

[Supplementary Material] Submodular Dictionary Learning for Sparse Coding

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1. Proofs of the Monotonicity and Submodularity Properties of Entropy Rate $\mathcal{H}(A)$

Recall our definition of $\mathcal{H}(A)$:

$$\mathcal{H}(A) = - \sum_i \mu_i \sum_j P_{i,j}(A) \log P_{i,j}(A) \quad (1)$$

where μ_i is the stationary probability of v_i in the stationary distribution $\boldsymbol{\mu}$ and $P_{i,j}(A)$ is the transition probability from v_i to v_j with respect to A .

1.1. Monotonicity

We prove that $\mathcal{H}(A)$ is monotonically increasing by showing $\mathcal{H}(A \cup \{a\}) \geq \mathcal{H}(A)$, for all $a \in E \setminus A$ and $A \subseteq E$. Without loss of generality, we assume $a = e_{1,2}$. The weights of the self loops for v_1 and v_2 are given by:

$$w_{1,1} = w_1 - \sum_{j: e_{1,j} \in A \cup \{a\}} w_{1,j}, \quad (2)$$

$$w_{2,2} = w_2 - \sum_{j: e_{2,j} \in A \cup \{a\}} w_{2,j}. \quad (3)$$

By the definition of entropy rate in (1), the increase of entropy rate due to the addition of a to A is computed as:

$$\begin{aligned} \mathcal{H}(A \cup \{a\}) - \mathcal{H}(A) &= - \sum_i \mu_i \sum_j P_{i,j}(A \cup \{a\}) \log P_{i,j}(A \cup \{a\}) \\ &\quad + \sum_i \mu_i \sum_j P_{i,j}(A) \log P_{i,j}(A) \\ &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log P_{i,j}(A \cup \{a\}) \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log P_{i,j}(A) \\ &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \\ &\quad - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i}{w_{all}} \\ &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \\ &\quad + \sum_i \frac{w_i}{w_{all}} \log \frac{w_i}{w_{all}} \left(\sum_j P_{i,j}(A \cup \{a\}) - \sum_j P_{i,j}(A) \right) \end{aligned} \quad (4)$$

$$\begin{aligned} &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \\ &\quad - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i}{w_{all}} \\ &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \\ &\quad + \sum_i \frac{w_i}{w_{all}} \log \frac{w_i}{w_{all}} \left(\sum_j P_{i,j}(A \cup \{a\}) - \sum_j P_{i,j}(A) \right) \end{aligned} \quad (5)$$

$$\begin{aligned} &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \\ &\quad - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i}{w_{all}} \\ &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \\ &\quad + \sum_i \frac{w_i}{w_{all}} \log \frac{w_i}{w_{all}} \left(\sum_j P_{i,j}(A \cup \{a\}) - \sum_j P_{i,j}(A) \right) \end{aligned} \quad (6)$$

$$\begin{aligned} &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \\ &\quad + \sum_i \frac{w_i}{w_{all}} \log \frac{w_i}{w_{all}} \left(\sum_j P_{i,j}(A \cup \{a\}) - \sum_j P_{i,j}(A) \right) \end{aligned} \quad (7)$$

Since $\sum_j P_{i,j}(A \cup \{a\}) = \sum_j P_{i,j}(A) = 1$, the last term in (7) becomes zero. Hence we have

$$\begin{aligned} \mathcal{H}(A \cup \{a\}) - \mathcal{H}(A) &= - \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A \cup \{a\}) \log \frac{w_i P_{i,j}(A \cup \{a\})}{w_{all}} \\ &\quad + \sum_i \sum_j \frac{w_i}{w_{all}} P_{i,j}(A) \log \frac{w_i P_{i,j}(A)}{w_{all}} \end{aligned} \quad (8)$$

We notice that in (8), all the terms associated with vertices other than v_1 and v_2 are canceled out if $a = e_{1,2}$. Thus,

$$\begin{aligned} \mathcal{H}(A \cup \{e_{1,2}\}) - \mathcal{H}(A) &= - \left\{ \frac{w_1}{w_{all}} P_{1,1}(A \cup \{e_{1,2}\}) \log \frac{w_1 P_{1,1}(A \cup \{e_{1,2}\})}{w_{all}} \right. \\ &\quad \left. + \frac{w_1}{w_{all}} P_{1,2}(A \cup \{e_{1,2}\}) \log \frac{w_1 P_{1,2}(A \cup \{e_{1,2}\})}{w_{all}} \right\} \\ &\quad + \left\{ \frac{w_1}{w_{all}} P_{1,1}(A) \log \frac{w_1 P_{1,1}(A)}{w_{all}} \right. \\ &\quad \left. + \frac{w_1}{w_{all}} P_{1,2}(A) \log \frac{w_1 P_{1,2}(A)}{w_{all}} \right\} \\ &\quad - \left\{ \frac{w_2}{w_{all}} P_{2,1}(A \cup \{e_{1,2}\}) \log \frac{w_2 P_{2,1}(A \cup \{e_{1,2}\})}{w_{all}} \right. \\ &\quad \left. + \frac{w_2}{w_{all}} P_{2,2}(A \cup \{e_{1,2}\}) \log \frac{w_2 P_{2,2}(A \cup \{e_{1,2}\})}{w_{all}} \right\} \\ &\quad + \left\{ \frac{w_2}{w_{all}} P_{2,1}(A) \log \frac{w_2 P_{2,1}(A)}{w_{all}} \right. \\ &\quad \left. + \frac{w_2}{w_{all}} P_{2,2}(A) \log \frac{w_2 P_{2,2}(A)}{w_{all}} \right\} \end{aligned} \quad (9)$$

Recall the definition of the transition probability:

$$P_{i,j}(A) = \begin{cases} 1 - \frac{\sum_{j': e_{i,j'} \in A} w_{i,j'}}{w_i} & \text{if } i = j, \\ \frac{w_{i,j}}{w_i} & \text{if } i \neq j, e_{i,j} \in A, \\ 0 & \text{if } i \neq j, e_{i,j} \notin A. \end{cases} \quad (10)$$

Note that $P_{i,j}(A) = 0$ if there is no edge connecting v_i and v_j . Hence, $P_{1,2}(A) = P_{2,1}(A) = 0$. From (2), (3) and the definition of $P_{i,j}$, (9) becomes:

$$\begin{aligned} \mathcal{H}(A \cup \{e_{1,2}\}) - \mathcal{H}(A) &= \frac{w_{1,1} + w_{1,2}}{w_{all}} \log \frac{w_{1,1} + w_{1,2}}{w_{all}} - \frac{w_{1,1}}{w_{all}} \log \frac{w_{1,1}}{w_{all}} - \frac{w_{1,2}}{w_{all}} \log \frac{w_{1,2}}{w_{all}} \\ &\quad + \frac{w_{2,2} + w_{2,1}}{w_{all}} \log \frac{w_{2,2} + w_{2,1}}{w_{all}} - \frac{w_{2,2}}{w_{all}} \log \frac{w_{2,2}}{w_{all}} - \frac{w_{2,1}}{w_{all}} \log \frac{w_{2,1}}{w_{all}} \\ &= f\left(\frac{w_{1,1}}{w_{all}} + \frac{w_{1,2}}{w_{all}}\right) - f\left(\frac{w_{1,1}}{w_{all}}\right) - f\left(\frac{w_{1,2}}{w_{all}}\right) \\ &\quad + f\left(\frac{w_{2,2}}{w_{all}} + \frac{w_{2,1}}{w_{all}}\right) - f\left(\frac{w_{2,2}}{w_{all}}\right) - f\left(\frac{w_{2,1}}{w_{all}}\right) \\ &\geq 0 \end{aligned} \quad (11)$$

$$\begin{aligned} &= f\left(\frac{w_{1,1}}{w_{all}} + \frac{w_{1,2}}{w_{all}}\right) - f\left(\frac{w_{1,1}}{w_{all}}\right) - f\left(\frac{w_{1,2}}{w_{all}}\right) \\ &\quad + f\left(\frac{w_{2,2}}{w_{all}} + \frac{w_{2,1}}{w_{all}}\right) - f\left(\frac{w_{2,2}}{w_{all}}\right) - f\left(\frac{w_{2,1}}{w_{all}}\right) \\ &\geq 0 \end{aligned} \quad (12)$$

$$\geq 0 \quad (13)$$

Note in (12), a convex function $f(x)$ in $(0,1)$ is defined as: $f(x) = x \log x$. It's easy to show that the convex function $f(x)$ is superadditive in $(0,1)$, *i.e.*,

$$\begin{aligned} f(x_1) + f(x_2) &= f\left((x_1 + x_2) \frac{x_1}{x_1 + x_2}\right) + f\left((x_1 + x_2) \frac{x_2}{x_1 + x_2}\right) \\ &\leq \frac{x_1}{x_1 + x_2} f(x_1 + x_2) + \frac{x_2}{x_1 + x_2} f(x_1 + x_2) \\ &= f(x_1 + x_2). \end{aligned} \quad (14)$$

Hence, inequality (13) holds, which completes the proof of the monotonically increasing property of $\mathcal{H}(A)$.

1.2. Submodularity

We prove $\mathcal{H}(A)$ is a submodular function by showing

$$\begin{aligned} \mathcal{H}(A \cup \{a_1\}) - \mathcal{H}(A) \\ \geq \mathcal{H}(A \cup \{a_1, a_2\}) - \mathcal{H}(A \cup \{a_2\}), \quad \forall a_1, a_2 \in E \setminus A \end{aligned} \quad (15)$$

Based on whether a_1, a_2 have a common vertex or not, we compare the value of $\mathcal{H}(A \cup \{a_1\}) - \mathcal{H}(A)$ with the value of $\mathcal{H}(A \cup \{a_1, a_2\}) - \mathcal{H}(A \cup \{a_2\})$ in two cases.

- **Case1:** a_1, a_2 share no common vertex. Without loss of generality, we assume $a_1 = e_{1,2}$ and $a_2 = e_{3,4}$. According to (9), adding a_1 to A causes the same weight changes as adding a_1 to $A \cup \{a_2\}$ because the addition of a_2 has no effect on the loop weights of v_1 and v_2 .

$$\begin{aligned} &\mathcal{H}(A \cup \{a_1, a_2\}) - \mathcal{H}(A \cup \{a_2\}) \\ &= \frac{w_{1,1} + w_{1,2}}{w_{all}} \log \frac{w_{1,1} + w_{1,2}}{w_{all}} - \frac{w_{1,1}}{w_{all}} \log \frac{w_{1,1}}{w_{all}} - \frac{w_{1,2}}{w_{all}} \log \frac{w_{1,2}}{w_{all}} \\ &+ \frac{w_{2,2} + w_{2,1}}{w_{all}} \log \frac{w_{2,2} + w_{2,1}}{w_{all}} - \frac{w_{2,2}}{w_{all}} \log \frac{w_{2,2}}{w_{all}} - \frac{w_{2,1}}{w_{all}} \log \frac{w_{2,1}}{w_{all}} \end{aligned} \quad (16)$$

Thus, $\mathcal{H}(A \cup \{a_1\}) - \mathcal{H}(A) = \mathcal{H}(A \cup \{a_1, a_2\}) - \mathcal{H}(A \cup \{a_2\})$

- **Case2:** a_1, a_2 share a common vertex. Without loss of generality, We assume $a_1 = e_{1,2}$ and $a_2 = e_{1,3}$. Then the new loop weights for vertex v_1 and v_2 are given by:

$$w'_{1,1} = w_1 - \sum_{j: e_{1,j} \in A \cup \{e_{1,2}, e_{1,3}\}} w_{1,j} = w_{1,1} - w_{1,3} \quad (17)$$

$$w'_{2,2} = w_2 - \sum_{j: e_{2,j} \in A \cup \{e_{1,2}, e_{1,3}\}} w_{2,j} = w_{2,2}, \quad (18)$$

where $w_{1,1}$ and $w_{2,2}$ here are given by (2) and (3).

Hence

$$\begin{aligned} &(\mathcal{H}(A \cup \{a_1\}) - \mathcal{H}(A)) - (\mathcal{H}(A \cup \{a_1, a_2\}) - \mathcal{H}(A \cup \{a_2\})) \\ &= \left\{ \frac{w_{1,1} + w_{1,2}}{w_{all}} \log \frac{w_{1,1} + w_{1,2}}{w_{all}} - \frac{w_{1,1}}{w_{all}} \log \frac{w_{1,1}}{w_{all}} - \frac{w_{1,2}}{w_{all}} \log \frac{w_{1,2}}{w_{all}} \right. \\ &\quad \left. + \frac{w_{2,2} + w_{2,1}}{w_{all}} \log \frac{w_{2,2} + w_{2,1}}{w_{all}} - \frac{w_{2,2}}{w_{all}} \log \frac{w_{2,2}}{w_{all}} - \frac{w_{2,1}}{w_{all}} \log \frac{w_{2,1}}{w_{all}} \right\} \\ &- \left\{ \frac{w'_{1,1} + w_{1,2}}{w_{all}} \log \frac{w'_{1,1} + w_{1,2}}{w_{all}} - \frac{w'_{1,1}}{w_{all}} \log \frac{w'_{1,1}}{w_{all}} - \frac{w_{1,2}}{w_{all}} \log \frac{w_{1,2}}{w_{all}} \right. \\ &\quad \left. + \frac{w_{2,2} + w_{2,1}}{w_{all}} \log \frac{w_{2,2} + w_{2,1}}{w_{all}} - \frac{w_{2,2}}{w_{all}} \log \frac{w_{2,2}}{w_{all}} - \frac{w_{2,1}}{w_{all}} \log \frac{w_{2,1}}{w_{all}} \right\} \end{aligned} \quad (19)$$

$$\begin{aligned} &= \left\{ \frac{w_{1,1} + w_{1,2}}{w_{all}} \log \frac{w_{1,1} + w_{1,2}}{w_{all}} - \frac{w_{1,1}}{w_{all}} \log \frac{w_{1,1}}{w_{all}} \right\} \\ &- \left\{ \frac{w'_{1,1} + w_{1,2}}{w_{all}} \log \frac{w'_{1,1} + w_{1,2}}{w_{all}} - \frac{w'_{1,1}}{w_{all}} \log \frac{w'_{1,1}}{w_{all}} \right\} \end{aligned} \quad (20)$$

$$= g\left(\frac{w'_{1,1} + w_{1,2}}{w_{all}}\right) - g\left(\frac{w'_{1,1}}{w_{all}}\right) \quad (21)$$

$$\geq 0 \quad (22)$$

From (20) to (21), the relationship between $w_{1,1}$ and $w'_{1,1}$ given in (17) is employed. And $g(x)$ in (21) is defined as:

$$g(x) = (x + \delta) \log(x + \delta) - x \log x \quad (23)$$

Here $\delta = \frac{w_{1,2}}{w_{all}}$. By taking advantage of the strictly increasing property of $g(x)$, we arrive at (22).

Showing the two cases above, we conclude that $\mathcal{H}(A)$ is a submodular function.

2. Proofs of the Monotonicity and Submodularity Properties of Discriminative Term $\mathcal{Q}(A)$

Recall our definition,

$$\mathcal{Q}(A) = \frac{1}{C} \sum_{i=1}^{N_A} \max_y N_y^i - N_A \quad (24)$$

where $\max_y N_y^i$ denotes the maximum element of the count vector $\mathbf{N}^i = [N_1^i, \dots, N_m^i]^t$ for cluster S_i , N_A is the number of connected components.

2.1. Monotonicity

We prove that $\mathcal{Q}(A)$ is monotonically increasing by showing:

$$\mathcal{Q}(A \cup \{a\}) \geq \mathcal{Q}(A), \quad (25)$$

for all $a \in E \setminus A$ and $A \subseteq E$.

Given any set of selected edges A and its corresponding graph partitioning $\mathcal{S}_A = \{S_1, \dots, S_{N_A}\}$, we are only interested in the nontrivial case in which the two vertices of a belong to different clusters. Otherwise the addition of edge a has no impact on the graph partitioning, *i.e.*, $\mathcal{Q}(A \cup \{a\}) - \mathcal{Q}(A) = 0$.

Without loss of generality, we assume $a = e_{1,2}$, v_1 and v_2 belong to S_i and S_j , respectively. The new graph partitioning $\mathcal{S}_{A \cup \{e_{1,2}\}}$ for $A \cup \{e_{1,2}\}$ is similar to the graph partitioning \mathcal{S}_A for A except one thing: clusters S_i and S_j are merged into one cluster S_* . Hence,

$$\begin{aligned} \mathcal{Q}(A \cup \{a = e_{1,2}\}) - \mathcal{Q}(A) &= \left(\frac{1}{C} \sum_{k=1}^{N_A-1} \max_y N_y^k - (N_A - 1)\right) \\ &\quad - \left(\frac{1}{C} \sum_{k=1}^{N_A} \max_y N_y^k - N_A\right) \\ &= \frac{1}{C} (\max_y [N_y^i + N_y^j] - \max_y N_y^i - \max_y N_y^j) + 1 \\ &= \frac{1}{C} (\max_y N_y^* - \max_y N_y^i - \max_y N_y^j) + 1 \end{aligned} \quad (26)$$

By definition,

$$C = \sum_i \sum_y N_y^i \geq \max_y N_y^i + \max_y N_y^j \quad (27)$$

and with

$$\max_y N_y^* \geq 0,$$

so (26) becomes

$$\mathcal{Q}(A \cup \{a\}) - \mathcal{Q}(A) \geq \frac{1}{C} (0 - C) + 1 = 0 \quad (28)$$

This completes the proof of monotonically increasing property of $\mathcal{Q}(A)$.

2.2. Submodularity

Before starting the proof of submodularity, we want to introduce the following two properties of a count vector $\mathbf{N}^i = [N_1^i, \dots, N_m^i]^t$.

(1) (Nonnegative) The elements of the count vector are all nonnegative, $N^i \geq 0, i = 1, \dots, N$.

(2) (Subadditivity) Given the new cluster S_* by merging clusters S_i and S_j , the count of the dominating class for cluster S_* is less than the sum of the counts of the dominating class for S_i and S_j , *i.e.*,

$$\max_y [N_y^i + N_y^j] \leq \max_y N_y^i + \max_y N_y^j, \quad (29)$$

with equality holds only when

$$\arg \max_y N_y^i = \arg \max_y N_y^j$$

Now we prove that $\mathcal{Q}(A)$ is submodular by showing

$$\begin{aligned} \mathcal{Q}(A \cup \{a_1\}) - \mathcal{Q}(A) &\geq \mathcal{Q}(A \cup \{a_1, a_2\}) - \mathcal{Q}(A \cup \{a_2\}) \\ &\quad \forall a_1, a_2 \in E \setminus A \end{aligned} \quad (30)$$

Again we consider only the nontrivial case in which edge a_1 combines two different subsets S_i and S_j . When $i = j$, $\mathcal{Q}(A \cup \{a_1\}) - \mathcal{Q}(A) = \mathcal{Q}(A \cup \{a_1, a_2\}) - \mathcal{Q}(A \cup \{a_2\}) = 0$.

Suppose the vertices of a_2 belong to clusters S_m, S_n , respectively. Based on the relationship among i, j, m, n ($i \neq j$), we discuss in the following four cases.

- **Case1 (trivial):** $m = n$, *i.e.*, the vertices of a_2 belong to the same cluster. Then adding a_2 has no effect on the graph:

$$\begin{aligned} \mathcal{Q}(A \cup \{a_2\}) &= \mathcal{Q}(A), \\ \mathcal{Q}(A \cup \{a_1, a_2\}) &= \mathcal{Q}(A \cup \{a_1\}) \end{aligned} \quad (31)$$

Thus $\mathcal{Q}(A \cup \{a_1\}) - \mathcal{Q}(A) = \mathcal{Q}(A \cup \{a_1, a_2\}) - \mathcal{Q}(A \cup \{a_2\})$.

- **Case2 (trivial):** $m \neq n$, $\{m, n\} = \{i, j\}$, *i.e.*, adding a_2 to the graph has the same effect as adding a_1 . Thus,

$$\mathcal{Q}(A \cup \{a_2\}) = \mathcal{Q}(A \cup \{a_1, a_2\}) \quad (32)$$

Together with monotonically increasing property in (28), we have

$$(\mathcal{Q}(A \cup \{a_1\}) - \mathcal{Q}(A)) \geq \mathcal{Q}(A \cup \{a_1, a_2\}) - \mathcal{Q}(A \cup \{a_2\}) = 0 \quad (33)$$

- **Case3:** $\{m, n\} \cap \{i, j\} = \emptyset$, *i.e.*, a_2 combines two clusters S_m, S_n that are not S_i, S_j .

$$\begin{aligned} &\mathcal{Q}(A \cup \{a_1, a_2\}) - \mathcal{Q}(A \cup \{a_2\}) \\ &= \frac{1}{C} \left\{ \max_y [N_y^i + N_y^j] + \max_y [N_y^m + N_y^n] \right. \\ &\quad \left. - \max_y N_y^i - \max_y N_y^j - \max_y [N_y^m + N_y^n] \right\} + 1 \end{aligned} \quad (34)$$

$$\begin{aligned} &= \frac{1}{C} \left\{ \max_y [N_y^i + N_y^j] - \max_y N_y^i - \max_y N_y^j \right\} + 1 \\ &= \mathcal{Q}(A \cup \{a_1\}) - \mathcal{Q}(A) \end{aligned} \quad (35)$$

- **Case4:** $m \in \{i, j\}$, and $n \notin \{i, j\}$. Without loss of generality, we assume $m = i, n = k \neq i, j$, *i.e.*, a_2 combines two subsets S_i, S_k .

$$\begin{aligned} &(\mathcal{Q}(A \cup \{a_1\}) - \mathcal{Q}(A)) - (\mathcal{Q}(A \cup \{a_1, a_2\}) - \mathcal{Q}(A \cup \{a_2\})) \\ &= \frac{1}{C} \left\{ \max_y [N_y^i + N_y^j] - \max_y N_y^i - \max_y N_y^j \right\} + 1 \\ &\quad - \frac{1}{C} \left\{ \max_y [N_y^i + N_y^j + N_y^k] - \max_y [N_y^i + N_y^j] - \max_y N_y^k \right\} - 1 \\ &= \frac{1}{C} \left\{ \left(\max_y [N_y^i + N_y^j] - \max_y N_y^i \right) \right. \\ &\quad \left. - \left(\max_y [N_y^i + N_y^k + N_y^j] - \max_y [N_y^i + N_y^k] \right) \right\} \end{aligned} \quad (36)$$

Based on the dominating class labels of cluster S_i, S_j and S_k , we compare the values of $(\max_y [N_y^i + N_y^j] - \max_y N_y^i)$ and $(\max_y [N_y^i + N_y^k + N_y^j] - \max_y [N_y^i + N_y^k])$ in the following three situations:

(a) $\arg \max_y N_y^i = \arg \max_y N_y^j$

In this case, S_i and S_j share the same dominating class. From (29) we have,

$$\max_y [N_y^i + N_y^j] - \max_y N_y^i = \max_y N_y^j \quad (37)$$

$$\max_y [N_y^i + N_y^k + N_y^j] - \max_y [N_y^i + N_y^k] \leq \max_y N_y^j \quad (38)$$

This implies that (36) is ≥ 0 .

(b) $\arg \max_y N_y^i \neq \arg \max_y N_y^j, \max_y N_y^i \geq \max_y N_y^j$

In this case S_i, S_j do not share the same dominating class, and the dominating class label of S_i will become the dominating class label for the merged cluster of S_i, S_j . Therefore, $\max_y [N_y^i + N_y^j] - \max_y N_y^i = 0$.

Note that the dominating class labels of S_j and S_k must not be the same. If S_j, S_k shares the same dominating class label and S_i has a different dominating class label, then according to the proposed greedy algorithm, the edge connecting S_j, S_k (referred to as a_3) must already exist in A before considering a_1, a_2 . However, cycle-free constraint requires that a_1, a_2, a_3 cannot exist at the same time. By this contradiction, we conclude that S_j, S_k must have different dominating class labels.

Moreover, taking $\arg \max_y N_y^i \neq \arg \max_y N_y^j$ into consideration, the dominating class, after merging S_i, S_j , and S_k , can only be either $\arg \max_y N_y^i$ or $\arg \max_y N_y^k$, in both case of which we have

$$\max_y [N_y^i + N_y^k + N_y^j] = \max_y [N_y^i + N_y^k], \quad (39)$$

which yields that $\max_y [N_y^i + N_y^j] - \max_y N_y^i = \max_y [N_y^i + N_y^k + N_y^j] - \max_y [N_y^i + N_y^k] = 0$. Thus, (36) is $= 0$.

(c) $\arg \max_y N_y^i \neq \arg \max_y N_y^j$, $\max_y N_y^i < \max_y N_y^j$

In this case, the dominating class label for S_j becomes the dominating class label for the merged cluster of S_i, S_j , *i.e.*,

$$\max_y [N_y^i + N_y^j] - \max_y N_y^i = \max_y N_y^j \quad (40)$$

Again according to (29),

$$\max_y [N_y^i + N_y^k + N_y^j] - \max_y [N_y^i + N_y^k] \leq \max_y N_y^j \quad (41)$$

which implies (36) is ≥ 0 .

From the discussion above we prove that (36) is always ≥ 0 , *i.e.*,

$$\mathcal{Q}(A \cup \{a_1\}) - \mathcal{Q}(A) \geq \mathcal{Q}(A \cup \{a_1, a_2\}) - \mathcal{Q}(A \cup \{a_2\}).$$

Summarizing the four cases above, we conclude that $\mathcal{Q}(A)$ is a submodular function.

3. Proof of Matroid

We claim that the cycle free constraint and the connected component constraint induce a matroid $\mathcal{M} = (E, \mathcal{I})$, where E is the edge set, and \mathcal{I} is the collection of subsets $A \subseteq E$ which satisfies (a) A is cycle-free, and (b) the graph partition from A has more than K connected components, *i.e.*, $N_A \geq K$.

\mathcal{M} satisfies the following three conditions:

- $\emptyset \in \mathcal{I}$: It's obvious that the empty set \emptyset induces no cycles. The graph associated with \emptyset has $N_\emptyset = |V|$ connected components, where the total number of nodes $|V| \geq K$. Therefore $\emptyset \in \mathcal{I}$.

- (Hereditary property): Assume $A \in \mathcal{I}$, and $B \subseteq A$. Denote the the graphs associated with edge set A, B as G_A and G_B respectively. Under our constraints (*i.e.*, $A \in \mathcal{I}$) G_A is cycle free, and $N_A \geq K$. B also satisfies $B \in \mathcal{I}$ because: (a) G_B is cycle free, since removing edges from G_A cannot create cycles. (b) $N_B \geq K$, since removing edges from G_A cannot decrease the number of connected components.
- (Exchange property): Suppose $A \in \mathcal{I}$, $B \in \mathcal{I}$, and $|A| < |B|$. Denote the the graphs associated with A, B as G_A, G_B respectively. Clearly G_A has $N_A = |V| - |A|$ connected components, and G_B has $N_B = |V| - |B|$ connected components, where $N_A > N_B$. This means G_B has fewer connected components than G_A , *i.e.*, G_B must contain some connected components, S_i , whose vertices are in two different connected components in G_A . Moreover, since S_i is connected, there must exist an edge $x \in B$ such that x connects two vertices in two different components in G_A . We can add that edge x without creating a cycle. Since $N_A \geq K$, $N_B \geq K$, and $N_A > N_B$, it must be true that $N_A \geq K + 1$. Moreover, adding one edge to a graph decreases the number of connected components by at most one. Hence $N_{A \cup \{x\}} \geq K$, which satisfies the connected component constraint. With that being said, for $A, B \in \mathcal{I}$, and $|A| < |B|$, there exists an element $x \in B - A$ such that $A \cup \{x\} \in \mathcal{I}$

With the three conditions satisfied, we conclude that $\mathcal{M} = (E, \mathcal{I})$ is a matroid.