Guidelines for the supervised learning of species interactions

Timothée Poisot 1,2

¹ Université de Montréal ² Québec Centre for Biodiversity Sciences

Correspondance to:

Timothée Poisot — timothee.poisot@umontreal.ca

This work is released by its authors under a CC-BY 4.0 license

Last revision: December 13, 2021

- 1. The prediction of species interaction networks is gaining momentum as a way to circumvent limitations in data volume. Yet, ecological networks are challenging to predict because they are typically small and sparse. Dealing with extreme class imbalance is a challenge for most binary classifiers, and there are currently no guidelines as to how predictive models can be trained.
- 2. Using simple mathematical arguments and numerical experiments in which a variety of classifiers (for supervised learning) are trained on simulated networks, we develop a series of guidelines related to the choice of measures to use for model selection, and the degree of unbiasing to apply to the training dataset.
- 3. Classifier accuracy and the ROC-AUC are not informative measures for the performance of interaction prediction. PR-AUC is a fairer assessment of performance. In some cases, even standard measures can lead to selecting a more biased classifier because the effect of connectance is strong. The amount of correction to apply to the training dataset depends as a function of the classifier and the network connectance.
- 4. These results reveal that training machines to predict networks is a challenging task, and that in virtually all cases, the composition of the training set needs to be experimented on before performing the actual training. We discuss these consequences in the context of the low volume of data.

- example on diagnostic test: rare events are hard to detect even with really good models
- summary of model challenges for networks
- Strydom et al. (2021) importance of drawing on traits + validation is challenging + comparing
- 4 across space
- 5 Binary classifiers are usually assessed by measuring properties of their confusion matrix, i.e. the
- 6 contingency table reporting true/false positive/negative hits. A confusion matrix is laid out as

$$\begin{pmatrix} tp & fp \\ fn & tn \end{pmatrix}$$

- 7 wherein tp is the number of interactions predicted as positive, tn is the number of non-interactions
- 8 predicted as negative, fp is the number of non-interactions predicted as positive, and fn is the number of
- 9 interactions predicted as negative. Almost all measures based on the confusion matrix express rates of
- error or success as proportions, and therefore the values of these components matter in a *relative* way. At a
- coarse scale, a classifier is accurate when the trace of the matrix divided by the sum of the matrix is close
- to 1, with other measures focusing on different ways in which the classifer is wrong.
- 13 The same approach is used to evaluate e.g. species distribution models (SDMs). Indeed, the training and
- evaluation of SDMs as binary classifiers suffers from the same issue of low prevalence. In a previous work,
- Allouche et al. (2006) suggested that κ was a better test of model performance than the True Skill Statistic
- (TSS), which we will refer to as Youden's informedness (or J); these conclusions were later criticized by
- Somodi et al. (2017), who emphasized that informedness' relationship to prevalence depends on
- assumptions about bias in the model, and therefore recommend the use of κ as a validation of
- 19 classification performance. Although this work offers recommendations about the comparison of models,
- 20 it doesn't establishes baselines or good practices for training on imbalanced ecological data. Within the
- 21 context of networks, there are three specific issues that need to be adressed. First, what values of
- 22 performance measures are we expecting for a classifier that has poor performance? This is particularly
- 23 important as it can evaluate whether low prevalence can lull us into a false sense of predictive accuracy.
- ²⁴ Second, independently of the question of model evaluation, is low prevalence an issue for *training*, and
- 25 can we remedy it? Finally, because the low amount of data on interaction makes a lot of imbalance
- ²⁶ correction methods (see e.g. Branco et al., 2015) hard to apply, which indicators can be optimized with the

- 27 least amount of positive interaction data?
- 28 In addition to the literature on SDMs, most of the research on machine learning application to life
- sciences is focused on genomics (which has very specific challenges, see a recent discussion by Whalen et
- al., 2021); this sub-field has generated largely different recommendations. Chicco & Jurman (2020)
- suggest using Matthews correlation coefficient (MCC) over F_1 , as a protection against over-inflation of
- predicted results; Delgado & Tibau (2019) advocate against the use of Cohen's κ , again in favor of MCC, as
- the relative nature of κ means that a worse classifier can be picked over a better one; similarly, Boughorbel
- et al. (2017) recommend MCC over other measures of performance for imbalanced data, as it has more
- desirable statistical properties. More recently, Chicco et al. (2021) temper the apparent supremacy of the
- 36 MCC, by suggesting it should be replaced by Youden's informedness (also known as J, bookmaker's
- accuracy, and the True-Skill Statistic) when the imbalance in the dataset may not be representative
- ³⁸ (Jordano, 2016a, which is the case as networks are under-sampled; 2016b), when classifiers need to be
- 39 compared across different datasets (for example when predicting a system in space, where undersampling
- varies locally; McLeod et al., 2021), and when comparing the results to a no-skill (baseline) classifier is
- important. As these conditions are likely to be met with network data, there is a need to evaluate which
- measures of classification accuracy respond in a desirable way.
- 43 A lot of binary classifiers are built by using a regressor (whose task is to guess the value of the interaction,
- 44 amd can therefore return somethins considered to be a pseudo-probability); in this case, the optimal value
- below which predicitions are assumed to be negative (i.e. the interaction does not exist) can be determined
- by picking a threshold maximizing some value on the ROC curve or the PR curve. The area under these
- 47 curves (ROC-AUC and PR-AUC henceforth) give ideas on the overall goodness of the classifier. Saito &
- 48 Rehmsmeier (2015) established that the ROC-AUC is biased towards over-estimating performance for
- 49 imbalanced data; on the contrary, the PR-AUC is able to identify classifiers that are less able to detect
- positive interactions correctly, with the additional advantage of having a baseline value equal to
- prevalence. Therefore, it is important to assess whether these two measures return different results when
- 52 applied to ecological network prediction.
- 53 We establish that due to the low prevalence of interactions, even poor classifiers applied to food web data
- will reach a high accuracy; this is because the measure is dominated by the accidental correct predictions
- of negatives. The F_1 score and positive predictive values are less sensitive to bias, but **TODO**

56 Baseline values

57 Intro

Definition of the performance measures

- 59 **K**
- 60 F_{β}
- 61 informedness
- 62 MCC
- 63 ROC-AUC
- 64 PR-AUC

65 Confusion matrix with skill and bias

- In this section, we will assume a network of connectance ρ , *i.e.* having ρS^2 interactions (where S is the
- species richness), and $(1-\rho)S^2$ non-interactions. Therefore, the vector describing the *true* state of the
- network is a column vector $\mathbf{o}^T = [\rho(1-\rho)]$ (we can safely drop the S^2 terms, as we will work on the
- 69 confusion matrix, which ends up expressing *relative* values).
- 70 In order to write the values of the confusion matrix for a hypothetical classifier, we need to define two
- characteristics: its skill, and its bias. Skill, here, refers to the propensity of the classifier to get the correct
- answer (i.e. to assign interactions where they are, and to not assign them where they are not). A no-skill
- classifier guesses at random, *i.e.* it will guess interactions with a probability ρ . The predictions of a no-skill
- classifier can be expressed as a row vector $\mathbf{p} = [\rho(1-\rho)]$. The confusion matrix **M** for a no-skill classifier
- is given by the element-wise product of these vectors $\mathbf{o} \odot \mathbf{p}$, *i.e.*

$$\mathbf{M} = \begin{pmatrix} \rho^2 & \rho(1-\rho) \\ (1-\rho)\rho & (1-\rho)^2 \end{pmatrix}.$$

In order to regulate the skill of this classifier, we can define a skill matrix **S** with diagonal elements equal to s, and off-diagonal elements equal to (1-s), and re-express the skill-adjusted confusion matrix as **M** \odot **S**, *i.e*.

$$\begin{pmatrix} \rho^2 & \rho(1-\rho) \\ (1-\rho)\rho & (1-\rho)^2 \end{pmatrix} \odot \begin{pmatrix} s & (1-s) \\ (1-s) & s \end{pmatrix}.$$

Note that when s = 0, $Tr(\mathbf{M}) = 0$ (the classifier is *always* wrong), when s = 0.5, the classifier is no-skill and guesses at random, and when s = 1, the classifier is perfect.

The second element we can adjust in this hypothetical classifier is its bias, specifically its tendency to over-predict interactions. Like above, we can do so by defining a bias matrix \mathbf{B} , where interactions are over-predicted with probability b, and express the final classifier confusion matrix as $\mathbf{M} \odot \mathbf{S} \odot \mathbf{B}$, *i.e.*

$$\begin{pmatrix} \rho^2 & \rho(1-\rho) \\ (1-\rho)\rho & (1-\rho)^2 \end{pmatrix} \odot \begin{pmatrix} s & (1-s) \\ (1-s) & s \end{pmatrix} \odot \begin{pmatrix} b & b \\ (1-b) & (1-b) \end{pmatrix}.$$

The final expression for the confusion matrix in which we can regulate the skill and the bias is

$$\mathbf{C} = \begin{pmatrix} s \times b \times \rho^2 & (1-s) \times b \times \rho(1-\rho) \\ (1-s) \times (1-b) \times (1-\rho)\rho & s \times (1-b) \times (1-\rho)^2 \end{pmatrix}.$$

In all further simulations, the confusion matrix \mathbf{C} is transformed so that it sums to 1.

86 What are the baseline values of performance measures?

In this section, we will change the values of b, s, and ρ , and report how the main measures discussed in the introduction (MCC, F_1 , κ , and informedness) are responding to issues with the classifier. Before we do so, it is important to explain why we will not focus on accuracy too much. Accuracy is the number of correct predictions (Tr(\mathbf{C})) divided by the sum of the confusion matrix. For a no-skill, no-bias classifier, accuracy is equal to $\rho^2 + (1 - \rho)^2$; for $\rho = 0.05$, this is ≈ 0.90 , and for $\rho = 0.01$, this is equal to ≈ 0.98 . In other words, the values of accuracy are expected to be so high that they are not really informatived (this is simply explained by the fact that for ρ small, $\rho^2 \ll (1 - \rho)^2$). More concerning is the fact that introducing

bias changes the response of accuracy in unexpected ways. Assuming a no-skill classifier, the numerator of accuracy becomes $b\rho^2 + (1-b)(1-\rho)^2$, which increases when b is low, which specifically means that at equal skill, a classifier that under-predicts interactions will have higher accuracy than an un-biased classifier. These issues are absent from balanced accuracy, but should nevertheless lead us to not report accuracy as the primary measure of network prediction success; moving forward, we will focus on other 98 measures. 99 In order to examine how MCC, F_1 , κ , and informedness change w.r.t. the imbalance, skill, and bias, we performed a grid exploration of the values of logit(s) and logit(b) linearly from -10 to 10, of ρ linearly in 101 [0, 0.5], which is within the range of usually observed connectance values for empirical food webs. Note 102 that at this point, there is no food web model to speak of; rather, the confusion matrix we discuss can be 103 obtained for any classification task. Based on the previous discussion, the desirable properties for a 104 measure of classifier success should be: an increase with classifier skill, especially at low bias; a 105 hump-shaped response to bias, especially at high skill, and ideally center around logit(b) = 0; an increase 106 with prevalence up until equiprevalence is reached.

[Figure 1 about here.]

108

120

In fig. 1, we show that none of the four measures satisfy all the considerations at once: F_1 increases with 109 skill, and increases monotonously with bias; this is because F_1 does not account for true negatives, and the 110 increase in positive detection masks the over-prediction of interactions. Informedness varies with skill, 111 reaching 0 for a no-skill classifier, but is entirely unsensitive to bias. Both MCC and κ have the same 112 behavior, whereby they increase with skill. κ peaks at increasing values of biass for increasing skill, i.e. is likely to lead to the selection of a classifier that over-predicts interactions. By contract, MCC peaks at the 114 same value, regardless of skill, but this value is not logit(b) = 0: unless at very high classifier skill, MCC 115 risks leading to a model that over-predicts interactions. In fig. 2, we show that all measures except F_1 give a value of 0 for a no-skill classifier, and are forced towars their correct maximal value when skill changes 117 (i.e. a more connected networks will have higher values for a skilled classifierd, and lower values for a classifier making mostly mistakes).

[Figure 2 about here.]

These two analyses point to the following recommendations: MCC is indeed more appropriate than κ , as

although sensitive to bias, it is sensitive in a consistent way. Informedness is appropriate at discriminating between different skills, but confounded by bias. F_1 is increasing with bias, and should not be prioritized 123 to evalue the performance of the model. The discussion of sensitivity to bias should come with a 124 domain-specific caveat: although it is likely that interactions documented in ecological networks are correct, a lot of non-interactions are simply unobserved; as predictive models are used for data-inflation 126 (i.e. the prediction of new interactions), it is not necessarilly a bad thing in practice to select models that 127 predict more interactions than the original dataset, because the original dataset misses some interactions. 128 Furthermore, the weight of positive interactions could be adjusted if some information about the extent of 129 undersampling exists (e.g. Branco et al., 2015). 130

Numerical experiments on training strategy

In the following section, we will generate random bipartite networks (this works without loss of generality 132 on unipartite networks), and train four binary classifiers (as well as an ensemble model using the sum of 133 ranged outputs from the component models) on 30% of the interaction data. Networks are generated by 134 picking a random infectiousness trait v_i for 100 species (from a B(6,8) distribution), and a resistance trait 135 h_i for 100 species (from a B(2, 8) distribution). There is an interaction between i and j when 136 $v_i - \xi/2 \le h_j \le v_i + \xi/2$, where ξ is a constant regulating the connectance of the network (there is an almost 1:1 relationship between ξ and connectance), and varies uniformly in [0.05, 0.35]. This model gives 138 fully interval networks that are close analogues to the bacteria-phage model of Weitz et al. (2005), with 139 both a modular structure and a non-uniform degree distribution. This model is easy to learn: when trained with features $[v_i, h_j, abs(v_i, h_i)]^T$ to predict the interactions between i and j, all four models 141 presented below were able to reach almost perfect predictions all the time (data not presented here) – this 142 is in part because the rule is fixed for all interactions. In order to make the problem more difficult to solve, we use $[v_i, h_i]$ as a feature vector, and therefore the models will have to uncover that the rule for 144 interaction is $abs(v_i, h_i) \le \xi$. 145 The training sample is composed of 30% of the 10^4 possible entries in the network, i.e. n = 3000. Out of these interactions, we pick a proportion ν (the training set bias) to be positive, so that the training set has 147 νn interactions, and $(1-\nu)n$ non-interactions. We vary ν uniformly in]0,1[. This allows to evaluate how the measures of binary classification performance respond to artificially rebalanced dataset for a given

network connectance. The rest of the dataset (n = 7000 pairs of species) is used as a testing set, on which all furher measures are calculated. Note that although the training set is balanced, the testing set is not, 151 and retains (part of) the imbalance of the original data. 152 The dataset used for numerical experiments is composed of 64000 such (ξ, ν) pairs, on which four 153 machines are trained: a decision tree regressor, a boosted regression tree, a ridge regressor, and a random 154 forest regressor. All models were taken from the MLJ.jl package (Blaom et al., 2020; Blaom & Vollmer, 155 2020) in Julia 1.7 (Bezanson et al., 2017). All machines use the default parameterization; this is an obvious deviation from best practices, as the hyperparameters of any machine require training before its 157 application on a real dataset. As we use 64000 such datasets, this would require 256000 unique instances 158 of tweaking thehyperparameters, which is not realistic. Therefore, we assume that the default 159 parameterizations are comparable across networks. All machines return a quantitative prediction, usually 160 (but not necessarilly) in [0, 1], which is proportional (but not necessarilly linearly) to the probability of an 161 interaction between *i* and *j*. 162 In order to pick the best adjacency matrix for a given trained machine, we performed a thresholding 163 approach using 500 steps on predictions from the testing set, and picking the threshold that maximized Youden's informedness, which is usually the optimized target for imbalanced classification. During the 165 thresholding step, we measured the area under the receiving-operator characteristic (ROC-AUC) and 166 precision-recall (PR-AUC) curves, as measures of overall performance over the range of returned values. 167 We report the ROC-AUC and PR-AUC, as well as a suite of other measures as introduced in the next 168 section, for the best threshold. The ensemble model was generated by summing the predictions of all 169 component models on the testing set (ranged in [0,1]), then put through the same thresholding process. 170 The complete code to run the simulations is given as an appendix; running the final simulation required 17 4.8 core days (approx. 117 hours). 172 After the simulations were completed, we removed all runs (i.e. pairs of ξ and ν) for which at least one of 173 the following conditions was met: the accuracy was 0, the true positive or true negative rates were 0, the connectance was larger than 0.25. This removes both the obviously failed model runs, and the networks 175 that are more densely connected compared to the connectance of empirical food webs (and are therefore 176 less difficult to predict, being less imbalanced; preliminary analyses of data with a connectance larger than 3 revealed that all machines reached consistently high performance).

79 Effect of training set bias on performance

189

195

In fig. 3, we present the response of MCC and informedness to (i) five levels of network connectance and 180 (ii) a gradient of training set bias, for the four component models as well as the ensemble. All models 181 reached a higher performance on more connected networks, and using more biased training sets (with the 182 exception of ridge regression, whose informedness decreased in performance with training set bias). In all 183 cases, informedness was extremely high, which is an expected consequence of the fact that this is the 184 value we optimized to determine the cutoff. MCC increased with training set bias, although this increase 185 became less steep with increasing connectance. Interestingly, the ensemble almost always outclassed its 186 component models. In a few cases, both MCC and informedness stared decreasing when the training set 187 bias got too close to one, which suggests that it is possible to over-correct the imbalance.

[Figure 3 about here.]

In fig. 4, we present the same information as fig. 3, this time using ROC-AUC and PR-AUC. ROC-AUC is always high, and does not vary with training set bias. On the other hand, PR-AUC shows very strong responses, increasing with training set bias. It is notable here that two classifiers that seemed to be performing well (Decision Tree and Random Forest) based on their MCC are not able to reach a high PR-AUC even at higher connectances. As in fig. 3, the ensemble outperforms its component models.

[Figure 4 about here.]

Based on the results presented in fig. 3 and fig. 4, it seems that informedness and ROC-AUC are not
necessarilly able to discriminate between good and bad classifiers (although this result may be an artifact
for informedness, as it has been optimized when thresholding). On the other hand, MCC and PR-AUC
show a strong response to training set bias, and may therefore be more useful at model comparison.

Required amount of positives to get the best performance

The previous results revealed that the measure of classification performance responds both to the bias in
the training set *and* to the connectance of the network; from a practical point of view, assembling a
training set requires to withold positive information, which in ecological networks are very scarce (and

typically more valuable than negatives, on which there is a doubt). For this reason, across all values of
connectance, we measured the training set bias that maximized a series of performance measures. When
this value is high, the training set needs to skew more positive in order to get a performant model; when
this value is about 0.5, the training set needs to be artificially balanced to optimize the model performance.
These results are presented in fig. 5.

[Figure 5 about here.]

209

215

The more "optimistic" measures (ROC-AUC and informedness) required a biasing of the dataset from
about 0.4 to 0.75 to be maximized, with the amount of bias required decreasing only slightly with the
connectance of the original network. MCC and PR-AUC required values of training set bias from 0.75 to
almost 1 to be optimized, which is in line with the results of the previous section, *i.e.* they are more
stringent tests of model performance.

[Figure 6 about here.]

When trained at their optimal training set bias, performance still had a significant impact on the
performance of some machines fig. 6. Notably, Decision Tree, Random Forest, and Ridge Regression had
low values of PR-AUC. In all cases, the Boosted Regression Tree was reaching very good predictions
(esepcially for connectances larger than 0.1), and the ensemble was almost always scoring perfectly. This
suggests that all the models are biased in different ways, and that the averaging in the ensemble is able to
correct these biases. We do not expect this last result to have any generality, and provide a discussion of a
recent exemple in which the ensemble was performing worse than its components models.

Do better classification accuracy result in more realistic networks?

In this last section, we generate a network using the same model as before, with S=50 species, a connectance of ≈ 0.16 ($\xi=0.19$), and a training set bias of 0.7. The prediction made on the complete dataset is presented in fig. 7. Visualizing the results this way highlights the importance of exploratory data analysis: whereas all models return a network with interactions laying mostly on the diagonal (as expected), the Ridge Regression is quite obviously biased. Despite this, we can see that the ensemble is close to the initial dataset.

The trained models were then thresholded (again by optimising informedness), and their predictions 231 transformed back into networks for analysis; specifically, we measured the connectance, nestedness 232 (REF), modularity (REF), and entropy (REF). The results are presented in tbl. 1. The random forest model 233 is an interesting instance here: it produces the network that looks the most like the original dataset, 234 despite having a very low PR-AUC, suggesting it hits high recall at the cost of low precision. Although the 235 ensemble was about to reach a very high PR-AUC (and a very high ROC-AUC), this did not necessarilly 236 translate into more accurate reconstructions of the structure of the network. This result bears elaborating. 237 Measures of model performance capture how much of the interactions and non-interactions are correctly 238 identified. As long as these predictions are not perfect, some interactions will be predicted at the "wrong" 239 position in the network; these measures cannot describe the structural effect of these mistakes. On the 240 other hand, measures of network structure can have the same value with interactions that fall at drastically different positions; this is in part because a lot of these measures covary with connectance, and 242 in part because as long as these values are not 0 or their respective maximum, there is a large number of 243 network configurations that can have the same value.

Table 1: Values of four performance metrics, and four network structure metrics, for the predictions presented in fig. 7. The values in **bold** indicate the best value for each column (including ties).

Model	MCC	Inf.	ROC-AUC	PR-AUC	Conn.	η	Q	Entropy
Decision tree	0.83	0.68	0.95	0.15	0.18	0.53	0.49	8.86
BRT	0.76	0.89	0.95	0.65	0.22	0.63	0.43	9.14
Random Forest	0.89	0.94	0.99	0.41	0.17	0.48	0.49	8.80
Ridge Regression	0.67	0.85	0.89	0.38	0.27	1.0	0.26	9.40
Ensemble	0.84	0.91	0.99	0.94	0.19	0.54	0.48	8.92
Data					0.16	0.45	0.49	8.71

²⁴⁵ Guidelines for the assesment of network predictive models

- The results presented here highlight an interesting paradox: larger networks (with lower connectance)
- require more training set bias in order to maximize model performance fig. 5, but are also more difficult to

```
predict according to MCC and PR-AUC fig. 6. This suggests that the task of network prediction will be
    difficult regardless of network size: by being limited by the frequency of interactions when the network is
249
    large, and by being limited by the number of interactions when the network is small. Nevertheless, based
250
    on the simulations and numerical experiments, it is possible to formulate a series of recommendations for
    the evaluation of network prediction models.
252
    First, because we should have more trust in reported interactions than in reported absences of interactions,
253
    we can draw on previous literature to recommend informedness as a measure to decide on a threshold
    (Chicco et al., 2021); this being said, because informedness is insensitive to bias, the model performance is
255
    better evaluated through the use of MCC fig. 3. Because F_1 is monotonously sensitive to classifier bias
256
    fig. 1 and network connectance fig. 2, MCC should be prefered as a measure of model evaluation.
    Second, because the PR-AUC responds more to network connectance fig. 6 and training set imbalance
258
    fig. 4, it should be used as a measure of model performance over the ROC-AUC. This is not to say that
259
    ROC-AUC should be discarded (in fact, a low ROC-AUC is a sign of an issue with the model), but that its
260
    interpretation should be guided by the PR-AUC value. This again echoes recommendations from other
261
    fields (Saito & Rehmsmeier, 2015).
262
    Thirdly, regardless of network connectance or measure to evaluate the model performance, as long as the
263
    network connectance is larger than \approx 0.1, artificially balancing the training set to have equiprevalence will
264
    give the best possible results. This was true for all models.
    Finally, it is noteworthy that the ensemble model was systematically better than the component models;
266
    even when poor models were included (Random Forest and Decision Tree), the ensemble was able to
267
    leverage the different biases expressed by the models to make an overall more accurate prediction. We do
    not expect that ensembles will always be better than single models. In a recent multi-model comparison,
269
    Becker et al. (2021) found that the ensemble was not the best model. There is no general conclusion to
270
    draw from this besides reinforcing the need to be pragmatic about which models should be included in the
    ensemble, or whether to use an ensemble at all. In a sense, the surprising peformance of the ensemble
272
    model should form the basis of the last recommendation: optimal training set bias and its interaction with
273
    connectance and binary classifier is, in a sense, an hyperparameter that should be assessed. The
    distribution of results in fig. 5 and fig. 6 show that there are variations around the trend; furthermore,
275
    networks with different structures than the one we simulated here may respond in different ways.
```

Acknowledgements: We acknowledge that this study was conducted on land within the traditional unceded territory of the Saint Lawrence Iroquoian, Anishinabewaki, Mohawk, Huron-Wendat, and Omàmiwininiwak nations. This research was enabled in part by support provided by Calcul Québec (www.calculquebec.ca) and Compute Canada (www.computecanada.ca) through the Narval general purpose cluster. TP is supported by a NSERC Discovery Grant and Discovery Acceleration Supplement,

and by a grant from the Institut de Valorisation des Données (IVADO).

References

282

301

302

Allouche, O., Tsoar, A., & Kadmon, R. (2006). Assessing the accuracy of species distribution models: 284 Prevalence, kappa and the true skill statistic (TSS). *Journal of Applied Ecology*, 43(6), 1223–1232. https://doi.org/10.1111/j.1365-2664.2006.01214.x 286 Becker, D., Albery, G. F., Sjodin, A. R., Poisot, T., Bergner, L., Dallas, T., Eskew, E. A., Farrell, M. J., Guth, 287 S., Han, B. A., Simmons, N. B., Stock, M., Teeling, E. C., & Carlson, C. J. (2021). Optimizing predictive 288 models to prioritize viral discovery in zoonotic reservoirs. bioRxiv, 2020.05.22.111344. 289 https://doi.org/10.1101/2020.05.22.111344 290 Bezanson, J., Edelman, A., Karpinski, S., & Shah, V. (2017). Julia: A Fresh Approach to Numerical 291 Computing. SIAM Review, 59(1), 65-98. https://doi.org/10.1137/141000671 292 Blaom, A. D., Kiraly, F., Lienart, T., Simillides, Y., Arenas, D., & Vollmer, S. J. (2020). MLJ: A Julia package 293 for composable machine learning. Journal of Open Source Software, 5(55), 2704. 294 https://doi.org/10.21105/joss.02704 295 Blaom, A. D., & Vollmer, S. J. (2020, December 31). Flexible model composition in machine learning and its 296 implementation in MLJ. http://arxiv.org/abs/2012.15505 297 Boughorbel, S., Jarray, F., & El-Anbari, M. (2017). Optimal classifier for imbalanced data using Matthews 298 Correlation Coefficient metric. *PloS One*, 12(6), e0177678. 299 https://doi.org/10.1371/journal.pone.0177678 300

Branco, P., Torgo, L., & Ribeiro, R. (2015, May 13). A Survey of Predictive Modelling under Imbalanced

Distributions. http://arxiv.org/abs/1505.01658

```
Chicco, D., & Jurman, G. (2020). The advantages of the Matthews correlation coefficient (MCC) over F1
       score and accuracy in binary classification evaluation. BMC Genomics, 21(1), 6.
304
       https://doi.org/10.1186/s12864-019-6413-7
305
    Chicco, D., Tötsch, N., & Jurman, G. (2021). The Matthews correlation coefficient (MCC) is more reliable
306
       than balanced accuracy, bookmaker informedness, and markedness in two-class confusion matrix
307
       evaluation. BioData Mining, 14, 13. https://doi.org/10.1186/s13040-021-00244-z
308
    Delgado, R., & Tibau, X.-A. (2019). Why Cohen's Kappa should be avoided as performance measure in
309
       classification. PloS One, 14(9), e0222916. https://doi.org/10.1371/journal.pone.0222916
310
    Jordano, P. (2016a). Chasing Ecological Interactions. PLOS Biol, 14(9), e1002559.
311
       https://doi.org/10.1371/journal.pbio.1002559
312
    Jordano, P. (2016b). Sampling networks of ecological interactions. Functional Ecology.
313
       https://doi.org/10.1111/1365-2435.12763
314
    McLeod, A., Leroux, S. J., Gravel, D., Chu, C., Cirtwill, A. R., Fortin, M.-J., Galiana, N., Poisot, T., & Wood,
315
       S. A. (2021). Sampling and asymptotic network properties of spatial multi-trophic networks. Oikos,
316
       n/a(n/a). https://doi.org/10.1111/oik.08650
317
    Saito, T., & Rehmsmeier, M. (2015). The Precision-Recall Plot Is More Informative than the ROC Plot
318
       When Evaluating Binary Classifiers on Imbalanced Datasets. PLOS ONE, 10(3), e0118432.
319
       https://doi.org/10.1371/journal.pone.0118432
320
    Somodi, I., Lepesi, N., & Botta-Dukát, Z. (2017). Prevalence dependence in model goodness measures with
321
       special emphasis on true skill statistics. Ecology and Evolution, 7(3), 863–872.
322
       https://doi.org/10.1002/ece3.2654
323
    Strydom, T., Catchen, M. D., Banville, F., Caron, D., Dansereau, G., Desjardins-Proulx, P., Forero-Muñoz,
324
       N. R., Higino, G., Mercier, B., Gonzalez, A., Gravel, D., Pollock, L., & Poisot, T. (2021). A roadmap
325
       towards predicting species interaction networks (across space and time). Philosophical Transactions of
326
       the Royal Society B: Biological Sciences, 376(1837), 20210063.
327
       https://doi.org/10.1098/rstb.2021.0063
328
    Weitz, J. S., Hartman, H., & Levin, S. A. (2005). Coevolutionary arms races between bacteria and
329
       bacteriophage. Proceedings of the National Academy of Sciences of the United States of America, 102(27),
330
```

```
9535-9540. https://doi.org/10.1073/pnas.0504062102
```

- Whalen, S., Schreiber, J., Noble, W. S., & Pollard, K. S. (2021). Navigating the pitfalls of applying machine learning in genomics. *Nature Reviews Genetics*, 1–13.
- https://doi.org/10.1038/s41576-021-00434-9

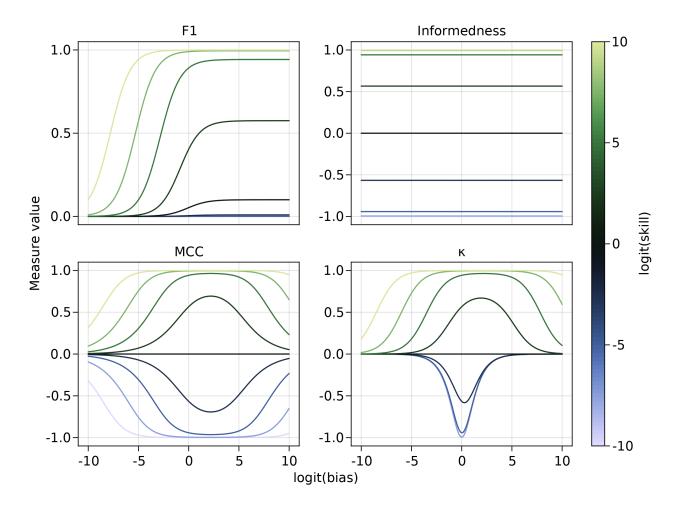


Figure 1: Consequences of changing the classifier skills (s) and bias (s) for a connectance $\rho=0.15$, on accuracy, F_1 , postive predictive value, and κ . Accuracy increases with skill, but also increases when the bias tends towards estimating *fewer* interactions. The F_1 score increases with skill but also increases when the bias tends towards estimating *more* interactions; PPV behaves in the same way. Interestingly, κ responds as expected to skill (being negative whenever s<0.5), and peaks for values of $b\approx0.5$; nevertheless, the value of bias for which κ is maximized in *not* b=0.5, but instead increases with classifier skill. In other words, at equal skill, maximizing κ would lead to select a *more* biased classifier.



Figure 2: As in fig. 1, consequences of changing connectance for different levels of classifier skill, assuming no classifier bias. Informedness, κ , and MCC do increase with connectance, but only when the classifier is not no-skill; by way of contrast, a more connected network will give a higher F_1 value even with a no-skill classifier.

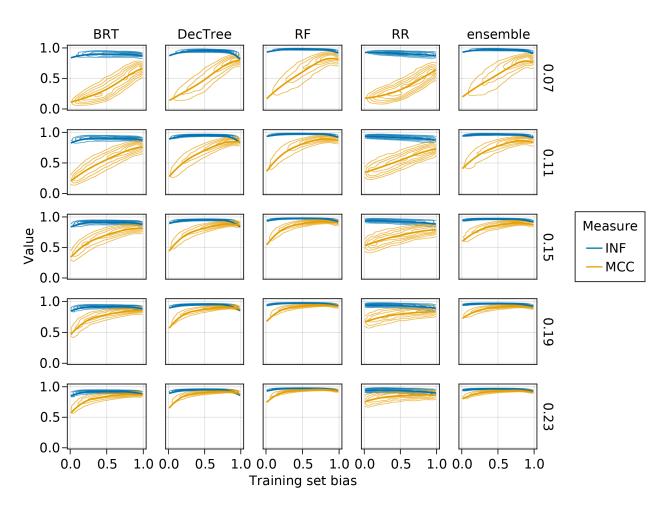


Figure 3: TODO

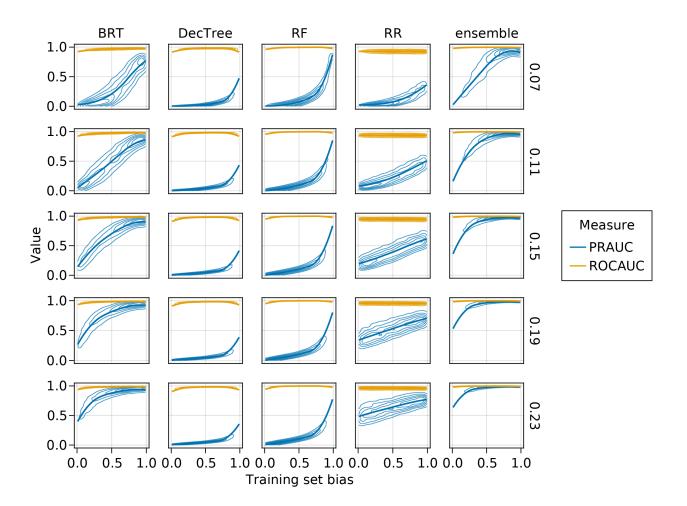


Figure 4: TODO

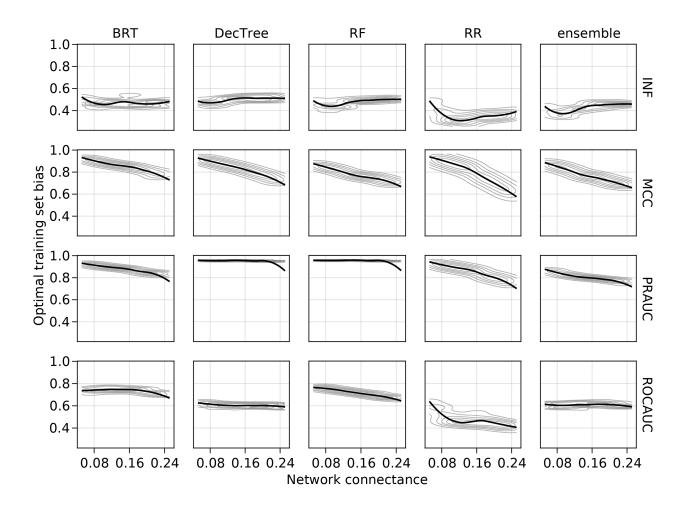


Figure 5: TODO

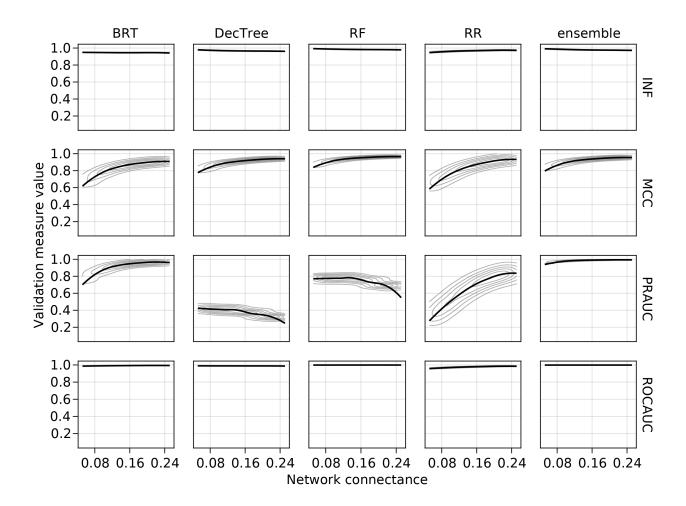


Figure 6: TODO

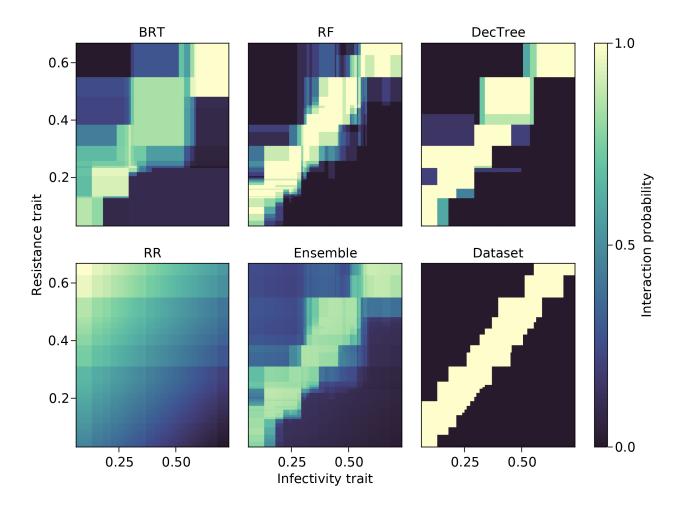


Figure 7: TODO