

A Cycle Constraint

O’Gorman et al. 2014 used $\sum_{a < b} \delta_{\text{trans}}^{(a,b,c)} R'_{a,b,c}$ as the cycle constraint of the Hamiltonian, and showed the

sufficient lower bound $\delta_{\text{lower}}^{(\text{full})} < \delta_{\text{trans}}^{(a,b,c)} = \delta^{(\text{full})} < \frac{\delta_{\text{trans}}^{(\text{full})}}{N-2}$, where $\delta_{\text{trans}}^{(a,b,c)} \in \mathbb{R}$, $R'_{a,b,c} = r'_{a,c} + r'_{a,b}r'_{b,c} - r'_{a,b}r'_{a,c} - r'_{b,c}r'_{a,c}$, and $r'_{n',n} = r_{n',n}$ if $n' < n$, $1 - r_{n,n'}$ otherwise. We replaced $\sum_{a < b} \delta_{\text{trans}}^{(a,b,c)} R'_{a,b,c}$ with $\sum_{a < b < c} \delta_{a,b,c}^{(\text{full})} R_{a,b,c}$ for simplicity, and set $\delta_{\text{trans}}^{(a,b,c)} = \frac{\delta_{a,b,c}^{(\text{full})}}{3}$ for the following reasons:

$$\begin{aligned}
\sum_{\substack{a,b,c \\ a < b}} R'_{a,b,c} &= \sum_{\substack{a,b,c \\ a < b}} (r'_{a,c} + r'_{a,b}r'_{b,c} - r'_{a,b}r'_{a,c} - r'_{b,c}r'_{a,c}) \\
&= \sum_{a < b < c} (r_{a,c} + r_{a,b}r_{b,c} - r_{a,b}r_{a,c} - r_{b,c}r_{a,c}) \\
&\quad + \sum_{a < c < b} (r_{a,c} + r_{a,b}(1 - r_{c,b}) - r_{a,b}r_{a,c} - (1 - r_{c,b})r_{a,c}) \\
&\quad + \sum_{c < a < b} ((1 - r_{c,a}) + r_{a,b}(1 - r_{c,b}) - r_{a,b}(1 - r_{c,a}) - (1 - r_{c,b})(1 - r_{c,a})) \\
&= \sum_{a < b < c} (r_{a,c} + r_{a,b}r_{b,c} - r_{a,b}r_{a,c} - r_{b,c}r_{a,c}) \\
&\quad + \sum_{a < c < b} (r_{a,b} + r_{a,c}r_{c,b} - r_{a,c}r_{a,b} - r_{c,b}r_{a,b}) \\
&\quad + \sum_{c < a < b} (r_{c,b} + r_{c,a}r_{a,b} - r_{c,a}r_{c,b} - r_{a,b}r_{c,b}) \\
&= 3 \sum_{a < b < c} (r_{a,c} + r_{a,b}r_{b,c} - r_{a,b}r_{a,c} - r_{b,c}r_{a,c}) \\
&= 3 \sum_{a < b < c} R_{a,b,c}.
\end{aligned}$$

B Sufficient Lower Bound

It is clear that

$$\delta_{\text{lower}}^{(Z)} = \max_n \max_{\lambda, \lambda'} \{ \max(-s_{1,\lambda,n}^{(Z)} - t_{\lambda,\lambda',n}^{(Z)}), \max(-s_{2,\lambda',n}^{(Z)} - t_{\lambda,\lambda',n}^{(Z)}) \} < \xi_{o,\lambda,\lambda',n}^{(Z)}$$

so that $\sum_{\lambda} p_{o,\lambda,n} \leq 1$ for all n, o . In addition, it does not lose its generality by assuming that $s_{1,\lambda,n}^{(Z)} + t_{\lambda,\lambda',n}^{(Z)} \leq s_{1,0,n}^{(Z)} + t_{0,\lambda',n}^{(Z)} = 0$, $s_{2,\lambda',n}^{(Z)} + t_{\lambda,\lambda',n}^{(Z)} \leq s_{2,0,n}^{(Z)} + t_{\lambda,0,n}^{(Z)} = 0$ for all λ, λ', n because $U_{o,0,n} = \phi$ is always most advantageous in the term of the DAG constraint.

Under these conditions and $\Lambda_{1,n}, \Lambda_{2,n} > 1$, the sufficient lower bound $\delta_{\text{lower}}^{(Z)}$ satisfies

$$\begin{aligned}
\delta_{\text{lower}}^{(\text{full})} &= \max\{0, \max_{n' \neq n} \max_{\mathbf{d}, \mathbf{n} \setminus d_{n',n}} (-H_{\text{score}}^{n(\text{full})}(\mathbf{d}, \mathbf{n} \mid d_{n',n} = 1) + H_{\text{score}}^{n(\text{full})}(\mathbf{d}, \mathbf{n} \mid d_{n',n} = 0))\} \\
&\leq \max_n \max_{\substack{o', o, \lambda \\ o' \neq o}} \max_{\mathbf{p}_{o', \cdot, n}} (-H_{\text{score}}^{n(Z)}(\mathbf{p}_{1, \cdot, n}, \mathbf{p}_{2, \cdot, n} \mid p_{o, \lambda, n} = 1) + H_{\text{score}}^{n(Z)}(\mathbf{p}_{1, \cdot, n}, \mathbf{p}_{2, \cdot, n} \mid p_{o, \cdot, n} = \mathbf{0})) \\
&= \max_n \max_{\lambda, \lambda'} \{ \max(-s_{1,\lambda,n}^{(Z)} - t_{\lambda,\lambda',n}^{(Z)}), \max(-s_{2,\lambda',n}^{(Z)} - t_{\lambda,\lambda',n}^{(Z)}) \} \\
&= \delta_{\text{lower}}^{(Z)}.
\end{aligned}$$

It is obvious that $\delta_{\text{lower}}^{(Z)}$ is also the sufficient bound when $\Lambda_{1,n} = 1$ or $\Lambda_{2,n} = 1$.

Correction and Apology. Equation (24) in the main text is a sufficient lower bound. However, the above result is better as a sufficient lower bound.