

Guidelines for the supervised learning of species interactions

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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.

1 example on diagnostic test: rare events are hard to detect even with really good models

2 summary of model challenges for networks - Strydom et al. (2021) importance of drawing on traits +

3 validation is challenging - Whalen et al. (2021) machine learning from genomics

4 Binary classifiers are usually assessed by measuring properties of their confusion matrix, *i.e.* the

5 contingency table reporting true/false positive/negative hits. The same approach is used to evaluate *e.g.*

6 species occurrence models (Allouche et al., 2006). A confusion matrix is laid out as

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

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

10 error or success as proportions, and therefore the values of these components matter in a *relative* way. At a

11 coarse scale, a classifier is *accurate* when the trace of the matrix divided by the sum of the matrix is close

12 to 1, with other measures focusing on different ways in which the classifier is wrong.

13 list of problems to solve - baseline values and response to bias - effect of training set bias on performance -

14 which models need the least amount of interactions to work

15 summary of the results

16 **Baseline values**

17 **Confusion matrix with skill and bias**

18 In this section, we will assume a network of connectance ρ , *i.e.* having ρS^2 interactions (where S is the

19 species richness), and $(1 - \rho)S^2$ non-interactions. Therefore, the vector describing the *true* state of the

20 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

21 confusion matrix, which ends up expressing *relative* values).

22 In order to write the values of the confusion matrix for a hypothetical classifier, we need to define two

23 characteristics: its skill, and its bias. Skill, here, refers to the propensity of the classifier to get the correct

24 answer (*i.e.* to assign interactions where they are, and to not assign them where they are not). A no-skill
 25 classifier guesses at random, *i.e.* it will guess interactions with a probability ρ . The predictions of a no-skill
 26 classifier can be expressed as a row vector $\mathbf{p} = [\rho(1 - \rho)]$. The confusion matrix \mathbf{M} for a no-skill classifier
 27 is given by the element-wise product of these vectors $\mathbf{o} \odot \mathbf{p}$, *i.e.*

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

28 In order to regulate the skill of this classifier, we can define a skill matrix \mathbf{S} with diagonal elements equal
 29 to s , and off-diagonal elements equal to $(1 - s)$, and re-express the skill-adjusted confusion matrix as
 30 $\mathbf{M} \odot \mathbf{S}$, *i.e.*

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

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

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

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

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

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

37 What are the baseline values of performance measures?

38 In this section, we will change the values of b and s for a given value of ρ , and see how the values of
39 common performance measures for binary classification are affected. Specifically, we will focus on four
40 quantities: the accuracy $((tp + tn)/(tp + tn + fp + fn))$, the *balanced* accuracy
41 $(tp/(2(tp + fn)) + tn/(2(tn + fp)))$, Youden's J $(tp/(tp + fn) + tn/(tn + fp) - 1)$, and the F_1 score
42 $(2tp/(2tp + fp + fn))$.

43 Justification of why these 4

44 Assuming a no-skill unbiased classifier ($s = 0.5$, *i.e.* $\mathbf{C} = \mathbf{M}$ after normalization), the accuracy is
45 $\rho^2 + (1 - \rho)^2$, the balanced accuracy is 0.5, Youden's J is 0, and $F_1 = \rho$. In other words, given a
46 connectance $\rho = 0.05$, we expect that a classifier guessing at random would still achieve an accuracy of
47 0.905; for a connectance of $\rho = 0.01$, this accuracy *increases* to over 0.98. In other words, networks with
48 fewer interactions have inherently higher accuracy, because it is easy to predict the overwhelming majority
49 of non-interactions right.

50 In order to examine how these values change w.r.t. the skill and bias, we performed a grid exploration of
51 the values of s (from 0 to 1), and of $\logit(b)$, and visualize the result for a connectance of **TODO**.

52 [Figure 1 about here.]

53 Numerical experiments

54 In the following section, we will generate random networks, and train four binary classifiers (as well as an
55 ensemble model using the sum of the outputs) on 30% of the interaction data. Networks are generated by
56 picking random generality g and vulnerability v traits for $S = 200$ species uniformly on the unit interval,
57 and assigning an interaction from species i to species j if $0.2g_i - \xi \leq v_j \leq 0.2g_i + \xi$, where ξ is a constant
58 regulating the connectance of the networks, and varies uniformly in $[5 \times 10^{-3}, 10^{-1}]$. This model gives
59 fully interval networks that are close analogues to the niche model (Williams & Martinez, 2000), but has
60 the benefit of only relying on two features (g_i, v_j) , and having the exact same rule for all interactions. It is,
61 therefore, a simple case which most classifiers should be able to learn.

62 The training sample is composed of 30% of the 4×10^4 possible entries in the network, *i.e.* $n = 12000$. Out

63 of these interactions, we pick a proportion ν (the training set bias) to be positive, so that the training set
 64 has νn interactions, and $(1 - \nu)n$ non-interactions. We vary ν uniformly in $]0, 1[$. This allows to evaluate
 65 how the measures of binary classification performance respond to artificially rebalanced dataset for a
 66 given network connectance. Note that both ξ and ν are sampled from a distribution rather than being
 67 picked on a grid; this is because there is no direct relationship between the value of ξ and the connectance
 68 of the simulated network, and therefore the precise value of ξ is not relevant for the analysis of the results.
 69 The dataset used for numerical experiments is composed of 20000 such (ξ, ν) pairs, on which four learners
 70 are trained: a decision tree regressor, a boosted regression tree, a ridge regressor, and a random forest
 71 regressor. All models were taken from the `MLJ.jl` package (Blaom et al., 2020; Blaom & Vollmer, 2020) in
 72 Julia 1.7 (Bezanson et al., 2017). In order to pick the best adjacency matrix for a given learner, we
 73 performed a thresholding approach using 500 steps on predictions from the testing set, and picking the
 74 threshold that maximized Youden’s informedness, which is usually the optimized target for imbalanced
 75 classification. During the thresholding step, we measured the area under the receiving-operator
 76 characteristic (ROC-AUC) and precision-recall (PR-AUC) curves, as measures of overall performance over
 77 the range of returned values. We report the ROC-AUC and PR-AUC, as well as a suite of other measures as
 78 introduced in the next section, for the best threshold. The ensemble model was generated by summing the
 79 predictions of all component models on the testing set (ranged in $[0, 1]$), then put through the same
 80 thresholding process. The complete code to run the simulations is given as an appendix.
 81 After the simulations were completed, we removed all runs (*i.e.* pairs of ξ and ν) for which at least one of
 82 the following conditions was met: the accuracy was 0, the true positive or true negative rates were 0, the
 83 connectance was larger than 0.2. This removes both the obviously failed model runs, and the networks
 84 that are more densely connected compared to the connectance of empirical food webs (and are therefore
 85 less difficult to predict, being less imbalanced).

Effect of training set bias on performance

Required amount of positives to get the best performance

Guidelines for prediction

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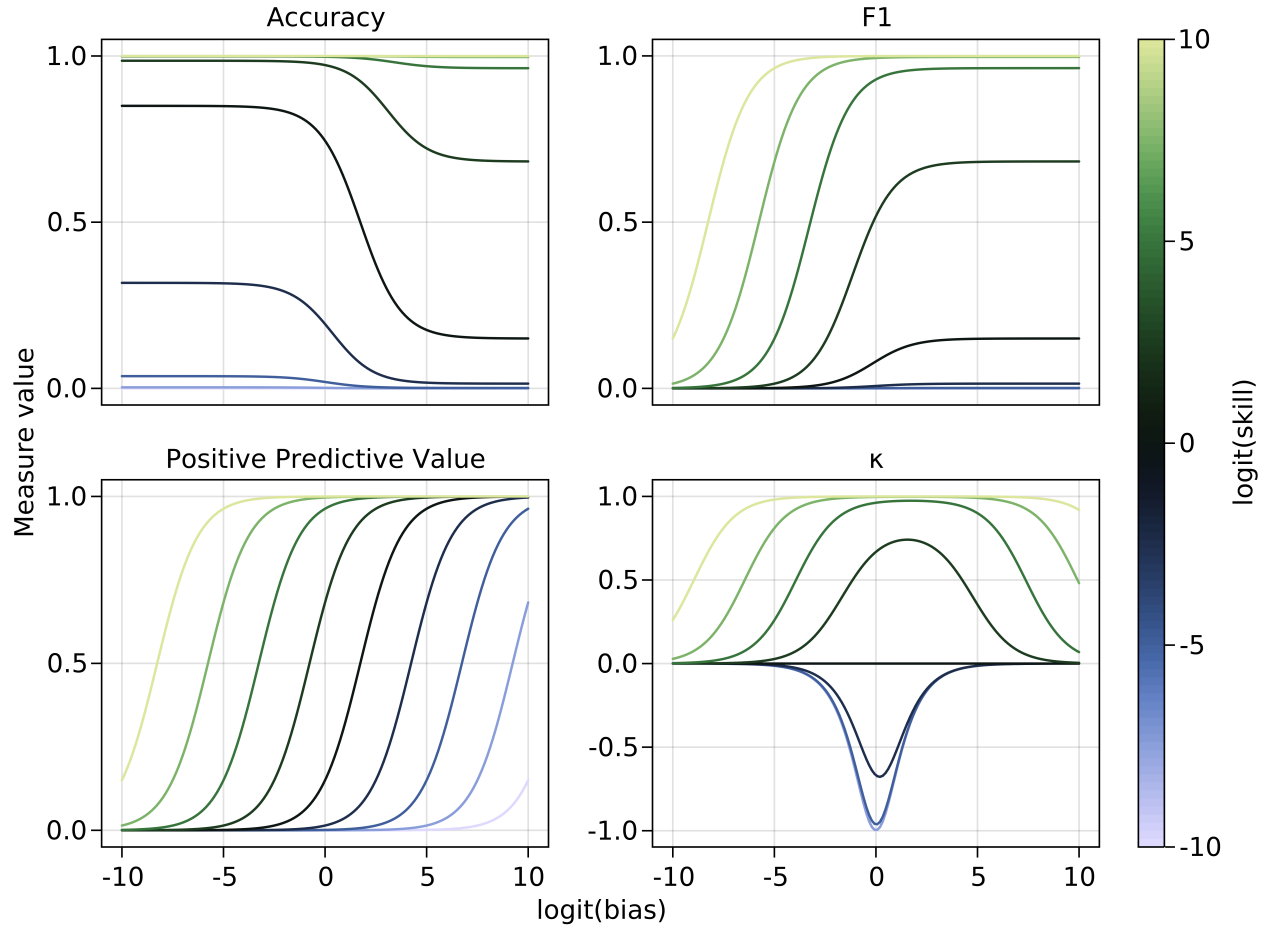


Figure 1: Consequences of changing the classifier skills (s) and bias (b) for a connectance $\rho = 0.15$, on accuracy, F_1 , positive predictive value, and κ . Accuracy increases with skill, but also increases when the bias tends towards estimating *fewer* interactions. The F_1 score increases with 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 $b \approx 0.5$; nevertheless, the value of bias for which κ is maximized is *not* $b = 0.5$, but instead increases with classifier skill. In other words, at equal skill, maximizing κ would lead to select a *more* bias classifier.