

Why do Motifs Occur in Engineering Systems?

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Abstract Recent years have witnessed new research interest in the study of complex systems architectures, in domains like biological systems, social networks etc. These developments have opened up possibility of investigating architectures of complex engineering systems on similar lines. Architecture of a system can be abstracted as a graph, wherein the nodes/vertices correspond to components and edges correspond to interconnections between them. Graphs representing system architecture have revealed motifs or patterns. Motifs are recurring patterns of 3-noded (or 4, 5 etc.) sub-graphs of the graph. Complex biological and social networks have shown the presence of some triad motifs far in excess (or short) of their expected values in random networks. Some of these over(under) represented motifs have explained the basic functionality of systems, e.g. in sensory transcription networks of biology overrepresented motifs are shown to perform signal processing tasks. This suggests purposeful, selective retention of these motifs in the studied biological systems. Engineering systems also display over(under) represented motifs. Unlike biological and social networks, engineering systems are designed by humans and offer opportunity for investigation based on known design rules. We show that over(under) represented motifs in engineering systems are not purposefully retained/avoided to perform functions but are a natural consequence of design by decomposition. We also show that biological and social networks also display signs of synthesis by decomposition. This opens up interesting opportunity to investigate these systems through their observed decomposition.

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1 Introduction

This section gives an introduction to the field of our research and an overview of insights proposed in this paper.

1.1 *Complex Systems Architecture*

Recent years have witnessed a growing interest in the study of complex systems architectures, in domains like biological systems and social networks [1]. Unifying principles have emerged [2]. Literature has commented on the hesitation of researchers in complex engineering systems, to look at their problems, in the light of emerging ideas in complex systems in general. “Engineering should be at the centre of these developments, and contribute to the development of new theory and tools” [3]; “Engineers seem a little bit indifferent as if engineering is at the edge of the science of complexity” [4].

Architecture is the fundamental structure of components of a system—the roles they play, and how they are related to each other and to their environment [5]. A layman definition of complexity refers to interconnected/interwoven components. Complexity of a system scales with the number of components, number of interactions, complexities of the components and complexities of interactions [6]. Complex engineering systems are synthesized from a large number of components coupled to each other, giving them a physical architecture. Architecture of a system (from any domain—say engineering, biology, sociology) can be abstracted as a network/graph, where the nodes/vertices correspond to components in the system and edges correspond to interconnection between them.

1.2 *Literature Survey*

In biology, over-represented motifs have led to interesting insights in the areas of protein–protein interaction prediction [7, 8]. For instance, in sensory transcription (protein–protein interaction) networks of biology the over-represented motif has been theoretically and experimentally shown to perform signal-processing tasks. This has led to the belief that over-represented motifs are simple building blocks of complex networks and can help understand the basic functionality of a system [7]. Importance of ideas related to motifs has recently become research interest in other domains.

Incremental ideas related to motifs have also been proposed in recent literature. Paulino et al. [9] proposed a different type of motif named ‘chain of motifs’ (that is, sequence of connected nodes with degree 2). They divided chains into

subdivisions named cords, rings etc. depending on the type of their extremities (e.g. open or connected). The main difference between these chain motifs and the motifs by Milo et al. [7] is that the former may involve a large number of vertices and edges. They calculated the statistics of chain of motifs for few biological networks and reported the appearance of chain motifs in these networks [9].

Milo et al. [10] proposed an approach to study similarity in the structure of networks based on the Motif Significance Profile (MSP) of their graphs. These profiles are seen to be highly correlated across systems of the same family (i.e., MSPs for all systems of same type are highly correlated, e.g. Sensory transcription network of *E. coli* and Yeast of Biology family are highly correlated). Due to the distinct motif signature indicated by systems, motif significance profile signatures have also been proposed as a classifier for systems [11]. In this paper, we proceed to investigate motifs and possible reasons for its occurrence in engineering systems [12].

1.3 New Insights

Unlike biological and social networks, engineering systems are designed by humans and offer opportunity for investigation based on known design rules. We show that over(under) represented motifs in engineering systems are not purposefully retained/avoided to perform functions but are a natural consequence of design by decomposition. We also show that biological and social networks also display signs of synthesis by decomposition.

2 Theoretical Background About Motifs

“Motifs are recurring sub-graphs of interactions from which the networks are built” [7]. If a graph/network representing a system has N nodes there are NC_3 3-node ‘triads’ in it. Some of these triads need not be connected and the rest that are connected are sub-graphs of the graph. Each 3-node sub-graph will correspond to one of 13 possible motifs (Fig. 1).

Each of the NC_3 triplets, if a sub-graph, will assume the pattern of one of the 13 motifs and one can count the occurrence of each motif in a graph and define a vector, of size 13 $n = \{n_i, i = 1 \text{ to } 13\}$. In a network, the count for a particular motif may be high, which by itself is not considered important. It is possible that such high count for that motif is unavoidable for a network synthesized using the N nodes that preserve the degree distribution of the real network. To investigate this, randomized networks are created [7] using same N nodes, i.e., the number of nodes and their degree distribution is preserved. A large number of randomized networks ($i = 1$ to m) will define a vector of means, $\mu = \{\mu_i, i = 1 \text{ to } 13\}$ and a vector of standard deviations of motif counts, $\sigma = \{\sigma_i, i = 1 \text{ to } 13\}$. For the real network one can check the motif significance profile (MSP) of all the 13 motifs by a vector $Z = \{Z_i, i = 1 \text{ to } 13\}$

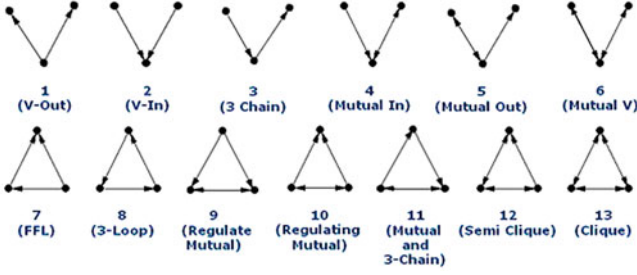


Fig. 1 All 13 patterns (motifs) for 3 node sub-graphs. The numbers are motif-ids and within brackets are nomenclature

$$[Z = (n_i - \mu_i) / \sigma_i \quad \text{for } i = 1 \text{ to } 13] \quad (1)$$

In simple words, Motif Significance Profile (MSP) is the vector (of size 13 for 3-node motifs) of the extent of over(under)-representation of all 13 motifs in a system. For a normally distributed random number, $-3 \leq Z_i \leq 3$ implies a rare occurrence (beyond $\pm 3\sigma$ limit). Any motif with its $Z_i > 2$ is considered an over-represented motif and any motif with its $Z_i < -2$ is an under-represented motif [7].

Milo et al. [10] argue that Z is influenced by the size of the network and propose normalisation of Z to make it largely independent of network size. Thus, the normalised significance profile vector, W is defined as $W = \{W_i, i = 1 \text{ to } 13\}$ where $W_i = Z_i / |Z|$.

3 Motifs in Engineering Systems

This section gives an introduction to the field of our research and an overview of insights proposed in this paper.

3.1 Details of Systems

We have gathered architecture data for more than 100 diverse engineering systems ranging from mechanical, software and electronic circuits. In this paper we consider 38 arbitrarily chosen systems from literature and study their architectures. Systems considered range from aircraft engine [13], softwares [14], electronic circuits [15, 16], robot [17], refrigerator [18], bacteria *E. coli* [19], yeast *S. cerevisiae* [19], language networks [19]. These 38 systems are of vastly different sizes (ranging from minimum 16 components to maximum 23,843 components). We extracted architecture data from these datasets by developing some tools for parsing/filtering from the raw data. Table 1 briefly identifies each of the 38 systems for the data.

Table 1 38 systems considered for study

S.no	System name	Nodes	S.no	System name	Nodes
1	Digital fractional multiplier (s208)	122	20	Traffic control system (s400)	186
2	Digital fractional multiplier (s420)	252	21	PLD (s820)	312
3	Digital fractional multiplier (s838)	512	22	Traffic control system (s382)	182
4	<i>E.coli</i>	423	23	ALU (74181)	87
5	Yeast	688	24	PLD (s832)	310
6	Apword	1,096	25	ECAT (c499)	243
7	Linux	5,420	26	ALU (c880)	443
8	Mysql	1501	27	ALU (c7552)	3,718
9	Vtk	778	28	PLD (s641)	433
10	Xmms	1,097	29	ECAT (c1908)	913
11	Traffic control system (s444)	205	30	ALU (c3540)	1,719
12	PLD (s713)	447	31	Traffic control system (s562)	217
13	ALU (c2670)	1,350	32	Aircraft Engine	54
14	ECAT (c1355)	1,355	33	Refrigerator	16
15	Forward logic chips (s9234)	5,844	34	Robot	28
16	Forward logic chips (s13207)	8,651	35	English	7,724
17	Forward logic chips (s15850)	10,383	36	French	9,424
18	Forward logic chips (s38417)	23,843	37	Japanese	3,177
19	Forward logic chips (s38584)	20,717	38	Spanish	12,642

In electronic circuits, nodes represent component gates and edges represent the flow of digital signals between gates. In case of software systems, nodes represent classes and edges represent directed collaboration relationships between classes. In mechanical systems, nodes represent physical components and edges represent exchange of energy, material or signal between components. In case of biological systems, nodes represent genes and edges represent direct transcription interactions. In case of languages, each word in a passage is a node and each edge represents word adjacency in the passage.

3.2 Motif Experiment and Results

We create 1,000 random networks for each considered system using same N nodes, i.e. number of nodes and their degree distribution is preserved (we have proposed a method named ‘switching method’ for doing this. The details of this method along with its comparison with existing method from literature are archived in our website [20]). We estimate the μ and σ of motifs of these random networks based on 1,000 random networks. For 10 arbitrarily chosen systems we create 10,000 and then 1,00,000 random networks to confirm that μ and σ of motifs counts based on 1,000 random cases are converged values. The further observations and analysis made in this paper is based on 1,000 random networks for each system.

For each real network we compute the significance of each of the 13 motifs of 3-noded sub-graphs, $Z_i = (n_i - \mu_i) / \sigma_i$ for $i = 1$ to 13. For example, the digital fractional multiplier s838 has $n = [860, 1100, 0, 401, 0, 0, 0, 0, 40, 0, 0, 0, 0]$, $\mu = [856.9, 1213.7, 0, 397.9, 3.1, 0, 0, 0, 1.1, 0, 0, 0, 0]$, $\sigma = [1.8, 3.6, 0, 1.8, 1.8, 0, 0, 0, 1, 0, 0, 0, 0]$ and therefore $Z = [1.72, -31.89, 0, 1.72, -1.72, 0, 0, 0, 37.1, 0, 0, 0, 0]$. One shall note the under-representation of motif id 2 and the over-representation of motif id 9 in the above example. We found all the systems that we studied had some or the other motif over-represented or under-represented. Z vectors are in fact computed for 3-noded, 4-noded and 5-noded sub-graphs. The results of 3-noded are available at [21] and the results of 4-noded, 5-noded are available at our website [20]. (It may be noted that the size of Z vector for 4-noded is 199 and for 5-noded is 9,364). Further study in this paper is restricted to 3-noded sub-graphs only.

3.3 What Causes Over(Under)-Represented Motifs?

All systems studied, including engineering systems, display over(under)-represented motifs; i.e., counts of some motifs in the real system are far in excess or short of their expected counts (beyond $+3\sigma$) in random graphs created using the same nodes. Such motif counts represent highly improbable events. In naturally evolving biological or social systems such motif presence can be attributed to deliberate retention to create useful functionality. But engineering systems are designed and the design process does not address functionality through motifs. So, why do over(under)-represented motifs appear in engineering systems?

4 What Causes Over-Represented Motifs

Engineering systems are designed by humans and offer opportunity for investigation based on known design rules. All engineering systems display over (under) represented motifs and they are rare events as per accepted interpretations. If designers of engineering systems explicitly retain/avoid motifs for the purpose of meeting system design requirements or system design objective, the rarity would have got explained. But we know these motifs are not retained/avoided by designers for any specific purpose. This prompts us to look for an interpretation that renders the motifs counts in a system as probable events. Thus we look for design rules that are responsible for the motifs counts in engineering systems. The motif counts when viewed without regard to those design rules will appear as rare events, but when viewed with regard to those design rules will appear as probable events. Artzy-Randrup et al. [20, 23] have argued that motifs can arise by various mechanisms other than evolutionary selection for function and highlighted for the first time that a rule in synthesis can influence motif counts in a system. They

showed that a rule like “the probability of preferential connection to other nodes falling off with the physical distance between nodes” can explain the over-represented motif in neural-connectivity map of a nematode *Caenorhabditis elegans*. But that design rule was unable to reproduce the full motif significance profiles [7].

One major design rule in complex engineering systems is ‘design by decomposition’ that is invoked to conquer complexity. System is decomposed into sub-systems (and recursively so for very complex systems) such that nodes within each sub-system are densely inter-connected and nodes from across sub-systems are sparsely inter-connected. We investigate impact of design by decomposition on motif counts in engineering systems. Consider an arbitrarily chosen engineering system—digital fractional multiplier s832 [16]. It has $N = 512$ nodes with each node having specific in-degree and out-degree and has a motif count vector of n , i.e. $n = n_i$, $i = 1$ to 13 is the count of 13 motifs in s832. We first study expected motif counts, of random graphs synthesized monolithically, i.e. without decomposition, from these 512 nodes. This is referred to as single cluster configuration and designated by $c = 1$. Large number of such randomized graphs are created by inter-connecting all node pairs such that the degree distribution of nodes and the count of 2 node sub-graphs as in the real network are retained in the random graphs. A vector of means of motif counts, $\mu_1 = \mu_{1,i}$ where $i = 1$ to 13 and a vector of standard deviations, $\sigma_1 = \sigma_{1,i}$ where $i = 1$ to 13 are defined. Here the subscript 1 of μ and σ refers to $c = 1$. The motif significance profile (MSP) vector [10] which we have defined in Sect. 2 as, $Z_1 = (n - \mu_1)/\sigma_1$ is computed. Some elements of Z_1 have values outside of ± 3 (From the picture (1) of Fig. 2 it can be seen that $Z_{1,2} < -3$ is under-represented and $Z_{1,9} > +3$ is over-represented). With regard to these over(under) represented motifs we can take a stand that a rare event is being witnessed. But such a stand becomes not justifiable when similar rare events are witnessed for all systems. So we take the alternate stand, that the event witnessed does not belong to configuration $c = 1$ and proceed to investigate other configurations.

We then create two cluster configurations out of same 512 nodes to represent two sub-systems. Each cluster has roughly $N/2 = 256$ nodes. We create large number of random graphs by inter-connecting edges of node pairs within a cluster with higher probability ($p = 0.9$) than node pairs across clusters ($p = 0.1$) along with preserving degree distribution of nodes and the count of 2 node sub-graphs as in the real network. Vector of means of motif count, μ_2 and vector of standard deviations, σ_2 are estimated. We now define MSP as $Z_2 = (n - \mu_2)/\sigma_2$ for this

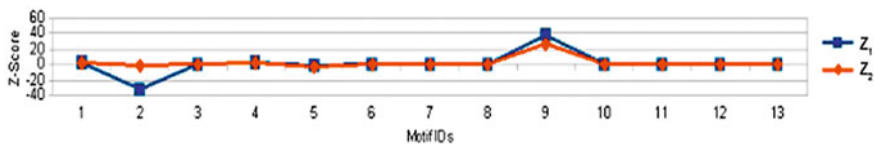


Fig. 2 MSP for Z_1 and Z_2 of digital fractional multiplier s832

$c = 2$ configuration. Motif significance profile vector Z_2 for clustered case (configuration $c = 2$) is significantly different from Z_1 (configuration $c = 1$). Motif id 2 ceases to be under-represented, while motif id 9 is continues to be over-represented whilst all other motif ids continue to be near zero. We similarly study cluster numbers $c = 3, 4, 5$, etc. and observe a clear dependence of motif significance profile vector, Z_c to clustering.

Let us assume that the real system is synthesized by the designer with k sub-systems. Since k for the s832 system is not known we use the following approach: We first use Walktrap Community Detection algorithm by Pons and Latapy [23] to find the best possible sub-systems grouping for a given k , from $k = 1$ to $k = N$. In order to choose the best k out of this, we use the system modularity index proposed by Newman and Girvan [24]. The modularity index calculates how modular is a given division of a graph into subgraphs. The system modularity index for clusters $k = 1$ to $k = N$ is computed and shown in Fig. 3.

When $k = 1$ all nodes are in one subsystem and have same probability to be connected to each other. When $k = N$ each node is a separate cluster and has same probability to get connected to each other node. The similarity of modularity index for $k = 1$ and $k = N$ is explained. Modularity index is highest for $k = 38$ suggesting that s832 is designed with $k = 38$ sub-systems. We show MSP for $k = 38$ as $Z_{38} = (n - \mu_{38})/\sigma_{38}$, in comparison with Z_1 in the Fig. 4. Z_{38} has no over(under)-represented motifs and hence no rare events.

We now repeat the process for aircraft engine [25] for which $N = 54$. The number of clusters present is discovered as $k = 5$ (Fig. 5).

Sosa et al. [25] have reported the number of modular sub-systems in aircraft engines as 6, which is close to what we discover here. Z_1 and Z_5 are computed for aircraft engine and compared in the Fig. 6. It can be seen that extent of over(under)-represented motifs in Z_5 as reduced significantly compared to Z_1 . We have repeated this exercise for other engineering systems to confirm the above

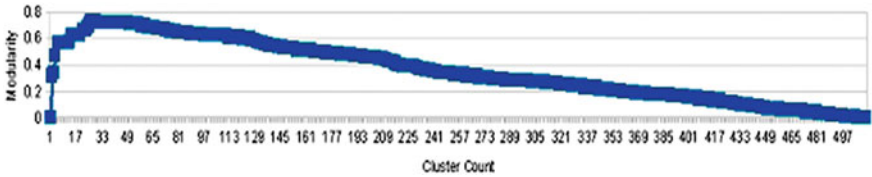


Fig. 3 System modularity index for various clusters sizes of s832

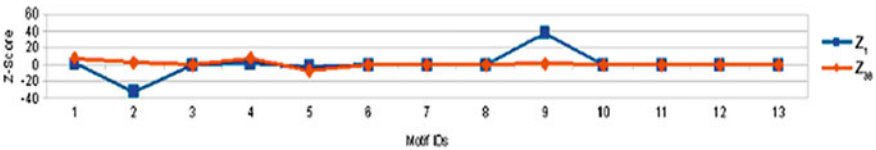


Fig. 4 MSP for Z_1 and Z_k (here $k = 38$) of digital fractional multiplier s832

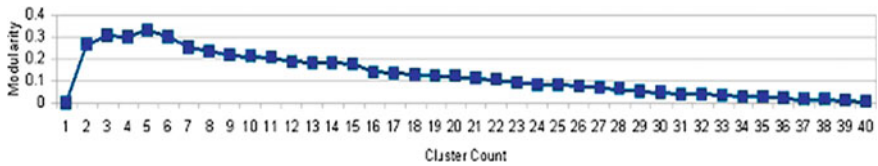


Fig. 5 System modularity index for aircraft engine [12] peaks at $k = 5$

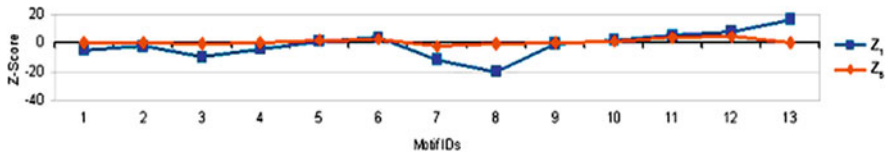


Fig. 6 MSP for Z_1 and Z_k (here $k = 5$) of aircraft engine

observation (the results are archived in our website [20]). We conclude that over(under) represented motifs observed are merely an outcome of comparing motif counts in a real system synthesized by decomposition to mean motif counts of random networks synthesized monolithically. Over(under) represented motifs do not show up if motif counts in the real system are compared to mean motif counts of random networks synthesized by decomposition. Randomization does not try to mimic exact nodes that go into each cluster or even exact number of nodes in each cluster, but has roughly equal number of nodes randomly picked in each cluster. But such randomization still shows remarkable likeness in motif count to real system.

5 Impact of Our Observations on Biological and Social Networks

Engineering systems are invariably designed through decompositions and it is evident that observed motif counts are a natural consequence of design by decomposition. With this backdrop of understanding for engineering system we now investigate biological systems and social networks.

We first investigate *E. coli* [19] for clustering and discover that it is not a connected graph and actually a collection of 28 sub-graphs not connected to each other. We investigate this collection of 28 sub-graphs to discover 49 subgraphs¹ (Fig. 7). We estimate Z_k for $k = 28$ and 49 and compare it with Z_1 (Fig. 8) and find a reduction in the extent of over(under) representation of the significant

¹ Out of the 28 sub-graphs, the big enough ones are decomposed further to discover 49 sub-graphs.

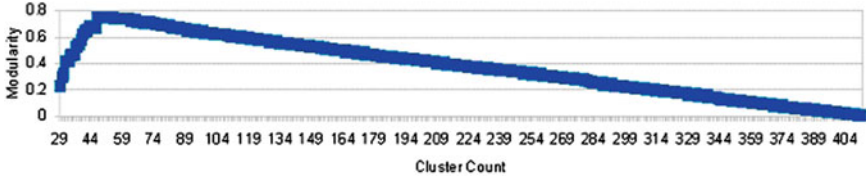


Fig. 7 System modularity index for *E. coli* [19] peaks at $k = 49$

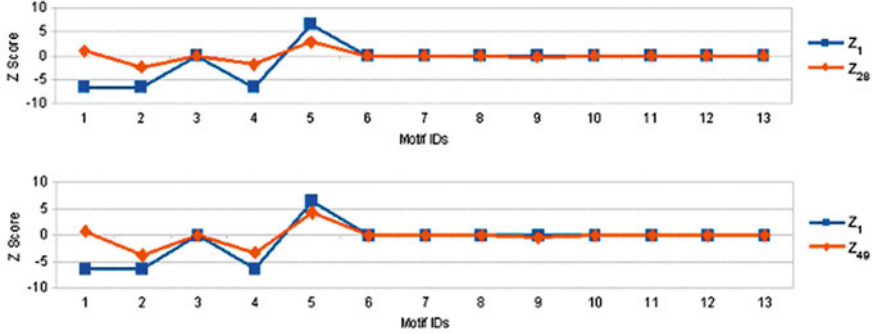


Fig. 8 MSP for Z_1 and Z_k (here $k = 28, k = 49$) of *E. coli*

motifs, though the reduction is not as dramatic as in engineering systems. There could be other rules apart from clustering that are present in these systems that may further reduce the extent of over(under) representation.

It is not clear why a bio-logical system must have sub-systems (clusters). Previous researchers have studied the role of over-represented motifs in a bio-logical system. We feel it could be more revealing to investigate role of clustering. What function do clusters of specific nodes with dense interconnections perform in biological system may lead to interesting and useful findings.

We finally investigate a social network, representing games played between American (NCAA) college football teams during the year 2000. Radicchi et al. [26] have reported the number of modular teams in football system under study as 9, which is same as what we discover here $k = 9$ (Fig. 9). We estimated Z_9 and compared it with Z_1 (Fig. 10). It can be seen that extent of over(under)-represented motifs in Z_9 has reduced significantly (almost close to zero indicating no rare

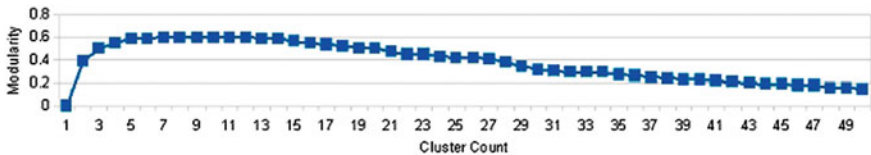


Fig. 9 System modularity index for football [20] peaks at $k = 9$

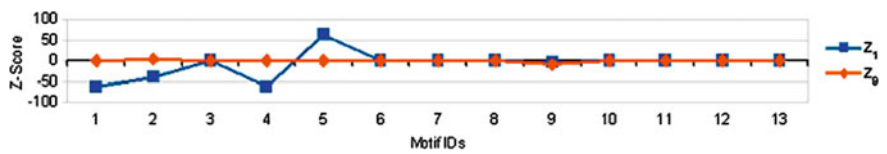


Fig. 10 MSP for Z_1 and Z_2 (here $k = 9$) of football

events) compared to Z_1 . This again implies that over(under) represented motifs observed are merely an outcome of comparing motif counts in a real system synthesized by decomposition to mean motif counts of random networks synthesized monolithically.

6 Computational Aspects

All the code that we have developed as part of this research as a software framework named CASMot. Some computational aspects about this framework are mentioned in Table 2.

Table 2 Computational aspects related to CASMot

<i>Features</i>	
Functionalities supported by CASMot framework	Automated scripts to convert raw domain specific data to network, discover over(under)-represented motifs, create MSP, Create CCP, perform decomposition Analysis.
<i>Software</i>	
Operating system	Debian Linux with kernel version 2.6
Programming language	Statistical R, Erlang, Bash shell scripting
Lines of code	48539
Main software paradigm	Functional programming using map-reduce architecture
<i>Hardware</i>	
CPU1	Eight core CPU 2 nos with a processing speed of 1.5 GHz
CPU2	Dual core CPU 5 nos with a processing speed of 1.5 GHz
RAM1	2 GB in the dual core machines
RAM2	16 GB in the eight core machines
Hard disc	80 GB in the dual core machines 500 GB in the eight core Machines
<i>Computational effort</i>	
After harnessing the computing capacity of both the hardware computational effort to run motif experiments	Computations required to generate MSPs of the 38 systems took roughly 850 h (approximately 35 days)

The reader is requested and encouraged to refer to our webpage [20] for the algorithms used for producing clustered random graphs, how to use our distributed software framework named CASMot for doing motif experiments etc.

7 Conclusion

Ideas related to complex system architectures may give insight into previously complex and poorly understood phenomena in engineering domains. Barabasi [27] argues that, “The science of networks is experiencing a boom. But despite the necessary multi-disciplinary approach to tackle the theory of complexity, scientists remain largely compartmentalised in their separate disciplines”. The application of this complex system architectures theory is still in infancy and has very recently entered into study of engineering systems or their design. We have shown that over(under) represented motifs in engineering systems are not purposefully retained/avoided to perform functions but are a natural consequence of design by decomposition. We also have shown that biological and social networks also display signs of synthesis by decomposition. This is shown by considering 38 arbitrarily chosen systems ranging from—biology systems, languages, electronic circuits, software systems and mechanical engineering systems. This study has thrown some new insights about Classification of Systems from Component Characteristics.

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