Entropy of random graph ensembles constrained with generalised degrees

ES Roberts†‡ and ACC Coolen†§
† Institute for Mathematical and Molecular Biomedicine, King’s College London, Hodgkin Building, London SE1 1UL, United Kingdom
‡ Randall Division of Cell and Molecular Biophysics, King’s College London, New Hunts House, London SE1 1UL, United Kingdom
§ London Institute for Mathematical Sciences, 35a South St, Mayfair, London W1K 2XF, United Kingdom

PACS numbers: 87.18.Vf, 89.70.Cf, 89.75.Fb, 64.60.aq
E-mail: ekaterina.roberts@kcl.ac.uk ton.coolen@kcl.ac.uk

Abstract. Generalised degrees provide a natural bridge between local and global topological properties of networks. We define the generalised degree \((k,m)\) to be the number of neighbours of a node within one and two steps respectively. Tailored random graph ensembles are used to quantify and compare topological properties of networks in a systematic and precise manner, using concepts from information theory. We calculate the Shannon entropy of random graph ensembles constrained with a specified generalised degree distribution. We find that the outcome has a natural connection with the degree-degree correlation which is implied by specifying a generalised degree distribution. We demonstrate how generalised degrees can be used to qualitatively and quantitatively describe a network.

1. Introduction

A network is a way of displaying and analysing data. It is interesting to observe how simple local properties can give rise to global topology - for example a critical degree value triggering the inevitable formation of a giant connected component [1], or a preferential attachment growth model creating a fat tailed degree distribution [2]. Understanding these relationships allows insights into the features and origins of real networks. It can also protect against the risk of reporting spurious patterns that are mathematical consequences of already known properties.

We advocate rigorously quantifying topological patterns by viewing them as constraints on a random graph ensemble. This provides a way to measure and compare topological features from the very rational point of view of whether they are present in a large or small number of possible networks.

A previous paper [3] considered tailored random graph ensembles with controlled degree distribution and degree-degree correlations; [4] covered the case of directed networks. In each case, the strategy is to calculate the Shannon entropy. Related quantities such as complexity and information-theoretic distances naturally follow. Subsequent papers were devoted to the numerical generation of graphs [5] from the proposed ensemble families and applications to molecular biology [6].
In the present paper, we extend this work by calculating, in leading order, the Shannon entropy of random graph ensembles constrained with a specified distribution of generalised degrees. The generalised degree distribution gives the probability of finding a node with any given size of first and second neighbourhood. The Shannon entropy provides a way of quantifying how restrictive the constraint is on the ensemble. This analysis is complemented with a qualitative study of generalised degree distributions. The results obtained show that general degrees form an interesting bridge between local statistics, global topology and motifs.

2. Generalised Degrees

Generalised degrees are a natural generalisation of simple degrees. They constitute a much more specific topological signature. Consider Figure 1 which illustrates how certain motifs have characteristic generalised degrees, and Figure 2 which shows the generalised degrees of three popular network topologies.

It will be shown in section 4 that the generalised degree has a close connection with the correlations between connected degrees. This links with the concept of the assortativity of the network - whether high degree nodes are likely to be connected to other high degree nodes, or to low degree nodes.

Hence it can be seen that this deceptively simple local constraint imposes strong conditions on the overall topology of the network. The numerical results based on parameters from real biological datasets are given in section 7; applying the formula derived in section 5 shows that specifying a generalised degree distribution is typically an onerous constraint.

The premise of the tailored graphs approach is that the most rational way to study a network’s overall topology is to view the particular network at hand as a realisation of a particular set of topological constraints. Specifying the generalised degree provides much greater control over the global topology of the networks in the ensemble.

2.1. Brief review of literature on generalised degrees

The concept of a generalised degree was discussed in [7] and references therein. Various relationships were derived using generating functions.

An alternative definition, presented by the authors of [8], measured the number of direct neighbours $s$ of a subset of $t$ nodes. The authors of [8] derive conditions based on their definition of general degrees which can ensure that (for some given $m$ and $d$) there are at least $m$ internally disjoint paths of length at most $d$. The diameter of the network is an obvious corollary - the smallest $d$ corresponding to $m \geq 1$. These results can be applied to questions of robustness of networks.

In combinatorics, the generalised degrees concept appears in Seymour’s Second Neighbourhood Conjecture, which asserts that in every simple directed graph there exists a vertex $v$ whose second out-neighbourhood contains at least as many vertices as its first out-neighbourhood.

The authors of [9] studied the spectral density of random graphs with hierarchically constrained topologies. This includes consideration of generalised degrees, as well as more general community structures. Using the replica method, in a similar way to [10], they achieve a form analogous to equation (5). They proceed numerically from that point, hence our approach to an analytical solution presented in section 5 is entirely novel.
Figure 1. Some simple networks and their generalised degree heatmap. The first degree is on the x axis and the second degree is on the y axis. The colour at any co-ordinate indicates the frequency of occurrence of that pair of values. The plots are smoothed.

In the first network - a simple chain - every node has the same generalised degree: (2, 4). The generalised degree heatmap has a single peak.

The second network - a star - has generalised degree distribution \( p(k, m) = \delta_{k,m,1(99, 99)} \frac{1}{100} + \delta_{k,m,1(1, 99)} \frac{99}{100} \). There is a visible peak at (1, 99). This peak is deformed due to smoothing with the peak at (99, 99) (which is too faint to see in its own right).

The final network is a Cayley tree. Every interior node has generalised degree (3, 9). View the Cayley tree as being grown one layer at a time (i.e. at every layer attach two new nodes to each node in the preceding layer), for \( n \) steps. The final two layers will have irregular generalised degree values (since they lack any further outwards neighbours) - being (1, 3) and (3, 6) for the final and penultimate layer respectively. Their relative frequencies can be calculated by summing a geometric series, and correspond to the three peaks shown.
3. Specifying the problem

3.1. Definitions

We consider ensembles of non-directed random graphs. Each graph is defined by a symmetric matrix \( c = \{c_{ij}\} \), with \( i, j \in \{1, \ldots, N\} \) and with \( c_{ij} \in \{0, 1\} \) for all \((i, j)\). Two nodes \( i \) and \( j \) are connected by a link if and only if \( c_{ij} = 1 \). We put \( c_{ii} = 0 \) for all \( i \). For simplicity we shall assume that there are no isolated nodes \( (p(k_i = 0) = 0) \). The first degree, \( k_i(c) \) and the second degree \( m_i(c) \), are defined

\[
\begin{align*}
 k_i(c) &= \sum_j c_{ij} \\
 m_i(c) &= \sum_{jk} c_{ij}c_{jk} = \sum_j c_{ij}k_j(c)
\end{align*}
\]

(1)

The first degree \( k_i \) counts the number of links to site \( i \). The second degree \( m_i \) counts the number of distinct two-step paths originating from node \( i \).

We can now define our random graph ensemble. We first draw all pairs \((k_i, m_i) \in \mathbb{N}^2 \) for all \( i = 1 \ldots N \) independently at random from a given joint distribution \( p(k, m) \), and define the two vectors \( k = (k_1, \ldots, k_N) \) and \( m = (m_1, \ldots, m_N) \). We then generate with uniform probabilities all graphs that meet the topological demands that \( k(c) = k \) and \( m(c) = m \)

\[
p(c) = \sum_k \sum_m p(k, m) p(c|k, m) \quad p(k, m) = \prod_i p(k_i, m_i) \quad p(c|k, m) = Z^{-1}(k, m) \prod_i \left( \delta_{k_i,k(c)} \delta_{m_i,m(c)} \right)
\]

(2)

\[
p(c|k, m) = Z^{-1}(k, m) \prod_i \left( \delta_{k_i,k(c)} \delta_{m_i,m(c)} \right)
\]

\[
Z(k, m) = \sum_c \prod_i \left( \delta_{k_i,k(c)} \delta_{m_i,m(c)} \right)
\]

Equivalently

\[
p(c) = Z^{-1}(k(c), m(c)) \prod_i p(k_i(c), m_i(c))
\]

(3)
Entropy of random graph ensembles constrained with generalised degrees

For this ensemble with prescribed topological features we wish to calculate, in leading order in the system size $N$, the Shannon entropy per node

$$S = -N^{-1} \sum_{\mathbf{c}} p(\mathbf{c}) \log p(\mathbf{c})$$ (4)

From this, in turn, follows the effective number $N$ of such graphs, via $N = e^S$.

3.2. Intermediate answer

Appendix A sets out the calculation to the point where the method diverges from that used in [14]. This takes the calculation to the intermediate form set out below.

$$S = \bar{k} \left( 1 + \log \left( \frac{N}{\bar{k}} \right) \right) - \sum_{\mathbf{c}} p(k, m) \log \left( \frac{p(k, m)}{\pi(k)} \right) + \sum_{(k,m)} p(k, m) \log \left[ \sum_{\xi_1, \xi_2} \gamma(k, \xi_1) \delta_{m, \sum_1^k \xi_1} \right] + \epsilon_N$$ (5)

The symbol $\bar{k}$ indicates the average degree; $\pi(k)$ is the Poissonian distribution with the same average degree. The sum in the final term should be read as the sum over all sets of $k$ integers $\xi_1...\xi_k$. The unknown expression $\gamma(\cdot, \cdot)$ complies with the self-consistency relation below.

$$\gamma(k, k') = \sum_{m} \frac{k'}{k} p(k', m') \left[ \frac{\sum_{\xi_1, \xi_2} \delta_{m', \sum_1^{k-1} \xi_2} \prod_{\xi_1}^{k-1} \gamma(k', \xi_2)}{\sum_{\xi_1, \xi_2} \delta_{m', \sum_1^{k'} \xi_2} \prod_{\xi_1}^{k'} \gamma(k', \xi_2)} \right]$$ (6)

The self-consistency equation (6) does not yield to a straightforward solution. Hence, equation (5) is unsatisfying because it can only be evaluated numerically, or in certain special cases. Without a physical interpretation of $\gamma$, this intermediate answer is limited in how much insight it can provide.

4. Implied generalised degree-degree correlation

Correlations between the generalised degrees of connected nodes can be expressed as

$$W(\bar{k}, \bar{k}' | \mathbf{c}) = \frac{\sum_{ij} c_{ij} \delta_{\bar{k}, \bar{k}'} \delta_{\bar{k}', \bar{k}'}}{\sum_{ij} c_{ij}}$$ (7)

where $\bar{k} = (k, m)$. We can calculate the average of this quantity in our ensemble with a specified generalised degree distribution.

$$W(\bar{k}, \bar{k}') = \lim_{N \to \infty} \sum_{\mathbf{c}} p(\mathbf{c}) p(\bar{k}) W(\bar{k}, \bar{k}' | \mathbf{c})$$ (8)

where

$$p(\mathbf{c}) p(\bar{k}) = \sum_{|\bar{k}_1, \bar{k}_2|} \frac{\prod_{i} (\delta_{\bar{k}_i, \bar{k}'_i}(\mathbf{c}))}{\prod_{i} (\delta_{\bar{k}_i, \bar{k}'_i}(\mathbf{c}))} \prod_{i} p(\bar{k}_i)$$

Expand this expression

$$W(\bar{k}, \bar{k}') = \frac{1}{kN} \sum_{rs} \sum_{|\bar{k}_1, \bar{k}_2|} \left[ \prod_{i} p(\bar{k}_i) \delta_{\bar{k}_i, \bar{k}'_i} \right] \frac{\sum_{\mathbf{c}} c_{rs} \prod_{i} (\delta_{\bar{k}_i, \bar{k}'_i}(\mathbf{c}))}{\prod_{i} (\delta_{\bar{k}_i, \bar{k}'_i}(\mathbf{c}))}$$ (9)

Appendix B sets out in detail the key steps of the calculation. In leading order, the integral evaluates to

$$W(\bar{k}, \bar{k}') = \frac{k}{(kN)^2} \sum_{rs} \sum_{|\bar{k}_1, \bar{k}_2|} \left[ \prod_{i} p(\bar{k}_i) \delta_{\bar{k}_i, \bar{k}'_i} \right] \gamma^*(\bar{k}, \bar{k}') \gamma^*(\bar{k}', \bar{k})$$ (10)
for

$$\gamma^*(\vec{k}, k) = \frac{\sum_{\{\xi_1, \ldots, \xi_k\}} \prod_{i=1}^{k-1} \gamma(k', \xi_i) \delta_{m' \sum \xi_i}}{\sum_{\{\xi_1, \ldots, \xi_k\}} \prod_{i=1}^{k} \gamma(k', \xi_i) \delta_{m' \sum \xi_i}}$$  \hspace{1cm} (11)$$

satisfying

$$\sum_{m'} k' \frac{p(\vec{k})}{k} \gamma^*(\vec{k}, k) = \gamma(k, k')$$  \hspace{1cm} (12)$$

whereupon we can simplify

$$W(\vec{k}, \vec{k}') = \gamma^*(\vec{k}, k') \gamma^*(\vec{k}, k) \frac{kk' p(\vec{k}) p(\vec{k}')}{k^2}$$  \hspace{1cm} (13)$$

We can very easily take the marginal of the object \(W\) using the relation for \(\gamma^*\)

$$\sum_{m, m'} W(\vec{k}, \vec{k}') = W(k, k') = \gamma(k, k') \gamma(k', k)$$  \hspace{1cm} (14)$$

This relationship is elegant and, at first glance, surprising. Considering this further, however, it becomes clear that a specified generalised degree distribution will essentially induce a non-trivial degree-degree correlation function that, in the limit, will indeed be shared by all members of the ensemble. It would be possible to write down various combinatorial relationships - and it is interesting and encouraging that the statistical mechanics route naturally discovers the same links.

Section 5 will use equation (13) to eliminate the undetermined \(\gamma\) term from equation (5). An interesting alternative route would have been to use equation (13) in order to describe \(\gamma\) in terms of topological observables. The form of the self-consistency equation (6) is strongly suggestive of a natural interpretation of \(\gamma\) in terms of conditional probabilities associated with links in the network.

5. Completing the solution

The aim is to resolve equation (5) into observable quantities. Consider the term

$$\Gamma = \sum_{(k, m)} \frac{p(k, m) \log \left[ \sum_{\{\xi_1, \ldots, \xi_k\}} \prod_{i=1}^{k} \gamma(k, \xi_i) \delta_{m \sum \xi_i} \right]}{N}$$  \hspace{1cm} (15)$$

Observe that at this point of the calculation, the effect of factorising across nodes has been to break the expression down into terms which, for every generalised degree \((k, m)\), enumerate all the possible ways of dividing \(m\) second neighbours between \(k\) first neighbours. The term inside the logarithm sums over all configurations \([k : \xi_1 \ldots \xi_k]\) which meet the condition \(\sum_{i=1}^{k} \xi_i = m\).

To formalise this idea, re-aggregate the expression to write

$$\Gamma = \frac{1}{N} \log \left[ \prod_{(k, m)} \sum_{\{\xi_1, \ldots, \xi_k\}} \prod_{i=1}^{k} \gamma(k, \xi_i) \delta_{m \sum \xi_i} \right]$$  \hspace{1cm} (16)$$

observing that \(Np(k, m)\) can be assumed to be an integer by construction, since we would typically have taken the statistics from a real network. This multiplies out to

$$\Gamma = \frac{1}{N} \log \left[ \sum_{\{\xi'_1, \ldots, \xi'_k\}} \sum_{\{\xi''_1, \ldots, \xi''_k\}} \ldots \sum_{\{\xi''_{k_1}, \ldots, \xi''_{k_{m}}\}} \prod_{i=1}^{k} \gamma(k, \xi_i^i) \delta_{m \sum \xi_i^i} \right]$$  \hspace{1cm} (17)$$
where the frequency with which any pair \((k, m)\) appears is given by \(Np(k, m)\).

This can be restated as

\[
\Gamma = \frac{1}{N} \log [\Gamma_1 + \Gamma_2 + \ldots + \Gamma_X]
\]  

(18)

where each of the \(\Gamma_*\) is a product of \(N\) terms of type \(\gamma\). A typical term would be

\[
\gamma(k_1, \xi_1)\gamma(k_1, \xi_2)\ldots\gamma(k_1, \xi_i)\gamma(k_2, \xi_i')\gamma(k_2, \xi_i')\ldots\gamma(k_N, \xi_i')\gamma(k_N, \xi_i')
\]  

(19)

We can now see that the separate terms \(\Gamma_1, \Gamma_2, \ldots, \Gamma_X\) precisely enumerate all the permutations of degrees and neighbour-degrees for networks with a generalised degree sequence consistent with any pair \((k, m)\) appearing \(Np(k, m)\) times.

If we identify the \(\xi\) as actual degrees and \(\gamma(k, k')\) with an actual edge in the network, then a necessary and sufficient condition for graphicality can be immediately deduced: in equation (19) every \(\gamma(k, k')\) must have a matching \(\gamma(k', k)\). This can be seen by construction. Every edge in the network going from \(k_i \rightarrow k_i\) will give a contribution of \(\gamma(k_i, k_i)\) when counted in the \(j = i\) term, and a contribution of \(\gamma(k_i, k_i)\) when counted in the \(j = i_2\) term. If this can be done, then it defines a network. If it cannot be done, then it proves that no network can be drawn with that sequence of degree and neighbour-degrees.

This insight allows the expression to be substantially simplified, since we already know that \(\gamma(k, k')\gamma(k', k) = W(k', k)\) where \(W(k', k)\) is the correlation between degrees of connected nodes. Hence, we now claim that a typical term will look like

\[
W(a, b)W(c, d)W(e, f)W(g, h)\ldots W(x, y)W(m, n)W(s, t)
\]

where a network is graphical. We disregard non-graphical terms. This step is in keeping with the natural interpretation of the problem, but not rigorously proved to be valid.

We can use our knowledge of the average quantities in the ensemble to deduce that for any arbitrary \(\alpha\) and \(\beta\) the term \(W(\alpha, \beta)\) will appear in this sequence \(N\) times.

The number of \(\Gamma\) terms is equation (18) is \(\mathcal{P}\). This could be expected to be equal to \(\mathcal{P} = \prod_{k,m} [\mathcal{P}_{k,m}]^{Np(k,m)}\) where \(\mathcal{P}_{k,m}\) is equal to the number of partitions of \(m\) into \(k\) terms. However, if the probability density function does not have compact support, then some of the \(\xi\) correspond to degrees which have zero probability - and so \(\mathcal{P}(\star, \xi) = 0\). In this case, the number of partitions is more accurately written as \(\mathcal{P}_{k,m} = \sum_{\{\xi_i\}} \delta_{\xi_i,m} \prod_i (1 - \delta_{p(\xi_i),0})\). This enumerates the number of \(\Gamma\) terms in 18. However, some of these sequences will not be graphical, so this is an upper bound.

So we have reached

\[
\Gamma = \frac{1}{N} \log \left[ \mathcal{P} \prod_{k,k'} W(k, k')^{\frac{k}{2}} W(k, k') \right]
\]  

(20)

\[
\Gamma = \frac{k}{2} \sum_{k,k'} W(k, k') \log W(k, k') + \sum_{k,m} p(k, m) \log \mathcal{P}_{k,m}
\]

where the factor of \(1/2\) compensates for over counting. An upper bound can be provided for the final term: \(\mathcal{P}_{k,m} \leq \sum_{\{\xi_i\}} \delta_{\xi_i,m} \prod_i (1 - \delta_{p(\xi_i),0})\), or \(\mathcal{P}_{k,m} \leq (n^{-1})^{m-k+1}\) if \(p(\xi) > 0\) for all \(\xi \leq m-k+1\).

Accordingly, the full expression for the entropy per node will be

\[
S = \frac{k}{2} \left( 1 + \log \left( \frac{N}{k} \right) \right) - \sum_k p(k, m) \log \left( \frac{p(k, m)}{\pi(k)} \right)
\]

(21)

\[
+ \frac{k}{2} \sum_{k,k'} W(k, k') \log W(k, k') + \sum_{k,m} p(k, m) \log \mathcal{P}_{k,m} + \epsilon_N
\]
6. Validation

The restrictiveness of the generalised degree constraint means that it is easy to find examples where the Shannon entropy can be obtained directly. This is useful to validate equation (21). Additionally, where the self consistency equation (6) can be solved, this can be checked against the final terms of equation (21). Appendix D provides several such examples. Figures D1, D2, D3 and D4 illustrate the validation examples.

6.1. Comparison with the maximum entropy ensemble specified by simple degrees only

The flat distribution corresponds to

$$p(m|k) = \sum_{\xi(m)} \prod_{i=1}^{k} p(\xi_{i}) \xi_{s}$$

where $m{\xi}$ describes a set of partitions of $m$ into $k$. This case will also have factorising $W$.

It can be shown (see e.g. [7]) that the flat ensemble defined by the degree distribution only is given by

$$p_{flat}(k, m) = p(k) \frac{k}{\sum_{m}^{m} \xi_{k} \prod_{s=1}^{k} \xi_{s}}$$

(22)

For the expression in equation (5) to be consistent with earlier results, it must collapse back to the degree-only case - as derived in [3] - for $p(k, m) = p_{flat}(k, m)$.

To validate the intermediate result given by equation (5), the final form achieved for generalised degrees less the final form achieved for simple degrees must leave a remainder satisfying

$$\sum_{k,m} p(k, m) \log \Gamma(k, m) - \sum_{k,m} p(k, m) \log p(m|k) = 0$$

(23)

where

$$\Gamma(k, m) = \sum_{\xi_{1}, \ldots, \xi_{k}} \prod_{s=1}^{k} \gamma(k, \xi_{s}) \delta_{m, \sum_{s=1}^{k} \xi_{s}}$$

(24)

Substitute in the result above $p(m|k) = \sum_{\xi(m)} \prod_{s=1}^{k} \frac{\xi_{s} p(\xi_{s})}{k}$. This implies $\gamma(k, \xi_{s}) = \frac{\xi_{s} p(\xi_{s})}{k}$. This satisfies the self-consistency relationship (6).

Since the connected node degrees are independent in this case, it is valid to write

$$\sum_{k,m} p(k, m) \log \left( \sum_{\xi(m)} \prod_{s=1}^{k} \frac{\xi_{s} p(\xi_{s})}{k} \right) = \sum_{k,m} p(k, m) \log \mathcal{P}_{km} + \sum_{\xi} \xi p(\xi) \log \left( \frac{\xi p(\xi)}{k} \right)$$

which is consistent with the final result in equation (21).

7. Numerical results

Specifying the generalised degree distribution is an onerous restriction on a random graph ensemble. This was justified intuitively in section 2. As an illustration, Figure 4 shows this numerically by applying equation (21) to random graph ensembles tailored to the topology of real biological networks, whose generalised degrees are shown in Figure 3. Appendix C gives some details of implementation.

The results show that, generally, incorporating the generalised degree constraint in the definition of the ensemble results in substantial reduction in the associated Shannon entropy. The magnitude of this reduction correlates well with a qualitative inspection of the heatmaps of the associated generalised degrees. Specifically, comparing qualitatively confirms that
there is greater complexity due to generalised degree where the generalised degree shows greater divergence from the maximum entropy simple degree distribution. Figure 5 combines Figure 3 with Figure 4 to allow for direct visual comparison of the qualitative features of the generalised degree distribution obtained from these datasets with the quantitative value for the complexity associated with the same distribution (based on equation (21)).

8. Conclusion

We have derived, in leading order, an expression for the Shannon entropy of random graph ensembles constrained by the number of direct neighbours and the number of neighbours within two steps.

Approaching the calculation directly is known to lead to a self-consistency equation which resists solution (e.g. [9, 14]). In this paper, this difficulty was avoided by taking the conceptual step of identifying that the objects appearing in the final unresolved term precisely enumerate possible allocations of neighbouring degrees. By excluding non-graphical cases, the series can be summed in terms of a topological observable: the degree-degree correlation. This provides a neat link to previous work, and shows that generalised degrees are indeed the next step in the sequence of hierarchical topological constraints studied by e.g. [14].

The exclusion of the non-graphical cases was not able to be rigorously justified.
However, it is within the spirit of the problem, and the final expression performs well under testing. The final expression takes the form of a term expressing the entropy of an ensemble constrained by a specified number of neighbours, and the specified degrees of those neighbours, plus a term reflecting the configurational entropy. The configurational entropy arises from the number of different ways that a second neighbourhood of size \( m \) can be made up from the degrees of the \( k \) neighbours of the node. To evaluate this factor accurately, graphicality would need to be incorporated into the analysis. Nonetheless, an upper-bound expression is provided, which already demonstrates a very material reduction in entropy under this constraint.

In this paper, the constraint was expressed in terms of the total number of first neighbours and second neighbours. Given the way that the result appears to enumerate all possible wirings, it would be interesting to directly calculate the entropy of a random graph ensemble constrained by specifying the composition \( \{k; \xi_1, \ldots, \xi_k\} \) of the neighbourhood of every node. This is a subset of an ensemble which has generalised degree \( (k, m) \) for \( m = \sum_{s=1}^{k} \xi_s \), specified for every node. One would expect to be able to relate one to the other, by viewing the generalised degree ensemble as the union of all the ensembles which have compliant neighbourhood compositions.

Another natural generalisation would be to consider neighbourhoods with a wider radius: for example, specifying the number of neighbours within one, two and three steps of every node. The algebra would be quite complicated, but the substance of the result is likely to be the same: relating the number of neighbours within successively larger number of steps with
Figure 5. This plot compares the calculated value for the complexity associated with the generalised degree constraint with the appearance of the generalised degree heatmap plot. From left to right along the x-axis the bars correspond to data from [15, 16, 17, 18, 19, 20]. The y-axis gives the complexity per bond associated with the ‘generalised degrees’ constraint (as taken from the corresponding dataset). This data is equivalent to subtracting the level of the fourth bar from the level of the second bar in figure 4 and then normalising by dividing by the average degree $\bar{k}$. The bars are reordered from largest to smallest for easier comparison. By inspection, it can be seen that there is a trend in the images which corresponds to intuitive expectation. The heatmaps are smoothed; the x-axis corresponds to the first degree and the y-axis corresponds to the second degree; the intensity of the colour indicates the likelihood of that pair of values.

The challenge in modelling a real network is to isolate the essential features, but to allow sufficient residual freedom. For any particular network, it would be possible to define a tightening sequence of topological descriptors, which will ultimately define a family of one. With the generalised degree constraint, we have taken a step closer to providing a set of descriptors that nearly uniquely define the network. It is a stimulating alternative viewpoint to consider a network to be described by its topological constraints, rather than the more traditional connectivity list.
Acknowledgements

ESR gratefully acknowledges financial support from the Biotechnology and Biological Sciences Research Council of the United Kingdom.

References

[1] Dorogovtsev SN, Goltsev AV, Mendes JF. Critical phenomena in complex networks. Reviews of Modern Physics. 2008;80(4):1275.
[2] Albert R, Barabási AL. Statistical mechanics of complex networks. Reviews of modern physics. 2002;74(1):47.
[3] Annibale A, Coolen ACC, Fernandes LP, Fraternali F, Kleinjung J. Tailored graph ensembles as proxies or null models for real networks I: tools for quantifying structure. Journal of Physics A: Mathematical and Theoretical. 2009;42(48):485001.
[4] Roberts ES, Coolen ACC, Schlitt T. Tailored graph ensembles as proxies or null models for real networks II: results on directed graphs. Journal of Physics A Mathematical General. 2011 Jan;44(26):5002.
[5] Roberts ES, Coolen ACC. Unbiased degree-preserving randomization of directed binary networks. Physical Review E. 2012 Apr;85:046103.
[6] Fernandes LP, Annibale A, Kleinjung J, Coolen ACC, Fraternali F. Protein networks reveal detection bias and species consistency when analysed by information-theoretic methods. PloS one. 2010 Aug;5(8):e12083.
[7] Newman M. Networks: an introduction. OUP Oxford; 2009.
[8] Faudree RJ, Gould RJ, Lesniak LM. Generalized degrees and Menger path systems. Discrete Applied Mathematics. 1992 Jul;37-38:179–191.
[9] Newman M. Networks: an introduction. OUP Oxford; 2009.
[10] Bianconi G, Coolen AC, Vicente CJP. Entropies of complex networks with hierarchically constrained topologies. Physical Review E. 2008;78(1):016114.
[11] Erdos P, Renyi A. On the evolution of random graphs. Publ Math Inst Hung Acad Sci. 1960;5:17–61.
[12] Albert R, Barabási AL. Emergence of Scaling in Random Networks. Science. 1999;286(5439):509–512.
[13] Watts DJ, Strogatz SH. Collective dynamics of ‘small-world’ networks. Nature. 1998 Jun;393(6684):440–442.
[14] Coolen ACC, De Martino A, Annibale A. Constrained Markovian dynamics of random graphs. Journal of Statistical Physics. 2009;136(6):1035–1067.
[15] Titz B, Rajagopala SV, Goll J, Häuser R, McKevitt MT, Palzkill T, et al. The binary protein interactome of Treponema pallidum—the syphilis spirochete. PLoS One. 2008;3(5):e2292.
[16] Ewing RM, Chu P, Elisma F, Li H, Taylor P, Clinnie S, et al. Large-scale mapping of human protein–protein interactions by mass spectrometry. Molecular systems biology. 2007;3(1).
[17] Arifuzzaman M, Maeda M, Itoh A, Nishikata K, Takita C, Suito R, et al. Large-scale identification of protein–protein interaction of Escherichia coli K-12. Genome research. 2006;16(5):686–691.
[18] Rual JF, Venkatesan K, Hao T, Hirozane-Kishikawa T, Dricot A, Li N, et al. Towards a proteome-scale map of the human protein–protein interaction network. Nature. 2005;437(7062):1173–1178.
[19] LaCount DJ, Vignali M, Chettier R, Phansalkar A, Bell R, Hesselberth JR, et al. A protein interaction network of the malaria parasite Plasmodium falciparum. Nature. 2005;438(7064):103–107.
[20] Ito T, Chiba T, Ozawa R, Yoshida M, Hattori M, Sakaki Y. A comprehensive two-hybrid analysis to explore the yeast protein interactome. Proceedings of the National Academy of Sciences of the United States of America. 2001 Apr;98(8):4569–4574.
Appendix A. Initial canonical steps to calculate Shannon entropy of random graph ensembles constrained with a specified general degree distribution

Please refer to Section 3.1 for starting point of this calculation and preliminary definitions. This section outlines the first steps of the solution, which are common with e.g. [3].

Appendix A.1. Expand the expression in order to identify the complicated term

We work out (4) for the ensemble (2), focusing on the leading order in $N$. We demand that the distribution $p(k, m)$ from which the local topology characteristics $(k_i, m_i)$ are drawn does not depend on $N$, so that with the law of large numbers one obtains

$$
S = N^{-1} \sum_c p(c) \log Z(k(c), m(c)) - N^{-1} \sum_i \sum_c p(c) \log p(k_i(c), m_i(c))
$$

We next focus on the first term. We abbreviate $\bar{k} = N^{-1} \sum \delta_{c,i,1}$ and define a Poissonian measure

$$
w(e|\bar{k}) = \prod_{i < j} \left[ \frac{\bar{k}}{N} \delta_{c,i,1} + \left(1 - \frac{\bar{k}}{N}\right) \delta_{c,i,0} \right]
$$

This measure is normalized, and depends on $c$ only via its average degree $\bar{k}(c)$, since

$$
w(e|\bar{k}) = \left[ \frac{\bar{k}}{N} \right]^{\sum_{\delta_{c,i,1}}} \left[ 1 - \frac{\bar{k}}{N} \right]^{\sum_{\delta_{c,i,0}}}
$$

Let us write the latter expression as $W(\bar{k}, \bar{k}(c))$. We may therefore write $Z(k, m)$ as

$$
Z(k, m) = \sum_c \frac{w(e|\bar{k})}{W(\bar{k}, \bar{k}(c))} \prod_i \left( \delta_{c_i,k_i(c)} \delta_{m_i,m(c)} \right)
$$

We thus obtain for the entropy the following expression, with $\langle .. \rangle_k$ denoting an average over the Poissonian measure with average connectivity $\kappa$, i.e. $\langle f(c) \rangle_k = \sum_c w(c|k) f(c)$,

$$
S = \frac{1}{N} \sum_{k,m} p(k, m) \log \left( \prod_i \left( \delta_{c_i,k_i(c)} \delta_{m_i,m(c)} \right) \right)_{\bar{k}} - \frac{1}{N} \sum_{k,m} p(k, m) \log W(\bar{k}, \bar{k}) - \sum_{k,m} p(k, m) \log p(k, m) + \epsilon_N
$$
are in an ‘all possible combinations’ combinatorial shape. 

It immediately follows that all the complexities of the problem are contained in the last line, which we abbreviate as

\[
\text{Entropy of random graph ensembles constrained with generalised degrees}
\]

\[\sum_{k,m} p(k,m) \log p(k,m)\]

\[\frac{1}{N} \sum_{k,m} p(k,m) \log \left( \prod_i \left( \delta_{k_i,k} \delta_{m_i,m} \right) \right) = \epsilon_N \tag{A.5}\]

**Appendix A.2. Expressing Kronecker \(\delta\) in Fourier Form**

All the complexities of the problem are contained in the last line, which we abbreviate as

\[\phi(k,m) = \frac{1}{N} \sum_{k,m} p(k,m) \log \left( \prod_i \left( \delta_{k_i,k} \delta_{m_i,m} \right) \right) \tag{A.6}\]

Using integral representations of the Kronecker \(\delta\)-functions allows us to write this nontrivial contribution to the entropy as

\[\phi(k,m) = \frac{1}{N} \sum_{k,m} p(k,m) \log \int_{-\pi}^{\pi} \prod_i \left[ \frac{d\omega_i d\psi_i}{4\pi^2} e^{i(k\omega_i + m\psi_i)} \right] L(\omega,\psi) \tag{A.7}\]

\[L(\omega,\psi) = \sum_c \prod_{i<j} \left[ \frac{k}{N} \delta_{c_{ij},1} + \left( 1 - \frac{k}{N} \right) \delta_{c_{ij},0} \right] e^{i\sum_j c_{ij}(\omega_i + \phi_j k_j)} \tag{A.8}\]

with \(\omega = (\omega_1, \ldots, \omega_N)\) and \(\psi = (\psi_1, \ldots, \psi_N)\).

By symmetry it is clear that \(\sum_{i<j} c_{ij}(\omega_i + \phi_j k_j) = \sum_{i<j} c_{ij}(\omega_i + \phi_i k_j + \omega_j + \phi_j k_j)\) so

\[L(\omega,\psi) = \sum_c \prod_{i<j} \left[ \frac{k}{N} \delta_{c_{ij},1} + \left( 1 - \frac{k}{N} \right) \delta_{c_{ij},0} \right] \exp\left[ -i c_{ij}(\omega_i + \phi_i k_j + \omega_j + \phi_j k_j) \right] \]

using the action of the \(\delta\)s, we reach:

\[L(\omega,\psi) = \sum_c \prod_{i<j} \left[ \frac{k}{N} \delta_{c_{ij},1} e^{-i(\omega_i + \phi_i k_j + \omega_j + \phi_j k_j)} - \delta_{c_{ij},0} \right] + \delta_{c_{ij},0} \right] \tag{A.9}\]

It is valid to exchange to exchange the order of the summation and the product, since we are in an ‘all possible combinations’ combinatorial shape.

\[L(\omega,\psi) = \prod_{i<j} \sum_{c_{ij}} \left[ \frac{k}{N} \delta_{c_{ij},1} e^{-i(\omega_i + \phi_i k_j + \omega_j + \phi_j k_j)} - \delta_{c_{ij},0} \right] + \delta_{c_{ij},0} \right] \tag{A.10}\]

\[= \prod_{i<j} \left[ \frac{k}{N} e^{-i(\omega_i + \phi_i k_j + \omega_j + \phi_j k_j)} - 1 \right] + 1 \]

Now express \(L(\omega,\psi)\) as the exponential of the logarithm. Taking the product outside the logarithm as a sum, and taking the leading order in \(N\) of the Taylor expansion for each term, it immediately follows that

\[L(\omega,\psi) = \exp \left[ \sum_{i<j} \frac{k}{2N} \left( e^{-i(\omega_i + \phi_i k_j + \omega_j + \phi_j k_j)} - 1 \right) + O(N^{-2}) \right] \tag{A.11}\]
Appendix A.3. Constructing special functions to bring down the site-specific variables

We now have a sum over site-specific variables. Define

\[ P(\omega, \psi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) = \frac{1}{N} \sum_{i} \delta(\omega - \omega_i) \delta(\phi - \phi_i) \delta_{i,k} \]  \hspace{1cm} (A.12)

By construction \( \sum_k \int P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) d\omega d\phi \equiv 1 \). So we can write

\[ L(\omega, \psi) = \exp \left[ \int d\omega d\phi \sum_{k,k'} P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) P(\omega', \phi', k'|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \left[ \frac{kN}{2} \exp \left(-i(\omega k' + \omega' k)\right) \right] e^{-\frac{2\pi}{N}} \right] \]

Before we proceed further we need to discretise \( L \) - this makes it easier to see how the next step works.

\[ L(\tilde{\omega}) = \exp \left[ \sum_{\omega, \phi, k} \Delta \omega \Delta \phi \Delta \phi' P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) P(\omega', \phi', k'|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \left[ \frac{kN}{2} \exp \left[-i(\omega \phi' + \omega' \phi)\right] \right] e^{-\frac{2\pi}{N}} \right] \]

Now - for every value of \( \omega, \phi, k \) apply the following relation \( \int dP(\omega, \phi, k) \delta \left[ P(\omega, \phi, k) - P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \right] \) in order to bring out the dependence on \( \epsilon \). This lets us replace every instance of \( P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \) with \( P(\omega, \phi, k) \).

\[ L(\tilde{\omega}) = \prod_{\omega, \phi, k} \int dP(\omega, \phi, k) \delta \left[ P(\omega, \phi, k) - P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \right] \exp \left\{ \Delta \omega \Delta \phi \Delta \phi' P(\omega, \phi, k) P(\omega', \phi', k') \left[ \frac{kN}{2} \exp \left[-i(\omega \phi' + \omega' \phi)\right] \right] e^{-\frac{2\pi}{N}} \right\} \]

Now we are going to express \( \delta \left[ P(\omega, \phi, k) - P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \right] \) in Fourier form

\[ \int dx \exp \left[i \frac{1}{2\pi} \left( P(\omega, \phi, k) - P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \right) \right] \]  \hspace{1cm} but in place of \( x \) we are going to use \( x = N \Delta \omega \Delta \phi \hat{P}(\omega, \phi, k) \) which also means we can substitute \( \frac{d}{x} = N \Delta \omega \Delta \phi \).

At this point we have the opportunity to spot that we have achieved a standard path integral form where we can write \( \prod_{\omega, \phi, k} N \Delta \omega \Delta \phi \hat{P}(\omega, \phi, k) dP(\omega, \phi, k) d\hat{P}(\omega, \phi, k) \) as \( dP d\hat{P} \).

We have arrived at the following form

\[ L(\tilde{\omega}) = \int \{dP d\hat{P}\} e^{\sum_{\omega, \phi, k} N \Delta \omega \Delta \phi \hat{P}(\omega, \phi, k) P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k})} \times e^{\frac{2\pi}{N}} \] \hspace{1cm} (A.13)

\[ \exp \left[ -\frac{kN}{2} \sum_{\omega, \phi, k} P(\omega, \phi, k) P(\omega', \phi', k') \left[ \frac{kN}{2} \exp \left[-i(\omega \phi' + \omega' \phi)\right] \right] e^{-\frac{2\pi}{N}} \right] \] \hspace{1cm} (A.14)

and restore the original delta function meaning of \( P(\omega, \phi, k|\tilde{\omega}, \tilde{\phi}, \tilde{k}) \).

Appendix A.4. Law of large numbers

Recall that our form of interest was

\[ \phi = N^{-1} \sum_{k,m} p(k, m) \log \left[ \int \prod_{i} \frac{d\omega_i e^{i\omega_i k}}{4\pi^2} L(\omega) \right] \] \hspace{1cm} (A.15)

We can pull out the site-specific variable
\[ \int \prod_i \left[ \frac{d\omega_i}{4\pi^2} e^{i(\omega_i \cdot \hat{\omega} - \hat{P}(\omega_i, \hat{k}))} \right] \]  

(A.16)

By symmetry this expression should not change under exchange of nodes, so we can re-write it as

\[ \prod_i \int \left[ \frac{d\omega_i}{4\pi^2} e^{i(\omega_i \cdot \hat{k} - \hat{P}(\omega_i, \hat{k}))} \right] = \exp \left( \sum_i \log \int \frac{d\omega_i}{4\pi^2} e^{i(\omega_i \cdot \hat{k} - \hat{P}(\omega_i, \hat{k}))} \right) \]  

(A.17)

which by the law of large numbers can be expressed as

\[ \exp \left[ N \sum_k p(k) \log \int \frac{d\omega}{4\pi^2} e^{i(\omega \cdot \hat{k} - \hat{P}(\omega, \hat{k}))} \right] \]  

(A.18)

Appendix A.5. Saddle point form

Which leads us to the following form for \( \phi \)

\[ \phi = \lim_{N \to \infty} N^{-1} \sum_k p(k) \log \int \{dPd\hat{P}\} e^{N\Psi[P, \hat{P}]} \]  

(A.19)

where

\[ \Psi[P, \hat{P}] = i \int_{-\pi}^{\pi} d\omega \sum_k P(\omega, k) \hat{P}(\omega, k) \]  

(A.20)

\[ + \frac{k}{2} \int d\omega d\omega' \sum_{k, k'} P(\omega, k) P(\omega', k') \exp[-i(\omega + \omega' + \phi k_1 + \phi' k_1)] \]

\[ - \frac{k}{2} \sum_k p(k) \log \int_{-\pi}^{\pi} \frac{d\omega}{4\pi^2} e^{i(\omega \cdot \hat{k} - \hat{P}(\omega, \hat{k}))} \]

Apart from the exponential in the second term, it is important to observe that all the elements of this expression are two component vectors: \( k = (k, m) \) represents the first and second neighbourhood of a node, \( \omega = (\omega, \phi) \) is the two component integration variable.

By a standard saddle point argument, the solution can be found by

\[ \phi = \text{extr}_{[P, \hat{P}]} \Psi[P, \hat{P}] \]  

(A.21)

via functional differentiation

Appendix A.6. Finding the extremum with functional differentiation

First make a substitution for easier manipulation \( Q = e^{-i\hat{P}} \) so that we can write

\[ \Psi[P, \hat{P}] = \int_{-\pi}^{\pi} d\omega \sum_k P(\omega, k) \log Q(\omega, k) \]  

(A.22)

\[ + \frac{k}{2} \int d\omega d\omega' \sum_{k, k'} P(\omega, k) P(\omega', k') e^{-i(\omega + \omega' + \phi k_1 + \phi' k_1)} - \frac{k}{2} \]

\[ + \sum_{(k, m)} p(k, m) \log \int_{-\pi}^{\pi} \frac{d\omega}{4\pi^2} e^{i\omega \cdot \hat{k}} Q(\omega, k) \]
Perform functional differentiation and setting \( \frac{\partial Q}{\partial P} = \frac{\partial P}{\partial Q} = 0 \)

\[
\log Q(\omega, k) = \tilde{k} \int d\omega' \sum_{k'} P(\omega', k') e^{-i(\omega + \omega' + \phi_k^* + \phi_{k'}^*)} 
\]

(A.23)

\[
P(\omega, k) = Q(\omega, k) \frac{p(k) e^{i\omega k}}{\int d\omega Q(\omega, k) e^{i\omega k}}
\]

Eliminate \( P(\omega, k) \) and define \( \gamma \) to satisfy

\[
Q = \exp \left( \tilde{k} \sum_{\zeta \in \mathbb{C}} \gamma(k, \zeta) e^{-i\omega \zeta} \right)
\]

which means that we require

\[
\sum_{\mu \in \mathbb{C}} \gamma(k, \mu) e^{-i\omega \mu} = \sum_{k'} \frac{\int d\omega' \exp \left( \tilde{k} \sum_{\zeta \in \mathbb{C}} \gamma(k', \zeta) e^{-i\omega' \zeta} \right) e^{i\omega' k'} e^{-(i(\omega' + \phi_{k'}^* + \phi_k^*))} p(k')} \int d\omega' \exp \left( \tilde{k} \sum_{\zeta \in \mathbb{C}} \gamma(k', \zeta) e^{-i\omega' \zeta} \right) e^{i\omega' k'}
\]

(A.24)

Compare coefficients of the free \( \omega \) to reach

\[
\gamma(k, \mu) = \delta_{\mu, 0} \sum_{k'} \frac{\int d\omega' \exp \left( \tilde{k} \sum_{\zeta \in \mathbb{C}} \gamma(k', \zeta) e^{-i\omega' \zeta} \right) e^{i\omega' k'} e^{-(i(\omega' + \phi_{k'}^* + \phi_k^*))} p(k')}{\int d\omega'' \exp \left( \tilde{k} \sum_{\zeta \in \mathbb{C}} \gamma(k', \zeta) e^{-i\omega'' \zeta} \right) e^{i\omega'' k'}}
\]

(A.25)

Do the integral on the bottom line by doing a series expansion of the exponential

\[
\int d\omega e^{i\omega k} \exp \left( \tilde{k} \sum_{\zeta \in \mathbb{C}} \gamma(k', \zeta) e^{-i\omega \zeta} \right) = \sum_{r=1}^{\infty} \frac{\tilde{k}^r}{r!} \int d\omega e^{i\omega k} \left( \tilde{k} \sum_{\zeta \in \mathbb{C}} \gamma(k', \zeta) e^{-i\omega \zeta} \right)^r
\]

\[
= \sum_{r=1}^{\infty} \frac{\tilde{k}^r}{r!} 4\pi^2 \sum_{\zeta \in \mathbb{C}} \sum_{\zeta' \in \mathbb{C}} \prod_{i=1}^{r} \gamma(k, \zeta) \delta_{k; \zeta, \zeta'}
\]

but this can be simplified further if we look back to equation (A.25), which requires \( \zeta_1 = 1 \) for \( \gamma \) to be non zero. Hence the bottom line of equation (A.25) is found to be

Bottom line = \( \frac{4\pi^2 \tilde{k}^r}{k_1!} \sum_{\zeta' \in \mathbb{C}} \prod_{i=1}^{r} \gamma(k, \zeta') \delta_{k; \zeta, \zeta'} \)

and by the same process the top line of equation (A.25) is found to be

Top line = \( \frac{4\pi^2 \tilde{k}^{r-1}}{(k_1 - 1)!} \sum_{\zeta' \in \mathbb{C}} \prod_{i=1}^{r-1} \gamma(k, \zeta') \delta_{k; \zeta, \zeta'} \)

Now we have an expression for \( \gamma \) at the point where \( P \) and \( \hat{P} \) maximise \( \Psi \). Write

\[
\Gamma = \exp \left( \tilde{k} \sum_{\zeta} \gamma(k, \zeta) e^{-i\omega \zeta} \right)
\]

so that

\[
P(\omega, k) = \frac{p(k) e^{i\omega k} \Gamma(\omega, k)}{\int_{\mathbb{R}} d\omega e^{i\omega k} \Gamma(\omega, k)}
\]
Define \( \Psi \). The first term of \( \Psi \) is disregarded from now on, since we have defined our ensemble to have no isolated nodes.

The entropy of random graph ensembles constrained with generalised degrees can be written as

\[
\Psi = - \sum_k p(k) \log \pi(k) + \sum_k p(k) \log \left[ \int \frac{\Sigma \, d\omega \, \sum_\xi p(k) e^{i\omega k} \Gamma(\omega, k)}{2} \right] \]

It is now necessary to evaluate all of the components of this expression.

\[
\int d\omega \, e^{i\omega k} \Gamma(\omega, k) = \frac{\tilde{k}^r}{r!} \int d\omega \, e^{i\omega k} \left( \sum_\xi \gamma(k, \xi) e^{-i\omega k} \right) = 4\pi^2 \left[ \delta_{k,0} + \frac{\tilde{k}^r}{k!} \theta(k - \frac{1}{2}) \prod_{i=1} \gamma(k, \xi_i) \delta_{m, \Sigma_i^\xi_i} \right]
\]

and with the same technique

\[
\int d\omega \, e^{i\omega k} \Gamma(\omega, k) \log \Gamma(\omega, k) = 4\pi^2 \frac{\tilde{k}^r}{(k-1)!} \theta(k - \frac{1}{2}) \prod_{i=1} \gamma(k, \xi_i) \delta_{m, \Sigma_i^\xi_i}
\]

where \( \theta \) is a heaviside function to distinguish the \( k = 0 \) case - which will be disregarded from now on, since we have defined our ensemble to have no isolated nodes. The first term of \( \Psi \) cancels down to \( \frac{1}{k^2} \). Combine this with the trailing \( \frac{1}{k^2} \) and re-write as \( \sum_k p(k) \log e^{i\omega k} - \sum_k p(k) \log \pi(k) \), and hence write the final form of \( \Psi \) as

\[
\Psi = - \sum_k p(k) \log \pi(k) + \sum_k p(k) \log \left[ \int \frac{\Sigma \, d\omega \, \sum_\xi p(k) e^{i\omega k} \Gamma(\omega, k)}{2} \right] \]

### Appendix A.7. Intermediate Answer

\[
S = \frac{\tilde{k}}{2} \left( 1 + \log \left( \frac{N}{\tilde{k}} \right) \right) - \sum_k p(k, m) \log \frac{p(k, m)}{\pi(k)}
\]

\[
\sum_{(k,m)} p(k, m) \log \left[ \prod_{(\xi_1, \ldots, \xi_k)} \gamma(k, \xi_s) \delta_{m, \Sigma_{s_i}^\xi_i} \right] + e_N
\]

where \( \gamma \) satisfies the self-consistency relation (\( m \) is used instead of \( k_2 \) for clarity)

\[
\gamma(k', \xi) = \delta_{\xi, 1} \sum_{k'} \frac{k'}{k} p(k') \frac{\sum_{\xi_1, \ldots, \xi_{k'-1}} \delta_{m', \Sigma_{s_i}^\xi_i} \gamma(k', \xi')} {\sum_{\xi_1, \ldots, \xi_{k'-1}} \delta_{m', \Sigma_{s_i}^\xi_i} \gamma(k', \xi')} \prod_{i=1}^{k'-1} \gamma(k', \xi')
\]

This can simplify a little bit. We can observe that in fact, \( \gamma \) depends on only two arguments: \( k_1, \xi_2 \). For convenience, relabel these as \( k, k' \) and rewrite the self consistency relation as

\[
\gamma(k, k') = \sum_{m'} \frac{k'}{k} p(k', m') \frac{\sum_{\xi_1, \ldots, \xi_{k'-1}} \delta_{m', \Sigma_{s_i}^\xi_i} \gamma(k', \xi')} {\sum_{\xi_1, \ldots, \xi_{k'-1}} \delta_{m', \Sigma_{s_i}^\xi_i} \gamma(k', \xi')} \prod_{i=1}^{k'-1} \gamma(k', \xi')
\]

### Appendix B. Implied generalised degree-degree correlation

Define

\[
W(k, \tilde{k} | c) = \frac{\sum_{ij} c_{ij} \delta_{k_i, \tilde{k_i}} \lambda_{ij} \lambda_{ij}} {\sum_{ij} c_{ij}}
\]
where \( \bar{k} = (k, m) \), the generalised degree. What is the average of this quantity in our ensemble with a specified generalised degree distribution? We can calculate this by looking at

\[
W(\bar{k}, \bar{k}') = \lim_{N \to \infty} \sum_c \text{prob}(c|\bar{k})W(\bar{k}, \bar{k}'|c)
\]  

(B.2)

where \( \text{prob}(c|\bar{k}) = \sum_{c' \in c} \frac{\prod \delta_{\bar{k}, \bar{k}'}(c)}{\prod p(\bar{k}')} \) Unpack this expression

\[
W(\bar{k}, \bar{k}') = \lim_{N \to \infty} \sum_c \sum_{\{k_i, \ldots, k_N\}} \frac{\prod \delta_{\bar{k}, \bar{k}'}(c)}{\prod p(\bar{k}')} \frac{\sum_{rs} c_{rs} \delta_{\bar{k}', \bar{k}'}(c)}{\sum_{ij} c_{ij}}
\]

\[
= \frac{1}{kN} \sum_{rs} \sum_{\{k_i, \ldots, k_N\}} \frac{\prod p(\bar{k}')} \frac{\sum c_{rs} \prod \delta_{\bar{k}', \bar{k}'}(c)}{\prod \delta_{\bar{k}, \bar{k}'}(c)}
\]

Focus on the difficult term, introducing the measure \( w(c|\bar{k}) = \prod_{i<j}(\frac{\bar{k}}{N} \delta_{c_{ij}, 1} + (1 - \frac{\bar{k}}{N}) \delta_{c_{ij}, 0}) \)

\[
I = \sum_c c_{rs} \frac{\prod_{i<j}(\frac{\bar{k}}{N} \delta_{c_{ij}, 1} + (1 - \frac{\bar{k}}{N}) \delta_{c_{ij}, 0}) \prod \delta_{\bar{k}', \bar{k}'}(c)}{\prod \delta_{\bar{k}, \bar{k}'}(c)}
\]

but I observe that I’ve already done this calculation.

\[
I = \int \frac{\text{d}w(\omega)k_L(\omega) e^{-\text{tr}(\omega k + \phi_{\bar{k}} + \phi_{\bar{k}'})}}{\text{d}w(\omega)k_L(\omega)}
\]

with \( L(\omega) \) defined as before. Since we are talking the large \( N \) limit, we can write this as

\[
I = \frac{\bar{k}}{N} (1 + O(N^{-1})) \int \frac{\text{d}w(\omega)k_L(\omega) e^{-\text{tr}(\omega k + \phi_{\bar{k}} + \phi_{\bar{k}'})}}{\text{d}w(\omega)k_L(\omega)}
\]

and follow the previous line of reasoning in order to achieve the form

\[
I = \frac{\bar{k}}{N} (1 + O(N^{-1})) \frac{\int \text{d}w(\omega)k_L(\omega) e^{-\text{tr}(\omega k + \phi_{\bar{k}} + \phi_{\bar{k}'})}}{\int \text{d}w(\omega)k_L(\omega)}
\]

We can now proceed with the same substitution that was previously helpful: \( e^{-\text{tr} \hat{\rho}} = Q(\omega, k) = \exp(\bar{k} \sum_{\xi \in \mathbb{Z}} \gamma(\xi, \xi)e^{-\text{im} \xi}) \). The integral \( \int \text{d}wQ(\omega, k)e^{-\text{tr}(\omega k + \phi_{\bar{k}} + \phi_{\bar{k}'})} \) evaluates by series expansion as

\[
\int \text{d}wQ(\omega, k)e^{-\text{tr}(\omega k + \phi_{\bar{k}} + \phi_{\bar{k}'})} = \sum_{\{\xi_1, \ldots, \xi_N\}} \prod \gamma(\xi_r, \xi_s) \delta_{m_r, \Sigma \xi_r} \frac{\bar{k}^N}{N!} \]

Hence, in leading order, the integral evaluates to

\[
I = \frac{\bar{k}}{N} k' k'' \sum_{\{\xi_1, \ldots, \xi_N\}} \prod_{r=1}^{k'} \gamma(\xi_r, \xi_s) \delta_{m_r, \Sigma \xi_r} \sum_{\{\xi_1, \ldots, \xi_N\}} \prod_{r=1}^{k''} \gamma(\xi_r', \xi_s') \delta_{m_r', \Sigma \xi_r'}
\]

\[
W(\bar{k}, \bar{k}') = \frac{k' k''}{(kN)^2} \sum_{rs} \sum_{\{k_i, \ldots, k_N\}} \prod p(\bar{k}) \delta_{\bar{k}, \bar{k}'} \gamma^*(\bar{k}', \bar{k}') \gamma^*(\bar{k}', \bar{k})
\]
Entropy of random graph ensembles constrained with generalised degrees

\[ \gamma^*(\vec{k}, k) = \sum_{\delta(\vec{k}, k) \prod_{i \neq k} \gamma(\vec{k}, k)} \left( \prod_{i \neq k} \gamma(\vec{k}, k) \right) \]

satisfying \( \sum_{m'} \vec{k} p(\vec{k}) \gamma^*(\vec{k}, k) = \gamma(k, k') \)

whereupon we can simplify

\[ W(\vec{k}, \vec{k}') = \gamma^*(\vec{k}, k') \gamma^*(\vec{k}, k) \frac{kk' p(\vec{k}) p(\vec{k}')}{(kN)^2} \sum_{rs} \delta_{\vec{k}, \vec{k}} \delta_{\vec{k}', \vec{k}'} \]

\[ = \gamma^*(\vec{k}, k') \gamma^*(\vec{k}, k) \frac{kk' p(\vec{k}) p(\vec{k}')}{(k)^2} \]

We can very easily take the marginal of the object \( W \) using the relation for \( \gamma^* \):

\[ \sum_{m,m'} W(\vec{k}, \vec{k}') = \gamma(k, k') \gamma(k', k) \]

which is in line with our earlier intuition, and serves to validate the preceding steps, e.g. since it shows we are correctly normalised.

Appendix C. Details of numerical implementation

There is no subroutine built into the C++ standard template library which calculates a factorial. Even for small values of \( x \), the size of \( x! \) can become unmanageable for the operating system. A simple factorial subroutine storing values as integers implemented on a 32bit system will fail at about 13!. Hence an object like \( \text{factorial} \) which is in line with our earlier intuition, and serves to validate the preceding steps, e.g. since it shows we are correctly normalised.

Additionally, the result found in 20 has the nuance that where the degree distribution does not have compact support, ‘impossible’ values must be excluded. Fortunately, it is possible to implement an iterative algorithm, which can efficiently calculate the final term, and can be directly adjusted to remove forbidden values.

Recall that the term which we wish to calculate from 20 is \( \sum_{k,m} p(k,m) \log \mathcal{P}_{k,m} \) where

\[ \mathcal{P}_{k,m} = \sum_{\vec{k}} \mathcal{U}_{k,m} \prod_{i \neq k} \left( 1 - \delta_{p(\vec{k}), 0} \right). \]

Observe that \( \mathcal{U}_{k,m} \) must satisfy

\[ \mathcal{U}_{k,m} = \sum_s \mathcal{U}_{k-1,m-s, \mathcal{I}(s)} \]

where \( \mathcal{I}(s) \) is an indicator: \( \mathcal{I}(s) = 1 - \delta_{p(\vec{k}), 0} \). That is to say, the number of configurations generalised degree \( (k,m) \) with a certain degree value \( s \) of the first neighbour is exactly the number of configurations with generalised degree \( (k-1,m-s) \) (i.e. considering as though the first neighbour was removed, since its degree value is known). Hence, the total number of configurations is calculated by summing over all values of \( s \).

We set up an iterative scheme as follows: populate row 1 with 0 or 1 depending if the degree \( i \) has a zero or non-zero probability. Populate row 2 as 1, 2, 3, 4,... However, wherever row 1 has a zero value, reduce the corresponding entry in row 2 by 1 instead of incrementing. This row can be interpreted as follows: the \( i \)th entry corresponds to the number of possible partitions of second degree \( i - 1 \) between 2 direct neighbours. This is consistent with C.1. Populate row 3 based on C.1. To populate row 4, we only need rows 1 and 3. Hence, we can release some memory by evaluating \( \sum_{k=1,2,m} p(k,m) \log \mathcal{U}_{k,m} \), storing this value, and releasing (i.e. over-writing) row 2. Note that the value of \( \mathcal{U}_{k,m} \) is read from the entry in row \( k \) entry.
m − k + 1. This scheme allows full accuracy to be maintained to much higher values of k and m - and allows direct adjustment for the case of ‘impossible’ degree values.

Appendix D. Validation

The entropy expression must satisfy certain properties. We can use these to check if our claimed answer (equation (21)) is plausible. Where there is a simple enough example to be enumerated directly, we expect to be able to reconcile the analytical expression for Z with counting \( \sum c \delta_{\vec{k},\vec{k}'(c)} \). Where the self consistency relation for \( \gamma \) can be solved directly, we expect to be able to reconcile the two forms of the \( \Gamma \) (the one involving \( \gamma \) terms, and the one involving \( W \) terms) We expect to retrieve the old simple degree result if we insert a ‘flat’ generalised degree distribution.

Appendix D.1. Ladder configuration

For this case (illustrated in figure D1), we find that \( \gamma(1,1) = 1, W(1,1) = 1 \) and \( \mathcal{P} = 1 \), so \( \Gamma = 0 \) calculated either way. To calculate \( S \) from first principles for this network we need to calculate \( p(c) = \prod_i p(k_i) \), where we have defined our ensemble as drawing degrees from \( p(k) = \delta_{k,1} \). As always, the core of the problem is in calculating \( Z(k) = \sum c_1 \delta_{1,k(c)} \) which is equivalent to counting the permutations of the network drawn above. There are \( N! \) orderings of the node, but this has to be divided by 2 since the bonds are symmetric and by \( N^2 \) since the order of the bonds is immaterial.

\[
\sum c p(c) \log(p(c)) = - \log \frac{N!}{2 \sqrt{\pi}} = - \log N! + \log 2 + \log N^2!
\]

which by Stirling’s approximation goes to \( \frac{N}{2} (\log N - 1) \) which corresponds to our analytical result in leading order in \( N \).

Appendix D.2. Wheel configuration

Consider an ensemble with generalised degrees consistent with figure D2. Based on the self consistency equations we find that \( \gamma(1,1) = \frac{1}{2} \) and so it follows:

\[
\Gamma = \frac{99}{100} \log \gamma(1,1) + \frac{99}{100} \log \gamma(s,1) = \frac{99}{100} \log \gamma(1,1) \gamma(s,1) = -\frac{k}{2} \log 2 \quad \text{(D.1)}
\]

We can immediately deduce the key parameters of this problem worked through as a starting point for an ensemble with given generalised degrees.

\[
\tilde{k} = 2 \times 99 \quad p(k,m) = \frac{\delta(k,m),(99,99)}{100} + \frac{99 \delta(k,m),(1,99)}{100}
\]
Figure D2. A validation example with two degree values - the wheel. In Appendix D.2 the partition function is evaluated directly and compared to the result using equation (21).

Let us work out $Z(k)$ for an arbitrary degree sequence drawn from our distribution. For the generalised degree case the only valid wiring is as illustrated: groups of 99 degree 1 nodes around a degree 99 node. To enumerate the ensemble, view the peripheral nodes as consecutively numbered; observe $99^{99}$ orderings of such a numbering - of which there are 99! equivalent permutations within each grouping. Hence, claim $Z(k) = \frac{99^{99}}{99!}$. So, directly calculated

$$\frac{1}{N} \log Z_{\text{enumerated}} = \frac{99}{100} \left( \log(N) + \log(99/100) - \frac{1}{100} \log 99! \right) - \frac{99}{100} \quad \text{(D.2)}$$

whereas picking up from the appropriate point in the calculation finds this quantity to be

$$\frac{1}{N} \log Z_{\text{analytical}} = \frac{k}{2} \left( 1 + \log \left( \frac{N}{k} \right) \right) + \sum p(k,m) \log \pi(k) + \Gamma$$

The $\pi(k)$ factors evaluate to

$$\log(\pi(1)) = \log \left( \frac{2 \times 99}{100} \right) - \bar{k}$$

$$\log(\pi(99)) = \log \left( \frac{2 \times 99}{100} \right)^{99} - \bar{k} - \log 99!$$

so, inserting equation (D.1) into D.2 shows that

$$\frac{1}{N} \log Z_{\text{analytical}} = -\frac{\bar{k}}{2} + \frac{k}{2} \log N + \frac{k}{2} \log \bar{k} - \frac{1}{100} \log 99! + \Gamma$$

which reconciles with the solution from first principles, as required.

Appendix D.3. A validation example with a more complicated degree-degree correlation

Consider a network based on figure D3 as a repeating motif. In fact, this is the only possible wiring of such a network that fulfils the generalised degree distribution required, up to permutation of nodes.

As previously, it is convenient to work with $\gamma^*(k',k) = \frac{\sum_{e_1,...,e_{k-1}} \Pi_{e<1} \gamma^{k'-1} \prod_{e<1} \gamma^{k'} e', e'' \prod_{e<1} \gamma^{k'}}{\sum_{e_1,...,e_{k-1}} \Pi_{e<1} \gamma^{k'-1} \prod_{e<1} \gamma^{k'} e', e'' \prod_{e<1} \gamma^{k'}}$

satisfying $\sum_{k'} \frac{k'}{k} p(k') \gamma^*(k',k) = \gamma(k,k')$.
But the example has been constructed so that (up to permutation) only one sequence is graphical: \{(1,1), (1,1), (1,3), (1,3), (1,3), (3,3)\...\} repeated \(N/6\) times. We can do the calculations for the small network only without loss of generality.

The self consistency relations are trivial in this example

\[
\gamma^2(1,1) = p(1,1) = \frac{1}{4}
\]

\[
\gamma(1,3)\gamma(3,1) = \frac{3p(3,3)}{k} = \frac{3}{8}
\]

from which it follows that \(\Gamma\) evaluated from equation (5) is

\[
\Gamma = \frac{\log \gamma(1,1)}{3} + \frac{\log \gamma(1,3)}{2} + \frac{\log \gamma(3,1)}{6}
\]

\[
= \frac{1}{6} \log \left[ \frac{1}{4} \left( \frac{3}{8} \right)^3 \right]
\]

Which evaluates to the same as the expression for \(\Gamma\) proposed in equation (21)

\[
\Gamma = \frac{k}{2} \sum_{k,k'} W(k,k') \log W(k,k') + \sum_{k,m} p(k,m) \log \left( \frac{m-1}{k-1} \right)
\]

\[
= \frac{8}{6^2} \left[ \frac{1}{4} \log \frac{1}{4} + \frac{3}{8} \log \frac{3}{8} + \frac{3}{8} \log \frac{3}{8} \right] + 0
\]

\[
= \frac{1}{6} \log \left[ \frac{1}{4} \left( \frac{3}{8} \right)^3 \right]
\]

as predicted.

A combinatorial argument can be used to calculate \(Z(k)\) in this case. Consider the network to be a combination of two sub networks. The sub-network of nodes degree \((1,1)\) has \(N/3\) nodes. Repeat the earlier strategy of counting the configurations by counting the number of labellings of the diagram \(\left( \frac{N}{3} \right)!\), and then dividing by the symmetries: \(2!\) since the pairs are symmetric and \((N/6)!\) since the order doesn’t matter. In the other subnetwork, there are \((N/2)!\) orderings of the peripheral nodes, divided by \((3)!^{N/6}\) symmetry factor (but the ‘order’ does matter, since this fixes the central node). Hence claim

\[
Z(k) = \frac{\frac{N}{3}! \frac{N}{3}!}{2! \frac{N}{6}! \frac{N}{3}!^{N/6}}
\]

If \(N = 6\), then \(Z(k) = \frac{21!}{12!3!} = 1\) as expected. If \(N = 12\), then \(Z(k) = \frac{432!}{272!153!3!^{12}} = \frac{6!}{27!3} = 60\) which can be corroborated directly.
Entropy of random graph ensembles constrained with generalised degrees

Working from first principles, it follows that

\[
\frac{1}{N} \log Z(k) = \frac{1}{3} \log \left(\frac{N}{3}\right) + \frac{1}{2} \log \left(\frac{N}{2}\right) - \frac{1}{6} \log \left(\frac{N}{6}\right) - \frac{1}{6} \log (12) - \frac{4}{6}
\]

\[
= \frac{4}{6} \log N - \frac{1}{3} [\log 3 + 2 \log 2] - \frac{2}{3}
\]

This matches the analytical result, evaluated with the help of equation (D.3).

Appendix D.4. A connected network example

\[
\begin{array}{c|cc}
 k & 1 & 4 \\
 m & 4 & 8 \\
p(k, m) & 2/3 & 1/3 \\
\end{array}
\]

Figure D4. A validation example based on a connected network. In Appendix D.4 the partition function is evaluated directly and compared to the result using equation (21).

Consider the ensemble of networks defined by the general degree sequence set out in figure D4. By combinatorics, argue that there are \(\frac{N}{3}!\) orderings of the centre nodes, and \(\frac{2N}{3}!\) orderings of the remaining nodes, divided by \(2^2\) for symmetry. Hence it follows that

\[
\frac{1}{N} \log Z(k, m) = \frac{1}{N} \log \left(\frac{N^{1+2N}}{2^2}\right)
\]

\[
= \frac{1}{3} \log \frac{N}{3} + \frac{2}{3} \log \frac{2N}{3} - \frac{1}{3} \log 2 - 1
\]

\[
= \log N - \log 3 + \frac{1}{3} \log 2 - 1
\]

Working using the analytical formula, note immediately that \(P_{k,m} = 1\) for all \(k, m\) appearing in the network (by construction), and \(\frac{1}{2} = 1\) so

\[
\frac{1}{N} \log Z(k, m) = \log N + \log (2 - 1) - \frac{2}{3} \log 2 - \log 3
\]

\[
= \log N + \frac{1}{3} \log 2 - \log 3 - 1
\]