

$$\rho_{i \rightarrow k}(c_i) = s(i, c_i) + s'(i, c'_i) + \sum_{k': k' \neq k} \alpha_{i \leftarrow k'}(c_i) + [c_i \in \text{neb}(i, c'_k)] \cdot \lambda_2 \cdot I \quad (20)$$

从惩罚函数传递给潜在代表点的 α -消息如下:

$$\alpha_{i \rightarrow k}(c_i) = \overbrace{\max_{J_1, \dots, J_{i-1}, J_{i+1}, \dots, J_N} \left[\Delta_k(J_1, \dots, J_{i-1}, c_i, J_{i+1}, \dots, J_N) + \sum_{i'} \rho_{i' \rightarrow k}(J_{i'}) \right]}^{\text{best possible configuration satisfying } \Delta_k \text{ given } c_i} \\ = \begin{cases} \overbrace{\left[[k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i': s(i', k) \leq \text{maxval}, \\ i' \neq k}} (\rho_{i' \rightarrow k}(k) + \lambda_2 \cdot I) + \sum_{i': i' \neq i, k} \max_{j'} \rho_{i' \rightarrow k}(j') \right]}^{\text{best configuration with or without cluster } k}, & \text{for } c_i = k = i, \\ \overbrace{\left[\sum_{i': i' \neq k} \max_{j': j' \neq k} \rho_{i' \rightarrow k}(j') \right]}^{\text{best configuration with no cluster } k}, & \text{for } c_i \neq k = i, \\ \overbrace{\left[\rho_{k \rightarrow k}(k) + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + \right]}^{k \text{ is an exemplar}} \\ \overbrace{\left[[k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i': s(i', k) \leq \text{maxval}, \\ i' \neq i, k}} (\rho_{i' \rightarrow k}(k) + \lambda_2 \cdot I) + \sum_{i': i' \neq i, k} \max_{j'} \rho_{i' \rightarrow k}(j') \right]}^{\text{best configuration of others}}, & \text{for } c_i = k \neq i \\ \max \begin{cases} \overbrace{\left[\max_{j': j' \neq k} \rho_{k \rightarrow k}(j') + \sum_{i': i' \neq i, k} \max_{j': j' \neq k} \rho_{i' \rightarrow k}(j') \right]}^{\text{best configuration with no cluster } k}, \\ \overbrace{\left[\rho_{k \rightarrow k}(k) [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i': s(i', k) \leq \text{maxval}, \\ i' \neq i, k}} (\rho_{i' \rightarrow k}(k) + \lambda_2 \cdot I) + \sum_{i': i' \neq i, k} \max_{j'} \rho_{i' \rightarrow k}(j') \right]}^{\text{best configuration with a cluster } k} \end{cases}, & \text{for } c_i \neq k \neq i \end{cases} \quad (21)$$

我们可将上述传递的两类消息变量看作一个关于 c_i 的变量和一个常量的和,即

$$\rho_{i \rightarrow k}(c_i) = \tilde{\rho}_{i \rightarrow k}(c_i) + \bar{\rho}_{i \rightarrow k} \quad (22)$$

$$\alpha_{i \leftarrow k}(c_i) = \tilde{\alpha}_{i \leftarrow k}(c_i) + \bar{\alpha}_{i \leftarrow k} \quad (23)$$

于是,上述公式(20)、公式(21)等价于:

$$\rho_{i \rightarrow k}(c_i) = s(i, c_i) + s'(i, c'_i) + \sum_{k': k' \neq k} \tilde{\alpha}_{i \leftarrow k'}(c_i) + \sum_{k': k' \neq k} \bar{\alpha}_{i \leftarrow k'}(c_i) + [c_i \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I \quad (24)$$

$$\alpha_{i \rightarrow k}(c_i) = \begin{cases} \left[[k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i': s(i', k) \leq \text{maxval}, \\ i' \neq k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i': i' \neq i, k} \max_{j'} \rho_{i' \rightarrow k}(j') \right], & \text{for } c_i = k = i \\ \sum_{i': i' \neq k} \max_{j': j' \neq k} \tilde{\rho}_{i' \rightarrow k}(j') + \sum_{i': i' \neq k} \bar{\rho}_{i' \rightarrow k}, & \text{for } c_i \neq k = i \\ \tilde{\rho}_{k \rightarrow k}(k) + \bar{\rho}_{k \rightarrow k} + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + \\ \left[[k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i': s(i', k) \leq \text{maxval}, \\ i' \neq i, k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i': i' \neq i, k} \max_{j'} \rho_{i' \rightarrow k}(j') \right], & \text{for } c_i = k \neq i \\ \max \begin{cases} \left[\max_{j': j' \neq k} \tilde{\rho}_{k \rightarrow k}(j') + \sum_{i': i' \neq i, k} \max_{j': j' \neq k} \tilde{\rho}_{i' \rightarrow k}(j') + \sum_{i': i' \neq i} \bar{\rho}_{i' \rightarrow k} \tilde{\rho}_{k \rightarrow k}(k) + \bar{\rho}_{k \rightarrow k} + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I \right] \\ \left[[k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i': s(i', k) \leq \text{maxval}, \\ i' \neq i, k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i': i' \neq i, k} \max_{j'} \rho_{i' \rightarrow k}(j') \right] \end{cases}, & \text{for } c_i \neq k \neq i \end{cases} \quad (25)$$

当 $c_i \neq k$ 时, $\rho_{i \rightarrow k}(c_i) = \tilde{\rho}_{i \rightarrow k}(c_i) + \bar{\rho}_{i \rightarrow k}$, 我们假设 $\bar{\rho}_{i \rightarrow k} = \max_{j: j \neq k} \rho_{i \rightarrow k}(j)$, 则有如下结论:

$$\max_{j': j' \neq k} \tilde{\rho}_{i \rightarrow k}(j') = 0, \max_{j'} \tilde{\rho}_{i \rightarrow k}(j') = \max(0, \tilde{\rho}_{i \rightarrow k}(k)) \quad (26)$$

类似地, 当 $c_i \neq k$ 时, $\alpha_{i \leftarrow k}(c_i) = \tilde{\alpha}_{i \leftarrow k}(c_i) + \bar{\alpha}_{i \leftarrow k}$, 假设 $\bar{\alpha}_{i \leftarrow k} = \alpha_{i \leftarrow k}$, 同样有:

$$\tilde{\alpha}_{i \leftarrow k}(c_i) = 0, \sum_{k': k' \neq k} \tilde{\alpha}_{i \leftarrow k'}(c_i) = \tilde{\alpha}_{i \leftarrow k}(c_i) \quad (27)$$

对于 $c_i=k$,公式(27)的和为 0.有了公式(26)和公式(27),我们可进一步对公式(24)和公式(25)进行简化:

$$\rho_{i \rightarrow k}(c_i) = \begin{cases} s(i, c_i) + s'(i, c'_i) + \sum_{k':k' \neq k} \bar{\alpha}_{i \leftarrow k'}(c_i) + [c_i \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I, & \text{for } c_i = k \\ s(i, c_i) + s'(i, c'_i) + \sum_{k':k' \neq k} \bar{\alpha}_{i \leftarrow k'}(c_i) + \sum_{k':k' \neq k} \bar{\alpha}_{i \leftarrow k'}(c_i), & \text{for } c_i \neq k \end{cases} \quad (28)$$

$$\alpha_{i \rightarrow k}(c_i) = \begin{cases} [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i':i' \neq i, k} \max(0, \tilde{\rho}_{i' \rightarrow k}(j')) + \sum_{i':i' \neq i, k} \bar{\rho}_{i' \rightarrow k}, & \text{for } c_i = k = i \\ \sum_{i':i' \neq i, k} \bar{\rho}_{i' \rightarrow k}, & \text{for } c_i \neq k = i \\ \tilde{\rho}_{k \rightarrow k}(k) + \bar{\rho}_{k \rightarrow k} + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq i, k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i':i' \neq i, k} \max(0, \rho_{i' \rightarrow k}(j')) + \sum_{i':i' \neq i, k} \bar{\rho}_{i' \rightarrow k}, & \text{for } c_i = k \neq i \end{cases} \quad (29)$$

$$\max \left[\begin{array}{l} \sum_{i':i' \neq i} \bar{\rho}_{i' \rightarrow k} \\ \tilde{\rho}_{k \rightarrow k}(k) + \bar{\rho}_{k \rightarrow k} + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq i, k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i':i' \neq i, k} \max(0, \rho_{i' \rightarrow k}(j')) + \sum_{i':i' \neq i, k} \bar{\rho}_{i' \rightarrow k} \end{array} \right], \quad \text{for } c_i \neq k \neq i$$

下面求解 $\tilde{\rho}_{i \rightarrow k}(c_i = k) = \rho_{i \rightarrow k}(c_i = k) - \bar{\rho}_{i \rightarrow k}$ 和 $\tilde{\alpha}_{i \leftarrow k}(c_i = k) = \alpha_{i \leftarrow k}(c_i = k) - \bar{\alpha}_{i \leftarrow k}$, 以得到更简单的迭代公式:

$$\begin{aligned} \tilde{\rho}_{i \rightarrow k}(c_i = k) &= \rho_{i \rightarrow k}(c_i = k) - \bar{\rho}_{i \rightarrow k} \\ &= \rho_{i \rightarrow k}(k) - \max_{j:j \neq k} \rho_{i \rightarrow k}(j) \\ &= s(i, c_i) + s'(i, c'_i) + \sum_{k':k' \neq k} \bar{\alpha}_{i \leftarrow k'} + [c_i \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I - \max_{j:j \neq k} \left[s(i, j) + s'(i, c'_j) + \tilde{\alpha}_{i \leftarrow j}(j) + \sum_{k':k' \neq k} \bar{\alpha}_{i \leftarrow k'} \right] \end{aligned} \quad (30)$$

$$\begin{aligned} \tilde{\alpha}_{i \leftarrow k}(c_i = k) &= \alpha_{i \leftarrow k}(c_i = k) - \bar{\alpha}_{i \leftarrow k} \\ &= \begin{cases} [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i':i' \neq i, k} \max(0, \tilde{\rho}_{i' \rightarrow k}(j')) + \sum_{i':i' \neq i, k} \bar{\rho}_{i' \rightarrow k} - \sum_{j':j' \neq k} \bar{\rho}_{j' \rightarrow k}, & \text{for } k = i \\ \tilde{\rho}_{k \rightarrow k}(k) + \bar{\rho}_{k \rightarrow k} + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq i, k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i':i' \neq i, k} \max(0, \rho_{i' \rightarrow k}(j')) + \sum_{i':i' \neq i, k} \bar{\rho}_{i' \rightarrow k} - \Omega, & \text{for } k \neq i \end{cases} \end{aligned} \quad (31)$$

这里的 Ω 可以表示为

$$\max \left[\begin{array}{l} \sum_{j':j' \neq k} \bar{\rho}_{j' \rightarrow k} \\ \tilde{\rho}_{k \rightarrow k}(k) + \bar{\rho}_{k \rightarrow k} + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq i, k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \bar{\rho}_{i' \rightarrow k} + \lambda_2 \cdot I) + \sum_{i':i' \neq i, k} \max(0, \rho_{i' \rightarrow k}(j')) + \sum_{i':i' \neq i, k} \bar{\rho}_{i' \rightarrow k} \end{array} \right].$$

从而,等式(31)可进一步化简为

$$\left\{ \begin{array}{l} [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \lambda_2 \cdot I) + \sum_{i':i' \neq i',k} \max(0, \tilde{\rho}_{i' \rightarrow k}(j')), \quad \text{for } k = i \\ \tilde{\rho}_{k \rightarrow k}(k) + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq i,k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \lambda_2 \cdot I) + \sum_{i':i \neq i',i,k} \max(0, \rho_{i' \rightarrow k}(j')) - \\ \max \left[0, \tilde{\rho}_{k \rightarrow k}(k) + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I + [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq i,k}} (\tilde{\rho}_{i' \rightarrow k}(k) + \lambda_2 \cdot I) + \sum_{i':i \neq i',i,k} \max(0, \rho_{i' \rightarrow k}(j')) \right], \end{array} \right. \quad (32)$$

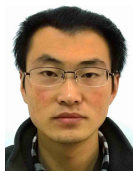
在更新过程中,当 $c_i \neq k$ 时, $\tilde{\rho}_{k \rightarrow i}(c_i)$ 和 $\tilde{\alpha}_{i \leftarrow k}(c_i)$ 并没有使用到(且注意到 $\tilde{\alpha}_{i \leftarrow k}(c_i \neq k) = 0$),因此,传递的消息可以认为是 $r(i, k) = \tilde{\rho}_{k \rightarrow i}(k)$ 和 $a(i, k) = \tilde{\alpha}_{i \leftarrow k}(k)$:

$$r(i, k) = s(i, k) + s'(i, k) + [k \in \text{neb}(c'_k)] \cdot \lambda_2 \cdot I - \max_{j:j \neq k} [s(i, j) + s'(i, j) + a(i, j)] \quad (33)$$

$$a(i, k) = \left\{ \begin{array}{l} [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq k}} (r(i', k) + \lambda_2 \cdot I) + \sum_{i':i' \neq i',k} \max(0, r(i'', k)), \quad k = i \\ \min \left[0, [k \in \text{neb}(c'_k)] \cdot \sum_{\substack{i':s(i',k) \leq \text{maxval}, \\ i' \neq i}} (r(i', k) + \lambda_2 \cdot I) + \sum_{i':i' \neq i'} \max(0, r(i'', k)) \right], \quad k \neq i \end{array} \right. \quad (34)$$

公式(34)就是文中给出的迭代公式.在迭代计算 $a(i, k)$ 更新时, $\min[0, \cdot]$ 的计算由如下等式得到:

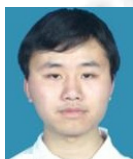
$$x - \max(0, x) = \min(0, x).$$



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