Analysis of Classification Algorithm on Hypergraph

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Abstract: Classification learning problem on hypergraph is an extension of multi-label classification problem on normal graph, which divides vertices on hypergraph into several classes. In this paper, we focus on the semi-supervised learning framework, and give theoretic analysis for spectral based hypergraph vertex classification semi-supervised learning algorithm. The generalization bound for such algorithm is determined by using the notations of zero-cut, non-zero-cut and pure component. Furthermore, we derive a generalization performance bound for near-zero-cut partition with optimal parameter λ.

Keywords: Classification algorithm, hypergraph, pure component, pure sub-hypergraph, scaling factor, tuning parameter.

1. INTRODUCTION

Spectral clustering of weighted graph, an important component of spectral graph theory and statistic learning theory, has been widely used in many fields, such as computer network, data mining, image segmentation and ontology similarity computation (see [1-7]). Hypergraph is a subset system for limited set, which is the most general discrete structure, and it is the generalization of the common graph. For many practical problems, adopting the concept of hypergraph is more usefully than adopting the concept of graph. At present, the model of hypergraph has been applied in many fields, such as: VLSI layout, electricity network topology analysis. The goal of classification algorithm on hypergraph is to divide vertices into several classes, and spectral method may play a key role in it (see [8-11]). Some applications on such classification can be referred in [12-18].

Let \( V=\{v_1, v_2, \ldots, v_m\} \) be a limited set, \( E \) is family of subset of \( V \), i.e., \( E \subseteq 2^V \). Then \( H=(V, E) \) is a hypergraph on \( V \). The element of \( V \) is called a vertex, the elements of \( E \) is called a hyperedge. Let \(|V| \) be the order of \( H \), \(|E| \) be the scale of \( H \).

\(|e|\) is basic number of hyperedge \( e \). \( r(H)=\max_j |e_j| \) is rank of hyperedge \( e \), and \( s(H)=\min_j |e_j| \) lower rank of hyperedge \( e \).

If \(|e|=k\) for each hyperedge \( e \) of \( E \) (that is \( r(H)=s(H)=k \)), then \( H \) is a \( k \)-uniform hypergraph. If \( k=2 \), then \( H \) is just a normal graph.

A hypergraph \( H \) is called a simple hypergraph or a sperner hypergraph, if any two hyperedges are not contained with each other. Let \( H'=(V, E') \) is a hypergraph on \( V \), if \( E' \subseteq E \), then \( H' \) is a part-hypergraph of \( H \). For \( S \subseteq V \), \( H[S]=\{e \subseteq E: e \subseteq S\} \) is called a sub-hypergraph of \( H \) induced by \( S \).

Hypergraph \( H \) can be represented by graph by using the set of vertices to represent the elements of \( V \). If \(|e_j|=2 \), using a continuous curve which attach to the elements of \( e_j \) to representing \( e_j \); If \(|e_j|=1 \), using a loop which contains \( e_j \) to represent \( e_j \); If \(|e_j| \geq 3 \), using a simple close curve which contains all the elements of \( e_j \) to represent \( e_j \).

In this paper, we assume \( H \) is a weighted hypergraph, each edge given a weight \( w(e) \). The degree of vertex \( v_j \) in hypergraph \( H \) is denoted as\n
\[
\deg_j(H) = \sum_{e \in E} w(e) h(v, e),
\]

where,

\[
h(v, e) = \begin{cases} 1, & \text{if } v \in e \\ 0, & \text{if } v \notin e \end{cases}
\]

Let \( \delta(e) = \sum_{v \in V} h(v, e) \). Then, the normalized laplacian \( L(H) \in \mathbb{R}^{m \times m} \) on hypergraph \( H \) is defined by:

\[
L_j(H) = \begin{cases} -\sum_{e \ni v_j} w(e) \frac{1}{\delta(e)} & \text{if } \deg_j(H) \text{ otherwise} \\ \deg_j(H) & \end{cases}
\]

Fixed \( m \) scaling factor \( \mathcal{S}_j \) (\( j=1, \ldots, m \) ) (Normally, we can choose \( \mathcal{S}=I \), or \( \mathcal{S}_j = \deg_j(H) \)). Let \( \mathcal{S} = \text{diag}(\mathcal{S}_j) \). Then \( \mathcal{S} \)-normalized Laplacian on hypergraph is given as:

\[
L_j(H) = \mathcal{S}^{-1/2}L(H)\mathcal{S}^{1/2}.
\]

The corresponding regularization is relying on:
\[ f_k^* L_x (H) f_k = \frac{1}{2} \sum_{i \in k} \frac{1}{\delta (e)} \sum_{j,j' \in e} w(e) \frac{f_{j,k} - f_{j',k}}{\sqrt{S_u} - \sqrt{S_v}}. \]

The definition of function \( f \) will be given later. It implies that, if vertices \( j, j' \) contained in the same hyperedge, then they have higher similarity and it is possible to be classified in the same class.

Now, we give the following definition for component on hypergraph: A sub-hypergraph \( H_0 = (V_0, E_0) \) of \( H \) is called pure component, if \( H_0 \) is connected, \( E_0 \) is induced by restricting \( E \) on \( V_0 \), and the labels \( y \) have identical values on \( V_0 \). A pure sub-hypergraph \( H' = \bigcup_{i \in I} H_i \) of \( H \) divides \( V \) into \( q \) disjoint sets \( V = \bigcup_{i \in I} V_i \) such that each sub-hypergraph \( H_i = (V_i, E_i) \) is a pure component. Denote by \( \lambda_i (H_i) = \lambda_i (L(H_i)) \) the \( i \)-th smallest eigenvalue of \( L(H_i) \).

For example, if all hyperedges of \( H \) which connect vertices with different labels are removed, then the resulting sub-hypergraph is a pure super-hypergraph. For each pure component \( H_i \), its first eigenvalue \( \lambda_i (H_i) \) is always zero. The second eigenvalue \( \lambda_2 (H_i) > 0 \) since \( H_i \) is connected.

Let \( Y \) be output space, which contain \( K \) possible values, and each value represents a class. Each vertex \( v_j \) on hypergraph corresponding to a output value \( y_j \). \( Z_n = \{ j : 1 \leq i \leq n \} \) is \( n \) indices random draw from \( \{ 1, \ldots, n \} \) uniformly and without replacement. Manually label the \( n \) vertices \( v_j \) with labels \( y_j \in Y \) and then automatically label the remaining \( m-n \) vertices. The aim of transductive classification learning on hypergraph is to estimate the labels on the remaining \( m-n \) vertices.

With fixed \( y = \{ y_1, \ldots, y_m \} \). The goal is to reconstruct it from subset of labels. In statistic learning theory setting, label \( y_j \) is regarded as vector in \( \mathbb{R}^K \); i.e., \( y_j = k \) means \( y_j \) is corresponding to vector \( f = \{ f_{j,1}, \ldots, f_{j,K} \} \), where \( k \)-th entry is 1, all others are 0. We can decode the corresponding label estimation \( \hat{y}_j \) as:

\[
\hat{y}_j = \hat{y}(f_j) = \arg \max_k \{ f_{j,k} : k = 1, \ldots, K \}.
\]

Let \( y_j \) be a true label, \( I() = \begin{cases} 1, & \text{if } \cdot \text{ is true} \\ 0, & \text{if } \cdot \text{ is false} \end{cases} \)

Then, the error for classification is:

\[
\text{err}(f_j, y_j) = I(\hat{y}(f_j) \neq y_j).
\]

For estimating the concatenated vector \( f = [f_j] = [f_{j,1}, \ldots, f_{j,k}] \in \mathbb{R}^m \) via a subset of labeled vertices, we need to impose restrictions using a quadratic regularizer:

\[
f^T Q f = \sum_{k=1}^m f_{j,k}^2.
\]

where, \( K \in \mathbb{R}^{m \times m} \) is full rank positive definite kernel matrix, \( f_k = \{ f_{j,1}, \ldots, f_{j,K} \} \in \mathbb{R}^m \); i.e., the predictive vector for each class \( k \) is regularized separately. Note that we use \( K \) to denote the kernel matrix and \( K \) to denote the number of classes.

For a fixed vector \( f \in \mathbb{R}^m \), we use loss function \( \phi(f_j, y_j) \) to measure the quality of its component \( f_j \). Thus, the empirical risk on \( Z_n \) subject to \( f^T Q f \) is given by:

\[
\hat{f} (Z_n) = \arg \min_{f \in \mathbb{R}^m} \frac{1}{n} \sum_{j \in Z_n} \phi (f_j, y_j) + \lambda f^T Q f,
\]

where, \( \lambda > 0 \) is a regularization parameter. We are interested in the following special class of loss function in this paper:

\[
\phi (f_j, y_j) = \sum_{k=1}^n \phi_0 (f_{j,k}, \delta_{k,y_j}),
\]

where,

\[
\delta_{a,b} = \begin{cases} 1, & a = b \\ 0, & a \neq b \end{cases}.
\]

Let \( \nabla_i \phi_0 (x, y) \) be a sub-gradient of \( \phi_0 (x, y) \) with respect to \( x \). We need the following assumption:

**Assumption 1:** There exist positive constants \( a, b, \) and \( c \) such that

1. \( \phi_0 (x, y) \) is non-negative and convex in \( x \).
2. When \( y = 0,1, \) and \( \phi_0 (x, y) \leq a, |\nabla_i \phi_0 (x, y)| \leq b. \)
3. \( c = \inf \{ x : \phi_0 (x, 1) \leq a \} - \sup \{ x : \phi_0 (x, 0) \leq a \} \).

We first give classification error on hypergraph as follows:

**Theorem 1.** Consider (1) with loss function satisfying Assumption 1. Then for \( \forall p > 0 \), the expected generalization error of the learning algorithm (1) on training samples \( Z_n \) (uniformly drawn without replacement form hypergraph vertices \( 1, \ldots, m \)) can be bounded by:

\[
E_{Z_n} \frac{1}{m-n} \sum_{j \in Z_n} \text{err}(\hat{f}_j (Z_n), y_j)
\]

\[
\leq \frac{1}{a} \inf_{f \in \mathbb{R}^m} \left[ \frac{1}{m} \sum_{j=1}^m \phi (f_j, y_j) + \lambda f^T Q f + \frac{\text{tr}_p (K)}{\lambda N} \right],
\]

where \( Z_n = \{ 1, \ldots, m \} \) - \( Z_a \),

\[
\text{tr}_p (K) = \left( \sum_{j=1}^m K_{j,j} \right)^{p/2},
\]

and \( K_{j,j} \) denoted as \( j \)-th diagonal entry of matrix \( K \).

2. **GENERALIZATION BOUND WITH HYPERGRAPH-CUT**

For fixed labeled \( y = \{ y_j \} = 1, \ldots, m \) on \( V \), the hypergraph cut for the \( S \)-normalized Laplacian \( L_S (H) \) as:
\[ \text{cut}(L, y) = \frac{1}{2} \sum_{e \in E} \sum_{(j, j') \in e} w(e) \left( \frac{1}{S_j} + \frac{1}{S_{j'}} \right) \]
\[ + \frac{1}{2} \sum_{e \in E} \sum_{(j, j') \in e} w(e) \left( \frac{1}{\sqrt{S_j}} - \frac{1}{\sqrt{S_{j'}}} \right)^2. \]

In the following section, we will apply Theorem 1 to analyze hypergraph learning by using hypergraph-cut.

The learning theoretical definition of hypergraph-cut penalizes a normalized version of between-class hyperedge weights on one hand, and penalizes within-class hyperedge weights when such a hyperedge connects two vertices with different scaling factors on the other hand. For un-normalized Laplacian, we delete the second term on the right hand side of hypergraph-cut definition, i.e., it only penalizes weights corresponding to edges connecting the vertices with different labels. Under such situation, the learning theoretical definition corresponds to the hypergraph-theoretical definition:
\[ \text{cut}(L, y) = \sum_{e \in E} \sum_{(j, j') \in e} w(e). \]

According to the learning theoretical hypergraph-cut definition, the generalization result for the estimator in (1) with \( K \) is defined as:
\[ K^{-1} = \alpha S^{-1} + L(H) = S^{-1/2} (\alpha I + L(H)) S^{-1/2}. \]

where, \( \alpha > 0 \) is called a tuning parameter in order to ensure that \( K \) is strictly positive definite. The corresponding regularization can be regarded as:
\[ f^T K f = \sum_{k=1}^{K} (\alpha \sum_{j=1}^{m} \frac{f_{jk}^2}{S_j} + \sum_{e \in E} \sum_{(j, j') \in e} w(e) \left( \frac{f_{jk}}{\sqrt{S_j}} - \frac{f_{j'k}}{\sqrt{S_{j'}}} \right)^2. \]

Usually, other trick is by setting \( K^{-1} = \alpha I + L(G) \). The corresponding conclusions are similar to that of (2).

Note that the bound of Theorem 1 depends on \( \lambda \) and \( K \), and this inspires us to consider the more detailed bound with optimal \( \lambda \). The assumption is stated as follows which is used for our analysis.

**Assumption 2** Consider (1) with regularization condition (2), \( \phi \) is loss function and satisfies Assumption 1 and \( \phi_0(0,0) = \phi_0(1,1) = 0. \)

The Assumption 2 on the loss function here holds for the least squares method and other standard loss functions such as SVM.

**Theorem 2** Consider (1) with Assumption 2 is satisfied. Then for any \( p > 0 \), there exists a sample independent regularization parameter \( \lambda \) such that the expected generalization error can be bounded by:
\[ E_{z_n} \frac{1}{m-n} \sum_{j \in Z_n} \text{err}(\hat{f}(Z_j), y_j) \leq \frac{C_p(a,b,c)}{n^{p/(p+1)}} \left( \text{cut}(L, y) \right)^{p/(p+1)} \text{tr}(K)^{1/(p+1)}, \]

where, \( s = \sum_{j=1}^{m} S_j^{-1} \).

In the following context, we will give some applications of examples for Theorem 2.

### 3. Algorithm Analysis Using Zero-Cut in Hypergraph

In this section, we consider an application of Theorem 2 for the normalized Laplacian with the zero-cut assumption that each connected component of the hypergraph has a single label. Under this assumption, our goal is to estimate the label for each connected component.

**Theorem 3** Consider (1) such with Assumption 2 and the regularization condition is \( K^{-1} = \alpha I + L. \) Assume that \( \text{cut}(L, y) = 0 \), and the hypergraph has \( q \) connected components with sizes \( m_1 \leq \ldots \leq m_q \). For any \( p > 0 \), let \( \alpha \rightarrow 0 \), and with optimal \( \lambda \), we obtain the generalization bound:
\[ E_{z_n} \frac{1}{m-n} \sum_{j \in Z_n} \text{err}(\hat{f}(j), y_j) \leq \frac{C_p(a,b,c)}{n^{p/(p+1)}} \left( \sum_{i} \frac{m}{m_i} \right)^{1/(p+1)} + O(\alpha), \]

where \( C_p \) is defined by (3). More specific, we get
\[ E_{z_n} \frac{1}{m-n} \sum_{j \in Z_n} \text{err}(\hat{f}(j), y_j) \leq \min \{ \frac{b}{ac}, \frac{b}{ac} \}, \]

Under the zero-cut assumption, when \( \alpha \rightarrow 0 \), the generalization error can be bounded as \( O\left( \frac{1}{n} \right) \). However, a faster convergence rate of \( O\left( \frac{1}{n} \right) \) can also be achieved, although the bound for generalization error depends on the inverse of the smallest component size through \( \frac{m}{m_i} \geq q, i.e., \) we can reach a better convergence at the \( O\left( \frac{1}{n} \right) \) level under the condition that the sizes of the components are balanced. If the component sizes are significantly different, the convergence may behave like \( O\left( \frac{1}{\sqrt{n}} \right) \).

### 4. Non-Zero Cut and Pure Components

We find the assumption that each connected component has only one label (i.e., the cut is zero) and it is too restrictive, and in many applications, this assumption is not reasonable. In this section, we relax the assumption and obtain similar bounds.

**Theorem 4.** Consider (1) with Assumption 2 is satisfied. Let \( H = \bigcup_{i=1}^{q} H_i \) be a pure sub-hypergraph of \( H \). For any
Theorem 4 can be regarded as a natural generalization of Theorem 3 for $p \geq 1$. As common graph, it quantitatively illustrates the importance of analyzing hypergraph learning by using a partition of the original hypergraph into well-connected pure components. The second eigenvalue $\lambda_2(H_j)$ measures how well-connected $H_j$ is. A more intuitive quantity that measures the connectedness of hypergraph $H=(V,E)$ is the isoperimetric number $h_{H_j}$ defined as

$$h_{H_j} = \inf_{S \subseteq V} \sum_{e \in S \setminus V-S,I \subseteq \{I \}} \frac{w(e)}{\delta(e) \min|S||V-S|}.$$ 

Similar as standard spectral graph theory [19], we can check that $\lambda_2(H_j) \geq \frac{2 \max \deg(H_j)}{h_{H_j}}$.

If the vertices are well-connected everywhere, then the isoperimetric number of hypergraph $H$ is large. Specifically, if $\deg(H)$ is of the order $|V|$, and $w(e)=1$ when $e \in E$, then

$$\sum_{e \in S \setminus V-S,I \subseteq \{I \}} \frac{w(e)}{\delta(e)}$$

is of the order $|S||V-S|$, and $h_{H_j}=O(|V|)$ for a well-connected hypergraph. Let $H'$ be a pure-sub-hypergraph of $H$ with well-behaved, i.e., each pure component $H_j$ of $H'$ is well-connected in the above sense. We infer that $\lambda_2(H_j) \geq \frac{1}{h_{H_j}}$ for some constant $u(H')$ which is independent on the vertex number of the pure components (but only how well-connected each pure component is). By such condition, we replace $\sum_{j=1}^n m_j \lambda_2(G_j)^p \sum_{j=1}^n m_j^{1-p}$ in Theorem 4 and get a simplified bound:

$$E_{Z_n} \frac{1}{m-n} \sum_{j \notin Z_n} \text{err}(\hat{f}_j, y_j) \leq C_p(a,b,c) \frac{\sum s_j(p) / m_j}{n^p + \rho(p+1)} \left( \frac{s}{\sqrt{m}} \right)$$

+ $\left( \frac{\text{cut}(L_{g,y})}{u(H') m} \right)^{2(p+1)}$

where

$$u(H') = \min \frac{\lambda_2(G_j)}{m_i}.$$

We consider the following two special situations: $p = 1$ and $p \to \infty$:

$$E_{Z_n} \frac{1}{m-n} \sum_{j \notin Z_n} \text{err}(\hat{f}_j, y_j) \leq 2 \max_{j \notin Z_n} (S_j / m_j) \frac{\sum s_j(1) / m_j}{n} \left( \frac{s}{\sqrt{m}} \right)$$

+ $\left( \frac{\text{cut}(L_{g,y})}{u(H') m} \right)^{2}$

(5)

These bounds can be regarded as the generalizations of those in Theorem 4. If we take $S=I$, then the number of pure components $q$ affects the $O(\frac{1}{\sqrt{n}})$ convergence rate in (4) as

$$\sum_{j=1}^q m_j^{1-p} = q.$$ If the vertices number of the components are balanced, better convergence at the $O(\frac{1}{n})$ level as in (5) can be achieved; otherwise, the convergence may just be as $O(\sqrt{\frac{q}{n}})$ level. This fact inspires a scaling matrix $S$ that compensates for the unbalanced vertices number of pure component, which we will discuss in the following context.

5. NEAR-ZERO-CUT PARTITION WITH OPTIMAL NORMALIZATION

We discuss a pure sub-hypergraph $H'=\bigcup_{j=1}^q H_j$ of $H$. If the scaling factors $S_j$ are nearly constant within each pure component, then using the Laplacian definition above, we infer a small regularization penalty for the hyperedges within a pure component and between the vertices with similarly output values (i.e., $f_{j,k} \approx f_{j,k}$). Thus, in the next context, we focus on finding the optimal scaling matrix $S$ such that $S_j$ is constant within each pure component $V_j$. Assume that we use $q$ numbers $[S_j]_{j=1}^q$ to quantify $S$ which satisfies $S_j = S_j$ for $j \in V_j$.

Consider the following quantity:
\[ cut(H', y) = \sum_{(i,j) \in \Delta(H', y)} w(e) \frac{1}{\delta(e)} \]
\[ + \sum_{j=1}^{2} \sum_{i \in \mathbb{V}_j} \sum_{\{i,j\} \in \mathbb{E}} w(e) \frac{1}{2\delta(e)} \]

Then, we have
\[ cut(L_{\mathbb{V}}, y) \leq \frac{cut(H', y)}{\min_{i} s_i}. \]

We assume that hyperedge weights are small if it contains vertices between pure components. Then, we can ensure that \( cut(H', y) \) is small as well.

With the \( O\left(\frac{1}{n}\right) \) convergence rate, we obtain from (5) that
\[ E_{\varepsilon_j} \frac{1}{m-n} \sum_{j \in \mathbb{Z}_2} \text{err}(\hat{f}_j, y_j) \leq \frac{b}{ac} \frac{\max(s_j / m_j)}{n} \left( \frac{\sum m_j}{s_j} + \frac{cut(H', y)}{u(H') \min_{i} s_i} \right)^2. \]

If \( cut(H', y) \) is small, then the right hand side of dominating term becomes \( \frac{\max(s_j / m_j)}{n} \sum m_j / s_j \), which can be optimized by choosing \( s_j = m_j \), and the resulting bound will be as follows:
\[ E_{\varepsilon_j} \frac{1}{m-n} \sum_{j \in \mathbb{Z}_2} \text{err}(\hat{f}_j, y_j) \leq \frac{b}{ac} \frac{1}{n} \left( \sqrt{q} + \frac{cut(H', y)}{u(H') \min_{i} s_i} \right)^2. \]

i.e., under the condition \( cut(H', y) \) is small, we can choose scaling factor \( \frac{s_j}{m_j} \approx m_j \) for each pure component such that the generalization bound is of the order \( O\left(\frac{1}{n}\right) \), which approximate to \( \frac{bq}{acn} \).

6. CONCLUSION

In our paper, we consider the semi-supervised learning framework, and obtain theoretic conclusions for spectral based hypergraph vertex classification of semi-supervised learning algorithm. The contribution of this article is two-fold: first, we deduce the generalization bound for such algorithm in terms of zero-cut, non-zero-cut and pure component; second, the generalization performance bound for near-zero-cut partition with optimal parameter \( \lambda \) is yielded. The result achieved in our paper illustrates the promising application prospects for algorithms using hypergraph model.

CONFLICT OF INTEREST

The authors confirm that this article content has no conflict of interest.

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