



## Subject Section

# Inferring Biological Function from Network Topology via Topological Ranking- Supplementary Material

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## Abstract

### 1 Biological Networks

Network	Type of nodes	No. Nodes	No. Edges	Link density
<i>GDN</i>	Gene	903	6,760	0.01659
<i>HDN</i>	Disease	516	1,118	0.009
<i>GDN<sub>GO</sub></i>	Gene	801	5,277	0.01647
<i>WGN</i>	Gene	554	137,918	0.897
<i>YD1</i>	Protein	990	4,687	0.01
<i>YD2</i>	Protein	1,443	6,993	0.007
<i>Y2H</i>	Protein	1,966	2,705	0.001

Table 1. Basic structural features of the considered biological networks

### 2 Topological measures

#### 2.1 Edges

##### 2.1.1 Incremental measures

**Topological Overlap Measure.** Given an edge  $(i, j)$ , the Topological Overlap Measure (TOM) and its Generalized version (GTOM $m$ ) (Ravasz *et al.*, 2002; Yip and Horvath, 2007) score the degree to which  $i$ 's and  $j$ 's neighbors overlap. The larger the overlap, the higher the weight assigned to  $(i, j)$ . TOM considers only the immediate neighbors, whereas GTOM $m$  includes all the neighbors at distance  $\leq m$ :

$$w_{ij} = \begin{cases} \frac{|N_m(i) \cap N_m(j)| + a_{ij}}{\min\{|N_m(i)|, |N_m(j)|\} + 1 - a_{ij}} & \text{if } i \neq j \\ 1 & \text{otherwise} \end{cases} \quad (1)$$

In Equation 1,  $N_m(i)$  denotes the set of  $i$ 's neighbors reachable with a shortest path of length at most  $m$  from  $i$ , and  $a_{ij} = 1$  if there exists an edge connecting vertices  $i$  and  $j$ ,  $a_{ij} = 0$  otherwise.

**Edge Clustering Value.** Similarly to TOM, Edge Clustering Value (ECV) (Wang *et al.*, 2011) quantifies how much the  $i$ 's and  $j$ 's neighborhood overlap:

$$w_{ij} = \frac{|N_1(i) \cap N_1(j)|^2}{|N_1(i)| \cdot |N_1(j)|}. \quad (2)$$

Unlike TOM which normalizes the size of common neighborhood over the smallest between  $i$  and  $j$  neighborhoods (see Equation 1), ECV is equal to 1 if and only if  $i$  and  $j$  have the same *exact* neighbors. It is worth noting that both TOM and ECV can be interpreted as a biological, neighborhood-normalized versions of Granovetter's *embeddedness* measure, historically used to characterize tie-strength in social networks (Marsden and Campbell, 1984).

**Dispersion.** For a given edge  $(i, j)$ , the Dispersion measure (Backstrom L, 2014) extends Granovetter's tie-strength measure (Marsden and Campbell, 1984), taking into account both the size and the *connectivity* of  $i, j$ 's common neighborhood. Intuitively, it quantifies of how "*not well*"-connected is the  $i, j$ 's common neighborhood within  $G_i$ , the subgraph induced by  $i$  and its neighbors. More formally, let  $G_i$  be the subgraph induced in  $G$  by  $\{i\} \cup N_1(i)$ . In  $G_i$ , let  $j$  be a neighbor of  $i$  (i.e.  $j \in N_1(i)$ ), and denote with  $C_{ij}^{(i)} = N_1(i) \cap N_1(j)$  the set of common neighbors of  $i$  and  $j$  within the induced subgraph  $G_i$ . The *absolute dispersion* (Backstrom L, 2014) is defined as follows:

$$disp(i, j) = \sum_{s, t \in C_{ij}^{(i)}} d_v(s, t) \quad (3)$$

where  $d_v$  is a boolean function such that  $d_v = 1$  if and only if  $s$  and  $t$  are not connected by a path of length  $\leq 2$  in  $G_i$ . The authors define two

enhanced versions of dispersion: *parametric* dispersion (Equation 4) and *recursive* dispersion (Equation 5):

$$param(i, j, \alpha, \beta, \gamma) = \frac{(disp(i, j) + \beta)^\alpha}{emb(i, j) + \gamma} \quad (4)$$

$$rec(i, j) \leftarrow \frac{\sum_{w \in C_{ij}^{(i)}} x_w^2 + 2 \sum_{s, t \in C_{ij}} d_v(s, t) x_s x_t}{emb(i, j)} \quad (5)$$

where  $emb(i, j)$  is equal  $|C_{ij}^{(i)}|$  (see details in (Backstrom L, 2014)). It is easy to show that both these measures are not symmetric. Since in our context we are considering undirected graphs, we unambiguously assign a weight to the edge  $(i, j)$  by defining and applying the following three variants:

1. **rec\_max**. Assigns a dispersion weight to edge  $(i, j)$  as  $w_{ij} = rec\_max(i, j) = MAX\{rec(i, j), rec(j, i)\}$ .

2. **rec\_min**. Assigns a dispersion weight to edge  $(i, j)$  as  $w_{ij} = rec\_min(i, j) = MIN\{rec(i, j), rec(j, i)\}$ .

3. **param\_sym**. Computes a *symmetric* parametric variant of  $w_{ij} = param(i, j, \alpha, \beta, \gamma)$  with parameters  $\alpha = 0.61$ ,  $\beta = 0$ ,  $\gamma = 5.0$  (i.e., parameters used by authors, see details in (Backstrom L, 2014)), considering the common neighborhood  $C_{ij}$  in  $G$  (and not in the induced subgraphs  $G_i, G_j$ , as in the original – non-symmetric – definition).

### 2.1.2 Decremental measures

**Edge Betweenness.** Given an edge  $e_{ij}$ , the Edge Betweenness (EB) (Girvan and Newman, 2002) is the fraction of shortest paths in the network  $\mathcal{N}$  containing the edge  $e_{ij}$ :

$$w_{ij} = \sum_{s, t \in V} \frac{\sigma_{st}(e_{ij})}{\sigma_{st}} \quad (6)$$

In Equation 6,  $\sigma_{st}$  represents the total number of shortest paths connecting nodes  $s, t$  ( $s \neq t$ ) in the network, whereas  $\sigma_{st}(e_{ij})$  counts only the shortest paths between the same nodes containing the edge  $e_{ij}$ . The higher  $w_{ij}$ , the more likely the edge  $e_{ij}$  acts as a *bridge* connecting separate communities, thus representing an *inter-community* edge.

**Edge Clustering Coefficient.** Given the edge  $e_{ij}$ , the Edge Clustering Coefficient (ECC3) (Radicchi et al., 2004) is the number of *triangles* the edge  $e_{ij}$  belongs to, divided by the number of triangles that might potentially include it:

$$w_{ij} = -\frac{z_{i,j}^3 + 1}{s_{i,j}^{(3)}} = -\frac{|N_1(i) \cap N_1(j)| + 1}{\min[ (|N_1(i)| - 1)(|N_1(j)| - 1) ]} \quad (7)$$

In Equation 7,  $z_{i,j}^3$  is the number of triangles built on the edge  $e_{ij}$  and  $s_{i,j}^{(3)}$  is the maximal possible number of them. The minus sign is explained as follows. Many triangles exists within dense communities. Therefore, the higher  $|w_{ij}|$  the more likely  $e_{ij}$  lies within a dense community, being an *intra-community* edge. Nevertheless, in order to identify communities (Radicchi et al., 2004) use  $|w_{ij}|$  in a Girvan-Newman fashion (Girvan and Newman, 2002): at each step of the divisive algorithm, edges with the *lowest*  $|w_{ij}|$  are removed, eventually splitting the original network into separate connected components. Here, we directly take the opposite of the original measure to rank first edges  $e_{ij}$  having the lowest  $|w_{ij}|$  (that is: the *inter-community* ones). These edges represent "less important" elements according to our framework.

**Edge Centrality Proximity Distance.** Edge Centrality Proximity Distance (ECPd) (De Meo et al., 2014) is based on the notion of Edge Centrality (Equation 9) as introduced in (DeMeo et al., 2012):

$$w_{ij} = 1 - \sqrt{\sum_{k=1}^n \frac{(L^\kappa(e_{ik}) - L^\kappa(e_{kj}))^2}{d(k)}} \quad (8)$$

$$L^\kappa(e) = \sum_{s \in V} \frac{\sigma_s^\kappa(e)}{\sigma_s^\kappa} \quad (9)$$

In Equation 8,  $L^\kappa(e_{ik})$  is the Edge Centrality, the fraction of times a random walker traverses the edge  $e_{ik}$  running through a random simple path of length at most  $\kappa$ . Thus,  $(L^\kappa(e_{ik}) - L^\kappa(e_{kj}))^2$  expresses a *proximity* between nodes  $i$  and  $j$ : the probability that a message propagated to node  $i$  reaches also node  $j$ , with node  $k$  being a common neighbor of the two. Therefore, Equation 8 represents a *distance* between nodes  $i$  and  $j$ : the higher  $w_{ij}$  the more likely the nodes  $i$  and  $j$  belong to different communities and  $e_{ij}$  being an inter-community edge.

## 2.2 Nodes

### 2.2.1 Incremental measures

**Node Clustering Coefficient.** Given a node  $i$ , Node Clustering Coefficient (NCC) (Watts, 1999) expresses how much densely connected is the  $i$ 's neighborhood. Let  $k_i$  be the number of neighbors of  $i$ , and let  $n_i$  be the number of edges connecting such neighbors:

$$x_i = \frac{2n_i}{k_i(k_i - 1)}. \quad (10)$$

In Equation 10, the denominator is equal to the maximum value for  $k_i$  (recall  $\mathcal{N}$  is an undirected graph). As a result, the greater the value of  $x_i$ , the closer the  $i$ 's neighborhood to be a clique.

**Eigenvector Centrality.** Given a node  $i$ , the Eigenvector centrality (EGC) (Bonacich, 1972) is a measure of topological "importance" (Brandes and Erlebach, 2005) for the node  $i$  in the network  $\mathcal{N}$ . Specifically, node  $i$  can acquire high centrality either by having a high degree or by being connected to other highly-important.

$$x_i = \frac{1}{\lambda} \sum_{j \in G} A_{ij} x_j \quad (11)$$

In Equation 11,  $\lambda$  is the largest positive eigenvalue of the adjacency matrix  $A$ , satisfying the equation  $A \mathbf{x} = \lambda \mathbf{x}$ , with  $\mathbf{x} = (x_1, x_2, \dots, x_n)$  being the vector of node centralities. Notably, Google's PageRank (Page et al., 1999) is a variant of Eigenvector Centrality.

### 2.2.2 Decremental measures

**Betweenness Centrality.** Given a node  $i$ , Node Betweenness (BC) (Freeman, 2012) quantifies the extent to which node  $i$  lies on *geodesic* (shortest) paths between other pairs of vertices:

$$x_i = \sum_{s \neq t \neq i} \frac{\sigma_{st}(i)}{\sigma_{st}} \quad (12)$$

In Equation 12,  $\sigma_{st}(i)$  represents the number of shortest paths from node  $s$  to node  $t$  that pass through  $i$ , whereas  $\sigma_{st}$  is the total number of shortest paths between the same nodes. Intuitively, the higher  $x_i$  the more likely  $i$  lies on a path between nodes in different communities.

**Subgraph Centrality.** Given a node  $i$ , Subgraph Centrality (SGC) (Estrada and Rodríguez-Velázquez, 2005) quantifies the centrality of node  $i$  based on the number of subgraphs it belongs to:

$$x_i = \sum_{k=0}^{\infty} \frac{(A^k)_{ii}}{k!} \quad (13)$$

Since each closed path is associated with a connected subgraph, EGC counts the number of closed walks in the network. In Equation 13,  $(A^k)_{ii}$  is the number of closed paths of length  $k$ , starting and ending on node  $i$ . Closed walks are weighted such that smaller walks are given higher weights (see (Estrada and Rodríguez-Velázquez, 2005)). Therefore, smaller subgraphs are given higher weights than larger ones, which makes SGC able to quantify the extent to which node  $i$  participates in network motifs within real-world networks. (Milo *et al.*, 2002; Yeager-Lotem *et al.*, 2004).

**$\kappa$ -Path Centrality.** Given a node  $i$ , the  $\kappa$ -Path Centrality (KPC) (Alahakoon *et al.*, 2011) is defined as the sum, over all possible source nodes  $s$ , of the probability that a message originating in  $s$  goes through  $i$ , assuming the message runs along random simple paths of length at most  $\kappa$ :

$$x_i = \sum_{s \neq i} \frac{\sigma_s^\kappa(i)}{\sigma_s^\kappa} \quad (14)$$

In Equation 14,  $\sigma_s^\kappa(i)$  is the number of messages originating at node  $s$  passing through node  $i$ , whereas  $\sigma_s^\kappa$  is the total number of messages originated from node  $s$ . Despite a similar formulation, KPC differs substantially from NB. In particular, KPC does not assume information flows necessarily across shortest paths, as NB does.

### 3 Algorithms

**Algorithm 1** Returns a *static* edge rank  $\mathcal{E}$  of network  $\mathcal{N}$ , based on the topological measure  $w$ .

```

1: function rank-static( $\mathcal{N}, w$ )
2:   for each  $(i, j) \in E$ 
3:     compute the weight function  $w(i, j)$ 
4:    $\mathcal{E} \leftarrow$  sort  $E$  in non-increasing order of weight
5:    $\mathcal{E} \leftarrow$  group edges of  $E$  with equal rank
6:   return  $\mathcal{E} = (E_1, E_2, \dots, E_k)$ 
7: end function
```

**Algorithm 2** Returns a *dynamic* edge rank  $\mathcal{E}$  of network  $\mathcal{N}$ , based on the topological measure  $w$ .

```

1: function rank-dynamic( $\mathcal{N}, w$ )
2:    $\mathcal{E} \leftarrow \emptyset$ 
3:    $i \leftarrow 1$ 
4:   while  $(|E| > 0)$  do
5:     for each  $(i, j) \in E$ 
6:       compute the weight function  $w(i, j)$ 
7:     Let  $E_i$  be the set of edges in  $E$  having maximum weight
8:     Append  $E_i$  to  $\mathcal{E}$  and delete edges in  $E_i$  from  $E$ 
9:      $i \leftarrow i + 1$ 
10:  end while
11:  return  $\mathcal{E} = (E_1, E_2, \dots, E_k)$ 
12: end function
```

ub

## 4 Benchmark Datasets

### 4.1 Protein-Protein Interaction Networks

**Yeast PPIN.** [(Daniele): TODO: briefly describe the networks Yeast-D1, Yeast-D2, Yeast Y2H and cite sources].

**Benchmarks for the Yeast PPIN.** We consider three reference sets of yeast complexes: Cmplx1 for YEAST-D1 (D1), Cmplx2 for YEAST-D2 (D2) and Cmplx3 for Y2H (Y2H), respectively. Cmplx1 includes 81 complexes of sizes at least 5, created from MIPS (Mewes *et al.*, 2000). Cmplx2 is made of 162 hand-curated complexes (size no less than 4 proteins) from MIPS (?). Finally, Cmplx3 includes 975 known and curated complexes from [(Daniele): TODO: source?].

## 5 Statistical Significance of a Topological Ranking

### 5.1 Precision, Recall and F-Measure Indices

### 5.2 Kendall index in Case of Ties

## 6 Results

### 6.1 Human and Gene Disease Networks

Definire Global Comparison

View Type	F	Rank Type	K_haus	EC test	TR test
I	ECV	static	0.921352		✓
I	GTOM2	static	0.263199	✓	✓
I	TOM	static	0.394417	✓	✓
I	kb_rec_max	static	0.512545		✓
I	kb_rec_min	static	0.157832		✓
I	kb_param_sym	static	0.109155		✓
I	ECV	dynamic	0.587569		✓
I	GTOM2	dynamic	0.258508	✓	✓
I	TOM	dynamic	0.387743	✓	✓
D	EB	static	0.904365		✓
D	ECC3	static	0.879348		✓
D	ECP	static	0.902387		✓
D	EB	dynamic	0.733648		✓
D	ECC3	dynamic	0.88796		✓

Table 2. **Global Comparison for the Human Disease Network HDNG using Edge Ranks.** The column *View Type* specifies the view, either (I)ncremental or (D)ecremental. The columns *F* and *Rank* give the topological measure together with the ranking type, respectively. Acronyms for the measures are in Section 2. *K\_haus* reports the corresponding normalized *K\_haus* distances obtained: the smaller the value, the more similar the topological ranking to the functional ranking. The final two columns indicate whether the EC and TR tests were passed.

### 6.2 Worm Disease Network

qui le tabelle che ha Greco di tutti tests su questo network

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View Type	F	Rank Type	K_haus	EC test	TR test
:GC_H D N E d g e s , e s u l t s h e i g h t I	NCC	static	0.558474	✓	✓
I	EGC	static	0.573012		✓
I	NCC	dynamic	0.432467	✓	✓
I	EGC	dynamic	0.673747		✓
D	NB	static	0.553613		✓
D	SGC	static	0.742343		
D	KPC	static	0.774174		
D	NB	dynamic	0.557036		✓
D	SGC	dynamic	0.664536		✓
D	KPC	dynamic	0.838758		

Table 3. Global Comparison for the Human Disease Network *HDNG* using Edge Equivalent Ranks. The legend is as in Table 2.

View Type	F	Rank Type	K_haus	EC test	TR test
I	ECV	static	0.96157		✓
I	GTOM2	static	0.126684	✓	✓
I	TOM	static	0.211708	✓	✓
I	kb_rec_max	static	0.398346		✓
I	kb_rec_min	static	0.058925		✓
I	kb_param_sym	static	0.037909		✓
I	ECV	dynamic	0.783565		✓
I	GTOM2	dynamic	0.126097	✓	✓
I	TOM	dynamic	0.210773	✓	✓
D	EB	static	0.784118		✓
D	ECC3	static	0.937585		✓
D	ECP	static	0.778692		✓
D	EB	dynamic	0.426541		✓
D	ECC3	dynamic	0.937758		✓

Table 4. Global Comparison for the Gene Disease Network *GDNG\_DS* using Edge Ranks. The legend is as in Table 2.

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View Type	F	Rank Type	K_haus	EC test	TR test
I	NCC	static	0.7739	✓	✓
I	EGC	static	0.457653		✓
I	NCC	dynamic	0.746356	✓	✓
I	EGC	dynamic	0.932883		✓
D	NB	static	0.243135		✓
D	SGC	static	0.954153		✓
D	KPC	static	0.984258		
D	NB	dynamic	0.223707		✓
D	SGC	dynamic	0.929725		✓
D	KPC	dynamic	0.98898		

Table 5. **Global Comparison for the Gene Disease Network *GDNG\_DS* using Edge Equivalent Ranks.** The legend is as in Table 2

View Type	F	Rank Type	K_haus	EC test	TR test
I	ECV	static	0.960733		✓
I	GTOM2	static	0.145038	✓	✓
I	TOM	static	0.240163	✓	✓
I	kb_rec_max	static	0.447846		✓
I	kb_rec_min	static	0.074278		✓
I	kb_param_sym	static	0.043585		✓
I	ECV	dynamic	0.764334		✓
I	GTOM2	dynamic	0.144126	✓	✓
I	TOM	dynamic	0.23884	✓	✓
D	EB	static	0.811777		✓
D	ECC3	static	0.934783		✓
D	ECP	static	0.80787		✓
D	EB	dynamic	0.452198		✓
D	ECC3	dynamic	0.938017		✓

Table 6. **Global Comparison for the Gene Disease Network *GDNG\_GODS* using Edge Ranks.** The legend is as in Table 2.

View Type	F	Rank Type	K_haus	EC test	TR test
I	NCC	static	0.801589	✓	✓
I	EGC	static	0.673495		✓
I	NCC	dynamic	0.767608	✓	✓
I	EGC	dynamic	0.936067		✓
D	NB	static	0.274195		✓
D	SGC	static	0.945941		✓
D	KPC	static	0.98083		
D	NB	dynamic	0.240112		✓
D	SGC	dynamic	0.919067		✓
D	KPC	dynamic	0.985727		

Table 7. **Global Comparison for the Gene Disease Network *GDNG\_GODS* using Edge Equivalent Ranks.** The legend is as in Table 2

View Type	F	Rank Type	K_haus	EC test	TR test
I	ECV	static	0.633149	✓	✓
I	GTOM2	static	0.628768	✓	✓
I	TOM	static	0.592387	✓	✓
I	kb_rec_max	static	0.548323		✓
I	kb_rec_min	static	0.667305		
I	kb_param_sym	static	0.682106		
I	ECV	dynamic	0.505902		✓
I	GTOM2	dynamic	0.629108	✓	✓
I	TOM	dynamic	0.592576	✓	✓
D	EB	static	0.556917		✓
D	ECC3	static	0.637379		✓
D	ECP	static	0.543236		✓
D	EB	dynamic	0.538452		✓
D	ECC3	dynamic	0.650556		

Table 8. **Global Comparison for the Gene Disease Network**  
*GDNG\_GOGO* using **Edge Ranks**. The legend is as in Table 2.

View Type	F	Rank Type	K_haus	EC test	TR test
I	NCC	static	0.529577	✓	✓
I	EGC	static	0.458644		✓
I	NCC	dynamic	0.508407	✓	✓
I	EGC	dynamic	0.635614		✓
D	NB	static	0.599601		✓
D	SGC	static	0.643931		✓
D	KPC	static	0.663018		
D	NB	dynamic	0.611015		✓
D	SGC	dynamic	0.623985		✓
D	KPC	dynamic	0.667948		

Table 9. **Global Comparison for the Gene Disease Network**  
*GDNG\_GOGO* using **Edge Equivalent Ranks**. The legend is as in  
Table 2