CS60021: Scalable Data Mining

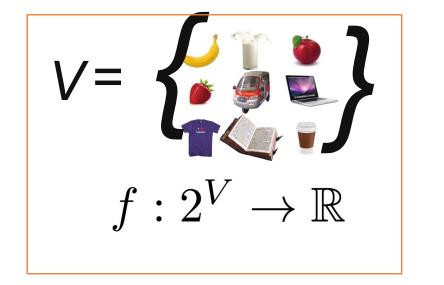
Subset Selection

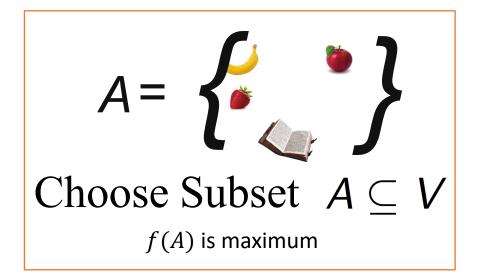
Sourangshu Bhattacharya

Submodular Subset Selection

Slides taken from IJCAI 2020 tutorial by Rishabh Iyer and Ganesh Ramakrishnan

Combinatorial Subset Selection Problems



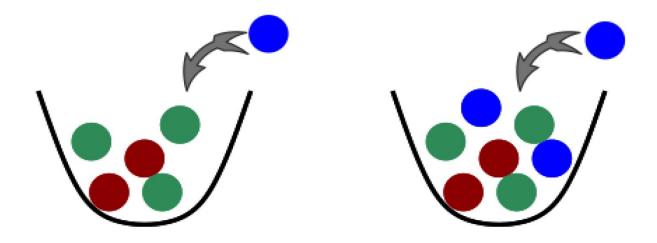


General Set function Optimization: very hard!

What if there is some special structure?

Submodular Functions

$f(A \cup v) - f(A) \ge f(B \cup v) - f(B)$, if $A \subseteq B$



Negative of a Submodular Function is a Supermodular Function!

f = # of distinct colors of balls in the urn.

Equivalent Definitions of Submodularity

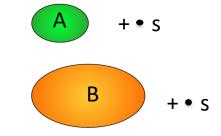
 $=f(A \cap B)$

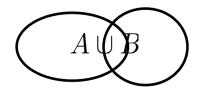
• Diminishing gains: for all $A, B \subseteq V$

 $= f(A_r) + 2f(C) + f(B_r) = f(A_r) + f(C) + f(B_r)$

 $f(A \cup v) - f(A) \ge f(B \cup v) - f(B)$, if $A \subseteq B$

• Union-Intersection: for all $A, B \subseteq V$ $f(A) + f(B) \ge f(A \cup B) + f(A \cap B)$

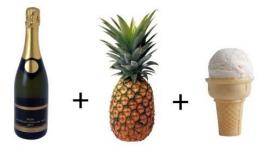




Modular Functions

• each element e has a weight w(e)

$$F(S) = \sum_{e \in S} w(e)$$



 $A \subset B$

 $F(A \cup e) - F(A) = w(e) = F(B \cup e) - F(B) = w(e)$

Modular Functions are both submodular and supermodular!

Monotone Submodular Functions

• A set function is called monotonic if $A \subseteq B \subseteq V \Rightarrow F(A) \leq F(B)$

Examples:

- Influence in social networks [Kempe et al KDD '03]
- For discrete RVs, entropy $F(A) = H(X_A)$ is monotonic: Suppose B=A \cup C. Then $F(B) = H(X_A, X_C) = H(X_A) + H(X_C | X_A) \ge H(X_A) = F(A)$
- Information gain: $F(A) = H(Y)-H(Y | X_A)$

Instantiations of Submodular Functions

Representation Functions

- Facility Location Function (k-mediods clustering)
- Graph Cut Family, Saturated Coverage

Diversity Functions

- Dispersion Functions (Min, Sum, Min-Sum)
- Determinantal Point Processes

Coverage Functions

- □ Set Cover Function
- Probabilistic Set Cover Function
- Feature Based Functions

Importance Functions

Modular Functions

Information Functions

- Mutual Information
- Entropy

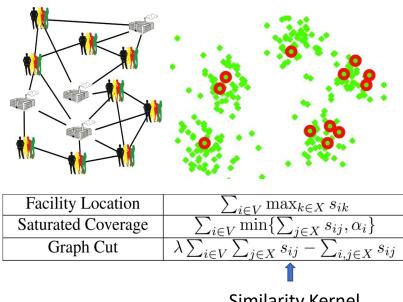
Discounted Cost Functions

- Clustered Concave over Modular Functions
- Cooperative Costs and Saturations

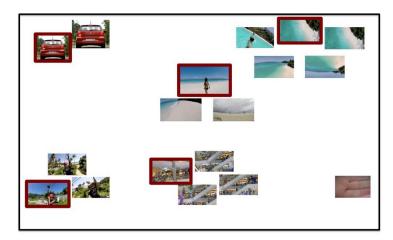
Complexity Functions

Bipartite Neighborhood Functions

Representation Functions



Similarity Kernel

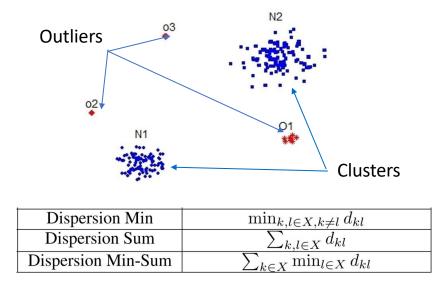


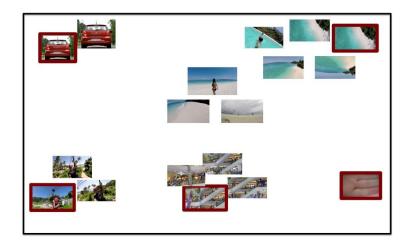
Representation Functions

Picks Centroids

lyer 2015, Kaushal et al 2019, Tschiatchek et al 2014, ...

Diversity Functions: Dispersion



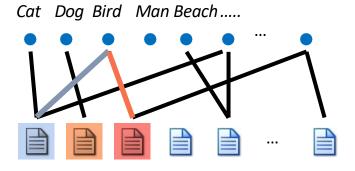


Diversity Functions Picks items as different as possible!

Dasgupta et al 2013, Chakraborty et al 2015

Dispersion Sum and Dispersion Min Not Submodular!

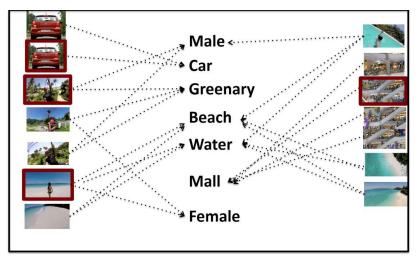
Coverage Functions



Set Cover Function

$$f(X) = w(\cup_{i \in X} U_i),$$

Concepts Covered by Instance i

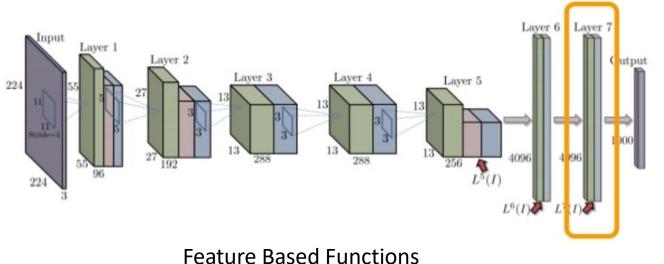


Coverage Functions

Select instances which "cover" alconcepts

Wolsey et al 1982, ...

Feature Based Functions



Achieve Uniformity in Feature Coverage

$$f_{fea}(S) = \sum_{u \in U} g(m_u(S)).$$

Wei-lyer et al 2014 ...

Total Contribution of Feature u in the Set of Images S

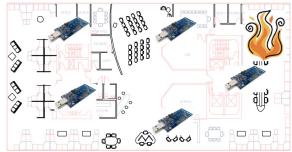
Information Functions

 X_1, \dots, X_n discrete random variables: $X_e \in \{1, \dots, m\}$ $F(S) = H(X_S) = \text{ joint entropy of variables indexed by } S$ $H(X_e) = \sum_{x \in \{1, \dots, m\}} P(X_e = x) \log P(X_e = x)$

$$A \subset B, e \notin B$$
 $F(A \cup e) - F(A) \ge F(B \cup e) - F(B)??$

$$\begin{split} H(X_{A\cup e}) - H(X_A) &= H(X_e | X_A) \\ &\leq H(X_e | X_B) \quad \text{``information never hurts''} \\ &= H(X_{B\cup e}) - H(X_B) \end{split}$$

discrete entropy is submodular!

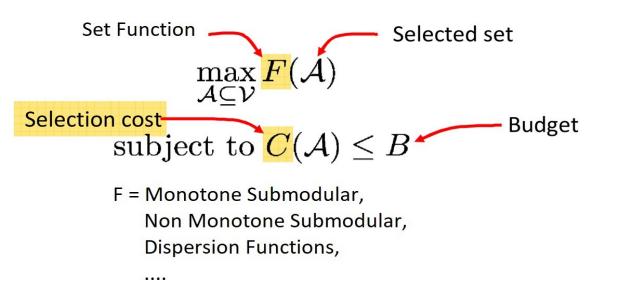


Entropy Mutual Information Information Gain

...

Krause et al 2008, ...

Master Optimization Problem



F Models:

- Diversity
- Representation
- Coverage

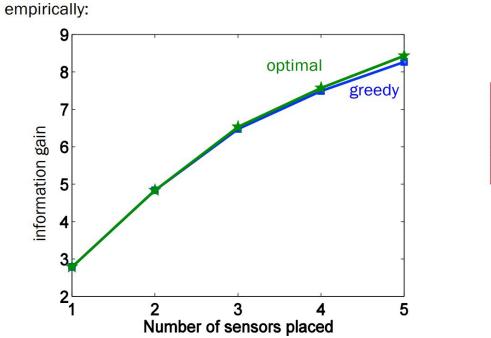
...

- Information
- Importance

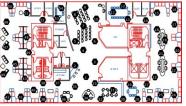
We shall study this and variants of this Master Optimization Problem!

Monotone Submodular Maximization

How good is Greedy in Practice?



sensor placement



How good is Greedy in Theory?

$$\max_{S} F(S) \text{ s.t. } |S| \le k$$

Theorem (Nemhauser, Fisher, Wolsey `78) F monotone submodular, S_k solution of greedy. Then $F(S_k) \geq \left(1 - \frac{1}{e}\right) F(S^*)$ optimal solution

No Poly-time algorithm can do better than this in the worst case!

Proof (Nemhauser et al 1978)

Let:

- $A_i = (v_1, v_2, \dots, v_i)$ be the the chain formed by the greedy algorithm, as defined above
- $A^* = (v_1^*, v_2^*, \dots, v_k^*)$ be the optimal solution, in an arbitrary order
- f be a monotone submodular function. Let $f \ge 0$ (Update on 04/25/2019: I thought this was w.l.o.g., but Andrey Kolobov pointed out that we actually need f to be non negative)
- $OPT = f(A^*)$, the value of the optimal solution.

We will prove that

$$f(A_k) \geq (1-1/e)OPT$$

Source: https://homes.cs.washington.edu/~marcotcr/blog/greedy-submodular/

Proof (Nemhauser et al 1978)

For all $i \leq k$, we have:

$$egin{aligned} f(A^*) &\leq f(A^* \cup A_i) & ext{Monotonicity} \ &= f(A_i) + \sum_{j=1}^k \Delta(v_j^* | A_i \cup \{v_1^*, v_2^*, \dots, v_{j-1}^*\}) & \ &\leq f(A_i) + \sum_{z \in A^*} \Delta(z | A_i) & ext{Using submodularity} & \ &\leq f(A_i) + \sum_{z \in A^*} \Delta(v_{i+1} | A_i) & v_{i+1} = argmax_{v \in V \setminus A_i} \Delta(v | A_i) & \ &= f(A_i) + k \Delta(v_{i+1} | A_i) & \end{aligned}$$

Rearranging the terms, we have proved that

$$\Delta(v_{i+1}|A_i) \geq rac{1}{k}(OPT - f(A_i))$$

Source: https://homes.cs.washington.edu/~marcotcr/blog/greedy-submodular/

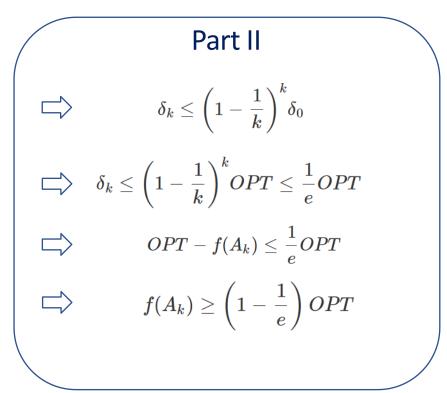
Proof (Nemhauser et al 1978)

Part I

Now we define $\delta_i = OPT - f(A_i)$. This implies $\delta_i - \delta_{i+1} = f(A_{i+1}) - f(A_i) = \Delta(v_{i+1}|A_i)$

Plugging this into our previous equation, we have:

$$igsquigarrow \delta_i - \delta_{i+1} \geq rac{1}{k} (\delta_i)$$
 $igsquigarrow \delta_{i+1} \leq (1-rac{1}{k}) \delta_i$



Source: https://homes.cs.washington.edu/~marcotcr/blog/greedy-submodular/

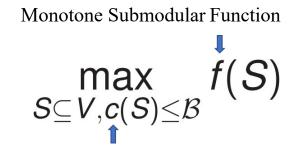
Monotone Submodular – Budget Constraints

$$\begin{array}{l} \max \ F(S) \ \text{s.t.} \ \sum_{e \in S} c(e) \leq B \\ 1. \ \text{run greedy:} \ S_{\text{gr}} \\ 2. \ \text{run a modified greedy:} \ S_{\text{mod}} \\ e^* = \arg \max \frac{F(S_i \cup \{e\}) - F(S_i)}{c(e)} \\ 3. \ \text{pick better of} \ S_{\text{gr}}, \ S_{\text{mod}} \\ \hline \end{array}$$

$$\begin{array}{l} \text{even better but less fast:} \\ partial enumeration \\ (Sviridenko, 2004) \text{ or} \\ \text{filtering} (Badanidiyuru \& Vondrák 2014) \end{array}$$

$$\begin{array}{l} \text{Sviridenko 2004:} \\ \bullet \ \text{Run the cost-sensitive} \\ \text{greedy algorithm starting} \\ \text{with all possible initial sets} \\ \{1,j,k\} \\ \bullet \ 0 \ n^3 \text{ initial complexity} \\ \bullet \ 1 \ (1/2) \text{ approximation} \end{array}$$

Summary: Greedy Algorithm Framework



Cost of Summary Subset S (e.g. size)

Problem Formulation

Initialization $S \leftarrow \emptyset$. **repeat** Pick an element $v^* \in \operatorname{argmax}_{v \in V \setminus S} \frac{f(v \cup S) - f(S)}{c(v)}$ Update $S \leftarrow S \cup v^*$ **until** Reaching the budget, i.e., c(S) > B**Greedy Algorithm**

Non-Monotone Submodular Functions

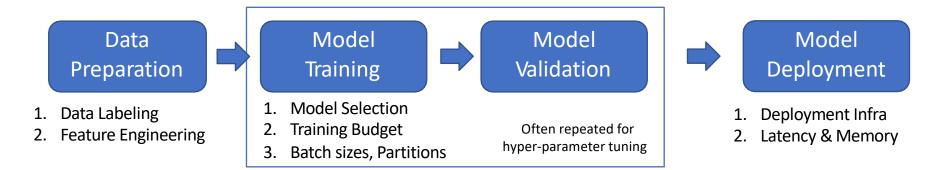
$$\max_{S} F(S) \text{ s.t. } |S| \le k$$

Start with $Y_0 = \emptyset$ for i = 1 to k do Let $M_i = \operatorname{argmax}_{X \subseteq V \setminus Y_{i-1}, |X| = k} \sum_{v \in X} f(v|Y_{i-1});$ Choose y as a uniformly random element in $M_i;$ $Y_i = Y_{i-1} \cup y;$ return Y_k .

Theorem (Buchbinder et al 2014): The Randomized Greedy Algorithm achieves a 1/e approximation guarantee for Non-Monotone Submodular Maximization subject to cardinality constraints!

Data subset selection

Make ML Data Efficient and Robust



Production Systems Constraints

- 1. Data Labeling => Time Consuming, Expensive, Noisy
- 2. Feature Selection => Latency & Memory
- 3. Model Training => Compute Intensive and Time Consuming
- 4. Hyper-Parameter Tuning/NAS => Very Time Consuming
- 5. Distribution Shift => Deployment vs Training

Can we train Models under these constraints without sacrificing on accuracy?

Data Subset Selection Setup

A Machine Learning model characterized by model parameters $\, heta$

Training Data: $\{(x_i, y_i), i \in \mathcal{U}\}$ Training log-likelihood function: $LL_T(\theta, \mathcal{U})$

Training a machine learning model often reduces to finding the parameters that maximizes a log-likelihood function for given training data empirically.

$$\theta^* = \operatorname*{argmax}_{\theta} LL_T(\theta, \mathcal{U})$$

Validation Data: $\{(x_i, y_i), i \in \mathcal{V}\}$ Validation log-likelihood function: $LL_V(\theta, \mathcal{V})$

Goal: Select a subset $S \subseteq \mathcal{U}$ such that the resulting model performs the **best**!

Requirements for optimal subset selection

- 1. The subset selection algorithm needs to be as fast as possible.
 - Subset Selection time <<<< Full training time

Example: Subset selection algorithm with negligible time complexity Training on 10 % Subset $\longrightarrow 10 \times$ Faster training

- 2. Theoretical guarantees of subset selection algorithm.
 - Can we show theoretical guarantees for subset selection algorithms?

Approaches for Data Subset Selection

Several different kinds of approaches studied in literature:

□ Approach 1: Use Submodular Functions as proxy functions for data subset selection

Approach 2: Choose data subset which approximates the gradient of the entire dataset

- □ Approach 3: Choose data subset which approximates the performance on full training dataset (or validation set) as a bi-level optimization!
- Approach 4: Choose data subset which minimizes a suitable divergence (e.g. KL divergence) between the distribution induced by the subset and full data!

Types of Data Selection

- □ Supervised (Using the labels)
- Unsupervised (No access to labels)
- □ Validation based (Access to a validation set for focusing on generalization)

Idea: Gradient Matching/ CoreSets

Can we obtain a weighted gradient of a **subset** of points that approximates the full gradient?

$$\sum_{i \in X_t} w_i^t \nabla_{\theta} L_T^i(\theta) \approx \nabla_{\theta} L(\theta)$$

Sivasubramaniam & Killamsetty et. al. 2021, Mirzasoleiman et al 2020

Gradient Matching/ CoreSets Convergence

Denote L_V as the validation loss, L_T as the full training loss, and L_T^i as the training loss on the i^{th} training example. Furthermore, assume that both losses have gradients bounded by σ_T and σ_V respectively, and that the parameters satisfy $||\theta^*||^2 \leq R^2$ (θ^* is the optimal parameter). Then letting L denote either the training or validation loss (with gradient bounded by σ), any data selection algorithm, defined via weights \mathbf{w}^t and subsets X_t for $t = 1, \dots, T$, and run with a learning rate $\alpha = \frac{R}{\sigma_T \sqrt{T}}$ satisfies:

$$\min_{t=1:T} L(\theta_t) - L(\theta^*) \le \frac{R\sigma_T}{\sqrt{T}} + \frac{R}{T} \sum_{t=1}^{T-1} \mathsf{Err}(\mathbf{w}^t, X_t, L, L_T, \theta_t)$$

where:

$$\mathsf{Err}(\mathbf{w}^t, X_t, L, L_T, \theta_t) = \left\| \sum_{i \in X_t} w_i^t \nabla_{\theta} L_T^i(\theta_t) - \nabla_{\theta} L(\theta_t) \right\|$$

Sivasubramaniam & Killamsetty et. al. 2021

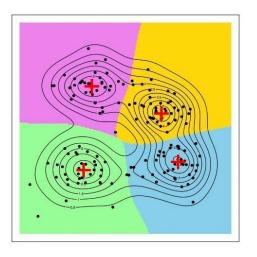
Gradient Matching: Main Idea

The theorem indicates that an effective data selection algorithm should try to have a low error $\text{Err}(\mathbf{w}^t, X_t, L, L_T, \theta_t)$ for $t = 1, \dots, T$. Thus, we can pose the problem as,

$$\mathbf{w}^{t}, X_{t} = \min_{\mathbf{w}, X: |X| \le k} \operatorname{Err}(\mathbf{w}, X, L, L_{T}, \theta_{t})$$
$$= \min_{\mathbf{w}, X: |X| \le k} \| \sum_{i \in X_{t}} w_{i}^{t} \nabla_{\theta} L_{T}^{i}(\theta_{t}) - \nabla_{\theta} L(\theta_{t}) \|$$

CRAIG as an upper bound

Facility location can be thought as an upper bound for this. Suppose we define $\pi_t^i \in \arg \min_{j \in X} \|\nabla_{\theta} L^i(\theta) - \nabla_{\theta} L_T^j(\theta)\|$, if $L = L_T$, then W = U otherwise if $L = L_V$ then W = V and $w_j = \sum_{i \in W} [\pi_t^i = j]$ then, for any θ_t we can write



$$\begin{aligned} \mathsf{Err}(\mathbf{w}, X, L, L_T, \theta_t) &= \left\| \nabla L(\theta_t) - \sum_{i \in X} w_i \nabla L_T^i(\theta_t) \right\| \\ &= \left\| \sum_{i \in W} \left(\nabla_{\theta} L_T^i(\theta_t) - \nabla_{\theta} L^{\pi_t^i}(\theta_t) \right) \right\| \\ &\leq \sum_{i \in W} \| \nabla_{\theta} L_T^i(\theta_t) - \nabla_{\theta} L^{\pi_t^i}(\theta_t) \|, \end{aligned}$$

Sivasubramaniam & Killamsetty et. al. 2021, Mirzasoleiman et al 2020

Directly Optimizing Gradient Error: GradMatch

Define the regularized version of our objective:

$$E_{\lambda}(X) = \min_{\mathbf{w}} \underbrace{\left\| \sum_{i \in X_t} w_t^i \nabla_{\theta} L_T^i(\theta_t) - \nabla_{\theta} L(\theta_t) \right\|^2 + \lambda ||\mathbf{w}^t||^2}_{E_{\lambda}(X_t, \mathbf{w}^t)}$$

This problem can be solved efficiently using Orthogonal Matching Pursuit (OMP) described as,

- 1. Find projection of $r = \nabla_{\theta} L_T^i(\theta_t)$ for each $i \in W$ along $\nabla_{\theta} L(\theta_t)$ and chose the *i* with whom projection is maximum and add it X
- 2. Solve linear regression problem to find w_t^i for $i \in Xs$.
- 3. Set $r = \nabla_{\theta} L(\theta_t) \sum_{i \in X_t} w_t^i \nabla_{\theta} L_T^i(\theta_t)$
- 4. Repeat the steps with new r until the $|r| < \epsilon$ or |X| < k(budget)
- 5. Return X, w_t

Orthogonal Matching Pursuit

The OMP algorithm Algorithm 1: OMP(A, b)Input: A, b **Result:** \mathbf{x}_k 1 Initialization $\mathbf{r}_0 = \mathbf{b}$, $\Lambda_0 = \emptyset$; 2 Normalize all columns of A to unit L_2 norm; 3 Remove duplicated columns in A; 4 for k = 1, 2, ... do Step-1. $\lambda_k = \operatorname*{argmax}_{j \notin \Lambda_{k-1}} \left| \langle \mathbf{a}_j, \mathbf{r}_{k-1} \rangle \right|;$ 5 Step-2. $\Lambda_k = \Lambda_{k-1} \cup \{\lambda_k\};$ 6 Step-3. $\mathbf{x}_k(i \in \Lambda_k) = \operatorname{argmin} \|\mathbf{A}_{\Lambda_k}\mathbf{x} - \mathbf{b}\|_2, \ \mathbf{x}_k(i \notin \Lambda_k) = 0;$ 7 Step-4. $\hat{\mathbf{b}}_k = \mathbf{A}\mathbf{x}_k;$ 8 Step-5. $\mathbf{r}_k \leftarrow \mathbf{b} - \hat{\mathbf{b}}_k$; 9 0 end

Convex DSS

Aim

- We study the problem of data efficient training of autonomous driving systems.
- Training using many frames on straight road sections may not be necessary. Frames at the turns turn out to be useful.



REDUNDANT

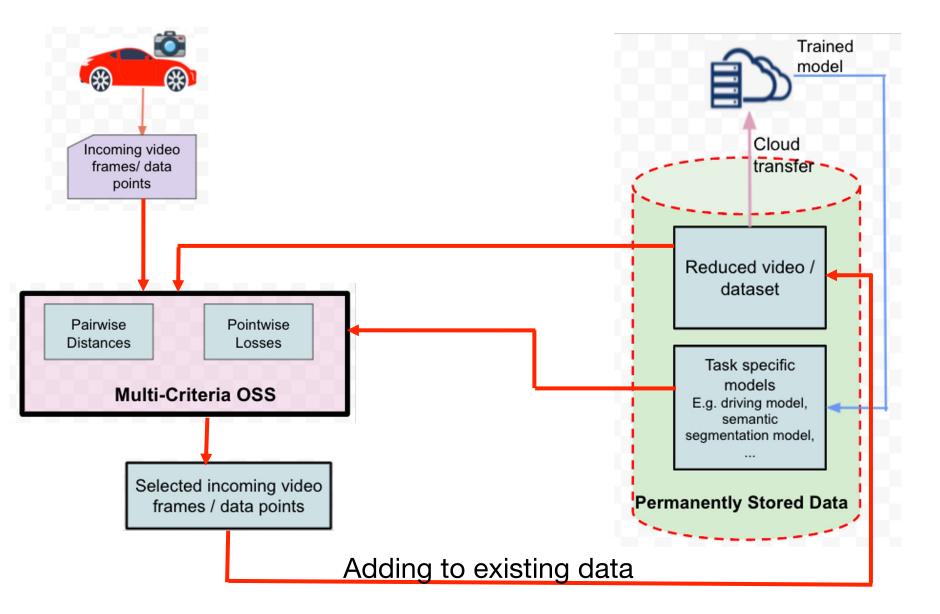


INFORMATIVE

Method	Train One-Turn	Test One-Turn
Uniform Skip	3/10	5/10

In the context of edge device deployment, multi-criteria online subset selection (OSS) framework can be useful in selecting informative frames, essential for an end-task.

Subset selection on Edge devices



High Level Idea

 Given a compression ratio, find out representatives which have the least dissimilarity with the left-out elements besides having the highest task-specific loss.

Problem Setup

- *X_t*: the set of incoming datapoints at time t (Size m)
- D: set of all data points (Size N)
- *R_t*: Reduced set of data at time t
- d_{ij} : Distance between data points I and j.
- z_{ij} : Indicator variable indicating that datapoint i is a representative for datapoint j.

Convex Subset Selection

• Original formulation in set notation:

$$\min_{\mathcal{S}\subseteq\mathcal{D}}\lambda|\mathcal{S}| + \sum_{j\in\mathcal{D}}\min_{i\in\mathcal{S}}d_{ij},$$

Formulation using indicator random variables z_{ij}:

Size regularizer
$$\begin{split} \min_{\{z_{ij}\}} \lambda \sum_{i \in \mathcal{D}} \mathrm{I}(\| \begin{bmatrix} z_{i1} \ z_{i2} \ \cdots \ \end{bmatrix} \|_p) + \sum_{j \in \mathcal{D}} \sum_{i \in \mathcal{D}} d_{ij} z_i \\ \mathrm{s.\,t.} \ z_{ij} \in \{0,1\}, \ \sum_{i=1}^N z_{ij} = 1, \ \forall \, i, j \in \mathcal{D}. \end{split}$$

• Convex relaxation:

 $0 \le z_{ij} \le 1$

Online Subset Selection

• At time t:

 R_{t-1} : old set (denoted by superscript o) X_t : in the new set (denoted by superscript n) R_t : the new reduced set that we are trying to compute using z_{ij} $R_t = R_{t-1} \cup \{i \in X_t | Z_{ij} = 1\}$

• Revised formulation:

$$J_{\text{enc}}' \triangleq \sum_{i \in \mathcal{E}_o} \sum_{j \in \mathcal{D}_n} d_{ij}^{o,n} z_{ij}^{o,n} + \sum_{i \in \mathcal{D}_n} \sum_{j \in \mathcal{D}_n} d_{ij}^{n,n} z_{ij}^{n,n},$$

 $\epsilon_o = R_{t-1}$ $D_n = X_t$

$$\min_{\mathcal{Z}'} J_{\text{enc}}' + \lambda \sum_{i \in \mathcal{D}_n} \mathrm{I}(\left\| \begin{bmatrix} z_{i1}^{n,n} & z_{i2}^{n,n} & \cdots \end{bmatrix} \right\|_p)$$
s.t. $z_{ij}^{o,n}, z_{ij}^{n,n} \in \{0,1\}, \ \forall i, j,$

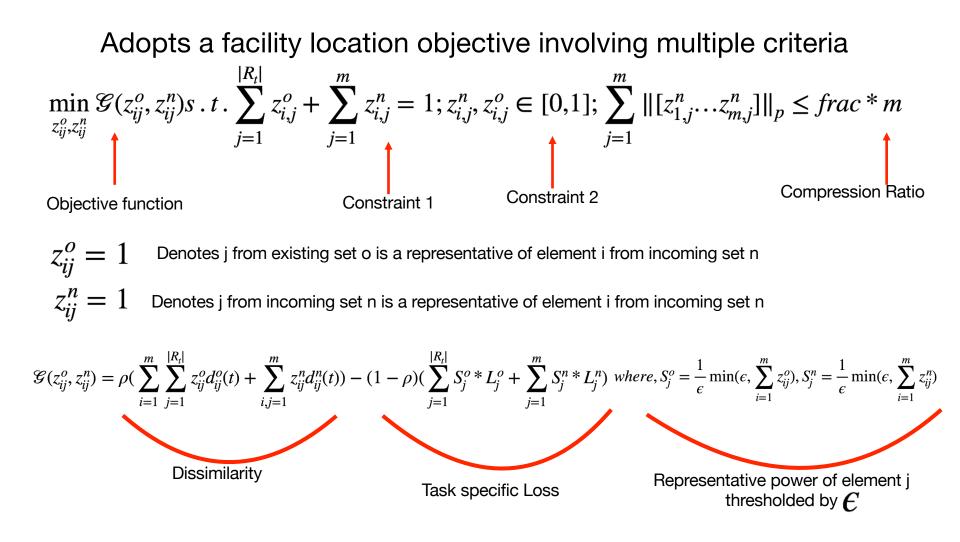
$$\sum_{i \in \mathcal{E}_o} z_{ij}^{o,n} + \sum_{i \in \mathcal{D}_n} z_{ij}^{n,n} = 1, \ \forall j \in \mathcal{D}_n,$$

High Level Idea

 Given a compression ratio, find out representatives which have the least dissimilarity with the left-out elements besides having the highest task-specific loss.

 Highest task-specific loss ensures having situational tasks needed to be learnt more by the model.

TMCOSS



Justification for thresholding

Theorem 1 Let z_{ij}^o and z_{ij}^n be the optimal solution for formulation 1. A new frame $j \in X_{t+1}$ is selected as a representative frame for at least one incoming frame $i \in X_{t+1}$, *i.e.* $z_{ij}^n = 1$, only if BOTH these conditions hold:

- For some incoming frame $i \in X_{t+1}$, $Q_{ij}^n < Q_{ij'}^n$, for all $j' \in X_{t+1}$ and $j' \neq j$
- For some incoming frame $i \in X_{t+1}, Q_{ij}^n < \frac{\sum_{i'=1}^m z_{i',k}^o Q_{i'k}^o + \lambda \|[z_{1,j}^n \dots z_{m,j}^n]\|_p}{\|\mathbf{z}_i^n\|_1}$

where
$$k = \arg \min_j \sum_{i=1}^m z_{i,j}^o Q_{i,j}^o$$
, and $\|\mathbf{z}_j^n\|_1 = \sum_{i'=1}^m z_{i'j}^n$

 $\rho = 0$

Corollary 1.1 Let z_{ij}^o and z_{ij}^n be the optimal solution for formulation 1. A new frame $j \in X_{t+1}$ is selected as a representative frame for at least one incoming frame $i \in X_{t+1}$, *i.e.* $z_{ij}^n = 1$, only if BOTH these conditions hold:

•
$$L_j^n > L_{j'}^n$$
 for all $j' \in X_{t+1}$ and $j' \neq j$

•
$$L_j^n > \frac{\sum_{i=1}^m z_{i,k}^o L_k^o - \lambda \|[z_{1,j}^n ... z_{m,j}^n]\|_p}{\|\mathbf{z}_j^n\|_1}$$

where $k = argmin_j \sum_{i=1}^{m} z_{i,j}^o Q_{i,j}^o$, and $\|\mathbf{z}_j^n\|_1 = \sum_{i'=1}^{m} z_{i'j}^n$

$\begin{aligned} & \text{Multi-criteria OSS (MCOSS)}^{1} \\ & \mathcal{Q}_{ij}^{n} = \rho d_{ij}^{n} - (1 - \rho) L_{j}^{n}; \\ & \mathcal{Q}_{ij}^{o} = \rho d_{ij}^{o} - (1 - \rho) L_{j}^{o} \\ & \min_{z_{ij}^{o}, z_{ij}^{n}} \sum_{i=1}^{m} \sum_{j=1}^{|R_{i}|} z_{ij}^{o} \mathcal{Q}_{ij}^{o} + \sum_{i,j=1}^{m} z_{ij}^{n} \mathcal{Q}_{ij}^{n} + \lambda \sum_{j=1}^{m} \| [z_{1,j}^{n} \dots z_{m,j}^{n}] \|_{p} \\ & s.t. \sum_{j=1}^{|R_{i}|} z_{i,j}^{o} + \sum_{j=1}^{m} z_{i,j}^{n} = 1, \forall i \in X_{t+1} z_{i,j}^{n}, z_{i,j}^{o} \in [0,1], \forall i,j \end{aligned}$

^{1.} Soumi Das, Sayan Mondal, Ashwin Bhoyar, Madhumita Bharde, Niloy Ganguly, Suparna Bhattacharya, Sourangshu Bhattacharya, "Multi-criteria onlineframe-subset selection for autonomous vehicle videos." Pattern Recognition Letters 133 (2020): 349-355.

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