Bayesian Model Selection on Random Networks

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Abstract

A general Bayesian framework for model selection on random network models regarding their features is considered. The goal is to develop a principle Bayesian model selection approach to compare different fittable, not necessarily nested, models for inference on those network realisations. The criterion for random network models regarding the comparison is formulated via Bayes factors and penalizing using the most widely used loss functions. Parametrizations are different in different spaces. To overcome this problem we incorporate and encode different aspects of complexities in terms of observable spaces. Thus, given a range of values for a feature, network realisations are extracted. The proposed principle approach is based on finding random network models such that a reasonable trade off between the interested feature and the complexity of the model is preserved, avoiding over-fitting problems.

Key words: Model Selection, Random Networks, HM-MCMC.

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1 Introduction

In this paper, we propose a general approach for generating and comparing random network models regarding their features. Given a random network model, we consider the joint distribution between the parameters and features of the model we are interested in and generate respective models that follows this distribution. By formulating the joint distribution we can find a part of distribution which captures a given desired distribution for either the parameters or the features. Different random network models capture differently parameters or features, sometimes not at all.

The researcher might be interested in observing a feature of the random network model (e.g. degree distribution or transitivity) and there is no obvious model that encodes the features you are interested in making it impossible or difficult to parametrize a model in terms of those features. He can only use models that understand, interpret, implement and can actually fit, because of computational, logistic tools, and carry out a secondary analysis if this random network model is appropriate for describing this feature. For example, SBM does not parametrize average path length but is pretty flexible model and you have the means to fit. We want to answer the following questions: Which model, that has the resources to fit, can capture the feature better? How limited is our description? Maybe the model is not powerful enough to say much things to represent the feature. We want a criteria that says if some features are well behaving. For instance, a researcher might be interested in degree distribution and suppose that he can only fit an Erdős-Rényi or a SBM model with certain parameters, degree density and number of blocks, respectively. Which one describes better a certain degree distribution?

Our research relates to the literature on intrinsic Bayes factor, model selection on parameters and features on random network models and the literature on informative prior elicitation. In [14] the authors are dealing with the elicitation of informative priors on
graph space that encode parameters and features. In [17] the author proposes a Bayesian framework for choosing the number of blocks as well as comparing it to the more elaborate degree-corrected block models, ultimately leading to a universal model selection framework capable of comparing multiple modeling combinations. In [16] they consider an approach based on the log likelihood ratio statistic and analyze its asymptotic properties under model misspecification in order to solve problems concerning estimating the latent node labels and the model parameters than the issue of choosing the number of blocks. They show the limiting distribution of the statistic in the case of underfitting is normal and obtain its convergence rate in the case of overfitting. In [12], the authors do not assume only community based penalties but any specific model for the network. They make a more general structural assumption of a model being approximately low rank, which holds for most popular network models. This is their limitation in contrast with our method. In [6] paper, the authors are limited in model selection under block models and its variants. They focus on a generic idea of network cross-validation. Cross-validation is a very popular and appealing method in many model selection problems. The adaptation to network data is usually through a node splitting procedure and has been considered by [9], [15], among others. In [17, 7] the author develop a Bayesian model selection criterion for stochastic block models which is inspired by BIC. In [4] the contribution of this paper is the development of a fully Bayesian model selection method based on a reversible jump Markov chain Monte Carlo algorithm which estimates the posterior probability for each competing model. Conceptually, the closest to our research framework is that of [10] where the authors design and implement MCMC algorithms for computing the maximum likelihood for four popular models: a power-law random graph model, a preferential attachment model, a small-world model, and a uniform random graph model. However there limitation is that their method is confined by those four models. Moreover, they do not use a loss function as in this we do in this paper.
Here we propose a methodology for generating and comparing random network models in such a way that the top model tend to produce posteriors that preserve simplicity and information for a certain feature when compared to posteriors obtained from models less favored by the comparison. The selection of random network models is obtained by decision theory approach. We make the case that the selection of random networks models implied by our approach are reasonably consistent with selection implied both by the most widely used loss functions functions for estimation and prediction.

The approach we propose is creating a joint distribution for a random network model which encapsulate both the parameters and features of the network. For this reason we use subsampling procedures by producing network instances for random network models and computing their joint feature distribution. Next, we are based on Bayesian model selection concepts and tools and we compare these models using a Bayesian model selection approach. The criterium for random network models regarding the comparison is formulated via Bayes factors of the most widely used loss functions. The rationale behind the proposed approach is to find random network models such that preserve the best possible trade of the information provided for the feature and the complexity of the model from the original data generating mechanism avoiding the problem of over-fitting. Thus, computational and Bayesian statistics enable us to generate and compare, in a principled way, random network models.

The paper proceeds as follows: In Section 2, we describe settings of the problem, we formulate them and give notation and definitions of networks and random networks. Furthermore, we present, briefly, subsampling and Bayes factors tools that are useful in the next sections. Then, in section 3, we focus in our main purpose of this paper which is how we use and compare random network models by using decision theory in order to preserve the needed amount of information for a certain given feature or number of features required
by Bayes factors. Conceptually and computationally, our methodology is presented. In section 4, for many random network models data analysis that gives experimental results involving decision theory is conducted showing the results of our approach. Finally, in section 5, we present with more details the limitation of the method and future work involving overlapping research areas.

2 Preliminaries

2.1 Random Networks

We define a network as a pair $G = (V, E)$, where $V$ denotes the set of nodes, and $E$ the set of edges $E \in V \times V$. We denote by $A_G$ the adjacency matrix of $G$. Let $N$ denote $|V|$. A network is called simple if at most one edge exists between each pair of nodes and no self-loops are allowed. A network is called undirected if the corresponding adjacency matrix is symmetric. A random network (or random graph model) is a probability model on the space of adjacency matrices. In this paper we consider random network models in the space of simple undirected networks, i.e., a distribution on the space of binary symmetric adjacency matrices. For the sake of simplicity, we are using the same symbol ($G$) for a network and a random network. We use $G(\omega)$ to denote a realization from the random network model. The simplest example of random network is Erdős-Rényi model, where each possible edge in the graph is included with a constant probability $p$.

2.2 Complexity of a Random network

A mathematical framework has been proposed for analyzing Random Network Models and for characterizing their complexity. Such framework allows the study of several network properties or features (link density, clustering coefficient, degree distribution, connectivity), and their relationship with the random network model complexity. For doing so, differ-
Figure 1: Penalizing in the space of parameters is complex as we can see. $a_1$ denotes the community structure. $a_2$ denotes the degree distribution and $a_3$ the network subcounts.

...ent entropy measures have been evaluated and their relationship has been assessed. The sample degree distribution entropy has shown to be correlated with the random network model entropy, providing a practical measurable indicator of complexity in real networks. Generally, link density, clustering coefficient, degree distributions and connectivity are computed and comparatively analyzed in order to illustrate their relationship with random network model complexity (Figure 1). The fundamental simulations have been performed by imposing varying values of the link density and triangle density parameters in ERGMs.

2.3 Bayes Factor

One of the central quantities in Bayesian learning is the evidence (or marginal likelihood), the probability of the data given the model $P(D \mid M_i)$ computed as the integral over the parameters $w$ of the likelihood times the prior. The evidence is related to the probability of the model, $P(M_i \mid D)$ through Bayes rule:

$$P(D \mid M_i) = \int P(D \mid w, M_i)P(w \mid M_i)dw, P(M_i \mid D) = P(D \mid M_i)P(M_i)P(D)$$ (1)
where it is not uncommon that the prior on models $P(M_i)$ is flat, such that $P(M_i \mid D)$ is proportional to the evidence. It is typically impossible to compute analytically. However, the model evidence is crucial for Bayesian model selection since it allows us to make statements about posterior model probabilities. The evidence discourages overcomplex models, and can be used to select the most probable model. It is also possible to understand how the evidence discourages overcomplex models and therefore embodies Occam’s Razor by using the following interpretation. The evidence is the probability that if you randomly selected parameter values from your model class, you would generate data set $D$. Models that are too simple will be very unlikely to generate that particular data set, whereas models that are too complex can generate many possible data sets, so again, they are unlikely to generate that particular data set at random. To the point, on computation, we will evaluate the different likelihood integrals in the Bayesian setting with a large-scale Monte Carlo procedure in almost any case of practical interest.

2.4 Intrinsic Expected Losses

As we mentioned in the introduction, many methods for model selection between random networks have been developed. All of them are penalizing based on one important attribute of the network which tries to measure the complexity of the network, as it is described in the previous subsection. Moreover, all of them select models from the same family of models e.g. are able to select which SBM fits better the data without overfitting them. Non of the mentioned methods are able to perform a principled universal model selection between two different random network models (e.g. compare a certain Barabasi-Albert model with a certain SBM).

To address the natural question of which model is best for a particular data set, we propose a model selection criterion for graph models and present a more flexible principle model selection criterion inspired by Bayesian Decision Theory penalizing with Expected
Losses of one or more specific features. The Bayes decision is simply the hypothesis with the larger posterior probability. The posterior expected loss of two models $M_1$ and $M_2$ are $K_1 \times P(M_1 \mid D)$ and $K_2 \times P(M_2 \mid D)$, respectively. The Bayes decision is again treat corresponding to the smallest posterior expected loss. In this Bayes test, the null hypothesis is rejected when:

$$\frac{K_1}{K_2} > \frac{P(M_1 \mid D)}{P(M_2 \mid D)}$$

In statistics and decision theory a loss function or cost function is a function that maps an event or values of one or more variables onto a real number intuitively representing some “cost” associated with the event. Simply, we formalize good and bad results with a loss function. The loss function determines the penalty for deciding how well a model is behaving in terms of the feature which is going to penalize it. Some examples involve: i) 0-1 loss function where $L(\hat{y}, y) = I(\hat{y} \neq y)$ and $I$ is the indicator function. ii) Quadratic Loss function where for a scalar parameter $\theta$, a decision function whose output $\hat{\theta}$ is an estimate of $\theta$, and a quadratic loss function $L(\theta, \hat{\theta}) = (\theta - \hat{\theta})^2$ and iii) absolute Loss function where for a scalar parameter $\theta$, a decision function whose output $\hat{\theta}$ is an estimate of $\theta$, and a quadratic loss function $L(\theta, \hat{\theta}) = |\theta - \hat{\theta}|$.

Since the choice of a particular loss function strongly influences the resulting inference, it seems necessary to rely on intrinsic losses when no information is available about the utility function of the decision-maker, rather than to call for classical losses like the squared error loss. Since this setting is quite similar to the derivation of non-informative priors in Bayesian analysis, we first recall the conditions of this derivation and deduce from these conditions some requirements on the intrinsic losses. For that reason intrinsic loss functions could be used.
2.5 Extracting Random graph information

We would like to define a prior such that, when sampling from the prior, we generate reasonable random networks. Here, reasonable is taken to mean that the networks should respect graph-theoretical properties that have been inferred by network properties. A general form of informative log linear distribution over graph is proposed by [14]. The random graph prior is defined as a distribution:

$$P(G) \propto \exp(\lambda \sum_i w_i f_i(G))$$

in which $\lambda$ is a strength parameter and the parameters $w_i$ tune the relative strengths of the individual concordance functions that capture several graph-theoretical properties of random network realization properties. Some examples of concordance functions are: individual edges, controlling the in-degree of graphs, higher-level Network features, degree distributions, priors on individual edges and priors on degrees counts.

2.6 Exchangeability and Concensus Monte Carlo

For estimating features from exchangeable models which are not straightforward to relate to the parametrization at hand, we extract the information about the feature included in the empirical graphon through the corresponding SBM of the model (each node/edge/measure-exchangeable model ([13], [3], [5], [8]) can be divided into parts in line with empirical graphon and described by it). This task is high dimensional (NP-complete) and in order to make it scalable we divide the model into $n \times n$ cells of 10 nodes each. When exchangeable or more generally model exchangeable parametric objects, through empirical graphon, are available then for estimating features from exchangeable models which are not analytically parametrized e.g. random networks producing diameters, we extract the information through [14]. Let $f(G)$ be a real-valued function on graphs that is increasing in the degree
to which graph $G$ agrees with prior beliefs (a “concordance function”). For potentially multiple concordance functions $f_i(G)$, we suggest a log-linear network prior of the form:

$$P(G) \propto \exp\left\{ \lambda \sum_{i=1}^{n^2} w_i f_i(G) \right\} = \prod_{i=1}^{n^2} \exp\{\lambda w_i f_i(G)\}$$

(4)

, where the $\exp\{\lambda w_i f_i(G)\}$ is one cell of the model which describes a submodel (e.g. one can be scale free distribution and the other follow a constant distribution).

Then, we merge all the networks into one each time, extracting the feature (parameter) ([18]). For this, we use consensus monte carlo ([2]), in order to merge the observables for each feature. Finally, we use all those merged observables using intrinsic loss functions for each feature. Obviously, this approach is computationally expensive, though it is scalable, due to model division in $n \times n$ squared cells (number of cores needed in Map-Reduce framework). Depending on the number of cores used we can reach complex networks up to 10,000 nodes.
3 Methodology

3.1 General Concepts

Suppose we have an observed feature (e.g. centrality) and we are given two different network models (e.g. SBM and Erdős-Rényi). What is the probability of observing the observed feature given the first model (e.g. SBM) compared with the probability of observing it given the second model (e.g. Erdős-Rényi model)? More specifically:

\[ BF = \frac{Pr(D_a | M_1)}{Pr(D_a | M_2)} \]

(5)

Here \( D_a \) are networks produced from the concordance function of centrality for a specific regime of centralities, \( M_1 = \) Centralities produced by a SBM with parameters \( K, z \) and \( M_2 = \) Centralities produced by an Erdős-Rényi with parameters \( \theta \). \( M_1 \) and \( M_2 \) are produced in the space of observables. We sample SBM and Erdős-Rényi models and for each realization we produce networks. For those networks we calculate their centralities. Given those networks we produce the distribution of centralities for this model (SBM or Erdős-Rényi respectively). Model comes from prior predictive (Figure 2) in random variable of centrality \( a \): \( Pr(a | K) \) for SBM and \( Pr(a | \theta) \) for Erdős-Rényi. If the observed feature is discrete (like diameter which is the maximum distance between nodes) then we are fine. If the observed feature is continuous we can compute posterior probability and use a smoothing method like a kernel density function to get the density.

Another thing we want to achieve is to provide a tool (figure 3) to formulate a question in terms of ranges, which can be useful for prior elicitation. In networks is very hard for practitioner to tell you information in terms of parameters (uncertainty in terms of parameters). Practitioners that are interested in specific ranges of features and once they have those ranges they can set candidates for the priors and see which one is more reasonable-better for those ranges. This tool is powerful in terms of flexibility way for looking of
ranges of features. So we are interested in answering how the prior of the network should be? That is very hard. Networks are very complicated objects and hard to be interpreted. Practitioners can look at the distribution of low dimensional features, get intervals that can be used in ways to calibrate your prior or to compare different models which could serve as a prior. We can achieve this by calculating the Bayes Factor:

$$BF = \frac{Pr(D | M_1)}{Pr(D | M_2)}$$ (6)

Here $D$ are general network data, $M_1 = \text{SBM}$ with parameters $K, z$ given $\hat{\alpha}$ and $M_2 = \text{Erd"{o}s-Rényi}$ with $\theta$ given $\hat{\alpha}$. $M_1$ and $M_2$ are produced in the space of observables. We sample SBM and Erdös-Rényi models and for each realization we produce networks.

For those networks we calculate their centralities. Given those networks we produce the distribution of centralities for this model (SBM or Erdös-Rényi respectively). Model comes from: $Pr(K, \hat{\alpha})$ in SBM and $Pr(\theta, \hat{\alpha})$ in Erdös-Rényi.

### 3.2 Model Selection of networks with respect to more than one feature.

Which model is better to fit to network data $D$? Model $M_1$ or model $M_2$? Until now we use the Bayesian factor test for constructing a principle Bayesian model selection test. How
do we combine three universal features such as community structure, degree distribution and network subcounts in a model selection test in a plausible principle way that makes sense? The penalty of the one might dominate the other and we might encounter problems where e.g. community structure is much more dominant than degree distribution or the opposite because of their values (large, small).

The Left Hand Side in (8), (9) and (10) is a number which absorbs (cancel out) any scaling problem from (11). You do not need to scale the axis every time to find the right portion of inclusion of each parameter’s penalty. Q.E.L. stands for the quadratic expected loss function in observable space. $D_{M_{1,2}}$ are the networks which are produced by the models $M_{1,2}$, respectively, and which we want to compare. We extract their features and compare them (Number of blocks, entropy of Degree distribution and number of Subgraph counts) which the corresponding features of the network data $D$. Which model could be fitted best regarding those three universal features? With this approach we do not encounter any problem regarding a dominance feature (scaling penalties) as in (5) which is derived if we directly use all the penalties from [1]

\[
\frac{Q.E.L(D_{M_1}, D)_{Blocks}}{Q.E.L(D_{M_2}, D)_{Blocks}} \propto \frac{P(M_1 \mid D)}{P(M_2 \mid D)} \tag{7}
\]

\[
\frac{Q.E.L(D_{M_1}, D)_{D.D.}}{Q.E.L(D_{M_2}, D)_{D.D.}} \propto \frac{P(M_1 \mid D)}{P(M_2 \mid D)} \tag{8}
\]

\[
\frac{Q.E.L(D_{M_1}, D)_{Motifs}}{Q.E.L(D_{M_2}, D)_{Motifs}} \propto \frac{P(M_1 \mid D)}{P(M_2 \mid D)} \tag{9}
\]

Summing the above 3 equations and divide by 3 we have:
Table 1: Real networks are constructed through Barabasi-Albert and Stochastic Block Model

| Local Feature          | Degree distribution through entropy |
|------------------------|-------------------------------------|
| Power Law              |                                     |
| SBM                    |                                     |

Table 2: Feature according to which we select a model

\[
\frac{Q.E.L(D_{M_1},D)_{Blocks}}{Q.E.L(D_{M_2},D)_{Blocks}} + \frac{Q.E.L(D_{M_1},D)_{D.D.}}{Q.E.L(D_{M_2},D)_{D.D.}} + \frac{Q.E.L(D_{M_1},D)_{Motifs}}{Q.E.L(D_{M_2},D)_{Motifs}} > \frac{P(M_1 | D)}{P(M_2 | D)}
\] (10)

4 Simulation Studies

We will perform three types of simulations. In all of them we will use Barabasi-Albert model and Stochastic Block Model. For the Barabasi-Albert model we will produce networks given the power law degree distribution sampling. For the Stochastic Block Model we will use [11] method. The three simulation setups are described below. The number of samples is N=100.

| Loss Function      | Expression               | Type of Inference |
|--------------------|--------------------------|-------------------|
| Quadratic Loss     | \( L(\theta, \hat{\theta}) = (\theta - \hat{\theta})^2 \) | point estimation |
| Absolute Loss      | \( L(\theta, \hat{\theta}) = | \theta - \hat{\theta} | \) | point estimation |

Table 3: Loss functions used for penalties
Table 4: Results of the loss functions

| Real Param | L.F. Ratio | Tested Parameters | Probabilities | Local Feature |
|------------|------------|-------------------|---------------|---------------|
| $\alpha$   | Q.L.=1493  | $P(\alpha = 2.9, 3.1 \mid D) = 0.67, P(K = 9) = 0.010$ | Power Law     |
| $\alpha$   | A.L.=0.0328| $P(\alpha = 2.9, 3.1 \mid D) = 0.67, P(K = 9) = 0.010$ | Power Law     |
| $K$        | Q.L.=31.082| $P(\alpha = 2.9, 3.1 \mid D) = 0.03, P(K = 9) = 0.37$ | SBM           |
| $K$        | A.L.=8.0287| $P(\alpha = 2.9, 3.1 \mid D) = 0.03, P(K = 9) = 0.37$ | SBM           |
| $\alpha = 3.2$ | Q.L.=0.8685| $P(\alpha = 2.9, 3.1 \mid D) = 0.02, P(K = 9) = 0.03$ | Power law and D.D. |
| $\alpha = 3.2$ | A.L.=0.241 | $P(\alpha = 2.9, 3.1 \mid D) = 0.02, P(K = 9) = 0.03$ | Power law and D.D. |

4.1 Simulation Set Up

As we can see from Table 5 when the data resemble more to a power law distribution it much more possible to select models that follow the power law distribution and have similar behaviour (their exponents are very close). On the other hand, when the network data are extracted from a SBM then it is much more likely to select models with a SBM with number of blocks close to one that the read network date were constructed. The same happened with degree equals to 0.4 but here the results are more ambiguous that in the other two cases. As we can observe from the last two rows from in the case of the combination of two loss functions, one for power law and one for the degree obviously the power law fraction dominates the degree distribution fraction. Still in that case power law distribution is much more possible to select models that follow the power law distribution and have similar behavior.

5 Discussion

Our methodology constitutes an attempt for comparing random network models regarding local features by using intrinsic Bayesian factor. We investigated how the following three interact: i) feature that you have phrase your scientific questions ii) features that are formulated by the model you are fitting and iii) features that can be retrieved more efficiently having sample size you have. For example: i) scientific question in terms of tran-
sitivity ii) you do not have a model that can be generated in terms of transitivity and iii) the compromise in terms of the feature what you want to capture and the model you can fit.

The need to compare random networks is fundamental to many fields, from the physical and life sciences to the social, behavioral, and economic sciences. This need is currently particularly significant in understanding information and incorporating complexity of random networks in network model selection. Although all model selection methods address the inevitable trade-off between goodness-of-fit and complexity, the manner in which they measure and penalize model complexity can differ substantially. The main advantage of our method is that it enables the statistician, for the first time, to compare random network models, both nested and non-nested and overcome the complexity problem. To this end, we have shown, through a comparative analysis of several rich and varied examples that the results obtained suggest that our method is both reasonable and universal.

The limitations of the approach in its current form include: i) Prior information of the data have to be incorporated to the complexity of the model in order to penalize the model, so it is reasonable the model to be related with the data ii) In multidimensional random network models computational costs might be an issue.

Future work includes: i) how can we reduce the cost of our algorithms in terms of complexity in high dimensional random network model features in the model selection ii) is it possible to create concordance function for every local feature regimes? ii) is there another way to penalize models due to features like e.g. modularity, motifs work or use two dimensional entropy of a graphon, as a penalty? iv) is it possible to connect asymptotically (e.g. through von Mises theorem) this approach for node-exchangeable models with the work in [16]?
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