Supplementary Text Reverse Engineering Molecular Hypergraphs

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I. Properties of Modified ODES

Our extended version of ODES is based on the following lemma. In this lemma and proof, we have used the same notation as in the ODES paper [1] for the convenience of the reader. In a connected graph, we define a *cut vertex* to be a vertex whose removal disconnects the graph into two or more connected components.

Lemma 1 *Let G be a connected edge-weighted graph where every edge has a positive weight that is at most 1. If G contains three or more nodes and has density $den(G) \geq 1/2$, then G contains at least one noncut vertex w whose removal from G does not decrease the density of G.*

Proof: The proof is trivial if there is no cut vertex in G. Let us assume that v is a cut vertex in G. Let S be the smallest connected component of $G - v$ and let A be the subgraph of G induced by the union of nodes in S and v. Let G have n vertices. We use $E(G)$ to denote the set of edges in G. Since v is not a cut vertex of A, there exists at least another such non-cut vertex (say, w) in A. Since w is not a cut vertex of A, it is not a cut vertex of G either. Moreover, w has the same neighbors in A and G. Therefore, the weighted degree $d(w)$ of w (in A as well as in G) is at the most the number of vertices in S, which is at most $n - 1/2$. Since the density of G is at least 0.5, we have

$$den(G) = \frac{2}{n(n-1)} \sum_{e \in E(G)} w(e) \geq \frac{1}{2}$$

Rearranging terms and combining with the bound on $d(w)$, we obtain

$$d(w) = \frac{n-1}{2} \leq \frac{2}{n} \sum_{e \in E(G)} w(e)$$

Cross-multiplying and subtracting both sides of the inequality from n times the total weight of the edges in G, we get

$$n \left(\sum_{e \in E(G)} w(e) - d(w) \right) \geq (n-2) \sum_{e \in E(G)} w(e)$$

Dividing each side by $(n-2)(n-1)n$, we get

$$\frac{2 \left(\sum_{e \in E(G)} w(e) - d(w) \right)}{(n-1)(n-2)} \geq \frac{2 \sum_{e \in E(G)} w(e)}{n(n-1)}$$

By definition, the left and right hand sides of this inequality are the density of $G - w$ and G, respectively, i.e.,

$$den(G - w) \geq den(G)$$

Since the removal of the non-cut vertex w from G cannot decrease the density of G, we have completed the proof. ■

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References

[1] J. Long and C. Hartman. ODES: an overlapping dense sub-graph algorithm. *Bioinformatics*, 26(21):2788–2789, 2010.