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 assesment 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 across space

Binary classifiers are usually assessed by measuring properties of their confusion matrix, *i.e.* the contingency table reporting true/false positive/negative hits. A confusion matrix is laid out as

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

wherein tp is the number of interactions predicted as positive, tn is the number of non-interactions predicted as negative, fp is the number of non-interactions predicted as positive, and fn is the number of 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.

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 classification performance. Although this work offers recommendations about the comparison of models, it doesn't establishes baselines or good practices for training on imbalanced ecological data. Within the context of networks, there are three specific issues that need to be adressed. First, what values of performance measures are we expecting for a classifier that has poor performance? This is particularly important as it can evaluate whether low prevalence can lull us into a false sense of predictive accuracy. Second, independently of the question of model evaluation, is low prevalence an issue for *training*, and can we remedy it? Finally, because the low amount of data on interaction makes a lot of imbalance correction methods (see *e.g.* Branco et al., 2015) hard to apply, which indicators can be optimized with the least amount of positive interaction data?

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 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 (Jordano, 2016a, which is the case as networks are under-sampled; 2016b), when classifiers need to be 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.

A lot of binary classifiers are built by using a regressor (whose task is to guess the value of the interaction, 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 curves (ROC-AUC and PR-AUC henceforth) give ideas on the overall goodness of the classifier. Saito & Rehmsmeier (2015) established that the ROC-AUC is biased towards over-estimating performance for 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 applied to ecological network prediction.

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**

Baseline values

Intro

Definition of the performance measures

κ

F_β

informedness

MCC

ROC-AUC

PR-AUC

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

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 $\mathbf{M}$ 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 $\mathbf{S}$ with diagonal elements equal to s, and off-diagonal elements equal to $(1-s)$, and re-express the skill-adjusted confusion matrix as $\mathbf{M} \odot \mathbf{S}$, *i.e.*

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

Note that when $s = 0$, $\text{Tr}(\mathbf{M}) = 0$ (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.

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 ($\text{Tr}(\mathbf{C})$) 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 measures.

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 $]0, 0.5]$, which is within the range of usually observed connectance values for empirical food webs. Note that at this point, there is no food web model to speak of; rather, the confusion matrix we discuss can be obtained for any classification task. Based on the previous discussion, the desirable properties for a measure of classifier success should be: an increase with classifier skill, especially at low bias; a hump-shaped response to bias, especially at high skill, and ideally center around logit(b) = 0; an increase with prevalence up until equiprevalence is reached.

[Figure 1 about here.]

In fig. 1, we show that none of the four measures satisfy all the considerations at once: F_1 increases with skill, and increases monotonously with bias; this is because F_1 does not account for true negatives, and the increase in positive detection masks the over-prediction of interactions. Informedness varies with skill, reaching 0 for a no-skill classifier, but is entirely unsensitive to bias. Both MCC and κ have the same 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 same value, regardless of skill, but this value is not logit(b) = 0: unless at very high classifier skill, MCC 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 (*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 to evalue the performance of the model. The discussion of sensitivity to bias should come with a 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 (*i.e.* the prediction of new interactions), it is not necessarilly a bad thing in practice to select models that predict more interactions than the original dataset, because the original dataset misses some interactions. Furthermore, the weight of positive interactions could be adjusted if some information about the extent of undersampling exists (*e.g.* Branco et al., 2015).

Numerical experiments on training strategy

In the following section, we will generate random bipartite networks (this works without loss of generality on unipartite networks), and train four binary classifiers (as well as an ensemble model using the sum of ranged outputs from the component models) on 30% of the interaction data. Networks are generated by picking a random infectiousness trait v_i for 100 species (from a $B(6,8)$ distribution), and a resistance trait h_j for 100 species (from a $B(2,8)$ distribution). There is an interaction between i and j when $v_i - \xi/2 \leq h_j \leq v_i + \xi/2$, 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 fully interval networks that are close analogues to the bacteria–phage model of Weitz et al. (2005), with both a modular structure and a non-uniform degree distribution. This model is easy to learn: when trained with features $[v_i, h_j, \text{abs}(v_i, h_j)]^T$ to predict the interactions between i and j, all four models presented below were able to reach almost perfect predictions all the time (data not presented here) – this is in part because the rule is fixed for all interactions. In order to make the problem more difficult to solve, we use $[v_i, h_j]$ as a feature vector, and therefore the models will have to uncover that the rule for interaction is $\text{abs}(v_i, h_j) \leq \xi$.

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 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, and retains (part of) the imbalance of the original data.

The dataset used for numerical experiments is composed of 64000 such (ξ, ν) pairs, on which four machines are trained: a decision tree regressor, a boosted regression tree, a ridge regressor, and a random forest regressor. All models were taken from the `MLJ.jl` package (Blaom et al., 2020; Blaom & Vollmer, 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 application on a real dataset. As we use 64000 such datasets, this would require 256000 unique instances of tweaking thehyperparameters, which is not realistic. Therefore, we assume that the default parameterizations are comparable across networks. All machines return a quantitative prediction, usually (but not necessarilly) in $[0, 1]$, which is proportional (but not necessarilly linearly) to the probability of an interaction between i and j.

In order to pick the best adjacency matrix for a given trained machine, we performed a thresholding 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 thresholding step, we measured the area under the receiving-operator characteristic (ROC-AUC) and precision-recall (PR-AUC) curves, as measures of overall performance over the range of returned values. We report the ROC-AUC and PR-AUC, as well as a suite of other measures as introduced in the next section, for the best threshold. The ensemble model was generated by summing the predictions of all component models on the testing set (ranged in $[0, 1]$), then put through the same thresholding process. The complete code to run the simulations is given as an appendix; running the final simulation required 4.8 core days (approx. 117 hours).

After the simulations were completed, we removed all runs (*i.e.* pairs of ξ and ν) for which at least one of 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 that are more densely connected compared to the connectance of empirical food webs (and are therefore 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).

Effect of training set bias on performance

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

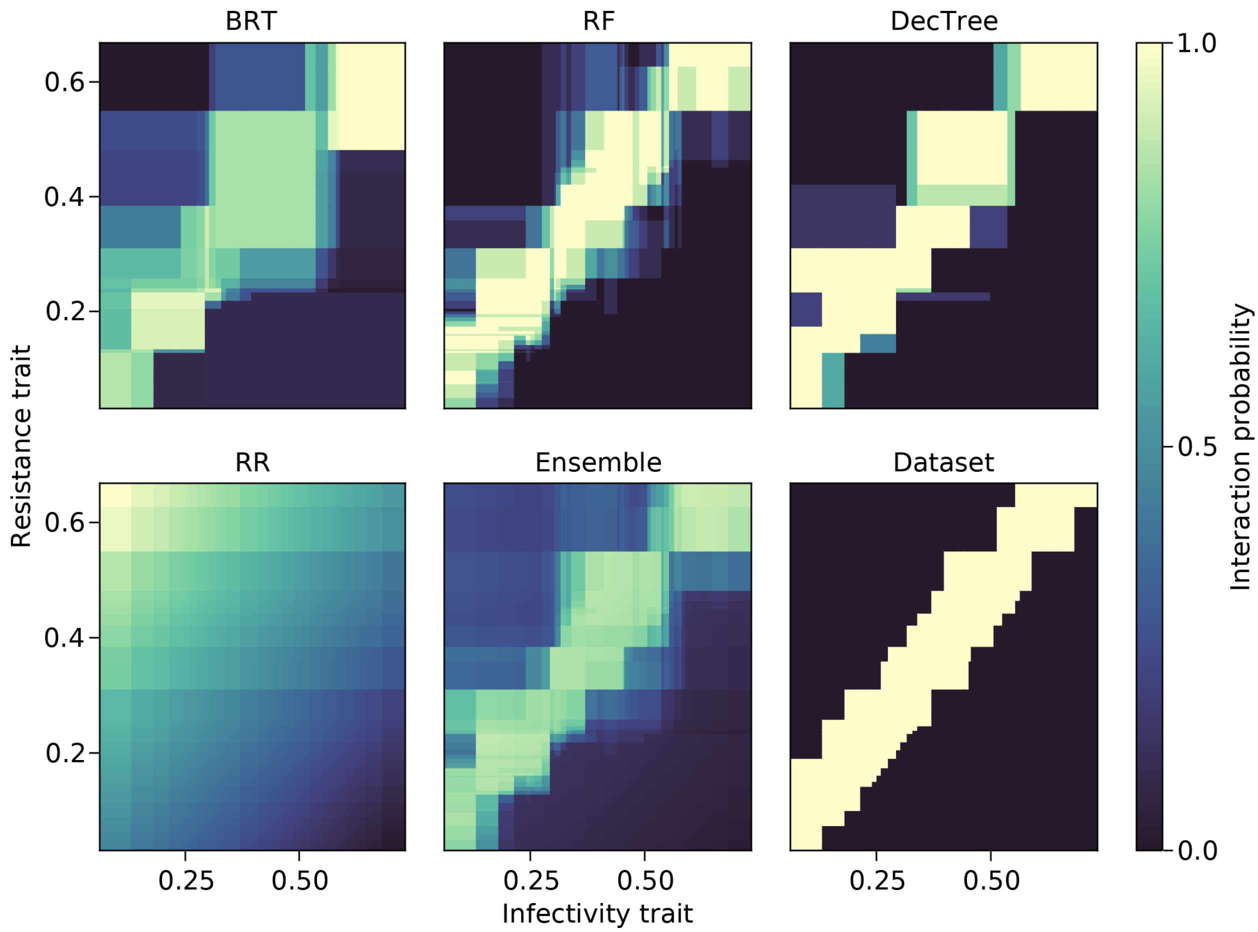
The more "optimistic" measures (ROC-AUC and informedness) required a biasing of the dataset from about 0.4 to 0.75 to be maximized, with the amount of bias required decreasing only slightly with the connectance of the original network. MCC and PR-AUC required values of training set bias from 0.75 to 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. **??**. 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 transformed back into networks for analysis; specifically, we measured the connectance, nestedness (REF), modularity (REF), and entropy (REF). The results are presented in the following table:

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

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 large, and by being limited by the *number* of interactions when the network is small. Nevertheless, based on the simulations and numerical experiments, it is possible to formulate a series of recommendations for the evaluation of network prediction models.

First, because we should have more trust in reported interactions than in reported absences of interactions, 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 better evaluated through the use of MCC fig. 3. Because F_1 is monotonously sensitive to classifier bias 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 fig. 4, it should be used as a measure of model performance over the ROC-AUC. This is not to say that ROC-AUC should be discarded (in fact, a low ROC-AUC is a sign of an issue with the model), but that its interpretation should be guided by the PR-AUC value. This again echoes recommendations from other fields (Saito & Rehmsmeier, 2015).

Thirdly, regardless of network connectance *or* measure to evaluate the model performance, as long as the network connectance is larger than ≈ 0.1, artificially balancing the training set to have equiprevalence will 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; even when poor models were included (Random Forest and Decision Tree), the ensemble was able to 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, Becker et al. (2021) found that the ensemble was *not* the best model. There is no general conclusion to 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 model should form the basis of the last recommendation: optimal training set bias and its interaction with 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, networks with different structures than the one we simulated here may respond in different ways.

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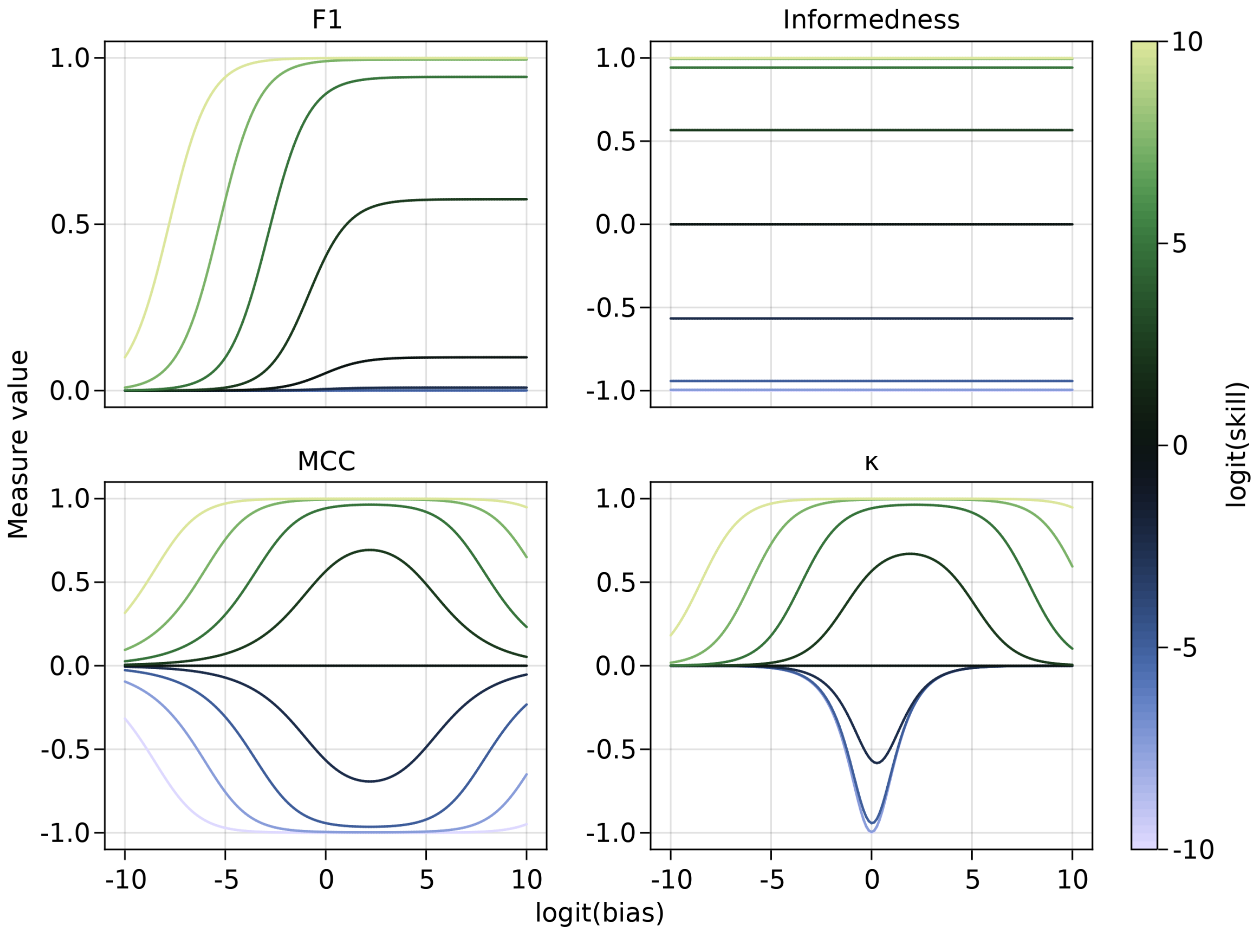

Figure 1: Consequences of changing the classifier skills (s) and bias (s) for a connectance $\rho = 0.15$, on accuracy, F_1, postive predictive value, and κ. Accuracy increases with skill, but also increases when the bias tends towards estimating *fewer* interactions. The F_1 score increases with skill 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 $b \approx 0.5$; 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.

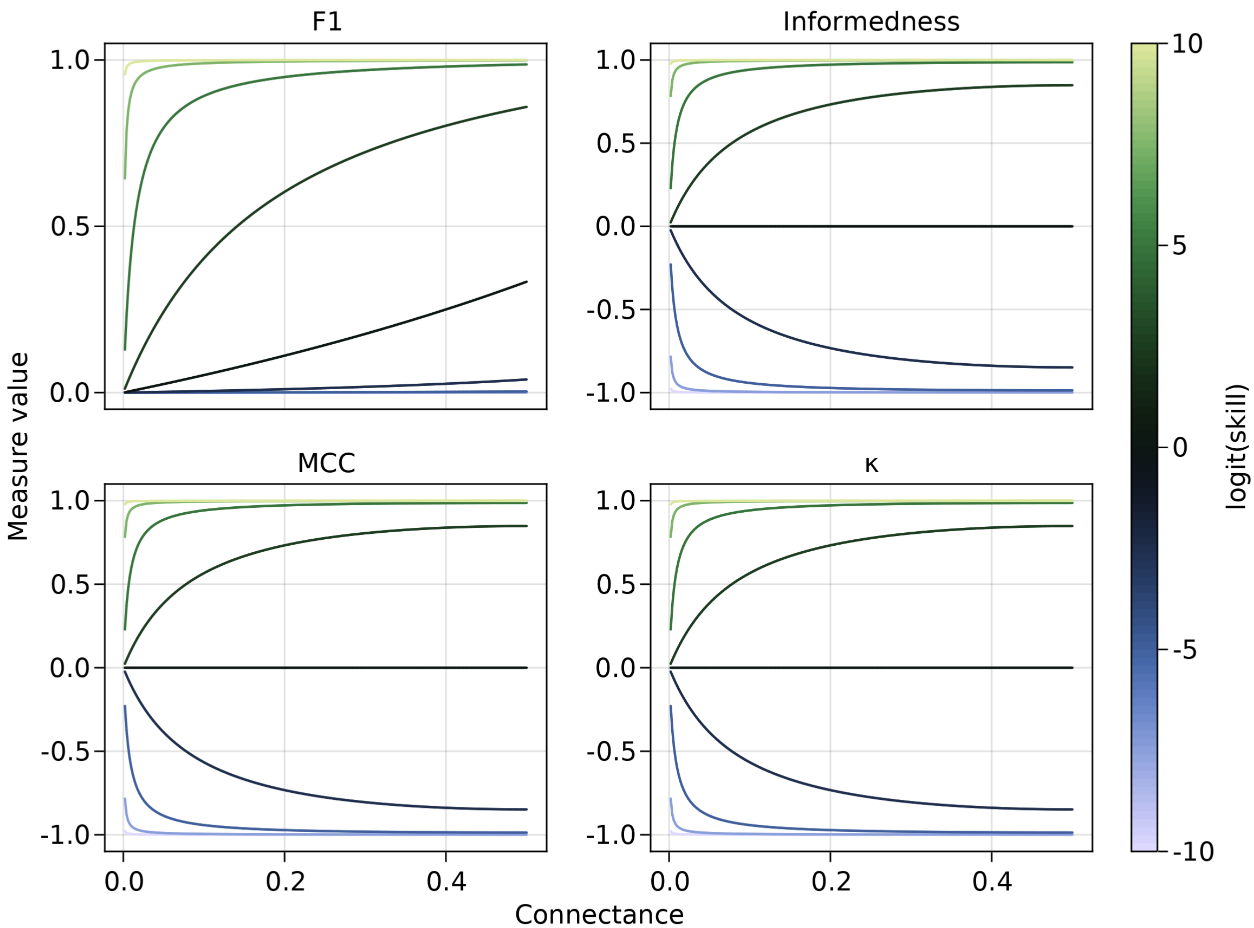

Figure 2: As in fig. 1, consequences of changing connectance for different levels of classifier skill, assuming no classifier bias. Informedness, κ, and MCC do increase with connectance, but only when the classifier is not no-skill; by way of contrast, a more connected network will give a higher F_1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

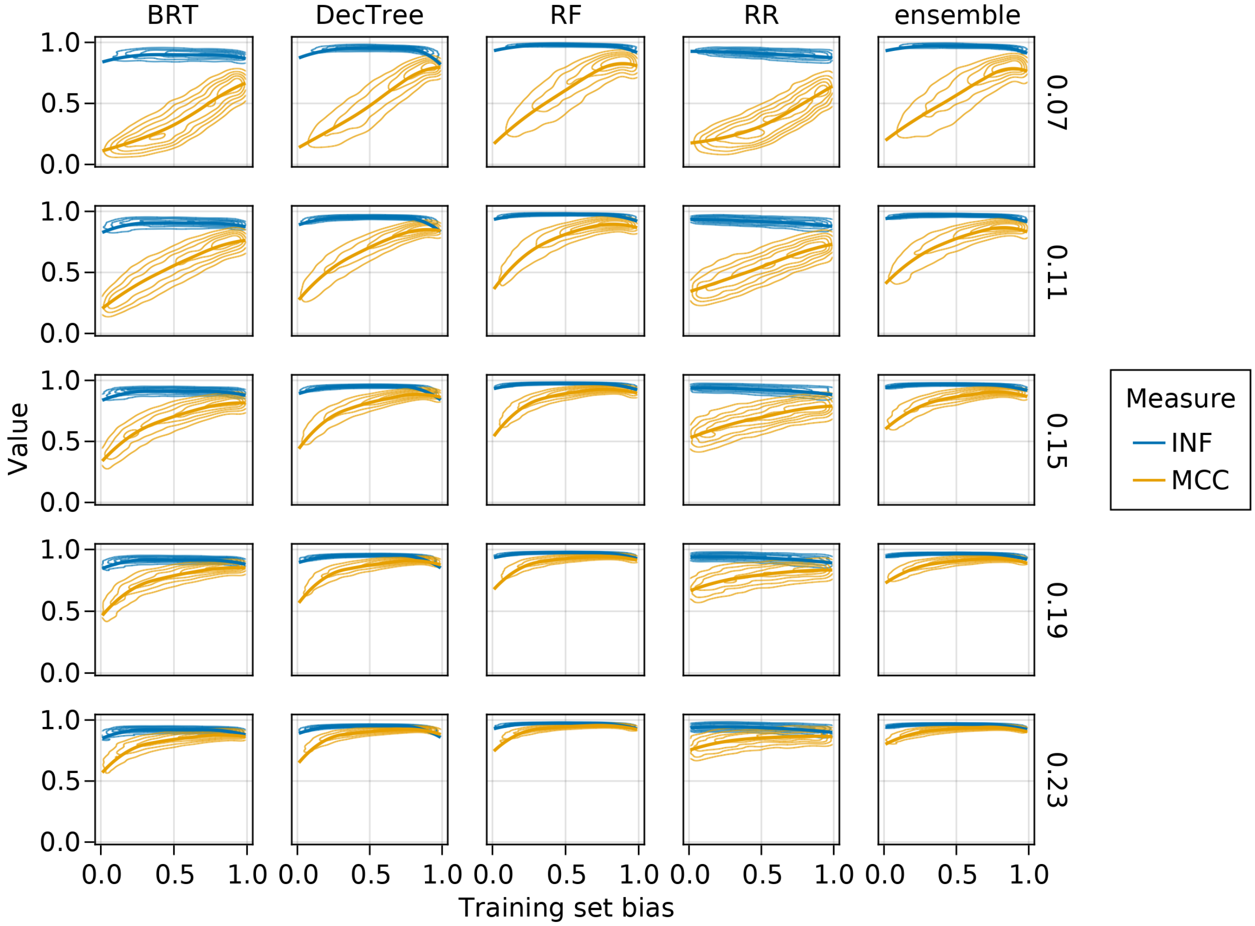

Figure 3: TODO

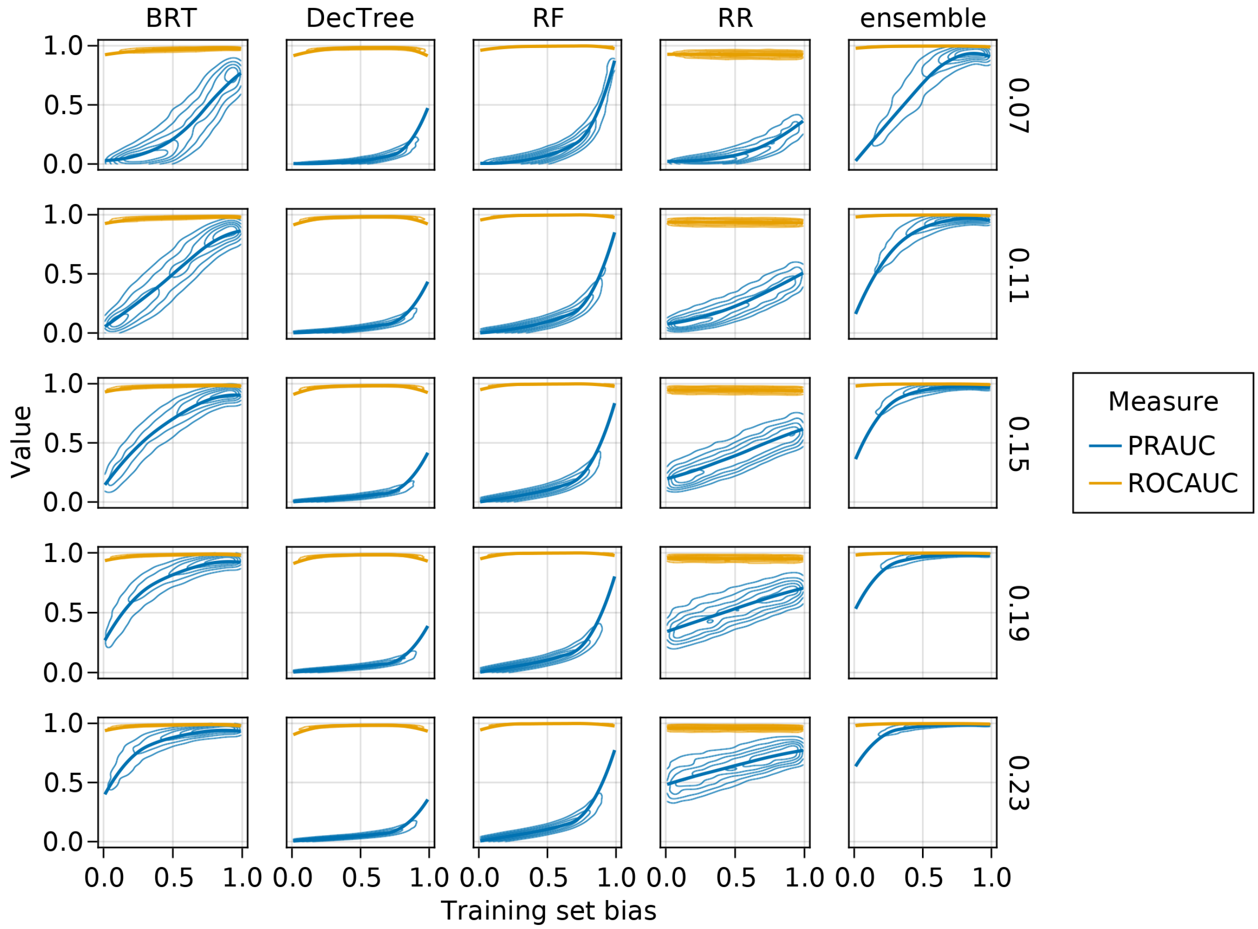

Figure 4: TODO

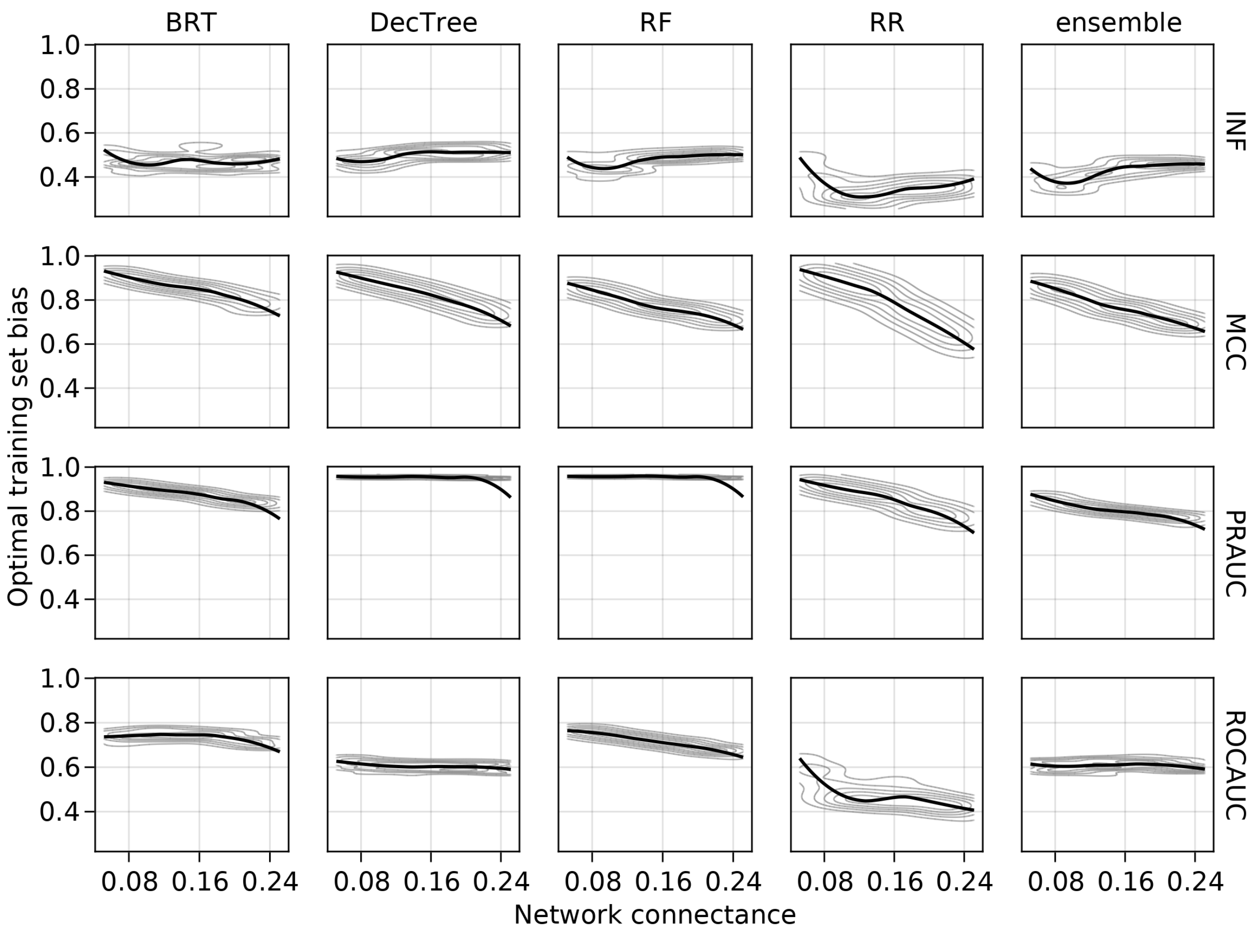

Figure 5: TODO

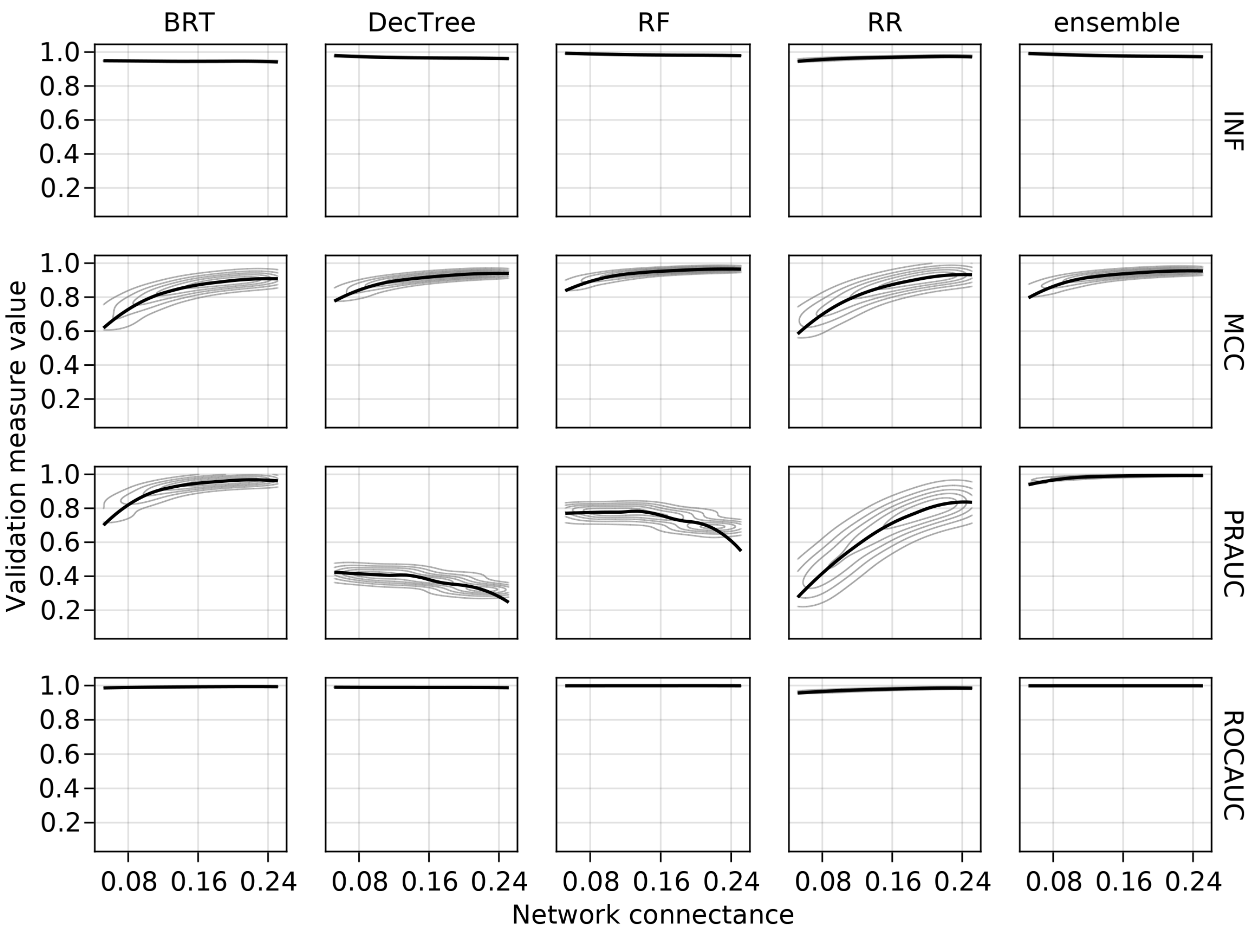

Figure 6: TODO