

Nonparametric Clustering from Energy Statistics

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Abstract

Energy statistics was proposed by Székely in the 80's inspired by the Newtonian gravitational potential from classical mechanics, and it provides a nonparametric test for equality of distributions. It was generalized to metric spaces of strong negative type, and more recently a connection with reproducing kernel Hilbert spaces (RKHS) was proposed. Although extensively used in statistics, it has not been previously incorporated in machine learning problems. Here we consider the problem of clustering data from an energy statistics theory perspective. We provide a precise mathematical formulation yielding a quadratically constrained quadratic program (QCQP), which we show to be equivalent to kernel k -means optimization problem. Thus, our results imply a first principles derivation of kernel k -means from energy statistics. Moreover, we also consider a weighted version of energy statistics applied to clustering, which is related to graph partitioning problems. To find local optimizers of such QCQP we consider an iterative algorithm based on Hartigan's method, which in this case has the same computational cost as kernel k -means algorithm but usually with better clustering performance. We provide carefully designed numerical experiments showing the superiority of this method compared to kernel k -means, standard k -means, and gaussian mixture models.

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I. INTRODUCTION

Energy statistics [1] is based on a notion of statistical potential energy between probability distributions, in close analogy to Newton’s gravitational potential in classical mechanics. It provides a nonparametric test for equality of distribution which is achieved under minimum energy. When probability distributions are different, this statistical potential energy diverges as sample size increases. Energy statistics has been applied to several goodness-of-fit hypothesis tests, multi-sample tests of equality of distributions, analysis of variance [2], nonlinear dependence tests through distance covariance and distance correlation, which generalizes the Pearson correlation coefficient, and hierarchical clustering [3] by extending Ward’s method of minimum variance. (We refer to [1] and references therein for an overview of energy statistics.) Moreover, an energy statistics formulation to clustering was already proposed in [4] which greatly motivated this paper.

Recently, distance covariance was generalized from Euclidean spaces to metric spaces of strong negative type [5]. Furthermore, a unifying framework establishing an equivalence between generalized energy distances to maximum mean discrepancies (MMD), which are distances between embeddings of distributions in reproducing kernel Hilbert spaces (RKHS), was established [6]. This provides the link between concepts used in energy statistics and concepts commonly used in machine learning, and form the basis of our approach.

The clustering problem has a long history in machine learning. The most used method is k -means [7–9], which is based on Lloyd’s heuristic [7] of assigning a data point to the cluster with closest center. The only statistical information about each cluster comes from its mean and thus it is sensitive to outliers. Moreover, k -means is strongly parametric, assuming that data is isotropically and normally distributed since it is a special case of gaussian mixture models (GMM) through the expectation maximization (EM) algorithm. Nevertheless, k -means works very well when data is linearly separable in Euclidean space, with a clear resolution of cluster centers and without significant overlap of the points belonging to different clusters.

To account for nonlinearities, kernel methods were introduced [10, 11]. A mercer kernel [12] is used to implicitly map data points to a RKHS, then clustering can be performed in the associated Hilbert space by using its inner product. This enables one to cluster way more complicated datasets, however, the kernel choice remains the biggest challenge since there

is no principled theory behind this. The well-known kernel k -means optimization problem is nothing but k -means in the feature space [11]. Furthermore, kernel k -means algorithm [13, 14] is still based on Lloyd’s heuristic [7] of using the mean of each cluster in the feature space. We refer the reader to [15] for a survey of clustering methods.

Although clustering from energy statistics was considered in [4], the precise optimization problem behind this approach remains elusive, as well as the connection to kernel methods. The main theoretical contribution of this paper is to fill this gap. Since the statistical potential energy is minimum when distributions are equal, the principle behind clustering is to maximize the statistical energy, enforcing probability distributions associated to each cluster to be different from one another. We provide a precise mathematical formulation to this statement, showing that there is only one possible optimization problem consistent with energy statistics. Moreover, we show that this is a quadratically constrained quadratic program (QCQP) in the associated RKHS. Our results immediately establish the connection to kernel methods used in machine learning, by showing that this QCQP is equivalent to kernel k -means optimization problem. The equivalence between kernel k -means, spectral clustering, and graph partitioning problems was already established in [13, 14]. We show how these connections arise from a weighted version of energy statistics.

Our algorithmic contribution is to use Hartigan’s method [16] to find local solutions of the above mentioned QCQP. This approach was also proposed in [4]. In this case, the resulting algorithm has the same time complexity as kernel k -means algorithm, however, the numerical results provide compelling evidence that this method is more accurate and robust than kernel k -means. This evidence is also supported by general theoretical results [17, 18]. Moreover, in our experiments we put in evidence the nonparametric aspect of energy statistics based clustering, which provides a default kernel, showing that it is able to perform accurately on data coming very different distributions, contrary to k -means and GMM for instance.

Our work is organized as follows. In section II we introduce the necessary background on energy statistics and RKHS. Section III contains the main theoretical results of this paper, where we consider a clustering theory based on energy statistics leading to a QCQP, which is NP-hard. We also show the equivalence to kernel k -means problem. In Section IV we generalize these results to a weighted version of energy statistics, which provides the connection with graph partitioning problems and spectral clustering. In Section V we

consider a simple example in one dimension, where we propose an algorithm which requires no initialization. In section VI we briefly review kernel k -means algorithm, and propose a new iterative algorithm based on Hartigan's method to solve this QCQP. Section VII contains some carefully designed numerical experiments indicating that this algorithm outperforms kernel k -means, standard k -means, and GMM/EM algorithms. Our final conclusions are presented in section VIII.

II. BACKGROUND ON ENERGY STATISTICS AND RKHS

In this section we introduce the main concepts from energy statistics and its relation to RKHS which form the basis of our work. For more details we refer the reader to [1] and [6].

Consider random variables in \mathbb{R}^D such that $X, X' \stackrel{iid}{\sim} P$ and $Y, Y' \stackrel{iid}{\sim} Q$, where P and Q are cumulative distribution functions with finite first moments. The quantity

$$\mathcal{E}(P, Q) \equiv 2\mathbb{E}\|X - Y\| - \mathbb{E}\|X - X'\| - \mathbb{E}\|Y - Y'\| \quad (1)$$

called *energy distance* [1] is rotational invariant and nonnegative, $\mathcal{E}(P, Q) \geq 0$, where equality to zero holds if and only if $P = Q$. Above, $\|\cdot\|$ denotes the Euclidean norm in \mathbb{R}^D . Energy distance provides a characterization of equality of distributions, and $\mathcal{E}^{1/2}$ is a metric on the space of distributions.

The energy distance can be generalized as, for instance,

$$\mathcal{E}_\alpha(P, Q) \equiv 2\mathbb{E}\|X - Y\|^\alpha - \mathbb{E}\|X - X'\|^\alpha - \mathbb{E}\|Y - Y'\|^\alpha \quad (2)$$

where $0 < \alpha \leq 2$. This quantity is also nonnegative, $\mathcal{E}_\alpha(P, Q) \geq 0$. Furthermore, for $0 < \alpha < 2$ we have that $\mathcal{E}_\alpha(P, Q) = 0$ if and only if $P = Q$, while for $\alpha = 2$ we have $\mathcal{E}_2(P, Q) = 2\|\mathbb{E}(X) - \mathbb{E}(Y)\|^2$ which shows that equality to zero only requires equality of the means, and thus $\mathcal{E}_2(P, Q) = 0$ does not imply equality of distributions.

It is important to mention that (2) can be even further generalized. Let $X, Y \in \mathcal{X}$ where \mathcal{X} is an arbitrary space endowed with a *semimetric of negative type* $\rho : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, which is required to satisfy

$$\sum_{i,j=1}^n c_i c_j \rho(X_i, X_j) \leq 0, \quad (3)$$

where $X_i \in \mathcal{X}$ and $c_i \in \mathbb{R}$ such that $\sum_{i=1}^n c_i = 0$. Then, \mathcal{X} is called a *space of negative type*. We can thus replace $\mathbb{R}^D \rightarrow \mathcal{X}$ and $\|X - Y\| \rightarrow \rho(X, Y)$ in the definition (1), obtaining the

generalized energy distance

$$\mathcal{E}(P, Q) \equiv 2\mathbb{E}\rho(X, Y) - \mathbb{E}\rho(X, X') - \mathbb{E}\rho(Y, Y'). \quad (4)$$

For spaces of negative type there exists a Hilbert space \mathcal{H} and a map $\varphi : \mathcal{X} \rightarrow \mathcal{H}$ such that $\rho(X, Y) = \|\varphi(X) - \varphi(Y)\|_{\mathcal{H}}^2$. This allows us to compute quantities related to probability distributions over \mathcal{X} in the Hilbert space \mathcal{H} . Even though the semimetric ρ may not satisfy the triangle inequality, $\rho^{1/2}$ does since it can be shown to be a legit metric.

There is an equivalence between energy distance, commonly used in statistics, and distances between embeddings of distributions in RKHS, commonly used in machine learning. This equivalence was established in [6]. Let us first recall the definition of RKHS. Let \mathcal{H} be a Hilbert space of real-valued functions over \mathcal{X} . A function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a reproducing kernel of \mathcal{H} if it satisfies the following two conditions:

1. $h_x \equiv K(\cdot, x) \in \mathcal{H}$ for all $x \in \mathcal{X}$.
2. $\langle h_x, f \rangle_{\mathcal{H}} = f(x)$ for all $x \in \mathcal{X}$ and $f \in \mathcal{H}$.

In other words, for any $x \in \mathcal{X}$ and any function $f \in \mathcal{H}$, there is a unique $h_x \in \mathcal{H}$ that reproduces $f(x)$ through the inner product of \mathcal{H} . If such a *kernel* function K exists, then \mathcal{H} is called a RKHS. The above two properties immediately imply that K is symmetric and positive definite. Indeed, notice that $\langle h_x, h_y \rangle = h_y(x) = K(x, y)$, and by definition $\langle h_x, h_y \rangle^* = \langle h_y, h_x \rangle$, but since the inner product is real we have $\langle h_y, h_x \rangle = \langle h_x, h_y \rangle$, or equivalently $K(y, x) = K(x, y)$. Moreover, for any $w \in \mathcal{H}$ we can write $w = \sum_{i=1}^n c_i h_{x_i}$, where $\{h_{x_i}\}_{i=1}^n$ is a basis of \mathcal{H} . It follows that $\langle w, w \rangle_{\mathcal{H}} = \sum_{i,j=1}^n c_i c_j K(x_i, x_j) \geq 0$, showing that the kernel is positive definite. If G is a matrix with elements $G_{ij} = K(x_i, x_j)$, this is equivalent to G being positive semidefinite, i.e. $v^\top G v \geq 0$ for any vector $v \in \mathbb{R}^n$.

The Moore-Aronszajn theorem [19] establishes the converse of the above paragraph. For every symmetric and positive definite function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, there is an associated RKHS \mathcal{H}_K with reproducing kernel K . The map $\varphi : x \mapsto h_x \in \mathcal{H}_K$ is called the *canonical feature map*. Given a kernel K , this theorem enables us to define an embedding of a probability measure P into the RKHS as follows: $P \mapsto h_P \in \mathcal{H}_K$ such that $\int f(x) dP(x) = \langle f, h_P \rangle$ for all $f \in \mathcal{H}_K$, or alternatively $h_P \equiv \int K(\cdot, x) dP(x)$. We can now introduce the notion of distance between two probability measures using the inner product of \mathcal{H}_K , which is called

the maximum mean discrepancy (MMD) and is given by

$$\gamma_K(P, Q) \equiv \|h_P - h_Q\|_{\mathcal{H}_K}. \quad (5)$$

This can also be written as [20]

$$\gamma_K^2(P, Q) = \mathbb{E}K(X, X') + \mathbb{E}K(Y, Y') - 2\mathbb{E}K(X, Y) \quad (6)$$

where $X, X' \stackrel{iid}{\sim} P$ and $Y, Y' \stackrel{iid}{\sim} Q$. From the equality between (5) and (6) we also have

$$\langle h_P, h_Q \rangle_{\mathcal{H}_K} = \mathbb{E}K(X, Y). \quad (7)$$

Thus, in practice, we can estimate the inner product between embedded distributions by averaging the kernel function over sampled data.

The following important result shows that semimetrics of negative type and symmetric positive definite kernels are closely related [21]. Let $\rho : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ and $x_0 \in \mathcal{X}$ an arbitrary but fixed point. Define

$$K(x, y) \equiv \frac{1}{2} [\rho(x, x_0) + \rho(y, x_0) - \rho(x, y)]. \quad (8)$$

Then, it can be shown that K is positive definite if and only if ρ is a semimetric of negative type (3). We have a family of kernels, one for each choice of x_0 . Conversely, if ρ is a semimetric of negative type and K is a kernel in this family, then

$$\begin{aligned} \rho(x, y) &= K(x, x) + K(y, y) - 2K(x, y) \\ &= \|h_x - h_y\|_{\mathcal{H}_K}^2 \end{aligned} \quad (9)$$

and the canonical feature map $\varphi : x \mapsto h_x$ is injective [6]. When these conditions are satisfied we say that the kernel K generates the semimetric ρ . If two different kernels generate the same ρ they are equivalent kernels.

Now we can state the equivalence between energy distance \mathcal{E} and inner products on RKHS, which is one of the main results of [6]. If ρ is a semimetric of negative type and K a kernel that generates ρ , then replacing (9) into (4), and using (6), yields

$$\mathcal{E}(P, Q) = 2 [\mathbb{E}K(X, X') + \mathbb{E}K(Y, Y') - 2\mathbb{E}K(X, Y)] = 2\gamma_K^2(P, Q). \quad (10)$$

Due to (5) we can compute the energy distance using the inner product of \mathcal{H}_K . Moreover, this can be estimated from a sample according to (7).

Finally, let us recall the main formulas from energy statistics for the test statistic of equality of distributions [1]. Assume we have data $\mathbb{X} = \{x_1, \dots, x_n\}$ where $x_i \in \mathcal{X}$ and \mathcal{X} is a space of negative type. Consider a disjoint partition $\mathbb{X} = \bigcup_{j=1}^k \mathcal{C}_j$, with $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$. Each expectation in (4) can be computed through the function

$$g(\mathcal{C}_i, \mathcal{C}_j) \equiv \frac{1}{n_i n_j} \sum_{x \in \mathcal{C}_i} \sum_{y \in \mathcal{C}_j} \rho(x, y) \quad (11)$$

where $n_i = |\mathcal{C}_i|$ is the number of elements in \mathcal{C}_i . The *within energy dispersion* is defined by

$$W \equiv \sum_{j=1}^k \frac{n_j}{2} g(\mathcal{C}_j, \mathcal{C}_j) \quad (12)$$

and the *between-sample energy statistic* is defined by

$$S \equiv \sum_{1 \leq i < j \leq k} \frac{n_i n_j}{2n} [2g(\mathcal{C}_i, \mathcal{C}_j) - g(\mathcal{C}_i, \mathcal{C}_i) - g(\mathcal{C}_j, \mathcal{C}_j)] \quad (13)$$

where $n = \sum_{j=1}^k n_j$. Given a set of distributions $\{P_j\}_{j=1}^k$, where $x \in \mathcal{C}_j$ if and only if $x \sim P_j$, the quantity S provides a *nonparametric test statistic* for equality of distributions [1]. When the sample size is large enough, $n \rightarrow \infty$, under the null hypothesis $H_0 : P_1 = P_2 = \dots = P_k$ we have that $S \rightarrow 0$, and under the alternative hypothesis $H_1 : P_i \neq P_j$ for at least two $i \neq j$, we have that $S \rightarrow \infty$. This test is nonparametric in the sense that it does not make any assumptions about the distributions P_j .

One can make the analogy that points $x \in \mathcal{C}_j$ form a massive body whose total mass is characterized by the distribution function P_j . The quantity S is thus a potential energy of the from $S(P_1, \dots, P_k)$ which measures how different the distribution of these masses are, and achieves the ground state $S = 0$ when all bodies have the same mass distribution. The potential energy S increases as bodies have different mass distributions.

III. CLUSTERING BASED ON ENERGY STATISTICS

This section contains the main theoretical results of this paper, where we formulate an optimization problem for clustering based on energy statistics and RKHS introduced in the previous section.

Due to the test statistic (13) for equality of distributions, the obvious criterion for clustering data is to maximize S , which makes each cluster as different as possible from

the other ones. In other words, given a set of points coming from different probability distributions, S should attain a maximum when each point is correctly classified as belonging to the cluster associated to its probability distribution. The following straightforward result shows that maximizing (13) is, however, equivalent to minimizing (12) which has a more convenient form.

Proposition 1. *Let $\mathbb{X} = \{x_1, \dots, x_n\}$ where each data point x_i lives in a space \mathcal{X} endowed with a semimetric $\rho : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ of negative type (3). For a fixed integer k , the partition $\mathbb{X} = \bigcup_{j=1}^k \mathcal{C}_j$, where $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$ for all $i \neq j$, maximizes (13) if and only if*

$$\min_{\mathcal{C}_1, \dots, \mathcal{C}_k} W(\mathcal{C}_1, \dots, \mathcal{C}_k), \quad (14)$$

where W is given by (12).

Proof. From (12) and (13) we have

$$\begin{aligned} S + W &= \frac{1}{2n} \sum_{\substack{i,j=1 \\ i \neq j}}^k n_i n_j g(\mathcal{C}_i, \mathcal{C}_j) + \frac{1}{2n} \sum_{i=1}^k \left[n - \sum_{j \neq i=1}^k n_j \right] n_i g(\mathcal{C}_i, \mathcal{C}_i) \\ &= \frac{1}{2n} \sum_{i,j=1}^k n_i n_j g(\mathcal{C}_i, \mathcal{C}_j) = \frac{1}{2n} \sum_{x \in \mathbb{X}} \sum_{y \in \mathbb{X}} \rho(x, y) = \frac{n}{2} g(\mathbb{X}, \mathbb{X}). \end{aligned} \quad (15)$$

Note that the right hand side of this equation only depends on the pooled data, so it is a constant independent of the choice of partition. Therefore, maximizing S over the choice of partition is equivalent to minimizing W . \square

For a given k , the clustering problem amounts to finding the best partition of the data by solving (14). Notice that this is a hard clustering problem, as partitions are disjoint. The problem (14) based on energy statistics was already proposed in [4]. However, it is important to note that this is equivalent to maximizing (13) which is the test statistic for equality of distributions. In the following we show what is the explicit optimization problem behind (14).

Let us formulate (14) in the corresponding RKHS. Based on (8) and (9), assume that the kernel $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ generates ρ . Let us define the Gram matrix

$$G \equiv \begin{pmatrix} K(x_1, x_1) & K(x_1, x_2) & \cdots & K(x_1, x_n) \\ K(x_2, x_1) & K(x_2, x_2) & \cdots & K(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ K(x_n, x_1) & K(x_n, x_2) & \cdots & K(x_n, x_n) \end{pmatrix}. \quad (16)$$

Let $Z \in \{0, 1\}^{n \times k}$ be the label matrix, with only one nonvanishing entry per row, indicating to which cluster (column) each point (row) belongs to. This matrix satisfy $Z^\top Z = D$ where the diagonal matrix $D = \text{diag}(n_1, \dots, n_k)$ contains the number of points in each cluster. Let us also introduce the rescaled matrix $Y \equiv ZD^{-1/2}$. In component form they are given by

$$Z_{ij} \equiv \begin{cases} 1 & \text{if } x_i \in \mathcal{C}_j \\ 0 & \text{otherwise} \end{cases} \quad Y_{ij} \equiv \begin{cases} \frac{1}{\sqrt{n_j}} & \text{if } x_i \in \mathcal{C}_j \\ 0 & \text{otherwise} \end{cases}. \quad (17)$$

Throughout the paper, we use the notation $M_{i\bullet}$ to denote the i th row of a matrix M , and $M_{\bullet j}$ denotes its j th column. Our next result shows the optimization problem (14) is NP-hard since it is a quadratically constrained quadratic program (QCQP).

Proposition 2. *The problem (14) is equivalent to*

$$\max_Y \text{Tr}(Y^\top G Y) \quad \text{s.t. } Y \geq 0, Y^\top Y = I, YY^\top e = e, \quad (18)$$

where $e = (1, 1, \dots, 1)^\top \in \mathbb{R}^n$ is the all-ones vector, and G is the Gram matrix (16).

Proof. From (9), (11), and (12) we have

$$W(\mathcal{C}_1, \dots, \mathcal{C}_k) = \frac{1}{2} \sum_{j=1}^k \frac{1}{n_j} \sum_{x, y \in \mathcal{C}_j} \rho(x, y) = \sum_{j=1}^k \sum_{x \in \mathcal{C}_j} \left(K(x, x) - \frac{1}{n_j} \sum_{y \in \mathcal{C}_j} K(x, y) \right). \quad (19)$$

Note that the first term is global so it does not contribute to the optimization problem. Therefore, minimizing (19) is equivalent to

$$\max_{\mathcal{C}_1, \dots, \mathcal{C}_k} \sum_{j=1}^k \frac{1}{n_j} \sum_{x, y \in \mathcal{C}_j} K(x, y). \quad (20)$$

But

$$\sum_{x, y \in \mathcal{C}_j} K(x, y) = \sum_{p=1}^n \sum_{q=1}^n Z_{pj} Z_{qj} G_{pq} = (Z^\top G Z)_{jj}, \quad (21)$$

where we used the definitions (16) and (17). Thus, the objective function in (20) is equal to $\text{Tr}(D^{-1} Z^\top G Z)$. Now we can use the cyclic property of the trace, and by the own definition of the matrix Z in (17), we obtain the following integer programming problem:

$$\max_Z \text{Tr} \left((ZD^{-1/2})^\top G (ZD^{-1/2}) \right) \quad \text{s.t. } Z_{ij} \in \{0, 1\}, \sum_{j=1}^k Z_{ij} = 1, \sum_{i=1}^n Z_{ij} = n_j. \quad (22)$$

Now we write this in terms of the matrix $Y = ZD^{-1/2}$. The objective function immediately becomes $\text{Tr}(Y^\top G Y)$. Notice that the above constraints imply that $Z^\top Z = D$,

where $D = \text{diag}(n_1, \dots, n_k)$, which in turn gives $D^{-1/2}Y^TYD^{-1/2} = D$, or $Y^TY = I$. Also, every entry of Y is positive by definition, $Y \geq 0$. Now it only remains to show the last constraint in (18), which comes from the last constraint in (22). In matrix form this reads $Z^Te = De$. Replacing $Z = YD^{1/2}$ we have $Y^Te = D^{1/2}e$. Multiplying this last equation on the left by Y , and noticing that $YD^{1/2}e = Ze = e$, we finally obtain $YY^Te = e$. Therefore, the optimization problem (22) is equivalent to (18). \square

Based on Proposition 2, to group data $\mathbb{X} = \{x_1, \dots, x_n\}$ into k clusters, we first compute the Gram matrix G and then solve the optimization problem (18) for $Y \in \mathbb{R}^{n \times k}$. The i th row of Y will contain a single nonzero element in some j th column, indicating that $x_i \in \mathcal{C}_j$. Problem (18) is NP-hard and there are few methods available to solve it directly, which is computational prohibitive even for small datasets. However, one can find approximate solutions by relaxing some of the constraints, or obtaining a relaxed SDP version of it. For instance, the relaxed problem

$$\max_Y \text{Tr}(Y^TGY) \quad \text{s.t. } Y^TY = I \quad (23)$$

has a well-known closed form solution $Y^* = UR$, where the columns of U contain the leading k eigenvectors of G corresponding to the k largest eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$, and $R \in \mathbb{R}^{k \times k}$ is an arbitrary orthogonal matrix. The resulting optimal objective function is given by $\max \text{Tr}(Y^{*\top}GY^*) = \sum_{i=1}^k \lambda_i$. One might then normalize and threshold the rows of Y^* , or better, following [22] one can normalize the rows of Y^* and apply standard k -means on this matrix where each row is considered as a data point. This is the procedure done in spectral clustering on a graph Laplacian matrix defined by a similarity matrix. However, computing eigenvectors of a very large matrix can be very expensive, and usually iterative methods are preferred. Moreover, this procedure is only guaranteed to converge if the normalized Y^* is positive semidefinite. In Section VI we will propose an iterative method to directly find approximate solutions to (18) that is guaranteed to converge and does not require that the similarities $K(x_i, x_j)$ be nonnegative.

The clustering problem (18) based on energy statistics is valid for data living in an *arbitrary* space of negative type, where a semimetric ρ , and thus the kernel (8), are assumed to be known. This clustering method is *nonparametric* since it does not make any assumptions about the distribution of the data, contrary to k -means and gaussian mixture models (GMM), for example. If one uses the standard energy distance defined

in (1), then $\rho(x, y) = \|x - y\|$ and this fixes the kernel through (8). In the same way, for data living in a more general metric space (\mathcal{X}, ρ) the corresponding semimetric ρ fixes the kernel. In practice, however, the clustering quality strongly depend on the choice of a suitable ρ which measures the similarity between data points, and is equivalent to choosing an appropriate kernel. The energy distance (2) fixes a family of choices $\rho(x, y) = \|x - y\|^\alpha$ with $0 < \alpha \leq 2$. If prior information is available one may choose a more appropriate ρ .

Relation to Kernel k -Means

One may wonder how energy statistics clustering relates to the well-known kernel k -means problem¹ which is extensively used in machine learning. For a positive semidefinite Gram matrix G , as defined in (16), there exists a map $\varphi : \mathcal{X} \rightarrow \mathcal{H}_K$ such that $K(x, y) = \varphi(x)^\top \varphi(y)$. The kernel k -means optimization problem, in the feature space, is defined by

$$\min_{\mathcal{C}_1, \dots, \mathcal{C}_k} \left\{ J(\mathcal{C}_1, \dots, \mathcal{C}_k) \equiv \sum_{j=1}^k \sum_{x \in \mathcal{C}_j} \|\varphi(x) - \varphi(\mu_j)\|^2 \right\}, \quad (24)$$

where $\mu_j = \frac{1}{n_j} \sum_{x \in \mathcal{C}_j} x$ is the mean of cluster \mathcal{C}_j in the ambient space. Notice that the above objective function is strongly tied to the idea of minimizing distances between points and cluster centers, which arises from k -means objective function. It was shown [13, 14] that problem (24) is equivalent to a QCQP in the same form as (18). The next result makes this explicit, showing that (14) and (24) are actually equivalent.

Proposition 3. *For a fixed kernel, the clustering optimization problem (14) based on energy statistics is equivalent to the kernel k -means optimization problem (24), and both are equivalent to (18).*

Proof. Notice that $\|\varphi(x) - \varphi(\mu_j)\|^2 = \varphi(x)^\top \varphi(x) - 2\varphi(x)^\top \varphi(\mu_j) + \varphi(\mu_j)^\top \varphi(\mu_j)$, therefore

$$J = \sum_{j=1}^k \sum_{x \in \mathcal{C}_j} \left(K(x, x) - \frac{2}{n_j} \sum_{y \in \mathcal{C}_j} K(x, y) + \frac{1}{n_j^2} \sum_{y, z \in \mathcal{C}_j} K(y, z) \right). \quad (25)$$

The first term is global so it does not contribute to the optimization problem. Notice that the third term gives $\sum_{x \in \mathcal{C}_j} \frac{1}{n_j^2} \sum_{y, z \in \mathcal{C}_j} K(y, z) = \frac{1}{n_j} \sum_{y, z \in \mathcal{C}_j} K(y, z)$, which is the same as the

¹ When we refer to kernel k -means problem we mean specifically the optimization problem (24), which should not be confused with kernel k -means algorithm that is just one possible recipe to solve (24).

second term. Thus, problem (24) is equivalent to

$$\min_{\mathcal{C}_1, \dots, \mathcal{C}_k} \left\{ J(\mathcal{C}_1, \dots, \mathcal{C}_k) = \max_{\mathcal{C}_1, \dots, \mathcal{C}_k} \sum_{j=1}^k \frac{1}{n_j} \sum_{x, y \in \mathcal{C}_j} K(x, y) \right\} \quad (26)$$

which is exactly the same as (20) from the energy statistics formulation. Therefore, once the kernel K is fixed, the function W given by (12) is the same as J in (24). The remaining of the proof proceeds as already shown in the proof of Proposition 2, leading to the optimization problem in the form (18). \square

The above result shows that kernel k -means problem is actually a consequence of energy statistics. In this vein, kernel k -means problem is part of a statistical framework where we are maximizing distances between probability distributions. The kernel function K arises from a semimetric ρ of negative type which defines the energy distance between distributions.

As shown in [13, 14], kernel k -means, spectral clustering, and graph partitioning problems such as ratio association, ratio cut, and normalized cut are all equivalent to a QCQP of the form (18). Thus one can use kernel k -means algorithm to solve these problems as well. This correspondence involves a weighted version of (18) that we demonstrate in the following.

IV. CLUSTERING BASED ON WEIGHTED ENERGY STATISTICS

We generalize the formulas from energy statistics to incorporate weights associated to each data point. Let $w(x)$ be a weight function associated to point $x \in \mathcal{X}$. We can generalize (11) as follows:

$$g(\mathcal{C}_i, \mathcal{C}_j) \equiv \frac{1}{s_i s_j} \sum_{x \in \mathcal{C}_i} \sum_{y \in \mathcal{C}_j} w(x) w(y) \rho(x, y), \quad s_i \equiv \sum_{x \in \mathcal{C}_i} w(x). \quad (27)$$

Now we replace this function in the formulas (12) and (13), with $n_i \rightarrow s_i$ and $n \rightarrow s$ where $s = \sum_{j=1}^k s_j$, to obtain a weighted version of energy test statistic. With these changes, Proposition 1 remains the unaltered, so the clustering problem becomes

$$\min_{\mathcal{C}_1, \dots, \mathcal{C}_k} \left\{ W(\mathcal{C}_1, \dots, \mathcal{C}_k) \equiv \sum_{j=1}^k \frac{s_j}{2} g(\mathcal{C}_j, \mathcal{C}_j) \right\} \quad (28)$$

where now g is given by (27). Let us define the following matrices and vector:

$$Y_{ij} \equiv \begin{cases} \frac{1}{\sqrt{s_j}} & \text{if } x_i \in \mathcal{C}_j \\ 0 & \text{otherwise} \end{cases}, \quad \mathcal{W} \equiv \text{diag}(w_1, \dots, w_n), \quad H \equiv \mathcal{W}^{1/2} Y, \quad \omega \equiv \mathcal{W} e, \quad (29)$$

where $w_i = w(x_i)$ and $e \in \mathbb{R}^n$ is the all-ones vector. Now we can show the analogous of Proposition 2 to the case of (28).

Proposition 4. *The weighted version of energy statistics clustering given by problem (28) is equivalent to*

$$\max_H \text{Tr} \{ H^\top (\mathcal{W}^{1/2} G \mathcal{W}^{1/2}) H \} \quad \text{s.t. } H \geq 0, H^\top H = I, HH^\top \omega = \omega, \quad (30)$$

where G is the Gram matrix (16) and the other quantities are defined in (29).

Proof. Replacing (9) and eliminating the global terms which do not contribute, the optimization problem (28) becomes

$$\max_{\mathcal{C}_1, \dots, \mathcal{C}_k} \sum_{j=1}^k \frac{1}{s_j} \sum_{x \in \mathcal{C}_j} \sum_{y \in \mathcal{C}_j} w(x)w(y)K(x, y). \quad (31)$$

This objective function can be written as

$$\begin{aligned} \sum_{j=1}^k \frac{1}{s_j} \sum_{p=1}^n \sum_{q=1}^n w_p w_q Z_{pj} Z_{qj} G_{pq} &= \sum_{j=1}^k \sum_{p=1}^n \sum_{q=1}^n \frac{Z_{jp}^\top \sqrt{w_p}}{\sqrt{s_j}} w_p^{1/2} G_{pq} w_q^{1/2} \frac{\sqrt{w_q} Z_{qj}}{\sqrt{s_j}} \\ &= \sum_{j=1}^k (H^\top \mathcal{W}^{1/2} G \mathcal{W}^{1/2} H)_{jj} \\ &= \text{Tr} (H^\top \mathcal{W}^{1/2} G \mathcal{W}^{1/2} H). \end{aligned} \quad (32)$$

To obtain the constraints, note that $H_{ij} \geq 0$ by definition, and

$$(H^\top H)_{ij} = \sum_{\ell=1}^n Y_{\ell i} \mathcal{W}_{\ell \ell} Y_{\ell j} = \frac{1}{\sqrt{s_i} \sqrt{s_j}} \sum_{\ell=1}^n w_\ell Z_{\ell i} Z_{\ell j} = \frac{\delta_{ij}}{s_i} \sum_{\ell=1}^n w_\ell Z_{\ell i} = \delta_{ij}, \quad (33)$$

therefore $H^\top H = I$. This is a constraint on the rows of H . To obtain a condition on the columns of H observe that

$$(H^\top H)_{pq} = \sqrt{w_p w_q} \sum_{j=1}^k \frac{Z_{pj} Z_{qj}}{s_j} = \begin{cases} \frac{\sqrt{w_p w_q}}{s_i} & \text{if both } x_p, x_q \in \mathcal{C}_i \\ 0 & \text{otherwise.} \end{cases} \quad (34)$$

Therefore, $(H^\top H \mathcal{W}^{1/2})_{pq} = \sqrt{w_p} w_q s_i^{-1}$ if both points x_p and x_q belong to the same cluster, which we denote by \mathcal{C}_i for some $i = 1, \dots, k$, and $(H^\top H \mathcal{W}^{1/2})_{pq} = 0$ otherwise. Thus, the p th line of this matrix is nonzero only on entries corresponding to points that are in the same cluster as x_p . If we sum over the columns of this line we obtain $\sqrt{w_p} s_i^{-1} \sum_{q=1}^n w_q Z_{qi} = \sqrt{w_p}$, or equivalently $HH^\top \mathcal{W}^{1/2} e = \mathcal{W}^{1/2} e$, which gives the constraint $HH^\top \omega = \omega$. \square

Connection with Graph Partitioning

The relation between kernel k -means and graph partitioning problems was already established [13, 14]. We repeat a similar analysis due to the relation of these problems to energy statistics and RKHS, which may provide a different perspective.

Consider a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{A})$ where \mathcal{V} is the set of vertices, \mathcal{E} the set of edges, and \mathcal{A} is an affinity matrix of the graph that measures the similarities between pairs of nodes. Thus, $\mathcal{A}_{ij} \neq 0$ if $(i, j) \in \mathcal{E}$, and $\mathcal{A}_{ij} = 0$ otherwise. We also associate weights to every vertex, $w_i = w(i)$ for $i \in \mathcal{V}$, and let $s_j = \sum_{i \in \mathcal{C}_j} w_i$, where $\mathcal{C}_j \subseteq \mathcal{V}$ is one partition of \mathcal{V} . Let

$$\text{links}(\mathcal{C}_\ell, \mathcal{C}_m) \equiv \sum_{i \in \mathcal{C}_\ell, j \in \mathcal{C}_m} \mathcal{A}_{ij}. \quad (35)$$

We want to partition the set of vertices \mathcal{V} into k disjoint subsets, $\mathcal{V} = \bigcup_{j=1}^k \mathcal{C}_j$. The generalized ratio association problem is given by

$$\max_{\mathcal{C}_1, \dots, \mathcal{C}_k} \sum_{j=1}^k \frac{\text{links}(\mathcal{C}_j, \mathcal{C}_j)}{s_j} \quad (36)$$

and maximizes the within cluster association. The generalized ratio cut problem

$$\min_{\mathcal{C}_1, \dots, \mathcal{C}_k} \sum_{j=1}^k \frac{\text{links}(\mathcal{C}_j, \mathcal{V} \setminus \mathcal{C}_j)}{s_j} \quad (37)$$

minimizes the cut between clusters. These two problems are equivalent, in analogous way as minimizing (12) is equivalent to maximizing (13), as shown in Proposition 1. Here this is due to the equality $\text{links}(\mathcal{C}_j, \mathcal{V} \setminus \mathcal{C}_j) = \text{links}(\mathcal{C}_j, \mathcal{V}) - \text{links}(\mathcal{C}_j, \mathcal{C}_j)$. Several graph partitioning methods [23–26] can be seen as a particular case of (36) or (37).

Consider (36), whose objective function can be written as

$$\sum_{j=1}^k \frac{1}{s_j} \sum_{p \in \mathcal{C}_j} \sum_{q \in \mathcal{C}_j} \mathcal{A}_{pq} = \sum_{j=1}^k \sum_{p=1}^n \sum_{q=1}^n \frac{Z_{jp}^\top}{\sqrt{s_j}} \mathcal{A}_{pq} \frac{Z_{qj}}{\sqrt{s_j}} = \text{Tr} (Y^\top \mathcal{A} Y), \quad (38)$$

with Z defined in (17) and Y in (29). To make the analogy with (30) explicit, problem (36) is equivalent to

$$\max_H \text{Tr} (H^\top \mathcal{W}^{-1/2} \mathcal{A} \mathcal{W}^{-1/2} H) \quad \text{s.t. } H \geq 0, H^\top H = I, H H^\top \omega = \omega. \quad (39)$$

Therefore, this is exactly the same problem as weighted energy statistics clustering (30) with $G = \mathcal{W}^{-1} \mathcal{A} \mathcal{W}^{-1}$. Assuming this matrix is positive semidefinite, this generates a semimetric

(9) for graphs given by

$$\rho(i, j) = \frac{\mathcal{A}_{ii}}{w_i^2} + \frac{\mathcal{A}_{jj}}{w_j^2} - \frac{2\mathcal{A}_{ij}}{w_i w_j} \quad \text{or} \quad \rho(i, j) = -\frac{2\mathcal{A}_{ij}}{w_i w_j} \quad (40)$$

for vertices $i, j \in \mathcal{V}$, and where in the second equation we assume the graph has no self-loops, i.e. $\mathcal{A}_{ii} = 0$. Using (40) in (11)–(13) allows one to use energy statistics theory for inference over populations of graphs.

V. TWO-CLASS PROBLEM IN ONE DIMENSION

Before stating a general algorithm to solve (18), let us first consider the simplest possible case which is one-dimensional data and a two-class problem. This will be useful to test energy statistics clustering on a simple setting.

Fixing $\rho(x, y) = |x - y|$ according to (1), we can actually compute (11) in $\mathcal{O}(n \log n)$ and find a direct solution to (14). This is done by noticing that

$$\begin{aligned} |x - y| &= (x - y)\mathbb{1}_{x \geq y} - (x - y)\mathbb{1}_{x < y} \\ &= x(\mathbb{1}_{x \geq y} - \mathbb{1}_{x < y}) + y(\mathbb{1}_{y > x} - \mathbb{1}_{y \leq x}) \end{aligned} \quad (41)$$

where we have the indicator function defined by $\mathbb{1}_A = 1$ if A is true, and $\mathbb{1}_A = 0$ otherwise. Let \mathcal{C} be a partition with n elements. Using the above distance in (11) we have

$$g(\mathcal{C}, \mathcal{C}) = \frac{1}{n^2} \sum_{x \in \mathcal{C}} \sum_{y \in \mathcal{C}} x(\mathbb{1}_{x \geq y} + \mathbb{1}_{y > x} - \mathbb{1}_{x \geq y} - \mathbb{1}_{x < y}). \quad (42)$$

The sum over y can be eliminated since each term in the parenthesis is simply counting the number of elements in \mathcal{C} that satisfy the condition of the indicator function. Assuming that we first order the data in \mathcal{C} , obtaining $\bar{\mathcal{C}} = [x_j \in \mathcal{C} : x_1 \leq x_2 \leq \dots \leq x_n]$, we can write (42) in the following simple form:

$$g(\bar{\mathcal{C}}, \bar{\mathcal{C}}) = \frac{2}{n^2} \sum_{\ell=1}^n (2\ell - 1 - n) x_\ell. \quad (43)$$

Note that the cost of computing (43) is $\mathcal{O}(n)$ and the cost of sorting the data is at the most $\mathcal{O}(n \log n)$. Assuming that each partition is ordered $\mathbb{X} = \bigcup_{j=1}^k \bar{\mathcal{C}}_j$ the within energy dispersion (12) can be written as

$$W(\bar{\mathcal{C}}_1, \dots, \bar{\mathcal{C}}_k) = \sum_{j=1}^k \sum_{\ell=1}^{n_j} \frac{2\ell - 1 - n_j}{n_j} x_\ell. \quad (44)$$

Algorithm 1 Approximate solution to (14) for a two-class problem in one dimension.

input data \mathbb{X}

output label matrix Z

- 1: sort \mathbb{X} obtaining $\bar{\mathbb{X}} = [x_1, \dots, x_n]$
 - 2: **for** $j \in [1, \dots, n]$ **do**
 - 3: Let $\bar{\mathcal{C}}_1^{(j)} = [x_i : i = 1, \dots, j]$ and $\bar{\mathcal{C}}_2^{(j)} = [x_i : i = j + 1, \dots, n]$
 - 4: $W^{(j)} \leftarrow W(\bar{\mathcal{C}}_1^{(j)}, \bar{\mathcal{C}}_2^{(j)})$ from (44)
 - 5: **end for**
 - 6: $j^* \leftarrow \arg \min_j W^{(j)}$
 - 7: $Z_{j\bullet} \leftarrow (1, 0)$ if $j \leq j^*$, and $Z_{j\bullet} \leftarrow (0, 1)$ otherwise, for $j = 1, \dots, n$
-

For a two-class problem we can use (44) to cluster data through a simple algorithm as follows. We first order the entire dataset $\mathbb{X} \rightarrow \bar{\mathbb{X}}$. Then we compute (44) for each possible split of $\bar{\mathbb{X}}$ and pick the point which gives the minimum value of W . This procedure is described in Algorithm 1. Notice that this method does not require any initialization, however, it only works for one-dimensional data with Euclidean distance. The total complexity of the algorithm is $\mathcal{O}(n \log n + n^2) = \mathcal{O}(n^2)$.

Assuming the true label matrix Z is available, a direct measure of how different the estimated matrix \hat{Z} is from Z , up to label permutations, is given by

$$\text{accuracy}(\hat{Z}) \equiv \max_{\sigma} \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^k \hat{Z}_{i\sigma(j)} Z_{ij} \quad (45)$$

where σ is a permutation of the k cluster groups. The accuracy is always between $[0, 1]$, where 1 corresponds to all points correctly clustered, and 0 to all points wrongly clustered. For a two-class problem with equal number of points in each cluster, the value $1/2$ correspond to chance.

Let us consider two simple experiments with equal number of points in each cluster. We plot the accuracy (45) versus the number of points in each cluster. The data is clustered using Algorithm 1, GMM through EM algorithm, and standard k -means algorithm. In the last two cases we use the initialization from k -means++ [27] and we run the algorithms few times choosing the result with best objective function value. Notice that Algorithm 1

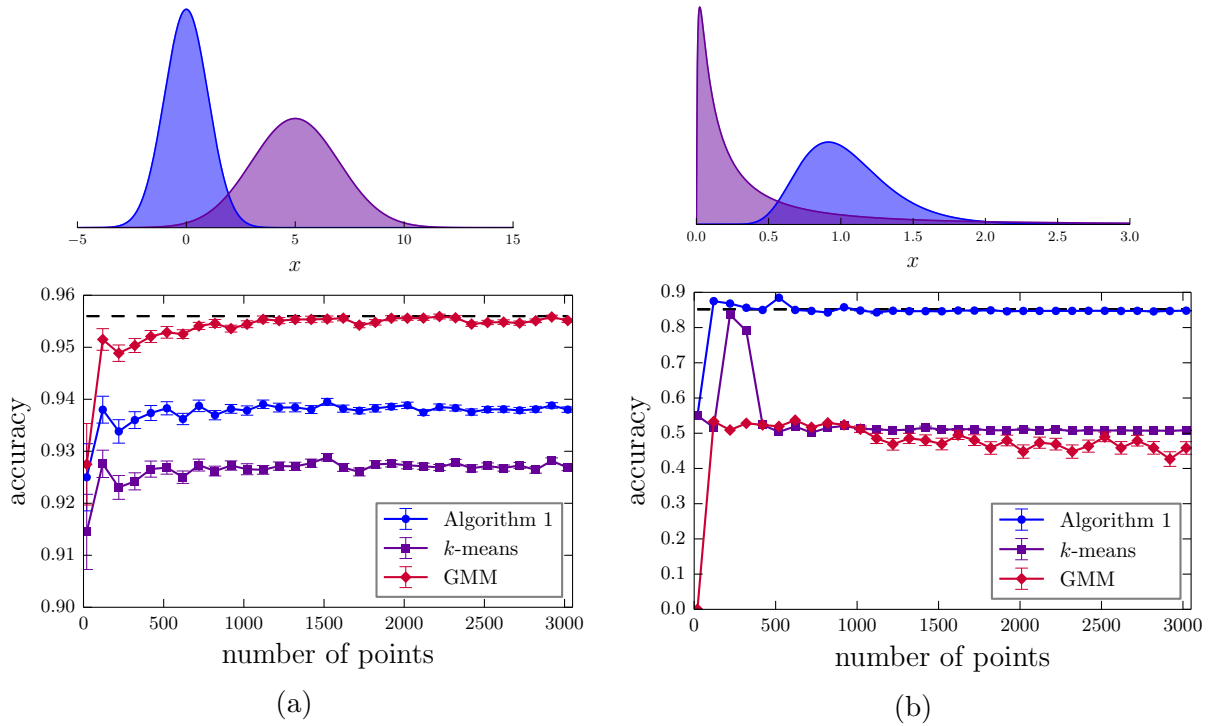


FIG. 1. Energy statistics clustering by Algorithm 1 compared to k -means and GMM/EM. We have the same number of points in both clusters, and for each case we sample 100 times from the distributions in the histograms. We plot the average value of (45) versus the total number of points (error bars are standard error). The dashed line indicates the best possible classification accuracy computed from Bayes error. (a) Data coming from (46), where the optimal accuracy is ≈ 0.956 . (b) Data from (47), where the optimal accuracy is ≈ 0.852 .

requires no initialization. Moreover, for each case we sample 100 times and show the average accuracy with error bars indicating the standard error. In Fig. 1a we sample data from two normal distributions, with equal number of points in each cluster:

$$x \sim \mathcal{N}(\mu_i, \sigma_i^2) \quad \text{with } \mu_1 = 0, \sigma_1 = 1 \text{ and } \mu_2 = 5, \sigma_2 = 2. \quad (46)$$

The optimal accuracy obtained from Bayes classification error is ≈ 0.956 , indicated by the dashed line in the plot. We see that the three methods perform closely, with a slight advantage of GMM as expected since it is the true model for the data. Energy statistics performs slightly better than k -means. In Fig 1b we consider two clusters with lognormal distributions:

$$\log x \sim \mathcal{N}(\mu_i, \sigma_i^2) \quad \text{with } \mu_1 = 0, \sigma_1 = 0.3 \text{ and } \mu_2 = -1.5, \sigma_2 = 1.5. \quad (47)$$

The optimal accuracy is ≈ 0.852 . In this case, Algorithm 1 provides a very accurate clustering while GMM and k -means basically cluster at chance. Sometimes GMM/EM was unable to estimate the parameters thus giving zero accuracy. These two simple experiments illustrate how energy statistics based clustering is nonparametric, being able to provide high quality clustering in settings where data comes from very different distributions.

VI. ITERATIVE ALGORITHMS FOR ENERGY STATISTICS CLUSTERING

In this section we introduce an iterative algorithm to find a local maximizer of (18). However, due to Proposition 3 we can also find an approximate solution by the well-known kernel k -means algorithm (see [13, 14]), which for convenience will also be restated in the present context.

Consider the optimization problem written in the form (20) as follows:

$$\max_{\{\mathcal{C}_1, \dots, \mathcal{C}_k\}} \left\{ Q = \sum_{j=1}^k \frac{Q_j}{n_j} \right\}, \quad Q_j = \sum_{x, y \in \mathcal{C}_j} K(x, y), \quad (48)$$

where Q_j represents an internal energy cost of cluster \mathcal{C}_j , and Q is the total energy cost where each individual cluster cost is weighted by the inverse of the number of its elements. For a data point x_i we denote its own energy cost with the entire cluster \mathcal{C}_ℓ by

$$Q_\ell(x_i) \equiv \sum_{y \in \mathcal{C}_\ell} K(x_i, y) = G_{i\bullet} \cdot Z_{\bullet\ell}, \quad (49)$$

where we recall that $G_{i\bullet}$ ($G_{\bullet i}$) denotes the i th row (column) of matrix G .

Kernel k -Means Algorithm

To optimize the kernel k -means objective function (25) we remove the global term and define the function

$$J^{(\ell)}(x_i) \equiv \frac{1}{n_\ell^2} Q_\ell - \frac{2}{n_\ell} Q_\ell(x_i) \quad (50)$$

which represents a cost depending on point x_i and cluster \mathcal{C}_ℓ . One thus assigns x_i to cluster \mathcal{C}_{j^\star} according to $j^\star = \arg \min_\ell J^{(\ell)}(x_i)$, for $\ell = 1, \dots, k$. This procedure is performed for every data point and repeated until convergence, i.e. until no new assignments are made. The entire procedure is in Algorithm 2. It can be shown that this algorithm converges provided G is positive semidefinite.

Algorithm 2 Kernel k -means algorithm to find an approximate solution to (18).

input number of clusters k , Gram matrix G , initial label matrix $Z = Z_0$

output label matrix Z

```

1:  $q \leftarrow (Q_1, \dots, Q_k)^\top$  have the costs of each cluster, according to (48)
2:  $n \leftarrow (n_1, \dots, n_k)^\top$  have the number of points in each cluster, obtained from  $D = Z^\top Z$ 
3: repeat
4:   for  $i = 1, \dots, n$  do
5:     let  $j$  be such that  $x_i \in \mathcal{C}_j$ 
6:      $j^* \leftarrow \arg \min_\ell J^{(\ell)}(x_i)$  according to (50), for  $\ell = 1, 2, \dots, k$ 
7:     if  $j^* \neq j$  then
8:       move  $x_i$  to  $\mathcal{C}_{j^*}$ :  $Z_{ij} \leftarrow 0$  and  $Z_{ij^*} \leftarrow 1$ 
9:       update  $n$ :  $n_j \leftarrow n_j - 1$  and  $n_{j^*} \leftarrow n_{j^*} + 1$ 
10:      update  $q$ :  $q_j \leftarrow q_j - 2Q_j(x_i)$  and  $q_{j^*} \leftarrow q_{j^*} + 2Q_{j^*}(x_i)$ 
11:    end if
12:  end for
13: until convergence

```

Notice that to compute the first term in (50) requires $\mathcal{O}(n_\ell)$ operations, and although the second term requires $\mathcal{O}(n_\ell^2)$ it only needs to be computed once outside loop through data points (step 1). Therefore, the time complexity Algorithm 2 is $\mathcal{O}(nk \max_\ell n_\ell) = \mathcal{O}(kn^2)$. For a sparse Gram matrix G having n' nonzero elements this complexity can be further reduced to $\mathcal{O}(kn')$.

Hartigan's Method for Energy Statistics Clustering

We now consider Hartigan's algorithm [16] applied to (48). This gives approximate solutions to (18). This approach was also proposed in [4]. The method is based on the change in the within energy statistic when moving a given data point to another cluster. Suppose point $x_i \in \mathcal{X}$ is currently assigned to cluster \mathcal{C}_j , yielding a total energy cost function (48) denoted by $Q^{(j)}$. Let us consider the change in the total energy by moving x_i to \mathcal{C}_ℓ .

Algorithm 3 Hartigan's method to find an approximate solution to (18).

input number of clusters k , Gram matrix G , initial label matrix $Z = Z_0$

output label matrix Z

```

1:  $q \leftarrow (Q_1, \dots, Q_k)^\top$  have the energy costs of each cluster, according to (48)
2:  $n \leftarrow (n_1, \dots, n_k)^\top$  have the number of points in each cluster, obtained from  $D = Z^\top Z$ 
3: repeat
4:   for  $i = 1, \dots, n$  do
5:     let  $j$  be such that  $x_i \in \mathcal{C}_j$ 
6:      $j^* \leftarrow \arg \max_{\ell} \Delta Q^{j \rightarrow \ell}(x_i)$ , for  $\ell = 1, 2, \dots, k$  and  $\ell \neq j$ 
7:     if  $\Delta Q^{j \rightarrow j^*}(x_i) > 0$  then
8:       move  $x_i$  to  $\mathcal{C}_{j^*}$ :  $Z_{ij} \leftarrow 0$  and  $Z_{ij^*} \leftarrow 1$ 
9:       update  $n$ :  $n_j \leftarrow n_j - 1$  and  $n_{j^*} \leftarrow n_{j^*} + 1$ 
10:      update  $q$ :  $q_j \leftarrow q_j - 2Q_j(x_i)$  and  $q_{j^*} \leftarrow q_{j^*} + 2(Q_{j^*}(x_i) + G_{ii})$ 
11:    end if
12:  end for
13: until convergence

```

Denote this new energy cost by $Q^{(\ell)}$. It is straightforward to see that

$$\begin{aligned} \Delta Q^{j \rightarrow \ell}(x_i) &\equiv Q^{(\ell)} - Q^{(j)} \\ &= \frac{1}{n_j - 1} \left[\frac{Q_j}{n_j} - 2Q_j(x_i) \right] - \frac{1}{n_\ell + 1} \left[\frac{Q_\ell}{n_\ell} - 2(Q_\ell(x_i) + K(x_i, x_i)) \right]. \end{aligned} \quad (51)$$

Thus, if $\Delta Q^{j \rightarrow \ell}(x_i) > 0$ we get closer to a maximum of (48) by moving x_i to \mathcal{C}_ℓ , otherwise we better keep x_i in \mathcal{C}_j . Based on this the algorithm goes as follows. We start with an initial configuration for the label matrix Z , then for each point x_i we compute the cost of moving it to another cluster, $\Delta Q^{j \rightarrow \ell}(x_i)$ for $\ell = 1, \dots, k$ with $\ell \neq j$. We then choose $j^* = \arg \max_{\ell} \Delta Q^{j \rightarrow \ell}(x_i)$. If $\Delta Q^{j \rightarrow j^*}(x_i) > 0$ we move x_i to cluster \mathcal{C}_{j^*} , otherwise we keep x_i in its original cluster \mathcal{C}_j . We update Z accordingly. The process is repeated until no points are assigned to new clusters. This whole procedure is described in Algorithm 3. Note that this ensures that the objective function is monotonically increasing at each iteration, and consequently the algorithm converges in a finite number of steps.

Computing G requires $\mathcal{O}(Dn^2)$ operations, where D is the dimension of each data point and n is the data size. However, both Algorithms 2 and 3 assume that G is given. There are more efficient methods to compute G , specially if it is sparse, but we will not consider this further and just assume that G is given. The computation of each cluster cost Q_j has complexity $\mathcal{O}(n_j^2)$, and overall to compute q we have $\mathcal{O}(n_1^2 + \dots + n_k^2) = \mathcal{O}(k \max_j n_j^2)$. These operations only need to be performed a single time. For each point x_i we need to compute $Q_j(x_i)$ once, which is $\mathcal{O}(n_j)$, and we need to compute $Q_\ell(x_i)$ for each $\ell \neq j$. The cost of computing (49) is $\mathcal{O}(n_j)$, thus the cost of step 8 in Algorithm 3 is $\mathcal{O}(k \max_j n_j)$ for $j = 1, \dots, k$. For the entire dataset this gives a time complexity of $\mathcal{O}(nk \max_j n_j) = \mathcal{O}(kn^2)$. This is the same cost as in kernel k -means, Algorithm 2. Again, if G is sparse this can be reduced to $\mathcal{O}(kn')$ where n' is the number of nonzero entries of G .

Some important properties of Hartigan's method are worth mentioning.

Theorem 5 (Telgarsky-Vattani [17]). *Hartigan's method has the cost function strictly decreasing in each iteration. Moreover, if $n > k$ then*

1. *the resulting partition has no empty clusters, and*
2. *the resulting partition has distinct means.*

Both condition above are not satisfied by Lloyd's method, and consequently by (kernel) k -means algorithm.

Theorem 6 (Telgarsky-Vattani [17]). *The set of local optima of Hartigan's method is a (possibly strict) subset of local optima of Lloyd's method.*

This means that Algorithm 2 cannot improve on a local optima of Algorithm 3. On the other hand, Algorithm 3 might improve on a local optima of Algorithm 2. Lloyd's method forms Voronoi partitions, while Hartigan's method groups data in regions formed by the intersection of spheres called circlonoi cells. It can be shown that the circlonoi cells are contained within a smaller volume of a Voronoi cell, and this excess volume grows exponentially with the dimension of \mathcal{X} [17, Theorems 2.4 and 3.1]. Points in this excess volume force Hartigan's method to iterate, contrary to Lloyd's method. Therefore, Hartigan's method can potentially escape local optima of Lloyd's method. Moreover, this improvement should be more prominent as dimension increases. Also, the improvement

grows as k increases. The empirical results of [17] show that an implementation of Hartigan’s method has comparable execution time as an implementation of Lloyd’s method, but no explicit complexity was provided. In our case, we showed that both Algorithms 2 and 3 have the same time complexity.

In [18] Hartigan’s method was applied to k -means problem with any Bregman divergence. They showed that the number of Hartigan’s local minima is upper bounded by $O(1/k)$ [18, Proposition 5.1]. In addition, they provide examples where *any* initial partition correspond to a local optima of Lloyd’s method, while the number of local optima in Hartigan’s is small and correspond to true partitions of the data. Empirically, the number of Hartigan’s local optima was considerably smaller than the number of Lloyd’s local optima. These results indicate that Hartigan’s method provides several advantages over Lloyd’s method. We will see this explicitly in the following numerical results where Algorithm 3 outperforms Algorithm 2 when using the same kernel.

VII. NUMERICAL EXPERIMENTS

In the experiments below we fix the semimetric according to the traditional energy distance (1), and the point $x_0 = 0$ is chosen in the corresponding kernel (8). We thus have

$$\rho(x, y) = \|x - y\|, \quad K(x, y) = \frac{1}{2} (\|x\| + \|y\| - \|x - y\|). \quad (52)$$

We will consider other kernels as well, but (52) will be considered the standard kernel for energy statistics and will always be present in every experiment for reference.

Let us briefly mention that we compared Algorithms 3 and 1 for several univariate distributions, and both perform almost indistinguishable regarding the clustering quality. We omit these results since we will analyse more interesting scenarios.

The main goal of the experiments shown in this section is to compare Algorithm 3, based on Hartigan’s method, to kernel k -means as described in Algorithm 2, based on Lloyd’s method. From the discussion in the previous section we expect Algorithm 3 to be superior than Algorithm 2. Another goal is to illustrate the nonparametric aspect of energy statistics. To this end we also compare Algorithm 3 to standard k -means and GMM/EM since these are the most used clustering algorithms in practice. Moreover, for every algorithm, we always

choose the initialization procedure from k -means++² [27]. Our measure of clustering quality will be the accuracy (45) based on the ground truth. Furthermore, in every experiment we sample data many times and show the average value of the accuracy, with error bars indicating standard error. Whenever possible, for reference, we also show the best possible accuracy obtained from a numerical estimation of Bayes classification error, which uses the true probability distribution of the data.

From the results of [17], the improvement of Hartigan’s method over Lloyd’s method should be more prominent in high dimensions. To analyse this we show how the algorithms degrade as the number of dimensions increase, while keeping the number of points in each cluster fixed. Consider two clusters with multivariate normal distributions given by

$$x \in \mathcal{C}_i \sim \mathcal{N}(\mu_i, \Sigma_i) \quad (i = 1, 2),$$

$$\mu_1 = \underbrace{(0, \dots, 0)}_{\times D}^\top, \quad \mu_2 = 0.7 \times \underbrace{(1, \dots, 1)}_{\times 10} \underbrace{(0, \dots, 0)}_{\times (D-10)}^\top, \quad \Sigma_1 = \Sigma_2 = I_D. \quad (53)$$

Note that the Bayes error is also kept fixed as D increases, given an optimal classification accuracy of ≈ 0.86 . We keep signal only the first 10 dimensions of μ_2 and increase D . For each D we sample 100 times, picking 100 points for each cluster. We apply each algorithm to the resulting data set and compute the average value of the accuracy (45). For both Algorithms 3 and 2 we use the standard kernel (52) from energy statistics. The results are shown in Fig. 2a, where error bars indicate the standard error. Notice that GMM/EM algorithm is unable to estimate the covariance matrix when the number of dimensions exceeds the number of points in each cluster. We see that Algorithm 3 performs better than all the other ones, and in particular it works better than kernel k -means as the number of dimensions increase. Note also that although GMM and k -means are parametric, they are consistent models for the above distributions. Now we consider the same experiment but with different covariances:

$$x \in \mathcal{C}_i \sim \mathcal{N}(\mu_i, \Sigma_i) \quad (i = 1, 2),$$

$$\mu_1 = \underbrace{(0, \dots, 0)}_{\times D}^\top, \quad \mu_2 = \underbrace{(1, \dots, 1)}_{\times 10} \underbrace{(0, \dots, 0)}_{\times (D-10)}^\top, \quad \Sigma_1 = I_D, \quad \Sigma_2 = \begin{pmatrix} \tilde{\Sigma} & 0 \\ 0 & I_{D-5} \end{pmatrix} \quad (54)$$

where $\tilde{\Sigma}_{jj} = j$ for $j = 1, \dots, 5$. The best possible accuracy from Bayes classification error is ≈ 0.95 . The results are shown In Figure 2b. In the experiments of Figure 2 we can see a

² Notice that we just use the initialization procedure and not the full k -means++ algorithm.

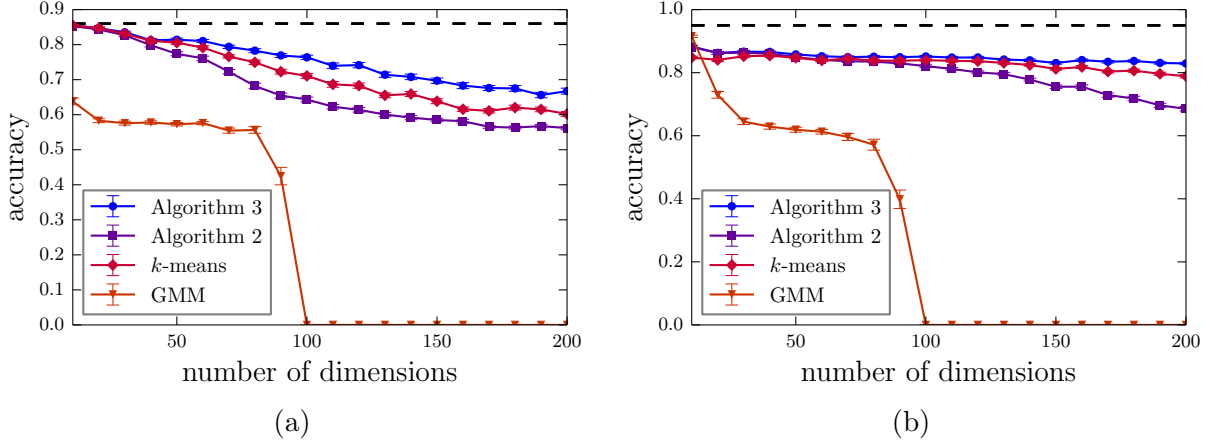


FIG. 2. Comparison of Algorithm 3, Algorithm 2, standard k -means and GMM/EM as the number of dimensions increase. We sample 100 times and show the average of (45) with error bars being standard error. We have two clusters with 100 points each. (a) Data distributed as in (53). The optimal accuracy from Bayes error is indicated by the dashed line which is ≈ 0.86 . (b) Data from (54). The optimal accuracy is ≈ 0.95 .

better performance of Algorithm 3 compared to the other ones, and in particular to kernel k -means, where we recall that both find approximate solutions to the same optimization problem (18). Notice that Algorithm 3 is more robust as the number of dimensions increase.

In Figure 3 we consider the effect of having unbalanced clusters. We generate data as

$$x \in \mathcal{C}_i \sim \frac{n_i}{N} \mathcal{N}(\mu_i, \Sigma_i) \quad (i = 1, 2), \quad \mu_1 = (0, 0, 0, 0)^\top, \quad \mu_2 = 1.5 \times (1, 1, 0, 0)^\top, \quad (55)$$

$$\Sigma_1 = I_4, \quad \Sigma_2 = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad n_1 = N - m, \quad n_2 = N + m, \quad N = 200.$$

We increase m , that is we make the clusters progressively more unbalanced, and plot the mean of (45) with standard errors, where we sample 100 times for each m . As expected, GMM works better than the other algorithms since it is a fuzzy clustering. We can see that the other methods based on hard assignments degrade similarly, and more rapidly than GMM. This indicates that a fuzzy version of Algorithm 3 should compensate for this effect.

Besides the standard kernel from energy statistics (52), associated to (1), let us consider two other semimetrics with their respective generating kernels,

$$\rho_{1/2}(x, y) = \|x - y\|^{1/2} \quad K_{1/2}(x, y) = \frac{1}{2} (\|x\|^{1/2} + \|y\|^{1/2} - \|x - y\|^{1/2}), \quad (56)$$

$$\rho_e(x, y) = 2 - 2e^{-\frac{1}{2}\|x-y\|} \quad K_e(x, y) = e^{-\frac{1}{2}\|x-y\|}. \quad (57)$$

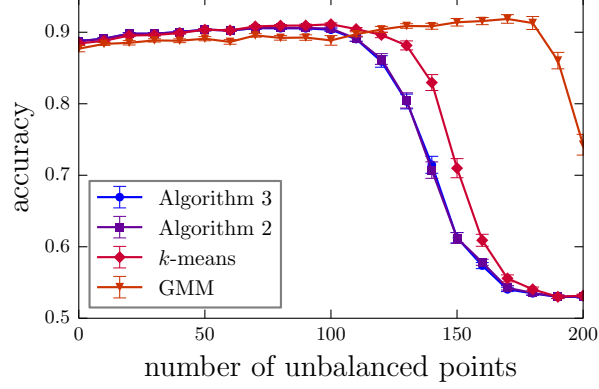


FIG. 3. Comparison of Algorithm 3, Algorithm 2, standard k -means and GMM/EM for data distributed as in (55), where we make the two clusters progressively more unbalanced.

The kernel (56) corresponds to the energy distance (2) with $\alpha = 1/2$. Now consider data normally distributed in $D = 20$ as follows:

$$x \in \mathcal{C}_i \sim \mathcal{N}(\mu_i, \Sigma_i) \quad (i = 1, 2),$$

$$\mu_1 = \underbrace{(0, \dots, 0)}_{\times 20}^\top, \quad \mu_2 = \frac{1}{2} \underbrace{(1, \dots, 1)}_5 \underbrace{(0, \dots, 0)}_{15}^\top, \quad \Sigma_1 = \frac{1}{2} I_{20}, \quad \Sigma_2 = I_{20}. \quad (58)$$

We sample an equal number of points for each cluster, which is increased. The optimal accuracy of (58) based on Bayes classification error is ≈ 0.90 . We repeat the same experiment as before but now using also the kernels (56) and (57). The results are shown in Figure 4a. Algorithm 3 performs better than all the other ones, and in particular the kernel (57) provides better results. As the number of points get large enough, GMM starts to approach optimal Bayes accuracy, as it should since it is consistent model to the distribution of the data. However, Algorithm 3 with kernel (57) achieves optimal accuracy with a much smaller number of points. Moreover, Algorithm 3 performs better than Algorithm 2 for any of the kernel choices. Standard k -means performs poorly on this example.

Consider the same parameters as in (58) but now with lognormal distribution, i.e.

$$\log x \in \mathcal{C}_i \sim \mathcal{N}(\mu_i, \Sigma_i) \quad (i = 1, 2). \quad (59)$$

The same previous experiment is now shown in Fig. 4b. We see that Algorithm 3 still performs accurately, while k -means works a little bit better than chance, and GMM is not even able to estimate the parameters. Again, the kernel (57) provides better results than

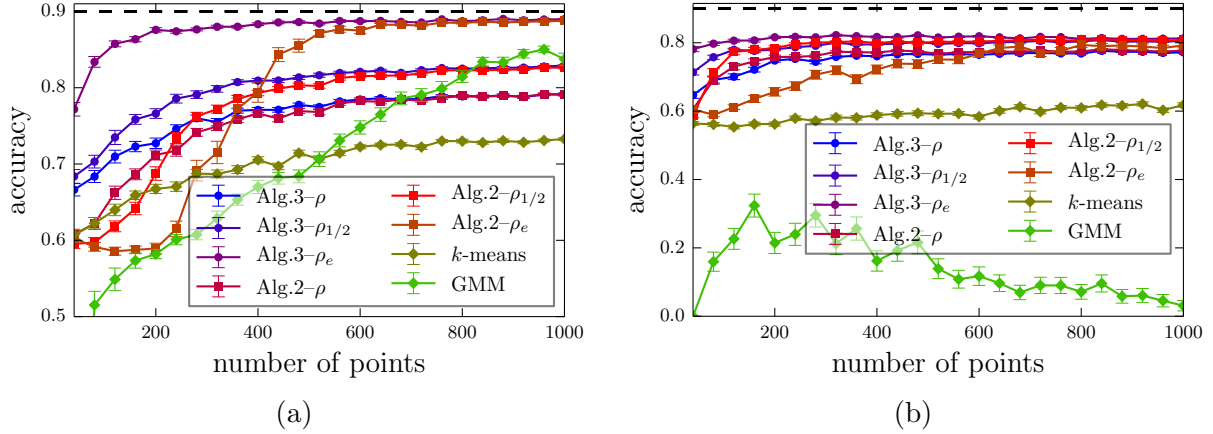


FIG. 4. Comparison of Algorithms 3 and 2 with kernels (52), (56) and (57), and also with k -means and GMM/EM. The optimal accuracy in both cases is ≈ 0.9 . We show average of (45) over 100 samples with standard error. (a) Data distributed as in (58). (b) Data distributed as in (59). These experiments illustrates how energy statistics based clustering is nonparametric.

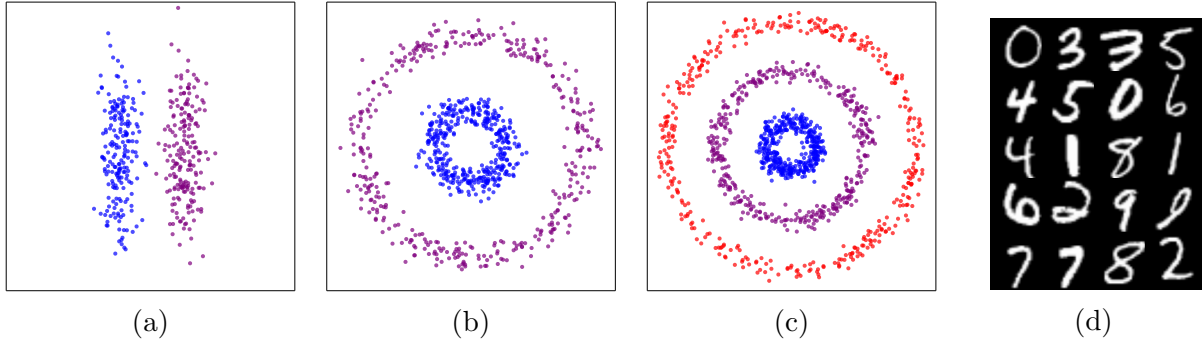


FIG. 5. (a) Parallel cigars, 200 points in each class. (b) Two concentric circles with noise, 400 points each. (c) Three concentric circles, 400 points each. Clustering for (a-c) is shown in Table I. (d) MNIST handwritten digits. Clustering on Table II.

(52) or (56). Algorithm 3 performs better than Algorithm 2 for every kernel choice. The experiments in Fig. 4 illustrates that energy statistics clustering is nonparametric.

Now we consider two dimensional data as illustrated in Fig 5(a-c) with the following choices of semimetric and corresponding generating kernel:

$$\rho_\alpha(x, y) = \|x - y\|^\alpha \quad K_\alpha(x, y) = \frac{1}{2} (\|x\|^\alpha + \|y\|^\alpha - \|x - y\|^\alpha), \quad (60)$$

$$\tilde{\rho}_\sigma(x, y) = 2 - 2e^{-\frac{\|x-y\|}{2\sigma}} \quad \tilde{K}_\sigma(x, y) = e^{-\frac{\|x-y\|}{2\sigma}}, \quad (61)$$

$$\hat{\rho}_\sigma(x, y) = 2 - 2e^{-\frac{\|x-y\|^2}{2\sigma^2}} \quad \hat{K}_\sigma(x, y) = e^{-\frac{\|x-y\|^2}{2\sigma^2}}. \quad (62)$$

		<i>Fig. 5a</i>		<i>Fig. 5b</i>		<i>Fig. 5c</i>
<i>Algorithm 3</i>	ρ_1	0.766 ± 0.066	ρ_1	0.522 ± 0.006	ρ_1	0.437 ± 0.030
	$\rho_{1/2}$	0.859 ± 0.062	$\rho_{1/2}$	0.524 ± 0.007	$\rho_{1/2}$	0.547 ± 0.026
	$\tilde{\rho}_2$	0.971 ± 0.015	$\tilde{\rho}_1$	0.9999 ± 0.0001	$\tilde{\rho}_2$	0.677 ± 0.003
	$\hat{\rho}_2$	0.998 ± 0.001	$\hat{\rho}_1$	0.597 ± 0.052	$\hat{\rho}_2$	0.645 ± 0.012
<i>Algorithm 2</i>	ρ_1	0.758 ± 0.069	ρ_1	0.516 ± 0.002	ρ_1	0.452 ± 0.030
	$\rho_{1/2}$	0.901 ± 0.060	$\rho_{1/2}$	0.524 ± 0.007	$\rho_{1/2}$	0.570 ± 0.016
	$\tilde{\rho}_2$	0.971 ± 0.015	$\tilde{\rho}_1$	0.9999 ± 0.0001	$\tilde{\rho}_2$	0.673 ± 0.002
	$\hat{\rho}_2$	0.998 ± 0.001	$\hat{\rho}_1$	0.528 ± 0.008	$\hat{\rho}_2$	0.640 ± 0.013
<i>k-means</i>		0.599 ± 0.046		0.521 ± 0.005		0.360 ± 0.004
<i>GMM</i>		0.9995 ± 0.0003		0.598 ± 0.018		0.479 ± 0.021

TABLE I. Clustering the data shown in Fig. 5 with Algorithms 3 and 2, besides k -means and GMM, for the kernels (60), (61) and (62). We sample the data 10 times and show the average accuracy (45) with standard error.

We apply both Algorithms 3 and 2, besides k -means and GMM, using the above kernels. The results are shown in Table I where the respective choice of parameters for the kernels are indicated. In the data shown in Fig. 5a the standard semimetrics from energy statistics, ρ_1 and $\rho_{1/2}$, are able to provide more accurate results compared to k -means. However, the gaussian kernel $\tilde{\rho}_2$ gives results very accurate results, similar to GMM, which is the true model of the data. In Fig. 5b we see that the choice of kernel is very sensitive, and only (61) was able to cluster accurately. The same kernel choice to the case of Fig. 5 still provides better results than the other choices, but the results are less accurate.

Next we consider the well-known MNIST handwritten digit dataset as illustrated in Fig. 5d. Each data point is an 8-bit gray scale image corresponding to one of the digits $\{0, 1, \dots, 9\}$. Each image forms a 784-dimensional vector. We consider subsets of these classes, where we sample 100 points for each class, and cluster the data using Algorithms 3 and 2. Besides the kernel (60), we consider the gaussian kernel (62) with the width computed from the data as

$$\sigma^2 = \frac{1}{n^2} \sum_{i,j=1}^n \|x_i - x_j\|^2 \quad (63)$$

where $\{x_i\}_{i=1}^n$ is the sampled dataset. The results are shown in Table II. Algorithm 3

		$\{0, 1, 2\}$	$\{0, 1, \dots, 4\}$	$\{0, 1, \dots, 6\}$	$\{0, 1, \dots, 8\}$
<i>Algorithm 3</i>	ρ_1	0.907 ± 0.007	0.866 ± 0.006	0.715 ± 0.013	0.616 ± 0.019
	$\rho_{1/2}$	0.918 ± 0.006	0.849 ± 0.025	0.711 ± 0.010	0.642 ± 0.009
	$\tilde{\rho}_\sigma$	0.900 ± 0.007	0.871 ± 0.005	0.719 ± 0.010	0.630 ± 0.016
<i>Algorithm 2</i>	ρ_1	0.914 ± 0.006	0.845 ± 0.023	0.664 ± 0.022	0.614 ± 0.014
	$\rho_{1/2}$	0.895 ± 0.011	0.822 ± 0.026	0.669 ± 0.021	0.591 ± 0.019
	$\tilde{\rho}_\sigma$	0.896 ± 0.007	0.869 ± 0.006	0.705 ± 0.016	0.646 ± 0.020
<i>k-means</i>		0.871 ± 0.015	0.840 ± 0.022	0.707 ± 0.012	0.634 ± 0.011

TABLE II. Clustering the data shown in Fig. 5d with Algorithms 3 and 2, and k -means. We use the kernel (60) with $\alpha \in \{1, 2\}$, and the gaussian kernel (62) with σ given by (63). For each subset of digits we sample 10 times and show the average accuracy (45) with standard error. We pick 100 points for each class.

performed slightly better than k -means, except for the last column where all the methods are comparable. Unsupervised clustering on MNIST dataset without any feature extraction or dimensionality reduction is not an easy task. For instance, the same experiment was performed in [28] where a low-rank transformation is learned then subsequently used in subspace clustering, providing very accurate results. One could explore analogous methods for learning a better representation of the data and subsequently apply Algorithm 3 for clustering.

VIII. CONCLUSION

We considered clustering from the perspective of energy statistics theory which provides a nonparametric test for equality of distributions. We showed that the clustering problem reduces to a quadratically constrained optimization problem (QCQP), as described in Proposition 2. Moreover, this problem is equivalent to kernel k -means optimization problem, once the kernel is fixed; see Proposition 3. Our results imply that kernel k -means is actually a consequence of energy statistics, and thus place this method into a principled statistical basis. We also considered a weighted version of energy statistics clustering which establishes connection with spectral clustering and graph partitioning problems.

We considered Algorithm 3 based on Hartigan’s method, and compared with kernel k -means described in Algorithm 2 which is based on Lloyd’s heuristic. Both have the same time complexity, however, the numerical results provide evidence that Algorithm 3 is more robust with a superior clustering performance. This is also theoretically supported as described in the end of Section VI.

In the same way that kernel k -means can be accelerated by exploring sparsity or sampling methods to approximate the Gram matrix, these techniques are also applicable to Algorithm 3. For instance, it would be interesting to explore the methods recently proposed in [29] to this case. Another fruitful avenue of exploration would be to find better methods to tackle the optimization problem (18).

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