Flexible Model Selection for Mechanistic Network Models via Super Learner

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Abstract

Application of network models can be found in many domains due to the variety of data that can be represented as a network. Two prominent paradigms for modeling networks are statistical models (probabilistic models for the final observed network) and mechanistic models (models for network growth and evolution over time). Mechanistic models are easier to incorporate domain knowledge with, to study effects of interventions and to forward simulate, but typically have intractable likelihoods. As such, and in a stark contrast to statistical models, there is a dearth of work on model selection for such models, despite the otherwise large body of extant work. In this paper, we propose a procedure for mechanistic network model selection that makes use of the Super Learner framework and borrows aspects from Approximate Bayesian Computation, along with a means to quantify the uncertainty in the selected model. Our approach takes advantage of the ease to forward simulate from these models, while circumventing their intractable likelihoods at the same time. The overall process is very flexible and widely applicable. Our simulation results demonstrate the approach’s ability to accurately discriminate between competing mechanistic models.

Keywords mechanistic network model, model selection, Super Learner, likelihood-free methods
1 Introduction

Many systems of scientific and societal interest can be represented as networks, and network models are used, among many other applications, to study social networks, communication patterns, scientific citations, as well as protein-protein interactions (Wasserman and Faust 1994; Pastor-Satorras and Vespignani 2007; Newman 2010; Lusher et al. 2012; Raval and Ray 2013). There are (at least) two prominent paradigms to the modeling of networks, which we refer to as the statistical approach and the mechanistic approach. In the statistical approach, one describes a model that specifies the likelihood of observing a given network, i.e., these are probabilistic models of data that take the shape of a network (Robins et al. 2007; Hoff et al. 2002; Goyal et al. 2014). In the mechanistic approach, one specifies a collection of domain-specific microscopic mechanistic rules, informed by scientific understanding of the problem, that are used to grow or evolve the network over time (Barabási and Albert 1999; Watts and Strogatz 1998; Solé et al. 2002; Vázquez et al. 2003; Klemm and Eguiluz 2002; Kumpula et al. 2007). For example, in the context of social networks, mechanisms of interest might include triadic closure or reciprocation of directed edges. Both modeling approaches provide distinct angles and advantages to our understanding of complex systems, and in both approaches one is interested in learning about the connection between microscopic and macroscopic structures. Both mechanistic and statistical models are indexed by parameters and calibration/inference on those parameters is expected to shed light on those micro/macro structures.

In mechanistic models, a particular generative mechanism may seem like a strong assumption in contexts where one does not directly observe the formation of the network, and where it is difficult to study microscopic interactions in isolation of the rest of the system. For example, it might be difficult to learn about the mechanistic rules that govern the formation or dissolution of ties in in-person interactions, whereas doing so in the setting of online social networks or calls in a cellular network (Viswanath et al. 2009; Onnela et al. 2007; Saramäki and Moro 2015) where every interaction can be recorded might be more feasible. In some biological networks the pairwise interactions between the actors are well understood both theoretically and experimentally, they can be studied in isolation, and these interactions are highly reproducible. For example, gene duplication is one of the main drivers of the evolution of genomes, it is well understood, and therefore perhaps not surprisingly, network models based on gene duplication were one of the first large-scale models used in systems biology (Raval and Ray 2013).

In comparison, statistical models may be a more appropriate approach in settings where domain specific understanding is not as readily available to guide the selection of mechanisms, or there are too many mechanisms and including all of them would not lead to insightful modeling. This is in line with the use of statistical modeling more broadly, where one of the goals might be to learn how different predictors are associated with the response, which is a problem that can be studied even if the true associations between response and predictors, let alone the underlying mechanisms, are unknown. Common statistical models have limitations in the structures they are able to accommodate (Goyal and Omela In progress), and fitting and sampling from some of these models can be difficult. For example, the popular class of exponential random graph models (ERGMs) may not always be consistent under sampling (Shalizi and Rinaldo 2013). Mechanistic models do not suffer from these limitations as much, since generation of network structures from a handful of mechanisms is usually computationally inexpensive, so it is relatively simple to sample/forward simulate (to simulate observations given parameter values) from a particular model.

Another advantage of mechanistic models is the ease with which one can incorporate domain knowledge
in the model. Since the modeler is in control of the mechanisms to include, one is able to encode relevant domain knowledge of known or hypothesized interactions between actors in the system as mechanistic rules. The duplication-divergence models in protein-protein interaction networks are good examples of this (Raval and Ray 2013). In statistical models, one is unable to model such interactions directly, and can only consider the types of networks structures one expects to observe due to these interactions.

While there is a very extensive literature on mechanistic models in network science, there is a dearth of work on model selection in mechanistic models (Middendorf et al. 2005; Omela and Mira In progress). The aim of this paper is to provide a framework for model selection for mechanistic network models. For instance, given a full model which has an array of different generative potential or plausible mechanisms, we are interested in selecting between different submodels each possessing only a subset of the mechanisms of the full model. Traditional likelihood-based model selection, frequentist or Bayesian, is not applicable to mechanistic models because in most cases their likelihood functions are unavailable in closed form. One of the reasons why the likelihood functions are intractable is that in mechanistic models one must consider all the possible paths to generate any one particular network realization, which leads to a combinatorial explosion save for the most trivial settings. As such, one must consider likelihood-free approaches.

A recent likelihood-free approach to both inference and model selection for problems with intractable likelihoods is Approximate Bayesian Computation (ABC) (Marin et al. 2012; Sunnåker et al. 2013; Lintusaari et al. 2016). As the name suggests, this Bayesian approach aims at calibrating the model parameters to obtain an approximate posterior distribution for the parameters of interest. Following Bayes theorem, the posterior is obtained by combining information from the prior distribution on parameters and the data set, as incorporated by the likelihood. ABC inference starts by generating samples of possible parameter values from the prior. For each sample from the prior, one forward simulates a pseudo data set according to the model for the data, where the nature of the model, statistical or mechanistic, is not relevant. Then, given a distance measure between data sets, one accepts only the generated pseudo data that are within a certain distance from the observed data. These accepted data sets are deemed “close” to the observed one, and the parameters sampled from the prior corresponding to these data sets form the approximation to the posterior distribution. Unless the data are discrete and of low dimension, it is usually necessary to base the distance measure on summary statistics of the data (Beaumont 2010). Model selection with ABC is similar but includes an additional layer of hierarchy and a prior for the candidate model indices (Grelaud et al. 2009). In fact, there is a scarcity of likelihood-free model selection methods outside the realm of ABC. Toni et al. (2009) extend the sequential Monte Carlo ABC of Sisson et al. (2007) to ABC model choice, while Lee et al. (2015) do so with the approach of Fearnhead and Prangle (2012). Other recent innovations include an adaptive approach (Stoehr et al. 2015) and a random forest-based approach (Pudlo et al. 2015).

The main difficulty in practice for ABC arises when selecting the summary statistics as well as the threshold on the distance. If the selected summary statistics are sufficient for the parameters of the model and the distance threshold is zero, i.e., only parameters that have generated data sets with values of summary statistics exactly matching those of the observed data set are retained, then these accepted parameter samples will be from the true posterior (Barber et al. 2013; Lintusaari et al. 2016). However, should one fall short on either of these accounts, then the accepted parameter samples will only be from an approximation to the true posterior. When available, relevant domain knowledge can be applied to guide the selection of “essentially sufficient” summary statistics, which incorporate features attributable to the inferential objects of interest. However, since likelihood-free approaches like ABC are only needed with analytically or computationally
intractable likelihoods, it will typically be difficult to find the sufficient statistics in the absence of domain knowledge, though there is previous work on how to select good summary statistics for an ABC procedure in such a setting (Drovandi et al. 2011; Prangle et al. 2014). As for the threshold on distance measure, the smaller the distance threshold, the lower the acceptance rate, and hence the greater the computational burden to generate a reasonable number of accepted samples. In fact, outside of using discrete summary statistics, it may be totally impractical to use a distance threshold of zero. As a result, the performance of ABC inference can suffer due to the inaccuracy of the resulting posterior (Sisson et al. 2007). ABC model choice suffers from these same issues with reference to the model index, which becomes an additional model parameter on which inference is required. Even if one were to select statistics that are marginally sufficient for the submodels, they may not be jointly sufficient for the full model and thus not be able to discriminate among the various models under comparison, save for some special cases (Grelaud et al. 2009; Robert et al. 2011). Lastly, if one does manage to select all the sufficient statistics and conduct model selection with ABC, the resulting ABC Bayes factor may have no correspondence to the true Bayes factor (Robert et al. 2011).

Instead of dealing with issues stemming from the inaccuracy of the ABC posterior and Bayes factor, we propose a procedure for model selection that borrows the data generation from candidate models from ABC. Just as in ABC model choice, the data forward simulated from each candidate model will be the basis for model selection as it becomes the training data for model selection, but rather than using a Bayesian approach, we propose to conduct model selection with the Super Learner (SL) (Polley et al. 2011; Van der Laan et al. 2007). Originally proposed for prediction in a regression setting, SL is an ensemble algorithm that makes a prediction by combining the predictions from a library of candidate algorithms. Given a particular loss function, SL aims to minimize the expected loss, called the risk. The discrete SL simply picks the candidate algorithm that has the lowest cross-validated risk over the training data, whereas the full SL creates the convex combination of the algorithm-specific estimates that has the lowest cross-validated risk. Given a bounded loss function, both the discrete and the full SL have the so-called oracle property, meaning that asymptotically (in the number of training data sets) they perform at least as well as the optimal candidate algorithm available in the library and as the optimal convex combination of the candidate algorithms, respectively (Van Der Laan and Dudoit 2003; Dudoit and van der Laan 2005).

Our proposed approach generalizes that of Pudlo et al. (2015), which is a random forest-based ABC approach for model selection that is fairly robust to the choice of summary statistics. Their approach measures performance with the prior error rate, which is the probability to select the wrong model averaged over the prior. First, in our approach, the choice of performance measure is flexible and can be encoded directly into the loss function. For example, the prior error rate implicitly weighs misclassification differently for each model due to the sensitivity to the choice of the prior. Should one desire a measure that does not discriminate between misclassification of different models, one can use a measure like the Area Under the receiver operating characteristic Curve (AUC) (Bradley 1997; Ling et al. 2003). Second, SL can make use of a host of candidate algorithms, including random forest, to perform the classification. Random forest is a very flexible algorithm, but it may not perform well in all settings. One can be more robust against this by having more candidate algorithms in the SL library. Thus, we can deem the random forest based ABC approach of Pudlo et al. (2015) a special case of our approach if we use the prior error rate as our performance measure, and include random forest as the sole algorithm in the SL library. To handle uncertainty in the selected model, we adapt the regression-based approach used in Pudlo et al. (2015).

Due to the intractable nature of the likelihood and the ease of forward simulating data, model selection
with mechanistic network models lends itself well to the flexibility of the SL framework. The rest of the paper is organized as follows. In Section 2, we provide a brief overview of SL as well as the procedure for model selection in the context of mechanistic network models. We also introduce and motivate a simple mechanistic network model as a proof of concept, and we then use this model in our subsequent simulations. In Section 3, we lay out the details of the simulations as well as the results and evaluate the performance of our approach. Finally, in Section 4, we conclude with further discussions and suggestions for future work.

2 Methods and Material

Given a particular loss function \( L \), SL, as introduced by Van der Laan et al. (2007), aims to minimize the expected loss \( E[L] \), known as the risk, with respect to the distribution of the training data with an algorithm for prediction composed of a library of candidate algorithms \( \{Q_l\} \). The procedure begins by partitioning the training data, with predictors \( X_t \), and outcome \( Y_t \), into \( V \) validation sets. When applied to model selection for mechanistic network models, summary statistics computed on forward simulated network realizations play the role of predictors in SL and network model indices play the role of outcome in SL. The predictors and outcome of the \( v \)th validation set are referred to as \( X_v^t \) and \( Y_v^t \), respectively, while those of the corresponding training set, i.e., the union of the remaining \( V - 1 \) validation sets, are referred to as \( X_v^{-v} \) and \( Y_v^{-v} \). Note the distinction between training data \( (X_t, Y_t) \) and training set \( (X_v^{-v}, Y_v^{-v}) \). For the \( v \)th validation set, each candidate algorithm \( Q_l \) of the library is trained on \( (X_v^{-v}, Y_v^{-v}) \). The resulting trained algorithm \( \hat{Q}_l^v \) is then evaluated at \( X_v^t \), giving prediction \( \hat{Y}_v^t \). After training each candidate algorithm on each training set and evaluating it on the corresponding validation set, a new data set \( Z = \{\hat{Y}_v^v, Y_v^v\} \) is formed with the cross-validated predicted outcomes \( \{\hat{Y}_v^v\} \) and the true outcome \( Y_v^v \) from all validation sets, where the former serves as the new predictor and the latter serves as the new outcome. \( Z \) is used to estimate the cross-validated risk. This cross-validation procedure is intended to prevent overfitting, and this new data set will be the basis for the final prediction algorithm.

To arrive at the final prediction via \( Z \), in the case of the discrete SL, the candidate algorithm with the smallest estimated cross-validated risk is chosen for final prediction. Assuming a regression setting and a squared error loss function, the cross-validated risk for the \( l \)th candidate algorithm can be estimated as

\[
\hat{E}[L(Q_l)] = \frac{1}{V} \sum_v \frac{1}{n_v} \sum_i (Y_v^{t,i} - \hat{Y}_v^{t,i})^2,
\]

where the first summation is over the \( V \) validation sets and the second is over the \( n_v \) observations in the \( v \)th validation set. In the case of the full SL, the estimated risk will be minimized over all convex combinations of the candidate algorithms. In the same regression setting with squared loss and a particular convex combination \( a \), where \( \sum_l a_l = 1 \) and \( a_l \geq 0 \), the cross-validated risk can be estimated as

\[
\hat{E}[L(a)] = \frac{1}{V} \sum_v \frac{1}{n_v} \sum_i (Y_v^{t,i} - \sum_l a_l \hat{Y}_l^{t,i})^2.
\]

Once the final prediction algorithm is determined, i.e., \( Q_{l^*} \), that achieves the smallest risk in the discrete SL or \( a^* \) in the full SL, each candidate algorithm is refit on the entire training data in order to predict an outcome for \( X_o \), the observed predictors. Each resulting trained algorithm \( \hat{Q}_l \) is then evaluated at \( X_o \), giving prediction \( \hat{Y}_{o,l} \). The final prediction is the \( \hat{Y}_{o,l^*} \) in the discrete SL, or \( \sum_l a_l^* \hat{Y}_{o,l} \) in the full SL. In the
classication setting, the \( \{ \hat{Y}_v \} \) are the algorithm-specific scores for each class and \( Y_v \) the true class, with \( \hat{E} [ L (Q_t) ] \) or \( \hat{E} [ L (\alpha) ] \) defined according to the chosen loss function. The final prediction \( \hat{Y}_{o,t} \) or \( \sum_l a_l \hat{Y}_{o,l} \) are then the scores for each potential class. Fig. 1 gives a visual representation of the SL framework.

Now, we introduce the procedure for mechanistic network model selection within the SL framework. In this setting, the SL will be based on training data forward simulated from each candidate mechanistic network model in order to predict the model index (outcome) from a set of chosen network statistics (predictors). Before generating the training data, one needs care when choosing the parameter values for the candidate models so that it is plausible for the candidate models to generate the observed network to predict for, assuming that one of the candidate models is the true model. This can be done by calibrating parameter values, e.g., through the ABC framework (Marin et al. 2012; Sunnåker et al. 2013; Lintusaari et al. 2016), so that the data generated from the candidate models match the observed data based on some summary statistics. In our simulations, we assume our models are already calibrated. This ensures the generated data from each candidate model is similar to the observed data in some way. Once the parameter values are determined, one can form the training data by combining statistics computed for data generated from each candidate model as predictors with their corresponding true model indices as the outcomes. Before going ahead with the SL procedure, one needs to determine the appropriate loss function for the setting. Since the prediction is for the model index, this is a classification problem, so a loss function like squared loss is no longer appropriate. Instead, we propose to use \( 1 - L_{AUC} \) as the loss function, where \( L_{AUC} \), also known as
“rank loss,” is the loss function associated with $AUC$, the area under the receiver operating characteristic curve. The $AUC$ is an appropriate measure of the quality of the classification since it does not depend on the distribution of the model index in the data for performance evaluation. The corresponding loss function is bounded, so the resulting SL will retain the oracle property.

Algorithm 1 lays out the procedure we propose for model selection using SL, and Fig. 2 is the corresponding schematic. In addition to selecting the candidate algorithms, one needs to select the all-important network summary statistics to both calibrate on, in step 1 in Algorithm 1, and to train the algorithms on, in steps 5 and 7 in Algorithm 1. As previously stated in Robert et al. (2011), even if the sufficient statistics of all submodels are selected, they may not be jointly sufficient for the full model. Since it will be difficult or impossible to achieve, sufficiency should not be the most important criterion in choosing these statistics, but rather their ability to characterize the similarities and differences between the candidate models and thus their ability to discriminate among models. Suppose one is trying to select between a full model and one of its submodels that has one of the mechanisms of the full model turned off. In this case, one needs to consider the characteristics of the network that the missing mechanism affects and those that it does not. The statistics chosen for calibrating the parameters in step 1 of Algorithm 1 should reflect the characteristics that are unaffected by the missing mechanism. Conversely, those chosen as predictors in steps 5 and 7 should reflect the characteristics affected by the missing mechanism. For instance, should the submodel be missing triadic closure, one would expect statistics related to clustering to be affected due to the
formation of triangles by triadic closure. On the other hand, the number of cycles of length greater than 3 should not be much affect by triadic closure. The ability to characterize these similarities and differences will determine the performance of the algorithm and, thus, should guide the selection of the summary statistics. Though the candidate models we consider here are nested, they do not need to be in general to use this framework. Finally, in step 8 of Algorithm 1, evaluating the trained SL on the predictors for the observed network gives a score to classify the observation. In binary classification, i.e., having two candidate models, one model will be nominally “negative” and represented by 0 in the training of the SL, while the other will be nominally “positive” and represented by 1. In this case, the score will be bounded between 0 and 1 with scores above a user-defined cutoff classified as 1, or the “positive” model, and vice versa. For example, a cutoff of 0.5 can be used for this binary situation, as we did in our simulations.

Algorithm 1 Steps for proposed mechanistic network model selection via SL

1. Calibrate the parameters for all candidate models with the observed network based on relevant statistics that highlight similarities between models
2. Select relevant statistics that highlight differences between models as predictors
3. Generate networks as training data from all models of interest
4. Split the training data into cross-validation sets
5. Train/evaluate each candidate algorithms on each training/validation pair based on selected predictors
6. Train SL on the results from each candidate algorithm
7. Train each candidate algorithm on the entire training data set
8. Classify/select model for observed network based on the results from steps 6 and 7 of this algorithm based on preselected cutoff on the score

In order to perform uncertainty quantification, i.e., to quantify the confidence in the model selected through Algorithm 1, we adapt a procedure for the same purpose from [Pudlo et al. (2015)](https://doi.org/10.1007/s11222-015-9452-4), for each element in the training data, one needs to produce an out-of-bag (OOB) classifier, i.e., a random forest classifier based only on trees that does not involve the given element. OOB shares similarities with cross-validation, which SL does in steps 1-3 in **Fig. 1**, but step 4 in **Fig. 1** involves the whole data set. So the base SL is not completely cross-validated. In addition, the SL does not involve the aggregation of multiple smaller elements like random forest, so truly OOB is not feasible with the SL. Instead, in the same spirit, we propose to first split the training data into B subsets \((X^b_i, Y^b_i)\). Then, the “OOB” classifier for any element in \((X^b_i, Y^b_i)\) can be defined as the SL trained on \((X^{-b}_i, Y^{-b}_i)\), i.e., the training data without \((X^b_i, Y^b_i)\). For each element of the training data, with \(I\) denoting the indicator function, one can compute \(W = I(\hat{M}^* = Y)\), where \(\hat{M}^*\) is the model selected by the corresponding “OOB” classifier and \(Y\) is the true model index. Now, one can build a regression model for \(P(\hat{M}^* = Y | X)\) by regressing \(W\), i.e., \(W\) computed for all elements of the training data, on the predictors \(X\). This regression model can be simply logistic regression or a SL with the correctly specified loss function. Lastly, one can take the fitted value of this regression model at \(X\), the predictors for the observed network, as the estimate for \(P(\hat{M}^* = Y_o | X_o)\), where \(Y_o\) is the unobserved true model index for the observed network.
2.1 Model for Proof of Concept

As a proof of concept for our framework for mechanistic model selection, we introduce a simple mechanistic model to demonstrate its performance. The basis for the model is the classic Erdős-Rényi (ER) model \cite{Erdos1959}. In the ER model, the number of nodes \( n \) is fixed, and there are two variants on how edges are placed in the graph. In one variant, sometimes called the \( G(n, p) \) model, each of the \( C(n, 2) \), \( n \) choose 2, possible edges are independent and included in the graph with probability \( p \), so the number of edges in the graph has a binomial distribution. In the other variant, sometimes called the \( G(n, m) \) model, the number of edges in the graph \( m \) is also fixed. In this case, the random graph has a uniform distribution over all \( C(C(n, 2), m) \) possible graphs with \( n \) nodes and \( m \) edges.

Our model takes elements from both variants of the ER model. The model generates random graphs with a fixed number of nodes and edges just like the second variant of the ER model, but each edge is added one at a time with a certain probability akin to the first variant. At each step of graph generation, we select a pair of unconnected nodes uniformly from all such node pairs, and we connect them with an edge with a given probability. This process is repeated until the required number of edges have been added. If the probability for adding each edge was always fixed, then this model would be the same as the second variant of the ER model. In our model, instead, there is a base probability \( p_0 \) for edge placement, but two additional mechanisms are included to allow this probability to vary. The first mechanism is triadic closure, where should connecting the two selected nodes with an edge close a triangle, then the probability will be increased by \( p_1 \) over the base probability for adding the edge. We dub the second mechanism “triadic closure plus,” where should connecting the two selected nodes with an edge close more than one triangle, then the probability will be further increased by \( p_2 \) for each potentially closed triangle in excess of one. Should the sum \( p_0 + p_1 + t_c p_2 \), where \( t_c \) is the number of closeable triangles, exceed 1, it will be interpreted as 1. Fig. 3 illustrates these two additional mechanisms. Though this model is fairly simple, both its mechanisms can be motivated in social networks. In a friendship network, the first mechanism corresponds to the idea that two people are more likely to become friends if they have a mutual friend, while the second mechanism further increases the likelihood for each additional mutual friend. As such, these mechanisms can also be related to the so-called weak ties hypothesis \cite{Granovetter1973}, and it has been shown, in large-scale communication networks, that a higher proportion of shared friends is associated with greater tie strength \cite{Omodei2007}.

3 Simulation and Results

We conduct simulation studies to assess the performance of our model selection framework. We will use SL to select between the full model with both triadic mechanisms vs. the submodel with only the “standard” triadic closure mechanism. Networks generated from both models have 100 nodes and a base edge probability of \( p_0 = 0.3 \). The probability of edge placement increases by \( p_1 = 0.1 \) for the first closed triangle and by \( p_2 \) for every subsequent triangle, and we vary \( p_2 \) over the values 0.005, 0.01, 0.03, and 0.05. We vary the number of edges for the two models for any particular simulation over the values 500, 1000, and 2000. As mentioned below, both the training data and the data for performance assessment come from the candidate models, so the models are already artificially “calibrated,” with matching values of \( p_0, p_1, \) and edge count. For a given number of edges, the variation of \( p_2 \) from 0.005 to 0.05 makes the differences caused by the additional
Fig. 3: The probability to add an edge between two unconnected nodes in our variant of the ER model with two additional mechanisms when there are no closeable triangles (left), when there is one closeable triangle (middle), and when there is more than one closeable triangle (right). $p_0$ is the base probability for edge placement, $p_1$ is the increase in the probability for closing at least one triangle, while $p_2$ is the increase for each additional closed triangle after the first

mechanism easier to detect. For a given value of $p_2$, the variation of the number of edges from 500 to 2000 means that there will be more opportunities for the additional mechanism to manifest itself, also making it easier to detect. The simulation studies iterate through each combination of values of $p_2$ and edge number to see the interplay between the two.

In the simulations, SL used a library of three candidate algorithms: k-nearest neighbors (KNN), support vector machine (SVM), and random forest (RF). These three algorithms are chosen largely for their ability to handle collinear predictors, which are often present in summary statistics for networks. Given an observed sample for classification, KNN determines which (user-defined) $k$ samples in the training data are closest to the observed sample, based on some distance measure in the predictor space, a common choice being the Euclidean distance. The predicted class is the most frequent class among the $k$-nearest neighbors. Unlike KNN, which essentially formulates a new decision rule for each observation, SVM seeks to formulate a single decision rule for all classifications by separating the space of the predictors with a set of hyperplanes that segregate the space class-wise. Heuristically, a good hyperplane is one that is farthest from any sample in the training data. Once the class-wise segregation of the predictor space is complete, a new data point is classified based on the class label of the subset of the predictor space it falls in. Lastly, RF seeks to create a set of decision trees (the “forest”) from the training data in order to arrive at the final prediction. To build each tree, a bootstrap sample of the training data is taken to form the root. Then, at each node, a subset of the predictors are selected, and a “best” split is determined for these predictors in order to form its daughter nodes. Typically, the quality of the split is measured by the amount of homogeneity in each daughter node. Given an observed sample, each tree is traversed and gives a class label for the sample. An observation is then classified as the most frequent amongst all the tree-wise decisions.

In addition to the library of candidate algorithms, choosing appropriate predictors is an important task for the user. As discussed in the previous sections, sufficient summary statistics are difficult to obtain in all
but the trivial mechanistic network models, and one should aim to use summary statistics that are likely able to characterize the differences between the candidate models. In the simulations presented, there are five summary statistics chosen as predictors. The first predictor is the triangle count, which is an obvious choice, since the additional mechanism in the full model will favor edges that close multiple triangles. The second is the average local clustering coefficient over all nodes. The local clustering coefficient of a node is a measure of how close its neighbors are to forming a complete subgraph by themselves, i.e., having every possible edge between any two neighbors. If the addition of an edge between nodes $a$ and $b$ will close multiple triangles, then, without loss of generality, from the point of view of node $a$, the addition of the edge would mean the addition of a single neighbor, $b$, and the addition of multiple edges amongst $a$’s updated set of neighbors between $b$ and the shared neighbors of $a$ and $b$. In scenarios with lower total edge counts, where the degree of either $a$ or $b$ is likely to be low, this could lead to a potentially large change in the local clustering coefficient. Lastly, the additional mechanism is a rich-getting-richer scheme in terms of the degree of a node, since the more closeable triangles a pair of nodes have, the higher their existing degrees, which further leads to a higher probability of both getting an increase to their degrees with an additional edge. Thus, this mechanism is likely to affect the degree distribution in the network. As a proxy to the full degree distribution, the three quartiles (25%, 50%, 75%) of the degree distribution are included as summary statistics and thus predictors.

The mechanistic model proposed in the previous section was coded in Python and based on the package NetworkX. The training of SL, with a 5-fold cross-validation, was done with the R package SuperLearner, which contains wrappers for the chosen candidate algorithms. The parameters for the candidate algorithms are kept at the default values. For a given combination of edge count and value for $p_2$, we generated 10,000 training samples from both the full model and the submodel as training data. Rather than using a separate sample to assess performance, the $AUC$ of SL as well as of each candidate algorithm was estimated via a 10-fold cross-validation. Note that this is a separate stage of cross-validation from that of the training of SL itself. First, the training data is partitioned into 10 validation sets, which are used for performance cross-validation. Then, for each of the 10 performance validation sets, a 5-fold cross-validated SL is trained on the union of the remaining 9 performance validation sets, and then used to predict the model index for the given performance validation set. The $AUC$ measure is computed for each of the 10 performance validation sets and averaged.

The cross-validated estimate of the $AUC$ for the full and discrete SL, and each candidate algorithm, for each scenario of the simulation studies are summarized in Fig. 4, with numerical results in Table 1 in the appendix. In general, performance decreases as the value of $p_2$ decreases, which is no surprise as the effect of the additional mechanism diminishes as $p_2$ gets smaller, and thus the two models are harder to distinguish. Performance also improves as the edge count increases, as the mechanism has more opportunities to manifest itself with more edges.

The simulation results seem to support the oracle properties of both the discrete and full SL. Indeed, in most scenarios, the discrete SL has the same cross-validated $AUC$ as the best performing candidate algorithm, with the full SL performing a little better, as expected. In these scenarios, the ordering of the candidate algorithms by performance is likely the same across each fold in the cross-validation. Thus, the discrete SL always picks the same candidate algorithm in each fold and has the same performance as the best candidate algorithm averaged across all folds. The full SL, in this case, takes a convex combination of the candidate algorithms in each fold and performs at least as well as, and likely better than, the best performing candidate algorithm in each fold. When averaged across the cross-validation folds, the full SL
Fig. 4: Cross-validated $AUC$ for each method: full SL (fSL, red), discrete SL (dSL, blue), support vector machine (SVM, grey), random forest (RF, grey), $k$-nearest neighbors (KNN, grey), in each simulation scenario clearly performs better, as evidenced by the simulations.

Still, there are a few scenarios where either or both of the discrete and full SL perform slightly worse than the best performing candidate algorithm. This occurs with edge count 500 and $p_2 \in \{0.005, 0.01, 0.03\}$. In these scenarios, there are several candidate algorithms that are quite close in performance, and the ordering of their performance is likely not constant across the folds. In this case, the discrete SL picks different candidate algorithms across the folds and the $AUC$ averaged across the folds may be worse than that of the best candidate algorithm. The full SL on the other hand weights different candidate algorithms most heavily across the folds, and the cross-validated $AUC$ can also end up worse than the best candidate algorithm.

In the scenarios where either or both of the discrete and full SL perform worse than the best candidate algorithm, they both still perform very close to the best candidate algorithm, with difference in $AUC$ only of the order of $10^{-3}$ or less. Since the oracle properties for both SLs are asymptotic results, some small deviations from asymptotic behaviors would be expected for finite samples. In the limit, the ordering of the performance of the candidate algorithms are likely to be constant across all folds, and both SLs are expected to perform no worse than the optimal candidate.

The best performing candidate algorithm varies between SVM and RF across the scenarios, which is not something known a priori, but both versions of SL are able to closely match or beat the best candidate algorithm. Although the differences between the best and worst performing candidate algorithms in the scenarios visited are not too great (biggest difference is about 0.1), it is still easy to see the manifestation.
of the oracle property, which would be even more valuable in scenarios with greater differences. Thus, when one particular candidate algorithm outperforms the rest, one can be confident that the discrete SL will select it, and the full version will weight it heavily. In cases when one is unlikely to fully grasp the significance of the various summary statistics as predictors or what learning algorithm would work best due to the complex nature of the data, it would be ideal to consider multiple candidate algorithms paired with different combinations of predictors and find an optimal mix. This makes SL well suited for model selection in mechanistic network models.

We implemented the proposed procedure for quantifying the uncertainty in the selected model on the simulated data. We assessed two scenarios, an easy one, with edge count 2000 and $p_2 = 0.005$, and a difficult one, with edge count 500 and $p_2 = 0.005$. For each scenario, we first define the $\hat{M}^*$ as 1, or the “positive” model, if the score given by the “OOB” SL is $>0.5$, and 0, or the “negative” model, otherwise. Then, we define $W$ as stated above, and build the regression model for $P(\hat{M}^* = Y|X)$ with a new SL with the appropriate loss function in order to maximize the corresponding binomial likelihood

$$\prod_i P(\hat{M}^*_i = Y_i|X_i)^{W_i}(1 - P(\hat{M}^*_i = Y_i|X_i))^{1-W_i}.$$ 

The new SL uses the same library of candidate algorithms as before. The average value of $P(\hat{M}^* = Y|X)$ for the two scenarios are 0.7090 for the easy scenario and 0.5341 for the difficult one. The average value for the easy scenario is noticeably higher than 0.5, while that of the difficult scenario is very close to 0.5, which is hardly better than a random guess. This reflects the $AUC$ simulation results as well as the distinguishability corresponding to the choice of edge count and $p_2$ we anticipated.

4 Discussion

Network models are used widely in many domains, and mechanistic models allow one to easily incorporate domain knowledge. However, due to the intractability of the likelihood of the typical mechanistic network models, likelihood-based model selection methods are not feasible. We propose a procedure that combines the Super Learner (SL) framework with the data generation of Approximate Bayesian Computation (ABC), allowing one to leverage the ease of generating data from mechanistic models via forward simulation, while quantifying uncertainty in the selected model.

While ABC provides one viable means for mechanistic network model selection, an accurate ABC posterior requires the knowledge of sufficient statistics, which are typically difficult to find in the case of intractable likelihoods. The lack of sufficiency and the distance thresholding inherent in ABC can cause inaccuracy in the approximation of the posterior distribution of the model index. In addition, the concatenation of the sufficient statistics of each submodel is not necessarily sufficient for the full model. This can lead to a lack of correspondence between the ABC Bayes factor and the true Bayes factor. Rather than relying on ABC to approximate the Bayes factor for model selection, which suffers from the lack of sufficiency, we proposed to use SL for model selection while borrowing the generation of pseudo-data from ABC.

With training data readily generated from each candidate model, SL seeks to build an optimal algorithm from a library of candidate algorithms. In this case, it seeks to build an optimal classifier from candidate algorithms to best discriminate between the available models with the given predictors, which are not necessarily sufficient. One is unlikely to know what classifiers paired with what predictors will perform
well, but with SL, one does not need to make this choice as SL will try to build the optimal classifier with all that is given. However, this does not mean that the quality of the predictors does not matter. The better the predictors are at characterizing the differences between the candidate models, the better SL performs. Though the ability to characterize the differences likely correlates with sufficiency, sufficiency in and of itself should not be the criterion for choosing the predictors. For mechanistic models, one can, and should, apply domain knowledge to select predictors.

The main difficulty of the proposed approach is that one needs to be sure that the candidate models could have plausibly generated the observed data, assuming one of the models under comparison is the true one. Furthermore, one needs to consider what characteristics of the data are unlikely to be affected by the different mechanisms of the candidate models, and then to calibrate the parameters of each candidate model based on these characteristics of the observed data. This will hopefully allow the differences in the candidate models to more clearly manifest themselves and ensure that the data generated from each candidate model are similar to the observed data in some aspects. Ideally, this also means that the data generated from the true model will match the observed data closely. However, there is no guarantee to this. In the current state, this part of the procedure is more an art than an algorithm.

The most immediate step for future work would be to make the calibrating of the parameters of the candidate models more concrete. Should this step be done incorrectly, one faces the danger of choosing the wrong model completely, even if the true model is included among the candidates.
## Appendix

| \(p_2\) | 0.005 | 0.01 | 0.03 | 0.05 |
|--------|-------|------|------|------|
| \(EC = 500\) | | | | |
| fSL    | 0.50786 | 0.51941 | 0.58896 | 0.65630 |
| dSL    | 0.50575 | 0.51950 | 0.58911 | 0.65585 |
| SVM    | 0.50097 | 0.49936 | 0.50504 | 0.55592 |
| RF     | 0.50826 | 0.51950 | 0.58911 | 0.65585 |
| KNN    | 0.50353 | 0.51158 | 0.56172 | 0.63093 |
| \(EC = 1000\) | | | | |
| fSL    | 0.57071 | 0.65993 | 0.90814 | 0.97895 |
| dSL    | 0.57055 | 0.65738 | 0.90445 | 0.97798 |
| SVM    | 0.50897 | 0.55834 | 0.90445 | 0.97586 |
| RF     | 0.57055 | 0.65738 | 0.90248 | 0.97798 |
| KNN    | 0.55596 | 0.64410 | 0.89605 | 0.97275 |
| \(EC = 2000\) | | | | |
| fSL    | 0.74179 | 0.90348 | 0.99839 | 0.99947 |
| dSL    | 0.73703 | 0.90067 | 0.99769 | 0.99917 |
| SVM    | 0.67271 | 0.90067 | 0.99709 | 0.99879 |
| RF     | 0.73703 | 0.89573 | 0.99769 | 0.99917 |
| KNN    | 0.72623 | 0.89077 | 0.99540 | 0.99751 |

### Table 1

| \(p_2\) | 0.005 | 0.01 | 0.03 | 0.05 |
|--------|-------|------|------|------|
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