

Classifying Complex Networks using Unbiased Local Assortativity

Mahendra Piraveenan^{1,2}, Mikhail Prokopenko² and Albert Y. Zomaya¹

¹ Centre for Distributed and High Performance Computing, School of Information Technologies,
The University of Sydney, NSW 2006, Australia

² CSIRO Information and Communications Technologies Centre, PO Box 76, Epping, NSW 1710, Australia
mikhail.prokopenko@csiro.au

Abstract

Assortativity is a network-level measure which quantifies the tendency of nodes to mix with similar nodes in a network. Local assortativity has been introduced as a measure to analyse the contribution of individual nodes to network assortativity. In this paper we argue that there is a bias in the formulation of local assortativity which favours low-degree nodes. We show that, after the bias is removed, local assortativity of a node can be interpreted as a scaled difference between the average excess degree of the node neighbours and the expected excess degree of the network as a whole. Finally, we study the local assortativity profiles of a number of model and real world networks, demonstrating that four classes of complex networks exist: (i) assortative networks with disassortative hubs, (ii) assortative networks with assortative hubs, (iii) disassortative networks with disassortative hubs, and (iv) disassortative networks with assortative hubs.

Introduction

Many complex systems are amenable to be described as networks, with a given number of nodes and connecting edges. These include ecological systems, author collaborations, metabolism of biological species, and interaction of autonomous systems in the Internet, among others (Solé and Valverde, 2004; Albert and Barabasi, 2002; Albert et al., 1999; Newman, 2003; Faloutsos et al., 1999). It has been a recent trend to study common topological features of such networks. Network diameter, clustering coefficients, modularity and community structure, information content are some features analysed in recent literature in this regard (Faloutsos et al., 1999; Alon, 2007; Lizier et al., 2009; Prokopenko et al., 2009). One such measure which has been analysed extensively is assortativity (Solé and Valverde, 2004; Newman, 2002; Albert and Barabasi, 2002; Newman, 2003; Callaway et al., 2001; Palsson, 2006; Maslov and Sneppen, 2002; Zhou et al., 2008; Bagler and Sinha, 2007; Vázquez, 2003). Having originated in ecological and epidemiological literature (Albert and Barabasi, 2002), the term ‘assortativity’ refers to the correlation between the properties of adjacent network nodes.

While similarity between adjacent nodes can be measured in a number of ways, the property that is of interest to us is

node degree. Based on degree-degree correlations, assortativity has been defined as a correlation function, and the level of assortative mixing has been measured quantitatively for a number of networks, including social, biological and technical networks (Solé and Valverde, 2004). The networks that have a positive correlation coefficient are called assortative: similar nodes tend to mix with each other in such networks. The networks characterised by a negative correlation coefficient are called disassortative: dissimilar nodes tend to connect predominantly in these networks. The precise local contribution of each node to the global level of assortative mixing can also be quantified (Piraveenan et al., 2008, 2009b, 2010). This quantity has been called ‘local assortativity’. Local assortativity measures the local contribution of each node to the global correlation coefficient which is the network assortativity. Local assortativity profiles (as distributions of local assortativity over nodes’ degrees) can also be constructed for various networks, and these profiles, in turn, can be used to classify networks (Piraveenan et al., 2008, 2009a). Two such classes of disassortative networks have been proposed in Piraveenan et al. (2008).

In this paper, we demonstrate that the formulation proposed for local assortativity in Piraveenan et al. (2008) has a bias, which favours low-degree nodes over hubs. This bias needs to be removed before networks can be analysed in terms of local assortativity. Therefore, our objective is two-fold: (i) to propose an unbiased formulation of local assortativity, and (ii) to characterise classes of networks in terms of this unbiased formulation. After presenting the unbiased formulation for local assortativity, we show that the classification of disassortative real-world networks that was proposed in Piraveenan et al. (2008) still holds, and in addition, there are two similar classes among assortative networks as well. The unbiased formulation also provides a clearer interpretation of what it means for a node to be locally assortative.

Definitions and Terminology

We need to introduce a number of definitions before removing the bias from the formulation of local assortativity. Consider a network with N nodes and M links. Assortativity for

such a network has been defined as a correlation function (Newman, 2002), in terms of the network's excess degree distribution $q(k)$, and link distribution $e_{j,k}$. The excess degree is the number of remaining links encountered when one reaches a node by traversing a link. The link distribution of the network is the joint probability distribution of the excess degrees of the two nodes at either end of a randomly chosen link. The formal definition of network assortativity is given by:

$$r = \frac{1}{\sigma_q^2} \left[\sum_{jk} jk (e_{j,k} - q(j)q(k)) \right] \quad (1)$$

where $e_{j,k}$ is the link distribution of the network and σ_q is the standard deviation of the excess degree distribution of the network, $q(k)$.

Since the expectation of the distribution $q(k)$ is given by $\sum_k kq(k)$, the assortativity of a network can also be written as:

$$r = \frac{1}{\sigma_q^2} \left[\left(\sum_{jk} jke_{j,k} \right) - \mu_q^2 \right] \quad (2)$$

where μ_q is the expectation of the distribution.

Local assortativity was motivated in Piraveenan et al. (2008) by calculating the contribution of each node to the above correlation coefficient. Therefore, the sum over all nodes is equal to network assortativity. Formally, local assortativity of a given node v was derived in Piraveenan et al. (2008) to be:

$$\rho_v = \frac{\alpha_v - \beta_v}{\sigma_q^2} = \frac{(j+1)(j\bar{k} - \mu_q^2)}{2M\sigma_q^2} \quad (3)$$

where j is the node's excess degree; \bar{k} is the average excess degree of its neighbours, $\sigma_q \neq 0$; the contribution α_v of the node v to the first term in (2), that is, to the sum $\sum_{jk} jke_{j,k}$ is

$$\alpha_v = (j+1) \frac{j\bar{k}}{2M} \quad (4)$$

and the contribution β_v of the node v to the second term in (2), that is, to μ_q^2 is

$$\beta_v = (j+1) \frac{\mu_q^2}{2M} \quad (5)$$

It can be shown that local assortativity satisfies the summation property:

$$r = \sum_{v=1}^N \rho_v \quad (6)$$

In particular,

$$\sum_{jk} jke_{j,k} = \sum_{v=1}^N \alpha_v \quad \text{and} \quad \mu_q^2 = \sum_{v=1}^N \beta_v \quad (7)$$

While the component α_v captures the precise contribution of each node to the term $\sum_{jk} jke_{j,k}$, the component β_v represents the contribution of each node to the term μ_q^2 with an imprecise scaling. Specifically, the scaling factor $(j+1)/2M$ in (5) is the correct scaling factor for μ_q , rather than μ_q^2 , and hence, β_v has a bias towards low-degree nodes (Piraveenan et al., 2010).

Unbiased local assortativity

The derivation of the correctly scaled (and hence, unbiased) contribution, $\hat{\beta}_v$, of a given node v to the term μ_q^2 is shown in Appendix A, yielding

$$\hat{\beta}_v = (j+1) \frac{j\mu_q}{2M} \quad (8)$$

where j is the node's excess degree, as before. Hence, the unbiased representation of local assortativity is given by

$$\hat{\rho}_v = \frac{\alpha_v - \hat{\beta}_v}{\sigma_q^2} = \frac{j(j+1)(\bar{k} - \mu_q)}{2M\sigma_q^2} \quad (9)$$

Let us compare the unbiased local assortativity $\hat{\rho}_v$ with that defined by (3). Specifically, the sign of the local assortativity (positive or negative) is determined by the difference between the average excess degree (\bar{k}) of the neighbours and the global average excess degree (μ_q). If the neighbours' average is higher, then the node is assortative. If the global average is higher, the node is disassortative. Therefore, the local assortativity can also be defined as a scaled difference between the average excess degree of the node's neighbours and the global average excess degree (the scale factor is proportional to the product of the node's degree and excess degree). In other words, a node tends to be locally assortative if it is surrounded by nodes with comparatively high degrees — hence, even though local assortativity is a property of a node, it is influenced by a node's 'locality', or neighbourhood.

The only difference between β_v defined by (5) and the unbiased $\hat{\beta}_v$ defined by (8) is that the network's mean μ_q , which is constant across nodes, is replaced by j , the node's excess degree. This means that there is a bias in the term (3) which favours low-degree nodes (with smaller j) and disfavours hubs (with larger j). In summary,

1. both the β_v proposed in Piraveenan et al. (2008) and $\hat{\beta}_v$ corrected in Piraveenan et al. (2010) adhere to summation rule $\sum \beta_v = \sum \hat{\beta}_v = \mu_q^2$.
2. $\hat{\beta}_v$ is higher for hubs and lower for low-degree nodes compared to β_v .

We will utilise average local assortativity plotted against degree. Average local assortativity $\bar{\rho}(d)$ can be calculated by averaging local assortativity quantities of all nodes with a

given degree d . For example, the difference between biased local assortativity profile $\rho(d)$ and unbiased local assortativity $\hat{\rho}(d)$ for *H. pylori* Protein Protein Interaction network is shown in the Appendix B.

We point out that local assortativity is a quantity that involves both degree and average (neighbour) degree, and as a result, the local assortativity profiles clearly differ from average degree profiles. In particular, an average degree profile always contains positive values that increase with the degree, while local assortativity profiles may contain both positive or negative values, increasing or decreasing with the degree.

Local assortativity in canonical networks

Regular lattice

For a lattice network each node has the same degree and excess degree, therefore the variance of the excess degree distribution is 0. Since there is only one type of nodes, the network is perfectly assortative ($r = 1$) and the local assortativity of all nodes is $1/N$, as shown in Figure 1.

Star network

A star graph is another extreme example of complex networks in terms of topology. In a pure star graph, any given link has a degree-one node at one end, with the excess degree zero. It can be shown that a star graph is perfectly disassortative ($r = -1$). Furthermore, any node in the star graph has either its excess degree as zero, or all of its neighbours' excess degrees as zero. It is easy to see that the term represented by equation (4) reduces to zero in all cases. Thus, the local assortativity reduces to

$$\rho = -\frac{j+1}{2M} \frac{\mu_q}{\sigma_q^2} \quad (10)$$

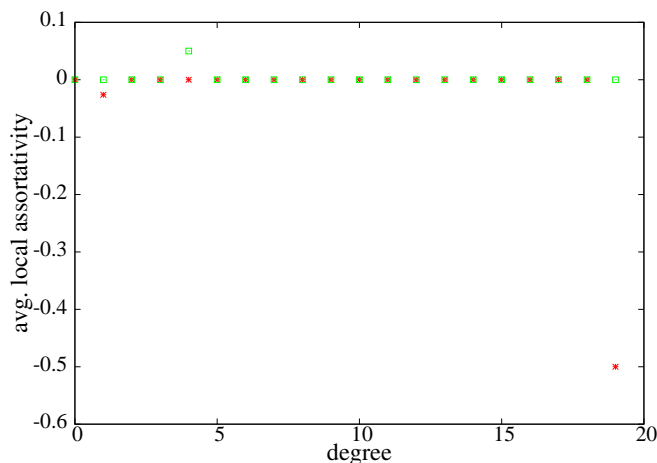


Figure 1: Local assortativity distribution, $\bar{\rho}(k)$ vs k , of a regular lattice with four nodes connecting to each node (squares), and of a star graph (stars). Network size in both cases is $N = 20$.

Figure 1 shows the local assortativity distribution for a pure star graph: the central node is much more locally-disassortative, as it connects with many dissimilar nodes, whereas the low-degree nodes are less locally-disassortative since they connect to only one dissimilar node.

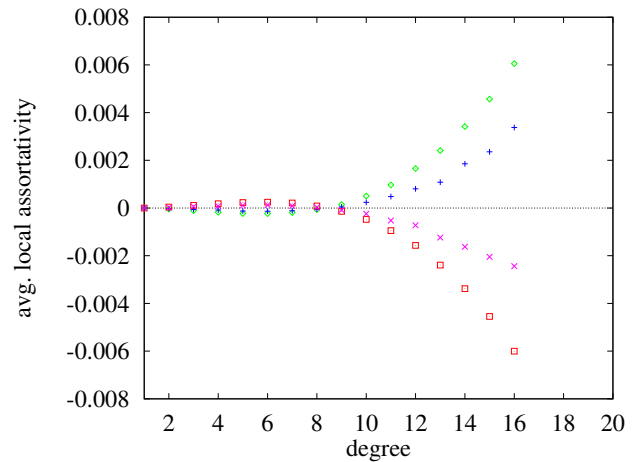


Figure 2: Local assortativity profile of scale-free networks ($N = 1000$ and $\gamma = 2.1$) with $r = 1.0$ (' \diamond '), $r = 0.5$ (' $+$ '), $r = -0.5$ (' \times ') and $r = -1.0$ (' \square ').

Classification of networks using unbiased local assortativity profiles

In this section we aim to classify both model and real-world networks using the unbiased local assortativity. Since local assortativity is a property of a node, it is possible to construct local assortativity distributions of networks (Piraveenan et al., 2008).

We begin the analysis by constructing model Barabási–Albert scale-free networks (Albert and Barabasi, 2002) of various assortativity levels and observing their local assortativity profiles. Specifically, we use the Assortative Preferential Attachment method (APA) (Piraveenan et al., 2007) to control the level of assortativity. Some of the results are shown in Figure 2 for network size $N = 1000$ and power law exponent $\gamma = 2.1$.

We could observe from Figure 2 that the profiles are symmetric with respect to the degree axis when assortativity is varied from $r = 1.0$ to $r = -1.0$ while other network parameters are kept constant. We also note that (i) globally assortative networks have assortative hubs and disassortative low-degree nodes, and (ii) globally disassortative networks have disassortative hubs and assortative low-degree nodes. That is, the overall assortativity of the network is matched by that of the hubs. Thus, we are able to classify the constructed model networks as either (i) assortative networks with assortative hubs, or (ii) disassortative networks with disassortative hubs. This is not surprising. However, one may ask whether there are also any disassortative networks with assortative hubs, as proposed in Piraveenan et al. (2008). To

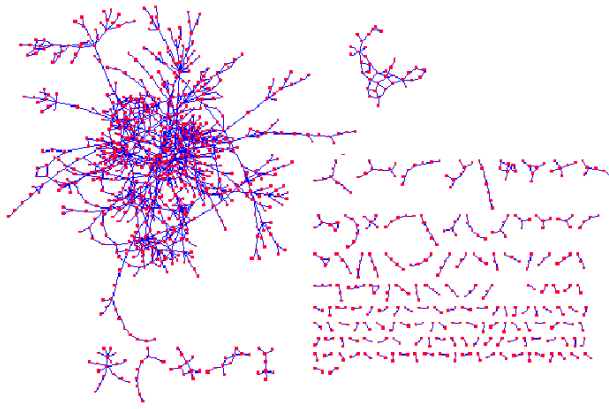


Figure 3: Example of an assortative network with assortative hubs. *H. sapiens* metabolic network; $N = 1288$, $\gamma \approx 2.32$, $r = 0.382$.

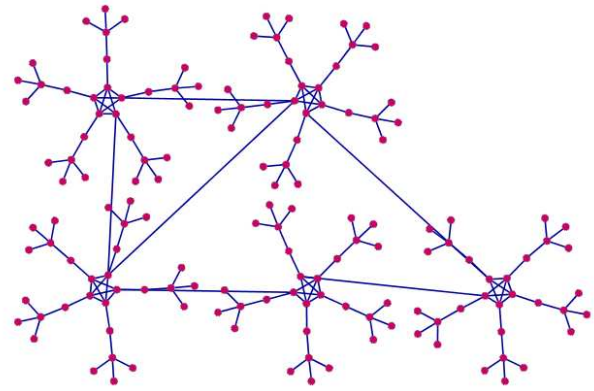


Figure 5: Example of a disassortative network with assortative hubs. A model network with $N = 150$, $r = -0.109$.

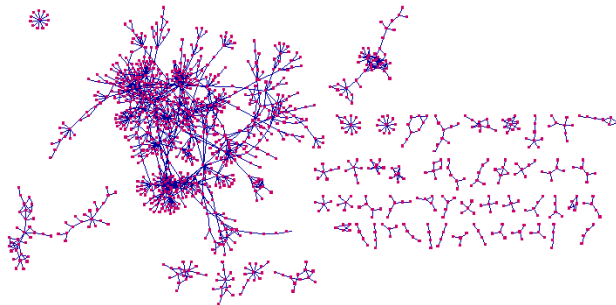


Figure 4: Example of an assortative network with disassortative hubs. *H. sapiens* Protein Protein Interaction network; $N = 1529$, $\gamma \approx 2.1$, $r = 0.075$.

answer this question, let us look at the model network given in Figure 5. This network is made up of a number of interconnected star-like subnetworks. Each subnetwork has a core of hubs that are densely connected to one another: this is the ‘rich club phenomenon’ (Zhou and Mondragón, 2004; Colizza et al., 2006). The rest of the subnetwork seems to have mostly disassortative connections. The subnetworks are then linked together with hub-to-hub connections, further reinforcing the rich-club phenomenon. The overall assortativity of the network is $r = -0.109$. However, as shown in Figure 9, the hubs are assortative. The embedded subnetworks pattern can be repeated on larger scales, retaining the assortative hubs with higher and higher degrees, while keeping the overall disassortativity. This example represents a third class, demonstrating that it is possible to have disassortative networks with assortative hubs.

The real-world networks we studied included most recent metabolic networks (KEGG database), citation networks, Protein-Protein Interaction (PPI) networks, food-webs, and Internet AS level networks among others. A list of the networks we analysed is shown in Table 1. We were able to

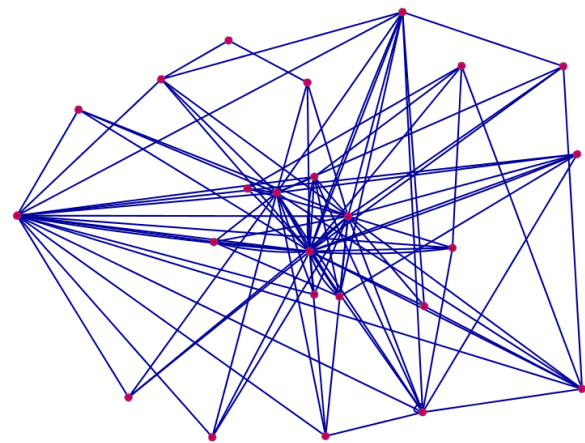


Figure 6: Example of a disassortative network with disassortative hubs. Crystal River D foodweb, $N = 24$, $r = -0.467$.

observe the following from our analysis.

Firstly, as in the case of model APA networks, some real-world assortative networks have assortative hubs (e.g., Figure 7; most other metabolic networks showed similar profiles). Also many real-world disassortative networks have disassortative hubs, e.g., one such food-web is shown in Figure 10. However, other assortative networks exhibit disassortative hubs, such as the PPI networks of *H. sapiens* shown in Figure 8. A number of other PPI networks displayed a similar profile. These networks represent the fourth class, namely the assortative networks with disassortative hubs.

Therefore, we can identify four classes of complex networks, namely: (i) assortative networks with assortative hubs, (ii) assortative networks with disassortative hubs, (iii) disassortative networks with disassortative hubs, (iv) disassortative networks with assortative hubs.

There are several examples of real-world networks for each of the first three cases, and we have shown representative examples in Figures 7, 8, and 10 respectively. We did

Network	assortativity r	class
Human metabolic (KEG, 2009)	0.382	assortative with assortative hubs
Chimpanzee metabolic (KEG, 2009)	0.398	assortative with assortative hubs
Rhesus monkey metabolic (KEG, 2009)	0.363	assortative with assortative hubs
Astro physics citation (Newman, 2009)	0.276	assortative with assortative hubs
Cond. mat. 2003 citation (Newman, 2009)	0.178	assortative with assortative hubs
Cond. mat. 2005 citation (Newman, 2009)	0.186	assortative with assortative hubs
Hep theory citation (Newman, 2009)	0.293	assortative with disassortative hubs
Net science citation (Newman, 2009)	0.46	assortative with disassortative hubs
H. sapiens PPI (PPI, 2009)	0.075	assortative with disassortative hubs
E. coli PPI (PPI, 2009)	0.056	assortative with disassortative hubs
Internet AS 1998 (CAI, 2009)	-0.198	disassortative with disassortative hubs
Internet AS 2008 (CAI, 2009)	-0.198	disassortative with disassortative hubs
Fruitfly PPI (PPI, 2009)	-0.21	disassortative with disassortative hubs
H. pylori PPI (PPI, 2009)	-0.235	disassortative with disassortative hubs
Mouse PPI (PPI, 2009)	-0.057	disassortative with disassortative hubs
Crystal River C (Batagelj and Mrvar, 2006)	-0.334	disassortative with disassortative hubs
Crystal River D (Batagelj and Mrvar, 2006)	-0.467	disassortative with disassortative hubs
Lower Chesapeake (Batagelj and Mrvar, 2006)	-0.391	disassortative with disassortative hubs
Scimet collaboration (Batagelj and Mrvar, 2006)	-0.03	disassortative with disassortative hubs
Smart grid collaboration (Batagelj and Mrvar, 2006)	-0.193	disassortative with disassortative hubs

Table 1: The networks studied and their classification.

not find any example of the fourth case among the networks we studied, however we have demonstrated that in theory such networks could exist, as shown in the profile in Figure 9, and real-world examples may yet be found as the range of networks studied is expanded.

We show the corresponding networks for each example in Figures 3, 4, 5, and 6 respectively. Note that the networks with assortative hubs and disassortative hubs are not always visually distinguishable, however, the local assortativity profiles are able to highlight an important topological difference in them.

While a detailed analysis of the classification results in the context of biological networks is out of scope for the paper, we briefly mention some possibilities. Assortative metabolic networks may have assortative hubs due to optimality in flux balance (Varma and Palsson, 1994): most metabolic reactions form chains ending with a regulatory decision in a hub, and the connections between hubs may optimise metabolic requirements for growth, utilising different pathways.

The hubs in food-webs could be disassortative because the separation between hubs plays an evolutionary role, maintaining sustainable food chains.

It is somewhat more complicated why the PPI networks that are assortative overall have disassortative hubs. On the one hand, many individual proteins may form a multi-

protein complex, and some of the proteins can participate in the formation of a variety of different protein complexes. Such high-interacting proteins are likely to be locally assortative. On the other hand, the anticorrelation in the node degree of connected nodes, i.e., the tendency of highly interacting nodes to be connected to low-interacting ones, has been reported previously (Maslov and Sneppen, 2002; Spirin and Mirny, 2003). In particular, Maslov and Sneppen argued that “this effect decreases the likelihood of cross talk between different functional modules of the cell and increases the overall robustness of a network by localizing effects of deleterious perturbations” (Maslov and Sneppen, 2002). These two alternatives are related to the distinction between protein complexes and functional modules (Spirin and Mirny, 2003): protein complexes are groups of proteins that interact with each other at the same time and place, forming a single multimolecular machine, while functional modules consist of proteins that participate in a particular cellular process while binding each other at a different time and place. Disassortative hubs are likely to be the proteins within functional modules. In addition, one may point out that there are artefacts of the high-throughput methods used to discover the interactions that may lead to low interaction coverage of certain protein types and obscure local assortativity profiles (Shoemaker and Panchenko, 2007a,b).

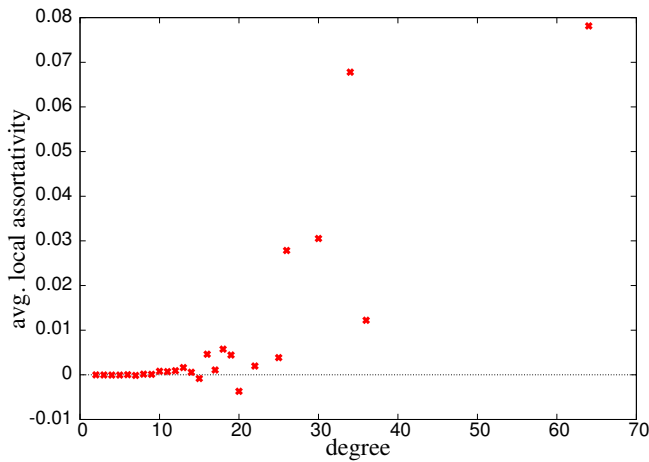


Figure 7: Local assortativity profile of *H. sapiens* metabolic network; $N = 1288$, $\gamma \approx 2.32$, $r = 0.382$.

Conclusions

We proposed an unbiased formulation for local assortativity in complex networks, and analysed the local assortativity profiles of some model and real-world networks in terms of this new formulation. We showed that a node's local assortativity is proportional to the difference between the average excess degree of its neighbours and the network's overall average excess degree. Specifically, a node is locally assortative if its neighbours have comparatively (i.e., compared with all nodes in the network) higher degrees. It is important to realise that the nodes with the highest local assortativity differ in general from the largest hubs (the nodes with the highest degrees).

Analyzing a range of model and real-world networks, we observed four classes of networks, namely: (i) assortative networks with assortative hubs, (ii) assortative networks with disassortative hubs, (iii) disassortative networks with disassortative hubs, and (iv) disassortative networks with assortative hubs. Real-world examples for the first three classes were identified, and a model network was constructed as an example for the fourth class.

The local assortativity profiles provide an additional quantitative tool for network analysis. These profiles highlight important topological differences in otherwise seemingly indistinguishable networks. This may help in studying diverse network properties and dynamics: e.g., (a) network growth may be modelled in such a way that the grown networks not only satisfy global characteristics, but also agree with required local assortativity profiles (Piraveenan et al., 2009b); (b) network robustness may be analysed in terms of an attack targeting the nodes with higher local assortativity; (c) motifs within networks can be studied via their average local assortativity, etc. One avenue for future work is to define local assortativity in directed networks, and apply this definition to directed biological networks, studying the role of the nodes with the highest local assortativity in regulatory processes (e.g., reaction cascades).

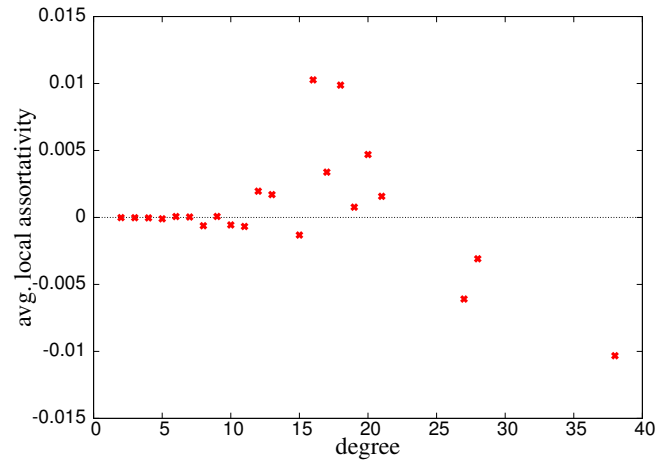


Figure 8: Local assortativity profile of *H. sapiens* Protein-Protein Interaction network; $N = 1529$, $\gamma \approx 2.1$, $r = 0.075$.

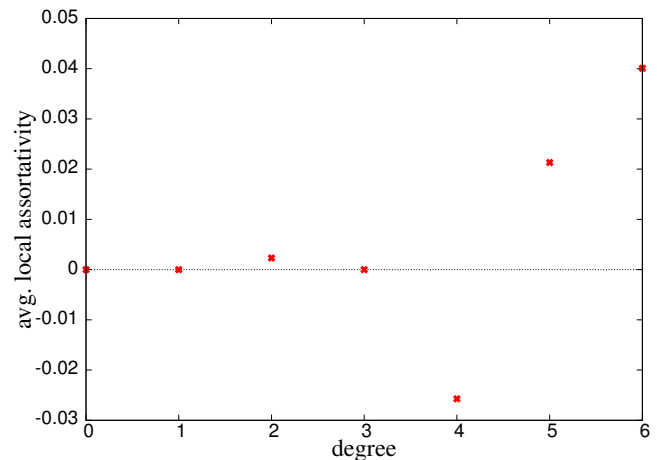


Figure 9: Local assortativity profile of the network shown in Figure 5; $N = 150$, $r = -0.109$.

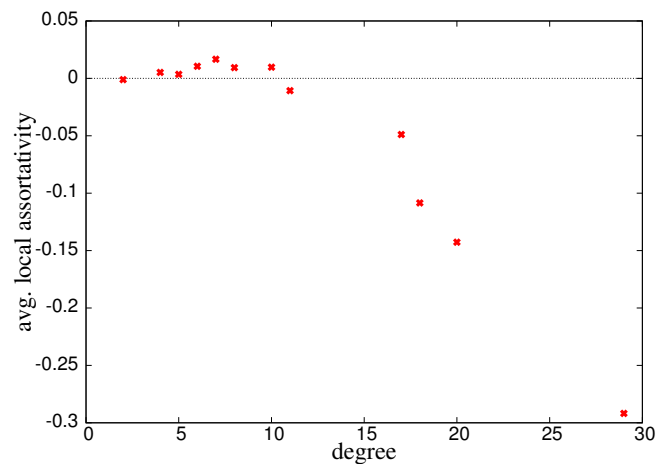


Figure 10: Local assortativity profile Chrystal River D food-web; $N = 24$, $r = -0.467$.

Acknowledgements

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Appendix A

To derive the contribution of each node to μ_q^2 we first look at the following equivalent definitions of μ_q :

$$\mu_q = \frac{1}{2M} \sum_{m=1}^M k_m \quad (11)$$

$$\mu_q = \frac{1}{2M} \sum_{v=1}^N k_v (1 + k_v) \quad (12)$$

where k is excess degree, m is a given edge and v is a given node of the network. We are especially interested in the latter form (12) since it makes it obvious what each node contributes to the term μ_q . It follows that

$$\mu_q = \frac{1}{2M} \left(\sum_{v=1}^N k_v + \sum_{v=1}^N k_v^2 \right) \quad (13)$$

yielding

$$\mu_q^2 = \frac{1}{4M^2} \left(\left(\sum_{v=1}^N k_v \right)^2 + \left(\sum_{v=1}^N k_v^2 \right)^2 + 2 \sum_{v=1}^N k_v \sum_{v=1}^N k_v^2 \right) \quad (14)$$

Now, let us consider a single node (without loss of generality, let it be the node 1 with excess degree k_1), and its contribution to each of the three summation terms in the expression above. Considering the first summation term, excess degree k_1 contributes to it as follows:

$$k_1^2 + 2(k_1 k_2 + k_1 k_3 + \dots + k_1 k_N) \quad (15)$$

Among these, terms such as $2k_1 k_j$ have to be ‘divided’ between node 1 and node j respectively. These are multiplication terms, and we assume that an equal division is appropriate. Therefore, the contribution of node 1 is:

$$k_1^2 + (k_1 k_2 + k_1 k_3 + \dots + k_1 k_N) = k_1 \sum_{j=1}^N k_j \quad (16)$$

Considering the second summation term in (14), we observe that the contribution of node 1 is $k_1^2 \sum_{j=1}^N k_j^2$. Let us analyse the contribution of node 1 to the third summation term in (14). The third summation term is given by

$$2 \sum_{i=1}^N k_i \sum_{j=1}^N k_j^2 = 2 \left(k_1 + \sum_{i=2}^N k_i \right) \left(k_1^2 + \sum_{j=2}^N k_j^2 \right) \quad (17)$$

where i, j are node indices. The contribution of node 1 to the third term is obtained by dividing terms such as $2k_1 k_j$ between node 1 and node j respectively:

$$2k_1^3 + k_1^2 \sum_{i=2}^N k_i + k_1 \sum_{j=2}^N k_j^2 = k_1 \sum_{j=1}^N k_j^2 + k_1^2 \sum_{j=1}^N k_j \quad (18)$$

Therefore, the total contribution of node 1, β_1 , to μ_q^2 is:

$$\beta_1 = \frac{k_1 \sum_{j=1}^N k_j + k_1^2 \sum_{j=1}^N k_j^2 + k_1 \sum_{j=1}^N k_j^2 + k_1^2 \sum_{j=1}^N k_j}{4M^2} \quad (19)$$

This can be further regrouped as

$$\beta_1 = \frac{k_1 + k_1^2}{4M^2} \left(\sum_{j=1}^N k_j + \sum_{j=1}^N k_j^2 \right) \quad (20)$$

Using equation (13) for μ_q , this can be reduced to:

$$\beta_1 = \frac{k_1 + k_1^2}{2M} \mu_q \quad (21)$$

Hence, the contribution of a node v to μ_q^2 is given by:

$$\hat{\beta}_v = (j + 1) \frac{j \mu_q}{2M} \quad (22)$$

where j is the excess degree of the node v . Thus, local assortativity is given by

$$\hat{\rho}_v = \frac{\alpha_v - \hat{\beta}_v}{\sigma_q^2} = \frac{j(j+1)(\bar{k} - \mu_q)}{2M\sigma_q^2} \quad (23)$$

Appendix B

The difference between the biased local assortativity profile $\rho(d)$, defined by (3), and the unbiased local assortativity $\hat{\rho}(d)$, defined by (9), for H. pylori Protein Protein Interaction network is shown in Figure 11. It is evident that $\hat{\rho}(d) < \rho(d)$ for the hubs, and more importantly, the hubs are now locally disassortative.

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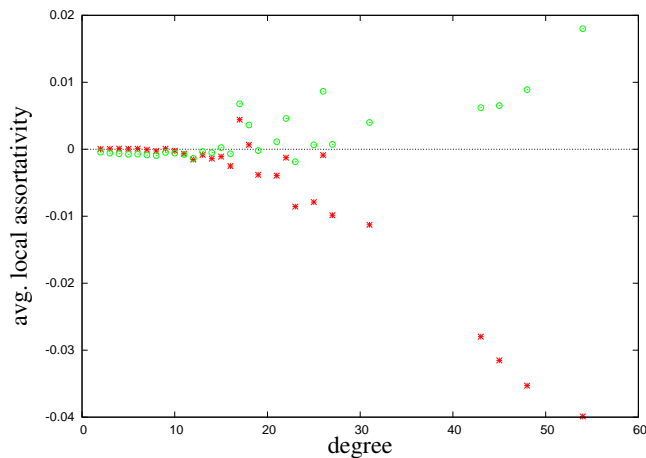


Figure 11: *H. pylori* Protein Protein Interaction network. Local assortativity profiles ρ ('o') and $\hat{\rho}$ (*); $N = 714$, $\gamma \approx 2.54$, $r = -0.235$.

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