# Clustering and Density Estimation for Streaming Data using Volume Prototypes

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**Abstract.** The authors have proposed *volume prototypes* as a compact expression of a huge data or a data stream, along with a one-pass algorithm to find them. A reasonable number of volume prototypes can be used, instead of an enormous number of data, for many applications including classification, clustering and density estimation. In this paper, two algorithms using volume prototypes, called VKM and VEM, are introduced for clustering and density estimation. Compared with the other algorithms for such a huge data, we showed that our algorithms were advantageous in speed of processing, while keeping the same degree of performance, and that both applications were available from the same set of volume prototypes.

## 1 Introduction

In these years, we often deal with an enormous amount of data or a data stream in a large variety of pattern recognition tasks. Such data require a huge amount of memory space and computation time for processing. So it is preferable to find a compact expression of data that is acceptable in time and space without losing characteristics of original datasets. For this goal, we have proposed *volume prototypes* [1,2] as an extension of conventional point prototypes. Each of volume prototypes is a geometric configuration that represents many data points inside.

Volume prototypes can be generated by a single-pass algorithm, and thus they are significantly effective for streaming data that can be accessed only once. As another advantage, volume prototypes typically converge to modes of the underlying distribution, so that we do not need to determine the number of prototypes beforehand. It suffices to take a sufficiently large number of initial prototypes, unlike mixture models.

In our earlier studies [1, 2], we conducted some experiments and analyzed a typical behavior of volume prototypes. In this paper, we investigate the applicability of volume prototypes. Especially, we try to apply volume prototypes to clustering and construction of mixture models.

## 2 Related Works

There have been many studies of clustering and density estimation for huge datasets or data streams.

Density estimation algorithms for a huge dataset are found in the literature [3–6]. Zhang *et al.* extended a kernel method to achieve a fast density estimation for very large databases [3]. Arandjelović and Cipolla realized a real-time density estimation by incremental learning of GMM [4]. The incremental EM algorithm [5] attempts to reduce the computational cost needed by EM algorithm. This is made by adopting partial E-steps. It divides a whole dataset into some blocks and performs a partial E-step on each block in a cyclic way. The lazy EM algorithm [6] has the same strategy with the incremental EM algorithm. However, it performs a partial E-step only on a significant subset of data.

Clustering methods for a huge dataset are also seen in the literature [7–10]. Charikar *et al.* proposed a one-pass clustering algorithm in a streaming model [7]. It produces a constant factor approximation of the solution of the *k*-median problem in storage space  $O(k \ poly \log n)$  for size *n* data. Bradley *et al.* showed an efficient clustering method for large databases [8]. Their method is based on classifying regions into three kinds of regions: the regions that must be maintained as they are, the regions that are compressive, and the regions that can be discarded. This algorithm requires at most one scan of the database. The algorithm BIRCH [9] by Zhang *et al.* achieves an efficient clustering for a huge dataset by constructing a CF-tree that is a hierarchical summary of clusters. Data is scanned only once to construct a CF-tree. The algorithm FEKM [10] by Goswami *et al.* produces almost the same clusters as the original *k*-means algorithm. Their algorithm is basically one-pass, and obtain clusters close to the correct clusters of the *k*-means with a few number of additional scans.

These approaches would be effective for a huge dataset in several situations. However, some of them require to keep a whole data and others require a constant number of rescanning of data or its reduced subset. If we are allowed to access each data only once, some of these methods are not available. One more important thing is that we do clustering for one goal, e.g., data compression, do density estimation for another goal, e.g., classification, and sometimes we do both. In this case, it is desirable to be able to carry out both efficiently. The goal of this paper is to show that our approach using volume prototypes gives one of possible solutions.

### **3** Algorithm for Volume Prototypes

In this section, we show the concrete algorithm VP to generate volume prototypes. The single-pass algorithm is shown in Fig. 1.

The outline is as follows. With multiple scans over the first N samples in different M orders, we obtain M seed prototypes (ME Step). Here N is relatively small, say N = 500, and M is taken to be ten times or so the number of expected modes, say M = 100. We bring up those seed prototypes by updating them using the samples fell in their acceptance regions (C Step). For *final prototypes*, we carry out prototype selection using greedy set covering to have L final prototypes.

## 3.1 Details

**Dataset:** We consider a data stream  $x_1, x_2, \ldots, x_N, x_{N+1}, \ldots$  of *d*-dimensional vectors.

**Inputs:**(Unlimited samples)  $x_1, x_2, \ldots, x_N, \ldots$ 

N is the number of samples for **ME Step**.

M is the number of seed prototypes.

- $N_v$  is the number of latest samples to be kept.
- $\theta$  is the value to determine radius r of the acceptance region.

Procedure for obtaining volume prototypes

#### ME (mode estimation) step:

Repeat M times the following for the first N samples.

- 1. Choose a random permutation  $\sigma$  to reorder the samples to  $x_{\sigma_1}, x_{\sigma_2}, \ldots, x_{\sigma_N}$ .
- 2. Initialize a prototype by the way described in the detailed description.
- 3. Use  $x_{\sigma_2}, \ldots, x_{\sigma_N}$  in order to update the *seed prototype* by the same way as 2.
- (using only the samples in the acceptance region (1)).

#### C (Convergence) step:

- For each sample  $x_i (i = N + 1, N + 2, ...)$  do the following.
  - 1. Update the seed prototypes in which  $x_i$  falls by (2)–(4).
  - 2. Keep the latest  $N_v$  samples.

#### **Exploit time:**

From M prototypes, select greedily  $L(\leq M)$  prototypes until no improvement is found for covering  $N_v$  samples. Count the number of samples falling in each prototype in  $N_v$  samples. Here a sample is divided by k when k prototypes share it.

Fig. 1. Volume Prototype Algorithm (VP).

- **Prototype:** Let  $p = (\mu, \Sigma, r, n)$  be a prototype. Here,  $\mu$  is the prototype center,  $\Sigma$  is the covariance matrix, r is the Mahalanobis radius and n is the number of samples inside the prototype.
- **Included Sample Set:** Let  $S_p$  be the set of data points inside prototype p, which is specified by  $S_p = \{x_i | (x_i \mu)' \Sigma^{-1} (x_i \mu) \le r^2\}$ . Then  $n = |S_p|$ . We approximate n by the number of samples used for updating the prototype.
- Acceptance Region: We specify the acceptance region  $A_p$  of prototype  $p = (\mu, \Sigma, r, n)$  by the acceptance Mahalanobis radius R as

$$\boldsymbol{A}_{p} = \{\boldsymbol{x} | (\boldsymbol{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \leq R^{2} \}.$$
(1)

Here,  $R(\geq r)$  is determined from r and n by  $R = r + \sqrt{\frac{\chi_d^2(0.95)}{n}}$ 

**Updating Procedure:** When a sample x falls into the acceptance region  $A_p^{(t)}$  of prototype  $p^{(t)}$  at (t + 1)th update,  $p^{(t)}$  is updated to  $p^{(t+1)}$  by

$$n^{(t+1)} = n^{(t)} + 1, (2)$$

$$\boldsymbol{\mu}^{(t+1)} = \frac{1}{n^{(t+1)}} \left( n^{(t)} \boldsymbol{\mu}^{(t)} + \boldsymbol{x} \right), \tag{3}$$

$$\boldsymbol{\Sigma}^{(t+1)} = \frac{1}{n^{(t+1)}} \left( n^{(t)} \boldsymbol{\Sigma}^{(t)} + \boldsymbol{x} \boldsymbol{x}' + n^{(t)} \boldsymbol{\mu}^{(t)} \boldsymbol{\mu}^{(t)\prime} - n^{(t+1)} \boldsymbol{\mu}^{(t+1)} \boldsymbol{\mu}^{(t+1)\prime} \right). (4)$$

The radius R of the acceptance region is also updated.

**Initialization of ME Step:** We initialize the center  $\mu^{(0)}$  and the covariance matrix  $\Sigma^{(0)}$  by  $\mu^{(0)} = x_1$  (the first element after random reordering) and  $\Sigma^{(0)} = \lambda^2 I$ . Here,  $\lambda^2 = \frac{1}{dN} \sum_{i=1}^N \min_{j \neq i, j \in \{1, 2, ..., N\}} ||x_i - x_j||^2$  ( $|| \cdot ||^2$  is the squared Euclidean norm) and I is the unit matrix. In addition, we set the initial value of  $n^{(0)}$  to  $n^{(0)} = d + 1$ .

## 4 Applications of Volume Prototypes

Volume prototypes are an intermediate representation between data and clusters, while they are more akin to data themselves. We can use them for costly applications instead of a large amount of original samples. In this section, we show two applications for clustering and density estimation.

Let us assume that we have a huge amount of data and they are represented by a reasonable number of volume prototypes. In the following, we consider the correspondence between a sample and a volume prototype. A big difference is that the latter has many samples in it and has a volume specified by a covariance matrix and a Mahalanobis radius.

#### 4.1 EM Algorithm with Volume Prototypes (VEM)

We consider first modeling of a given density by a finite mixture of Gaussian component densities. The number K of component densities is assumed to be given beforehand. Let the kth component be a Gaussian  $N(x; \nu_k, \Sigma_k)$ , where  $\nu_k$  is the mean,  $\Sigma_k$  is the covariance matrix. Then, the density is estimated by a mixture as f(x) = $\sum_{k=1}^{K} \pi_k N(x; \nu_k, \Sigma_k)$  with prior probabilities  $\pi_k$ . To estimate the parameter values from given volume prototypes, we show a volume prototype version (VEM) of EM algorithm. The concrete algorithm is shown in Fig. 2.

In the following, we use suffix j for volume prototypes and k for component densities. Thus, jth volume prototype is denoted by  $p_j = (\mu_j, \Sigma_j, n_j)$ , omitting the radius  $r_j$ .

In the Maximization step (M step), we estimate the mean and covariance of kth component density from the currently estimated membership value  $m_k(\mathbf{p})$  of a volume prototype  $\mathbf{p}$  to kth component. Here,  $\sum_{k=1}^{K} m_k(\mathbf{p}) = 1$ . The parameter values are estimated by the maximum likelihood estimators. The updating procedure is given as

$$\pi_k = \sum_j m_k(\boldsymbol{p}_j) n_j / \sum_j n_j, \quad \boldsymbol{\nu}_k = \sum_j m_k(\boldsymbol{p}_j) n_j \boldsymbol{\mu}_j / \sum_j m_k(\boldsymbol{p}_j) n_j$$
$$\Sigma_k = \sum_j m_k(\boldsymbol{p}_j) n_j \left\{ \Sigma_j + (\boldsymbol{\mu}_j - \boldsymbol{\nu}_k) (\boldsymbol{\mu}_j - \boldsymbol{\nu}_k)' \right\} / \sum_j m_k(\boldsymbol{p}_j) n_j.$$

In the Expectation step (E step), we re-estimate the membership values  $m_k(p)$  from the currently estimated K component densities. To do this, we use a kind of distance measure between p and kth component. In the original EM algorithm, Mahalanobis Inputs: *L* volume prototypes:  $p_1, p_2, ..., p_L$  ( $p_l = (\mu_l, \Sigma_l, n_l), l = 1, 2, ..., L$ ). *K* is the number of components. Outputs:  $f(x) = \sum_{k=1}^{K} \pi_k f_k(x; \theta_k)$  ( $f_k$  is a Gaussian with  $\theta_k = (\nu_k, \Sigma_k)$ ). Procedure for obtaining a mixture model Initialize step: Set randomly the membership  $m_k(p_l)$  for every *k*th component and *l*th prototype. Repeat the following M step and E step in turn until convergence. M step: For *k*th component (k = 1, 2, ..., K), update the following:  $\pi_k = \sum_l m_k(p_l)n_l/\sum_l n_l$   $\nu_k = \sum_l m_k(p_l)n_l\mu_l/\sum_l m_k(p_l)n_l$   $\Sigma_k = \sum_l m_k(p_l)n_l \{\Sigma_l + (\mu_l - \nu_k) (\mu_l - \nu_k)'\} / \sum_l m_k(p_l)n_l$ . E step: For *l*th prototype (l = 1, 2, ..., L), update the membership by  $m_k(p_l) = \pi_k(2\pi)^{-\frac{D}{2}} |\Sigma_k|^{-\frac{1}{2}} e^{-\frac{1}{2}(tr\Sigma_k^{-1}\Sigma_l + (\mu_l - \nu_k)'\Sigma_k^{-1}(\mu_l - \nu_k))}$ .

Fig. 2. Volume prototype EM algorithm (VEM).

**Inputs:** *L* volume prototypes:  $p_1, p_2, ..., p_L$ ; *K* is the number of clusters to be found. **Outputs:** *K* clusters specified by means  $\nu_1, \nu_2, ..., \nu_K$ . **Procedure** *K*-means with volume prototypes  $t \leftarrow 0$ . Choose the first *K* prototypes and assign their centers to  $\nu_1^{(0)}, \nu_2^{(0)}, ..., \nu_K^{(0)}$ .

Repeat the following until convergence.

Assign prototype  $\boldsymbol{p}_l(l = 1, 2, ..., L)$  to the nearest cluster  $C_s$  with  $\boldsymbol{\nu}_s^{(t)}$ . Here, the nearness between  $\boldsymbol{p}_l = (\boldsymbol{\mu}_l, \Sigma_l, n_l)$  and  $\boldsymbol{\nu}_s^{(t)}$  is measured by  $||\boldsymbol{\nu}_s^{(t)} - \boldsymbol{\mu}_l||$ .  $t \leftarrow t + 1$ . Update  $\boldsymbol{\nu}_k^{(t)}$  (k = 1, 2, ..., K) by  $\boldsymbol{\nu}_k^{(t)} = \frac{1}{N_k} \sum_{\boldsymbol{p}_l \in C_k} n_l \boldsymbol{\mu}_l$ , where  $N_k = \sum_{\boldsymbol{p}_l \in C_k} n_l$ .

Fig. 3. Volume prototype k-means algorithm (VKM).

distance between a sample x and mean  $\nu_k$  is used. Here, since p has a volume, we use the expected Mahalanobis distance on prototype p:

$$E_{X \in p_j} (X - \boldsymbol{\nu}_k)' \boldsymbol{\Sigma}_k^{-1} (X - \boldsymbol{\nu}_k)$$
  
=  $E_{X \in p_j} (X - \boldsymbol{\mu}_j + \boldsymbol{\mu}_j - \boldsymbol{\nu}_k)' \boldsymbol{\Sigma}_k^{-1} (X - \boldsymbol{\mu}_j + \boldsymbol{\mu}_j - \boldsymbol{\nu}_k)$   
=  $tr \boldsymbol{\Sigma}_k^{-1} \boldsymbol{\Sigma}_j + (\boldsymbol{\mu}_j - \boldsymbol{\nu}_k)' \boldsymbol{\Sigma}_k^{-1} (\boldsymbol{\mu}_j - \boldsymbol{\nu}_k).$ 

Then, with the prior probability  $\pi_k$ , the membership value is updated as

$$m_{k}(\boldsymbol{p}_{j}) = \pi_{k}(2\pi)^{-\frac{D}{2}} |\Sigma_{k}|^{-\frac{1}{2}} \cdot \exp\left\{-\frac{1}{2}\left(tr\Sigma_{k}^{-1}\Sigma_{j} + (\boldsymbol{\mu}_{j} - \boldsymbol{\nu}_{k})'\Sigma_{k}^{-1}(\boldsymbol{\mu}_{j} - \boldsymbol{\nu}_{k})\right)\right\}.$$

Here, we notice that the estimated Mahalanobis distance converges to the ordinal Mahalanobis distance  $(\mu_j - \nu_k)' \Sigma_k^{-1} (\mu_j - \nu_k)$  of a single point  $\mu_j$  under the assumption that  $\Sigma_j = \epsilon I$  and  $\epsilon \to 0$ . Therefore, this way of assigning membership values is an extension of the traditional E step.

#### 4.2 *k*-means Algorithm with Volume Prototypes (VKM)

It is also easy to make the k-means algorithm applicable to volume prototypes (VKM). Here, it is also assumed that the number K of clusters is determined beforehand.

When J volume prototypes  $\{p_j = (\mu_j, \Sigma_j, n_j)\}$  (j = 1, 2, ..., J) are combined into one, we have a combined volume prototype  $p = (\mu, \Sigma, n)$ :

$$n = \sum_{j=1}^{J} n_j, \quad \boldsymbol{\mu} = \sum_{j=1}^{J} \frac{n_j}{n} \boldsymbol{\mu}_j$$
$$\boldsymbol{\Sigma} = \sum_{j=1}^{J} \frac{n_j}{n} \left\{ \boldsymbol{\Sigma}_j + (\boldsymbol{\mu}_j - \boldsymbol{\mu})(\boldsymbol{\mu}_j - \boldsymbol{\mu})' \right\}$$
(5)

These hold even if  $\{p_j\}$  are samples  $\{x_j\}$  (easily verified with  $\Sigma_j = 0$ ,  $\mu_j = x_j$  and  $n_j = 1$ ).

For extending k-means using samples to the one using volume prototypes, all we need is to define the distance between a volume prototype and a cluster center. Under the assumption that a volume prototype (and all samples in it) belongs to one cluster only, the squared distance minimization criterion Q for samples in the original k-means can be used even for volume prototypes:

$$Q = \sum_{k=1}^{K} \sum_{\boldsymbol{x} \in C_{k}} ||\boldsymbol{x} - \boldsymbol{\nu}_{k}||^{2} = \sum_{k=1}^{K} \sum_{\boldsymbol{x} \in C_{k}} \operatorname{tr}(\boldsymbol{x} - \boldsymbol{\nu}_{k})(\boldsymbol{x} - \boldsymbol{\nu}_{k})' \quad (C_{k} \text{ is } k \text{th cluster})$$
$$= \sum_{k=1}^{K} \sum_{\boldsymbol{p}_{j} \in C_{k}} n_{j} \left( \operatorname{tr} \Sigma_{j} + ||\boldsymbol{\mu}_{j} - \boldsymbol{\nu}_{k}||^{2} \right) \quad (\text{Eq. (5)})$$
$$= \sum_{\boldsymbol{p}_{j}} n_{j} \operatorname{tr} \Sigma_{j} + \sum_{k=1}^{K} \sum_{\boldsymbol{p}_{j} \in C_{k}} n_{j} ||\boldsymbol{\mu}_{j} - \boldsymbol{\nu}_{k}||^{2}.$$

The first term is the irreducible error when volume prototypes are used. Therefore, when we adopt the k-means algorithm to find a sub-optimal solution of this optimization problem, we may assign a volume prototype to the nearest cluster in the distance  $||\boldsymbol{\mu}_j - \boldsymbol{\nu}_k||$ . By setting  $\frac{\partial Q}{\partial \boldsymbol{\nu}_k} = 0$ , we have the estimated mean for iteration:  $\boldsymbol{\nu}_k = \frac{1}{N_k} \sum_{j \in C_k} n_j \boldsymbol{\mu}_j$ , where  $N_k = \sum_{j \in C_k} n_j$ . The concrete algorithm is shown in Fig. 3.

In algorithm VKM, the cluster centers can be initialized by the first K prototypes. This strategy is effective because these K prototypes are already chosen in VP algorithm so as to cover as many samples as possible in order.

### **5** Experiments

In the following experiments, we used three 2-dimensional artificial datasets:

1. Circle: Two clusters. One cluster is concentrated on the origin and it is surrounded by the other cluster at a distance.

- 2. **4-Cross**: Four Gaussians that cross at four corners.
- 3. 5-Gaussian: Five Gaussians. Some of them are close.

In each dataset, 100,000 samples were generated according to a specified distribution. We chose M = 100 seed volume prototypes with radius  $r = \chi_2^2(0.9)$  in VP algorithm. The first N = 1000 samples were used for ME step and prototype selection.

The obtained volume prototypes are shown in Fig.4 (1st column). In Fig.4, only selected volume prototypes are shown. Therefore, the number L is rather less than M = 100. We can see that 1) the set of volume prototypes represents well the distribution, 2) they are located inside the distribution because of  $\theta = 0.9$ , and 3) the number (25, 23 and 24 in order) is quite smaller than the number  $10^5$  of samples.

#### 5.1 Experiment 1 : Clustering

We applied our VKM clustering method to the selected final prototypes. We compared it with a one-pass k-means algorithm, SKM (scalable k-means) [11]. SKM was applied to all the data. We examined two different numbers of clusters. The results are shown in Fig.4 (2nd and 3rd columns).

From Fig.4, we see:

- 1. When the specified number K of clusters is the same as that of the underlying distribution, the cluster centers are comparable between VKM and SKM.
- 2. If *K* is larger than the correct number, the cluster centers found by VKM are located inside the distribution compared with those by SKM.

#### 5.2 Experiment 2 : Mixture Models

Then, we applied our VEM method to the same selected final prototypes. We used the results of VKM for initializing the membership values of a mixture model. We compared it with the incremental EM algorithm [5]. In the incremental EM algorithm, the number of blocks over which a partial E-step was carried was set to 100. Two different numbers of components were examined. The results are also shown in Fig.4 (4th and 5th columns).

From Fig.4, we see the following:

- 1. The incremental EM and VEM are almost comparable when K is correct.
- 2. If *K* is larger, the components found by VEM are more safely secured than those of the incremental EM. Note that the number of components is automatically reduced to a near optimal number. This is because volume prototypes limit an excessive production of small, in the number of included samples, components (see the results of 4–Cross with K = 8 and 5–Gaussian with K = 10).
- 3. The components obtained by VEM are narrower than those of the incremental EM. This is because the components in VEM are generated from volume prototypes that give an inner approximation of the distribution.

In total, our VEM algorithm is more stable compared with the incremental EM algorithm.



Fig. 4. Results of clustering and mixture models in three datasets ( $\theta = 0.90$ ). In clustering, the cluster centers are shown as black dots. In mixture models, the covariance matrix of each component is shown.

#### 5.3 Computation Time

The calculation time is shown in Table 1. It is clear that our two algorithms of VKM and VEM are faster than SKM and the incremental EM algorithm, respectively, as long as we do not take into account the time consumed for obtaining volume prototypes. Even if we add the time for obtaining volume prototypes, VEM is faster than the incremental EM. The time advantage of VKM and VEM would be increased if we use a larger

Dataset	K	Time (sec.)				
		VP	VKM	SKM	VEM	Incremental EM
Circle	5	5.908	0.001	4.204	0.012	10.136
(25 prototypes)	10		0.004	4.216	0.048	19.133
4-Cross	4	7.440	0.001	2.204	0.028	7.732
(23 prototypes)	8		0.001	2.532	0.184	15.332
5-Gaussian	5	7.928	0.001	2.544	0.012	9.808
(24 prototypes)	10		0.008	3.520	0.104	18.825

Table 1. Time comparison in clustering and mixture models.

dataset, because VP is a completely one-pass algorithm. It should be noted that VKM and VEM are separately applicable to the same set of volume prototypes. In addition, we can try several values of K very efficiently with VKM and VEM for model selection.

## 6 Conclusions

In this paper, we have presented two algorithms for clustering and density estimation on the basis of volume prototypes which can be used instead of a huge data and obtained by a single-pass algorithm. The necessary number of volume prototypes is quite smaller than the number of given samples, therefore, our algorithms work very efficiently for a huge data or data streams.

One of proposed algorithms is a volume prototype version (VEM) of EM algorithm. It is for density estimation. Since each prototype has a volume, we extended the original algorithm so as to take into account the volume and the number of samples included. Another algorithm is a k-means algorithm for volume prototypes (VKM). In this algorithm, we developed a distance measure between a volume prototype and a cluster center as a natural extension of its point version.

We confirmed the efficiency of both algorithms in some experiments with 2 - dimensional artificial data. The main advantage of these algorithms is that we can carry out both algorithms in low cost, once volume prototypes are given. We will further investigate the applicability for high-dimensional real-world datasets.

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