Expansion of the conditional probability function in a network with nearest–neighbour degree correlations

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A useful property of a network that can be used to characterize many systems is the degree distribution. However, many complex networks exhibit higher–order degree correlations that must be studied through other means, such as clustering coefficients, the Newman $r$ factor, and the average nearest neighbour degree (ANND). In this paper we develop an expansion of the conditional probability that can be used to parameterize such degree correlations. The measures of degree correlations associated with this expansion can be used to signal the presence of non–linear correlations.
I. INTRODUCTION

Interest in the applications of networks to technological, biological, and social systems has grown significantly in recent years [1, 3]. One property of networks that has received much attention is the degree distribution, which characterizes the number of edges that connect a given node. Many networks show a power-law form of the degree distribution, while other networks may have an exponential or truncated power-law distribution. However, there is a further property of networks that is not completely captured by the degree distribution alone: it is found that most networks have a high degree of clustering, with nodes tending to share many common connections.

A number of ways have been developed to characterize such correlations. One standard approach was formulated by Newman [4–7], who introduced what is now called the Newman factor $r$. This number is essentially the Pearson correlation coefficient of degrees from connected vertices in a network and is fully defined by two–point correlations in a network. The Newman factor is normalized to lie in the interval $-1 \leq r \leq 1$, and is defined so that positive (negative) values indicate that vertices with the same (different) degree tend to be connected, which indicate assortative (disassortative) mixing. A Newman factor of 0 means no correlations are present. Most networks have a non-trivial (negative) values indicate that vertices with the same (different) degree tend to be connected, which indicate assortative

However, some of these measures may not completely capture all correlations that may be present in a network. For example, the Pearson correlation coefficient by definition only explores linear relationships between two variables [11]. In this paper, we develop a formalism that in principle can be used to measure higher–order non–linear correlations. We do this by examining an expansion of $P(k,k')$, the joint probability that an edge chosen at random connects vertices of degree $k$ and $k'$. In Section II we develop this expansion, through which we can define generalizations of the Newman $r$ factor and the ANND $k_{nn}(k)$ which are sensitive to non–linear correlations. The expansion developed in this section involves certain input coefficients; in Section III we show how to relate this expansion to one involving the specification of certain generalized ANND functions. In Section IV we use the results of Ref. [10] to show how these arise in defining clustering coefficients. In Section V we illustrate the use and effects of these generalizations in some simple examples. Section VI contains some brief conclusions.

II. EXPANSION OF THE CONDITIONAL PROBABILITY FUNCTION

Let $P(k)$ denote the probability of finding a node of degree $k$, $P(k'|k)$ the conditional probability that a vertex of degree $k$ is connected to a vertex of degree $k'$, and $P(k, k') = P(k'|k)P(k)$ be the joint probability that a randomly chosen edge connects vertices of degree $k$ and $k'$. These satisfy the normalization conditions

$$\sum_k P(k) = \sum_{k'} P(k'|k) = 1$$

as well as the detailed balance equation

$$kP(k'|k)P(k) = k'P(k|k')P(k')$$

Let us now introduce the edge distribution [7]

$$P_e(k) = \sum_{k'} P(k', k)$$

This allows us to express the joint probability $P(k', k)$ to the conditional probability $P(k'|k)$ as

$$P(k', k) = P(k'|k)P_e(k)$$

If we now define, for any function $f(k)$,

$$\langle f(k) \rangle = \sum_k f(k)P_e(k)$$

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we can relate the edge distribution \( P_e(k) \) to the degree distribution \( P(k) \) as

\[
P_e(k) = \frac{k}{k} P(k) \tag{6}
\]

In terms of \( P_e(k) \), the detailed balance condition of Eq. (2) becomes

\[
P(k'|k)P_e(k) = P(k|k')P_e(k') \tag{7}
\]

We now examine the form of the conditional probability \( P(k'|k) \). First note that, if the network were uncorrelated, we would have

\[
P_{nc}(k'|k) = \frac{k' P(k')}{k} = P_e(k') \tag{8}
\]

This suggests that we can put \( P(k'|k) \) into the form

\[
P(k'|k) = P_e(k') + Q(k'|k) \tag{9}
\]

for some function \( Q(k'|k) \). The detailed balance condition of Eq. (7) implies

\[
Q(k'|k)P_e(k) = Q(k|k')P_e(k') \Rightarrow Q(k'|k) = P_e(k')Q(k', k) \tag{10}
\]

where \( Q(k', k) = Q(k, k') \) is symmetric in \( k \) and \( k' \). With this, we can then put \( P(k'|k) \) of Eq. (9) into the form

\[
P(k'|k) = P_e(k') [1 + Q(k', k)] \tag{11}
\]

subject to the condition

\[
\sum_{k'} Q(k', k)P_e(k') = 0 \tag{12}
\]

which follows from Eq. (11).

Let us assume that we can expand the function \( Q(r, s) \) in in terms of symmetric polynomials of \( r \) and \( s \):

\[
Q(r, s) = E_0(r, s) + E_1(r, s) + E_2(r, s) + E_3(r, s) + E_4(r, s) + \ldots \tag{13}
\]

where

\[
E_0(r, s) = e_{00}^{(0)} \]

\[
E_1(r, s) = e_{11}^{(1)} (r + s) \]

\[
E_2(r, s) = e_{22}^{(2)} (r^2 + s^2) + e_{11}^{(2)} rs \]

\[
E_3(r, s) = e_{33}^{(3)} (r^3 + s^3) + e_{21}^{(3)} (r^2 s + rs^2) \]

\[
E_4(r, s) = e_{44}^{(4)} (r^4 + s^4) + e_{31}^{(4)} (r^3 s + rs^3) + e_{22}^{(4)} r^2 s^2 \tag{14}
\]

and \( e_{ij}^{(k)} \) are constant coefficients. The constraint of Eq. (12) will lead to conditions on certain coefficients of these expansions to a given order. This will allow us to write the expansion of \( Q(m, n) \) to the \( t \)th order as

\[
Q^{(t)}(r, s) = \sum_{i=1}^{t} \sum_{j=1}^{t} \alpha_{ij} v_i(r)v_j(s) \tag{15}
\]

where we have introduced

\[
v_n(k) = \frac{1}{\sqrt{\nu_{nn}}} [k^n - \langle k^n \rangle] \]

\[
\sigma_{ij} \equiv \langle (k^i - \langle k^i \rangle)(k^j - \langle k^j \rangle) \rangle = \langle k^i k^j \rangle - \langle k^i \rangle \langle k^j \rangle \tag{16}
\]

Note that \( \langle v_{ij} \rangle = 0 \) and \( \langle v_i v_j \rangle = 1 \) for \( i = 1, 2, \ldots, n \), but \( \langle v_i v_j \rangle \neq 0 \) for \( i \neq j \). Through the Gram–Schmidt procedure, we can develop an orthonormal basis \( u_i(k) \) satisfying \( \langle u_i \rangle = 0 \) and \( \langle u_i u_j \rangle = \delta_{ij} \) from the \( v_i(k) \) as

\[
u_i(k) = \frac{U_i(k)}{\sqrt{\langle U_i U_i \rangle}} \tag{17}
\]
where

\[ U_1(k) = v_1(k) \]
\[ U_2(k) = v_2(k) - (u_1 v_2) u_1(k) \]
\[ U_3(k) = v_3(k) - (u_1 v_3) u_1(k) - (u_2 v_3) u_2(k) \]
\[ \vdots \]
\[ U_n(k) = v_n(k) - \sum_{j=1}^{n-1} (u_j v_n) u_j(k) \]  \hspace{1cm} (18)

The relations of Eqs. (17, 18) allow us to express the \( v_i(k) \) in terms of the \( u_i(k) \):

\[ v_n(k) = \sum_{j=1}^{n} (u_j v_n) u_j(k) \]  \hspace{1cm} (19)

This allows us to express the expansion of \( Q(s, t) \) of Eq. (15) as

\[ Q^{(t)}(r, s) = \sum_{a=1}^{t} \sum_{b=1}^{t} \alpha_{ab} v_a(r) v_b(s) \]
\[ = \sum_{a=1}^{t} \sum_{b=1}^{t} \sum_{i=1}^{t} \sum_{j=1}^{t} \alpha_{ab} \langle u_i v_a \rangle \langle u_j v_b \rangle u_i(r) u_j(s) \]
\[ = \sum_{i=1}^{t} \sum_{j=1}^{t} \sum_{a=1}^{t} \sum_{b=1}^{t} \alpha_{ab} \langle u_i v_a \rangle \langle u_j v_b \rangle \theta(a - i) \theta(b - j) u_i(r) u_j(s) \]
\[ = \sum_{i=1}^{t} \sum_{j=1}^{t} \beta_{ij} u_i(r) u_j(s) \]  \hspace{1cm} (20)

where \( \theta(x) = 1 \) if \( x \geq 1 \) and zero otherwise, and

\[ \beta_{ij} = \sum_{a=1}^{t} \sum_{b=1}^{t} \alpha_{ab} \langle u_i v_a \rangle \langle u_j v_b \rangle \theta(a - i) \theta(b - j) \]  \hspace{1cm} (21)

The coefficients \( \beta_{ij} \) can be interpreted in terms of generalized correlation coefficients as follows. We have, from Eq. (20) and the fact that \( \langle u_i u_j \rangle = \delta_{ij} \), the relationship

\[ \sum_{r} \sum_{s} u_a(r) u_b(s) Q^{(t)}(r, s) P_a(r) P_b(s) = \beta_{ab} \]  \hspace{1cm} (22)

We now introduce a generalized \( a \)-th–order ANND \( k_{nn}^{(a)}(k) \) as

\[ k_{nn}^{(a)}(k) = \sum_{k'} u_a(k') P(k'|k) = \sum_{k'} u_a(k') Q^{(t)}(k', k) P_a(k') = \sum_{j=1}^{t} \beta_{aj} u_j(k) \]  \hspace{1cm} (23)

where we have used Eqs. (11, 20) and \( \langle u_i(k) \rangle = 0 \). This allows us to write \( Q^{(t)}(r, s) \) of Eq. (20) as

\[ Q^{(t)}(r, s) = \sum_{i=1}^{t} u_i(r) k_{nn}^{(i)}(s) = \sum_{i=1}^{t} k_{nn}^{(i)}(r) u_i(s) \]  \hspace{1cm} (24)

and also allows us to express Eq. (22) as

\[ \beta_{ab} = \langle k_{nn}^{(a)}(k) u_b(k) \rangle \]  \hspace{1cm} (25)

We can then use this to introduce generalized correlation coefficients \( r_{ab} \) to order \( t \):

\[ r_{ab} = \frac{\langle (k_{nn}^{(a)} - \langle k_{nn}^{(a)} \rangle) (u_b - \langle u_b \rangle) \rangle}{\sqrt{\langle (k_{nn}^{(a)} - \langle k_{nn}^{(a)} \rangle)^2 \rangle \langle (u_b - \langle u_b \rangle)^2 \rangle}} = \frac{\langle k_{nn}^{(a)} u_b \rangle}{\sqrt{\langle k_{nn}^{(a)} \rangle^2}} \equiv \frac{\beta_{ab}}{R_a} \]  \hspace{1cm} (26)
where \(a, b = 1, 2, \ldots, t\), we have used \(\langle k_{nn}^{(a)} \rangle = 0 = \langle u_i \rangle\), and we have defined

\[
R_a = \sqrt{\langle (k_{nn}^{(a)})^2 \rangle} = \sqrt{\sum_{j,k=1}^{t} \beta_{aj} \beta_{ak} \langle u_j u_k \rangle} = \sqrt{\sum_{j,k=1}^{t} \beta_{aj} \beta_{ak} \delta_{jk} \langle u_j u_k \rangle} = \sqrt{\sum_{j=1}^{t} \beta_{aj}^2} \tag{27}
\]

The definition of \(r_{ab}\) in Eq. (26) satisfies \(-1 \leq r_{ab} \leq 1\), which follows from the Cauchy–Schwarz inequality

\[
|\langle (X - \langle X \rangle)(Y - \langle Y \rangle) \rangle |^2 \leq \langle (X - \langle X \rangle)^2 \rangle \langle (Y - \langle Y \rangle)^2 \rangle \tag{28}
\]

for two variables \(X\) and \(Y\). We can then write the expansion of \(Q^{(1)}(r, s)\) of Eq. (20) as

\[
Q^{(1)}(r, s) = \sum_{a=1}^{t} \sum_{b=1}^{t} R_{ab} r_{ab} u_a(r) u_b(s) \tag{29}
\]

with the condition \(R_{a} r_{ab} = R_{b} r_{ba}\) coming from \(\beta_{ab} = \beta_{ba}\). Note that, to a given order \(t\), the \(r_{ab}\) are not independent, since by Eq. (26) we have \(r_{a1}^2 + r_{a2}^2 + \ldots + r_{at}^2 = 1\). This allows us to introduce \(t - 1\) hyperspherical angles \(\theta_{ak}\) and parameterize the \(r_{ab}\) as

\[
\begin{pmatrix}
r_{a1} \\
r_{a2} \\
r_{a3} \\
\vdots \\
r_{at} \\
r_{a(t-1)} \\
\end{pmatrix} = \frac{1}{R_a} \begin{pmatrix}
\beta_{a1} \\
\beta_{a2} \\
\beta_{a3} \\
\vdots \\
\beta_{at} \\
\beta_{a(t-1)} \\
\end{pmatrix} = \begin{pmatrix}
\cos \theta_{a1} \\
\sin \theta_{a1} \cos \theta_{a2} \\
\sin \theta_{a1} \sin \theta_{a2} \cos \theta_{a3} \\
\vdots \\
\Pi_{i=1}^{k-1} \sin \theta_{a1} \sin \theta_{a2} \cdots \sin \theta_{a(t-2)} \cos \theta_{a(t-1)} \\
\sin \theta_{a1} \cdots \sin \theta_{a(t-2)} \sin \theta_{a(t-1)} \\
\end{pmatrix} \tag{30}
\]

This form of the \(r_{ab}\), as appearing in the expansion of Eq. (20), makes it explicit that it is the combination of the \(\beta_{ab}\) parameters that appear in \(R_a\) that sets the scale for \(Q^{(1)}(r, s)\).

It is straightforward to see how the usual ANND \(k_{nn}(k)\), and related Newman correlation coefficient \(r\), are related to the generalized \(k_{nn}^{(a)}(k)\) of Eq. (23) and \(r_{ab}\) of Eq. (20). Suppose we keep only the leading-order \(t = 1\) term in the expansion of \(Q^{(1)}(r, s)\) in Eq. (13):\n
\[
Q^{(1)}(r, s) = \alpha_{11} v_1(r) v_1(s) \tag{31}
\]

where, from Eq. (16),

\[
v_1(k) = \frac{k - \langle k \rangle}{\sqrt{\sigma_{11}}} = \frac{k - \langle k \rangle}{\sqrt{(k^2) - \langle k \rangle^2}} \tag{32}
\]

In this case only the orthonormal basis vector \(u_1(k) = v_1(k)\) of Eq. (14) would arise, leading to the expansion

\[
Q^{(1)}(r, s) = \beta_{11} u_1(r) u_1(s) \tag{33}
\]

The only generalized ANND function of Eq. (23) that would appear would be

\[
k_{nn}^{(1)}(k) = \sum_{k'} u_1(k') P(k'|k) = \frac{1}{\sqrt{\sigma_{11}}} \sum_{k'} (k' - \langle k' \rangle) P(k'|k) = \frac{1}{\sqrt{\sigma_{11}}} \left[ \sum_{k'} k' P(k'|k) - \langle k \rangle \right] \tag{34}
\]

Since the standard ANND \(\bar{k}_{nn}(k)\) is defined as \(0\)

\[
\bar{k}_{nn}(k) = \sum_{k'} k' P(k'|k) \tag{35}
\]

which satisfies \(\langle \bar{k}_{nn}(k) \rangle = \langle k \rangle\), we then have the relationship

\[
k_{nn}^{(1)}(k) = \frac{1}{\sqrt{\sigma_{11}}} [\bar{k}_{nn}(k) - \langle k \rangle] = \frac{\bar{k}_{nn}(k) - \langle \bar{k}_{nn}(k) \rangle}{\sqrt{(k^2) - \langle k \rangle^2}} \tag{36}
\]
We can also relate the standard Newman correlation factor $r$ to the corresponding generalization of Eq. (26). The Newman factor $r$ can be written as [7]

$$r = \frac{1}{\langle k^2 \rangle - \langle k \rangle^2} \sum_{k', k} k'k \left[ P(k', k) - P_e(k')P_e(k) \right] =$$

$$= \frac{1}{\sigma_{11}} \left[ \sum_{k', k} k'k P(k'|k)P_e(k) - \langle k \rangle^2 \right] = \frac{1}{\sigma_{11}} \left[ \sum_k \bar{k}_{nn}(k)kP_e(k) - \langle k \rangle^2 \right] =$$

$$= \frac{1}{\sigma_{11}} ((\bar{k}_{nn}(k) - \langle \bar{k}_{nn}(k) \rangle)(k - \langle k \rangle))$$

(37)

where we have used Eq. (4) to relate the joint probability to the conditional probability, as well as $\langle \bar{k}_{nn}(k) \rangle = \langle k \rangle$. Using Eq. (36) to relate $\bar{k}_{nn}(k)$ to $k^{(1)}_{nn}(k)$, as well as Eq. (32) to relate $k$ to $u_1(k)$, we then have

$$r = \frac{1}{\sigma_{11}} (\sqrt{\sigma_{11}}^2 \langle k^{(1)}_{nn}(k)u_1(k) \rangle) = \langle k^{(1)}_{nn}(k)u_1(k) \rangle$$

(38)

The corresponding correlation coefficient of Eq. (26) that would appear to this order is

$$r_{11} = \frac{\langle (k^{(1)}_{nn} - \langle k^{(1)}_{nn} \rangle)(u_1 - \langle u_1 \rangle) \rangle}{\sqrt{\langle (k^{(1)}_{nn} - \langle k^{(1)}_{nn} \rangle)^2 \rangle} \sqrt{\langle (u_1 - \langle u_1 \rangle)^2 \rangle}} = \frac{\langle k^{(1)}_{nn}u_1 \rangle}{\sqrt{\langle k^{(1)}_{nn}^2 \rangle}} = \frac{\beta_{11}}{\langle k_{nn} \rangle}$$

(39)

which allows us to identify $r = \beta_{11} = r_{11}/|\beta_{11}|$. Note that, to this order, we have $r_{11} = \pm 1$, which simply reflects the fact that in the linear approximation there is perfect linear correlation or anti-correlation between $k^{(1)}_{nn}$ and $u_1$.

### III. SPECIFYING THE AVERAGE NEAREST NEIGHBOUR DEGREE

An alternate, but related, approach to the expansion discussed here has been formulated by Weber and Porto [7], who examined how one could expand the joint probability in terms of a particular functional form for the ANND $k_{nn}(k)$. In the current notation, this approach proceeds as follows. One begins with the functional form of Eq. (11) for the conditional probability:

$$P(k'|k) = P_e(k') \left[ 1 + Q(k', k) \right]$$

(40)

subject to the constraint of Eq. (12):

$$\sum_{k'} Q(k', k)P_e(k') = 0$$

(41)

One then assumes the symmetric function $Q(k', k)$ has the form

$$Q(k', k) = h(k')h(k)$$

(42)

and expresses the ANND $\bar{k}_{nn}(k)$ in terms of $h(k)$ as

$$\bar{k}_{nn}(k) = \sum_{k'} k'P(k'|k) = \langle k \rangle + \sum_{k'} k'h(k')P_e(k')h(k) = \langle k \rangle + \langle kh(k) \rangle h(k)$$

(43)

which allows one to infer

$$h(k) = \frac{\bar{k}_{nn}(k) - \langle k \rangle}{\langle kh(k) \rangle}$$

(44)

From this, one has

$$\langle kh(k) \rangle = \frac{\langle k\bar{k}_{nn}(k) - k(k) \rangle}{\langle kh(k) \rangle} \Rightarrow \langle kh(k) \rangle = \sqrt{\langle k\bar{k}_{nn}(k) \rangle - \langle k \rangle^2}$$

(45)
The function $Q(k', k)$ arising in the joint probability

$$Q(k', k) = \frac{(\bar{k}_{nn}(k') - \langle k \rangle)(\bar{k}_{nn}(k) - \langle k \rangle)}{(k \bar{k}_{nn}(k)) - \langle k \rangle^2} \tag{46}$$

is thus specified by $\bar{k}_{nn}(k)$. In order to respect the identity $\langle \bar{k}_{nn}(k) \rangle = \langle k \rangle$, we can parameterize $\bar{k}_{nn}(k)$ as

$$\bar{k}_{nn}(k) = \frac{\langle k \rangle}{\langle g(k) \rangle} g(k) \tag{47}$$

for a suitable function $g(k)$.

This approach can be related to the expansion considered here. To do this, we first cast the expansion of $Q(k', k)$ in Eq. (46) as

$$Q(k', k) = \frac{k^{(1)}_{nn}(k') k^{(1)}_{nn}(k)}{\langle k^{(1)}_{nn}(k) u_1(k) \rangle} \tag{48}$$

and the parameterization of $\bar{k}_{nn}(k)$ of Eq. (47) as

$$k^{(1)}_{nn}(k) = \frac{\langle k \rangle}{\sqrt{\sigma_{11}}} \left[ \frac{g(k)}{\langle g(k) \rangle} - 1 \right] \tag{49}$$

where Eqs. (22), (30) have been used. This is to be compared to the general expansion of Eq. (24):

$$Q^{(i)}(k', k) = \sum_{i=1}^{t} \sum_{j=1}^{t} \beta_{ij} u_i(k') u_j(k) = \sum_{i=1}^{t} u_i(k') k^{(i)}_{nn}(k) = \sum_{i=1}^{t} k^{(i)}_{nn}(k') u_i(k) \tag{50}$$

Rather than considering the $\beta_{ij}$ coefficients as input parameters to $Q^{(i)}(k', k)$, we could, in analogy with Eq. (47), specify the ANND $k^{(a)}_{nn}(k)$ by some function $f^{(a)}(k)$. In order to respect the normalization $\langle k^{(a)}_{nn}(k) \rangle = 0$, we write

$$k^{(a)}_{nn}(k) = \left[ f^{(a)}(k) - \langle f^{(a)}(k) \rangle \right] \tag{51}$$

Introducing

$$\sigma_{f^a} = \sqrt{\langle (f^{(a)}(k) - \langle f^{(a)}(k) \rangle)^2 \rangle} \tag{52}$$

we can write this as

$$k^{(a)}_{nn}(k) = \sigma_{f^a} \frac{f^{(a)}(k) - \langle f^{(a)}(k) \rangle}{\sigma_{f^a}} \equiv \sigma_{f^a} g^{(a)}(k) \tag{53}$$

so that $g^{(a)}(k)$ has zero mean and unit norm. We then expand $g^{(a)}(k)$ in terms of the orthonormal basis $u_a(k)$ to some order $t$:

$$g^{(a)}(k) = \sum_{b=1}^{t} c^{(a)}_b u_b(k) \tag{54}$$

with the coefficients $c^{(a)}_b$ given by $c^{(a)}_b = \langle u_b(k) g^{(a)}(k) \rangle$. Comparing this to the expansion of Eq. (22) of $k^{(a)}_{nn}(k)$ in terms of the $\beta_{ij}$ allows us to identify

$$\beta_{ab} = \sigma_{f^a} c^{(a)}_b = \sigma_{f^a} \langle u_b(k) g^{(a)}(k) \rangle \tag{55}$$

In this approach, the order $t$ to which one is working should be chosen so that the expansion in Eq. (54) of $g^{(a)}(k)$ in terms of the orthonormal basis $u_a(k)$ is accurate.

Note that, in analogy with the expansion of $Q(k', k)$ of Eq. (46) developed by Weber and Porto [7], we could consider in the present approach a generalization of the expansion of Eq. (24):

$$Q^{(i)}(k', k) = \sum_{i=1}^{t} k^{(i)}_{nn}(k') u_i(k) \rightarrow \sum_{i=1}^{t} \frac{k^{(i)}_{nn}(k') k^{(i)}_{nn}(k)}{\langle k^{(i)}_{nm}(k) u_i(k) \rangle} \tag{56}$$

As with any perturbative expansion, the potential advantages of this form over the expression of Eq. (24) will depend on these higher–order terms being small, in some sense, to the unperturbed case.
IV. CLUSTERING COEFFICIENTS

Clustering measures correlations among 3 nodes in a network, and so requires knowledge of the conditional probability $P(k',k''|k)$, which is the probability that a vertex of degree $k$ is simultaneously connected to two vertices of degree $k'$ and $k''$. For non–Markovian networks $P(k',k''|k)$ and $P(k'|k)$ are unrelated, but for Markovian networks, we have the relation $P(k',k''|k) = P(k'|k)P(k''|k)$, so knowledge of the two–point probability distribution is sufficient. As shown by Dorogovtsev [10], various measures of clustering in a network can be derived in this case taking into account degree correlations present in $P(k'|k)$. Three related clustering coefficients can be introduced:

- The degree–dependent local clustering coefficient $C(k)$:
  \[
  C(k) = \frac{\langle m_{nn}(k) \rangle}{k(k-1)/2}
  \] (57)

  where $\langle m_{nn}(k) \rangle$ is the average number of connections between the nearest neighbours of a vertex of degree $k$.

- The mean clustering coefficient $\overline{C}$:
  \[
  \overline{C} = \sum_k P(k)C(k)
  \] (58)

- The clustering coefficient $C$:
  \[
  C = \frac{\sum_k P(k)\langle m_{nn}(k) \rangle}{\sum_k P(k)k(k-1)/2} = \frac{1}{k(k-1)} \sum_k k(k-1)P(k)C(k)
  \] (59)

As shown in Ref. [10], assuming the size $N$ of the network is large and there is “weak” clustering, the degree–dependent local clustering coefficient $C(k)$ of Eq. (57) is given by

\[
C(k) = \frac{1}{Nk} \sum_{q,q'} P(q'|k)P(q|k) \frac{P(q'|q)}{P_e(q')} (q' - 1)(q - 1)
\] (60)

which, in terms of the expansion of $P(k'|k)$ in terms of the function $Q(k',k)$ through Eq. (11), can be written as

\[
C(k) = \frac{1}{Nk} \sum_{q,q'} P_e(q') [1 + Q(q', k)] P_e(q) [1 + Q(q, k)] [1 + Q(q', q)] (q' - 1)(q - 1)
\] (61)

The mean clustering coefficient $\overline{C}$ and the clustering coefficient $C$ then follow by Eqs. (58, 59). Note that, In the limit of an uncorrelated network ($Q(k', k) = 0$), we have

\[
C_{nc}(k) = \overline{C}_{nc} = C_{nc} = \frac{((k) - 1)^2}{Nk}
\] (62)

Thus, a $k$–dependence of $C(k)$, leading to differences between $C(k)$, $\overline{C}$, and $C$, signals the presence of nearest–neighbour degree correlations.

One can now use the expansion of $Q(m, n)$ of Eq. (20) in order to express these clustering coefficients in terms of the expansion parameters $\beta_{ab}$. We first do so for the local coefficient $C(k)$. When expanding Eq. (61), we see that there will be linear, quadratic, and cubic terms in $Q(m, n)$ present. The linear terms can be evaluated using only the properties $\langle u_a \rangle = 0$ and $\langle u_a u_b \rangle = \delta_{ab}$. However, for the quadratic and cubic terms, we will need to evaluate $\langle u_a u_b u_c \rangle$. This can be done as follows. Let us express the relations of Eqs. (18, 19) relating the basis vectors $u_a(k)$ and $v_n(k)$ as

\[
u_m(k) = \sum_{j=1}^m c_{mj}v_j(k)
\]

\[
v_n(k) = \sum_{j=1}^n d_{nj}u_j(k)
\] (63)

We then have

\[
u_a(k)u_1(k) = \sum_{j=1}^a c_{aj}v_j(k)u_1(k) = \sum_{j=1}^a c_{aj}v_j(k)v_1(k)
\] (64)
where we have used $u_1(k) = v_1(k)$. Using the definition of $v_n(k)$ in Eq. 66, we have
\[
v_j v_1 = \frac{1}{\sqrt{\sigma_{jj} \sigma_{11}}} \left[ k^j - \langle k^j \rangle \right] [k - \langle k \rangle]
\]
\[
= \frac{1}{\sqrt{\sigma_{jj} \sigma_{11}}} \left[ \sqrt{\sigma_{j+1,j+1}} v_{j+1} - \sqrt{\sigma_{jj}} \langle k^j \rangle v_j - \sqrt{\sigma_{11}} \langle k^j \rangle v_1 + \langle k^{j+1} \rangle - \langle k^j \rangle \right] \quad (65)
\]
In this we can then use the second relation of Eq. 63 in this equation to express the terms involving $v_j$ in terms of $u_i$, and then insert this into Eq. 64 in order to find $u_n u_1$ in terms of a series of terms linear in $u_i$. We find
\[
u_n(k) u_1(k) = \sum_{j=1}^{a} \frac{c_{aj}}{\sqrt{\sigma_{jj} \sigma_{11}}} \left[ \sqrt{\sigma_{j+1,j+1}} \sum_{m=1}^{j+1} d_{j+1,m} u_m(k)
\right.
\]
\[
- \sqrt{\sigma_{jj}} \sum_{m=1}^{j} d_{jm} u_m(k) - \sqrt{\sigma_{11}} \langle k^j \rangle u_1(k) + \langle k^{j+1} \rangle - \langle k^j \rangle
\]
\[
\left. \right] \quad (66)
\]
We then have
\[
\langle u_n u_b u_1 \rangle = \sum_{j=1}^{a} \frac{c_{aj}}{\sqrt{\sigma_{jj} \sigma_{11}}} \left[ \sqrt{\sigma_{j+1,j+1}} d_{j+1,b} - \sqrt{\sigma_{jj}} d_{jb} - \sqrt{\sigma_{11}} \langle k^j \rangle \delta_{b1} \right]
\]
\[
\equiv \gamma_{ab} \quad (67)
\]
Introducing the notation
\[
\langle f(q,k) \rangle_q = \sum_q P_c(q)f(q,k) \quad (68)
\]
for a function $f(q,k)$, one can then derive the following relations:
\[
\langle Q(q,k)u_1(q) \rangle_q = k_{1n}^{(1)}(k)
\]
\[
\langle Q(q,k) k_{nn}^{(a)}(q) \rangle_q = \sum_b \beta_{ab} k_{nn}^{(b)}(k)
\]
\[
\langle Q(q',q)Q(q',k) \rangle_q = \sum_a k_{nn}^{(a)}(q)k_{nn}^{(a)}(k)
\]
\[
\langle Q(q',q)Q(q',k) u_1(q') \rangle_q = \sum_{a,b} \gamma_{ab} k_{nn}^{(a)}(q)k_{nn}^{(b)}(k)
\]
\[
\langle Q(q,k)k_{nn}^{(a)}(q)u_1(q) \rangle_q = \sum_{b,c} \beta_{ac} \gamma_{bc} k_{nn}^{(b)}(k) \quad (69)
\]
Using $u_1(k) = \sqrt{\sigma_{11}} u_1(k) + \langle (k) - 1 \rangle$, we then find the following contributions to $C(k)$:
\[
\sum_{q,q'} P_c(q) P_c(q') (q-1)(q'-1) = [\langle (k) - 1 \rangle]^2
\]
\[
\sum_{q,q'} P_c(q) P_c(q') \left[ Q(q,k) + Q(q',k) + Q(q,q') \right] (q-1)(q'-1) = \sigma_{11} \beta_{11} + 2\sqrt{\sigma_{11}} \langle (k) - 1 \rangle k_{nn}^{(1)}(k)
\]
\[
\sum_{q,q'} P_c(q) P_c(q') \left[ Q(q,k)Q(q',k) + Q(q',k)Q(q,q') + Q(q,k)Q(q,q') \right] (q-1)(q'-1) = \sigma_{11} \left[ k_{nn}^{(1)}(k) \right]^2 + 2\sqrt{\sigma_{11}} \langle (k) - 1 \rangle \sum_a \beta_{1a} k_{nn}^{(a)}(k) + 2\sigma_{11} \sum_{a,b} \beta_{1b} \gamma_{ab} k_{nn}^{(a)}(k)
\]
\[
\sum_{q,q'} P_c(q) P_c(q') \left[ Q(q,k)Q(q',k) (q-1)(q'-1) = \sigma_{11} \sum_{a,b,c,d} \beta_{cd} \gamma_{ac} \gamma_{bd} k_{nn}^{(a)}(k) k_{nn}^{(b)}(k)
\]
\[
+ 2\sqrt{\sigma_{11}} \langle (k) - 1 \rangle \sum_{a,b,c} \beta_{ac} \gamma_{bc} k_{nn}^{(a)}(k) k_{nn}^{(b)}(k) + \langle (k) - 1 \rangle^2 \sum_{ab} \beta_{ab} k_{nn}^{(a)}(k) k_{nn}^{(b)}(k) \right)
\]
\[
(70)
\]
We then find the local clustering coefficient $C(k)$, normalized to the non-correlated value $C_{nc}$ of Eq. (62), can be written as

$$\frac{C(k)}{C_{nc}} = 1 + F + \sum_a G_a k_{nn}^{(a)}(k) + \sum_{a,b} H_{ab} k_{nn}^{(a)}(k) k_{nn}^{(b)}(k)$$  \hspace{1cm} (71)$$

where

$$F = \frac{\sigma_{11} \beta_{11}}{(\langle k \rangle - 1)^2}$$

$$G_a = \frac{2\sqrt{\sigma_{11}}}{(\langle k \rangle - 1)} [\delta_{1a} + \beta_{1a}] + \frac{2\sigma_{11}}{(\langle k \rangle - 1)^2} \sum_b \beta_{1b} \gamma_{ab}$$

$$H_{ab} = \beta_{ab} + \frac{2\sqrt{\sigma_{11}}}{(\langle k \rangle - 1)} \sum_c \beta_{ac} \gamma_{bc} + \frac{\sigma_{11}}{(\langle k \rangle - 1)^2} \left[ \delta_{1a} \delta_{1b} + \sum_{c,d} \beta_{cd} \gamma_{ac} \gamma_{bd} \right]$$  \hspace{1cm} (72)$$

To calculate the clustering coefficient $C$ of Eq. (59), we will need

$$\langle k_{nn}^{(a)}(k) u_1(k) \rangle_k = \beta_{a1}$$

$$\langle k_{nn}^{(a)}(k) k_{nn}^{(b)}(k) \rangle_k = \sum_c \beta_{ac} \beta_{bc}$$

$$\langle k_{nn}^{(a)}(k) k_{nn}^{(b)}(k) u_1(k) \rangle_k = \sum_{c,d} \beta_{ac} \beta_{bd} \gamma_{cd}$$ \hspace{1cm} (73)$$

This leads to

$$\frac{C}{C_{nc}} = 1 + F + \frac{\sqrt{\sigma_{11}}}{(\langle k \rangle - 1)} \sum_a G_a \beta_{a1} + \sum_{a,b,c} H_{ab} \beta_{ac} \beta_{bc} + \frac{\sqrt{\sigma_{11}}}{(\langle k \rangle - 1)} \sum_{a,b,c,d} H_{ab} \beta_{ac} \beta_{bd} \gamma_{cd}$$  \hspace{1cm} (74)$$

In order to get a qualitative sense of the behaviour of $C(k)$ of Eq. (71) and $C$ of Eq. (74), let us assume that the expansion parameters $\beta_{ab}$ are small, such that we need only keep terms up to linear order in them. Since by the definition of Eq. (23) the generalized ANND $k_{nn}^{(a)}(k)$ is linear in $\beta_{ab}$, we find the local clustering coefficient $C(k)$ of Eq. (71) could be approximated as

$$\frac{C(k)}{C_{nc}} \approx 1 + \frac{\sigma_{11} \beta_{11}}{(\langle k \rangle - 1)^2} + \frac{2\sqrt{\sigma_{11}}}{(\langle k \rangle - 1)} k_{nn}^{(1)}(k)$$ \hspace{1cm} (75)$$

while the corresponding approximation of the clustering coefficient $C$ of Eq. (74) is

$$\frac{C}{C_{nc}} \approx 1 + \frac{3\sigma_{11} \beta_{11}}{(\langle k \rangle - 1)^2}$$ \hspace{1cm} (76)$$

In the next section we consider a couple of examples to illustrate the behaviour of various quantities discussed in this and the previous sections. The full numerical results for the clustering coefficients suggest that, for for small $\beta_{ab}$, this linear approximation just considered gives at least give a fairly good qualitative picture for how the clustering coefficients behave. In particular, from Eq. (61), the local degree-dependent clustering coefficient $C(k)$ has a $k$-dependence that follows approximately that of the first-order ANND $k_{nn}^{(1)}(k)$ (compare Fig. 1 and Fig. 5) and also Fig. 8 and Fig. 9. As well, the clustering coefficient $C$ of Eq. (74) is increased/decreased slightly, relative to the non-correlated value, for positive/negative $\beta_{11}$, corresponding to assortative/dis assortative mixing (see the discussion immediately following, respectively, Fig. 8 and Fig. 9).

V. EXAMPLES

In order to illustrate the relative size of the effects considered in the previous sections, in this Section we examine two examples of explicit choices of the parameters $\beta_{ab}$ in the expansion of $Q(k', k)$ of Eq. (11). In keeping with the spirit of a perturbative approach, we expect that, if we keep relatively few terms in the expansion, the corrections to the uncorrelated case $Q(k', k) = 0$ will be small in some sense. In both cases we use a degree distribution function
\( P(k) \sim k^\gamma \), with \( \gamma = -1.2 \), and consider degrees \( 1 \leq k \leq 40 \). The uncorrelated joint probability \( P_{nc}(q|k) = P_e(q) \) appears as in Fig. 1.

![FIG. 1. The uncorrelated conditional probability \( P_{nc}(q|k) \) for \( P(k) \sim k^\gamma \), with \( \gamma = -1.2 \).](image1)

The first case will be one exhibiting assortative mixing. For this we choose a single linear term \( \beta_{11} = 0.07 \). The function \( Q(q,k) \) appears in Fig. 2 while the conditional probability \( P(q|k) = P_e(q)[1 + Q(q,k)] \) appears in Fig. 3.

![FIG. 2. The expansion function \( Q(q,k) \) for \( \beta_{11} = 0.07 \).](image2)
As expected with assortative mixing, we see from the conditional probability of Fig. 3 that there is an increased likelihood of nodes with the same degree to be connected. Fig. 4 shows the generalized ANND of Eq. (23); in this case, only $k_{nn}^{(1)}(k)$ will be non-zero, and it is a linear function.

The only non-zero correlation coefficient $r_{ab}$ of Eq. (26) is $r_{11} = 1$, as expected, since the linear correlation is perfect in this case. Finally, in Fig. 5 we plot the degree-dependent local clustering coefficient $C(k)$ of Eq. (57), which has been normalized to the uncorrelated value $C_{nc}$ of Eq. (62).
FIG. 5. The degree–dependent local clustering coefficient $C(k)/C_{nc}$ for $\beta_{11} = 0.07$, normalized to the uncorrelated value.

Corresponding to this $C(k)$, we find the mean clustering coefficient $\overline{C}$ of Eq. (68), normalized to $C_{nc}$, to be $\overline{C}/C_{nc} = 0.94$, while the clustering coefficient $C$ of Eq. (59), also normalized to $C_{nc}$, to be $C/C_{nc} = 1.10$; this represents about a 10% change from the uncorrelated state.

The second case we examine will be one exhibiting disassortative mixing. For this we consider including both linear and quadratic terms in the expansion of $Q(q, k)$, and we choose $\beta_{11} = -0.07$, $\beta_{12} = 0.02 = \beta_{21}$, and $\beta_{22} = -0.04$. The function $Q(q, k)$ appears in Fig. 6 while the conditional probability $P(q|k) = P_c(q)[1 + Q(q, k)]$ appears in Fig. 7.

FIG. 6. The expansion function $Q(q, k)$ for $\beta_{11} = -0.07$, $\beta_{12} = 0.02 = \beta_{21}$, and $\beta_{22} = -0.04$. 
FIG. 7. The conditional probability $P(q|k)$ for $\beta_{11} = -0.07$, $\beta_{12} = 0.02 = \beta_{21}$, and $\beta_{22} = -0.04$.

As expected with disassortative mixing, in this case we see from the conditional probability of Fig. 7 that there is an increased likelihood of nodes of different degree to be connected. Fig. 8 shows the generalized ANND of Eq. (20); in this case, both $k^{(1)}_{nn}(k)$ and $k^{(2)}_{nn}(k)$ will be non–zero.

FIG. 8. The first–order ANND $k^{(1)}_{nn}(k)$ and second–order ANND $k^{(2)}_{nn}(k)$ for $\beta_{11} = -0.07$, $\beta_{12} = 0.02 = \beta_{21}$, and $\beta_{22} = -0.04$.

It is found that the only non–zero correlation coefficients $r_{ab}$ of Eq. (26) are $r_{11} = -0.96$, $r_{12} = 0.27$, $r_{21} = 0.45$, and $r_{22} = -0.89$. Finally, in Fig. 9 we plot the degree–dependent local clustering coefficient $C(k)$ of Eq. (57), which has been normalized to the uncorrelated value $C_{nc}$ of Eq. (62).
Corresponding to this $C(k)$, we find the mean clustering coefficient $\bar{C}$ of Eq. (58), normalized to $C_{nc}$, to be $\bar{C}/C_{nc} = 1.08$, while the clustering coefficient $C$ of Eq. (59), also normalized to $C_{nc}$, to be $C/C_{nc} = 0.91$; this represents about a 10% change from the uncorrelated state.

VI. CONCLUSIONS

We have examined an expansion of the conditional probability $P(k',k) = P_e(k')[1+Q(k',k)]$ about the uncorrelated case $P_{nc}(k'|k) = P_e(k')$ in terms of symmetric polynomials in $k'$ and $k$. Setting aside the question of convergence, we find a systematic expansion is possible, and will involve expansion coefficients $\beta_{ab}$. Having specified these coefficients up to a certain order, the usual measures of nearest–neighbour degree correlations – the Average Nearest Neighbour Degree ANND, Pearson–inspired correlation coefficients, and various clustering coefficients – can be calculated. In the present case, since non–linear terms in the expansion would in principle appear, appropriate generalizations of these measures of degree correlations were introduced.

One possible use for the type of expansion discussed in this paper might be as a means to estimate qualitatively the effect of nearest–neighbour degree correlations in models describing the evolution of states of nodes on specific networks – for example, the propagation of disease on the network. This can be formulated in terms of the equations governing the evolution of probabilities. This can come by formulating the equations governing the evolution in terms of probabilities. To see this in a general sense, let $\rho_{X,k}$ be the probability that a node of degree $k$ is in a state $X$ at time $t$. A differential equation describing the time evolution of $\rho_{X,k}$ might then contain terms such as

$$\frac{d \rho_{X,k}}{dt} = g\rho_{X,k}\rho_{Y,k} + \ldots$$

which would describe how the transition $X \rightarrow Y$ in the system, parameterized by a rate $g$, affects the probability $\rho_{X,k}$. Nearest–neighbour degree correlations could be incorporated into this model by consideration of the interaction term

$$\frac{d \rho_{X,k}}{dt} = gk\rho_{X,k}\Theta_{Y,k} + \ldots$$

where

$$\Theta_{Y,k} = \sum_{k'} \frac{k' - 1}{k'} P(k'|k)\rho_{Y,k'}$$
is the probability that a neighbour of the node, chosen randomly from amongst its $k$ neighbours, is in a state $Y$. Thus, specifying a conditional probability function $P(k'|k)$ that differs from the uncorrelated case $P_{uc}(k'|k) = P_e(k')$ would allow one to see the effects of different types of degree correlations in this model.

If one is to use the expansion of $Q(k', k)$ of Eq. (20) in specifying a conditional probability $P(k'|k)$ containing correlations, one must decide on the values of the expansion parameters $\beta_{ab}$ to use, and at what point does one know that enough terms have been kept. A mild constraint on the expansion is that, being a perturbative expansion, the corrections about the unperturbed case should be small, and that inclusion of higher–order effects should not affect significantly the results of the presumably more important lower–order terms. An equivalent statement of this is that, for a given set of parameters, changing them slightly would not change the overall qualitative picture. It may be possible, by examining classes of real networks, to be able to say something about the relative magnitude of the various $\beta_{ab}$ coefficients. However, if one wanted just a qualitative estimate of the relative effects of such degree correlations in the model under consideration, then one could consider a “small” number of terms in this expansion with “small” values of the $\beta_{ab}$ parameters, where “small” in this context is defined through the constraint that the effects do not significantly alter the uncorrelated case. The examples of Section V show that a reasonable set of parameters can be chosen which incorporate various types of degree correlations. Such an approach would not allow one to say anything quantitative about a real network, but it would allow one to decide, with some degree of confidence, whether or not inclusion of degree correlations in the model might lead to significant effects, and thus would be worthy of further, more detailed, study.

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