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The CCB-ID approach to tree species mapping with airborne imaging spectroscopy

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Background. Biogeographers assess how species distributions and abundances affect the structure, function, and composition of ecosystems. Yet we face a major challenge: it is difficult to precisely map species across landscapes. Novel Earth observations could obviate this challenge. Airborne imaging spectrometers measure plant functional traits at high resolution, and these measurements can be used to identify tree species. Plant traits are often highly conserved within species, and highly variable between species, which provides the biophysical basis for species mapping. In this paper I describe a trait-based approach to species identification with imaging spectroscopy, *CCB-ID*, which was developed as part of a NIST-sponsored ecological data science evaluation (ECODSE).

Methods. These methods were developed using NEON airborne imaging spectroscopy data. CCB-ID classifies tree species using trait-based reflectance variation and decision tree-based machine learning models, approximating a morphological trait and dichotomous key method traditionally used in botanical classification. First, outliers were removed using a spectral variance threshold. The remaining samples were transformed using principal components analysis and resampled by species to reduce common species biases. Gradient boosting and random forest classifiers were trained using the transformed and resampled feature data. Prediction probabilities were then calibrated using sigmoid regression, and sample-scale predictions were averaged to the crown scale.

Results. This approach performed well according to the competition metrics, receiving a rank-1 accuracy score of 0.919, and a cross-entropy cost score of 0.447 on the test data. Accuracy and specificity scores were high for all species, but precision and recall scores were variable for rare species. PCA transformation improved accuracy scores compared to models trained using reflectance data, but outlier removal and data resampling exacerbated class imbalance problems.

Discussion. CCB-ID accurately classified tree species using NEON imaging spectroscopy data, reporting the best classification scores among participants. However, it failed to overcome several well-known species mapping challenges, like precisely identifying rare species. Key takeaways include (1) training models to maximize metrics beyond accuracy (e.g. recall) could improve rare species predictions, (2) within-genus trait variation may drive spectral separability, precluding efforts to distinguish between functionally convergent species, (3) outlier removal and data resampling exacerbated class imbalance problems, and should be carefully implemented, (4) PCA transformation greatly improved model results, and (5) feature selection could further improve species classification models. CCB-ID is open source, designed for use with NEON data, and available to support future species mapping efforts.

The CCB-ID approach to tree species mapping with airborne imaging spectroscopy

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Abstract

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Methods. These methods were developed using NEON airborne imaging spectroscopy data. *CCB-ID* classifies tree species using trait-based reflectance variation and decision tree-based machine learning models, approximating a morphological trait and dichotomous key method traditionally used in botanical classification. First, outliers were removed using a spectral variance threshold. The remaining samples were transformed using principal components analysis and resampled by species to reduce common species biases. Gradient boosting and random forest classifiers were trained using the transformed and resampled feature data. Prediction probabilities were then calibrated using sigmoid regression, and sample-scale predictions were averaged to the crown scale.

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Discussion. *CCB-ID* accurately classified tree species using NEON imaging spectroscopy data, reporting the best classification scores among participants. However, it failed to overcome several well-known species mapping challenges, like precisely identifying rare species. Key takeaways include (1) training models to maximize metrics beyond accuracy (e.g. recall) could improve rare species predictions, (2) within-genus trait variation may drive spectral separability, precluding efforts to distinguish between functionally convergent species, (3) outlier removal and data resampling exacerbated class imbalance problems, and should be carefully implemented, (4) PCA transformation greatly improved model results, and (5) feature selection could further improve species classification models. *CCB-ID* is open source, designed for use with NEON data, and available to support future species mapping efforts.

1 Introduction

2 When you get down to it, biogeographers seek to answer two key questions: where are
3 the species, and why are they where they are? Answering these simple questions has proven
4 remarkably difficult. The former reflects a data gap; we do not have complete or unbiased
5 information on where species occur. This is known as the ‘Wallacean shortfall’ (Whittaker et al.,
6 2005; Bini et al., 2006). Addressing the latter, however, does not necessarily require data; the
7 drivers of species abundances and their spatial distributions can be derived from ecological
8 theory (McGill, 2010). But evaluating these theoretical predictions does require data. Testing
9 generalized theories of species distributions requires continuously-mapped presences and
10 absences for many individuals across large areas. And while field efforts can assess fine-scale
11 distribution patterns, they are often restricted to small extents. Mapping organism-scale species
12 distributions over landscapes could help fill the data gaps that preclude addressing these key
13 biogeographic questions. One remote sensing dataset holds the promise to do so: airborne
14 imaging spectroscopy.

15 Airborne imaging spectrometers measure variation in the biophysical properties of soils
16 and vegetation at fine grain sizes across large areas (Goetz et al., 1985). In vegetation mapping
17 contexts, imaging spectroscopy can map plant structural traits, like leaf area index and leaf angle
18 distribution (Broge & Leblanc, 2001; Asner & Martin, 2008), and plant functional traits, like
19 growth and defense compound concentrations (Kokaly et al., 2009; Asner et al., 2015). These
20 traits tend to be highly conserved within tree species, and highly variable between species (i.e.,
21 interspecific trait variation is often much greater than intraspecific trait variation; (Townsend et
22 al., 2007; Asner et al., 2011). This trait conservation provides the conceptual and biophysical
23 basis for species mapping with imaging spectroscopy. Indeed, airborne imaging spectroscopy has
24 been used to map crown-scale species distributions across large extents in several contexts

25 (Fassnacht et al., 2016). These approaches have been applied in temperate (Baldeck et al., 2014)
26 and tropical ecosystems (Hesketh & Sánchez-Azofeifa, 2012), using multiple classification
27 methods (Ferret & Asner, 2013) and multiple sensors (Clark, Roberts & Clark, 2005; Colgan et
28 al., 2012; Baldeck et al., 2015). However, this wide range of approaches has not yet identified a
29 canonical best practice for tree species identification.

30 In this paper I describe an approach to tree species classification using airborne imaging
31 spectroscopy data that builds on the above methods to advance the discussion on best practices.
32 This approach was developed as a submission to a NIST-sponsored ecological data science
33 evaluation competition (ECODSE; <https://ecodse.org>). This competition had participants use
34 airborne imaging spectroscopy data, collected by the National Ecological Observatory Network's
35 Airborne Observation Platform (NEON AOP), to identify tree crowns to the species level. The
36 work described below was submitted under the team name of the Stanford Center for
37 Conservation Biology (Stanford CCB), and has since been formalized under the moniker *CCB-*
38 *ID* (<https://github.com/stanford-ccb/ccb-id>). First, I describe the CCB-ID approach to tree
39 species classification using airborne imaging spectroscopy data. Next, I review its successes and
40 shortcomings in the context of this competition. Finally, I highlight key opportunities to improve
41 future imaging spectroscopy-based species classification approaches. The goals of this work are
42 to improve NEON's operational tree species mapping efforts and to reduce barriers for
43 addressing key data gaps in biogeography.

44 **Materials & Methods**

45 The CCB-ID approach was inspired by botanical and taxonomic approaches to species
46 classification. In the field, botanists can use plant morphological features and a dichotomous key
47 to identify tree species. These features often include variations in reproductive traits (e.g.,

48 flowering bodies, seeds), vascular traits (e.g., types of woody and non-woody tissue), and foliar
49 traits (e.g., waxy or serrated leaves). The dichotomous key approach hierarchically partitions
50 species until each can be identified using a specific combination of traits.

51 Species classification with imaging spectroscopy is rather restricted, in comparison;
52 imaging spectrometers can only measure a subset of plant traits. Furthermore, the inter- and
53 intraspecific variation in this subset of traits is rarely known *a priori*, precluding the use of a
54 standard dichotomous key. Imaging spectroscopy approaches to species classification instead
55 rely on distinguishing species-specific variations in canopy reflectance signal. However, several
56 confounding factors drive variation in canopy reflectance data, including (1) measurement
57 conditions (e.g., sun and sensor angles), (2) canopy structure (e.g., leaf area index or leaf angle
58 distribution), (3) leaf morphology and physiology (i.e., plant functional traits), and (4) sensor
59 noise. Measurement conditions and canopy structure tend to drive the majority of variation; up to
60 79-89% of spectral variance is driven by within-crown variation (Baldeck & Asner, 2014; Yao et
61 al., 2015). Unfortunately, this variation does not help distinguish between species. Interspecific
62 spectral variation is instead driven by functional trait variation (Asner et al., 2011).
63 Disentangling trait-based variation from measurement and structure-based variation is thus
64 central to mapping species with airborne imaging spectroscopy.

65 CCB-ID classifies tree species using trait-based reflectance variation with decision tree-
66 based machine learning models. This approach approximates a morphological trait and
67 dichotomous key model, and is described in the following sections. The first section describes
68 the outlier removal and data transformation procedures. The second section describes how the
69 training data were resampled to reduce biases towards common species. The third section
70 describes model selection, training, and probability calibration. The fourth section describes the

71 model performance metrics, and the final section describes two analyses performed post-
72 ECODSE submission.

73 The data from NEON included the following data products: 1) Woody plant vegetation
74 structure (NEON.DP1.10098); 2) Spectrometer orthorectified surface directional reflectance -
75 flightline (NEON.DP1.30008); 3) Ecosystem structure (NEON.DP3.30015); and High-resolution
76 orthorectified camera imagery (NEON.DP1.30010). These data were provided by the ECODSE
77 group (2017; <https://ecodse.org>). All analyses were performed using the Python programming
78 language (Oliphant, 2007; <https://python.org>) and the following open source packages: NumPy
79 (der Walt, Colbert & Varoquaux, 2011; <http://numpy.org>), scikit-learn (Pedregosa et al., 2011;
80 <http://scikit-learn.org>), pandas (McKinney et al., 2010; <https://pandas.pydata.org>), and matplotlib
81 (Hunter, 2007; <https://matplotlib.org>). The python scripts used for these analyses have been
82 uploaded to a public GitHub repository (<https://github.com/stanford-ccb/ccb-id>), including a
83 build script for a Singularity container to ensure computational replicability (Kurtzer, Sochat &
84 Bauer, 2017).

85 *Data preprocessing*

86 The canopy reflectance data were preprocessed using two steps: outlier removal and
87 dimensionality reduction. In the outlier removal step, the reflectance data were spectrally subset,
88 transformed using PCA, then thresholded to isolate spurious values. First, reflectance values
89 from the blue region of the spectrum (0.38-0.49 μm) and from noisy bands (1.35-1.43 μm , 1.80-
90 1.96 μm , and 2.48-2.51 μm) were removed. These bands correspond to wavelengths dominated
91 by atmospheric water vapor, and do not track variations in plant traits (Gao et al., 2009; Asner et
92 al., 2015). Next, these spectrally-subset samples were transformed using PCA. The output
93 components were whitened to zero mean and unit variance, and outliers were identified using a

94 three-sigma threshold. Samples with values outside of +/- three standard deviations from the
95 means (i.e., which did not fall within 99.7% of the variation for each component) for the first 20
96 principal components were excluded from analysis. These samples were expected to contain
97 non-vegetation spectra (e.g., exposed soil), unusually bright or dark spectra, or anomalously
98 noisy spectra (Féret & Asner, 2014). The outlier-removed reflectance profiles for each species
99 are shown in Figure 1.

100 Once the outliers were removed, the remaining spectra were transformed using PCA.
101 This was not performed on the already-transformed data from the outlier removal process, but on
102 the outlier-removed, spectrally-subset reflectance data. PCA transformations are often applied to
103 airborne imaging spectrometer data to handle the high degree of correlation between bands, and
104 these transformations are highly sensitive to input feature variation (Jia & Richards, 1999).
105 Furthermore, transforming reflectance data into principal components can isolate the variation
106 driven by measurement conditions from variation driven by functional traits, which is critical for
107 distinguishing between species. And though trait-based variation drives a small proportion of
108 total reflectance signal, a single trait can be expressed in up to 9 orthogonal components (Asner
109 et al., 2015). After the transformation, the first 100 components were used as feature vectors for
110 the species classification models. This threshold was arbitrary; it was set to capture the majority
111 of biologically-relevant components and to exclude noisy components.

112 *Class imbalance*

113 Class imbalance refers to datasets where the number of samples per-class are not evenly
114 distributed among classes. Imbalanced data sets are common in classification contexts, but can
115 lead to problems if this imbalance is not addressed. Training classification models with
116 imbalanced data can select for models that overpredict common classes when model

117 performance is based on metrics like accuracy. The ECODSE data were imbalanced: after outlier
118 removal, these data contained a total of 6,034 samples from 9 classes (8 identified species, one
119 ‘other species’ class). The most common species, *Pinus palustris*, contained 4,026 samples (66%
120 of the samples) and the rarest species, *Liquidambar styraciflua*, contained 62 samples (1% of the
121 samples).

122 These data were resampled prior to analysis to reduce the likelihood of overpredicting
123 common species. Resampling was performed by setting a fixed number of samples per class,
124 then undersampling or oversampling each class to that fixed number. This fixed number was set
125 to 400 samples to split the difference of two orders of magnitude between the rarest and the most
126 common classes. This number was arbitrary, but it approximates the number of per-species
127 samples recommended in Baldeck & Asner (2014). To create the final training data, classes with
128 fewer than 400 samples were oversampled with replacement, and classes with more than 400
129 samples were undersampled without replacement. The final training data included 400 samples
130 for each of the 9 classes (3,600 samples total), where each sample contained a feature vector of
131 the principal components derived from the outlier removed, spectrally subset canopy reflectance
132 data.

133 *Model selection, training, and probability calibration*

134 The CCB-ID approach used two machine learning models: a gradient boosting classifier
135 (GBC) and a random forest classifier (RFC; (Friedman, 2001; Breiman, 2001)). These models can
136 fit complex, nonlinear relationships between response and feature data, can automatically handle
137 interactions between features, and have built-in mechanisms to reduce overfitting. They were
138 selected because they perform well in species mapping contexts (Elith, Leathwick & Hastie,
139 2008), in remote sensing contexts (Pal, 2005), and in conjunction with PCA transformations

140 (Rodríguez, Kuncheva & Alonso, 2006). Furthermore, these models are built as ensembles of
141 decision trees, resembling the dichotomous key employed by botanists. Unlike a dichotomous
142 key, these models were trained to learn where to split the data since the trait variation that
143 distinguishes species was not known *a priori*.

144 These models were fit using hyper-parameter tuning and probability calibration
145 procedures. Model hyper-parameters were tuned by selecting the parameters that maximized
146 mean F1 scores in 5-fold cross-validation using an exhaustive grid search. The following
147 parameters were tuned for both models: number of estimators, maximum tree depth, minimum
148 number of samples required to split a node, and minimum node impurity split threshold. The
149 learning rate and node split quality criterion were also tuned for GBC and RFC, respectively. All
150 samples were used for hyper-parameter tuning, and the best model hyper-parameters (i.e., the
151 hyper-parameters that maximized mean F1 scores in cross validation) were used to fit the final
152 models.

153 Accurately characterizing prediction probabilities is essential for error propagation and
154 for assessing model reliability, and prediction probabilities were calibrated once the final hyper-
155 parameters were selected. Well-calibrated probabilities should scale linearly with the true rate of
156 misclassification (i.e., should not be under or overconfident in predictions). Some ensemble
157 methods, like RFC, tend to be poorly calibrated; their variance can skew high probabilities away
158 from one, and low probabilities away from zero, since they average their predictions from a set
159 of weak learners, which individually have high misclassification rates but gain predictive power
160 post-ensemble. This results in sigmoid-shaped reliability diagrams (DeGroot & Fienberg, 1983;
161 Niculescu-Mizil & Caruana, 2005).

162 To reduce these probability biases, prediction probabilities were calibrated using sigmoid
163 regression for both RFC and GBC. The data were first randomly split into three subsets: model
164 training (50%, or 200 samples per class), probability calibration training (25%, or 100 samples
165 per class), and model testing (the remaining 25%). Each classifier was fit using the model
166 training subset and the tuned hyper-parameters. Prediction probabilities were calibrated with
167 sigmoid regression, using the probability training subset and internal 3-fold cross validation to
168 assess the calibration. Calibrated model performance was assessed using the holdout test set.
169 After these assessments, the final models were fit using the model training data, then calibrated
170 using the full probability training and testing data (i.e., the full 50% of samples not used in initial
171 model training).

172 *Model assessment*

173 During model training, performance was assessed on a per-sample basis using model
174 accuracy and log loss scores. Model accuracy calculates the proportion of correctly classified
175 samples in the test data (Figure 2). High model accuracy scores are desirable. Log loss assesses
176 whether the prediction probabilities were well calibrated, penalising incorrect and uncertain
177 predictions. Low log loss scores indicate that misclassifications occur at rates close to the rates
178 predicted by the reported probabilities. During model testing, performance was assessed using
179 rank-1 accuracy and cross entropy cost (Marconi et al., 2018). Rank-1 accuracy was calculated
180 based on which species ID was predicted with the highest probability. The cross entropy score is
181 similar to the log loss function, but was scaled using an indicator function. These can be
182 interpreted in similar ways to accuracy and log loss; high rank-1 accuracy and low cross entropy
183 scores are desirable.

184 Secondary model testing metrics were calculated for each species using the test data.
185 These included model specificity, precision, and recall (Figure 2). These metrics reveal model
186 behavior that accuracy scores may obscure. Specificity assesses model performance on non-
187 target species, penalizing overprediction of the target species (i.e., a high number of false
188 positives). Precision also penalizes overprediction, but assesses the rate of overprediction relative
189 to the rate of true positive predictions. Recall calculates the proportion of true positive
190 predictions to the total number of positive observations per species. Higher values are desirable
191 for each. These metrics were calculated to aid interpretation, but were not used to formally rank
192 model performance.

193 Performance during model training was assessed at the sample scale, but the competition
194 evaluation metrics were calculated using crown-scale prediction probabilities. To address this
195 scale mismatch, prediction probabilities were first calculated for each sample in a crown using
196 both GBC and RFC models. These sample-scale probabilities were then averaged by crown.

197 *Further analyses*

198 Two post-submission analyses were performed to assess how PCA transformations
199 affected model performance. Prior to these analyses, I bootstrapped the original model fits to
200 assess their variance. I then compared these bootstrapped fits to models trained with the
201 spectrally-subset reflectance data instead of the PCA transformed data. Next, I compared models
202 trained using a varying number of principal components. These models were trained using n_{pcs}
203 $\in \{10, 20, \dots, 345\}$ as the input features, with 345 being the maximum number of potential
204 components after spectral subsetting. These comparisons assessed whether the PCA
205 transformations improved model performance, and how changing the amount of spectral

206 variation in the feature data affected performance. These analyses were each bootstrapped 50
207 times.

208 **Results**

209 CCB-ID performed well according to the ECODSE competition metrics, receiving a
210 rank-1 accuracy score of 0.919, and a cross-entropy cost score of 0.447 on the test data. These
211 were the highest rank-1 accuracy and the lowest cross-entropy cost scores among participants. A
212 confusion matrix with the classification results is reported in Table 1. In addition to the high
213 rank-1 accuracy and low cross entropy cost scores, the CCB-ID model performed well according
214 to the secondary crown-scale performance metrics. These secondary metrics calculated a mean
215 accuracy score of 0.979, mean specificity score of 0.985 , mean precision score of 0.614, and
216 mean recall score of 0.713 across all species. The per-species secondary metrics are summarized
217 in Figure 3. These results were calculated using the categorical classification predictions (i.e.,
218 after assigning ones to the species with the highest probabilities, and zeros to all other species).
219 The probability-based confusion matrix and classification metrics are reported in Table S1 and
220 Figure S1, respectively.

221 During model training, outlier removal excluded 797 samples from analysis. After
222 removal, the first principal component contained 78% of the explained variance. However, this
223 component did not drive model performance; it ranked 7th and 11th in terms of ranked feature
224 importance scores for GBC and RFC. Model accuracy scores, calculated on the 25% training
225 data holdout, were 0.933 for GBC and 0.956 for RFC. Log loss scores, calculated prior to
226 probability calibration, were 0.19 for GBC, and 0.47 for RFC. After probability calibration, log
227 loss scores were 0.24 for GBC and 0.16 for RFC. The per-class secondary metrics reported a

228 mean specificity score of 0.987, mean precision score of 0.908, and mean recall score of 0.907
229 across all species.

230 The post-submission analyses found PCA transformations improved model accuracy.
231 Models fit using the original methods calculated mean bootstrapped accuracy scores of 0.944 (s
232 = 0.009) for GBC and 0.955 (s = 0.008) for RFC. Models fit using the spectrally-subset
233 reflectance data as features calculated mean accuracy scores of 0.883 (s = 0.012) for GBC and
234 0.877 (s = 0.011) for RFC, and mean log loss scores of 0.46 (s = 0.03) for GBC and 0.48 (s =
235 0.03) for RFC. For the models fit using varying numbers of principal components, mean model
236 accuracies declined and mean log loss scores increased after including more than 20 components
237 as features (Figure 4).

238 Discussion

239 The CCB-ID approach accurately classified tree species using NEON imaging
240 spectroscopy data, reporting the highest rank-1 accuracy score and lowest cross-entropy cost
241 score among ECOSDE participants. These scores compare favorably to other imaging
242 spectroscopy-based species classification efforts (Fassnacht et al., 2016). The crown-scale test
243 results highlight the potential to develop species mapping methods that approximate botanical
244 and taxonomic approaches to classification. However, this method failed to overcome several
245 well-known species mapping challenges, like precisely identifying rare species. Below, I discuss
246 some key takeaways, and suggest opportunities to improve future imaging spectroscopy-based
247 species classification approaches.

248 The high per-species accuracy scores indicate a high proportion of correctly classified
249 crowns in the test data. However, accuracy can be a misleading metric in imbalanced contexts.
250 Since seven of the nine classes had six or fewer crowns in the test data (out of 126 total test

251 crowns), classification metrics weighted by the true negative rate (i.e., accuracy and specificity)
252 were expected to be high if the majority class were correctly predicted. Metrics weighted instead
253 by the true positive rate (i.e., precision and recall) showed much higher variation across rare
254 species, as a single misclassification greatly alters these metrics when there are few observed
255 crowns (Figure 3). Due to the small sample size, it is difficult to assess if these patterns portend
256 problems at larger scales. For example, there were two observed *Acer rubrum* crowns in the test
257 data, yet only one was correctly predicted. Was the misclassified crown an anomaly? Or will this
258 low precision persist across the landscape, predicting *Acer rubrum* occurrences at half its actual
259 frequency? The latter seems unlikely, in this case; the low cross entropy and log loss scores
260 suggest misclassified crowns were appropriately uncertain in assigning the wrong label (Table
261 S1). However, since airborne species mapping is employed to address large-scale ecological
262 patterns where precision is key (e.g., in biogeography, macroecology, and biogeochemistry), we
263 should be assessing classification performance on more than one or two crowns per species.

264 Model performance between and within taxonomic groups revealed some notable
265 patterns. *Quercus* and *Pinus* individuals (i.e., Oaks and Pines) accounted for 120 of the 126 test
266 crowns and there was high fidelity between them; only one *Quercus* crown was misclassified as
267 *Pinus*, and two *Pinus* crowns were misclassified as *Quercus*. From a botanical perspective, this
268 makes sense; these genera exhibit very different growth forms (i.e., different canopy structures
269 and foliar traits), and should thus be easy to distinguish in reflectance data. However, *Quercus*
270 and *Pinus* showed different within genus patterns. *Quercus* crowns were never misclassified as
271 other *Quercus* species, yet there were several within-*Pinus* misclassifications. This may be
272 because *Quercus* species tightly conserve their canopy structures and foliar traits (Cavender-
273 Bares et al., 2016), while *Pinus* species may express trait plasticity. *Pinus* species maintain

274 similar growth forms (i.e., their needles grow in whorls bunched through the canopy), limiting
275 opportunities to identify species-specific structural variation. Furthermore, they are distributed
276 across the varying climates of the southern, eastern, and central United States, suggesting some
277 degree of niche plasticity. If this plasticity is expressed in each species' functional traits, then
278 convergence among species may then preclude trait-based classification efforts. Quantifying the
279 extent to which foliar traits are conserved within and between species and genera will be
280 essential for assessing the potential for imaging spectroscopy to map community composition
281 across large extents.

282 The post-submission analyses revealed further notable patterns. First, PCA
283 transformation increased mean model accuracy scores compared to the spectrally-subset
284 reflectance data. I suspect this is because the models could focus on the spectral variation driven
285 by more biologically meaningful components instead of searching for that signal in the
286 reflectance spectrum where the majority of variation is driven by abiotic factors. The low feature
287 importance scores of the first principal component support this interpretation. The first
288 component in reflectance data is typically driven by brightness (i.e., not a driver of interspecific
289 variation) and contained 78% of the explained reflectance variance, but ranked low in feature
290 importance for both models. This preprocessing transformation approximates the 'rotation forest'
291 approach developed by Rodríguez, Kuncheva & Alonso (2006). They found PCA transformation
292 improved tree-based ensemble models in several contexts, and they suggested retaining all
293 components to maintain the dimensionality of the input features. However, the analysis that
294 varied the number of feature components showed model accuracy decreased when including
295 more than 20 components (Figure 4). This suggests that using all components could overfit to
296 noise. Performing feature selection on transformed data may help overcome this. Feature

297 selection has been applied to reflectance data to find the spectral features that track functional
298 trait variation (Feilhauer, Asner & Martin, 2015), and I believe it could help identify trait-based
299 components that discriminate between species. Furthermore, other transformation methods may
300 be more appropriate than PCA; principal components serve only as proxies to functional traits in
301 this context. Transforming reflectance data directly into trait-based features could improve
302 species classification efforts, improve model interpretability, and further develop the biophysical
303 basis for species mapping with imaging spectroscopy.

304 Despite the successes of CCB-ID, there were a few missteps in model design and
305 implementation. For example, outlier removal and resampling were employed to obviate class
306 imbalance problems but may instead have exacerbated them. First, the PCA-based outlier
307 removal excluded samples based on deviation from the mean of each component. However,
308 since the transformations were calculated using imbalanced data, the majority of the variance
309 was driven by variation in the most common class. This means outlier removal excluded samples
310 that deviated too far from the mean-centered variance weighted by *Pinus palustris*. Indeed, 533
311 of the 797 samples excluded from analysis (67%) were from non-*P. palustris* species (which
312 comprised only 37% of the full dataset). This removed up to 45% of samples from the rarest
313 species (*Liquidambar styraciflua*), reducing the spectral variance these models should be trained
314 on to better identify rare species. This suggests, for rare species, outlier removal should either be
315 skipped or implemented using other methods (e.g., using spectral mixture analysis to identify
316 samples with high soil fractions).

317 Data resampling further exacerbated the class imbalance problem. By setting the
318 resampling threshold an order of magnitude above the least sampled class, the rarest species
319 were oversampled nearly tenfold in model training. This inflated per-class model performance

320 metrics by double-counting (or more) correctly classified samples for oversampled species.
321 These metrics were further inflated as a result of how the train/test data were split. The split was
322 performed after resampling, meaning the train/test data for oversampled species were likely not
323 independent. This invalidated their use as true test data, and further overestimated performance
324 during model training. This is unequivocally bad practice; I call this “user error.” Undersampling
325 the common species was also detrimental. Excluding samples from common species meant the
326 models were exposed to less intraspecific spectral variation during training, a key source of
327 variance the models should recognize. This made it more difficult for the models to distinguish
328 inter and intraspecific variation. Assigning sample weights (e.g., proportional to the number of
329 samples per class) and using actually independent holdout data could obviate these issues. These
330 will be implemented in future versions of CCB-ID. However, these need not be the only updates
331 to this method; CCB-ID is an open source, freely available project ([https://github.com/stanford-](https://github.com/stanford-ccb/ccb-id)
332 [ccb/ccb-id](https://github.com/stanford-ccb/ccb-id)), and I invite you to to use it and improve it.

333 **Conclusions**

334 It wasn't always possible to classify tree species from airplanes; now it is. Airborne
335 imaging spectrometers can identify trees at crown scales across large areas, and these data are
336 now publicly available through NEON. However, there is currently no canonical imaging
337 spectroscopy-based species mapping approach, limiting opportunities to explore key patterns in
338 biogeography. CCB-ID was developed to identify best practices for species classification in this
339 context, and to further the conversation on how to implement these practices. CCB-ID performed
340 well within the scope of the ECODSE competition, reporting the highest rank-1 accuracy and
341 lowest cross entropy scores among participants, but further testing is necessary to identify
342 whether this method can scale to other regions (e.g., to high diversity forests). I hope CCB-ID

343 will be used to improve future species mapping efforts, and to pursue answers to biogeography's
344 great mysteries of where the species are, and why they are there.

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Figure 1 (on next page)

Per-species canopy reflectance profiles

Canopy reflectance profiles for the eight tree species analyzed, with mean reflectance values in black and ± 1 standard deviation values in color. The bottom right panel shows the mean reflectance values for each species, with each color corresponding to the individual species panels. Though the mean reflectance signals show high interspecific variation, the high intraspecific variation complicates classification efforts.

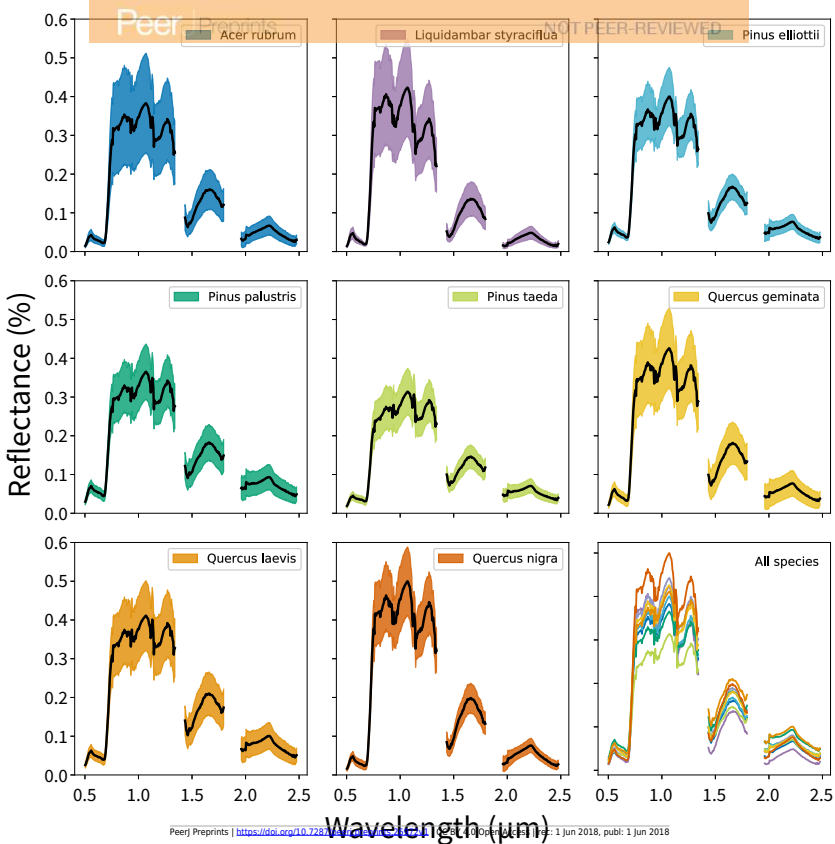
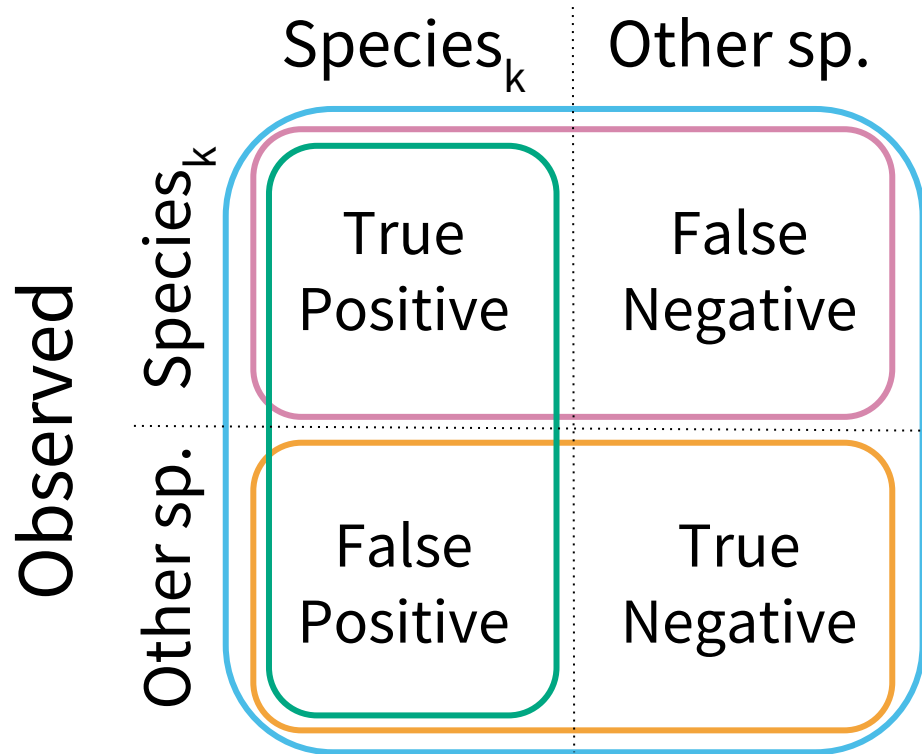


Figure 2 (on next page)

Model performance metrics

Visual representation of the classification model metrics calculated on a per-species basis. A confusion matrix was computed for each species, and each metric was calculated in a one-vs.-all fashion.

Predicted



Accuracy

$$= \frac{TP + TN}{TP + TN + FP + FN}$$



Specificity

$$= \frac{TN}{TN + FP}$$



Precision

$$= \frac{TP}{TP + FP}$$



Recall

$$= \frac{TP}{TP + FN}$$

Figure 3(on next page)

CCB-ID model performance

Per-species secondary performance metrics from the test data. These metrics were calculated using the binary confusion matrix reported in Table 1. Metrics weighted by the true negative rate (i.e., accuracy and specificity) were high for all species since the models correctly predicted the most common species, *Pinus palustris*. However, metrics weighted by the true positive rate (i.e., precision and recall) were much more variable since there were only 1 to 6 observed crowns for 7 of the 9 species (*P. palustris* and *Quercus laevis* had 84 and 23 crowns, respectively). This penalized misclassifications of rare species. These metrics were re-calculated using the per-crown prediction probabilities, and can be found in Figure S1.

Model performance on testing data

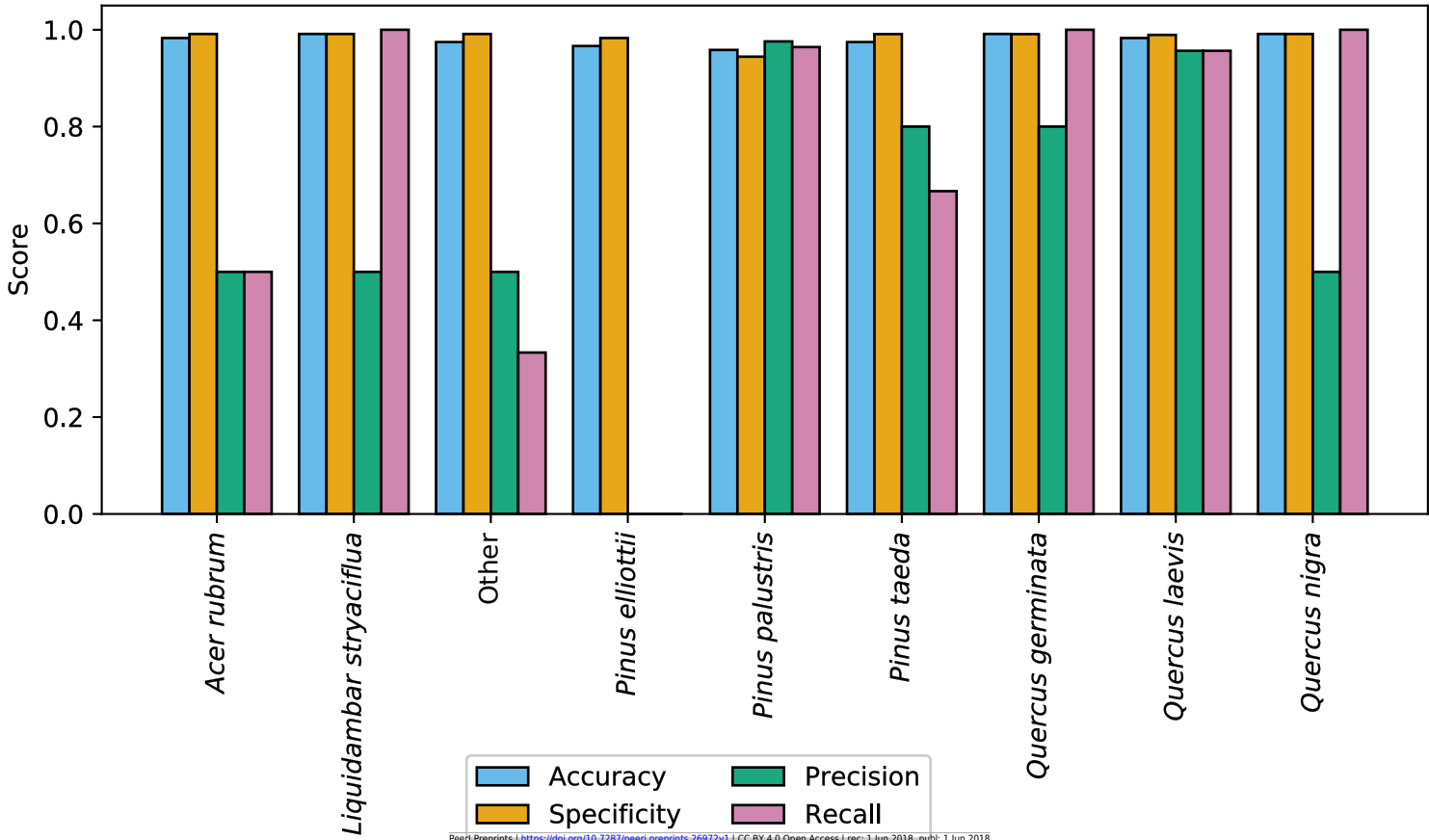


Figure 4(on next page)

Spectral variance and model performance

The effects of increasing spectral variance on model performance through altering the number of principal component features. These plots show the mean (solid) and standard deviation (shaded) of (A) model accuracy and (B) log loss scores for each classification method. Scores were calculated on holdout data from the training set, not the competition test data. These results suggest that using all available spectral variance (i.e., all principal components) may decrease model performance. Using feature selection to identify components that track variation in plant traits may prevent overfitting to noisy features.

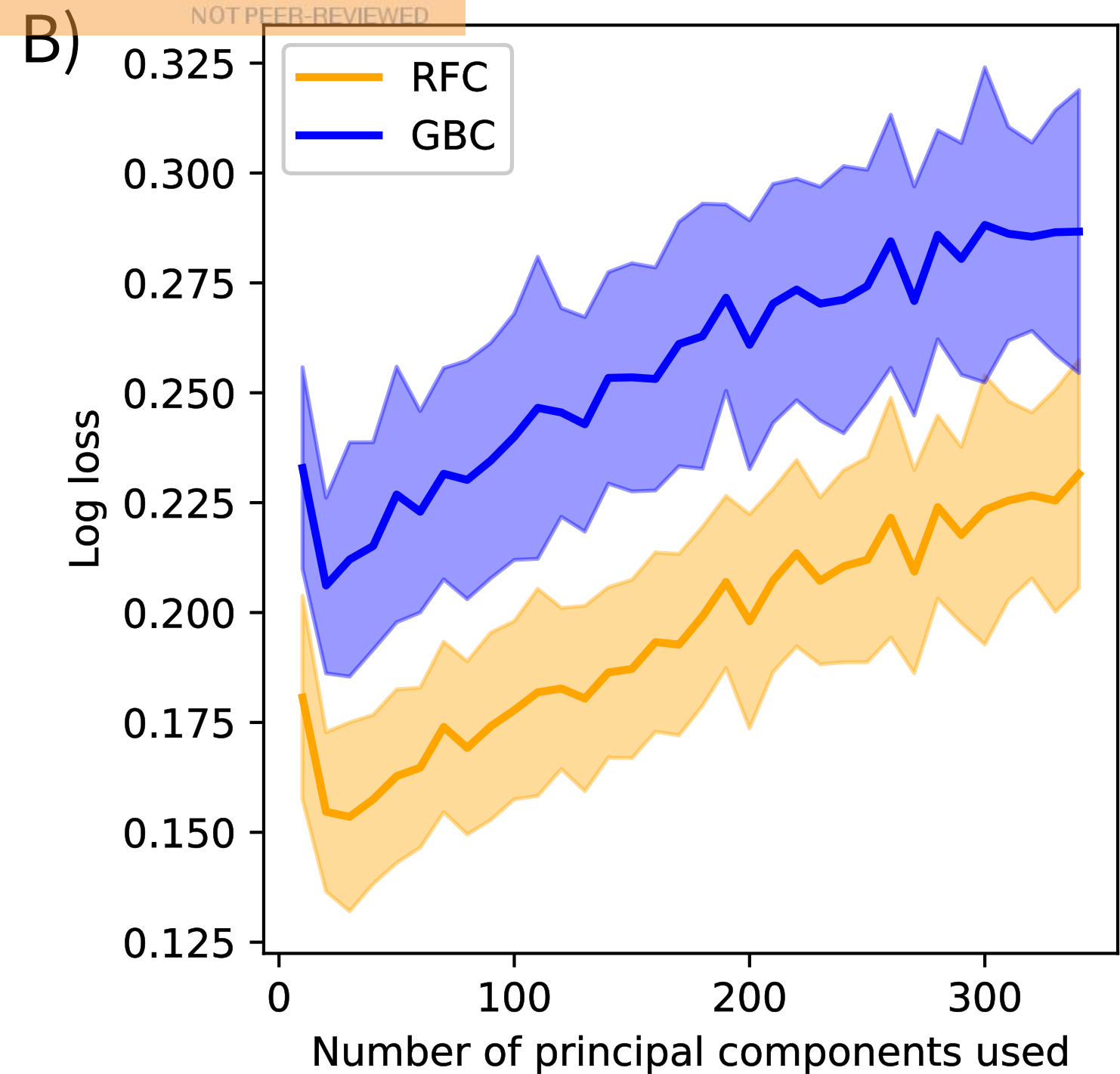
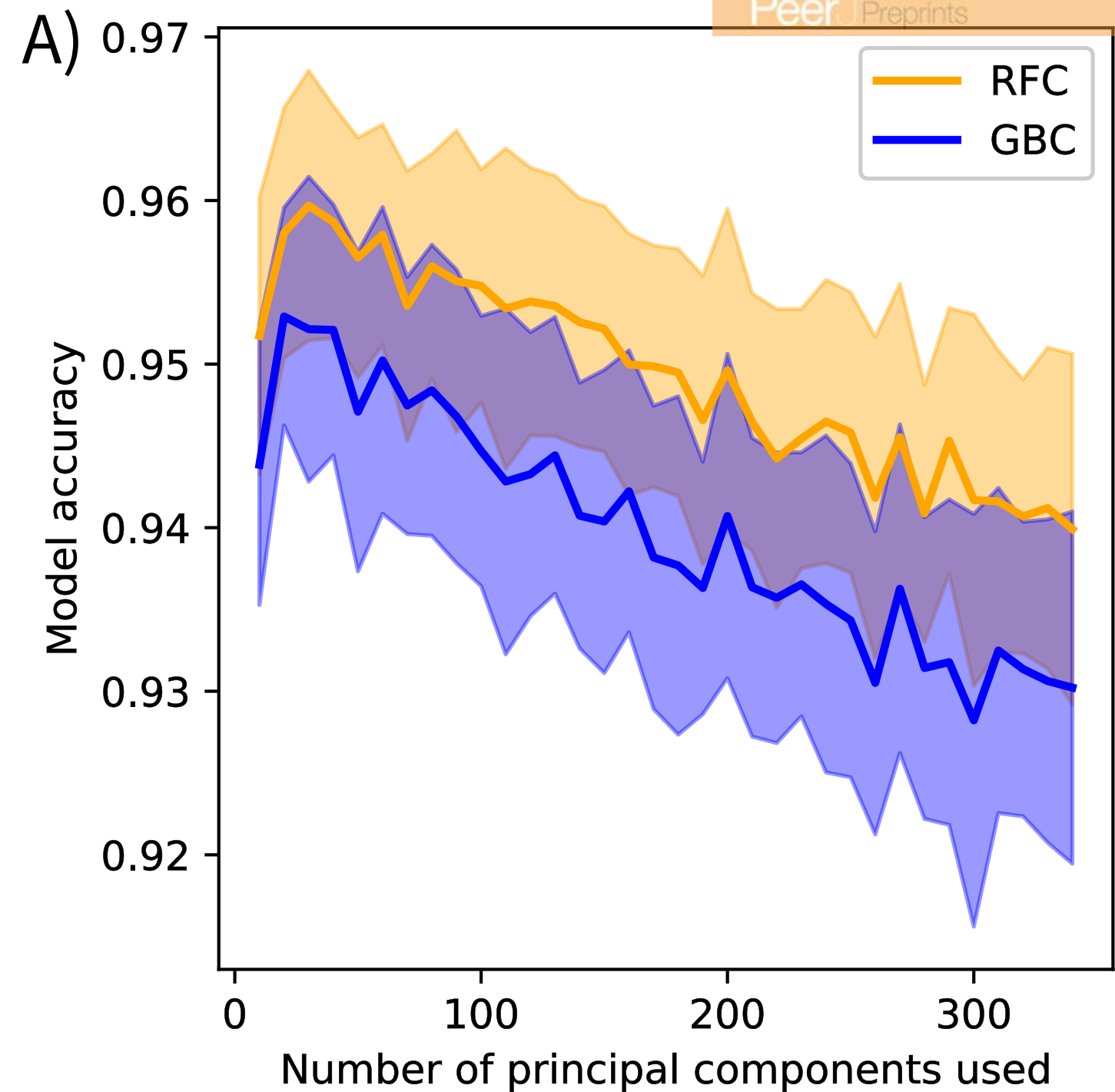


Table 1 (on next page)

Confusion matrix of classification results

Binary classification results of the CCB-ID model on the competition test data.

					Predicted					
	Species ID	Acer rubrum	Liquidambar styraciflua	Other	Pinus elliottii	Pinus palustris	Pinus taeda	Quercus germinata	Quercus laevis	Quercus nigra
	Acer rubrum	1	0	0	0	0	0	0	0	1
	Liquidambar styraciflua	0	1	0	0	0	0	0	0	0
	Other	1	1	1	0	0	0	0	0	0
Actual	Pinus elliottii	0	0	0	0	1	1	0	0	0
	Pinus palustris	0	0	0	2	81	0	0	1	0
	Pinus taeda	0	0	1	0	0	4	1	0	0
	Quercus germinata	0	0	0	0	0	0	4	0	0
	Quercus laevis	0	0	0	0	1	0	0	22	0
	Quercus nigra	0	0	0	0	0	0	0	0	1