Nonparametric Clustering from Energy Statistics

Guilherme França[*] and Joshua T. Vogelstein[†]

Johns Hopkins University

Abstract

Energy statistics provides a nonparametric test for equality of distributions. It was proposed by Székely in the 80's inspired by the Newtonian gravitational potential from classical mechanics. The idea is to associate a statistical potential energy to observations, such that minimum energy is achieved under the null hypothesis of equality of distributions. Energy statistics was further generalized to probability distributions on arbitrary metric spaces, and more recently, a connection with kernels in RKHS was established. Nevertheless, although extensively used by the statistics community, energy statistics has not been previously incorporated in machine learning problems. In this paper, we consider the problem of clustering data from an energy statistics theory perspective. We provide a precise mathematical formulation, yielding a quadratically constrained quadratic optimization problem (QCQP). We show that this is equivalent to kernel k-means optimization problem, however, energy statistics is able to fix the kernel choice. This clustering method is nonparametric, and if prior information is available it can be easily incorporated in the kernel construction. We propose an iterative algorithm to find local optimizers of this QCQP problem, based on the change in the statistical energy of moving points to different clusters. This algorithm is different but has the same computational cost as kernel k-means algorithm. We then compare this algorithm with well-known kernel k-means, standard k-means, and GMM algorithms by providing carefully designed numerical experiments. The results show that, in general, this method outperforms these most used clustering algorithms.

[*] guifranca@gmail.com

[†] jovo@jhu.edu

I. INTRODUCTION

Energy statistics is based on the energy distance between probability distributions, which provides a notion of statistical potential energy to statistical observations, in close analogy to Newton's gravitational potential energy in classical mechanics. We refer the reader to [1], and references therein, for an overview. It has been applied to several goodness-of-fit hypothesis tests, multi-sample tests of equality of distributions, analysis of variance [2], and (nonlinear) dependence tests through distance covariance and distance correlation, which generalizes the Pearson correlation coefficient. Moreover, energy statistics was applied to hierarchical clustering [3] by extending Ward's method of minimum variance.

More recently, the distance covariance was generalized from Euclidean spaces to metric spaces of strong negative type [4]. 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 provided [5]. This important work establishes the link between techniques commonly used in the statistics literature, regarding energy statistics, and techniques commonly used in machine learning.

Given a dataset $\mathbb{X} = \{x_1, x_2, \dots, x_n\}$, where each datapoint lives in a generic space $x_i \in \mathcal{X}$, the k-clustering problem consists in grouping these points into k groups $\{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_k\}$, such that points belonging to the same group are more "similar" to each other than to points in other groups. This intuitive notion already assumes a "metric" able to measure the similarity between datapoints. Clustering is an unsupervised method, and one of the most important problems in machine learning since it provides the first step towards automatically constructing labels for previously unseen data. The most used algorithms are by far k-means and gaussian mixture models (GMM) through expectation maximization (EM) algorithm. Both are parametric, making strong assumptions about the distribution of the data (normality), and the space where data lie is Euclidean, $\mathcal{X} = \mathbb{R}^D$, hence the similarity is based on Euclidean metric, $\|x_i - x_j\|^2 = (x_i - x_j)^\top (x_i - x_j) = \sum_{\ell=1}^{D} (x_{i,\ell} - x_{j,\ell})^2$. These algorithms provide a good clustering when data is linearly separable in Euclidean space.

To account for nonlinearly separable data, which may possibly live in an arbitrary non-Euclidean space, kernel methods are usually employed. If a Mercer kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is available [6], which is a symmetric and positive definite function, it guarantees that there exists a map $\varphi : \mathcal{X} \to \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space. Thus, one can compute similarities through the inner product and perform clustering in the feature space $\mathcal{H}$. The nice thing about this is that the map φ is only used implicitly, i.e. one does not need to know φ, since the inner product can be computed only based on the kernel $K(\cdot, \cdot)$, a convenient technique known as kernel trick. The well-known kernel k-means problem is exactly k-means in the feature space [7, 8] (see also [9] for a survey of clustering methods). It exploits the nonlinear structure provided by a kernel function to perform clustering in datasets that are not linearly separable in their original space $\mathcal{X}$. As it stands, kernel k-means is an heuristic approach in the sense that it is not derived from a statistical theory. Moreover, the choice of kernel is crucial, and there is no systematic theory for this. One must rely on ad hoc methods.

In this paper, we consider how to perform clustering based on energy statistics theory. The original goal is to provide a nonparametric clustering method, since energy distance is nonparametric. The basis of our work is the theory developed in [5]. Based on this and on the multi-sample test for equality of distributions from energy statistics, we show that there is only one function that provides the clustering optimization problem. We then show that this clustering optimization problem reduces to a quadratically constrained quadratic problem (QCQP). This optimization problem has the same form as kernel k-means, spectral clustering, and some well-known graph partitioning problems [10]. This lead us to show that energy statistics based clustering is actually equivalent to kernel k-means optimization problem. However, energy statistics fixes a kernel to begin with. Furthermore, these results can be seen as a first-principle derivation of kernel k-means from energy statistics, which thus bring these kernel based clustering methods into a unifying mathematical theory. We also provide an iterative algorithm, different but with the same complexity as kernel k-means algorithm. The numerical results indicate that this method is more accurate and robust.

Our work is organized as follows. In section II we review the necessary background on energy statistics and RKHS. Section III contains the main results of this paper where we consider a clustering theory based on energy statistics, leading to a QCQP which is NP-hard. In section IV we consider a simple example in one dimension, where we propose an algorithm which requires no initialization. In section V we briefly review kernel k-means algorithm, and propose a new iterative algorithm to solve this QCQP. Section VI contains some carefully designed numerical experiments indicating that this algorithm outperforms kernel k-means, standard k-means, and GMM algorithms. Our conclusions are in section VII.

II. BACKGROUND ON ENERGY STATISTICS AND RKHS

In this section we briefly review the main concepts from energy statistics and its relation to reproducing kernel Hilbert spaces (RKHS) which form the basis of our work. For more details we refer the reader to [1] (and references therein) and also [5].

Consider random variables in $\mathbb{R}^D$ such that $X, X' \overset{iid}{\sim} P$ and $Y, Y' \overset{iid}{\sim} Q$, where P and Q are cumulative distribution functions with finite first moments. The quantity [1]

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

called *energy distance*, is rotational invariant and nonnegative, $\mathcal{E}(P,Q) \ge 0$, 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,

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

where $0 < \alpha \le 2$. This quantity is also nonnegative, $\mathcal{E}_\alpha(P,Q) \ge 0$. 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 $\mathcal{E}_2(P,Q) = 2\|\mathbb{E}(X) - \mathbb{E}(Y)\|^2$, showing 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 a space endowed with a *semimetric of negative type* $\rho : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, which is required to satisfy

$$\sum_{i,j=1}^{n} \alpha_i \alpha_j \rho(X_i, X_j) \le 0, \tag{3}$$

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

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

For spaces of negative type, there exists a Hilbert space $\mathcal{H}$ and a map $\varphi : \mathcal{X} \to \mathcal{H}$ such that $\rho(X,Y) = \|\varphi(X) - \varphi(Y)\|^2_{\mathcal{H}}$, which 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 [5]. We first recall the definition of RKHS. Let $\mathcal{H}$ be a Hilbert space of real-valued functions over $\mathcal{X}$. A function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ 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 since this inner product is real, $\langle h_x, h_y \rangle^* = \langle h_y, h_x \rangle = \langle h_x, h_y \rangle$, we immediately have that the kernel is symmetric, $K(y, x) = K(y, x)$. 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 $\langle w, w \rangle_{\mathcal{H}} = \sum_{i,j=1}^n c_i c_j K(x_i, x_j) \ge 0$, 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 semi-definite: $\boldsymbol{v}^\top G\, \boldsymbol{v} \ge 0$ for any vector $\boldsymbol{v} \in \mathbb{R}^n$.

The Moore-Aronszajn theorem [11] establishes the converse of the above paragraph. For every symmetric and positive definite function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, 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: $P \mapsto h_P \in \mathcal{H}_K$ 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 $\mathcal{H}_K$. This is called the maximum mean discrepancy (MMD) and is given by

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

which can also be written as [12]

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

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

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

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

The following important result shows that semimetrics of negative type and symmetric positive semidefinite kernels are closely related [13]. Let $\rho : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, and $x_0 \in \mathcal{X}$ an arbitrary but fixed point. Define

$$K(x, y) = \tfrac{1}{2} \left[\rho(x, x_0) + \rho(y, x_0) - \rho(x, y) \right]. \tag{8}$$

Thus, it can be shown that K is positive definite if and only if ρ is a semimetric of negative type (3). Here 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

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

and the canonical feature map $\varphi : x \mapsto h_x$ is injective [5]. 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 [5]. If ρ is a semimetric of negative type and K a kernel that generates ρ, then replacing (9) into (4), and using (6), yields

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

Since $\gamma_k^2(P, Q) = \| h_P - h_Q \|^2_{\mathcal{H}_K}$ we can compute the energy distance using the inner product of $\mathcal{H}_K$. Moreover, this can be computed from the data according to (7).

Finally, let us recall the main formulas for test statistics 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 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

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

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

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

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

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

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, $n \to \infty$, under the null hypothesis $H_0 : P_1 = P_2 = \cdots = P_k$ we have that $S \to 0$, and under the alternative hypothesis $H_1 : P_i \neq P_j$ for at least two $i \neq j$, we have that $S \to \infty$. 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 every data point $x \in \mathcal{C}_j$ form a massive body, whose total mass is characterized by the distribution function P_j. Then S is a potential energy of the from $S(P_1, \ldots, P_k)$ which measures how different are these mass distributions, and achieves the ground state $S = 0$ when all bodies have the same mass distribution. The potential energy S increases as each body has different mass distribution than the other ones.

III. CLUSTERING BASED ON ENERGY STATISTICS

This section contains the main 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 The following straightforward result shows that maximizing (13) is equivalent to minimizing (12), which has a more convenient form.

Proposition 1. *Let $\mathbb{X} = \{x_1, \ldots, x_n\}$ where each data point x_i lives in a space $\mathcal{X}$ endowed with a semimetric $\rho : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ of negative type* (3)*. For a fixed integer k, the partition*

$\mathbb{X} = \bigcup_{j=1}^{k} \mathcal{C}_j$, *where* $\mathcal{C}_i \cap C_j = \emptyset$ *for all* $i \neq j$, *maximizes* (13) *if and only if*

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

where W *is given by* (12).

Proof. From (12) and (13), and recall that $n = \sum_{i=1}^{k} n_i$, we have

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

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. □

Thus, 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 assignment clustering problem.

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

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

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 $D = \operatorname{diag}(n_1,\dots,n_k)$ contains the number of points in each cluster. We also introduce the rescaled matrix $Y \equiv Z D^{-1/2}$. In component form they are given by

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

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

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

$$\max_{Y} \operatorname{Tr}\left(Y^{\top} G\, Y\right) \qquad s.t.\ Y \geq 0,\ Y^{\top} Y = I,\ Y Y^{\top} \boldsymbol{e} = \boldsymbol{e}, \tag{18}$$

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

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

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

Note that the first term does not contribute to the optimization problem, since it is a global term that does not depend which partition is chosen. Therefore, minimizing (19) is equivalent to

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

But

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

where we used the definitions (16) and (17). Thus the objective function in (20) is equal to $\operatorname{Tr}\left(D^{-1} Z^{\top} G Z\right)$. 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 programing problem:

$$\max_{Z} \operatorname{Tr}\Big(\big(Z D^{-1/2}\big)^{\top} G \big(Z D^{-1/2}\big) \Big) \quad \text{s.t. } Z_{ij} \in \{0,1\},\ \textstyle\sum_{j=1}^{k} Z_{ij} = 1,\ \sum_{i=1}^{n} Z_{ij} = n_j. \tag{22}$$

Now we write this in terms of the matrix $Y = Z D^{-1/2}$. The objective function immediately becomes $\operatorname{Tr}\left(Y^{\top} G\, Y\right)$. Notice that the above constraints imply that $Z^{T} Z = D$, where $D = \operatorname{diag}(n_1, \ldots, n_k)$, which in turn gives $D^{-1/2} Y^{T} Y D^{-1/2} = D$, or $Y^{\top} Y = I$. 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 $Z^{T} \boldsymbol{e} = D \boldsymbol{e}$. Replacing $Z = Y D^{1/2}$ we have $Y^{\top} \boldsymbol{e} = D^{1/2} \boldsymbol{e}$. Multiplying this last equation on the left by Y, and noticing that $Y D^{1/2} \boldsymbol{e} = Z \boldsymbol{e} = \boldsymbol{e}$, we finally obtain $Y Y^{\top} \boldsymbol{e} = \boldsymbol{e}$. Thus, the optimization problem (22) is equivalent to (18) . □

Based on Proposition 2, to group data $\{x_1, \ldots, x_n\}$ 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 ith row of Y will contain a single nonzero element in some jth 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 the problem. For instance, the relaxed problem

$$\max_{Y} \operatorname{Tr}\left(Y^\top G\, Y\right) \quad \text{s.t. } Y^\top Y = I \tag{23}$$

has a well-known closed form solution given by $Y^\star = UR$, where the columns of U contain the leading k eigenvectors of G corresponding to the k largest eigenvalues $\{\lambda_1, \dots, \lambda_k\}$, and $R \in \mathbb{R}^{k\times k}$ is an arbitrary orthogonal matrix. The resulting optimal objective function is thus given by $\max \operatorname{Tr}\left(Y^{\star\top} G\, Y^\star\right) = \sum_{i=1}^k \lambda_i$. One might then normalize and threshold the rows of $Y^\star$, or even better, following [14] we can normalize the rows of Y and apply standard k-means on this matrix where each row is considered as a datapoint. This same procedure usually done in spectral clustering on the (normalized) Laplacian of the graph defined by a similarity matrix. However, computing eigenvectors of a very large matrix can be problematic, and usually iterative methods are preferred.

It is important to note that the previous theory for clustering based on energy statistics hold for data living in an *arbitrary space of negative type*. 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. Moreover, this approach *does not require* the concept of the *cluster mean* which can be ill-defined for some types of data, such as images for instance, and thus it should also be robust to outliers. This method is quite general and makes very few assumptions about the data. If one uses the traditional energy distance (1), then $\rho(x, y) = \|x - y\|$ and this fixes the kernel choice through (8). In practice, however, the clustering quality strongly depend on the choice of a suitable ρ which is what measures the similarity between different data points, and is equivalent to choosing an appropriate kernel. Nevertheless, if prior knowledge is available for choosing ρ, or equivalently K, this can easily be taken into account.

One may wonder how energy statistics clustering relates to the well-known kernel k-means problem. We now address this question. For a positive semidefinite G, there exists a map $\varphi : \mathcal{X} \to \mathcal{H}_K$ such that $K(x, y) = \varphi(x)^\top \varphi(y)$. The kernel k-means optimization problem, in feature space, is defined by

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

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. It is known [10] 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, once the kernel is fixed.

Proposition 3. *The clustering problem* (14) *based on energy statistics is equivalent to the kernel k-means 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

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

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 second term. Thus the kernel k-means optimization problem is

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

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). □

It was shown [10] that 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). Actually, in general, this corresponds to a weighted version of (18) which reads $\operatorname{Tr}\left(Y^\top W^{1/2} G\, W^{1/2} Y\right)$, where $W = \operatorname{diag}(w(x_1),\dots,w(x_n))$ and $w(\cdot)$ is a weight attributed to each data point. Our previous results show that energy statistics based clustering is also equivalent to these problems. The advantage of energy statistics compared to kernel k-means is that the semimetric ρ is supposed to be fixed. Moreover, from a theoretical perspective, it brings the clustering problem into a formal statistical theory based on distances between probability distributions and embeddings in RKHS. There was no a priori reason to expect that clustering based on energy statistics would be equivalent to the kernel k-means problem (24).

IV. 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 also be useful later for comparison with the more general iterative algorithm.

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

$$\begin{aligned} |x - y| &= (x - y)\mathbb{1}_{x \geq y} - (x - y)\mathbb{1}_{x<y} \\ &= x\left(\mathbb{1}_{x\geq y} - \mathbb{1}_{x<y}\right) + y\left(\mathbb{1}_{y>x} - \mathbb{1}_{y\leq x}\right), \end{aligned} \tag{27}$$

where we have the indicator function defined as $\mathbb{1}_A = 1$ 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

$$g\left(\mathcal{C}, \mathcal{C}\right) = \frac{1}{n^2} \sum_{x\in\mathcal{C}} \sum_{y\in\mathcal{C}} x\left(\mathbb{1}_{x\geq y} + \mathbb{1}_{y>x} - \mathbb{1}_{x\geq y} - \mathbb{1}_{x<y}\right). \tag{28}$$

The sum over y can be eliminated since the term in parenthesis is simply counting the number of elements in $\mathcal{C}$ that satisfy the conditions of the indicator functions. Assuming that we first order the data in the partition, obtaining $\bar{\mathcal{C}} = [x_j \in \mathcal{C} : x_1 \leq x_2 \leq \cdots \leq x_n]$, we can write (28) in the following simple form:

$$g\left(\bar{\mathcal{C}}, \bar{\mathcal{C}}\right) = \frac{2}{n^2} \sum_{\ell=1}^{n} (2\ell - 1 - n)x_\ell. \tag{29}$$

Note that the cost of computing this 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 $\mathbb{X} = \bigcup_{j=1}^{k} \bar{\mathcal{C}}_j$, but notice that the entire data set $\mathbb{X}$ does not need to be necessarily ordered, the within energy dispersion (12) can be written as

$$W\left(\bar{\mathcal{C}}_1, \ldots, \bar{\mathcal{C}}_k\right) = \sum_{j=1}^{k} \sum_{\ell=1}^{n_j} \frac{2\ell - 1 - n_j}{n_j} x_\ell. \tag{30}$$

For a two-class problem, we can use (30) to cluster data through a simple algorithm as follows. We first order the entire dataset $\mathbb{X} \to \bar{\mathbb{X}}$. Then we compute (30) 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 $\mathcal{O}(n \log n + n^2) = \mathcal{O}(n^2)$.

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

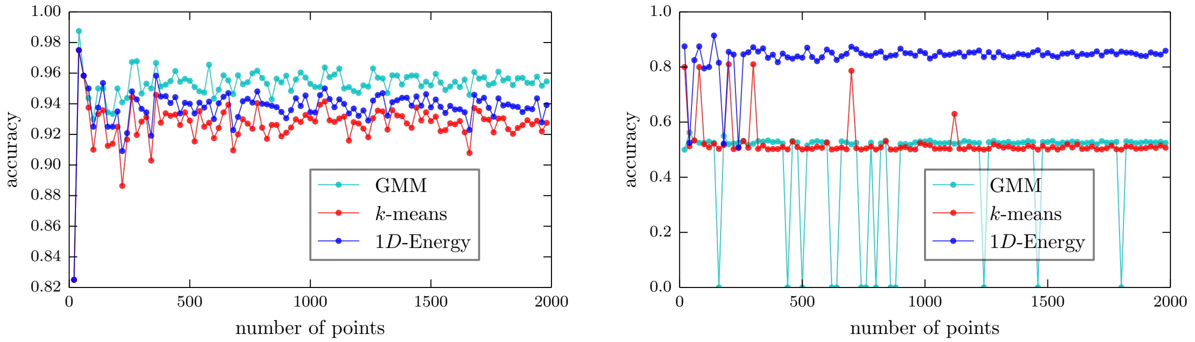
```
input  data $\mathbb{X}$
output  label matrix $Z$
sort $\mathbb{X}$ obtaining $\bar{\mathbb{X}} = [x_1, \dots, x_n]$
for $j \in [1, \dots, n]$ do
    Let $\bar{\mathcal{C}}_1^{(j)} = [x_i : i = 1, \dots, j]$ and $\bar{\mathcal{C}}_2^{(j)} = [x_i : i = j+1, \dots, n]$
    $W^{(j)} \leftarrow W\big(\bar{\mathcal{C}}_1^{(j)}, \bar{\mathcal{C}}_2^{(j)}\big)$ from (30)
end for
$j^\star \leftarrow \arg\min_j W^{(j)}$
$Z_{j\bullet} \leftarrow (1,0)$ if $j \le j^\star$, and $Z_{j\bullet} \leftarrow (0,1)$ otherwise, for $j = 1, \dots, n$
```

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

$$\text{accuracy}(\hat{Z}) = \max_{\sigma} \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} \hat{Z}_{i\sigma(j)} Z_{ij} \tag{31}$$

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.

Before proposing a more general iterative algorithm to (18), let us consider two simple experiments with equal number of points in each cluster. We keep increasing the number of points in the clusters for each experiment, and cluster the data using Algorithm 1. We also cluster the same data set with GMM, through EM algorithm, and with k-means. In both of these cases we use the initialization from k-means++ [15] and we run the algorithms few times with different initializations and choose the answer with best objective function value. We use (31) to measure the clustering quality. In Fig. 1a we have data from normal distributions, where we can see that all the three methods perform closely, with a slight advantage of GMM, as expected, since it is the right model for the data. However, as shown in Fig 1b, for lognormal distributions, Algorithm 1 provides a huge improvement compared to both GMM and k-means which basically cluster at chance. The zero accuracy values for



(a)

(b)

FIG. 1. We cluster data using Algorithm 1 ($1D$-Energy in the plots), GMM, and k-means. We use (31) to evaluate cluster quality. Both clusters have the same number of points, which are increased in each experiment. (a) $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1,\sigma_1)+\mathcal{N}(\mu_2,\sigma_2)\right)$ with $\mu_1=0$, $\mu_2=5$, $\sigma_1=1$, and $\sigma_2=2$. (b) $x \sim \frac{1}{2}\left(e^{\mathcal{N}(\mu_1,\sigma_1)}+e^{\mathcal{N}(\mu_2,\sigma_2)}\right)$ with $\mu_1=0$, $\mu_2=-1.5$, $\sigma_1=0.3$, and $\sigma_2=1.5$.

GMM happened when EM algorithm was unable to estimate the parameters. These two simple experiments illustrate how energy statistics based clustering is nonparametric, since it is able to provide high quality clustering in settings where data comes from very different distributions.

V. ITERATIVE ALGORITHM FOR ENERGY STATISTICS CLUSTERING

In this section we will introduce a new iterative algorithm to find a local maximizer of the QCQP (18), however, due to Proposition 3 we can also find an approximate solution by the well-known kernel k-means algorithm, which for convenience will also be restated in the present context. First, let us introduce some base notation.

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

$$\max_{\{\mathcal{C}_1,\dots,\mathcal{C}_k\}} \left\{ Q = \sum_{j=1}^{k} \frac{Q_j}{n_j} \right\}, \qquad Q_j = \sum_{x,y\in\mathcal{C}_j} K(x,y), \tag{32}$$

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 $\mathcal{C}_\ell$ by

$$Q_\ell(x_i) \equiv \sum_{y\in\mathcal{C}_\ell} K(x_i,y) = G_{i\bullet}\cdot Z_{\bullet\ell}, \tag{33}$$

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

A. Kernel *k*-Means Algorithm

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

$$J^{(\ell)}(x_i) \equiv -\frac{2}{n_\ell} Q_\ell(x_i) + \frac{1}{n_\ell^2} Q_\ell, \tag{34}$$

which represents a cost depending on point x_i and cluster $\mathcal{C}_\ell$. 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 complete algorithm is shown in Algorithm 2. It can be shown that this algorithm converges provided G is positive semidefinite. Although our notation looks a little different than the standard kernel k-means found in the literature [10], this is precisely the same algorithm but written in a more concise and explicit way.

Notice that to compute the first term in (34) 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 the data points loop in Algorithm 2 (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 $\mathcal{O}(kn')$.

B. Energy Cost Algorithm

Now let us consider a different algorithm, which is based on the change in the within energy statistics when moving a given data point to a different cluster. Suppose we have a data point $x_i \in \mathcal{X}$ which is currently assigned to cluster $\mathcal{C}_j$, yielding a total energy cost function (32) denoted by $Q^{(j)}$. Let us consider the change in the total energy cost by moving x_i to cluster $\mathcal{C}_\ell$. Denote the new energy cost after moving x_i to $\mathcal{C}_\ell$ by $Q^{(\ell)}$. It is straightforward to see that

$$\begin{aligned} \Delta Q^{j\to\ell}(x_i) &\equiv Q^{(\ell)} - Q^{(j)} \\ &= \frac{1}{n_j - 1}\left[\frac{Q_j}{n_j} - 2Q_j(x_i)\right] - \frac{1}{n_\ell + 1}\left[\frac{Q_\ell}{n_\ell} - 2\big(Q_\ell(x_i) + K(x_i, x_i)\big)\right]. \end{aligned} \tag{35}$$

Thus, if $\Delta Q^{j\to\ell}(x_i) > 0$ we get closer to a maximum of (32) by moving x_i to $\mathcal{C}_\ell$, otherwise we better keep x_i in $\mathcal{C}_j$. Based on this we propose an algorithm where the iterates are performed as follows. We start with an initial configuration for the label matrix Z, then for each point

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 $Z$
$\boldsymbol{q} \leftarrow (Q_1, \dots, Q_k)^\top$ have the costs of each cluster, according to (32)
$\boldsymbol{n} \leftarrow (n_1, \dots, n_k)^\top$ have the number of points in each cluster, obtained from $D = Z^\top Z$
repeat
  for $i = 1, \dots, n$ do
    let $j$ be such that $x_i \in \mathcal{C}_j$
    $j^\star \leftarrow \arg\min_\ell J^{(\ell)}(x_i)$ according to (34), for $\ell = 1, 2, \dots, k$
    if $j^\star \neq j$ then
      move $x_i$ to $\mathcal{C}_{j^\star}$: $Z_{ij} \leftarrow 0$ and $Z_{ij^\star} \leftarrow 1$
      update $\boldsymbol{n}$: $n_j \leftarrow n_j - 1$ and $n_{j^\star} \leftarrow n_{j^\star} + 1$
      update $\boldsymbol{q}$: $q_j \leftarrow q_j - 2Q_j(x_i)$ and $q_{j^\star} \leftarrow q_{j^\star} + 2Q_{j^\star}(x_i)$
    end if
  end for
until convergence
```

x_i we compute the cost of moving it to another cluster, $\Delta Q^{j\to\ell}(x_i)$ for $\ell = 1, \dots, k$ with $\ell \neq j$. We then choose $j^\star = \arg\max_\ell \Delta^{j\to\ell}(x_i)$. If $\Delta Q^{j\to j^\star}(x_i) > 0$ we move x_i to cluster $\mathcal{C}_{j^\star}$, otherwise we keep x_i in its original cluster $\mathcal{C}_j$. We update Z accordingly. The process is repeated until convergence, i.e. until no points are assigned to new clusters. This whole procedure is described in Algorithm 3. Note that (35) assures that the objective function is monotonically increasing at each iteration.

Notice that 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 previous algorithms assume that G is given. There are more efficient methods to compute G, specially if it is sparse. 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 $\boldsymbol{q}$ we have $\mathcal{O}(n_1^2 + \cdots + n_k^2) = \mathcal{O}(k \max_j n_j^2)$. These operations, however, only need to be performed a single time. Now 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

Algorithm 3 Energy cost 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: $\boldsymbol{q} \leftarrow (Q_1, \dots, Q_k)^\top$ have the energy costs of each cluster, according to (32)
 2: $\boldsymbol{n} \leftarrow (n_1, \dots, n_k)^\top$ 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:     $j^\star \leftarrow \arg\max_\ell \Delta Q^{j \to \ell}(x_i)$, for $\ell = 1, 2, \dots, k$ and $\ell \neq j$
 7:     if  $\Delta Q^{j \to j^\star}(x_i) > 0$  then
 8:       move $x_i$ to $\mathcal{C}_{j^\star}$: $Z_{ij} \leftarrow 0$ and $Z_{ij^\star} \leftarrow 1$
 9:       update $\boldsymbol{n}$: $n_j \leftarrow n_j - 1$ and $n_{j^\star} \leftarrow n_{j^\star} + 1$
10:       update $\boldsymbol{q}$: $q_j \leftarrow q_j - 2Q_j(x_i)$ and $q_{j^\star} \leftarrow q_{j^\star} + 2\left(Q_{j^\star}(x_i) + G_{ii}\right)$
11:     end if
12:   end for
13: until convergence
```

cost of computing (33) 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.

VI. 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 associated kernel (8). We thus have

$$\rho(x, y) = \|x - y\|, \qquad K(x, y) = \tfrac{1}{2}\left(\|x\| + \|y\| - \|x - y\|\right). \tag{36}$$

We will consider other semimetrics/kernels as well, but the above will be considered the standard kernel for energy statistics and will always be present in every experiment as a reference. Notice that this is a convention, we could have chosen any other semimetric as the standard. One of the main goals of the following experiments is to compare Algorithm 3 to kernel k-means algorithm, described in Algorithm 2. Thus, for every kernel used in Algorithm 3, we also use the same kernel in Algorithm 2. Another goal is to compare Algorithm 3 with k-means and GMM (through expectation maximization algorithm), as these are the most used clustering algorithms in practice. Since for synthetic data the true labels are available, our measure of clustering quality will be (31). Moreover, for all algorithms, we always choose the initialization from k-means++ [15].

We first consider clustering in high dimensions and analyze how the algorithms degrade as the number of dimensions increase, while keeping the number of points in each cluster fixed. The Bayes error is also kept fixed as ambient dimension increases. In Figure 2a we have data generated from D-variate normal distributions as follows:

$$\begin{aligned} & x \sim \tfrac{1}{2}\left[\mathcal{N}(\mu_1,\Sigma_1)+\mathcal{N}(\mu_2,\Sigma_2)\right], \\ & \mu_1 = (\underbrace{0,\dots,0}_{\times D})^\top, \quad \mu_2 = 0.7\times(\underbrace{1,\dots,1}_{\times 10},\underbrace{0,\dots,0}_{\times(D-10)})^\top, \quad \Sigma_1=\Sigma_2=I_D. \end{aligned} \tag{37}$$

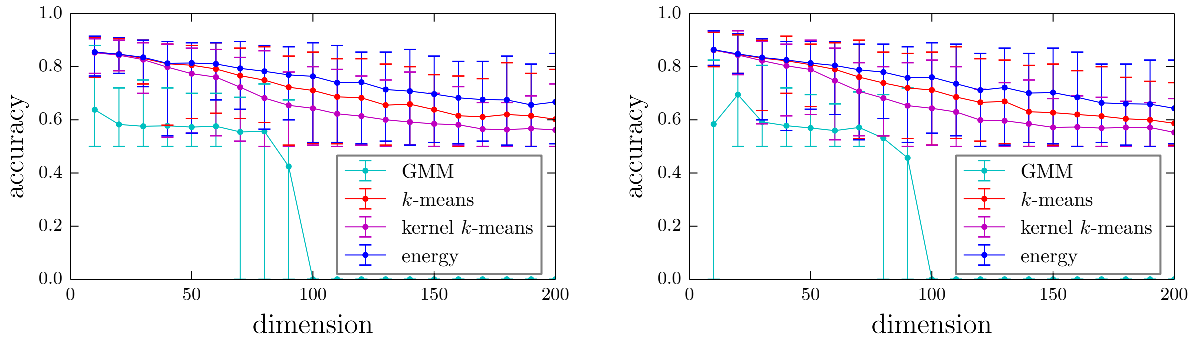
We only keep signal in in the first 10 dimensions of μ_2, and keep increasing the ambient dimension D. For each D, we perform 100 experiments, obtaining the clustering accuracy for each algorithm. We can see that GMM is not able to estimate the covariance matrix when the number of dimensions exceeds the number of points in each cluster, so it gives zero accuracy for $D \gtrsim 100$. In Figure 2b we have the same type of experiment but with

$$\begin{aligned} & x \sim \tfrac{1}{2}\left[\mathcal{N}(\mu_1,\Sigma_1)+\mathcal{N}(\mu_2,\Sigma_2)\right], \\ & \mu_1 = (\underbrace{0,\dots,0}_{\times D})^\top,\ \mu_2 = 0.7\times(\underbrace{1,\dots,1}_{\times 10},\underbrace{0,\dots,0}_{\times(D-10)})^\top,\ \Sigma_1=I_D,\ \Sigma_2=\left(\begin{smallmatrix} \frac{1}{2}I_{10} & 0 \\ 0 & I_{D-10}\end{smallmatrix}\right). \end{aligned} \tag{38}$$

Therefore, for both experiments shown in Figure 2 we can see a better performance of Algorithm 3 compared to the other ones, in particular compared to kernel k-means algorithm, where we recall that both aim at optimizing the same problem (see Proposition 3). Also, notice that k-means and GMM are consistently the right model for this dataset, so it is hard to perform better than these algorithms in this current setting. Notice that Algorithm 3 is more robust as the ambient dimension increases.

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

$$\begin{aligned} & x \sim \frac{n_1}{N}\mathcal{N}(\mu_1,\Sigma_1)+\frac{n_2}{N}\mathcal{N}(\mu_2,\Sigma_2), \quad \mu_1=(0,0,0,0)^\top,\ \mu_2 = 1.5\times(1,1,0,0)^\top, \\ & \Sigma_1 = I_4, \quad \Sigma_2 = \left(\begin{smallmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{smallmatrix}\right), \quad n_1 = N-m, \quad n_2 = N+m, \quad N=200. \end{aligned} \tag{39}$$



(a)

(b)

FIG. 2. Effect of increasing the ambient dimension while keeping Bayes error fixed, for two clusters with normally distributed data with 100 points in each cluster. (a) We increase D as described in (37). The blue line correspond to Algorithm 3, while the magenta line corresponds to kernel k-means, Algorithm 2. (b) The same but with data following (38). One notices that Algorithm 3 is more robust than the other ones.

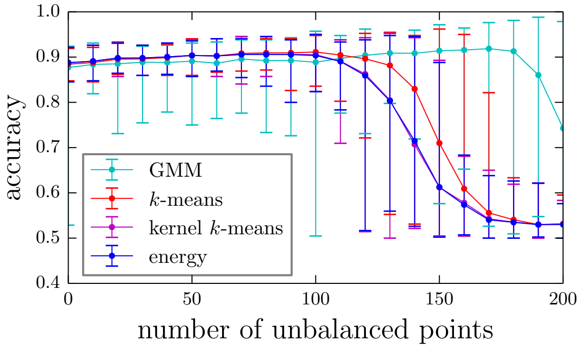


FIG. 3. Previous algorithms for unbalanced clusters, according to (39).

We then increase m, i.e. we make the clusters progressively more unbalanced. We generate 100 experiments for each m, and plot the clustering accuracy versus m. As expected, GMM works better than the other algorithms in the case of unbalanced clusters. This is mostly due to its soft assignments. 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 energy statistics clustering should compensate for this effect.

Now, besides (36) we consider two other semimetrics:

$$\rho_{1/2}(x,y) = \|x-y\|^{1/2}, \qquad K(x,y) = \tfrac{1}{2}\left(\|x\|^{1/2} + \|y\|^{1/2} - \|x-y\|^{1/2}\right), \tag{40}$$

$$\rho_e(x,y) = 2 - 2e^{-\|x-y\|/2}, \qquad K(x,y) = e^{-\|x-y\|/2}. \tag{41}$$

In Figure 4a we have data in 20 dimensions distributed as

$$\begin{gathered} x \sim \tfrac{1}{2}\left[\mathcal{N}(\mu_1,\Sigma_1) + \mathcal{N}(\mu_2,\Sigma_2)\right], \\ \mu_1 = (\underbrace{0,\dots,0}_{\times 20})^\top, \quad \mu_2 = \tfrac{1}{2}(\underbrace{1,\dots,1}_{5},\underbrace{0,\dots,0}_{15})^\top, \quad \Sigma_1 = \tfrac{1}{2}I_{20}, \quad \Sigma_2 = I_{20}. \end{gathered} \tag{42}$$

We increase the number of points in each cluster and show the clustering accuracy with different algorithms. The new semimetrics (40) and (41) are indicated in the legend. One can see that Algorithm 3 performs better than all the other ones, and in particular (41) provides better results. As the number of datapoints get large enough, GMM starts to be as accurate as clustering based on energy statistics, as it should since it is consistent model to the data. In Figure 4b, however, we use the same parameters as in (42) but now with data log-normally distributed:

$$x \sim \tfrac{1}{2}\left[e^{\mathcal{N}(\mu_1,\Sigma_1)} + e^{\mathcal{N}(\mu_2,\Sigma_2)}\right]. \tag{43}$$

We see that clustering based on energy statistics still performs accurately for this kind of data, while k-means works a little bit better than chance, and GMM is not even able to estimate the parameters. Again, (41) provides slightly better results than (36) or (40). Notice also that Algorithm 3 performs better than Algorithm 2. Both experiments in Figure 4 shows that energy statistics clustering is nonparametric, since it is able to cluster data coming from very different distributions.

VII. CONCLUSION

In this paper we have considered clustering from the perspective of energy statistics, which provides a nonparametric test for equality of distributions. Based on this, we showed that the clustering problem reduces to a quadratically constrained optimization problem (QCQP), as described in Proposition 2. Moreover, we showed that clustering based on energy statistics is equivalent to kernel k-means optimization problem, once the kernel is fixed; see Proposition 3. Our results imply that kernel k-means approach to clustering

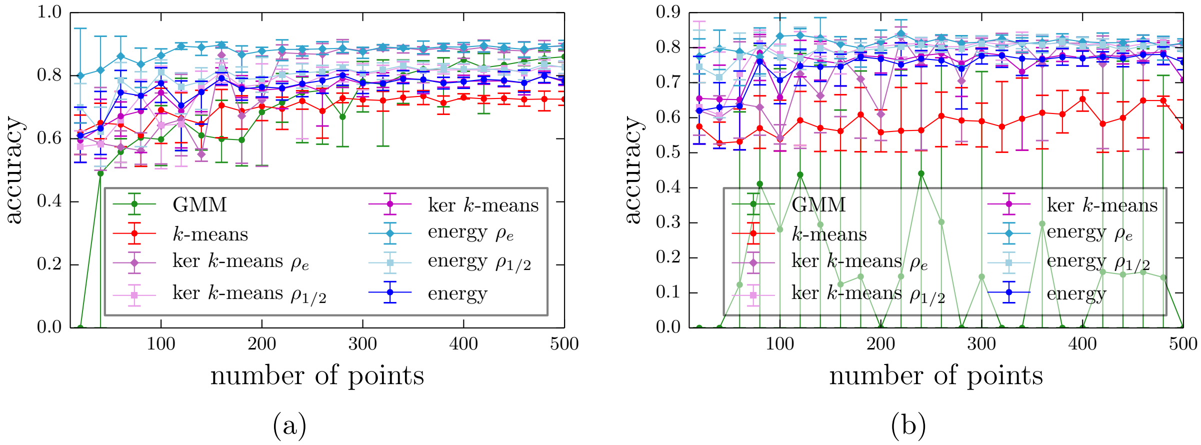


FIG. 4. (a) Data normally distributed as in (42). We increase the number of points in each cluster to illustrate the statistical consistency of the algorithms. (b) The same experiment but for data following (43). In both experiments, for each case we run every algorithm 100 times and show the average results. One can see the better performance of energy statistics clustering, Algorithm 3, and in particular by using the semimetric (41). These two figures illustrate that energy statistics clustering is nonparametric since it works well for very different distributions.

is actually a consequence of energy statistics theory, and thus place this method into a principled statistical basis. As already known [10], this approach is related to spectral clustering, and graph partitioning problems. Therefore, all these problems may be seen as arising naturally from energy statistics clustering. It is important to mention that energy statistics clustering, as formulated here, is valid for arbitrary metric spaces of negative type, and makes no assumptions about the distribution of the data. Moreover, it does not rely on the concept of a cluster mean, even implicitly.

We also proposed Algorithm 3 as an alternative to the well-known kernel k-means algorithm (see Algorithm 2), where both have the same time complexity. The numerical results show that Algorithm 3 might provide better clustering accuracy and is more robust than kernel k-means algorithm. Since there exists a huge literature about kernel k-means, and approximation methods to make it faster, with applications to several artificial and real data, we limited ourselves to analyze few but carefully designed experiments, which illustrates the advantages of Algorithm 3.

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