## Fast and exact search for the partition with minimal information loss

Shohei Hidaka ${ }^{1 *}$, Masafumi Oizumi ${ }^{2,3}$,<br>1 Japan Advanced Institute of Science and Technology, Nomi-shi, Ishikawa, Japan<br>2 Araya Inc., Minato-ku, Tokyo, Japan<br>3 RIKEN Brain Science Institute, Wako-shi, Saitama, Japan<br>*shhidaka@jaist.ac.jp

## Supporting information 2: Extension to $k$-partition algorithm

The Queyranne's algorithm [1] works on minimization of $g(U)=f(U)+f(V \backslash U)$ with respect to non-empty set $U \subset V$ or $g((U, V \backslash U)=f(U)+f(V \backslash U)$ over bi-partition $(U, V \backslash U)$ with an arbitrary submodular set function $f$. Here we show a recursive method extending this symmetric submodular search over a set of bi-partitions to that of 3 -partitions. The following argument will be easily extended to that of $k$-partition.

First let us denote the set of $k$-partitions of a given set $V$ by
$P_{k, V}:=\left\{\left(M_{0}, M_{1}, \ldots, M_{k-1}\right) \mid \bigcup_{i} M_{i}=V, M_{i} \cap M_{j}=\emptyset\right.$ for any $i \neq j$ and, $M_{i} \neq \emptyset$ for every $\left.i\right\}$
For a submodular system $(V, f)$ of a given underlying set $V$ and a submodular set function $f: 2^{V} \mapsto \mathbb{R}$, we consider minimization of function $g: P_{3, V} \mapsto \mathbb{R}$ of the form

$$
\begin{equation*}
g\left(\left(M_{0}, M_{1}, M_{2}\right)\right)=\sum_{i=0}^{2} f\left(M_{i}\right)+c \tag{1}
\end{equation*}
$$

where $c \in \mathbb{R}$ is a constant. This is an extension of the bi-partition function algorithm to minimize this $k$-partition function by employing Queyranne's algorithm.

By defining $f(M):=H(M)$ for $M \subseteq V,(V, f)$ is a submodular system, and the information loss function is written with a constant $c=-f(V)$ by

$$
g\left(\left(M_{0}, M_{1}, M_{2}\right)\right)=\sum_{i=0}^{2} f\left(M_{i}\right)-f(V)
$$

For the special case $k=2, g\left(\left(M_{0}, M_{1}\right)\right)=I\left(M_{0} ; M_{1}\right)$, this is identical to the minimal loss of information introduced in this study.

Our argument below does not depend on any specific form of a particular
submodular function $f$, as long as the objective function takes the form in (1). The basic idea is to reduce the original objective function $g: P_{3, V} \mapsto \mathbb{R}$ to a set function

$$
\begin{equation*}
g_{3, V}(U):=f_{V}(U)+h_{2, V}(U) \tag{2}
\end{equation*}
$$

where for any $\emptyset \subset U_{1} \subset U_{2}, f_{U_{2}}\left(U_{1}\right):=f\left(U_{1}\right)+f\left(U_{2} \backslash U_{1}\right)$ and $h_{1, U_{2}}\left(U_{1}\right):=0$ and

$$
h_{2, U_{2}}\left(U_{1}\right):=\left\{\begin{array}{ll}
\min \begin{cases}\min _{\emptyset \subset U^{\prime} \subset U_{2} \backslash U_{1}} g_{2, U_{2} \backslash U_{1}}\left(U^{\prime}\right) \\
\min _{\emptyset \subset U^{\prime} \subset U_{1}} g_{2, U_{1}}\left(U^{\prime}\right)\end{cases} & \left(\min \left(\left|U_{1}\right|,\left|U_{2} \backslash U_{1}\right|\right)>1\right)  \tag{3}\\
\min _{\emptyset \subset U^{\prime} \subset U_{2} \backslash U_{1}} g_{2, U_{2} \backslash U_{1}}\left(U^{\prime}\right) & \left(\left|U_{1}\right|=1\right) \\
\min _{\emptyset \subset U^{\prime} \subset U_{1}} g_{2, U}\left(U^{\prime}\right) & \left(\left|U_{2} \backslash U_{1}\right|=1\right)
\end{array} .\right.
$$

This function (2) can be interpreted as recursive bi-partitioning across multiple stages: The first partition $(U, V \backslash U)$ of the set $V$ is made on $f_{V}$, and the second partition ( $U^{\prime}, \bar{U}^{\prime}$ ) of either $U$ or $V \backslash U$ on $h_{k-1}$, and so forth. For $|U|=1$ or $|V \backslash U|=1$, there is only one set for which the second partition can be made, otherwise smaller one of either $f_{U}\left(M_{0}\right)$ or $f_{V \backslash U}\left(M_{0}\right)$ has the solution. For $k=2, g_{2, V}(U)=f_{V}(U)$, and minimization of $f_{V}(U)$ over the set of bi-partitions of $V$ can be computed by the Queyranne's algorithm.

If this function $g_{3, V}$ is symmetric and submodular, we can apply the Queyranne's algorithm to this function at every recursive step above. Then, the minimum of $g_{3, V}(\hat{U})$ is identical to $g\left(\left(\hat{U}, M_{0}, M_{1}\right)\right)$ with the 3 -partition is ( $\left.\hat{U}, \hat{M}_{0}, \hat{M}_{1}\right)$ such that

$$
\hat{U}=\underset{\emptyset \subset U \subset V}{\arg \min } g_{3, V}(U) \text { and }\left(\hat{M}_{0}, \hat{M}_{1}\right)=\underset{\left(M_{0}, M_{1}\right) \in P_{2, V \backslash \hat{U}}}{\arg \min } h_{2}\left(M_{0}, M_{1}\right)
$$

or $\left(V \backslash \hat{U}, \hat{M}_{0}, \hat{M}_{1}\right)$ such that

$$
\hat{U}=\underset{\emptyset \subset U \subset V}{\arg \min } g_{3, V}(U) \text { and }\left(\hat{M}_{0}, \hat{M}_{1}\right)=\underset{\left(M_{0}, M_{1}\right) \in P_{2, \hat{U}}}{\arg \min } h_{2}\left(M_{0}, M_{1}\right) .
$$

As $g_{k, V}$ is obviously symmetric by definition, our main question now is whether it is submodular. The lemma following states that it is submodular.
Lemma 1. For a given submodular system $(V, f)$, the function $g_{3, V}: 2^{V} \mapsto \mathbb{R}$ is submodular.

The proof of Lemma 1 needs Lemma 2 which is stated after the proof.
Proof. For a pair of set $X, Y \subseteq V$ and $k>2$, consider the difference

$$
\Delta:=g_{3, V}(X)+g_{3, V}(Y)-g_{3, V}(X \cup Y)-g_{3, V}(X \cap Y)
$$

and

$$
\Delta_{h}:=h_{3, V}(X)+h_{3, V}(Y)-h_{3, V}(X \cup Y)-h_{3, V}(X \cap Y)
$$

As $\Delta-\Delta_{h} \geq 0$ due to submodularity of the function $f, \Delta_{h} \geq 0$ implies $\Delta \geq 0$ for any $k$. We show $\Delta_{h} \geq 0$ as follows. Now we will show that $\Delta_{h} \geq 0$, by using the fact that any function $g_{2, U}$ for $U \subseteq V$ is submodular.

Let us denote the minimizer of $g_{3, X}$ by

$$
[X]:=\underset{\emptyset \subset W \subset X}{\arg \min } g_{3, X}(W) .
$$

For all three cases of the function $h$ (3), we consider the case below as the lower bound for $\Delta_{h}$, and the other cases follow the essentially same argument:

$$
\Delta_{h} \geq g_{3, X}([X])+g_{3, Y}([Y])-g_{3, X \cup Y}([X \cup Y])-g_{3, X \cap Y}([X \cap Y])
$$

By definition, $g_{3, X}([X]) \leq g_{3, X}(W)$ for any non-empty $W \subset X$, and thus for any

$$
\Delta_{h, 3} \geq g_{3, X}([X])+g_{3, Y}([Y])-g_{3, X \cup Y}(W)-g_{3, X \cap Y}(Z) .
$$

By Lemma 2, $\Delta_{h} \geq 0$ due to submodularity of $g_{2, U}$ for any $U \subseteq V$.

The last line in the proof of Lemma 1 is shown as follows.
Lemma 2. For an arbitrary submodular system $(V, f), f(\emptyset)=0$ and $\emptyset \subset W \subset Z \subseteq V$, write

$$
f_{Z}(W):=f(W)+f(Z \backslash W)
$$

For any given pair of partitions $(W, \bar{W}) \in P_{2, X \cup Y}$ and $(Z, \bar{Z}) \in P_{2, X \cap Y}$, there is some pair $(A, \bar{A}) \in P_{2, X}$ and $(B, \bar{B}) \in P_{2, Y}$ which holds the inequality

$$
f_{X}(A)+f_{Y}(B) \geq f_{X \cup Y}(W)+f_{X \cap Y}(Z)
$$

Vice versa, for any given pair of partitions $(A, \bar{A}) \in P_{2, X}$ and $(B, \bar{B}) \in P_{2, Y}$, there is some pair $(W, \bar{W}) \in P_{2, X \cup Y}$ and $(Z, \bar{Z}) \in P_{2, X \cap Y}$ which holds the inequality above.

This lemma states about a kind of submodularity on the bi-partition function $f_{X}$ by existence of some pair $W$ and $Z$ for any pair $A$ and $B$ or vice versa. The proof of Lemma 2 is beyond the scope of this section, and will be reported elsewhere.

The Lemma 1 states that Queyranne's algorithm can be used to minimize the symmetric submodular set function $g_{m, U}\left(U^{\prime}\right)$ with respect to non-empty $U^{\prime} \subset U$ at each step of the function $g_{k, V}(U)$. This observation further applies recursively for a $k$-partition problem, which can be reduced to the minimization of $(k-1)$-partition problem by defining an appropriate function. As minimization of a $k$-partition function includes the minimization of $(k-1)$-partition function, the computational time of this recursive algorithm for the minimal $k$-partition of $n$ elements would take the order $O\left(n^{3(k-1)}\right)$.

## References

1. Queyranne M. Minimizing symmetric submodular functions. Mathematical Programming. 1998;82(1-2):3-12.
