Multiclass sub-pixel target detection using functions of multiple instances

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ABSTRACT

The Multi-class Convex-FUMI (Multi-class C-FUMI) method is developed and described. The method is capable of learning prototypes for multiple target classes from hyperspectral imagery. Multi-class C-FUMI is a non-traditional supervised learning method based on the Functions of Multiple Instances (FUMI) concept. The FUMI concept differs significantly from traditional supervised by the assumption that only functions of target patterns are available. Moreover, these functions are likely to involve other non-target patterns. In this paper, data points which are convex combinations of multiple target and several non-target prototypes are considered. Multi-class C-FUMI learns the target and non-target patterns, the number of non-target patterns, and the weights (or proportions) of all the prototypes for each data point. For hyperspectral image analysis, the target and non-target prototypes estimated using Multi-class C-FUMI are the endmembers for the target and non-target (background) materials. For this method, training data need only binary labels indicating whether a data point contains or does not contain some proportion of a target endmember; the specific target proportions for the training data are not needed. After learning the target prototype using the binary-labeled training data, target detection is performed on test data. Results showing sub-pixel target detection on highly mixed simulated hyperspectral data generated from the ASTER spectral library are presented.

Keywords: sub-pixel, target detection, unmixing, endmember, hyperspectral

1. INTRODUCTION

The FUMI concept is a generalization of Multiple Instance Learning (MIL) methods.$^1$–$^6$ In MIL, training data are divided into positive and negative “bags.” A bag is defined to be a multi-set of data points. A positive bag includes at least one target point. In each positive bag, the exact number of data points belonging to the target class is unknown. Negative bags are composed entirely of non-target data points. The MIL methods are effective for learning target concepts and developing classifiers for cases where accurate sample-level labeled training data is unavailable.

The FUMI framework can be related to the MIL framework by treating each data point as being a function of a positive or negative bag. FUMI methods learn target and non-target prototypes given a set of data points that are some unknown function of the target and non-target prototypes. Suppose there is a given data set $X = \{x_1, x_2, ..., x_N\}$ where each data point is some unknown function of prototypes, $x_i = f(B_i, P_i)$ where $P_i$ are the set of parameters for $x_i$, and $B_i$ is the “bag” of prototypes that contribute in a non-negligible way to the data point $x_i$.

The C-FUMI (Convex FUMI) algorithm$^7$ was the first algorithm to implement the FUMI concept. C-FUMI assumes each data point is a convex combination of target and non-target prototypes. The C-FUMI algorithm was then extended to the Weighted C-FUMI algorithm.$^8$ Weighted C-FUMI weights terms associated with target and non-target training data points based on the number of target and non-target

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data points are found in a training data set. The weighted C-FUMI algorithm is appropriate in cases where there are significantly more non-target training points than target training points by weighting terms in the objective associated with target training points higher than the corresponding non-target terms.

In this paper, the specific case that is considered is that each data point is assumed to be a convex combination of target and non-target prototypes, as shown in Equation 1 where the set of prototypes, \( \mathbf{E} \), with non-zero weights for data points \( \mathbf{x}_i \) define the bag \( \mathbf{B}_i \). Each training point \( \mathbf{x}_i \) is given a binary label for each target type, \( l(\mathbf{x}_i, t) \) where \( l(\mathbf{x}_i, t) = 1 \) if \( \mathbf{b}_t \in \mathbf{B}_i \) and \( l(\mathbf{x}_i, t) = 0 \) if \( \mathbf{b}_t \notin \mathbf{B}_i \). After learning target prototypes using the binary-labeled training data, target detection can be performed on test data.

\[
\mathbf{x}_i = \sum_{t=1}^{T} l(\mathbf{x}_i, t) \mathbf{p}_t \mathbf{e}_t + \sum_{k=T+1}^{M+T} p_{ik} \mathbf{e}_k
\]

where \( \mathbf{x}_i \) is a data point, \( \mathbf{e}_t \) is a target prototype \( t = 1, \ldots, T \), \( \mathbf{e}_k \) is a non-target prototype for \( k = T + 1, \ldots, M+T \) and \( p_{ik} \) is the weight (or proportion value) of the \( k \)th prototype in data point \( i \). The proportions are constrained to sum-to-one and be greater than zero.

\[
\sum_{t=1}^{T} p_{it} + \sum_{k=T+1}^{M+T} p_{ik} = 1, \quad p_{it} \geq 0, \quad p_{ik} \geq 0
\]

Endmember detection and spectral unmixing are common tasks in hyperspectral image (HSI) analysis.\(^9\) Given an HSI analysis task, the target and non-target prototypes estimated using C-FUMI methods are the target and background endmembers.

The exact proportion values for the training data are not needed. Therefore, multi-class C-FUMI\(^7\) learns the spectral shape of target endmembers given mixed training data without prior knowledge of the proportions of each target in every training point. In the following section, the multi-class C-FUMI algorithm is developed. In addition to learning prototypes, the multi-class C-FUMI algorithm learns the number of non-target endmembers needed for a data set and determines the proportions of endmembers for each data point. Experimental results, discussion and future work sections are found in Sections 3 and 4.

2. THE MULTI-CLASS C-FUMI ALGORITHM

The multi-class C-FUMI Algorithm is an extension of the Weighted C-FUMI algorithm\(^7,8\) which is, in turn, an extension of the Sparsity Promoting Iterated Constrained Endmembers (SPICE) algorithm.\(^9\) In SPICE, endmembers and proportions are iteratively updated by minimizing the objective function in Equation 3 where \( \gamma_k = \frac{1}{\sum_{i=1}^{N} p_{ik}} \) using the proportions from the previous iteration and \( \Gamma \) is a parameter used to control the degree of sparsity.

\[
G = (1 - \mu) \sum_{i=1}^{N} \left\| \mathbf{x}_i - \sum_{k=1}^{M} p_{ik} \mathbf{e}_k \right\|_2^2 + \frac{\mu}{2} \sum_{k=1}^{M} \sum_{j=1}^{M} \left\| (\mathbf{e}_k - \mathbf{e}_j) \right\|_2^2 + \sum_{k=1}^{M} \frac{\gamma_k}{\Gamma} \sum_{i=1}^{N} p_{ik}
\]

The first term of this objective computes the squared error between the input data and the estimate found using the current prototypes (or endmembers) and proportions. The second term produces endmembers that provide a tight fit around the data. The third term is a sparsity promoting term used to determine \( M \), the number of endmembers needed to describe the input data. This objective is updated iteratively using alternating optimization on the endmembers and proportions.

The SPICE algorithm is an unsupervised algorithm to learn the proportions, the endmembers, and the number of endmembers, \( M \), for a given unlabeled dataset. The multi-class C-FUMI (and C-FUMI or Weighted C-FUMI) algorithm extends the SPICE algorithm by using the binary labeled training points to learn and distinguish the specific target endmembers from the remaining non-target background endmembers. The target endmembers found can then be used for detection in test data. The multi-class C-FUMI algorithm extends weighted C-FUMI by estimating multiple target endmembers.
For negatively labeled training data, the proportion value associated with the target prototype is constrained to be zero. Therefore, the objective function for Weighted C-FUMI can be written as shown in Equation 4 where $l(x_i)$ is 1 when $x_i$ is in the target class and 0 otherwise.

$$F = (1 - \mu) \sum_{i=1}^{N} w_{max}(l(x_i,t)) \left\| \left( x_i - \sum_{k=1}^{T} l(x_i)p_{it}\mathbf{e}_t - \sum_{k=T+1}^{M+T} p_{ik}\mathbf{e}_k \right) \right\|_2^2 + \frac{\mu}{2} \sum_{k=1}^{M+T} \sum_{j=1}^{M+T} ||(\mathbf{e}_k - \mathbf{e}_j)||_2^2$$

$$+ \sum_{k=T+1}^{M+T} \gamma_k \sum_{i=1}^{N} p_{ik} + \sum_{i=1}^{N} \sum_{t=1}^{T} \frac{1}{\sigma^2 l(x_i,t)(p_{it} - 1)^2}$$

Often, there are many more non-target training pixels than target training pixels, to emphasize the target training data a weight is placed on their error terms in the objective function to enhance their contribution to the estimate of the target and background endmembers. The value for $w_{l(x_i,t)}$ is 1 when $x_i$ is a background pixel and is $\frac{\alpha N_b}{N_t}$ where $N_b$ is the number of background training samples and $N_t$ is the number of target training samples for pixels that contain some proportion of target. Therefore, if the parameter $\alpha$ is set to 1, then the weight on the target points is scaled such that the collection of target points has the same influence on the first term as the collection of non-target training points. Furthermore, $\alpha$ can be set to larger than 1 to further emphasize the importance of target training data over background data.

The final term in the multi-class C-FUMI objective function encourages the proportions associated with target endmembers in target pixels to be large. This term can be viewed as a prior distribution placed on the target proportion values where the prior is a truncated Gaussian centered at 1. The weight of this term is determined by $\alpha$ which is a fixed parameter.

The multi-class C-FUMI algorithm updates the target and non-target endmembers, proportions, and number of endmembers by iteratively minimizing the objective function in Equation 4. In order to update both target and non-target endmembers, the proportions for all data points are held constant and Equation 4 is minimized by setting the derivative of the objective with respect to each endmember to zero and solving for the endmember value. When updating proportions, endmembers are held constant and Equation 4 is minimized subject to the constraints in Equation 2. Since this is a quadratic objective with linear constraints, a quadratic programming step is used to update the proportions. The sparsity promoting term (the 4th term in the objective) is used to determine the number of non-target endmembers needed. This term drives the proportions associated with unneeded non-target endmembers to zero. Then, the unneeded endmembers can be removed with no effect on the squared error terms. The objective function is iteratively minimized until some stopping criterion is reached such as convergence or a maximum number of iterations.

After learning target and non-target prototypes, target detection on test data can be carried out. Given the prototypes and test data, the proportions for all the prototypes for the given test data are computed by minimizing the residual sum of squared errors subject to the constraints in Equation 2 using a quadratic programming step. The proportion value for the target endmember is used as the detection statistic.

3. EXPERIMENTAL RESULTS

Multi-class C-FUMI was applied to simulated data generated from four endmembers selected from the ASTER spectral library. Endmembers correspond to Borate, Carbonate, Chloride and Sulfate. Simulated data was generated by drawing proportions from Dirichlet distributions with the following mean distribution values, $[0.6, 0.2, 0.2], [0.08, 0.1, 0.1], [0.4, 0.4, 0.05, 0.05], [0, 0.7, 0.3]$, and $[0, 0.1, 0.9]$. The first two proportion values correspond to the target endmembers, Borate and Carbonate, respectively. None of the training data were pure pixels of either target endmember or either of the background endmembers. For training data, 950 pixels were generated; 50 pixels containing target 1 and background, 50 pixels containing target 2 and background, 50 pixels containing target 1, target 2 and background and 800 pixels containing only background were generated. For testing data, 1800 pixels were generated in the same fashion. Using the test data, the multi-class C-FUMI algorithm was used to estimate endmember spectra.
was run with the following parameter settings: \( \mu = 0.01, \gamma = 1, \alpha = 2, \) and \( \sigma = 0.5. \) The algorithm was run with 20 initial background endmembers. Multi-class C-FUMI correctly pruned the background endmember set down to 2 background endmembers. Figure 1 shows the true and estimated endmembers using the multi-class C-FUMI algorithm. As can be seen, the estimated endmembers correspond well to the true endmembers.

![Figure 1](Image)

Figure 1. Comparison of true endmembers (solid) and estimated endmembers (dashed) found using the Multi-class C-FUMI algorithm.

4. DISCUSSION AND FUTURE WORK

In this paper, a multi-class sub-pixel target detection algorithm that is based on the functions of multiple instances framework is presented. The proposed method estimated target and non-target prototypes from a binary labeled training data set. Future work for extending this method will include the use of sparsity promoting priors to encourage each data point to have non-zero proportions associated with a small number of endmembers. In many datasets, pixels are often associated with a small number of endmembers. Also, for image data, spatial information may be incorporated to help improve results. Finally, investigations into methods to have the target endmembers have as unique of a spectral shape from background endmembers as possible are being conducted. The use of non-linear mixing models, as opposed to the linear mixing model, will also be investigated.

REFERENCES


