Multi-way Clustering Using Super-symmetric Non-negative Tensor Factorization

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ABSTRACT

We consider the problem of clustering data into $k \geq 2$ clusters given complex relations — going beyond pairwise — between the data points. The complex n-wise relations are modeled by an n-way array where each entry corresponds to an affinity measure over an n-tuple of data points. We show that a probabilistic assignment of data points to clusters is equivalent, under mild conditional independence assumptions, to a super-symmetric non-negative factorization of the closest hyper-stochastic version of the input n-way affinity array. We derive an algorithm for finding a local minimum solution to the factorization problem whose computational complexity is proportional to the number of n-tuple samples drawn from the data. We apply the algorithm to a number of visual interpretation problems including 3D multi-body segmentation and illumination-based clustering of human faces.

1. INTRODUCTION

We address the fundamental problem of grouping feature vectors (points) on the basis of multi-wise similarity or coherency relationships among n-tuples of points. The case of pairwise ($n = 2$) relationships has drawn much attention in statistical, graph theoretical and computer vision literature. For example, a clustering task of a collection of points $\mathbf{x}_1, ..., \mathbf{x}_m$ in Euclidean space R^n may be induced by a symmetric "affinity" matrix $K_{ij} = e^{-\|\mathbf{x}_i - \mathbf{x}_j\|^2/\sigma^2}$ which would serve as the input to a process aimed at assigning the m points into $k \geq 2$ classes — either "hard" assignments (a point ending up assigned exclusively to one class) or "soft" assignments by generating a probability $g_{r,s} = P(y_s = r \mid \mathbf{x}_s)$ of point $\mathbf{x}_s$ being assigned to class (cluster) C_r where $y_s \in \{1, ..., k\}$, $s = 1, ..., m$, are the corresponding (unknown) labels. The desired membership probabilities form an $m \times k$ non-negative "partition" matrix $G = [\mathbf{g}_1, ..., \mathbf{g}_k]$, where a hard clustering entails $G^\top G = I$. Therefore, the clustering process based on a (symmetric) pairwise similarity relationship starts with an input $m \times m$ matrix K with the goal of finding a stochastic $m \times k$ matrix $G \geq 0$, and if a hard clustering is desired then in addition one should have $G^\top G = I$. The greatly popular "spectral" clustering technique, for example, relaxes the non-negativity constraint and looks for the k leading eigenvectors of a normalized version of K as a new coordinate system which in ideal settings would map the original coordinates of the points to k points in R^k, one per each cluster [10, 11]. Graph theoretical methods perform normalization on the affinity matrix (producing the Laplacian of K) whereby the second smallest eigenvector splits the points into two clusters [15, 8], and more recently it was shown that conditionally independent statements $y_i \perp y_j \mid \mathbf{x}_i, \mathbf{x}_j$ and $y_i \perp \mathbf{x}_j \mid \mathbf{x}_i$ lead to the finding that $K = GG^\top$ which also underlies the k-means formulation of clustering [20].

It has been recently pointed out by a number of authors [1, 5, 21] that for many computer vision and machine learning applications a pairwise affinity relationship among points does not capture the complexity of the problem. For example, if a parametric model requires d points for a definition, then $n \geq d + 1$ points can be used to provide an affinity value by taking the square residual error Δ^2 of the least-squares fit of the n points to the model and translating it into a probability value $\kappa(\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}) = e^{-\Delta^2/\sigma^2}$, where $1 \leq i_1, ..., i_n \leq m$. The affinities form an n-way (tensor) super-symmetric array $K_{i_1,...,i_n} = \kappa(\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n})$ which like as above is the input for a clustering of the m points into $k \geq 2$ clusters, i.e., of forming the $m \times k$ stochastic matrix $G \geq 0$. Computer vision applications for parametric models include (i) 3D-from-2D multi-body segmentation where under an affine model one would need $n \geq 5$ points to determine an affinity value [17] and under a perspective model $n \geq 9$ points are required [9]; (ii) segmenting 3D objects taken from the same pose but under varying illumination conditions — for matte surfaces ignoring self-shadowing one would need $n \geq 4$ pictures for determining an affinity, i.e., the likelihood that the four pictures are of the same 3D surface [13], and (iii) multi-model selection in general. Non-parametric applications include clustering articles into different topics on the basis of authors alone where the affinity degree n is determined by the maximal number of articles written by a single author [21].

We address in this paper the problem of clustering m points into $k \geq 2$ clusters given an n-way super-symmetric affinity array $K \in [m] \times .. \times [m] = [m]^{\times n}$. We will first describe the state of the art in this domain and then proceed to describe our contribution.

1.1 Previous Work on n-way Clustering

Clustering from an n-way affinity array is new to computer vision and machine learning (existing publications are few months old [1, 5, 21]) but has been a topic of extensive research in VLSI and PCB clustering placement since the early 70s. A convenient representation of the problem is given by a *hypergraph* where the vertices correspond to the points (circuit elements in VLSI) to be clustered into $k \geq 2$ parts and the hyper-edges (nets connecting circuit elements) correspond to subsets of vertices where the degree n of an edge is the number of vertices spanned by it. An edge can also be associated with a weight. Thus a complete hypergraph with m vertices and uniform degree n has m^n hyper-edges and if the hypergraph is undirected then there are only $\binom{m}{n}$ different hyper-edges (the order of vertices spanned by an edge does not matter).

Fig. 1a illustrates the one-to-one mapping between a uniform

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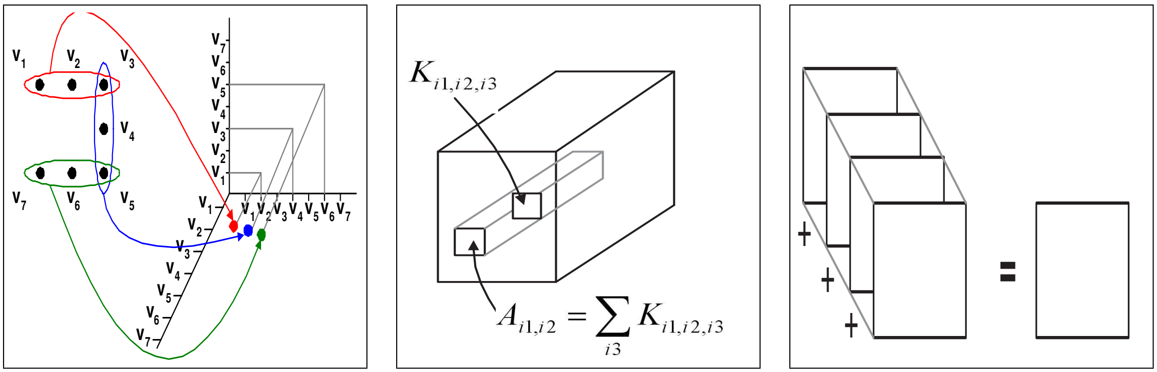

(a) (b) (c)

Figure 1: *(a) the hypergraph and tensor representations of a triadic affinity relation (see text); (b,c) the projection paradigm forming a graph from the original hypergraph (see text).*

degree hypergraph (of degree three) and 3-way array K. A hyper-edge spans three vertices $1 \leq i_1, i_2, i_3 \leq 7$ and corresponds to the entry K_{i_1,i_2,i_3} of the tensor. If the hyper-edges are weighted then K_{i_1,i_2,i_3} is equal to the weight, otherwise the entries of K are binary. An undirected hypergraph corresponds to a super-symmetric tensor $K_{i_1,i_2,i_3} = K_{\sigma(i_1,i_2,i_3)}$ where $\sigma(i,j,k)$ is a permutation of three letters S_3. In fact we only need to store the entries $1 \leq i_1 < i_2 < i_3 \leq 7$ — but this would be addressed later in the technical sections.

The techniques employed by the VLSI/PCB community for hypergraph partitioning into clusters are largely heuristic in nature. The techniques center around two main paradigms: (i) local update of a given clustering solution by means of vertex swapping — known as the FM and KL techniques [6, 3], and (ii) a multilevel paradigm which proceeds by generating a sequence of successively coarser (by means of vertex mergers) hypergraphs followed by a clustering of the coarsest hypergraph (which contains only k vertices). The clustering result from the coarsest hypergraph is projected to the next finer level and is subjected to the local KL/FM refinement update and projected upwards again — for a review see [2].

The recent work coming out from the vision and machine learning communities [1, 5, 21] are all very similar to each other and take the approach of finding an approximate graph that best resembles the original hypergraph. For example, if H is the $m \times \binom{m}{n}$ hypergraph incident matrix, then [5] computes the graph adjacency $m \times m$ matrix $HH^\top$ whose entries H_{ij} correspond to the sum of all hyper-edges weights which are incident to vertices v_i, v_j of the hypergraph, whereas [21] performs a multiplicative normalization with the vertices degrees (the sum of weights incident to a vertex) as part of creating a Laplacian of the hypergraph. Both are consistent with graph theoretical research which define hypergraph Laplacians by summing up all the weights incident to pairs of vertices [12]. Once a graph has been created the authors then perform the clustering using graph techniques — the popular being spectral clustering or normalized cuts.

The idea of projecting the hypergraph onto a graph is not without merit. The basis for doing so lies in the assumption that it is possible to define a pairwise affinity given higher-order affinities. Consider, for example, clustering lines. Since any two points define a line we would need to rely on a 3rd-order affinity relationship K_{i_1,i_2,i_3} thus the affinity between points $\mathbf{x}_i$ and $\mathbf{x}_j$ would be $A_{i,j} = \sum_{i_3} K_{i,j,i_3}$ (see Fig. 1b). If the line passing through $\mathbf{x}_i, \mathbf{x}_j$ is dense with points and the number of lines (clusters) in the data is relatively small then indeed one should expect $A_{i,j}$ to be high — and vice versa if $\mathbf{x}_i, \mathbf{x}_j$ are not supported by a line of data points then A_{ij} should be low. What in fact is being performed is a projection of the 3D cube along one of its axis (any axis will do since the cube is super-symmetric) to form a 2D array (see Fig. 1c).

Naturally, the projection from a high-order affinity array to a pairwise affinity would have a high SNR for *simple* problems. Problems with a small number of clusters having a high number of points per cluster relative to the affinity degree would benefit from the projection approach. Generally, however, a projection induces information-loss and the pairwise affinities will get increasingly obscured with increasing affinity degree — and since we have here a "curse of dimensionality" effect, a rapid decline of pairwise affinity SNR is expected with increasing problem complexity.

1.2 Contribution of our Approach

Rather than performing a projection we work with the full affinity tensor. Our approach enables us to define any affinity degree we desire — including one obtained by projection of the original tensor to a lower degree one, and in particular to a pairwise affinity. Starting from a super-symmetric tensor K of any degree, we show that a general probabilistic argument on conditional independence introduces a simple connection between K and the desired $m \times k$ partition matrix $G \geq 0$. The connection is two fold (i) the "balancing" requirement on the cluster sizes requires K to be hyper-stochastic, and (ii) G is obtained by a super-symmetric non-negative factorization (SNTF) of K. The algorithm we derive for performing the SNTF is based on a positive-preserving gradient descent scheme. The scheme also supports partial sampling of the affinity tensor which is necessary since it is practically impossible to fill in, or even store, a full high-degree affinity array. The complexity of the update step is $O(mkp)$ where $p \leq \binom{m}{n}$ is the number of samples.

The work presented here is an outgrowth of our algebraic treatment of pairwise affinity clustering showing that K is completely positive [20] and of a general treatment of tensor ranks and conditional independence with latent variables [14].

2. PROBABILISTIC CLUSTERING FROM N-WAY AFFINITY ARRAYS

Let $\mathbf{x}_i \in R^d$, $i = 1, ..., m$, be points which we wish to assign to k clusters $C_1, .., C_k$ and let $y_i \in \{1, ..., k\}$ be the associated (unknown) labels. We assume that we have a way to measure the probability, which for now is simply an affinity measure in the range

$[0, 1]$, that any n-tuple of points $\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}$, $1 \le i_j \le m$, belong to the same cluster. For example, if we know that the clusters are defined as $n-1$ dimensional subspaces, then $k(\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}) = e^{-\Delta}$, where Δ is the volume defined by the n-tuple, would be a reasonable measure of n-tuple affinity because $k(\cdot) = 1$ when the points are linearly dependent (i.e., live in an $l < n$ dimensional subspace) and approaches zero as the volume increases.

Given the affinities $k(\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n})$, which form an n-way array K indexed by $K_{i_1,...,i_n}$, we wish to assign a probability $g_{r,s} = P(y_s = r \mid \mathbf{x}_s)$ of point $\mathbf{x}_s$ belonging to cluster C_r. The desired membership probabilities form an $m \times k$ matrix $G = [\mathbf{g}_1, ..., \mathbf{g}_k]$, thus our goal is to find G given K. We will derive below an algebraic constraint on the n-way array K and relate it, by means of factorization and linear constraints, to the desired matrix G.

Consider the labels y_i as hidden variables and assume that

$$y_1 \perp ... \perp y_m \mid \mathbf{x}_1, ..., \mathbf{x}_m,$$

i.e., that the labels are independent of each other given the data points, and that

$$y_i \perp \{\mathbf{x}_1, ..., \mathbf{x}_{i-1}, \mathbf{x}_{i+1}, ..., \mathbf{x}_m\} \mid \mathbf{x}_i,$$

namely that given $\mathbf{x}_i$ its label y_i is independent from all other data points[1]. The probability that $\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}$ belong to cluster C_r, $P(y_{i_1} = r, ..., y_{i_n} = r \mid \mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n})$ is factorized:

$$P(y_{i_1} = r, ..., y_{i_n} = r \mid \mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}) = P(y_{i_1} = r \mid \mathbf{x}_{i_1}) \cdots P(y_{i_n} = r \mid \mathbf{x}_{i_n}).$$

The probability that the n-tuple are clustered together is given by marginalization:

$$K_{i_1,...,i_n} = \sum_{r=1}^{k} P(y_{i_1} = r \mid \mathbf{x}_{i_1}) \cdots P(y_{i_n} = r \mid \mathbf{x}_{i_n}) = \sum_{r=1}^{k} g_{r,i_1} \cdots g_{r,i_n},$$

which translate to the fact that K should be a rank=k super-symmetric tensor:

$$K = \sum_{r=1}^{k} \mathbf{g}_r^{\otimes n}, \quad \mathbf{g}_r \ge 0,$$

where $\mathbf{g}^{\otimes n}$ denotes the rank-1 tensor $\mathbf{g} \otimes \mathbf{g} \otimes ... \otimes \mathbf{g}$. In other words, the cluster assignment probabilities are related to a non-negative super-symmetric factorization of the input n-way array K. To complete the algebraic relation between K and G we need to consider the constraints on K such that the n-way affinity array will indeed represent a distribution:

PROPOSITION 1. *Given uniform priors on the distribution of data points and labels, i.e., $P(\mathbf{x}_i) = 1/m$ and $P(y_i = j) = 1/k$ for all $i = 1, ..., m, j = 1, ..., k$, the n-way array K must be hyper-stochastic:*

$$\sum_{i_1,..,i_{j-1},i_{j+1},...,i_n} K_{i_1,...,i_n} = \left(\frac{m}{k}\right)^{n-1} \mathbf{1}, \quad j = 1, ..., n$$

where $\mathbf{1}$ *is the m-dimensional vector* $(1, ..., 1)$.

Proof: From the definition of G we have that the rows sum to 1: $\sum_r P(y_s = r \mid \mathbf{x}_s) = \sum_r g_{rs} = 1$. Using Bayes rule and the uniform prior assumption we can see that the columns sum to m/k:

$$\sum_{i=1}^{n} P(y_i = r \mid \mathbf{x}_i) = \frac{m}{k} \sum_i P(\mathbf{x}_i \mid y_i = r) = \frac{m}{k}.$$

The rows and columns sums propagate to a (scaled) hyper-stochastic constraint on K:

$$\sum_{i_1,..,i_{j-1},i_{j+1},...,i_n} K_{i_1,...,i_n}$$

$$= \sum_{r=1}^{k} g_{r,i_j} \sum_{i_1,..,i_{j-1},i_{j+1},...,i_n} g_{r,i_1} \cdots g_{r,i_{j-1}} g_{r,i_{j+1}} \cdots g_{r,i_n}$$

$$= \sum_{r=1}^{k} g_{r,i_j} (\sum_{i_1} g_{r,i_1}) \cdots (\sum_{i_{j-1}} g_{r,i_{j-1}})$$

$$(\sum_{i_{j+1}} g_{r,i_{j+1}}) \cdots (\sum_{i_n} g_{r,i_n})$$

$$= \left(\frac{m}{k}\right)^{n-1} \sum_{r=1}^{k} g_{r,i_j} = \left(\frac{m}{k}\right)^{n-1}$$

□

Note that the hyper-stochasticity constraint is "balanced partitions" in disguise. The uniform prior assumption in fact constraints the dataset to form k "balanced" clusters. Combining the two results above suggests the following optimization procedure: (i) find a hyper-stochastic approximation F to the input affinity array K, and (ii) given F, perform a super-symmetric non-negative tensor factorization (SNTF), i.e., find $\mathbf{g}_1, ..., \mathbf{g}_k \ge 0$ that minimize the Frobenius[2] norm $\|F - \sum_r \mathbf{g}_r^{\otimes n}\|^2$.

Finding a hyper-stochastic approximation to K can be done by repeating a normalization step which is an extension of the symmetrized Sinkhorn [16] rows and columns normalization procedure for matrices. The following proposition forms a normalization algorithm which converges to a super-symmetric hyper-stochastic array:

PROPOSITION 2. *For any non-negative super-symmetric n-way array $K^{(0)}$, iterating the process:*

$$K^{(t+1)}_{i_1,...,i_n} = \frac{K^{(t)}_{i_1,...,i_n}}{(a_{i_1} \cdots a_{i_n})^{1/n}},$$

where

$$a_i = \sum_{i_2,...,i_n} K_{i,i_2,...,i_n}, \quad i = 1, ..., m$$

converges to a hyper-stochastic array.

Proof: See Appendix B. □

Before we proceed to derive the SNTF algorithm it may be instructive to examine the pairwise, $n = 2$, affinity case, i.e., K is a non-negative symmetric matrix. Our results above say that $K = GG^\top$ and that prior to factorizing K we should normalize it by replacing it with $F = D^{-1/2} K D^{-1/2}$ where D is a diagonal matrix holding the row sums of K. If we iterate this normalization procedure we will obtain a doubly-stochastic approximation to K. This is consistent with [20] which argues that the conditional independence statements $y_i \perp y_j \mid \mathbf{x}_i, \mathbf{x}_j$ and $y_i \perp \mathbf{x}_j \mid \mathbf{x}_i$ lead to the finding that $K = GG^\top$ which also underlies the k-means, spectral clustering and normalized cuts approaches. To be concrete, the symmetric factorization $F = GG^\top$ can be represented as maximizing $trace(FGG^\top) = trace(G^\top FG)$. If we would like a "hard" clustering, i.e., each point must belong to one and only cluster then we should add $G^\top G = I$ and if we ignore the non-negativity constraint we obtain the result that the columns of G are

[1] We will later see that these assumptions underly the existing spectral pairwise ($n = 2$) clustering approaches, therefore we are not loosing any power of expression conventionally employed in the pairwise affinity case. Also weaker conditional independence assumptions would suffice — those defined on n-subsets, however for purposes of clarity we will stay with the stronger version

[2] entries with repeating indices can be ignored — we will come back to that later and define a reduced semi-norm.

the k leading eigenvectors of $D^{-1/2}KD^{-1/2}$. In other words, the conditional independence assumptions we made at the start are already built-in into the conventional pairwise affinity treatment — we have simply acknowledged them and extended them beyond pairwise affinities.

3. THE SNTF ALGORITHM

We are given a n-way affinity array $K \in [d1] \times .... \times [d_n]$ with $d_i = m$ being the number of data points to be clustered. An entry $K_{i_1,...,i_n}$ with $1 \leq i_j \leq m$ denotes the (un-normalized) probability of the n-point tuple $\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}$ to be clustered together. The tensor K is super-symmetric because the probability $K_{i_1,...,i_n}$ does not depend on the order of the n points. Furthermore, we can ignore entries with repeating indices and focus only on the case $i_1 \neq ... \neq i_n$ (this is crucial for the success of the algorithm). For practical reasons, we would like to store only a single representative of each n-tuple (instead of $n!$ entries), thus we focus only on the entries $i_1 < i_2 < ... < i_n$. Accordingly, we define the order-restricted Frobenius (semi) norm:

$$\|K\|_o^2 =< K, K >_o= \sum_{1\leq i_1<i_2<...<i_n\leq m} K^2_{i_1,...,i_n},$$

where $< A, B >_o$ is the inner-product (restricted to strictly ascending order) operation. Note that when K is super-symmetric then

$$\|K\|_o^2 = \frac{1}{n!} \sum_{i_1\neq ...\neq i_n} K^2_{i_1,...,i_n}$$

which is the restriction of the Frobenius norm to non-repeating indices. As mentioned in the previous section, we pass K through a normalization process and obtain a normalized version denoted by F. Our goal is to find a non-negative matrix $G_{m\times k}$ whose columns are denoted by $\mathbf{g}_1, ..., \mathbf{g}_k$ such as to minimize the following function:

$$f(G) = \frac{1}{2}\|F - \sum_{j=1}^{k} \mathbf{g}_j^{\otimes n}\|_o^2,$$

We derive below a positive-preserving update rule: $g_{r,s} \leftarrow g_{r,s} - \delta_{rs}\partial f/\partial g_{r,s}$. We start with the derivation of the partial derivative $\partial f/\partial g_{r,s}$. The differential df is derived below:

$$\begin{aligned}
df &= d\frac{1}{2} < F - \sum_{j=1}^{k} \mathbf{g}_j^{\otimes n} \ , \ F - \sum_{j=1}^{k} \mathbf{g}_j^{\otimes n} >_o \\
&=< \sum_{j=1}^{k} \mathbf{g}_j^{\otimes n} - F \ , \ d(\sum_{j=1}^{k} \mathbf{g}_j^{\otimes n}) >_o \\
&=< \sum_{j=1}^{k} \mathbf{g}_j^{\otimes n} - F \ , \ \sum_{j} (d\mathbf{g}_j) \otimes \mathbf{g}_j^{\otimes(n-1)} + ... + \mathbf{g}_j^{\otimes(n-1)} \otimes d\mathbf{g}_j >_o
\end{aligned}$$

The partial derivative with respect to $g_{r,s}$ (the s'th entry of $\mathbf{g}_r$) is:

$$\frac{\partial f}{\partial g_{rs}} =< \sum_{j=1}^{k} \mathbf{g}_j^{\otimes n} - F \ , \ \mathbf{e}_s \otimes \mathbf{g}_r^{\otimes(n-1)} + ... + \mathbf{g}_r^{\otimes(n-1)} \otimes \mathbf{e}_s >$$

where $\mathbf{e}_s$ is the standard vector $(0, 0, .., 1, 0, ..0)$ with 1 in the s'th coordinate. It will be helpful to introduce the following notation: let $1 \leq i_2 < ... < i_n \leq m$ and let $1 \leq s \leq m$ be different from $i_2, ..., i_n$, then $s \rightarrow i_2, .., i_n$ is an ascending n-tuple index (i.e., s is inserted into $i_2, ..., i_n$ in the appropriate position). Thus, for example:

$$< F, \mathbf{a}\otimes\mathbf{b}\otimes\mathbf{b}+\mathbf{b}\otimes\mathbf{a}\otimes\mathbf{b}+\mathbf{b}\otimes\mathbf{b}\otimes\mathbf{a} >_o= \sum_{i_1\neq i_2<i_3} F_{i_1\rightarrow i_2,i_3} a_{i_1} b_{i_2} b_{i_3}$$

Using the above short-hand notation, the partial derivative becomes:

$$\begin{aligned}
\frac{\partial f}{\partial g_{r,s}} &= \sum_{j=1}^{k} g_{j,s} \sum_{s\neq i_2<...<i_n} \prod_{q=2}^{n} g_{j,i_q} g_{r,i_q} \\
&- \sum_{s\neq i_2<...<i_n} F_{s\rightarrow i_2,..,i_n} \prod_{q=2}^{n} g_{r,i_q} \qquad (1)
\end{aligned}$$

We will be using a "positive preserving" gradient descent scheme $g_{rs} \leftarrow g_{rs} - \delta_{rs}\partial f/\partial g_{rs}$. Following [7] we set the gradient step size δ_{rs} as follows:

$$\delta_{rs} = \frac{g_{rs}}{\sum_{j=1}^{k} g_{j,s} \sum_{s\neq i_2<...<i_n} \prod_{q=2}^{n} g_{j,i_q} g_{r,i_q}} \qquad (2)$$

After substitution of eqn. 2 into the gradient descent equation we obtain a multiplicative update rule:

$$g_{rs} \leftarrow \frac{g_{rs} \sum_{s\neq i_2<...<i_n} F_{s\rightarrow i_2,..,i_n} \prod_{q=2}^{n} g_{r,i_q}}{\sum_{j=1}^{k} g_{j,s} \sum_{s\neq i_2<...<i_n} \prod_{q=2}^{n} g_{j,i_q} g_{r,i_q}} \qquad (3)$$

The update rule preserves positivity, i.e., if the initial guess for G is non-negative and F is super-symmetric and non-negative, then all future updates will maintain non-negativity. The proof that the update rule reduces $f(G)$ and converges to a local minima is presented in Appendix A.

There are a couple of noteworthy points to make. First, by removing from consideration entries in F that correspond to repeated indices makes the energy function $f(g_{r,s})$ be quadratic (when all other entries of G are fixed) which in turn is the key for the update rule above to reduce the energy at each step. Second, each sample of n points corresponds to $n!$ entries of the affinity tensor K which makes any algorithm for processing K unpractical as simply recording the measurements is unwieldy. The scheme we presented above records only the $\binom{m}{n}$ entries $1 \leq i_1 < ... < i_n \leq m$ instead of m^n in return for keeping a lexicographic order during measurement recording and during the update process of $g_{r,s}$ (access to $F_{s\rightarrow i_2,...,i_n}$).

Next, for large arrays, the need to sample all the possible (ordered) n-tuples out of m points introduces an excessive computational burden. In fact, it is sufficient to sample only a relatively small fraction of all n-tuples for most clustering problems. The sampling introduces vanishing entries in K that do not correspond to low affinity of the corresponding n-tuple but to the fact that the particular tuple was not sampled — those should be weighted-out in the criteria function $f(G)$. A "weighted" version of the scheme above requires merely a straightforward modification of the update rule as described next.

3.1 Weighting-out Unsampled Entries

Let $W_{i_1,...,i_n} \geq 0$, $i_1 < ... < i_n$, be a weight associated with the entry $K_{i_1,...,i_n}$. In particular we are interested in the binary weighting scenario where the weight is zero if the n-tuple $\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}$ was not sampled and '1' otherwise. We define the (reduced) weighted norm:

$$\|K\|_w^2 =< K, K >_w= \sum_{1\leq i_1<i_2<...<i_n\leq m} W_{i_1,...,i_n} K^2_{i_1,...,i_n}.$$

The partial derivative then becomes:

$$\begin{aligned}
\frac{\partial f}{\partial g_{r,s}} &= \sum_{j=1}^{k} g_{j,s} \sum_{s\neq i_2<...<i_n} W_{s\rightarrow i_2,...,i_n} \prod_{q=2}^{n} g_{j,i_q} g_{r,i_q} \\
&- \sum_{s\neq i_2<...<i_n} W_{s\rightarrow i_2,...,i_n} F_{s\rightarrow i_2,..,i_n} \prod_{q=2}^{n} g_{r,i_q}
\end{aligned}$$

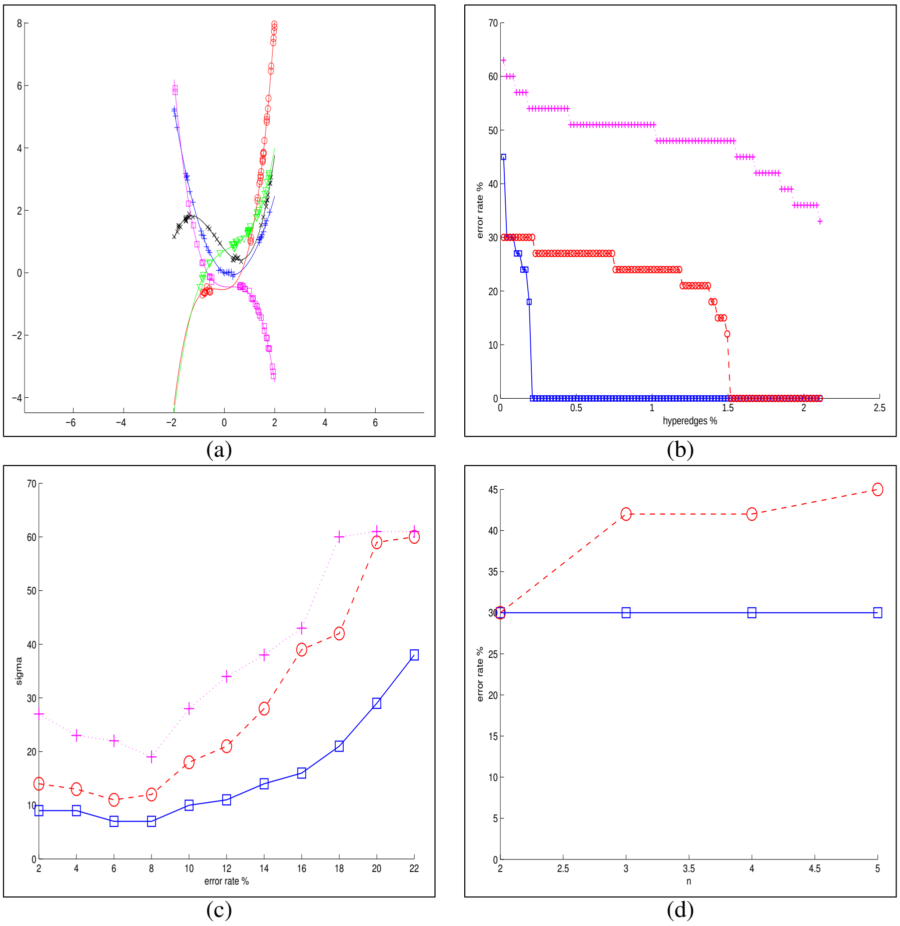

Figure 2: *Synthetic study of clustering $m = 200$ points arranged in $k = 5$ 3rd-order curves (i.e., affinity degree is $n = 5$). See text for details on each display.*

and the update rule becomes:

$$g_{rs} \leftarrow \frac{g_{rs}\sum_{s\neq i_2<\ldots<i_n} W_{s\rightarrow i_2,\ldots,i_n} F_{s\rightarrow i_2,..,i_n}\prod_{q=2}^{n} g_{r,i_q}}{\sum_{j=1}^{k} g_{j,s}\sum_{s\neq i_2<\ldots<i_n} W_{s\rightarrow i_2,\ldots,i_n}\prod_{q=2}^{n} g_{j,i_q} g_{r,i_q}} \qquad (4)$$

3.2 Summary: the n-way Clustering Algorithm

The n-way clustering algorithm is summarized as follows: We are given points $\mathbf{x}_1, ..., \mathbf{x}_m$ and an affinity measure $0 \leq \kappa(\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}) \leq 1$ that operates on an n-tuple of points. Our goal is to obtain a probabilistic measure $g_{r,s} = P(y_s = r \mid \mathbf{x}_s)$ where $s = 1, ..., m$ and $r = 1, ..., k$ and $y_s \in \{1, ..., k\}$ is the label associated with point $\mathbf{x}_s$.

1. Construct K: sample n-tuples $\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n}$, $i_1 < ... < i_n$, and set $K_{i_1,...,i_n} = k(\mathbf{x}_{i_1}, ..., \mathbf{x}_{i_n})$. Set $W_{i_1,...,i_n} = 1$.
2. Normalize K: apply the iterative normalization scheme which generates F (Prop. 2).
3. Factor F: starting with an initial guess for $G \geq 0$, iteratively update the entries $g_{r,s}$ one at at a time using eqn. 4 until convergence is reached.

Note that only sampled entries participate in the algorithm, therefore the complexity of each update step (eqn. 4) is a constant factor of the number of samples. The complexity of the algorithm is $O(mkp)$ where $p \leq \binom{m}{n}$ is the number of samples (number of non-vanishing entries of W).

4. EXPERIMENTS

We begin by studying the performance of the SNTF algorithm on synthetic data compared to the graph projection methods [1, 5, 21]. A comparative study of graph projection against outlier rejection algorithms (like RANSAC) and the multi-level hypergraph partitioning algorithms used in the VLSI community was presented in [1] showing a significant advantage to graph projection. Therefore we will focus our comparative study on the performance relationship between SNTF and graph projection.

The graph projection approximates the original hypergraph with a graph followed by spectral clustering. In practice, when the affinity degree n is large one needs to use sampling, i.e., during the projection (clique expansion and clique averaging in [1]) not all hyper-edges are used since their number grows exponentially with the affinity degree ([5] addressed the sampling issue). We expect the graph projection to work well when the problem is "simple", i.e., when a projection from $\binom{m}{n}$ hyper-edges to $\binom{m}{2}$ edges can be done with minimal information loss – in those cases it is worthwhile to reduce the problem size from a hypergraph to a graph rather than working directly with the full affinity tensor. On the other hand, when the number of points is large or when the affinity degree is high, one would expect a significant information-loss

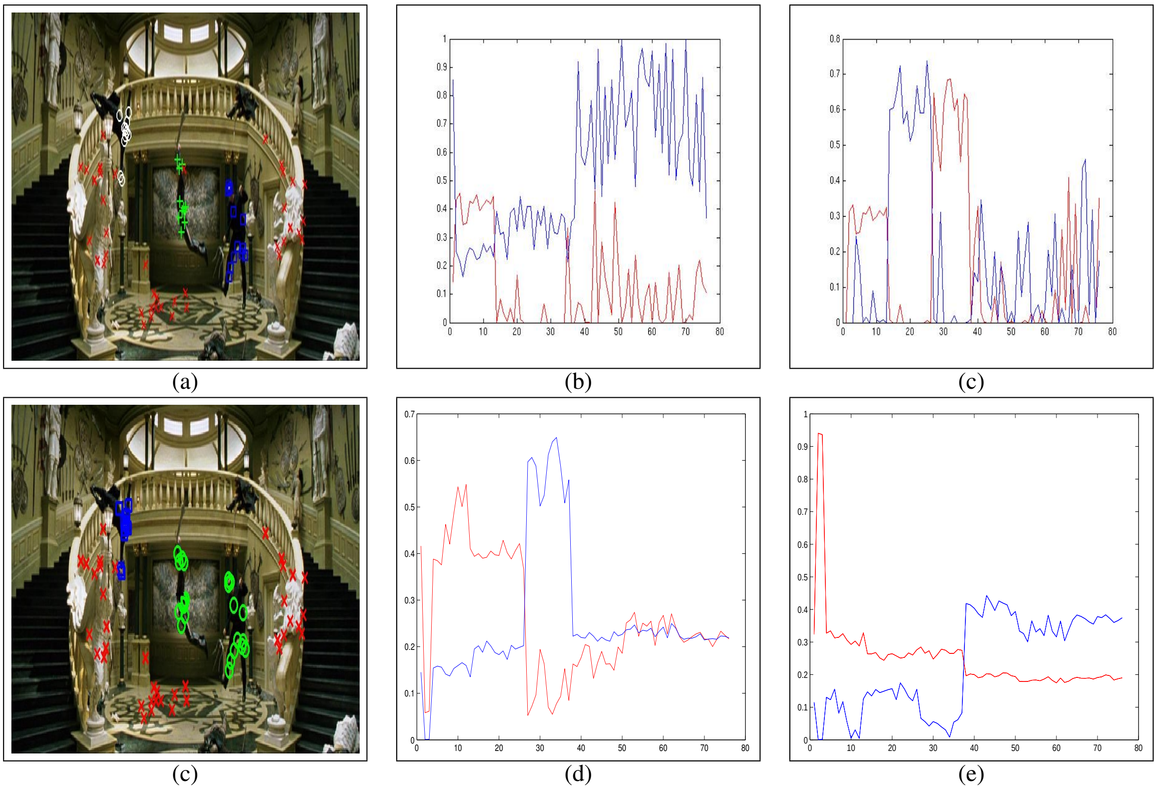

Figure 3: *3D-from-2D motion segmentation. (a) shows a picture with 76 points over four separate bodies, (b,c) show the resulting four columns of the partition matrix G using SNTF with a 9-way affinity array. The bottom row shows the results after projecting the affinity array onto a matrix. The projection resulted in significant information-loss which caused performance degradation.*

during projection with a resulting degraded performance.

In our first experiment we generated $m = 200$ points in the 2D plane laying on $k = 5$ 3rd-order polynomials with added Gaussian noise. The number of hyper-edges (entries of the affinity tensor K) is $\binom{200}{5}$ and since a 3rd-order 1D polynomial is determined by four coefficients we have $n = 5$. We ran SNTF, graph projection using Normalized-Cuts (NC) and graph projection using SNTF (i.e., the same algorithm described in this paper but for $n = 2$). We varied the runs according to the sampling percentage ranging from $0.02\% - 2.5\%$ of sampled hyper-edges. Fig. 2a shows the input data and Fig. 2b shows the clustering error percentage of the three runs per sampling (upper graph corresponds to NC, middle to SNTF with $n = 2$, lower to SNTF on the original affinity tensor). The error of the SNTF is indeed higher than the graph projection when the sampling is very low (0.02%), i.e., when the affinity tensor is very sparse and thus the projection onto a graph (matrix) does not suffer from information-loss. As the sampling rate increases the performance of the SNTF on $n = 5$ original affinity tensor significantly outperforms both graph projection runs and reaches perfect clustering much earlier (0.2% compared to 1.5% sampling). Fig. 2c compares the error rate of SNTF and graph projections (NC and SNTF with $n = 2$) using 0.15% sampling rate while varying σ used in computing the affinity from the residual Δ, i.e., $e^{-\Delta^2/\sigma^2}$. One can see that the SNTF on the original affinity degree $n = 5$ consistently outperforms clustering over graph projections — regardless of the clustering technique (NC upper graph and SNTF middle graph).

It is possible to use the SNTF framework in coarse-to-fine manner by generating affinity tensors of degree $q = 2, 3, ..., n$ by means of projection. Starting from $q = 2$ (graph) we recover the partition matrix G and use it as the initial guess for the SNTF of level $q + 1$ and so forth. In other words, the SNTF framework allows the flexibility to work with projections of the original affinity tensor, but instead of being limited to a projection onto a graph we could work with any affinity degree. Fig. 2d shows the percentage of error on the same data but with 0.02% sampling (where we have seen that the graph projection has the upper-hand) using the coarse-to-fine approach. One can see that the error remains fixed compared to an increasing error for each projection level when the SNTF does not use the resulting partition matrix of the previous level as an initial guess. This also confirms that there is a tradeoff between the complexity of the energy landscape introduced in high-degree affinities and the information loss introduced by aggressive projections. Ideally, one should work with a projection to the smallest affinity degree with minimal information loss. The advantage of the SNTF framework is that we are free to choose the affinity degree, whereas with graph projection the affinity degree is set to $n = 2$.

We move next to a 3D motion segmentation experiment. Fig. 3a shows a frame from "Matrix Reloaded" where we track 76 points arranged on four different moving bodies: the background (moving due to camera motion) and three separate people moving independently from the background motion. The points were tracked across two successive frames and our task is to perform a segmentation (clustering) of the points and assign each point to the proper moving body. It is well known that under perspective projection each pair of matching points p_i, p'_i in the image plane represented in homogenous coordinates satisfy a bilinear constraint: $p'^{\top}_i F p_i = 0$ where F is a 3×3 matrix iff the corresponding 3D points are part

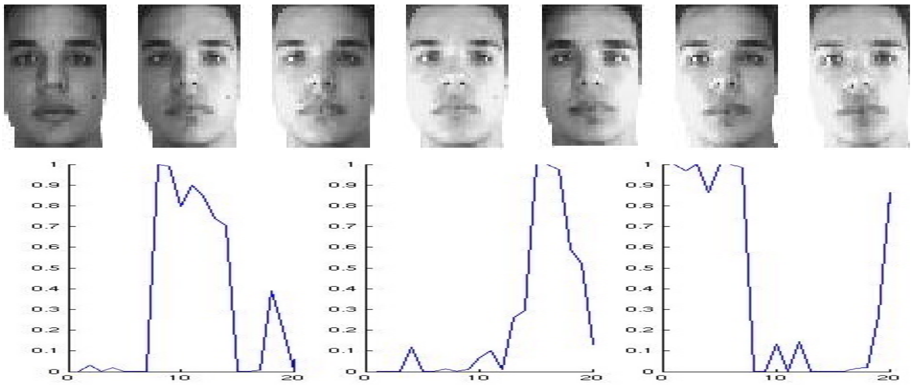

Figure 4: *Segmenting faces under varying illumination conditions. See text.*

of a single moving object [9]. Therefore, in the affinity ”language” we would need $n = 9$ points in order to obtain an affinity measurement, i.e., the likelihood that the 9-tuple arise form the same moving object. The affinity tensor has $\binom{76}{9}$ entries and we sample roughly $10,000$ entries from it with a proximity bias, i.e., once a point is sampled the next point is biased towards close points according to a Normal distribution. We ran SNTF with $k = 4$ clusters on the 9-degree (sampled) affinity tensor. Fig. 3b,c shows the four columns of the partition matrix G. Recall that the entries of each column represent the assignment probability of the corresponding point to the cluster associated with the column. A successful clustering (if the data is not ambiguous) will induce a distribution of values in G such that each row has a single maximal point. Once can clearly see that the values of G induce a clear-cut segmentation of the points to four separate bodies and the assignments are shown in Fig. 3a as varying color and shape (circles, crosses, squares and pluses). This particular segmentation problem is sufficiently challenging both for the graph projection approach and to the geometric-specific methods of [19, 18]. With regard to graph projection, the projection from a 9-degree affinity to a pairwise affinity is very aggressive with significant information-loss. Fig. 3e,f shows the four columns of G recovered from SNTF with $n = 2$ (followed by a projection) — one can see that one of the moving bodies got lost.

Finally we ran an experiment on segmenting faces under varying illumination conditions. It is well known that under certain surface property assumptions (Lambertian) the space of pictures of a 3D object ignoring cast-shadows lie in a 3D subspace [13]. In the affinity ”language” we would need a 4th-degree affinity measured over quadruples of pictures. Fig. 4 shows a sequence of pictures of a person under varying illumination conditions adopted from the AR dataset. We had 21 pictures spanning three different persons and we ran SNTF using 4-degree affinity tensor with $k = 3$ clusters. The three columns of the partition matrix G are shown in the bottom display. The pictures are unambiguously assigned to the correct person. Similar results of comparable quality were also obtained by graph projection.

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APPENDIX

A. PROOF OF CONVERGENCE: THE UPDATE RULE

Let $f(g_{rs})$ be the energy as a function of g_{rs} (all other entries of G remain constant) and let g'_{rs} be the updated value according to eqn. 3. We wish to show that if we make a gradient descent with a step size δ_{rs} given by eqn. 2 (which as we saw leads to a positive-preserving update), then $f(g'_{rs}) \leq f(g_{rs})$. They key is that δ_{rs} is smaller than the inverse second derivative:

PROPOSITION 3. *The update scheme $g'_{rs} = g_{rs} - \delta_{rs}\partial f/\partial g_{rs}$, with δ_{rs} given by eqn. 2 and the partial first derivative is given by eqn. 1, reduces the optimization function, i.e., $f(g'_{rs}) \leq f(g_{rs})$.*

Proof: The second derivative is:

$$\frac{\partial^2 f}{\partial g_{rs}\partial g_{rs}} = \sum_{s\neq i_2<\ldots<i_n} \prod_{q=2}^{n} g_{r,i_q}^2,$$

and the step size δ_{rs} satisfies:

$$\begin{aligned}\delta_{rs} &= \frac{g_{rs}}{\sum_{j=1}^{k} g_{j,s} \sum_{s\neq i_2<\ldots<i_n} \prod_{q=2}^{n} g_{j,i_q} g_{r,i_q}} \\ &\leq \frac{g_{rs}}{\cdot g_{r,s} \sum_{s\neq i_2<\ldots<i_n} \prod_{q=2}^{n} g_{r,i_q}^2} \\ &= \frac{1}{\partial^2 f/\partial g_{rs}\partial g_{rs}}\end{aligned}$$

The Taylor expansion of $f(g_{rs}+h)$ with $h = -\delta_{rs}\partial f/\partial g_{rs}$ is:

$$f(g'_{rs}) = f(g_{rs}) - \delta_{rs}(\frac{\partial f}{\partial g_{rs}})^2 + \frac{1}{2}\delta_{rs}^2(\frac{\partial f}{\partial g_{rs}})^2 \frac{\partial^2 f}{\partial g_{rs}\partial g_{rs}},$$

from which follows:

$$f(g_{rs}) - f(g'_{rs}) = \delta_{rs}(\frac{\partial f}{\partial g_{rs}})^2(1 - \frac{1}{2}\delta_{rs}\frac{\partial^2 f}{\partial g_{rs}\partial g_{rs}}) \geq 0,$$

since $\delta_{rs}\partial^2 f/\partial g_{rs}\partial g_{rs} \leq 1$. □

We apply the update rule in a Gauss-Seidel fashion according to a lexicographic scan of the entries of G. Since the energy is lower-bounded, twice differentiable, and is monotonically decreasing via the update rule, yet cannot decrease beyond the lower bound (i.e., positive preserving), then the process will converge onto a local minimum of the optimization function $\frac{1}{2}\|F - \sum_{j=1}^{k} g_j^{\otimes n}\|^2$ with entries with repeated indices ignored.

B. PROOF OF CONVERGENCE: NORMALIZATION SCHEME

We prove the following proposition:

For any non-negative super-symmetric n-way array $K^{(0)}$, without vanishing slices, iterating the process:

$$K^{(t+1)}_{i_1,\ldots,i_n} = \frac{K^{(t)}_{i_1,\ldots,i_n}}{(a_{i_1}\cdots a_{i_n})^{1/n}}, \tag{5}$$

where

$$a_i = \sum_{i_2,\ldots,i_n} K_{i,i_2,\ldots,i_n}, \quad i = 1,\ldots,m$$

converges to a hyper-stochastic array.

Proof: we define the *hyper-permanent* (following the definition of hyper-determinant [4]):

$$hperm(K) = \sum_{\sigma_2\in S_m}\cdots\sum_{\sigma_n\in S_m}\prod_{i=1}^{m} K_{i,\sigma_2(i),\ldots,\sigma_n(i)},$$

where S_m is the permutation group of m letters. Let K' be the n-way array following one step of the normalization step described in eqn. 5. We have:

$$\prod_{i=1}^{m}(a_1 a_{\sigma_2(i)}\cdots a_{\sigma_n(i)})^{1/n} = \prod_{i=1}^{m}(a_i^n)^{1/n} = \prod_{i=1}^{m} a_i,$$

from which we can conclude that:

$$hperm(K') = \frac{1}{\prod_{i=1}^{m} a_i} hperm(K).$$

To show that the normalization scheme monotonously increases the hyper-permanent of the n-way array we need to show that $\prod_{i=1}^{m} a_i \leq 1$. From the arithmetic-geometric means inequality it is sufficient to show that $\sum_{i=1}^{m} a_i \leq m$. From the definition of a_i we have:

$$\sum_{i=1}^{m} a_i = \sum_{i,i_2,\ldots,i_n} K_{i,i_2,\ldots,i_n}\frac{1}{(a_i a_{i_2}\cdots a_{i_n})^{1/n}}. \tag{6}$$

From the arithmetic-geometric means inequality $(\prod_{i=1}^{m} x_i)^{1/m} \leq (1/m)\sum_i x_i$, replace x_i with $1/a_i$ (recall that $a_i > 0$) and obtain:

$$\frac{1}{(a_1 a_2\cdots a_m)^{1/m}} \leq \frac{1}{m}\sum_{i=1}^{m}\frac{1}{a_i},$$

and in general for any n-tuple $1 \leq i_1 < \ldots < i_n \leq m$:

$$\frac{1}{(a_{i_1}\cdots a_{i_n})^{1/n}} \leq \frac{1}{n}(\frac{1}{a_{i_1}} + \ldots + \frac{1}{a_{i_n}}). \tag{7}$$

By substituting the inequality eqn. 7 into eqn. 6 while noting that:

$$\begin{aligned}&\sum_{i,i_2,..,i_n} K_{i,i_2,\ldots,i_n}\frac{1}{a_{i_j}} \\ &= \sum_{i_j=1}^{m}\frac{1}{a_{i_j}}\sum_{i,i_2,\ldots,i_{j-1}i_{j+1},\ldots,i_n} K_{i,i_2,\ldots,i_{j-1}i_{j+1},\ldots,i_n} \\ &= m,\end{aligned}$$

we obtain that $\sum_i a_i \leq m$ as required. Therefore, we conclude so far that each step of the normalization scheme increases the hyper-determinant of the previous step. The hyper-permananet is bounded from above since:

$$hperm(K) \leq \prod_{i=1}^{m} a_i \leq 1,$$

therefore the process must converge. The process converges when $hperm(K') = hperm(K)$ which can happen only of $a_1 = \ldots = a_m = 1$. □