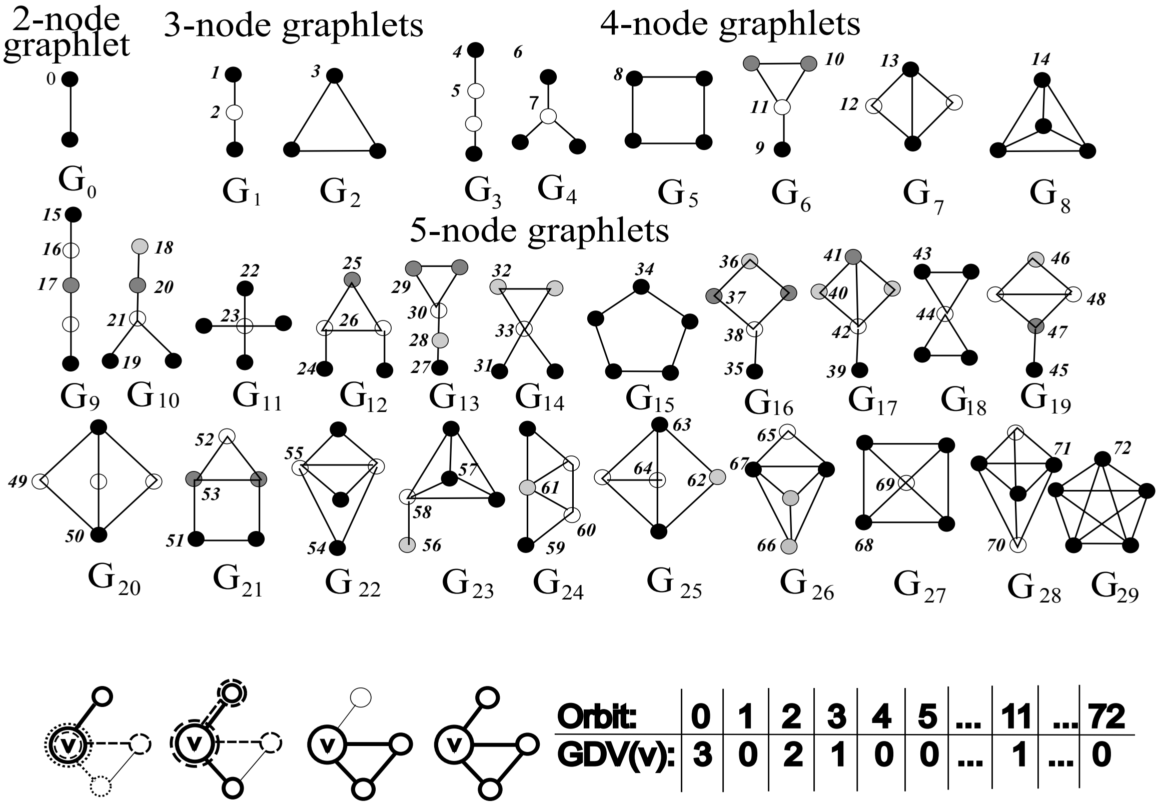
Supplementary Figures



Orbit:	0	1	2	3	4	5	...	11	...	72
GDV(v):	3	0	2	1	0	0	...	1	...	0

Figure 1: **Above**: Graphlets with 2 to 5 nodes denoted by $G_0, G_1, G_2, \ldots, G_{29}$ and their automorphism orbits $i \in 0, 1, 2, \ldots, 72$. Nodes within a graphlet belonging to the same orbit (i.e. invariant under the ”symmetry group”) are represented by the same shade. **Below**: An illustration of a GDV vector of a node v. Node touches G_0 graphlet, orbit 0 three times (first panel), middle node of a graphlet G_1, orbit 2, two times (second panel), a graphlet G_2 (third panel), a middle node of a graphlet G_6, orbit 11, (fourth panel) and no other orbits.

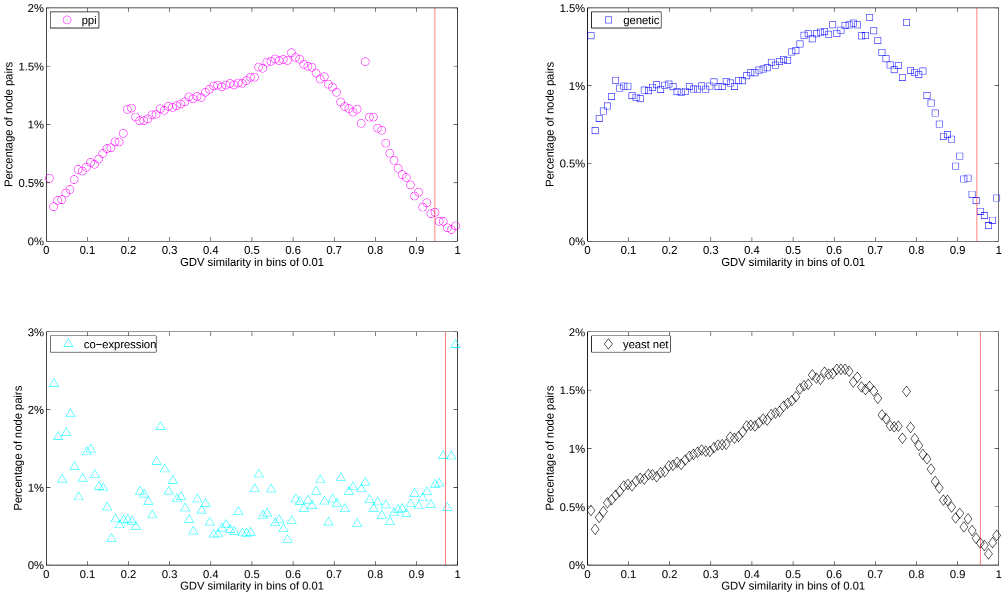


Figure 2: **GDV similarity distributions**: Distribution of gene pairs according to their GDV similarity in four different networks of *Saccharomyces cerevisiae*: (A) protein-protein interaction (PPI) network; (B) genetic interaction (GI) network; (C) gene co-expression network; (D) integrated function network (YeastNet). Vertical red line represents a threshold for a given distribution obtained by selecting top 1% of the most similar gene pairs (corresponding to a p-value of 0.01).

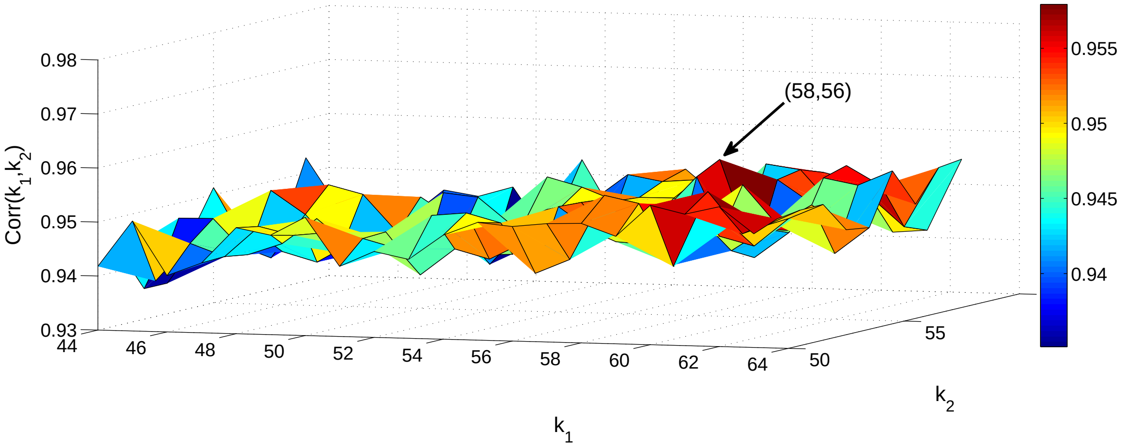


Figure 3: **Estimation of rank parameters by computing cophenetic correlation coefficient**: For each pair $(k_1^{(i)}, k_2^{(j)})$ of ranks, depicted in the (x, y) plane we compute averaged cophenetic correlation coefficient for two data sets - *genes* and *GO terms*. Averaged coefficient is represented on the z axis. We identified a set of parameters $(k_1, k_2) = (58, 56)$, as our optimal ranks, for which there is a maximum value of cophenetic correlation coefficient (a peak on this 3D color plot). Around this value, correlation coefficient significantly drops.

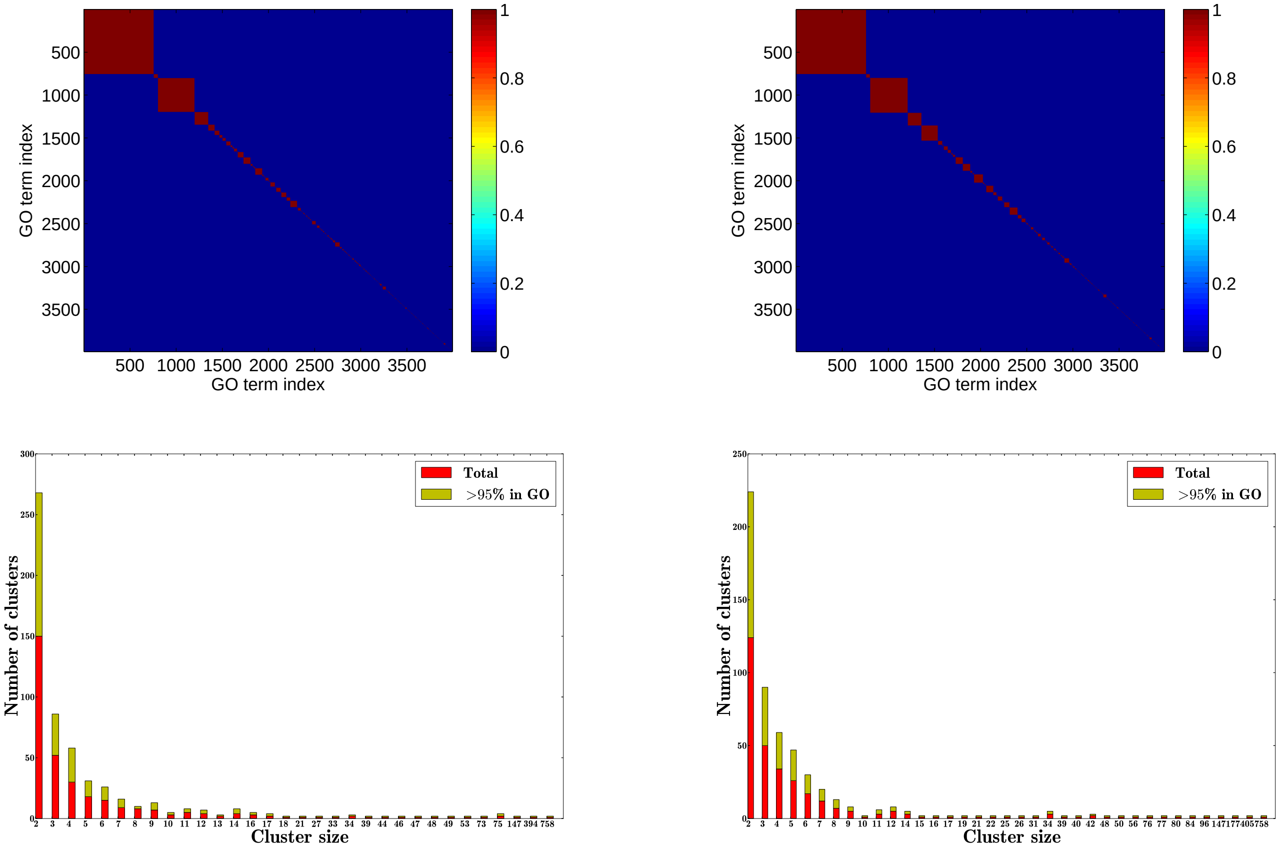


Figure 4: **Top panels**: Block diagonal form of consensus matrix obtained by running the algorithm only on network data (**left**) and on network data including GDV similarity constraints (**right**). Each consensus matrix is computed by averaging different connectivity matrices obtained by repeating the factorization process for 20 different random initial conditions. Highly reliable term-term associations are denoted within blocks of a matrix. **Bottom panels**: Distribution of cluster sizes for network data (**left**) and network + GDV similarity constraints (**right**). Number of clusters with a given size is represented with red bars while the number of clusters of the same size containing more than 90% of terms directly connected in GO is represented with yellow bars.