Theorem 1: *Incorporating multiple contexts reduces the probability of feature duplication among nodes, thereby enhancing the discriminative power of the 1-WL test.* Specifically,

$$P_{\text{conflict}}^{\text{single}} \geq P_{\text{conflict}}^{\text{multi}} \tag{1}$$

where $P_{\text{conflict}}^{\text{single}}$ and $P_{\text{conflict}}^{\text{multi}}$ represent the probabilities of feature conflict between two distinct nodes in single-feature graphs and multi-feature graphs, respectively.

Proof

We begin with the definition of feature conflict probability: For a graph with n nodes, the probability of feature conflict is defined as:

$$P_{\text{conflict}} = \frac{\text{Number of conflicting pairs}}{\text{Total number of node pairs}} \tag{2}$$

The total number of node pairs is given by:

$$\binom{n}{2} = \frac{n(n-1)}{2} \tag{3}$$

Next, we analyze the single-feature case, as (2) shows. Let the feature space size for single features be k. The probability of assigning the same feature to a pair of nodes is:

$$P(h_u^{(0)} = h_v^{(0)}) = \frac{1}{k}, \quad u \neq v \tag{4}$$

The number of conflicting pairs is:

$$\text{Conflicting pairs}_{\text{single}} = \sum_{x \in \mathcal{H}_{\text{single}}} \binom{n_x}{2} \tag{5}$$

where n_x is the number of nodes with feature x. Assuming uniform distribution, $n_x = \frac{n}{k}$, we have:

$$\text{Conflicting pairs}_{\text{single}} = k \cdot \binom{\frac{n}{k}}{2} = k \cdot \frac{\frac{n}{k} \cdot (\frac{n}{k} - 1)}{2} \tag{6}$$

Simplifying:

$$\text{Conflicting pairs}_{\text{single}} = \frac{n(n-k)}{2k} \tag{7}$$

Thus, the conflict probability is:

$$P_{\text{conflict}}^{\text{single}} = \frac{\text{Conflicting pairs}_{\text{single}}}{\binom{n}{2}} = \frac{n-k}{k(n-1)} \tag{8}$$

Next, we infer the multi-feature case, as (7) shows. Let the feature space size grow exponentially with dimension d, i.e., $k_d = k^d$. The probability of assigning the same feature vector to a pair of nodes is:

$$P(h_u^{(0)} = h_v^{(0)}) = \frac{1}{k^d} \tag{9}$$

The number of conflicting pairs is:

$$\text{Conflicting pairs}_{\text{multi}} = \frac{n(n-1)}{2k^d} \tag{10}$$

Thus, the conflict probability is:

$$P_{\text{conflict}}^{\text{multi}} = \frac{\text{Conflicting pairs}_{\text{multi}}}{\binom{n}{2}} = \frac{1}{k^d} \tag{11}$$

Finally, as (11) shows, since $k^d \gg k$ for $d > 1$, it follows that:

$$P_{\text{conflict}}^{\text{multi}} = \frac{1}{k^d} \ll \frac{n-k}{k(n-1)} = P_{\text{conflict}}^{\text{single}} \tag{12}$$

Thus we can prove equation 1.