 0.5 s, whose durations total 29.4 minutes. Co-added pixel values are downloaded from the spacecraft with the remainder of the processing performed on Earth. After calibration, light curves are produced using simple aperture photometry and subjected to cotrending to remove systematic noise (Smith et al. 2012; Stumpe et al. 2012).

2.2. Transiting Planet Search (TPS)

The Kepler pipeline (Jenkins et al. 2010a) is a data reduction pipeline used for translating the raw pixel data into potential transiting planet detections. In particular, this paper concerns itself with the last two modules of the pipeline: those that identify TCEs and their subsequent transit model fitting. The TPS (Jenkins et al. 2010b) module takes as input the systematic error-corrected light curve for a star; searches a parameter space of possible transit signatures; and outputs a TCE or says that one does not exist on the target star. This produces a smaller list of stars that have TCEs. This subset of target stars is then given to the “data validation” module, which fits this initial TCE to a transit model using the geometric transit model described by Mandel & Agol (2002) with the limb-darkening coefficients of Claret & Bloemen (2011). Data validation then gaps the transit signature from the light curve and uses the TPS to find additional TCEs on the same target star. This process repeats until no more TCEs are found on a star or a processing timeout has been reached.

The TPS algorithm detects transit-like features in light curves by applying a noise-compensating, wavelet-based matched filter (Jenkins 2002). TPS characterizes the PSD of the observation noise as a function of time to implement a whitening filter in the wavelet domain. The trial transit pulse is whitened and correlated against the whitened flux time series.

Features with correlations above the threshold of 7.1σ are flagged as potential TCEs and subjected to additional tests in TPS to guard against false alarms (Seader et al. 2013).

The algorithm searches a parameter space of varying transit duration \(D \in \{1.5, 2.0, 2.5, 3.0, 3.5, 4.5, 5.0, 6.0, 7.5, 9.0, 10.5, 12.0, 12.5, 15.0\} \text{ hr}\), which produces a Single Event Static (SES) time series that is the significance of the detection of the reference transit pulse centered on that particular time for each \(D\). This is computed as \(\text{SES}(t) = \frac{N(t)}{\sqrt{\mathcal{D}(t)}}\), where \(N(t)\) is the correlation time series; that is, how well the reference transit pulse correlates with the light curve. The quantity, \(\sqrt{\mathcal{D}(t)}\), is the expected S/N of a signal that exactly matches the template pulse. The Combined Differential Photometric Precision is \(1 \times 10^{-6} / \sqrt{\mathcal{D}(t)}\) ppm and encapsulates the effect of the observation noise on the detectability of the reference transit pulse as a function of time.

A Multiple Event Static (MES) is constructed that characterizes a significant detection in a search over varying orbital periods \(p\) and epochs (phase) \(t_0\) by folding \(N(n)\) and \(\mathcal{D}(n)\). A MES > 7.1σ may produce a TCE if it also passes additional statistical tests described by Seader et al. (2013). If several permutations of \((t_0, p, D)\) would produce a TCE, then TPS only reports the event with the maximum MES as the TCE for the target star. Diagnostics such as MES and SES are the basis of some of the attributes used in the training set (see Section 5.3). The minimum MES, which can be negative if the light curve is anti-correlated with the reference transit pulse, is also computed. This is referred to as the MESmin. An event with a negative MESmin would look like a repeated brightening above the median flux.

In addition to detecting PCs and AFPs, TPS often generates a TCE for non-transiting phenomena. NTPs are caused by instrumental, systematic noise (Caldwell et al. 2010), and stars with high variability, such as “heartbeat” stars (Thompson et al. 2012). Many NTPs have periods with approximately one year in duration as the electronics associated with the instrumental signatures rotates back into the same observing field. Unfortunately, this part of parameter space corresponds to the habitable zone of Sun-like stars.

2.3. Data Validation

Data validation (Wu et al. 2010) is a set of algorithms that performs tests to determine the suitability of the TCE as a PC. In particular, data validation fits the transiting portion of the light curve to a transit model using the geometric transit model described by Mandel & Agol (2002), with the limb-darkening coefficients of Claret & Bloemen (2011), and constructs a set of diagnostic tests to help determine the nature of the TCE. Data validation also attempts to locate the actual source of the transits (Bryson et al. 2013) in order to determine if the actual transit signal is being induced by a source offset from the target star. This can be caused by background eclipsing binaries, optical ghosts of bright stars with periodic signatures, or other unresolved contamination (Coughlin et al. 2014). Data validation constructs difference images between the in-transit and out-of-transit images for the target. The centroid of the difference image is then the center of the transit source. If the difference image is significantly offset from the out-of-transit centroid, then a background eclipsing binary may have produced the transit-like signal. Using the transit centroid offset from the position of the target star in the Kepler Input...
3. RANDOM FORESTS

3.1. Introduction

A random forest itself is an ensemble of decision trees. Each tree votes for the classification of an unknown object based on a vector of attributes (real valued random variables) that describe the object in question. The classification the forest assigns to an object is the plurality vote of the random forest. A decision tree is a directed graph where each internal vertex in the graph is a binary test; in this case, the tests are inequalities. If the test is true, then one branch is taken otherwise the other branch is taken. Leaf vertices indicate classifications. The trees in the random forest are constructed in such a way that tested attributes are randomly selected, so each tree makes a different set of tests. Figure 1 shows a simplified, hypothetical random forest.

3.2. Notation

$X$ represents the set of random variables that describe a TCE. Sometimes we refer to $X$ as the attributes of the TCEs. When we need to refer to a particular random variable without naming it, we use $x_i$ or some other subscript. Thus the set of a TCE’s attributes could be referred to as $X = \{ x_1, ..., x_A \}$, where $A$ is the number of attributes of $X$. The instantiation of the set of all the random variables for all the TCEs under consideration is $X$. When referring to the set of instantiations for a particular TCE we use $x$. The constant, $s_i$, is used to split $X$ into two different subsets. The subscript $i$ refers to a split made on the $i$th attribute. $Y$ refers to the set of all classes to which a TCE might belong; these are sometimes known as labels. A particular label is denoted $y_i \in Y$ and there are $C = |Y|$ distinct classes. For this classification problem, $Y = \{ y_1, y_2, y_3 \} = \{ \text{PC}, \text{AFP}, \text{NTP} \}$. $Y$ refers to the instantiation of all the labels for all the TCEs under consideration, $y$ is the instantiation for a particular TCE (usually in the training set). The set $\mathcal{L}$ is a set of instantiations of all the attributes $X$ and their labels $Y$; that is, attributes that describe all the TCEs and the TCEs’ labels. $\mathcal{L}$ is also known as the training set. The size of the training set is $N = |\mathcal{L}|$: the number of labeled TCEs.

When a split is generated, one subtraining set contains all of the TCEs with an attribute less than the split, $\mathcal{L}_l = \{ x_i < s \}$. The other subtraining set is composed of all the TCEs greater than or equal to the split $\mathcal{L}_r = \{ x_i \geq s \}$. The number of TCEs in each of these respective subtraining sets is then $N_l$ and $N_r$.

The purpose of classification is to assign an estimated label, $\hat{y}$, given an instantiation of attributes $x$. A classification function, $h$, generates a prediction for a set of attribute instantiations, $h: x \to \hat{y}$.

3.3. Decision Trees

As an example, Equation (1) is a simple, makeshift classification function. The training set consists of only two attributes to describe a TCE and two splits.

$$h(MES_{\text{min}}/MES_{\text{max}}, \Delta_{\text{centroid}}) = \begin{cases} \text{classify TCE as NTP, if} & \frac{MES_{\text{max}}}{MES_{\text{min}}} < s_1 \\ \text{classify as PC, if} & \Delta_{\text{centroid}} < s_2 \\ \text{classify as AFP, otherwise} & \end{cases} \tag{1}$$

$\Delta_{\text{centroid}}$ is the difference between the star’s KIC position and its mean out-of-transit centroid in arc seconds. $MES_{\text{min}}$ is the minimum MES discovered by the TPS, indicating repeated events above the baseline stellar flux. $MES_{\text{max}}$ is the highest MES discovered by TPS. A TCE representing a strong transit detection should have a high ratio of these two attributes. This is the second attribute in Section 5.3. TCEs caused by background eclipsing binaries should show an offset from their catalog position, so a high $\Delta_{\text{centroid}}$ value is cause to classify a TCE as an AFP.

Optimizing the parameters $s_1, s_2$ for the minimal misclassification rate of $h$ yields a misclassification error rate of 0.0886. The misclassification error rate is simply the number of incorrect classifications divided by the size of the training set ($N$). A logical next step to reduce the error rate would be to consider additional attributes that would discriminate TCEs. The Classification and Regression Tree (CART) algorithm (Breiman et al. 1984) can construct a recursive nesting of the conditional tests of arbitrary depth. These are sometimes visualized as a tree of conditionals called a decision tree. When building a decision tree, CART minimizes the following function for all splits $s_i$ under consideration:

$$\Delta I(\mathcal{L}, s_i) = N \log(I(\mathcal{L}_l)) - N_l \log(I(\mathcal{L}_l)) - N_r \log(I(\mathcal{L}_r)) \tag{2}$$

$P(y_i)$ is the frequency of class $y_i$ in $\mathcal{L}$. Function $I$ is an impurity function ($I: \mathcal{L} \to \mathbb{R}$) chosen so that it is maximum when all $P(y_i)$ are approximately equal, and zero when any $P(y_i) = 1$. $\mathcal{L}_i$ is the subset of $\mathcal{L}$ consisting of the training examples where the attribute $x_i$ is less than the threshold $s$. The members of $\mathcal{L}_i$ depend only on the ordering of the attributes relative to the split. This implies attribute transformations that are class independent and do not change the ordering of training examples, which result in the same $\mathcal{L}_i$. For example, log $x_i$ would not change the results of any splits. When CART is selecting a split for the training set, it iterates over all $x_i$ to find the attribute with the largest $\Delta I$. 

![Figure 1. Hypothetical, simplified random forest. Left branches are taken if the inequality is satisfied, otherwise the right branch is taken. A TCE with the attribute vector of $x = (2, 0.2, 4, 11, 5, 0.3, 6.1)$ is classified. Bold, green lines indicate the paths taken in the decision trees. The individual decision trees have voted [PC, AFP, PC, PC] yielding a classification of PC for the forest as a whole.](image-url)
One possible definition for $I$ is an information function:

$$I_L(L) = -\sum_{i=1}^{C} P(y_i | L) \log_2 [P(y_i | L)],$$

(3)

where $P(y_i | L)$ is the probability of a given class, $y_i$ given the training set $L$. So, when a split is selected using Equation (2), we are maximizing the information loss of the split. A perfect split would result in the members of $L_i$ and $L_r$ being of the same class, and therefore all the information would have been lost since $I_L(L_i) = 0$ and $I_L(L_r) = 0$.

In practice the Gini impurity function:

$$I_G(L) = \sum_{i=1}^{C} P(y_i | L) [1 - P(y_i | L)]$$

(4)

$I_G$ is used because it is faster to compute and usually results in the same split. $I_G$ is the sum of the misclassification probabilities. That is, the probability of guessing class $y_i$ for some example in $L$, when the label is actually some other class. Breiman et al. (1984) discusses other impurity functions. Figure 2 gives an example of $\Delta I$ evaluated at every possible split. Splitting the training set occurs between the attribute values with the maximum $\Delta I$.

Splitting the training set happens recursively so that $L_i$ and $L_r$ are then the training set for the next level of the decision tree. Tree construction ends when a split would result in a training set with instances of only a single class and impurity has fallen to zero. This generates the leaf vertex that assigns a class $\hat{y}$ to $x$ when the tree is evaluated.

3.4. Random Forest Description

The forest is a set of base, decision tree classifiers \{h_1, ..., h_r, ..., h_{N_{\text{tree}}}\}. Each tree, $h_k(x)$, is trained on $L_k$, which is a bootstrap replica of $L$ known as a bag. Each bag is about $2/3$ the size of the training data set. The observations not contained in the bag, $\overline{L}_k$, are known as the out-of-bag data. The number of trees $N_{\text{tree}}$ is one of two tunable parameters for this algorithm. For this problem we use $N_{\text{tree}} = 15,000$. Each tree’s misclassification error can be evaluated on its out-of-bag data to provide an unbiased estimate of the misclassification error of the random forest. Unlike other classification algorithms, the random forest allows us to estimate the misclassification error rate without having to resort to cross-validation to eliminate overfitting. Section 5.2.2 discusses how this out-of-bag error can be used to estimate the importance of various attributes.

Unlike any individual decision tree, the random forest has bounded error. That is, the overall misclassification error converges to this error bound. In order to prove this, Breiman (2001), makes the assumption that individual trees make their decisions independently of other trees. When a split is made during the construction of $h_k$, a random subset of attributes are considered for the split, rather than all attributes. $m_{\text{try}}$ is the number of attributes that are selected randomly during a split. These two techniques (i.e., bootstrap sampling and choosing a random subset of attributes at each split) break the correlation among the decision trees in the forest so that they approach the ideal of independent classifiers.

The random forest’s error is bounded by the equation,

$$\text{Err}_{\text{RF}} \leq \bar{p} (1 - g^2)/g^2.$$

(5)

Where $g$ is the strength of the the random forest. This is the average difference between the proportion of votes for the correct class and the maximum proportion of votes for any other class over all of $L$. $\bar{p}$ is the correlation among all the pairs of trees of the random forest over all of $L$ after the function

$$R(k) = \begin{cases} 1, h_k(x) = y \\ -1, h_k(x) = \text{the most common misclassification of } x \\ 0, \text{ otherwise} \end{cases}$$

(6)

has been applied to the classification of each tree on the training data.

The error bounds of the random forest then depend on how correlated the decisions of the trees are with each other and how well the forest as a whole separates between the correct class and the next best classification. Breiman (2001) contains a proof for convergence of the random forest to these error bounds.

Equations (5) and (6) imply that correlated attributes also produce correlated errors, which can cause a higher generalization error. In Section 5.2.4 we remove correlated attributes.

4. TRAINING SET AND UNKNOWN SET

4.1. Introduction

The TCE catalog contains the ephemerides of all the TCEs under consideration. This is separated into known ephemerides, which constitute the training set, and unknown ephemerides. Labeling of the TCEs naturally falls out of this process.

4.2. TCE Catalog

The TCE catalog used is from the first 12 quarters of Kepler data, as described by Tenenbaum et al. (2013). This TCE catalog contains a total of 18,407 TCEs. The TCE ephemerides are correlated with the ephemerides of known planets, PCs, and AFP from the NASA Exoplanet Archive. We use the

6 http://exoplanetarchive.ipac.caltech.edu
cumulative KOI catalog that was available on 2013 June 25 for the training data ephemerides. An older KOI catalog is used purposefully in order to more closely examine the generalization of the random forest (Section 7.2).

In this particular run of the Kepler pipeline, 2126 target stars that generate TCEs were excluded from consideration. The majority of these excluded stars are known eclipsing binaries from the Prša et al. (2011) catalog. Planets that have very short periods and relatively deep transits are identified as harmonics and removed by TPS (e.g., Kepler-10 b Batalha et al. 2011). These are not accounted for in the TCE catalog because they are not found by the Kepler pipeline. Planets with large transit timing variations and planets whose existence can only be inferred by transit timing variations (e.g., Kepler-19 b, c; Ballard et al. 2011) are also not in the TCE catalog. There are some cases where TPS has identified multiple TCEs for a single eclipsing binary. When this occurs, the TCEs usually have a period that is an integer multiple of an accompanying TCE on the same target star. No attempt is made to match these TCEs to the source eclipsing binary, and so they are considered to be unlabeled and not used in the training set.

4.3. Non-Transiting Phenomena

For quarter one through quarter 12 of the Kepler data, the TCERT reviewed all of the TCEs that were not caused by previously known Kepler objects of interest. Each TCE was examined by two or more people (vetters) to see if it had one of the following problems: stellar variability, instrumental effects, or anomalous behavior. A TCE is considered a product of stellar variability if it shows sinusoidal activity especially outside the primary transit event. Stellar variability with periods longer than the transit durations is not of concern because this is removed from the light curve before searching for transits. Instrumental noise is defined as a TCE exhibiting a transit-like signature that was apparently caused by spacecraft systematics, such as those induced by periodic spacecraft operations and uncorrected transient events such as radiation damage and cosmic ray hits. In some cases anomalous TCEs occur if there was insufficient data to make a classification, or if the transit did not appear at the expected position in the light curve. This step in the process of TCE vetting is known as triage.

A TCE in the training set is identified as an NTP if the vetters where unanimous in their decision to reject the TCE as a new KOI. This means that every vetter needed to identify one of the problems listed in the previous paragraph. This process yielded 11,304 TCEs that are in the class NTP. Since these TCEs were identified from the pipeline run, their ephemerides did not require matching against a known catalog.

More information about the TCERT process can be found in Batalha et al. (2013), Burke et al. (2014), and Rowe et al. (2015). A KOI can be a confirmed or validated exoplanet (confirmed or validated by one of several methods), a PC, an AFP, or undispositioned. A PC has a convincing transit-like signature in the light curve for the target star, but may lack additional information needed to confirm it as an exoplanet. Confirmed and statistically validated planets are also in the class PC. The class of AFP includes eclipsing binaries, background eclipsing binaries, and unresolved contamination from other astrophysical sources. We drop undispositioned Kepler objects of interest from the training set. Eight of the PCs in the Q1-Q12 public Kepler objects of interest catalog maintained by the NASA Exoplanet Archive have been corrected to AFPs with information that was available at a later date.

After ephemeris matching, our training set has 2879 PCs and 393 AFPs. This likely underrepresents the true population of AFPs because many AFPs were excluded from our pipeline run (see Section 4.2).

4.5. Priors

The random forest algorithm is not a Bayesian technique. Its knowledge of $P(y)$ is inferred directly from the frequencies of the classes present in the training set, not through assumption (or knowledge) of some continuous probability function $P$(AFP) when computed this way is problematic in this data set because this class is underrepresented in the training data (see Section 4.2). So the estimate of $P$(AFP) is likely to underestimate the true $P$(AFP).

$P$(NTP) is highly dependent on the algorithm used to detect TCEs; the periodic, instrumental noise present; and the population of target stars. The most comprehensive alternative attempt at discovering planets in the Kepler data is detailed in Petigura et al. (2013). In this alternative pipeline 16,227 TCEs were detected. So it would seem that transit detection algorithms lead to an abundance of false detections.

$P$(PC) conflates the detectability of planets with the actual occurrence rates of planets within our galaxy. Detectability is most influenced by the the S/N, which is proportional to the square root of the number of transits. Section 7.1 partially addresses the signal-to-noise issues. We discuss how the random forest fares when the training data is restricted to shorter-period TCEs, but is asked to predict against longer-period TCEs. The Kepler team is still in the process of assessing the detection rate (DR) of the pipeline.

Our approach to dealing with priors is to take the frequency of different classes as is and then to reweigh the votes of the random forest to account for the effects of an underrepresented frequency of AFP. Sections 7.2 and 7.3 discuss how the classifier fares with these corrected priors on an expanded data set with more known classifications.

4.6. Matching Ephemerides

We match the ephemeris contained in the KOI catalog to the TCE catalog in order to identify labels for training data. Additionally, this algorithm is also used to compute correlations with other TCEs. This turns out to be an important attribute for class AFP and NTP (Section 5).

For each KOI $K_j$, we identify all the TCEs $J_i$ where $C_i = C_j$ (the set of TCEs and Kepler objects of interest that are on the same target star). We identify the best match to the KOI in the following way. We compute the Pearson’s correlation
5. ATTRIBUTES

5.1. Missing Attribute Values

In some cases attribute values are not available. This can occur because information is missing in stellar catalogs, the data validation fit fails to converge, or a processing timeout is reached. Several methods of dealing with missing data were investigated: using sentinel values, imputing missing values, and training different classifiers for each subset of missing data. Imputing missing values involves substituting reasonable values for the missing data. During training, class-conditional values of mean, median, and most common are used. During prediction, the non-conditional version of those functions are used to fill the values for the unclassified TCEs. Training multiple classifiers involves identifying those subsets of attributes that are commonly defined. A sentinel value is a special value that is not commonly seen in the distribution of the attribute; we use –1. Using a sentinel value turns out to be the simplest method with the lowest error rate. Internally, when stellar parameters are not available, data validation uses the Sun’s parameters. For example, when stellar radius is not available data validation assumes that the unknown radius is 1 $R_\odot$.

5.2. Attribute Pruning

5.2.1. Introduction

The initial attribute set contains 237 attributes that are based on the wavelet matched filter used by TPS, transit model fitting, difference image centroids, and some additional tests.

The principle of parsimony says we should prefer a classifier that uses fewer attributes to one that uses more attributes. Also, should many attributes have poor strength, which is poor prediction value, then their presence in the training set will cause degradation of classification performance. Finally, attributes that are correlated with each other can cause the random forest’s error bound to be weaker than it might otherwise be (Equation (5)). For these reasons we remove attributes from our initial training set.

5.2.2. Importance

An importance function returns an estimate the importance of an attribute relative to other attributes, $Q: x_i \rightarrow \mathbb{R}$. Attributes can be ranked by their importance; a measure of how much the attribute influences the error rate of the random forest. This is computed by using the out-of-bag data, permuting the values of the attribute among the out-of-bag TCEs, and recomputing the error rate for the tree. The importance is then the mean increase in error over all the trees in the random forest when the value of the attribute has been permuted. Random permutations are used so that values come from the same distribution, but are no longer correlated with any classes.

Sometimes we want to refer to the class-conditional importance $Q(x_i | y)$; that is, we want to measure how important a variable is to predicting a particular class rather then the importance over all classes. When comparing the importance of an attribute with other attributes, we use the maximum of all the class-conditional importances for each attribute, which is represented as $\max_i(Q(x_i | y_i))$. In this way, an attribute that is important for discriminating only one class will not be discarded in Section 5.2.3.
5.2.3. Removing Weak Attributes

In order to identify weak attributes we must first know what the importance of a weak attribute looks like. To do this we add an attribute that is generated with a random number generator to the training set and then measure the importance of this random attribute. We trained 151 random forests, each with a different randomly generated attribute. This gives us an estimate of the importance of a random attribute, \( Q(x_{\text{random}}) \). We choose a cutoff of \( 6\sigma \) of \( Q(x_{\text{random}}) \) above zero importance; this turns out to be 5E-5. Attributes that have a maximum, class-conditional importance less than this threshold are dropped. This removes 35 attributes.

5.2.4. Removing Correlated Attributes

Equation (5) implies that removing correlated attributes can decrease the error rate of the random forest because it will decorrelate errors. To remove correlated attributes, we compute the matrix of the absolute values of Pearson’s correlation coefficients, \( \rho_{ij} \), from our matrix of attributes. \( \theta_{ij} \) is a correlation threshold, attributes \((x_i, x_j)\) whose \( \rho_{ij} \) is greater than this threshold are considered significantly correlated.

For each pair of attributes \((x_i, x_j)\), if \( \rho_{ij} \geq \theta_{ij} \), then we drop one or the other attribute. The attribute that has the lower of the two class-conditional importances \( \max_c(Q(x_i|y)) \) is dropped.

To estimate \( \theta_{ij} \), we trained a random forest by imposing various values of \( \theta_{ij} \in [0.15, 1.0] \) in 0.05 increments. We verified that the out-of-bag error (Section 3.4) differs by only 5E-4 in the interval \( \theta_{ij} \in [0.35, 1.0] \). Removing one of a pair of attributes with lower values of \( \theta_{ij} \) increases the out-of-bag error. Therefore reducing the attribute correlation threshold does not produce any significant decrease in misclassification error. However, this still allows us to reduce the number of attributes used by the random forest to produce a more parsimonious training set.

At the minimum out-of-bag error, \( \theta_{ij} = 0.55 \) and there are 77 attributes that meet our thresholds. The 10 most important of these attributes are described in detail in Section 5.3.

5.3. Most Important Attributes

We discuss the top 10 most important attributes in this section. This cutoff is arbitrary for the sake of brevity. The range of attribute importance of the top 10 attributes is from 7.5% increase in out-of-bag error down to a 5.3% increase in out-of-bag error. For the purpose of ranking attributes by importance we use the maximum of the class-conditional importances.

Figures 5 and 6 have the class-conditional attribute distributions for these attributes.

1. The maximum ephemeris correlation, \( \rho_{\text{match}} \) (Equation (7)), is computed for a TCE against all the other TCEs on the same star. If there is only one TCE on the same star then this value is zero. When the ephemerides of TCEs on the same star are highly correlated it is an indication that a secondary eclipse may be present and has been detected as a TCE. For NTPs this may indicate that a similar source of instrumental noise has been detected with a slightly different phase.

2. The absolute value of the ratio of the maximum MES to the minimum MES (see Section 2.2) found over all search periods. When this value is near 1 it indicates that the periodic events lower than the median flux are of similar statistical significance to similar events greater than the median flux. This attribute attempts to eliminate TCEs that are problematic with respect to stellar variability and instrumental noise.

3. The SNR for the all-transit model fit. This is the transit depth normalized by its uncertainty.

4. MES scaled by SES auto-correlation statistic; MES(1 − R). The expected SES time series should have negligible auto-correlation strength, \( R \), beyond the transit duration time scale. This expectation is not always met in practice for the Kepler flux time series, having residual astrophysics and systematics remaining after the detrending and whitening filter is applied.

To identify targets with enhanced auto-correlation strength beyond the expectation, we begin with the SES time series assuming a 10.5 hr transit duration, and remove cadences with bad data. The remaining good cadences are separated into blocks of 4250 cadences (similar to a single Kepler observing quarter). For each block of 4250 cadences, the auto-correlation is calculated out to lag 1050, and we calculate the fraction of the lags where the auto-correlation value is above or below the 95% or 5% expectation, respectively. We simulate the expected auto-correlation value through 150 k Monte Carlo trials. A Monte Carlo trial starts with a random realization of a zero-mean, unit-variance Gaussian vector of length 4250, with a moving average applied with a 10.5 hr window size. The Monte Carlo trial roughly corresponds to the expectation for the SES time series in the null case. We measure the auto-correlation on the Monte Carlo trials to empirically estimate the 5% lower and 95% upper bound expectation at each lag.

The expectation for a null result (well behaved) SES time series is an auto-correlation strength of 0.05; meaning 5% of the lags for a typical SES time series are above the expectation set by the Monte Carlo simulation. As values approach 1.0 for the auto-correlation strength, the SES is demonstrating very large variability and systematics remaining after the detrending and whitening filter is applied.

\[
\theta_{ij} = \frac{1}{2} \left(1 + \cos\left(\frac{\pi x}{L}\right)\right)
\]

where the auto-correlation value is above or below the expected auto-correlation value through 150 k Monte Carlo trials. A Monte Carlo trial starts with a random realization of a zero-mean, unit-variance Gaussian vector of length 4250, with a moving average applied with a 10.5 hr window size. The Monte Carlo trial roughly corresponds to the expectation for the SES time series in the null case. We measure the auto-correlation on the Monte Carlo trials to empirically estimate the 5% lower and 95% upper bound expectation at each lag.

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amounts of auto-correlation and can violate an underlying assumption of the detection statistics. We use the median of the auto-correlation strength across all the blocks to scale the detection statistic, $R$.

5. The $\chi^2$ for the all-transit model fit. This is the raw $\chi^2$ value (i.e., not scaled by the degrees of freedom).

6. Same as attribute 5, but this only considers the odd numbered transits. Comments about odd and even transits made in attribute 7 apply equally here as well. The Kolmogorov–Smirnov test shows the importance of this attribute is significantly greater than the all-transit-fit version of this attribute (attribute 5) for class NTP with $p \ll 0.001$.

7. The ratio of the fitted planet's semimajor axis to the star radius for only the even numbered transits.

Sampling only the even transits (or conversely the odd transits) may have the effect of skipping or including quarters of data that are more problematic. During the

Figure 5. Class-conditional distributions of attributes 1 through 6. If an attribute's domain extends to zero or negative numbers, a small constant has been added so that it can be log scaled. $\Delta f$ (Equation (2)) is plotted to show where a split might be made if it was the first split in a decision tree.
second quarter of operation *Kepler* experienced a number of safe modes causing thermal transients. During the fourth quarter one of the CCDs modules failed. During the eighth quarter a number of safe modes occurred. *Kepler* experienced a coronal mass ejection event during the 12th quarter.

In order to see if the importance of this attribute was due to the randomness of the random forest, we trained 40 random forests and then tested the distributions of the importances for this attribute versus the distribution of the importances of the all-transit-fit version. The Kolmogorov–Smirnov test shows that the importance of this attribute is significantly greater than the all-transit-fit version of this attribute for class NTP with $p < 0.001$.

Additionally we computed the importance of this attribute for every TCE. The TCEs that show this attribute as having higher importance than the all-transit-fit version of this attribute tend to have longer periods; greater than four days. This also corresponds with the somewhat bimodal distribution of NTPs, which tend to be more prevalent at relatively shorter and longer periods, as shown in the plot of attribute 7 in Figure 6. There is a weak negative correlation of $-0.22$ (Pearson’s correlation coefficient) with the effective temperature of the target star.

8. The uncertainty of the angular offset on the plane of the sky between the best-fit centroids from the difference image and the KIC position by averaging over all quarters. The KIC position is subtracted from the difference image centroid. TCEs with large offsets from the KIC position are believed to be caused by background eclipsing binaries or some other events that are not on the target star.

9. The significance of attribute 8 rather than the uncertainty itself.

10. The proportion of the light curve that was missing during this TCE’s transit. We use an already detrended light curve that is median detrended with a window three times the transit duration. This is folded on the TCE ephemeris. The detrended light curve is binned with a bin width of half a transit duration for bins within four transit durations of the transit center. This attribute is the fraction of the bins that have any data contributing to them. A value of less than one indicates the TCE is overlapping with a region of data that are missing when phase folded on the ephemeris.

---

**Figure 6.** Class-conditional distributions of attributes 7 through 10. If an attribute’s domain extends to zero or negative numbers, a small constant has been added so that it can be log scaled. $\Delta I$ (Equation (2)) is plotted to show where a split might be made if it was the first split in a decision tree.
6. CLASSIFICATION RESULTS

6.1. Assessment

When assessing classification performance, we use the out-of-bag error (Section 3.4) rather than cross validation (the common approach for estimating the misclassification rate). We tuned the number of trees in the random forest so that the out-of-bag errors are close to the leave-one-out-cross-validation votes. When \( N_{\text{trees}} = 1000 \) out-of-bag votes have a correlation with the leave-one-out-cross-validated votes of 0.90; when \( N_{\text{trees}} = 3000 \) this correlation becomes 0.998. We use \( N_{\text{trees}} = 15,000 \), because this allows us some margin of error and is still computationally tractable. Since each TCE used for training is out-of-bag a random number of times, the votes are normalized by the number of trees for which the training TCE was out-of-bag, so that \( \sum_{i=1}^{C} v_i = 1 \).

The number of attributes considered for any split of the training set is known as \( m_{\text{try}} \) (Section 3.4). The value of \( m_{\text{try}} \) suggested by Liaw & Wiener (2002) is \( \lfloor \sqrt{A} \rfloor \), where \( A \) is the number of attributes. In practice, the random forest is not very sensitive to changes in \( m_{\text{try}} \). For our final 77 attributes \( m_{\text{try}} = 9 \).

We are able to achieve an out-of-bag error rate of 2.19%.

6.2. Optimal Loss Function

It is possible to stop here and use this vote tuple to assess the performance, but we also weigh the votes so they minimize the out-of-bag error. We do this in a manner that allows us to change the our assumptions about the priors.

We compute the confusion rate matrix. The columns of a confusion matrix indicate the predicted classes, while the rows indicate the actual class. An entry in the diagonal indicates the count of correct classifications, off-diagonal entries indicate misclassifications of various kinds. For the ideal confusion matrix, the sum of the diagonal elements is equal to the number of items in the training set. A confusion rate matrix is a rate rather than a count of classifications. For the ideal confusion rate matrix, the diagonal would be the frequency of the classes present in the training set.

The out-of-bag votes are \( v_i(l) \) for class \( y_i \) for TCE \( l \in \mathcal{L} \). The votes are weighted by \( \Omega = \omega_1, \omega_2, \omega_3 \). The function \( I: y \to 0, 1 \), is an indicator function that returns 1 for correct classifications, otherwise it returns 0. Parameter \( \omega_0 \) is not a free parameter and is set to 1. The confusion rate matrix is defined as

\[
\zeta_{ij}(\Omega) = \frac{1}{|\mathcal{I}|} \sum_{l \in \mathcal{L}} I(y_j = \arg \max_{i=1}^{C} \{ \omega_i v_i(l) \}).
\]

We followed the methodology of Landgrebe & Duin (2007) and chose an \( \Omega \) that minimizes following the loss function representing the Bayes costs for the given set of weights:

\[
L(\Omega) = \sum_{i=1}^{C} P(y_i) \left( \sum_{j=1, j \neq i}^{C} \zeta_{ij}(\Omega) S_{ij} \right) - \sum_{i=1}^{C} P(y_i) \zeta_{ii}(\Omega) S_{ii},
\]

where \( S_{ij} \) is the cost matrix, and \( \zeta_{ij} \) is the confusion rate matrix specifying the fraction of objects with label \( i \) classified as class \( j \) by the classifier with class weights \( \Omega \). In this paper we set the cost matrix to have zeros along its diagonal and ones elsewhere. This corresponds to minimizing the total number of misclassifications. A logarithmically spaced grid is used to search for values of \( \Omega \) that minimize Equation (9). Prior probabilities, \( P(y_i) \), of classes are estimated from the frequency of the classes in the training set.

At the optimal values of \( \Omega \) the random forest is able to achieve out-of-bag error of 1.34%, which is an improvement of 0.85% over the unweighted version. The resulting confusion matrix is presented in Table 1. The diagonal elements of a confusion matrix represent correct classifications. Off-diagonal elements are errors. The error rate can be computed from the confusion matrix by summing all the off-diagonal elements and then dividing by the sum of all matrix elements.

From the weighted out-of-bag votes we produce a Receiver Operating Characteristic (ROC) curve that shows DR as a function of the false positive rate. To generate the curve, we calculate the false positive rate at vote thresholds in \( 0.01 \) increments in the interval \([0, 1]\). A vote threshold of one is accepting a classification only when all trees are unanimous and a zero vote threshold is accepting every classification for the class under examination. A vote threshold of zero indicates that an instance of the class will never be misclassified, but also guarantees a high false positive rate. The DR is the number of instances of the class that are correctly classified, divided by the number present in the training data. The false alarm rate (FAR) is the number of misclassifications, divided by the number of instances of the undesirable classes detected in the training set. The Area Under the Curve (AUC) is the integrated area under the ROC curve. This is a useful metric when comparing classifiers. A classifier with a superior AUC will have some trade off between DR and FAR that results in a higher DR/FAR ratio than one with a lower AUC. For more information on the ROC, see Fawcett (2004). PCs versus AFP show an orbital period dependent ROC curve, see Figure 7. This is likely caused by a lower DR for Kepler at longer periods and therefore less training data at longer periods for all classes.

6.3. Comparison With Other Classification Algorithms

In addition to the random forest, we also tried other well-known classification algorithms that are often used as benchmarks for other classification problem domains: k-nearest neighbors (k-NN) and naive Bayes.

The k-NN algorithm (Duda et al. 2001) has the advantage that it is simple, explainable, and provides bounded error, but in a different manner than the random forest. With a training set of finite size, k-NN would converge to no more than twice the error bounds of a Bayesian classifier, with perfect knowledge of the joint probability distribution function of all the attributes. k-NN classifies an unknown using the minimum distance to some example in the training set. The Euclidean distance function between points in the attribute space is used. The notion of distance in can be broadened to include the class

| Training Set Class | PC | AFP | NTP |
|--------------------|----|-----|-----|
| PC                 | 2843 | 8 | 28 |
| AFP                | 98  | 271| 24 |
| NTP                | 25  | 12 | 11.267 |
of the k-nearest neighbors instead of just a single nearest neighbor. For our problem this turns out not to be useful; optimal \( k \) turns out to be \( k = 1 \). Other values of \( k \) turn out to have classification performance that is very close to random.

An identical training set is used for RF and k-NN, except that the attributes are log scaled. To assess k-NN performance we use leave-one-out cross validation. Unfortunately, since \( k = 1 \), it is not possible to plot an ROC curve for k-NN because its classification space is just a single point (Figure 8).

A naive Bayes classifier assigns a classification by choosing the class with the highest probability given the evidence. This algorithm has the advantage that it is simple, explainable, and provides probabilities rather than votes.

\[
i^* = \arg \max_j P(y_j | x_u)
\]

\[
P(y_j | x) = P(y_j) \prod_{j=1}^A \frac{P(x_j|y_j)}{P(x_j)},
\]

where \( x \) refers to the attributes of the unknown TCE and \( A \) is the number of attributes. Prior probabilities, \( P(y_j) \), of classes are estimated from the frequency of the classes in the training set. Probability distributions, \( P(x_j|y_j) \), are estimated using a kernel density estimator. We use a Gaussian kernel with Silverman’s rule-of-thumb bandwidth as described in Feigelson & Babu (2012). The implication of Equation (10) is that our attributes are independent from one another; it is naive after all.

We use leave-one-out cross validation to estimate the classification performance. The resulting error rates for k-NN and naive Bayes are 3.15% and 2.73%, respectively. Performance of all classification algorithms described in this paper is presented for the purpose of discriminating between PC \( \cup \) AFP versus NTP in Figure 8.

These results show that while other classification algorithms have better than random performance, they do not perform as well as the random forest.

7. APPLICATION TO TRANSIT SURVEYS

7.1. Classifying Against Longer Orbital Periods Than Training Data

A transit survey such as Kepler will initially discover larger, shorter-period planets. As the survey continues it will find smaller, longer-period planets. This poses a potential issue to the supervised machine-learning algorithm because a portion of parameter space it is trained on may no longer be representative of the population as a whole. We look at what happens to classification errors when we only have successively smaller amounts of training data and for shorter orbital periods.

Figure 9 shows the error rates achieved when limiting the amount of training data used to less than some orbital period. The abscissa is the log orbital period. The ordinate is the portion of the TCEs retained for training that have orbital periods less than the abscissa. The value plotted is log of the misclassification error of all the data that was not used for training.

![Figure 7. Period dependent ROC curve for PC vs. AFP. For all orbital periods the AUC is 0.9522 ± 0.0080. For the orbital period bins \( p \leq 10, 10 < p \leq 100, \) and \( p > 100 \) the AUC are 0.9568 ± 0.0094, 0.9484 ± 0.0193, and 0.8229 ± 0.0730, respectively.](image)

![Figure 8. Comparison of random forest, naive Bayes, and k-NN. AUC = 0.9991 for random forest and 0.9894 for naive Bayes. k-NN (when \( k = 1 \)) does not produce a ranking of predictions and so is represented as a single point in the trade space between detection rate and false alarm rate.](image)

![Figure 9. The effects of limiting the amount of training data used to less than some orbital period. The abscissa is the log orbital period. The ordinate is the portion of the TCEs retained for training that have orbital periods less than the abscissa. The value plotted is log of the misclassification error of all the data that was not used for training.](image)
and the out-of-bag error. The mean out-of-bag error of the three random forests is used to estimate the error surface in Figure 9.

At a period of 16 days and training data fraction of zero, no training data longer than 16 days is used to train the random forests. The error rate for this orbital period is 3.13%. If we were then expanding our search to longer periods, we would only need to add 5% of the TCEs with periods longer than 16 days in order to have the error rates fall to 1.56%. Therefore adding a small, but uniformly sampled (with respect to orbital period) portion of the unknown TCEs to the training set can yield a large reduction in misclassification error.

### 7.2. Predictions on Later TCERT Detections

The TCE catalog contains 3831 TCEs that are not labeled with our ephemeris matching algorithm. Of these, 1487 have since been given dispositions by the TCERT using somewhat different techniques from the original training set, which were methods described in Coughlin et al. (2014). We now look at the classification predictions on this later set of TCEs that were not in the training set. Table 2 contains the confusion matrix of the random forest predictions.

We looked at a random sample of a small number of AFPs that were misclassified as PCs. The vast majority of these were determined by the TCERT to be AFPs based on information that was not available in the training set of attributes. These classifications are based on the presence of significant secondary eclipses, indicating an eclipsing binary. Another source of false positives is direct PRF contamination. In these cases the light from a nearby, but out-of-aperture star, induces a transit signal on the target star and our existing attributes are not able to detect the off-aperture false positive.

AFPs that are misclassified as NTP are partially due to a labeling problem that the TCERT will remedy in the future: the KOI table generated by TCERT homogenizes all kinds of non-planetary TCEs into one category: false positive. Non-planet TCEs that are astrophysical in nature and those that are instrumental both receive the false positive label, which is why there is not a NTP row in Table 2.

### 7.3. Using Corrected Priors

The priors used in our training set are much different compared with the test set used in Section 7.2. Using Equation (9) we can reweigh the votes of the trained classifier to correct for the eclipsing binaries that were omitted from the run of the Kepler pipeline, and so do not appear (see Section 4.2). Table 3 shows improvement when more realistic priors are used. Table 4 is the combined confusion matrix representing the TCEs in Tables 1 and 3 (with different priors).

With priors reflecting more eclipsing binaries, the total error from Table 4 is 5.85%. When the errors between AFPs and NTPs are ignored we have an error rate of 2.81%, which is more relevant for planet detection.

### 8. CONCLUSION

Machine learning techniques offer a way to automate some stages of exoplanet discovery. In this paper we have demonstrated that the random forest algorithm is quite good at distinguishing between systematic noise, eclipsing binary and exoplanet candidate signatures. As seen in Table 4, classifications have a low overall error rate (5.85%), and when ignoring distinctions between AFP and noise, the error rate falls to 2.81%.

When used to predict on longer orbital periods than the training data, the overall error rate increases. This can be mitigated by sampling a small percentage of the most recent TCE detections, classifying them, and adding them to the training set. There are some populations of AFP that have been identified using other methods; with attributes not available in the training data set. The random forest often confuses these astrophysical false positive TCEs with PCs and NTP (Table 2). In the future we intend to add additional attributes that would help separate out the AFP. Newer versions of the TPS software can detect weak secondary eclipses that would indicate the presence of an eclipsing binary. Transit signatures induced by off-aperture sources can be identified by performing photometry on the local background pixels of the target stars. Transits detected in this aperture should not have a similar significance to the transits detected on the target stars.

The Kepler mission is currently working to estimate the completeness of the pipeline using injected transits (Christian et al. 2013). Using injected transits as training data will allow us to assess the accuracy of human and machine classification efforts. We look forward to the continued revision and applications of these automated classification methods on subsequent Kepler pipeline runs, and these methods can be readily applied to large transit surveys in the future, such as TESS (Ricker et al. 2014).

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