A MEAN FIELD GAMES MODEL FOR FINITE MIXTURES OF BERNOULLI AND CATEGORICAL DISTRIBUTIONS

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Abstract. Finite mixture models are an important tool in the statistical analysis of data, for example in data clustering. The optimal parameters of a mixture model are usually computed by maximizing the log-likelihood functional via the Expectation-Maximization algorithm. We propose an alternative approach based on the theory of Mean Field Games, a class of differential games with an infinite number of agents. We show that the solution of a finite state space multi-population Mean Field Games system characterizes the critical points of the log-likelihood functional for a Bernoulli mixture. The approach is then generalized to mixture models of categorical distributions. Hence, the Mean Field Games approach provides a method to compute the parameters of the mixture model, and we show its application to some standard examples in cluster analysis.

1. Introduction. Finite mixture models, given by convex combinations of probability density functions (PDFs in short)

$$\pi(x) = \sum_{k=1}^{K} \alpha_k \pi_k(x), \quad \text{with } \alpha_k \in [0, 1], \quad \sum_{k=1}^{K} \alpha_k = 1, \quad (1)$$

are an important mathematical tool in statistical analysis of data. Introduced by the biometrician K. Pearson [20], due to their flexibility, they are employed in a large variety of fields as astronomy, biology, genetic, medicine, marketing and engineering (see [26, Chapter 6-7], [25]). In cluster analysis, a classical problem in unsupervised
Machine Learning consisting in the repartition of a data set into subgroups with similar characteristics, finite mixture models can be used in order to determine the intrinsic structure of clustered data when no information, except for the observed values, are available. For a detailed description of the theory of mixture models and applications, see [10, 18, 25].

Given a data set \( \mathcal{X} \) representing the measurements of a phenomena, whose different values are related to the membership to unknown categories, a corresponding finite mixture model is built by assuming that the data have been generated by a random variable \( X \), whose unknown probability distribution \( \pi \) can be described as in (1).

The parameters of the mixture (1) are in general unknown and the aim is to determine them in such a way that they optimally fit the given data set \( \mathcal{X} \). To this end, different methods can be employed such as the graphical method [24], the Bayesian method [25] and the likelihood estimator [4]. The latter one, which is the starting point of our analysis, generates a tough quantity to be maximized, which is usually computed by means of the Expectation Maximization (EM in short) algorithm (see [3]). In our approach, we characterize the optimal parameters of a mixture model through a multi-population Mean Field Games (MFG in short) system, a coupled system of differential or difference equations which characterizes the Nash equilibria in the framework of stochastic games with a very large number of agents. The MFG theory has been introduced simultaneously by Lasry-Lions [17] and Huang-Caines-Malhamé [16] and it has been successfully applied to different fields, such as economics, biology, environmental policy, etc. (for a plain introduction, see [14]). Recently, its scope has been broadened to Machine Learning applications. In [7], it is proposed a numerical scheme for MFG problems based on tools from neural networks, whereas in [9] the authors recast some deep learning techniques as mean-field optimal control problems. Concerning unsupervised Machine Learning, we refer to [8, Chapter 2] and [21] where multi-population MFG systems are studied in connection with cluster problems.

In [1], we developed a MFG approach to finite mixture models defined over a continuous random variable \( X \). Data points are interpreted as agents and the aim is to subdivide the whole population, described by a PDF \( \pi(x) \), in \( K \) sub-populations, described by PDFs \( \pi_k \) and mixing coefficients \( \alpha_k \), on the basis of some similar characteristics appropriately encoded in the cost functional of the control problems of the different populations. As a result, we end up with a multi-population ergodic Mean Field Games in \( \mathbb{R}^d \) which, in the particular case of a quadratic cost, characterizes the critical points of the log-likelihood functional for a mixture of Gaussian distributions.

In this paper, we focus on a mixture model for a discrete random variable \( X \) described by a Bernoulli distribution or, more generally, by a categorical one. We assume that the sub-populations can be discriminated on the basis of a single specific characteristic taking only one of \( S \) different values (the case of several different characteristics will be discussed further on in the paper).

Given a data set \( \mathcal{X} = \{x_1, \ldots, x_N\} \), in order to characterize the components of the mixture model, i.e. the PDFs \( \pi_k \) and the weights \( \alpha_k \), we introduce the \( K \)-populations finite state MFG system.
\[ V_k(i) = \min_{P_{ij} \geq 0} \sum_{j=1}^{S} P_{ij} \left( c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta_k) + V_k(j) \right) - \lambda_k, \]

\[ \pi_k(i) = \sum_{j=1}^{S} P_{kj} \pi_k(j), \]

\[ \pi_k(i) \geq 0, \sum_{i=1}^{S} \pi_k(i) = 1, \sum_{i=1}^{S} V_k(i) = 0, \]

\[ \alpha_k = \frac{1}{N} \sum_{n=1}^{N} \gamma_k(x_n), \]

for \( i \in \{1, \ldots, S\} \). The term \( c(P_{ij}) \) is a transition cost between the states \( i \) and \( j \) and \( \varepsilon \log(P_{ij}) \) is an entropy penalization term which forces the agents to diversify their transition choices. Each of the \( K \) sub-populations is characterized by a quadruple \((V_k, \lambda_k, \pi_k, \alpha_k)\), with the couple \((V_k, \lambda_k)\) solving an ergodic Hamilton-Jacobi-Bellman equation and with the probability distribution \( \pi_k \) solving a Fokker-Planck equation where the transition matrix \( P_{kj} \), composed of the rows \( P_{kj} = \{P_{kj} \}_{j=1}^{S} \), is such that

\[ P_{kj} = \arg \min_{P_{ij} \geq 0} \sum_{j=1}^{S} P_{ij} \left( c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta_k) + V_k(j) \right). \]

The vector \( \theta_k \in \mathbb{R}^{S} \) represents the average value of the data set with respect to the distribution \( \pi_k \) and therefore depends on the solution of (2). Interaction among the sub-populations is encoded in the weights \( \alpha_k \) and in the coupling cost \( F(i, \theta_k) \), which depend on the responsibilities

\[ \gamma_k(x_n) = \frac{\alpha_k \pi_k(x_n)}{\pi(x_n)} \quad k = 1, \ldots, K, x_n \in \mathcal{X}. \]

These quantities play a crucial role and, in cluster analysis, can be used to assign a point to the class with the highest \( \gamma_k \) (see Section 2 for some more details on the game theoretic interpretation of (2)).

Relying on the theory for finite states MFG system developed in [13], we prove that the system (2) admits a solution \((V_k, \lambda_k, \pi_k, \alpha_k)\), \( k = 1, \ldots, K \). Moreover we show that, for \( S = 2 \), (2) characterizes the critical points of the maximum log-likelihood functional for a mixture of Bernoulli distributions and therefore gives an alternative way to compute the critical points of the log-likelihood functional. We show an application of this method to the computation of the optimal parameters for mixture models related to some standard examples in cluster analysis, such as digit classification.

We remark that the goal of the paper is to provide a new perspective to a class of problems which, up to now, have been considered in the classical framework of finite dimensional optimization. For a linear cost \( c \) and \( \varepsilon = 0 \), the algorithm described in Section 5 is equivalent to the classical EM algorithm and, in general, it is not computationally competitive with other algorithms for cluster analysis. But our model is feasible to be generalized in several directions and, in a forthcoming paper, we plan to study more general costs, possibly depending on the state variable, in order to exploit in a deeper way the structure of the data set.

The paper is organized as follows. In Section 2, we briefly review the finite mixture model theory, with the corresponding EM algorithm, and the theory of finite state discrete time Mean Field Games problems. In Section 3, we introduce
the MFG model for a Bernoulli random variable and we show the connection with the maximization of the log-likelihood functional. In Section 4, we generalize the model of the previous section to a mixture of categorical distributions and we prove existence of a solution to the MFG system. In Section 5, we apply the MFG model to some standard problems in cluster analysis. In Appendix A, we prove some results for a finite-state stationary MFG system we use in the previous sections.

2. A short introduction to mixture models and finite state discrete time Mean Field Games problems. In this section, we review the parametric mixture model and the corresponding EM algorithm for the optimization of the parameters. We also give a short description of the game theoretic interpretation of the MFG system (2).

Mixture models and EM algorithm. Let $X$ be a random variable, univariate or multivariate and consider a sample $X = \{x_1, \ldots, x_N\}$ of size $N$ of $X$, where the sample space $S$ can be discrete or continuous. Let $p(x)$ be the unknown distribution of $X$, defined with respect to an appropriate reference measure on $S$. We assume that $X$ comes from a finite mixture model, i.e. $p(x)$ can be written as a convex combination of PDFs $p_k$ as
\[
p(x) = \sum_{k=1}^{K} \alpha_k p_k(x), \quad x \in S,
\]
where $K$, the number of the components of $p$, is supposed to be known a priori and $\alpha_k$, the weights or mixing coefficients, satisfy $\sum_{k=1}^{K} \alpha_k = 1$ and $\alpha_k \geq 0$. How to determine the number $K$ of PDFs in the mixture model is an unresolved issue and, in general, a combination of criteria and experimental analysis is used to guide the decision (see [10, Chapter 6]).

Usually, it is assumed that the components of the mixture (3) belong to the same parametric family of density distributions, i.e. they can be written as $p_k(x) = p(x; \Theta_k)$, where $\Theta_k$ is the parameter which defines the $k$-th PDF. For example, in the Gaussian mixture model, $p(x; \Theta_k) = \mathcal{N}(x; \mu_k, \Sigma_k)$ are Gaussian distributions of parameters $\Theta_k = (\mu_k, \Sigma_k)$ where $\mu_k, \Sigma_k$ are the mean and covariance matrix; in the Bernoulli mixture model, $p(x; \Theta_k) = \mathcal{B}(x; \mu_k)$ are Bernoulli distributions of parameter $\Theta_k = \mu_k$. The aim is to find the parameters $\alpha = (\alpha_1, \ldots, \alpha_K)$ and $\Theta = (\Theta_1, \ldots, \Theta_K)$ which give the best representation of the sample $X$. This can be achieved through the maximization of the log-likelihood functional
\[
\mathcal{L}(\alpha, \Theta; X) = \sum_{n=1}^{N} \log \left( \sum_{k=1}^{K} \alpha_k p(x_n; \Theta_k) \right)
\]
By writing the necessary condition for the extrema of (4), we have
\[
\frac{\partial \mathcal{L}}{\partial \alpha_k} = \sum_{n=1}^{N} \frac{p(x_n; \Theta_k)}{\sum_{j=1}^{K} \alpha_j p(x_n; \Theta_j)} - \lambda = 0,
\]
\[
\frac{\partial \mathcal{L}}{\partial \Theta_k} = \sum_{n=1}^{N} \frac{\alpha_k}{\sum_{j=1}^{K} \alpha_j p(x_n; \Theta_j)} \cdot \frac{\partial p(x_n; \Theta_k)}{\partial \Theta_k} = 0.
\]
where $\lambda$ is a Lagrange multiplier which takes into account the constraint for the mixing coefficients. The Expectation-Maximization algorithm is an iterative procedure for the computation of a solution of the previous system. We shortly describe
its derivation. Firstly, it is introduced a latent, or hidden, \(K\)-dimensional random variable \(Y = (Y_1, \ldots, Y_K)\), with \(Y_k \in \{0, 1\}\) and \(\sum_{k=1}^{K} Y_k = 1\), saying which component of the mixture (3) has generated a given sample point \(x_n\). More specifically, we assume that, for each observed point \(x_n \in \mathbb{R}^D\), there exists a corresponding unobserved one \(y_n \in \mathbb{R}^K\) such that, if the point \(x_n\) has been generated by the \(k\)-component of the mixture, then \(y_{n,k} = 1\) and \(y_{n,j} = 0\) for \(j \neq k\). Hence \(Y\) is a multinomial random variable and we assume that \(P(Y_k = 1) = \alpha_k\). A simple application of Bayes’ Theorem allows to compute the responsibility, i.e. the probability of \(Y\) given \(X\),

\[
\gamma_k(x_n) := P(Y_k = 1|X = x_n) = \frac{\alpha_k p(x_n; \Theta_k)}{\sum_{j=1}^{K} \alpha_j p(x_n; \Theta_j)} .
\]

Multiplying (5) by \(\alpha_k\) and summing over \(k\) we get that \(\lambda = N\), hence replacing (7) in (5) we get a first condition for an extremum of (4)

\[
\alpha_k = \frac{1}{N} \sum_{n=1}^{N} \gamma_k(x_n). \tag{8}
\]

Using (7) in (6), we have

\[
\sum_{n=1}^{N} \gamma_k(x_n) \frac{\partial \log(p(x_n; \Theta_k))}{\partial \Theta_k} = 0 . \tag{9}
\]

Since the coefficients \(\alpha_k\) in (8) depend on \(\Theta_k\) via the responsibilities \(\gamma_k\), the equations (8) and (9) do not provide a closed form solution for the parameters.

However, they suggest the following iterative scheme which alternates two steps. Starting from some arbitrary initialization \((\alpha^{(0)}, \Theta^{(0)})\), at \(h\)-iteration we perform the following steps: in the Expectation step (E-step in short), using the current values \((\alpha^{(h)}, \Theta^{(h)})\) of the parameters, we compute the responsibilities by means of formula (7) with \(\Theta^{(h)}\) and \(\alpha^{(h)}\) in place of \(\Theta\) and \(\alpha\). In the Maximization step (M-step in short), given the responsibilities as in the E-step, we compute the new parameters \((\alpha^{(h+1)}, \Theta^{(h+1)})\) by means of (8) and (9). It can be proved that at each iteration (E-step, M-step), the log-likelihood function increases its value. For more details see [3], [4, Chapter 9].

For specific parametrized families of distributions, such as Gaussian and Bernoulli distributions, it is possible to get explicit formulas for the parameters \(\Theta_k\). Computed the responsibility \(\gamma_k^{(h+1)}(x)\) by means of (7) in the E-step, in the M-step we have the following explicit formulas

\[
\alpha_k^{(h+1)} = \frac{1}{N} \sum_{n=1}^{N} \gamma_k^{(h+1)}(x_n)
\]

and, for a Gaussian mixture,

\[
\mu_k^{(h+1)} = \frac{\sum_{n=1}^{N} \gamma_k^{(h+1)}(x_n)x_n}{\sum_{n=1}^{N} \gamma_k^{(h+1)}(x_n)},
\]

\[
\Sigma_k^{(h+1)} = \frac{\sum_{n=1}^{N} \gamma_k^{(h+1)}(x_n)(x_n - \mu_k^{(h+1)})(x_n - \mu_k^{(h+1)})^t}{\sum_{n=1}^{N} \gamma_k^{(h+1)}(x_n)}.
\]
for a Bernoulli mixture,
\[
\mu_k^{(h+1)} = \frac{\sum_{n=1}^{N} \gamma_k^{(h+1)}(x_n)x_n}{\sum_{n=1}^{N} \gamma_k^{(h+1)}(x_n)},
\]

Remark 1. Equations (8) and (9) also characterize the necessary conditions for the extrema of the functional
\[
\tilde{L} = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_k(x_n)(\log(\alpha_k) + \log p(x_n; \Theta_k)),
\]
where \(\gamma_k\) is as in (7), which provides a different, but equivalent approach to the optimization of the mixture model for a given data set (see [4, Chapter 9.3]).

Mean Field Games. Following [5, 13], we give a short interpretation of system (2) in terms of a control problem for a distribution of agents. For simplicity of notations, we will consider the case of a single population, i.e. \(K = 1\).

We first describe the finite horizon problem. Given two natural numbers \(S, T \geq 1\), representing respectively the number of possible states for the agents and the total duration of the process, a solution of the MFG problem is a sequence of pairs \(\{(\pi_t, V_t)\}_{t=0}^{T}\) where \(\pi_t \in \mathbb{R}^S\), \(\pi_t(i) \in [0, 1]\) and \(\sum_{i=1}^{S} \pi_t(i) = 1\), is a probability vector describing the distribution of the agents among the \(S\) states at time \(t\); the components of the value function \(V_t \in \mathbb{R}^S\) represent the expected cost for an agent in the corresponding state at time \(t\). The family of vectors \(\{(\pi_t, V_t)\}_{t=0}^{T}\) must satisfy certain optimality conditions we are going to explain. Given an initial distribution of the agents \(\bar{\pi}_0\), the evolution of the population follows the law
\[
\pi_{t+1}(i) = \sum_{j=1}^{S} P_t^{ij} \pi_t(j), \quad t = 0, \ldots, T - 1,
\]
where the transition matrix \(P^t\) is a \(S \times S\) stochastic matrix with \(P_t^{ij}\) representing the probability that an agent at the state \(i\) moves in the state \(j\). Given the terminal cost \(\bar{V}^T \in \mathbb{R}^S\), the matrix \(P^t, t = 0, \ldots, T - 1\), is obtained by minimizing the cost functional
\[
J^t(i, P) = \sum_{j=1}^{S} P_{ij} \left( c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta) + V^{t+1}(j) \right)
\]
with the value function defined by \(V^t(i) = \inf_P [J^t(i, P)]\), \(i, \ldots, S\). The pairs \(\{(\pi_t, V^t)\}_{t=0}^{T}\) satisfy
\[
\begin{aligned}
V^t(i) &= \min_{P_t \colon P_{ij} \geq 0, \sum_j P_{ij} = 1} \left\{ \sum_{j=1}^{S} P_{ij} \left( c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta) + V^{t+1}(j) \right) \right\}, \\
\pi^{t+1}(i) &= \sum_{j=1}^{S} P_t^{ij} \pi^t(j), \\
V^T &= \bar{V}^T, \quad \pi^0 = \bar{\pi}^0,
\end{aligned}
\]
for \(t = 0, \ldots, T - 1\). The previous system is given by a backward Hamilton-Jacobi-Bellman equation for the value function and a forward Fokker-Planck equation for the distribution of agents with the corresponding final and initial condition.

The stationary MFG system, see (2) for \(K = 1\), is obtained by considering the
The long-run average cost is:

\[ J(i, \{ P^t \}_{t \in \mathbb{N}}) = \limsup_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T} \sum_{j=1}^{S} P^t_{ij} \left( c(P^t_{ij}) + \varepsilon \log(P^t_{ij}) + F(i, \theta) \right). \]

In this case, the ergodic cost \( \lambda \) is given by the infimum of \( J(i, \{ P^t \}_{t \in \mathbb{N}}) \) and it is independent of the state \( i \), while \( \pi \) represents the invariant distribution of the process. Note that the solution of the stationary Hamilton-Jacobi-Bellman equation is defined up to an additive constant and therefore the normalization condition \( \sum_{j=1}^{S} V(j) = 0 \) is added.

In the multi-population system (2), each population satisfies a control problem as before, and the interaction among the different populations is given by the value \( \theta_k \) and the mixing coefficients \( \alpha_k \).

3. A Mean Field Games approach to Bernoulli mixture models. In this section, we describe a Mean Field Games approach for a mixture of multivariate Bernoulli distributions. This method is used to cluster high-dimensional binary data. In order to explain the technique, we start describing an application of the previous model to the classification of handwritten digits (see [4, Cap. 9]). Consider a database \( \mathcal{X} = \{ x_1, \ldots, x_N \} \) of images representing handwritten digits of \( K \) numbers between 0 and 9. Each image, which is originally given by a square of \( \sqrt{D} \times \sqrt{D} \) pixels in grey scale, is turned in a binary vector \( x = (x_1, \ldots, x_D) \), of size \( D \), by setting the elements whose value exceeds \( 1/2 \) to state 1 and the remaining to state 0, with 1 corresponding to a white pixel, 0 to a black one. Assuming to know \( K \), the aim is to subdivide the data set \( \mathcal{X} \) in \( K \) clusters, where each cluster is represented by the component \( \pi_k \) of a mixture of Bernoulli distributions and an image is attributed to the cluster which maximizes the responsibility. In a second phase, these clusters can be used to identify the digit corresponding to a new image, but we will not consider this problem here. In Figure 1, we see some samples of digits taken from database MNIST [19]. We suppose that the digits are the i.i.d.

![Figure 1. Samples of hand-written digits from the MNIST database](image-url)
Bernoulli distributions

\[ \pi(x) = \sum_{k=1}^{K} \alpha_k \pi_k(x), \]  
\[ (11) \]

where each measure \( \pi_k \), defined by

\[ \pi_k(x) = \prod_{d=1}^{D} \pi_k^d(x^d), \quad x = (x^1, \ldots, x^D) \in \{0,1\}^D \]
\[ (12) \]

\[ \pi_k^d(x^d) = (\mu_k^d)^{x^d} (1-\mu_k^d)^{1-x^d}, \quad x^d \in \{0,1\} \]

represents the distribution of a specific digit in the \( k \)th cluster. The aim is to design a \( K \)-populations MFG system to find the unknown parameters \( \alpha = (\alpha_1, \ldots, \alpha_K) \in \mathbb{R}^K \) and \( \mu = (\mu_1, \ldots, \mu_K) \in \mathbb{R}^{K \times D} \) with \( \mu_k = (\mu_k^1, \ldots, \mu_k^D) \), in such a way that the measure \( \pi \) in (11) optimally fits the data set \( \mathcal{X} \). Following the analysis described in Section 2, we introduce a \( K \)-dimensional latent random variable \( Y \) that specifies which element of the mixture (11) has generated a given data point \( x_n \) and, for \( x_n \in \mathcal{X} \), we define the responsibilities

\[ \gamma_k(x_n) = \frac{\alpha_k \pi_k(x_n)}{\pi(x_n)} \quad k = 1, \ldots, K. \]

Note that \( \gamma_k(x_n) \) are defined in terms of the unknown measure \( \pi \). Given the responsibilities, we define the average value of the data set \( \theta_k = (\theta_k^1, \ldots, \theta_k^D) \in \mathbb{R}^D \) with respect to the \( k \)th component of the mixture by

\[ \theta_k^d = \frac{\sum_{n=1}^{N} \gamma_k(x_n) x_n^d}{\sum_{n=1}^{N} \gamma_k(x_n)}, \quad d = 1, \ldots, D. \]
\[ (13) \]

By definition, \( \theta_k^d \in [0,1] \). For each \( d = 1, \ldots, D \), we consider the following 2-states \( K \)-populations MFG system

\[
\begin{cases}
V_k^d(0) = \min_{p \in [0,1]} \{ p \left( -\frac{1-p}{2} + \epsilon \log(p) + V_k^d(0) \right) \\
\quad \quad + (1-p) \left( -\frac{q}{2} + \epsilon \log(1-p) + V_k^d(1) \right) \} - \lambda_k^d + (\theta_k^d)^2 \\
V_k^d(1) = \min_{q \in [0,1]} \{ (1-q) \left( -\frac{q}{2} + \epsilon \log(1-q) + V_k^d(0) \right) \\
\quad \quad + q \left( -\frac{1-q}{2} + \epsilon \log(q) + V_k^d(1) \right) \} - \lambda_k^d + (1-\theta_k^d)^2 \\
\pi_k^d(0) = \rho \pi_k^d(0) + (1-q) \pi_k^d(1) \\
\pi_k^d(1) = (1-p) \pi_k^d(0) + q \pi_k^d(1) \\
\pi_k^d \geq 0, \quad \sum_{x \in \{0,1\}} \pi_k^d(x) = 1, \quad \sum_{x \in \{0,1\}} V_k^d(x) = 0.
\end{cases}
\]
\[ (14) \]

where the values \((p,q)\) in the second couple of equations are given by controls realizing the minimum in the first couple of equations. The family of MFG systems (14) is completed with the global coupling condition

\[ \alpha_k = \frac{1}{N} \sum_{n=1}^{N} \gamma_k(x_n). \]
\[ (15) \]

For each \( d = 1, \ldots, D \) fixed, the unknowns in the \( K \)-populations MFG system (14) are the couple \((V_k^d, \lambda_k^d)\), with \( V_k^d \in \mathbb{R}^2 \) and \( \lambda_k^d \in \mathbb{R} \), solving the Hamilton-Jacobi-Bellman equation, and the binomial distributions \( \pi_k^d \), solving the Fokker-Planck
equation, while the weights \( \alpha_k \in [0, 1] \) are global unknowns, independent of the index \( d \). It is important to observe that also the transition matrix

\[
P = \begin{bmatrix} p & 1-p \\ 1-q & q \end{bmatrix},
\]

(16)
in the Fokker-Planck equation depends on \( k \) and \( d \) and, under appropriate assumptions (see Section 4), is univocally determined by the couple of controls \( p, q \) which minimize the first two Hamilton-Jacobi equations.

For \( d \) fixed, the coupling cost \((\theta_d^k)^2, (1 - \theta_d^k)^2\) is defined in such a way that a population described by the density function \( \pi_d^k \) distributes in the two states \( \{0, 1\} \) so that its expected value \( \mu_d^k \) is as close as possible to the average value \( \theta_d^k \) of the data set. Hence this forces the expected value of the \( k \)-th component \( \pi_k \) of the mixture to be close to the average of \( X \), given the occurrence of the event \( Y_k = 1 \).

Note that the value \( \theta_d^k \) depends on the responsibilities \( \gamma_k \), see (13), and therefore, in turn, on the complete distribution \( \pi \). Hence, the systems (14) are coupled also with respect to the index \( d \) by means of the quantities \( \theta_d^k \). Indeed, the covariance matrix of (11) is not diagonal (see [4, Equation (9.50)]) and the model can capture correlation among the components of the mixture. The well-posedness of problem (14) and (15) will be discussed in Section 4 in the more general setting of the categorical distributions.

We now show the connection between the multi-population MFG system (14) and the functional (10), which, in the case of a multivariate Bernoulli distribution (12), is plainly given by

\[
\hat{L}(\alpha, \mu; \mathcal{X}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_n(x_n) \left( \log(\alpha_k) + \sum_{d=1}^{D} (x_n^d \log(\mu_d^k) + (1 - x_n^d) \log(1 - \mu_d^k)) \right)
\]

(17)

for \( \alpha = (\alpha_1, \ldots, \alpha_K), \mu = (\mu_1, \ldots, \mu_K) \in \mathbb{R}^{K \times D} \), where \( \mu_k = (\mu_1^k, \ldots, \mu_D^k), k = 1, \ldots, K \). Note that, since the log-likelihood has to be maximized, we are interested in the critical values of \( \hat{L}(\alpha, \mu; \mathcal{X}) \) for the values of the parameters \( \alpha_k, \mu_k^d \) inside the interval \((0, 1)\). By (17), the necessary conditions (8) and (9) can be computed explicitly in terms of responsibilities and they are given by

\[
\left\{ \begin{array}{l}
\mu_d^k = \frac{\sum_{n=1}^{N} \gamma_n(x_n) x_n^d}{\sum_{n=1}^{N} \gamma_n(x_n)} \\
\alpha_k = \frac{1}{N} \sum_{n=1}^{N} \gamma_n(x_n).
\end{array} \right.
\]

(18)

In the next proposition, we show that a Bernoulli mixture satisfying (18) can be always obtained as a solution of the MFG system (14) with \( \varepsilon = 0 \). Moreover, a solution of problem (14) and (15) with \( \varepsilon = 0 \) gives a mixture satisfying (18).

**Proposition 1.** We have

(i) Let \( \pi(x) = \sum_{k=1}^{K} \alpha_k \pi_k(x) \), with \( \pi_k \) as in (12), be a Bernoulli mixture satisfying (18). Then, the family of quadruples \( (V_k, \lambda_k, \pi_k, \alpha_k), k = 1, \ldots, K, \)
with
\[ V_k = (V_k^1, \ldots, V_k^P), \quad V_k^d(x) = \left(\frac{1-2\mu_k^d}{2}\right)^x \left(\frac{2\mu_k^d-1}{2}\right)^{1-x}, \quad x \in \{0, 1\}, \]
\[ \lambda_k = (\lambda_k^1, \ldots, \lambda_k^P), \quad \lambda_k^1 = 0, \]
\[ \pi_k = (\pi_k^1, \ldots, \pi_k^P), \quad \pi_k^d(x) = (\mu_k^d)^x (1-\mu_k^d)^{1-x}, \quad x \in \{0, 1\}, \]

(19)
is a solution of (14) and (15) with \( \epsilon = 0 \) and \( \theta_k^d \) as in (13).

(ii) Let \( \{(V_k, \lambda_k, \pi_k, \alpha_k)\}_{k=1}^K \) be a solution of the MFG system (14) and (15) with \( \epsilon = 0 \) and \( \theta_k^d \) as in (13). Then \( \pi(x) = \sum_{k=1}^K \alpha_k \pi_k(x) \) is a Bernoulli mixture verifying (18).

Proof. (i) Consider a mixture \( \pi \) defined as in (11) and (12) and satisfying (18). Then, each component \( \pi_k^d \) satisfies the 2-states Fokker-Planck equation
\[
\begin{align*}
\pi_k^d(0) &= p \pi_k^d(0) + (1-q) \pi_k^d(1) \\
\pi_k^d(1) &= (1-p) \pi_k^d(0) + q \pi_k^d(1) \\
\pi_k^d &\geq 0, \quad \sum_{x \in \{0, 1\}} \pi_k^d(x) = 1
\end{align*}
\]
(20)
where the transition matrix \( P \) is defined as in (16) with \( p = 1-\mu_k^d \), \( q = \mu_k^d \). We observe that by condition (18), the expected values \( \theta_k^d \) in (14), defined in (13), coincide with \( \mu_k^d \). Therefore the couple \( (V_k^d(x), \lambda_k^d) = \left((1-2\mu_k^d)^x \left(\frac{2\mu_k^d-1}{2}\right)^{1-x}, 0\right), \quad x \in [0, 1] \) satisfies the first and second equation of system (14) with \( \epsilon = 0 \) and with optimal controls given by \( p^* = 1-\mu_k^d \) and \( q^* = \mu_k^d \).

In addition, the homogeneous condition \( \sum_{x \in \{0, 1\}} V_k^d(x) = 0 \) is fulfilled.

Hence, we conclude that the transition matrix \( P \) in (20) is given by the optimal controls \( p^* \) and \( q^* \) and therefore (19) is a solution of (14) with \( \epsilon = 0 \).

(ii) Let \( \{(V_k, \lambda_k, \pi_k, \alpha_k)\}_{k=1}^K \) be a solution of the MFG system (14) and (15) with \( \epsilon = 0 \). Then, since \( (V_k^d, \lambda_k^d) \) is the solution to Hamilton-Jacobi-Bellman equation
\[
\begin{align*}
V_k^d(0) &= \min_{p \in [0,1]} \{p(1-p) + V_k^d(0)\} \\
&\quad + (1-p)(-\frac{1}{2} + V_k^d(1)) - \lambda_k^d + (\theta_k^d)^2 \\
V_k^d(1) &= \min_{q \in [0,1]} \{(1-q)(-\frac{1}{2} + V_k^d(0)) \\
&\quad + q(1-q) + V_k^d(1)\} - \lambda_k^d + (1-\theta_k^d)^2, \\
\sum_{x \in \{0,1\}} V_k^d(x) &= 0,
\end{align*}
\]
we have \( (V_k^d, \lambda_k^d) = \left((1-2\mu_k^d)^x \left(\frac{2\mu_k^d-1}{2}\right)^{1-x}, 0\right) \) with the optimal controls \( p \) and \( q \) given by
\[ p = 1-\theta_k^d, \quad q = \theta_k^d \]
(21)
It follows that, given the transition matrix \( P \) as in (16) with \( p,q \) as in (21), the solution to the Fokker-Planck equation (20) is a Bernoulli distribution \( \pi_k^d(x) \) of parameter \( \mu_k^d = \theta_k^d \). Therefore, by (13), \( \mu_k^d \) satisfies the first condition in (18). Moreover, since the coefficients \( \alpha_k \) are given by (15), also the second condition in (18) is satisfied. \( \square \)
Remark 2. If \( \varepsilon > 0 \), then it is possible to show that the MFG system (14) characterizes the critical points of the functional

\[
\tilde{L}_\varepsilon(\alpha, \mu; \mathcal{X}) = \sum_{n=1}^N \sum_{k=1}^K \gamma_k(x_n) \left( \log(\alpha_k) + \sum_{d=1}^D x_n^d \log(f_\varepsilon(\mu_k^d)) \right) + \left(1 - x_n^d\right) \log(f_\varepsilon(1 - \mu_k^d))
\]

where

\[
f_\varepsilon(\mu) = \mu + \frac{\varepsilon}{2} \log \left( \frac{\mu}{1 - \mu} \right).
\]

Note that \( f_\varepsilon(\mu) \in (0, 1) \) for \( \mu \in (\delta_\varepsilon, 1 - \delta_\varepsilon) \), for some appropriate constant \( \delta_\varepsilon \in (0, 1) \) with \( \lim_{\varepsilon \to 0^+} \delta_\varepsilon = 0 \). Hence the functional \( \tilde{L}_\varepsilon \) is defined for \( \mu \in (\delta_\varepsilon, 1 - \delta_\varepsilon) \) and, for \( \varepsilon > 0 \), the MFG system (14) gives non degenerate multinomial Bernoulli distributions.

4. A Mean Field Games approach to mixture models of categorical distributions. In the classification of handwritten digits previously described, the components of the random variable \( X \), which generates the data set \( \mathcal{X} \), can take only one of two possible values, i.e. 0 and 1 corresponding to a white or a black pixel. In other models, see for example the Fashion-MNIST dataset [11], a discrete random variable can take only one of a certain number \( S \) of mutually exclusive states. In this case, \( X \) is called a categorical random variable. In this section, we introduce a MFG approach to the optimization of the parameters for a mixture of categorical distributions, i.e. discrete probability measures associated with a categorical random variable.

We denote by \( S = \{1, \ldots, S\} \) the state space of a component \( X_d \) of \( X \). A probability measure on the state space \( S \) can be identified with a vector \( p \in \mathbb{S} \), where \( \mathbb{S} = \{p = (p(1), \ldots, p(S)) : p(i) \geq 0, \sum_{i=1}^S p(i) = 1\} \) is the probability simplex. The set of the \( S \times S \) stochastic matrices is identified with \( \mathbb{S}^S \).

We assume that the data set \( \mathcal{X} \) is generated by the i.i.d. observations of a random variable \( X \) in \( \mathbb{R}^D \), whose components \( X_d \) are mutually independent categorical random variables with values in \( S \). In order to find a representation of the distribution of \( X \), we consider the mixture

\[
\pi(x) = \sum_{k=1}^K \alpha_k \pi_k(x), \quad x = (x^1, \ldots, x^D) \in \mathcal{S}^D,
\]

where each measure \( \pi_k \) is given by

\[
\pi_k(x) = \prod_{d=1}^D \pi_k^d(x^d),
\]

with \( \pi_k^d \in \mathbb{S}, \quad d = 1, \ldots, D, \) a categorical distribution. Note that (23) is consequence of the assumption that the components of \( X \) are mutually independent. We denote with \( \mathcal{P} \) the space of the multinomial categorical measures, i.e. the space of the measures defined as in (23). We also identify a measure \( \pi_k \) on \( \mathcal{S}^D \) with a vector \( \pi_k = (\pi_1^k, \ldots, \pi_D^k) \) such that \( \pi_k^d \in \mathbb{S} \).

Remark 3. The Fashion-MNIST dataset is composed of grey-scale, 28 \times 28 pixels images of 10 different types of fashion products. In this case we have \( D = 784 \), corresponding to the pixels of the images, \( S = 256 \), corresponding to the grey-scale
levels of a single pixel, and \( K = 10 \), corresponding to the different fashion objects in the dataset.

Given the data set \( \mathcal{X} = \{ x_n \} \), for \( k = 1, \ldots, K \) we define the responsibilities by

\[
\gamma_k(x_n) = \mathbb{P}[Y_k = 1|X = x_n] = \frac{\alpha_k \pi_k(x_n)}{\pi(x_n)} \quad n = 1, \ldots, N.
\]

(24)

and the vector \( \theta_k = (\theta_k^1, \ldots, \theta_k^D) \in \mathbb{S}^D \), \( \theta_k^d = (\theta_k^d(1), \ldots, \theta_k^d(S)) \in \mathbb{S} \), by

\[
\theta_k^d(i) = \frac{\sum_{n=1}^N \gamma_k(x_n)[x_n^d = i]}{\sum_{n=1}^N \gamma_k(x_n)} \quad i = 1, \ldots, S
\]

(25)

(here the Iverson brackets \( [x_n^d = i] \) evaluate 1 if the realization of the random variable \( X^d \) corresponding to the \( n^{th} \) entry of the data set \( \mathcal{X} \) assumes state \( i \), 0 otherwise). The vector \( \theta_k \) represents the weighted probabilities of the random variable \( X^d \) with respect to the \( k^{th} \) component of the mixture computed on the data set \( \mathcal{X} \). For \( k = 1, \ldots, K \), \( d = 1, \ldots, D \) and \( i = 1, \ldots, S \), we consider the multi-population MFG system

\[
\begin{align*}
V_k^d(i) &= \min_{P_{ij} \geq 0, \sum_{P_{ij}} = 1} \left\{ \sum_{j=1}^S P_{ij} \left( c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta_k^d(j)) \right) \right\} - \lambda_k^d, \\
\pi_k^d(i) &= \sum_{j=1}^S P_{ij} \pi_k^d(j), \\
\pi_k^d(i) &\geq 0, \quad \sum_{i=1}^S \pi_k^d(i) = 1, \quad \sum_{i=1}^S V_k^d(i) = 0, \\
\alpha_k &= \frac{1}{N} \sum_{n=1}^N \gamma_k(x_n),
\end{align*}
\]

(26)

where the transition matrix \( P_k \) in the Fokker-Planck equation is composed of rows \( P^d_i = \{ P^d_{ij} \}_{j=1}^S \) which realize the minimum in the Hamilton-Jacobi-Bellman equation. Note that, for the optimal values of \( P_i \), \( c(P_{ij}) \) is a transition cost from the state \( i \) to the state \( j \) and the entropy penalization term \( \varepsilon \log(P_{ij}) \) enforces the agent to diversify their choices, so that \( P_{ij} > 0 \) for any \( i, j = 1, \ldots, S \). We assume that \( c \in \mathcal{C}^1([0,1]) \) with \( pc(p) \) convex for \( p \in [0,1] \) and \( F : \mathbb{S} \times \mathbb{S} \to \mathbb{R} \) is such that \( F(i, \cdot) \) is bounded and continuous for all \( i \in S \).

A solution of (26) is a family of quadruples \( \{ V_k, \lambda_k, \pi_k, \alpha_k \} \), \( k = 1, \ldots, K \), where

\[
\begin{align*}
V_k &= (V_k^1, \ldots, V_k^D), & \quad V_k^d &= (V_k^d(1), \ldots, V_k^d(S)) \in \mathbb{R}^S, & d = 1, \ldots, D; \\
\lambda_k &= (\lambda_k^1, \ldots, \lambda_k^D), & \quad \lambda_k^d \in \mathbb{R}, & d = 1, \ldots, D; \\
\pi_k &= (\pi_k^1, \ldots, \pi_k^D), & \quad \pi_k^d &= (\pi_k^d(1), \ldots, \pi_k^d(S)) \in \mathbb{S}, & d = 1, \ldots, D; \\
\alpha_k &= 0, & \quad \alpha_k \in [0,1].
\end{align*}
\]

As observed in the previous section, for fixed \( d \in \{ 1, \ldots, D \} \), (26) gives a \( K \)-populations MFG system on a \( S \)-states space. The system is globally coupled by means of the vectors \( \theta_k^d \), which depend on the full measure \( \pi \) via the responsibilities \( \gamma_k \), and by means of the weights \( \alpha_k \). Note that, a priori, the responsibilities are not well defined since \( \pi \) could vanish for some \( x_n \in \mathcal{X} \). However, we will prove in Theorem 4.1 that, due to the entropy penalization term, there exists a solution of (26) for which \( \pi \) cannot vanish on the data set \( \mathcal{X} \) and therefore \( \gamma_k \) and \( \theta_k^d \) are well defined.

**Theorem 4.1.** For any \( \varepsilon > 0 \), there exists a solution \( \{ V_k, \lambda_k, \pi_k, \alpha_k \} \), \( k = 1, \ldots, K \), of (26).
Proof. We define the

$$D = \left\{ (\alpha, \pi) = (\alpha_1, \ldots, \alpha_K, \pi_1, \ldots, \pi_K) : \alpha_k \in [0, 1], \sum_{k=1}^K \alpha_k = 1, \right\}$$

$$\pi_k = \prod_{d=1}^D \pi^d_k \in \mathcal{P}, \min_{i \in S} \pi^d_k(i) \geq \delta > 0, d = 1, \ldots, D \right\},$$

(27)

where $\delta$ is a constant to be fixed later. It is easy to see that $D$ is a convex and compact set with respect to the topology of $\mathbb{R}^K \times (\mathcal{S}^D)^K$. We define a map $\Psi$ on $D$ in the following way:

Given $(\alpha, \pi) \in D$, we set for $k = 1, \ldots, K$

$$\gamma_k(x_n) = \frac{\alpha_k \pi_k(x_n)}{\sum_{k=1}^K \alpha_k \pi_k(x_n)}, \quad n = 1, \ldots, N \quad (28)$$

and

$$\theta^d_k(i) = \frac{\sum_{n=1}^N \gamma_k(x_n) [x^d_n = i]}{\sum_{n=1}^N \gamma_k(x_n)}, \quad d = 1, \ldots, D \quad (29)$$

where $$\pi_k \in \mathcal{P}, \min_{i \in S} \pi_k(i) \geq \delta > 0, \quad \forall x \in \mathcal{S}^D, \quad (28)$$

and $\theta^d_k = (\theta^d_k(1), \ldots, \theta^d_k(S))$.

Note that, since $\min_{i \in S} \pi^d_k(i) \geq \delta > 0$, then $\pi_k(x) \geq \delta^D$ for any $x \in \mathcal{S}^D$, and therefore

$$\sum_{k=1}^K \alpha_k \pi_k(x_n) \geq \delta^D, \quad n = 1, \ldots, N. \quad (30)$$

Hence $\gamma_k$ and $\theta^d_k$ in (28) and (29) are well defined. For each $d = 1, \ldots, D$, we consider the $K$-populations $S$-states space MFG system

$$\begin{cases}
V^d_k(i) = \min_{P_{ij} \geq 0} \left\{ \sum_{j=1}^S P_{ij} \left[ c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta^d_k) + V^d_k(j) \right] \right\} - \lambda^d_k \\
\rho^d_k(i) = \sum_{j=1}^S P_{ij} \rho^d_k(j) \\
\rho^d_k(i) \geq 0, \quad \sum_{i=1}^S \rho^d_k(i) = 1, \quad \sum_{i=1}^S V^d_k(i) = 0
\end{cases}$$

(31)

for $i = 1, \ldots, S$, where the transition matrix $P^k$ in the Fokker-Planck equation is composed of rows $P^k = \{P^k_{ij}\}_{j=1}^S$ which realize the minimum in the Hamilton-Jacobi-Bellman equation. Since the coefficients $\theta^d_k(i)$ are given (see (29)), the previous systems are not coupled with respect to the index $d$. By Theorem A.4, for any $d = 1, \ldots, D$, there exists a unique solution $(V^d_k, \lambda^d_k, \rho^d_k)$ to (31) with

$$\min_{i \in S} \rho^d_k(i) \geq C(\varepsilon) > 0, \quad k = 1, \ldots, K. \quad (32)$$

Set $\rho = (\rho_1, \ldots, \rho_K)$, where for any $k = 1, \ldots, K$ the vector $\rho_k = (\rho^d_k, \ldots, \rho^D_k) \in \mathcal{P}$ has components given by the solutions $\rho^d_k$ of (31), and

$$\beta_k = \frac{1}{N} \sum_{n=1}^N \gamma_k(x_n).$$

Then, the map $\Psi$ is defined by $\Psi(\alpha, \pi) = (\beta, \rho)$. Fixing the constant $\delta$ in (27) smaller than the constant $C(\varepsilon)$ in (32), then it follows that $\Psi$ maps the set $D$ into itself. We prove that $\Psi$ is a continuous map on $D$ with respect to the topology of $\mathbb{R}^K \times (\mathcal{S}^D)^K$. Consider a sequence $((\alpha^{(h)}, \pi^{(h)}), D, h \in \mathbb{N}$, converging to $(\alpha, \pi) \in D$.
and denote by \((\rho^{(h)}, \beta^{(h)}), (\rho, \beta)\) the corresponding images by means of \(\Psi\). Given the vector \((\theta^{d(h)}_k)\) whose components are defined by

\[
(\theta^{d(h)}_k(i)) = \frac{\sum_{n=1}^{N} \gamma^{(h)}_k(x_n)[x_n = i]}{\sum_{n=1}^{N} \gamma^{(h)}_k(x_n)}, \quad k = 1, \ldots, K, \quad d = 1, \ldots, D,
\]

and recalling (30), it is immediate that \((\theta^{d(h)}_k(i)) \to \theta^{d(i)}(i)\) for \(h \to \infty\), hence \((\theta^{d(h)}_k) \to \theta^d_k\) for \(h \to \infty\) for any \(k = 1, \ldots, K, \quad d = 1, \ldots, D\). By continuity, \(F(i, (\theta^{d(h)}_k))\) converges to \(F(i, \theta^d_k)\). By Lemma A.2 and A.3, it follows that the vectors \(P_i^{(h)}\), which attain the minimum in the first equation of (31) for \(((V^{d(h)}_k), (\lambda^{d(h)}_k))\), converge to the corresponding vector \(P_i\) which attains the minimum in the first equation of (31) for \(((V^d_k), (\lambda^d_k))\). Since the transition matrices \(P^{(h)}\), composed of the rows \(P_i^{(h)}\), \(i = 1, \ldots, S\), converge to the transition matrix \(P\), composed of the rows \(P_i\), \(i = 1, \ldots, S\), it follows that the corresponding invariant distribution \((\rho^{d(h)}_k)\) converge to \(\rho^d_k\), \(d = 1, \ldots, D\) and therefore \((\rho_k)^{(h)} = \prod_{d=1}^{D} (\rho^{d(h)}_k)\) converges to \(\rho_k = \prod_{d=1}^{D} \rho^d_k\). Moreover, recalling (32), it follows that \(\beta^{d(h)}_k\) converges to \(\beta_k\). Hence the map \(\Psi\) is continuous.

By the Brouwer’s fixed point Theorem, there exists \((\alpha, \pi) \in \mathcal{D}\) such that \(\Psi(\alpha, \pi) = (\alpha, \pi)\) and therefore a solution to (26).

Note that, in this framework, it is, in general, not reasonable to obtain uniqueness for the system (26), since the log-likelihood functional can not be concave. This also corresponds to the fact that, in cluster analysis, there may be several admissible partitions of a given data set. As for the case \(S = 2\), see Proposition 1, it is possible to show that, identifying the state \(i \in S\) with the vertex of coordinate

\[
T_i = (0, \ldots, 1_i, \ldots, 0)
\]

of the simplex in \(\mathbb{R}^S\), taking \(c(p) = -(1-p)/2\) and \(F(i, \theta)\) equal to the square of distance of \(\theta\) from \(T_i\), then the solutions of the MFG system (26) for \(\varepsilon = 0\) are associated with the critical points of the the log-likelihood functional for a mixture of categorical distributions.

**Remark 4.** Theorem 4.1 provides an existence result to the MFG system (26) only for \(\varepsilon > 0\). For \(\varepsilon = 0\), estimate (32) no longer holds and (30) no longer applies. Therefore, it is not guaranteed that the responsibilities \(\gamma_k\) in (24) are well defined. On the other hand, for \(\varepsilon \to 0\), it is possible to prove that, up to a subsequence, the vector \(\theta^d_k\), defined in (25) converges to a vector \(\tilde{\theta}^d_k \in \mathcal{S}\) and, moreover, the solution of (26) converges to a solution of (26) with \(\varepsilon = 0\) and cost \(F(i, \tilde{\theta}^d_k)\). The point is that we cannot characterize \(\tilde{\theta}^d_k\) by a formula equivalent to (25) since again we cannot exclude that the responsibilities \(\gamma_k\), corresponding to the solution of the limit system, vanish for some value \(x_n \in \mathcal{X}\).

**Remark 5.** For the simplicity of the notation, we assumed that all the components \(X^d\) of the random variable \(X\), which generates the data set, are \(S\)-dimensional categorical random variables. Nevertheless, it is possible to assume that they have state spaces of different dimension \(S_d\), for each \(d = 1, \ldots, D\). In this case, also the MFG systems (26) are defined on states spaces of dimension \(S_2\) and the results of this section can be easily reformulated in this more general framework.
5. Numerical approximation and examples. In this section we present the main idea for the numerical solution of the MFG system (26), then we apply the resulting algorithm to some classical tests in cluster analysis. For the reader’s convenience, we recall the MFG system here: for $k = 1, \ldots, K$, $d = 1, \ldots, D$ and $i = 1, \ldots, S$,

$$
\begin{align*}
V^d_k(i) &= \min_{\pi_{ij} \geq 0, \sum_j \pi_{ij} = 1} \left\{ \sum_{j=1}^S \pi_{ij} (c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta_k^d) + V^d_k(j)) \right\} - \lambda^d_k, \\
\pi^d_k(i) &= \sum_{j=1}^S P_{ij} \pi^d_k(j), \\
\pi^d_k(i) &\geq 0, \sum_{i=1}^S \pi^d_k(i) = 1, \sum_{i=1}^S V^d_k(i) = 0,
\end{align*}
$$

As discussed in Section 4, this system depends on the dimension $S$ of the state space, the number $K$ of populations, and also on the number $D$ of components of the categorical random variable associated to the mixture. This yields a possibly huge non linear problem of size $S \times K \times D$, which is fully coupled, since the parameters $\theta_k$, $k = 1, \ldots, K$, appearing in the cost $F$ depend, through the responsibilities $\gamma_k$, on the whole mixture $\pi$. Moreover, each Hamilton-Jacobi-Bellman equation in the system includes an optimization problem for the optimal controls in the transition matrix $P$.

Following the strategy of the classical EM algorithm, we can mitigate the computational efforts by reducing the above system to $P$ independent sub-systems of size $S$. More precisely, we devise the following iterative procedure, in which each iteration is split into two steps: starting from an arbitrary guess $\alpha_k^{(0)}$, $\pi_k^{(0)}$ for the components of the mixture (22), iterate on $h \geq 0$:

E-step: for $k = 1, \ldots, K$ compute the new responsibilities and weights

$$
\gamma_k^{(h+1)}(x_n) = \frac{\alpha_k^{(h)} \pi_k^{(h)}(x_n)}{\sum_{k=1}^K \alpha_k^{(h)} \pi_k^{(h)}(x_n)}, \quad \alpha_k^{(h+1)} = \frac{1}{N} \sum_{n=1}^N \gamma_k^{(h+1)}(x_n),
$$

and the parameters $\theta_k$ of the components of the mixture

$$
(\theta_k^d)^{(h+1)}(i) = \frac{\sum_{n=1}^N \gamma_k^{(h+1)}(x_n) P_{ij}^d}{\sum_{n=1}^N \gamma_k^{(h+1)}(x_n)}, \quad d = 1, \ldots, D, \quad i = 1, \ldots, S.
$$

M-step: for $k = 1, \ldots, K$, $d = 1, \ldots, D$ solve the $S$-state space MFG sub-system

$$
\begin{align*}
V^d_k(i) &= \min_{\pi_{ij} \geq 0, \sum_j \pi_{ij} = 1} \left\{ \sum_{j=1}^S \pi_{ij} (c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, (\theta_k^d)^{(h+1)}) + V^d_k(j)) \right\} - \lambda^d_k, \\
\pi^d_k(i) &= \sum_{j=1}^S P_{ij} \pi^d_k(j), \\
\pi^d_k(i) &\geq 0, \sum_{i=1}^S \pi^d_k(i) = 1, \sum_{i=1}^S V^d_k(i) = 0,
\end{align*}
$$

to obtain the new mixture components $\pi_k^{(h+1)}$. 

For a fixed tolerance $\tau > 0$, convergence can be checked by evaluating in a suitable norm the condition $\|\theta^{(h+1)} - \theta^{(h)}\| < \tau$. For instance one can reinterpret $\theta^{(h)}$ as a vector in $\mathbb{R}^{S \times K \times D}$ and simply take the Euclidean norm.

Note that in this EM-like formulation, the coupling is all embedded in the E-step, whereas the M-step can be completely parallelized. Moreover, each MFG subsystem indexed by $(k, d)$ is also decoupled, since the dependency of $(\theta_k^d)^{(h+1)}$ on $\pi$ is frozen at the previous iteration. Hence, the building block of the algorithm is just a simple linear system with linear constraints.

This results in a linear system in the $\theta$-norm the condition

$$\sum_{i=1}^{S} V(i) = 0,$$

where the transition matrix $P$ in the Fokker-Planck equation is composed of rows $P_i = \{P_{ij}\}_{j=1}^{S}$ which realize the minimum in the HJB equation. For the Hamilton-Jacobi-Bellman equation, we employ a standard policy iteration algorithm. More precisely, starting from a guess for the optimal transition matrix $P^{(0)}$, we introduce an inner iteration $m \geq 0$ by taking $P^{(m)}$ as minimizer:

$$V^{(m)}(i) = \sum_{j=1}^{S} P^{(m)}_{ij} \left( c(P^{(m)}_{ij}) + \varepsilon \log(P^{(m)}_{ij}) + F(i, \theta(i)) + V^{(m)}(j) \right) - \lambda^{(m)},$$

$$\sum_{i=1}^{S} V^{(m)}(i) = 0.$$

This results in a linear system in the $S + 1$ unknowns $(V^{(m)}(1), \ldots, V^{(m)}(S), \lambda^{(m)})$, whose solution is then plugged back in the optimization problem for $P$ to get $P^{(m+1)}$:

$$P^{(m+1)} = \arg\min_{P_{ij} \geq 0, \sum_j P_{ij} = 1} \left\{ \sum_{j=1}^{S} P_{ij} \left( c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta(i)) + V^{(m)}(j) \right) \right\}$$

Iterations on $m$ are performed up to convergence $\|P^{(m+1)} - P^{(m)}\| < \tau$.

Note that, under the assumptions made on the transition cost, each optimization problem for $P$ is convex with linear constraints $\sum_{i=1}^{S} P_{ij} = 1$, and it can be readily solved with classical algorithms.

Finally, the optimal transition matrix $P$ is plugged in the Fokker-Planck equation, yielding again a simple linear system with linear constraints.

We have to remark that, at present, the proposed algorithm is just heuristic, supported by numerical evidence only, and a complete proof for its convergence is still under investigation. While convergence of the policy iteration method for Hamilton-Jacobi-Bellman equations is a quite well established subject in the literature, at least in the continuous setting (see [2, 12, 15, 23, 22]), a policy iteration method for MFG systems seems new and not much explored yet (see [6]). Here, further difficulties appear in the additional coupling with the expectation step of the algorithm. Nevertheless, we stress that, at this early stage, the aim of the present work is to provide a new perspective to cluster analysis, more than introduce a new method computationally competitive with classical algorithms. We believe that a better understanding of the proposed MFG formulation of the problem, including
the case of more general costs, and an analysis on how these choices affect the resulting clusterization, could reveal additional features of the data set, exploiting its structure in a deeper way.

We now consider some classical examples in cluster analysis, in order to show that the MFG approach produces reasonable results. It is important to remark that the solution of the full $K$-populations MFG system is in general not unique, hence the numerical solution obtained with the proposed algorithm depends on the choice of the initial guess $\alpha^{(0)}_k$, $\pi^{(0)}_k$, for $k = 1, \ldots, K$. In the following experiments we always choose $\alpha^{(0)}_k = 1/K$, while $\pi^{(0)}_k$ is built using random numbers in $(0,1)$. Moreover, we choose the costs $c(p) = -(1-p)/2$ and $F(i, \theta) = |\theta - T_i|^2$, identifying the state $i \in S$ with the vertex of coordinate $T_i = (0, \ldots, 1, \ldots, 0)$ of the simplex in $\mathbb{R}^S$. We also set $\varepsilon = 0.05$ in order to justify the computational efforts of our algorithm, namely ensuring that our solution does not coincide with the explicit one produced by the EM algorithm for $\varepsilon = 0$. A detailed comparison with the EM and other classical algorithms, including convergence rates and performance tests, is beyond the scope of the present paper, and it will be addressed in a more computational oriented work.

We first consider the case of Bernoulli mixtures, i.e. $S = 2$, taking as dataset the MNIST database of handwritten digits [19], see Figure 1. We recall that the database contains 60000 images of the digits $\{0, \ldots, 9\}$, each composed by $28 \times 28$ pixels in 256 grey levels, that we turn (via hard-threshold) in monochrome images and represent by binary vectors of size $D = 784$. Moreover, we remark that each sample in the database is already labelled by the number of the corresponding digit, that we use to check the correctness of the clusterization. To this end, given $1 \leq K \leq 10$, we select $K$ digits $d_1, \ldots, d_K$ in $\{0, \ldots, 9\}$, and we run our algorithm to compute the Bernoulli parameters $\mu_k$ of the mixture components, for $k = 1, \ldots, K$. Then we introduce a matrix $H$ of size $K \times K$, whose entries are obtained as follows. For each sample $x$ of type $d_k$, we compute the corresponding responsibilities $\gamma_1(x), \ldots, \gamma_K(x)$, and we accumulate these values in the $k$-th row of $H$, normalizing their sum with respect to the number of samples in $d_k$. More precisely, for $k, j = 1, \ldots, K$

$$H_{kj} = \frac{1}{|d_k|} \sum_{x \in d_k} \gamma_j(x)$$

provides the averaged probability, for a sample of type $d_k$, of belonging to the cluster $j$. Up to a permutation of the rows, namely a reordering of the mixture components, we can always assume that the maximal values of $H$ correspond to the diagonal entries, so that digits of type $d_k$ will belong, with the highest probability, to the cluster $k$. In a perfect clusterization, $H$ is clearly the identity matrix, but we recall that each Bernoulli distribution $\pi_k$ is built as a joint probability of all the observed pixel values (12). Since the samples of type $d_k$ can be very different from each other, and also share some similarity with samples of other types (see Figure 2), we can never expect such a sharp partition.

For visualization purposes we represent each row of the matrix $H$ as a histogram, reporting on the $x$-axis the type $d_k$, for $k = 1, \ldots, K$, and assigning $K$ different colors to the values $H_{kj}$ for $j = 1, \ldots, K$, corresponding to the $K$ clusters $C_1, \ldots, C_K$. Moreover, since the state space dimension is $S = 2$, we can conveniently represent the parameters $\mu_k \in [0, 1]^D$ of the corresponding Bernoulli distributions in the mixture, for $k = 1, \ldots, K$, as grey scale images.
Let us start with the case $K = 2$, choosing the digits 1, 3. In Figure 3, we show the clusterization histogram and the corresponding Bernoulli parameters, observing that the samples of the two digits are very well separated.

![Figure 3. Clusterization histogram for digits 1, 3 and the corresponding Bernoulli parameters.]

We now choose the digits 3, 5, and we show the results in Figure 4. In this case, we observe that the clusterization is slightly ambiguous, since, in average, the samples of the two types are more similar to each other (see the corresponding Bernoulli parameters). In the histogram we clearly see a repartition of about 60% and 40% (and viceversa) between the two clusters.

![Figure 4.](image)

We finally consider the case $K = 5$ with even digits 0, 2, 4, 6, 8. In Figure 5, we observe that the chosen digits are, in average, different from each other, so that they are quite well clusterized.

It is worth noting that the greatest error in the cluster assignment correspond to digit 6, which indeed shares about 15% of its samples with the cluster of the digit 2. Looking at the corresponding Bernoulli parameters, we readily see that the
two images have very similar vertical alignments, and also a quite large overlapping bottom region. In particular, the Bernoulli parameter for the digit $2$ is visibly more diffused, and this reflects the inhomogeneity of the corresponding samples. Similar considerations also apply to the pairs of digits $2, 4$ and $4, 8$, with errors in the cluster assignment below 10%.

We now consider the case of categorial distributions, i.e. $S > 2$, taking as dataset the Fashion-MNIST database [11], see Figure 6.

The database contains 60000 images of ten categories of fashion products, namely \{T-shirt, Trouser, Pullover, Dress, Coat, Sandal, Shirt, Sneaker, Bag, ...\}.
Figure 6. Samples of fashion products from the Fashion-MNIST database

\textbf{Boot}, each composed by $28 \times 28$ pixels in 256 grey levels. We turn these images (via hard-thresholding) in images with $S$ grey levels, and represent them by vectors in $\mathbb{R}^D$, where $S = \{1, \ldots, S\}$ and $D = 784$. As in the previous tests, we use the label associated to each sample in the database to build the clusterization histogram. Moreover, we visualize the parameters $\theta_k(i) \in [0, 1]^D$ of the corresponding categorical distributions in the mixture, for $i = 1, \ldots, S$ and $k = 1, \ldots, K$, as grey scale images, i.e. averaging the values with respect to $i$ as $\bar{\theta}_k = \frac{1}{S} \sum_{i=1}^{S} \theta_k(i)$.

In this example, clusterization is very challenging. To give an idea of the issues, we set $S = 32$ and compute separately ten “ideal” categorical distributions associated to the dataset, by simply averaging the pixel values of all the samples of a same type. The result is shown in Figure 7.

Figure 7. Averaged categorical distributions for the Fashion-MNIST database

We clearly see that types \textbf{Pullover}, \textbf{Coat} and \textbf{Shirt} are almost indistinguishable. Moreover, they all have a very large overlap region with the type \textbf{T-shirt}, but also with the types \textbf{Trouser} and \textbf{Dress}. Finally, we observe that the samples of type \textbf{Sandal} are so different from each other that the corresponding distribution is completely smoothed out. As one can expect, such drawbacks dramatically affect the quality of the clusterization, but they also suggest how the present model could be improved, for instance including in the cost functions some geometric correlation between the image pixels. This direction of research is currently under development.
We conclude this section with the following tests, which confirm the above considerations. We set $K = 2$ and choose the types \textbf{T-shirt} and \textbf{Trouser}. In Figure 8, we show the resulting clusterization histogram and the corresponding categorical parameters.

Despite the clusterization being still “acceptable” (in average more than 60% of samples correctly assigned to the corresponding clusters), we clearly observe a weird mixing of the two types. On the other hand, choosing types which are substantially different from each other, we end up with a good clusterization. This is the case for the example shown in Figure 9, where we set $K = 4$ and choose the types \textbf{Dress}, \textbf{Sneaker}, \textbf{Bag} and \textbf{Boot}.

![Figure 8. Clusterization histogram for types T-shirt, Trouser and the corresponding categorical parameters.](image)

![Figure 9. Clusterization histogram for types Dress, Sneaker, Bag, Boot and the corresponding categorical parameters.](image)
### Appendix A. A two-states ergodic MFG system

In this section, we study some properties of a particular MFG system we need for the analysis performed in Section 4. In this case, the cost in the Hamilton-Jacobi-Bellman equation does not depend on the distribution of the population, hence the coupling term is only in the Fokker-Planck equation which characterizes the stationary distribution. Here we mainly follow the notations in [13].

Given a matrix $P \in S^S$, we denote with $P_i$ the $i$-th row of $P$. For $\varepsilon > 0$, we consider MFG system

\[
\begin{align*}
V(i) &= \min_{P_i: P_{ij} \geq 0, \sum_j P_{ij} = 1} \left\{ \sum_{j=1}^S P_{ij} \left( c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta) + V(j) \right) \right\} - \lambda \\
\pi(i) &= \sum_{j=1}^S P_{ij} \pi(j) \\
\pi(i) &\geq 0, \sum_{i=1}^S \pi(i) = 1, \sum_{i=1}^S V(i) = 0
\end{align*}
\]

for $i = 1, \ldots, S$, where $\varepsilon > 0$ and the components of the vector $\theta = (\theta(1), \ldots, \theta(S)) \in S$ are fixed parameters and the transition matrix $P$ in the Fokker-Planck equation is composed of the rows

\[
P_i = \{P_{ij}\}_{j=1}^S
\]

which realize the minimum in the Hamilton-Jacobi-Bellman equation. The transition cost from the state $i$ to the state $j$ is given by

\[C^c(P_{ij}, \theta) = c(P_{ij}) + \varepsilon \log(P_{ij}) + F(i, \theta), \quad i, j = 1, \ldots, S.
\]

We assume that the cost function $c \in C^1([0, 1])$ with $pc(p)$ convex for $p \in [0, 1]$ and $F: S \times S \to \mathbb{R}$ is such that $F(i, \cdot)$ is bounded and continuous for all $i \in S$.

The average cost in the state $i$ for a given choice of the transition matrix $P$ is defined by

\[e_i(P, V) = \sum_{j=1}^S (C^c(P_{ij}, \theta) + V(j)) P_{ij} \quad i = 1, \ldots, S
\]

and we denote with $e(P, V)$ the corresponding $S$-dimensional vector. Note that $e_i(P, V)$ depends only on the $i$-th row of the matrix $P$.

We introduce the definition of Nash minimizer for $e(P, V)$ (see [13, Definition 1]). Given the stochastic matrix $P \in S^S$ and a probability vector $q \in S$, we denote with $\mathcal{R}(P, q, i)$ the stochastic matrix obtained by replacing the $i$-th row of $P$ with the vector $q$.

**Definition A.1.** Given a cost vector $V \in \mathbb{R}^S$, a stochastic matrix $P$ is said to be a Nash minimizer for $e(P, V)$ if for each $i = 1, \ldots, S$, $q \in S$, it holds

\[e_i(P, V) \leq e_i(\mathcal{R}(P, q, i), V).
\]

**Proposition 2.** For each vector $V \in \mathbb{R}^S$, there exists a unique Nash minimizer $P$ for $e(P, V)$.

**Proof.** As proved in [13, Theorem 1], existence of a Nash minimizer $P$ follows by the continuity and convexity of the cost $e_i(P, V)$ with respect to the vector $P_i$, $i = 1, \ldots, S$. Moreover, a straightforward computation gives that the function $g: S^S \to S^S$, defined by $g_{ij}(P) = \partial e_i(P, V) / \partial P_{ij}$, is diagonally convex, i.e. for all
$P^1, P^2 \in \mathcal{S}^S$, $P^1 \neq P^2$, it holds
\[
\sum_{ij} (P^1_{ij} - P^2_{ij})(g_{ij}(P^1) - g_{ij}(P^2)) > 0.
\]
Indeed, for any $i, j \in \{1, \ldots, S\}$ and $P \in \mathcal{S}^S$, we have
\[
\frac{\partial \varepsilon_i(P,V)}{\partial P_{ij}} = P_{ij}(c_i(P_{ij}) + \varepsilon \frac{1}{P_{ij}}) + c_{ij}(P_{ij}) + \varepsilon \log(P_{ij}) + V(j) + F(i, \theta).
\]
Hence,
\[
(P^1_{ij} - P^2_{ij})(g_{ij}(P^1) - g_{ij}(P^2)) = \varepsilon(P^1_{ij} - P^2_{ij}) \log \left( \frac{P^1_{ij}}{P^2_{ij}} \right)
+ P^1_{ij}c_i(P^1_{ij}) - P^2_{ij}c_i(P^2_{ij}) - (P^2_{ij}c_i(P^1_{ij}) + c(P^1_{ij})) - (P^1_{ij}c_i(P^1_{ij}) + c(P^2_{ij})) - (P^2_{ij} - P^1_{ij})) > 0,
\]
because of the monotonicity of $\log(p)$ and the convexity of $pc(p)$ for $p \in [0, 1]$. By [13, Theorem 2], we get the uniqueness of the Nash minimizer.

We now prove that $\pi$ has positive mass for any state $i = 1, \ldots, S$. This is a crucial result for the existence of a solution to the multi-population MFG system studied in Section 4. We need some preliminary results.

**Lemma A.2.** For any vector $\theta \in \mathcal{S}$, there exists a unique solution $(\lambda_\theta, V_\theta)$ to the Hamilton-Jacobi-Bellman equation
\[
\begin{cases}
V(i) = \min_{P_i} \left\{ \frac{\sum_{j=1}^{S} (C^c(P_{ij}, \theta) + V(j)) P_{ij}}{P_i} \right\} - \lambda \\
\sum_{i=1}^{S} V(i) = 0.
\end{cases}
\]
Moreover, if $\theta \to \bar{\theta}$, then $(\lambda_\theta, V_\theta)$ converges to $(\lambda_{\bar{\theta}}, V_{\bar{\theta}})$.

**Proof.** Existence and uniqueness of a solution to (34) follows from [13, Proposition 8 and Theorem 4]. Indeed, since the cost in the Hamilton-Jacobi-Bellman equation is independent of the distribution $\pi$, the assumptions of Proposition 8 and Theorem 4 in [13] are trivially satisfied. The convergence of $(\lambda_\theta, V_\theta)$ to $(\lambda_{\bar{\theta}}, V_{\bar{\theta}})$ follows by the continuity of the costs $e_i(P, V)$ with respect to $\theta$ and the uniqueness of the solution to (34).

Proposition 2 and the continuity of the average cost $e_i(P, V)$ implies the continuity of the Nash minimizer (see [13, Proposition 1]).

**Lemma A.3.** The Nash minimizer $P(V)$ is a continuous function of $V$.

**Theorem A.4.** For any vector $\theta \in \mathcal{S}$, there exists a unique solution $(V_\theta, \lambda_\theta, \pi_\theta) \in \mathbb{R}^S \times \mathbb{R} \times \mathcal{S}$ to (33). Moreover, there exists a positive constant $c(\varepsilon) \in (0, 1)$ such that, for each $\theta \in \mathcal{S}$ and for each $i = 1, \ldots, S$
\[
\pi_\theta(i) \geq c(\varepsilon) > 0.
\]

**Proof of Theorem A.4.** Note that, because of the particular structure of the system (33), Propositions 2 and A.2 immediately ensure existence and uniqueness of a solution to (33).

To show (35), we argue by contradiction assuming that there exists a sequence $\theta_n \in \mathcal{S}$ such that $\pi_{\theta_n}(i_n) \to 0$ for $n \to \infty$. Since the state space is finite we assume
that, up to a subsequence, \( i_n = i \) for any \( n \). Let \( \theta \in S \) be such that, up to a subsequence, \( \theta_n \rightarrow \theta \). By Lemma A.2 and A.3, it follows that \( P(V_{\theta_n}) \rightarrow P(V_{\theta}) \), where \( P(V_{\theta_n}) \) and \( P(V_{\theta}) \) are the Nash minimizers corresponding to the solution of (34) with \( \theta_n \) and, respectively, with \( \theta \). By the equation
\[
\pi_{\theta_n} = \pi_{\theta_n} P(V_{\theta_n}),
\]
satisfied by the invariant distribution associated to \( P(V_{\theta_n}) \), we get that, up to a subsequence, \( \pi_{\theta_n} \) converges to \( \bar{\pi} \in S \) satisfying
\[
\bar{\pi} = \bar{\pi} P(V_{\theta}),
\]
with \( \pi(i) = 0 \). But, because of entropy regularization term, all the entries \( P_{ij} \) of the transition matrix \( P(V_{\theta}) \) are strictly positive, hence \( P \) is a positive matrix and the associated invariant distribution satisfies \( \pi(i) > 0 \) for each \( i = 1, \ldots, S \). By the contradiction, we obtain 35.

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