## Greedy Modality Selection via Approximate Submodular Maximization (Supplementary material)

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## **1 PRELIMINARY FOR MISSING PROOFS**

**Proposition 1.1.** Let  $X, Y \in \{0, 1\}$  be random variables,  $\mathcal{H}$  be the class of functions of X such that  $\forall h \in \mathcal{H}, h(X) \in [0, 1]$ , and  $\ell(\cdot, \cdot)$  be the cross-entropy loss. We have:

$$\inf_{h \in \mathcal{H}} \mathbb{E}[\ell(Y, h(X))] = H(Y \mid X) \tag{1}$$

*Proof.* Let  $x, \hat{y}$  be the instantiation of  $X, \hat{Y}$  respectively, where  $\hat{Y} \coloneqq h(X)$ .  $\mathbb{1}(\cdot)$  denotes the indicator function, and  $D_{\mathrm{KL}}(\cdot \parallel \cdot)$  denotes the Kullback–Leibler divergence.

$$\mathbb{E}_{\mathcal{D}}[\ell(Y, h(X))] = \mathbb{E}_{X, Y}[-\mathbb{1}(Y=1)\log\hat{Y} - \mathbb{1}(Y=0)\log(1-\hat{Y})]$$
(2)

$$= -\mathbb{E}_{X}[\mathbb{E}_{Y|x}[\mathbb{1}(Y=1)\log\hat{y} + \mathbb{1}(Y=0)\log(1-\hat{y})]]$$
(3)

$$= -\mathbb{E}_{X}[\Pr(Y=1 \mid x) \log \hat{y} + \Pr(Y=0 \mid x) \log(1-\hat{y})]$$
(4)

$$= \mathbb{E}_{X} \left[ \Pr(Y = 1 \mid x) \log \frac{1}{\hat{y}} + \Pr(Y = 0 \mid x) \log \frac{1}{1 - \hat{y}} \right]$$
(5)

$$= \mathbb{E}_X[\Pr(Y=1 \mid x) \log \frac{\Pr(Y=1 \mid x)}{\hat{y}} + \Pr(Y=0 \mid x) \log \frac{\Pr(Y=0 \mid x)}{1-\hat{y}}]$$
(6)

$$+\mathbb{E}_{X}[-\Pr(Y=1 \mid x)\log\Pr(Y=1 \mid x) - \Pr(Y=0 \mid x)\log\Pr(Y=0 \mid x)]$$
(7)

$$\mathbb{E}_X[D_{\mathrm{KL}}(\Pr(Y \mid x) \parallel h(x))] + \mathbb{E}_X[H(Y \mid x)]$$
(8)

$$= D_{\mathrm{KL}}(\Pr(Y \mid X) \parallel h(X)) + H(Y \mid X)$$
(9)

Since  $H(Y \mid X) \ge 0$  and is unrelated to h(X),  $\mathbb{E}_{\mathcal{D}}[\ell(Y, h(X))]$  is minimum when  $h(X) = \Pr(Y \mid X)$ .

## 2 MISSING PROOFS

**Proposition 2.1.** Given  $Y \in \{0,1\}$  and  $\ell(Y,\hat{Y}) \coloneqq \mathbb{1}(Y=1)\log \hat{Y} + \mathbb{1}(Y=0)\log(1-\hat{Y}), f_u(S) = I(S;Y).$ 

*Proof.* By Definition 3.1 and Proposition 1.1, we have:

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$$f_u(S) = \inf_{h \in \mathcal{H}} \mathbb{E}[\ell(Y, c)] - \inf_{h \in \mathcal{H}} \mathbb{E}[\ell(Y, h(S))]$$
(10)

$$=H(Y \mid c) - H(Y \mid S) \tag{11}$$

$$=H(Y) - H(Y \mid S) \tag{12}$$

$$=I(S;Y) \tag{13}$$

\*Equal contribution.

**Proposition 2.2.**  $\forall M \subseteq N \subseteq V$ ,  $I(N;Y) - I(M;Y) = I(N \setminus M;Y \mid M) \ge 0$ .

*Proof.* Let  $N := \{X_1, ..., X_n\}, M := \{X_1, ..., X_m\}, n \ge m.$ 

$$I(N;Y) - I(M;Y) = \sum_{i=1}^{n} I(X_i;Y \mid X_{i-1},...,X_1) - \sum_{i=1}^{m} I(X_i;Y \mid X_{i-1},...,X_1)$$
(14)

$$= \sum_{i=m+1}^{n} I(X_i; Y \mid X_{i-1}, ..., X_1)$$
(15)

$$= I(N \setminus M; Y \mid M)$$

$$\geq 0$$
(16)
(17)

**Proposition 2.3.** Under Assumption 2.1, I(S;Y) is  $\epsilon$ -approximately submodular, i.e.,  $\forall A \subseteq B \subseteq V, e \in V \setminus B$ ,  $I(A \cup \{e\}; Y) - I(A; Y) + \epsilon \ge I(B \cup \{e\}; Y) - I(B; Y).$ 

*Proof.* For subset A, we have:

$$I(A \cup \{e\}; Y) - I(A; Y) = I(\{e\}; Y \mid A)$$
(18)

$$= I(\{e\}; Y, A) - I(\{e\}; A)$$
(19)

$$= I(\{e\}; Y) + I(\{e\}; A \mid Y) - I(\{e\}; A)$$
(20)

Similarly,  $I(B \cup \{e\}; Y) - I(B; Y) = I(\{e\}; Y) + I(\{e\}; B \mid Y) - I(\{e\}; B)$ . Given Assumption 2.1 holds, we denote  $I(\{e\}; A \mid Y) = \epsilon_A$  and  $I(\{e\}; B \mid Y) = \epsilon_B$  where  $\epsilon_A, \epsilon_B \leq \epsilon$ . In the worst case where  $\epsilon_A = 0$ , absolute submodularity is still satisfied if  $\epsilon_B \leq I(\{e\}; B) - I(\{e\}; A)$ , i.e.,

$$I(B \cup \{e\}; Y) - I(B; Y) = I(\{e\}; Y) + I(\{e\}; B \mid Y) - I(\{e\}; B)$$
(21)

$$= I(\{e\}; Y) - I(\{e\}; B) + \epsilon_B$$
(22)

$$\leq I(\{e\};Y) - I(\{e\};B) + I(\{e\};B) - I(\{e\};A) = I(A \cup \{e\};Y) - I(A;Y)$$
(23)

But if  $\epsilon_B > I(\{e\}; B) - I(\{e\}; A)$ , the submodularity above will not hold. However, because  $\epsilon_B \leq \epsilon$ , we can define approximate submodularity characterized by the constant  $\epsilon \ge 0$ . Specifically:

$$I(B \cup \{e\}; Y) - I(B; Y) = I(\{e\}; Y) + I(\{e\}; B \mid Y) - I(\{e\}; B)$$
(24)

$$= I(\{e\}; Y) - I(\{e\}; B) + \epsilon_B$$
(25)

$$\leq I(\lbrace e \rbrace; Y) - I(\lbrace e \rbrace; B) + \epsilon \tag{26}$$

$$\leq I(\{e\};Y) - I(\{e\};A) + \epsilon$$
(27)

$$\leq I(\{e\};Y) - I(\{e\};A) + \epsilon_A + \epsilon \tag{28}$$

$$\leq I(A \cup \{e\}; Y) - I(A; Y) + \epsilon \tag{29}$$

**Theorem 2.1.** Under Assumption 2.1, let  $q \in \mathbb{Z}^+$ , and  $S_p$  be the solution from Algorithm 1 at iteration p, we have:

$$I(S_p; Y) \ge (1 - e^{-\frac{p}{q}}) \max_{S:|S| \le q} I(S; Y) - q\epsilon$$
(30)

*Proof.* Let  $S^* \coloneqq \max_{S:|S| \le q} I(S;Y)$  be the optimal subset with cardinality at most q. By Proposition 3.2,  $|S^*| = q$ . We order  $S^*$  as  $\{X_1^*, ..., X_q^*\}$ . Then for all positive integer  $i \le p$ ,

$$I(S^*;Y) \le I(S^* \cup S_i;Y) \tag{31}$$

$$= I(S_i; Y) + \sum_{j=1}^{q} I(X_j^*; Y \mid S_i \cup \{X_{j-1}^*, ..., X_1^*\})$$
(32)

$$= I(S_i; Y) + \sum_{j=1}^{q} (I(\{X_j^*, ..., X_1^*\} \cup S_i; Y) - I(\{X_{j-1}^*, ..., X_1^*\} \cup S_i; Y))$$
(33)

$$\leq I(S_i; Y) + \sum_{j=1}^{q} (I(\{X_j^*\} \cup S_i; Y) - I(S_i; Y) + \epsilon)$$
(34)

$$\leq I(S_i; Y) + \sum_{j=1}^{q} (I(S_{i+1}; Y) - I(S_i; Y) + \epsilon)$$
(35)

$$\leq I(S_i;Y) + q(I(S_{i+1}) - I(S_i;Y) + \epsilon)$$
(36)

Eq. (31) is from Proposition 3.2, Eq. (32) and Eq. (33) are by the chain rule of mutual information, Eq. (34) is from Proposition 3.3, Eq. (35) is by the definition of Algorithm 1 that  $I(S_{i+1}; Y) - I(S_i; Y)$  is maximized in each iteration *i*. Let  $\delta_i := I(S^*; Y) - I(S_i; Y)$ , we can rewrite Eq. (36) into  $\delta_i \le q(\delta_i - \delta_{i+1} + \epsilon)$ , which can be rearranged into  $\delta_{i+1} \le (1 - \frac{1}{q})\delta_i + \epsilon$ .

Let  $\delta_0 = I(S^*; Y) - I(S_0; Y)$ . Since  $S_0 = \emptyset$ , we have  $\delta_0 = I(S^*; Y)$ . By the previous results, we can upper bound the quantity  $\delta_p = I(S^*; Y) - I(S_p; Y)$  as follows:

$$\delta_p \le (1 - \frac{1}{q})\delta_{p-1} + \epsilon \tag{37}$$

$$\leq (1 - \frac{1}{q})((1 - \frac{1}{q})\delta_{p-2} + \epsilon) + \epsilon$$
(38)

$$\leq (1 - \frac{1}{q})^p \delta_0 + (1 + (1 - \frac{1}{q}) + \dots + (1 - \frac{1}{q})^{p-1})\epsilon$$
(39)

$$= (1 - \frac{1}{q})^p \delta_0 + (\frac{1 - (1 - \frac{1}{q})^{p-1+1}}{1 - (1 - \frac{1}{q})})\epsilon$$
(40)

$$= (1 - \frac{1}{q})^p \delta_0 + (q - q(1 - \frac{1}{q})^p)\epsilon$$
(41)

$$\leq (1 - \frac{1}{q})^p \delta_0 + q\epsilon \tag{42}$$

$$\leq e^{-\frac{p}{q}}\delta_0 + q\epsilon \tag{43}$$

Eq. (39) to Eq. (41) is through the summation of the geometric series  $1 + (1 - \frac{1}{q}) + ... + (1 - \frac{1}{q})^{p-1}$ . Eq. (43) is by the inequality  $1 - x \le e^{-x}$  for all  $x \in \mathbb{R}$ . Substitute the definitions of  $\delta_p$  and  $\delta_0$  into Eq. (43) completes the proof.

**Corollary 2.1.** Assume conditions in Theorem 3.1 hold, there exists optimal predictor  $h^*(S_p) = \Pr(Y \mid S_p)$  such that

$$\mathbb{E}[\ell_{01}(Y, h^*(S_p))] \le \mathbb{E}[\ell_{ce}(Y, h^*(S_p))] \le H(Y) - (1 - e^{-\frac{p}{q}})I(S^*; Y) + q\epsilon$$
(44)

*Proof.* Denote the quantity  $(1 - e^{-\frac{p}{q}}) \max_{S:|S| \le q} I(S; Y) - q\epsilon$  from Theorem 3.1 as letter b. By the definition of mutual information, we have  $H(Y \mid S_p) \le H(Y) - b$ . Following Proposition 1.1,  $\inf_{h:S_p \to [0,1]} \mathbb{E}[\ell_{ce}(Y, h(S_p))] \le H(Y) - b$ . In other words,  $\exists h^* = \Pr(Y \mid S_p) \ s.t. \ \mathbb{E}[\ell_{ce}(Y, h^*(S_p))] \le H(Y) - b$ .

When the predictor is probabilistic (i.e., h(X) = 0 if and only if  $h(X) \le 0.5$ ),  $\ell_{01}(Y, \hat{Y}) = \mathbb{1}(Y \neq \hat{Y})$  naturally extends to  $Y \mathbb{1}(\hat{Y} \le 0.5) + (1 - Y) \mathbb{1}(\hat{Y} > 0.5)$ , which is upper bounded by  $\ell_{ce}(Y, \hat{Y})$  for all  $(Y, \hat{Y})$ . Therefore, for the same  $h^*$  as

above, we have:

$$\mathbb{E}[\ell_{01}(Y, h^*(S_p))] \le \mathbb{E}[\ell_{ce}(Y, h^*(S_p))] \le H(Y) - b$$
(45)

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**Corollary 2.2.** Assume conditions in Theorem 3.1 hold. There exists optimal predictors  $h_1^* = \Pr(Y \mid S_p)$ ,  $h_2^* = \Pr(Y \mid S^*)$  such that

$$\mathbb{E}[\ell_{ce}(Y, h_1^*(S_p))] - \mathbb{E}[\ell_{ce}(Y, h_2^*(S^*))]$$

$$\leq e^{-\frac{p}{q}}I(S^*; Y) + q\epsilon$$
(46)

*Proof.* Following Theorem 3.1, and denote  $\arg \max_{S:|S| \le q} I(S; Y)$  as  $S^*$ , we have:

$$I(S_p; Y) \ge (1 - e^{-\frac{p}{q}}) \max_{S:|S| \le q} I(S; Y) - q\epsilon$$
(47)

$$\implies H(Y) - H(Y \mid S_p) \ge (1 - e^{-\frac{p}{q}})(H(Y) - H(Y \mid S^*)) - q\epsilon$$

$$\tag{48}$$

$$\implies H(Y \mid S_p) - H(Y \mid S^*) \le e^{-\frac{r}{q}} (H(Y) - H(Y \mid S^*)) + q\epsilon \tag{49}$$

$$\implies H(Y \mid S_p) - H(Y \mid S^*) \le e^{-\frac{\nu}{q}} (I(S^*;Y)) + q\epsilon$$
(50)

Using Proposition 1.1 completes the proof.

**Proposition 2.4.** Under Assumption 2.1, I(S;Y) is  $\epsilon$ -approximately sub-additive for any  $S \subseteq V$ , i.e.,  $I(S \cup S';Y) \leq I(S;Y) + I(S';Y) + \epsilon$ .

Proof.

$$I(S \cup S'; Y) = I(S; Y) + I(S'; Y \mid S)$$
(51)

$$= I(S;Y) + I(S \cup Y;S') - I(S;S')$$
(52)

$$= I(S;Y) + I(S';Y) + I(S;S' \mid Y) - I(S;S')$$
(53)

$$\leq I(S;Y) + I(S';Y) + \epsilon \tag{54}$$

Eq. (53) to Eq. (54) because  $I(S; S' | Y) \le \epsilon$  by Assumption 2.1, and I(S; S') is always non-negative.

**Proposition 2.5.** Under Assumption 3.1, I(S;Y) is  $\epsilon$ -approximately super-additive for any  $S \subseteq V$ , i.e.,  $I(S \cup S';Y) \ge I(S;Y) + I(S';Y) - \epsilon$ .

*Proof.* Similarly to the proof of Proposition 3.4, we have:

$$I(S \cup S'; Y) = I(S; Y) + I(S'; Y) + I(S; S' \mid Y) - I(S; S')$$
(55)

$$\geq I(S;Y) + I(S';Y) - \epsilon \tag{56}$$

Eq. (55) to Eq. (56) because  $I(S; S') \leq \epsilon$  by Assumption 3.1, and  $I(S; S' \mid Y)$  is non-negative.

**Proposition 2.6.** If conditions in Proposition 3.4 and Proposition 3.5 hold, we have  $I(X_i; Y) - \epsilon \le \phi_{I,X_i} \le I(X_i; Y) + \epsilon$  for any  $X_i \in V$ .

*Proof.* By Proposition 3.4 and Proposition 3.5, for any  $X_i \in V$  and  $S \subseteq V$ , we have:

$$I(X_i;Y) - \epsilon \le I(S \cup \{X_i\};Y) - I(S;Y) \le I(X_i;Y) + \epsilon$$
(57)

Let's first apply the right inequality in Eq. (57) to Definition 2.2. Because  $I(X_i; Y) + \epsilon$  is independent of S, we can simplify the calculation of the upper bound of  $\phi_{I,X_i}$  as follows.

$$\phi_{I,X_i} = \sum_{S \subseteq V \setminus \{X_i\}} \frac{|S|!(|V| - |S| - 1)!}{|V|!} (I(S \cup \{i\}; Y) - I(S; Y))$$
(58)

$$\leq \sum_{S \subseteq V \setminus \{i\}} \frac{|S|!(|V| - |S| - 1)!}{|V|!} (I(X_i; Y) + \epsilon)$$
(59)

$$=\sum_{|S|=0}^{|V|-1} {|V|-1 \choose |S|} \frac{|S|!(|V|-|S|-1)!}{|V|!} (I(X_i;Y)+\epsilon)$$
(60)

$$=\sum_{|S|=0}^{|V|-1} \frac{(|V|-1)!}{|S|(|F|-1-|S|)!} \frac{|S|!(|V|-|S|-1)!}{|V|!} (I(X_i;Y)+\epsilon)$$
(61)

$$=\sum_{|S|=0}^{|V|-1} \frac{1}{|V|} (I(X_i;Y) + \epsilon)$$
(62)

$$=I(X_i;Y) + \epsilon \tag{63}$$

Applying the same procedure to the left inequality in Eq. (57) to Definition 2.2, we have  $\phi_{I,X_i} \ge I(X_i; Y) - \epsilon$ . Combining both results completes the proof.

**Proposition 2.7.** Under Assumption 2.1,  $\forall X_i \in V$ , we have  $I(X_i; Y) \leq \phi_{I,X_i}^{mci} \leq I(X_i; Y) + \epsilon$ .

*Proof.* By Proposition 3.3,  $I(\cdot; Y)$  would be approximately submodular under Assumption 2.1, thus:

$$I(X_i; Y) + \epsilon = I(\emptyset \cup X_i; Y) - I(\emptyset; Y) + \epsilon$$
(64)

$$\geq \max_{S \subseteq V} I(S \cup X_i; Y) - I(S; Y) = \phi_{I, X_i}^{mci}$$
(65)

On the other hand, if  $\arg \max_{S \subseteq V} I(S \cup X_i; Y) - I(S; Y) = \emptyset$ , we have  $\phi_{I,X_i}^{mci} = I(\emptyset \cup X_i; Y) - I(\emptyset; Y) = I(X_i; Y)$ . If  $\arg \max_{S \subseteq V} I(S \cup X_i; Y) - I(S; Y)$  is some non-empty subset A, we have  $\phi_{I,X_i}^{mci} = I(A \cup X_i; Y) - I(A; Y) \ge I(\emptyset \cup X_i; Y) - I(\emptyset; Y)$ . In this case,  $\phi_{I,X_i}^{mci} \ge I(X_i; Y)$ . Combining both inequalities completes the proof.