Clustering through the optimal transport barycenter problem

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Abstract

The problem of clustering a data set is formulated in terms of the Wasserstein barycenter problem in optimal transport. The objective proposed is the maximization of the variability attributable to class, further characterized as the minimization of the variance of the Wasserstein barycenter. Existing theory, which constrains the transport maps to rigid translations, is generalized to include affine transformations, which are proved optimal for the purpose of clustering. The resulting non-parametric clustering algorithms include $k$-means as a special case and have more robust performance, demonstrated by comparisons with popular clustering algorithms on both artificial and real-world data sets.

Keywords: Clustering, optimal transport, Wasserstein barycenter, explanation of variability

AMS Subject classification: 62H30, 49M30

1 Introduction

Clustering a data set $\{x_i\}$ consists of assigning to each sample $x_i \in X$ a label $k_i \in [1, K]$ based on some notion of similarity among data points. The objective of clustering can be conceptualized from various overlapping perspectives:

1. Class discovery: one seeks a scheme that classifies the data set, discovering whether it is naturally divided into distinct groups. Such discovery may be of independent interest and lead to further research onto the meaning of such partition. For instance, if a clinical study reveals that patients respond to a medical treatment following one of three different patterns, one will further inquire into what biological conditions determine the pattern that a given patient will follow.

2. Dimensionality reduction: the samples $x_i$ may lie in a high-dimensional space $X$, making their storage, transmission and analysis potentially costly. Replacing $x_i$ by $k_i$ is a dimensional reduction procedure that mitigates these problems. From a human user’s perspective, the entries of a vector $x_i$ may provide little intuition, while its label $k_i$ may be easier to grasp.

3. Explanation of variability: part of the difference among the various samples $x_i$ can be attributed to the class to which they belong. Thus the task of finding clusters finds a natural complement in determining what makes these clusters different, such as their mean, their covariance, the value of a particular combination of their components or of a set of functions of independent interest. In either case, we are explaining part of the variability in the data in terms of its partition into classes.

4. Removal of the effect of confounding factors: The component of the variability in the data that has been attributed to its partition into classes can be removed as one does with other confounding factors, such as the batch effect in biostatistics, making the resulting filtered data suitable for further analysis.

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The problem of removing from the data the variability associated with classes that have already been assigned adopts a natural formulation in terms of optimal transport. Presumably the data points of each class \( k \) represent an underlying probability \( \rho_k(x) \), with various distinct \( \rho_1, \ldots, \rho_K \). Then removing the variability attributable to class is paramount to mapping the points \( \{x_i\} \) through class-dependent maps \( y = Y_k(x) \) such that the resulting \( \{y_i = Y_k(x_i)\} \) have an underlying distribution \( \mu(y) \) that is independent of \( k \) (for otherwise part of the variability explainable by the classes would not have been removed.) Moreover, one would prefer to use maps \( Y_k \) that, while satisfying the aforementioned condition, deform the data minimally, so that only the variability due to class is removed. If one quantifies the deformation associated to the map with the expected value of a pointwise “transportation” cost \( c(x, Y_k(x)) \), one arrives at the Wasserstein barycenter problem:

\[
\min_{Y_k} D = \sum_{k=1}^{K} P_k \int c(x, Y_k(x)) \, d\rho_k(x), \quad Y_k \# \rho_k = \mu,
\]

where the \( P_k > 0 \) are weights attached to each class, such as the proportions of samples that they contain.

As described, this procedure comes after clustering, as it assumes that each sample \( x_i \) has already been assigned to a class \( k_i \). However, it can also be invoked to define an objective function for the clustering process itself: one should assign the samples to classes in such a way as to minimize the unexplained variability, i.e. the variability left in \( \mu \).

When posed in this framework, the clustering problem contains two layers of optimization. The inner layer consists of finding a representative for a given collection of distributions or data points, when a class assignment is given. It corresponds to the real-world problems of “removing batch effects”, “pooling data’ or “supervised unlearning” \([22]\). This layer is effectively modeled by the Wasserstein barycenter problem, where filtering out class distinctions corresponds to transporting distinct data sets onto a common representative, and avoiding information loss corresponds to minimizing transportation cost.

The outer layer of optimization determines the class assignment, an unsupervised learning problem. The effectiveness of learning is measured by the amount of uncertainty removed, calculated as the difference between the variance before and after the “supervised unlearning” of the inner layer. This approach can be compared to the task of data compression, and we can entertain the hypothesis that, when the brain receives some perceptive input, it looks for tentative categorizations or class assignments, then compresses the data accordingly in the cognitive space, and eventually selects the representation that is most space- or time-efficient.

This framework was first proposed in \([22]\), which showed that, if one quantifies the variability in \( \mu \) through the trace of the covariance matrix, uses as cost \( c(x, y) \) the squared Euclidean distance, and restricts the maps \( Y_k \) to rigid displacements, this formulation becomes equivalent to \( k \)-means. Yet, this idea can be extended much further, for instance by quantifying the variability in \( \mu \) in alternative ways, using cost functions different from the square distance, and allowing more general transport maps.

This article develops in detail the next natural step, which replaces the rigid translations of \([22]\) by general affine maps. Moreover, it proves that the affine maps are already optimal for the purpose of clustering, that is, the minimum variability achievable using arbitrary transport maps or couplings can be obtained through affine maps alone, when one adopts the variance as a measure of variability and the square distance as transportation cost.

The literature on clustering data sets is vast and rich, including a broad array of diverse methodologies which we cannot possibly summarize here. The purpose of this article is not so much to build one new method for clustering, but rather to develop a conceptual paradigm that characterizes clustering as a procedure for the reduction of variability in data, which can be formulated naturally in terms of the Wasserstein barycenter problem with hidden class assignment. The main contribution is to extend the proposal in \([22]\), which derives \( k \)-means using rigid translation as transport maps, to incorporate the more general affine maps, and to show the optimality of this extension. As such, this article opens the way to considering more general characterizations of variability, as well as to moving from discrete to continuous class assignments. Along the way, it develops an optimal-transport-based numerical procedure for clustering that is shown to compare favorably with more standard approaches.

The plan of this article is as follows. After this introduction, section \([2]\) summarizes the elements that we need from the Wasserstein barycenter problem. Section \([3]\) introduces optimal affine transport (i.e. the optimal transport barycenter problem restricted to affine maps) and proves its optimality. Section \([4]\) describes
factor discovery –i.e. class assignment– with affine maps, its solution via gradient descent, its relation to
$k$-means and its reduction and simplification in various scenarios. Section 4 compares the performance of the
various variants of the method, $k$-means and fuzzy $k$-means on synthetic and real world data. Finally section
6 summarizes the work and sketches some directions of current research.

2 The Wasserstein Barycenter problem

Let $\mathcal{P}_2(\mathbb{R}^d)$ be the space of Borel probability measures in $\mathbb{R}^d$ with finite second moments, and by $\mathcal{P}_{2,ac}(\mathbb{R}^d)$
the subspace of absolutely continuous measures. Given $\rho_1, \ldots, \rho_K \in \mathcal{P}_2(\mathbb{R}^d)$ and corresponding weights $P_k$
(positive and satisfying $\sum_{k=1}^{K} P_k = 1$), we seek to remove the variability attributable to the classes $1, \ldots, K$
by transporting these $\rho_k$ to a weighted barycenter $\mu$. The Monge-formulation of this problem seeks a measure $\mu$ and corresponding transport maps $Y_1, \ldots, Y_K$ that minimize “information distortion”, captured by the the
total transportation cost

$$D = \sum_{k=1}^{K} P_k \int_{\mathbb{R}^d} c(x, Y_k(x)) d\rho_k(x),$$

where the cost function $c$ is taken to be the squared Euclidean distance $||x - y||^2$, and each $Y_k$ satisfies
$Y_k \# \rho_k = \mu$. The Kantorovich relaxation is given by

$$\min_{\mu, \pi_k} \sum_{k=1}^{K} P_k \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\pi_k(x, y)$$

(1)

where $\pi_k$ is a coupling with marginals $\rho_k$ and $\mu$. This linear-programming problem has dual [22]

$$\max_{\phi_k, \psi_k} \sum_{k=1}^{K} P_k \int \phi_k(x) d\rho_k(x)$$

(2)

subject to the constraints $\phi_k + \psi_k \leq P_k c$ and $\sum_{k=1}^{K} \psi_k \geq 0$, which can be simplified into

$$\forall(x_1, \ldots x_K), \sum_k \phi_k(x_k) \leq \sum_{k,l} P_k P_l ||x_k - x_l||^2.$$

It is known that the barycenter exists for $\rho_1, \ldots, \rho_K \in \mathcal{P}_2(\mathbb{R}^d)$, and if some $\rho_k \in \mathcal{P}_{2,ac}(\mathbb{R}^d)$ then the
barycenter is unique [4] and absolutely continuous [13]. If furthermore $\rho_1, \ldots, \rho_K \in \mathcal{P}_{2,ac}(\mathbb{R}^d)$, then the
Monge problem can solved by transport maps of the form [22]

$$Y_k = x - P_k^{-1} \nabla \phi_k(x).$$

3 Optimal affine transport

One way to relax the barycenter problem is to restrict $\phi_k$ to the set of convex quadratic functions $\mathcal{F}$, which
prevents over-fitting in data-based implementation and eases computation. The constraints of (2) allow us
to set $\psi(y) = \min_{\phi} (P_k c(x, y) - \phi(x))$, which is also a convex quadratic function. Thus, the constraints of the
Kantorovich formulation [1] can be weakened into

$$\forall k, \forall \phi \in \mathcal{F}, \int_{\mathbb{R}^d} \phi(x) d\rho_k(x) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \phi(x) d\pi_k(x, y)$$

$$\forall \psi \in \mathcal{F}, \int_{\mathbb{R}^d} \psi(y) d\mu(y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \psi(y) d\pi_k(x, y)$$

(4)

Consequently, the marginals of the coupling $\pi_k$ only need to match $\rho_k$ and $\mu$ in their first and second mo-
ments, namely their mean and covariance matrix. The transport map according to (3) becomes an affine map.
Given the barycenter $\mu$, we can solve for the maps $Y_k$. By applying a suitable preconditioning $\rho_k^* = F \# \rho_k$ and $\mu^* = G \# \mu$, the composite map

$$Y_k = G^{-1} \circ Y_k^* \circ F$$

will be optimal if the map $Y_k^*$ is the optimal transport map from $\rho_k^*$ to $\mu^*$. By [15], if $G, F$ are restricted to affine maps, then the following is an admissible pair

$$F(x) = \Lambda_1^{1/4} Q^T \Sigma_k^{-1/2} (x - \bar{x}_k), \quad G(y) = \Lambda_1^{1/4} Q^T \Sigma_k^{-1/2} (y - \bar{y})$$

where $\bar{x}_k, \bar{y}, \Sigma_k, \Sigma_y$ are the means and covariances of $\rho_k$ and $\mu$, and $\Sigma_k^{-1/2} \Sigma_y \Sigma_k^{-1/2} = QAQ^T$ is an eigendecomposition (By matrix square root, we always mean the principal square root with positive eigenvalues). Since $Y_k$ is affine, $Y_k^*$ must also be affine. Since the preconditioning has already pushed $\rho_k$ and $\mu$ to have the same mean and covariance matrix, whereas any nontrivial affine $Y_k^*$ would alter the mean or the covariance, $Y_k^*$ must be the identity in order to satisfy (4). It follows that

$$Y_k(x) = G^{-1} \circ F = \Sigma_k^{-1/2} (\Sigma_k^{-1/2} \Sigma_y \Sigma_k^{-1/2})^{1/2} \Sigma_k^{-1/2} (x - \bar{x}_k) + \bar{y}.$$  

An alternative derivation can be found in [17].

Next, we derive in Theorem 3.1 the form of the barycenter’s covariance $\Sigma_y$, and then show that this covariance can be achieved through affine maps. Since the performance of clustering depends only on variability, which we quantify as $\text{Tr}[\Sigma_y]$, it follows that affine transport maps are sufficient to solve the clustering problem.

We apply techniques from [14] to characterize the barycenter $\mu$ using the total cost formula [1]. Define the random variables $X_k \sim \rho_k, Y \sim \mu$ and the weighted average $\bar{X} = \sum_{k=1}^K P_k X_k$. Then

$$\min_{\mu, \pi} D = \min_{\mu, \pi} \mathbb{E} \left[ \sum_{k=1}^K P_k ||X_k - Y||^2 \right] = \min_{\mu, \pi} \mathbb{E} \left[ \sum_{k=1}^K P_k \left( ||X_k - \bar{X}||^2 + ||Y - \bar{X}||^2 \right) \right].$$

Hence we can set $Y = \bar{X}$, and in particular, the barycenter’s mean is given by the weighted sum

$$\bar{y} = \sum_{k=1}^K P_k \bar{x}_k. \quad (5)$$

In the following derivation, we assume that all $\bar{x}_k = 0$ since they only contribute constant terms. Denote by $\Pi(\rho_1, \ldots \rho_K) \subseteq \mathbb{P}(\mathbb{R}^d)$ the set of all couplings of $\rho_1, \ldots \rho_K$. The problem is now equivalent to

$$\max_{\pi \in \Pi(\rho_1, \ldots \rho_K)} \mathbb{E} \left[ \sum_{k=1}^K P_k \langle X_k, \bar{X} \rangle \right] = \max_{\pi} \text{Tr}[\Sigma_y] \quad (6)$$

and we can bound the left hand side by

$$\max_{\pi} \mathbb{E} \left[ \sum_{k=1}^K P_k \left( \frac{1}{2} X_k^T [\Sigma_k^{-1/2} (\Sigma_k^{1/2} \Sigma_y \Sigma_k^{1/2})^{1/2} \Sigma_y^{-1/2}] X_k + \frac{1}{2} \bar{X}^T [\Sigma_y^{-1/2} (\Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2})^{1/2} \Sigma_y^{-1/2}] \bar{X} \right) \right],$$

which follows from the Cauchy-Schwartz inequality and the identity

$$[\Sigma_k^{-1/2} (\Sigma_k^{1/2} \Sigma_y \Sigma_k^{1/2})^{1/2} \Sigma_k^{-1/2}]^{-1} = \Sigma_y^{-1/2} (\Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2})^{1/2} \Sigma_y^{-1/2}.$$

Then

$$\max_{\pi} \text{Tr}[\Sigma_y] \leq \max_{\pi} \text{Tr} \left[ \sum_{k=1}^K P_k \left( \frac{1}{2} (\Sigma_k^{1/2} \Sigma_y \Sigma_k^{1/2})^{1/2} + (\Sigma_k^{1/2} \Sigma_y \Sigma_k^{1/2})^{1/2} \right) \right]$$

$$= \max_{\pi} \text{Tr} \left[ \sum_{k=1}^K P_k (\Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2})^{1/2} \right]. \quad (7)$$
Intuitively, if we define an updating function on covariance matrices

$$F(\Sigma_y) := \sum_{k=1}^{K} P_k (\Sigma_1^{1/2} \Sigma_k \Sigma_y^{1/2})^{1/2}$$  \hspace{1cm} (8)$$
then given any coupling \( \pi \) with \( \Sigma_y \), if \( F(\Sigma_y) \) can be realized by some \( \pi' \), then \( \pi' \) is a potentially better solution that increases \( I \). The following theorem confirms this intuition:

**Theorem 3.1.** Given \( \rho_1, \ldots, \rho_K \in \mathcal{P}_2(\mathbb{R}^d) \), the solution set of the matrix equation \( \Sigma_y = F(\Sigma_y) \) contains a maximizer of \( I \), which is the covariance of some barycenter. In particular, if some \( \rho_k \in \mathcal{P}_2,ac(\mathbb{R}^d) \), then the unique positive-definite solution of \( \Sigma_y = F(\Sigma_y) \) is the covariance of the unique barycenter.

We present our proof in Appendix A. Versions of this result were given in [14] and [18], and [4] also offered a proof for the case when the \( \rho_k \) are Gaussian.

A useful result from [3] is that when some covariance \( \Sigma_k \) is positive-definite (e.g. when some \( \rho_k \) is absolutely continuous), the unique positive-definite solution \( \Sigma_y \) can be calculated through the following iteration scheme:

$$\Sigma(n + 1) := \Sigma(n)^{-1/2} \left( \sum_{k=1}^{K} P_k \Sigma(n)^{1/2} \Sigma_k \Sigma(n)^{1/2} \right)^{1/2} \Sigma(n)^{-1/2}$$ \hspace{1cm} (9)$$
where the initial \( \Sigma(0) \) is some arbitrary positive-definite matrix, and \( \Sigma(n) \) converges to \( \Sigma_y \).

Now we can prove the effectiveness of affine transport maps. Denote by \( G(\mathbb{R}^d) \) the set of non-degenerate Gaussians (or more generally, any location-scatter family \( \subseteq \mathcal{P}_2,ac(\mathbb{R}^d) \)), and by \( S^+(d) \) the set of positive definite matrices. Then, the space \( G(\mathbb{R}^d) \) equipped with the quadratic Wasserstein metric is equivalent to

$$\left( G(\mathbb{R}^d), W_2 \right) \cong (\mathbb{R}^d \times S^+(d), D_\mathcal{G})$$

where \( \mathbb{R}^d \times S^+(d) \) represents the mean and covariance that uniquely determine a Gaussian, and \( D_\mathcal{G} \) is the metric

$$D_\mathcal{G}((m_1, \Sigma_1), (m_2, \Sigma_2)) \equiv \sqrt{||m_1 - m_2||^2 + Tr[\Sigma_1 + \Sigma_2 - 2(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2})^{1/2}]^2}$$

We can further define a “forgetful map” \( f : \mathcal{P}_2,ac(\mathbb{R}^d) \rightarrow \mathbb{R}^d \times S^+(d) \) by

$$f(\rho) = (\text{mean}, \text{covariance matrix})$$

which “forgets” all information on \( \rho \) except its first two moments. In particular, the equivalence class \( f^{-1}(f(\rho)) \) contains the Gaussian \( \mathcal{N}(f(\rho)) \).

**Corollary 3.1.** The forgetful \( f \) preserves the Wasserstein barycenter, that is, given any \( \rho_1, \ldots, \rho_K \in \mathcal{P}_2,ac(\mathbb{R}^d) \) and weights \( \rho_1 \ldots, \rho_K \), their \( W_2 \)-barycenter \( \mu \) is mapped by \( f \) to the \( D_\mathcal{G} \)-barycenter of \( f(\rho_1) \ldots, f(\rho_K) \).

**Proof.** Equation [5] and Theorem 3.1 has fixed \( f(\mu) \), the mean and covariance of the barycenter. By Theorem 6.1 from [4], \( \mathcal{N}(f(\mu)) \) is exactly the barycenter of the Gaussians \( \mathcal{N}(f(\rho_k)) \).

**Remark 3.1.** As described in the next section, the clustering problem can be posed as the minimization of the barycenter’s variance. Thus, the only relevant data are \( f(\mu) \), which depend only on \( f(\rho_k) \), so it is sufficient to restrict our attention to the equivalence classes \( f^{-1}(f(\rho_k)) \) and the maps between these classes. It is straightforward to show that these are affine maps, and therefore affine maps are sufficient for the optimization of the clustering problem.

In summary, the optimal affine transport maps \( Y_k(x) = \alpha_k x + \beta_k \) are given by

$$\begin{cases} \bar{y} = \sum_{k=1}^{K} P_k \bar{x}_k \\ \Sigma_y = F(\Sigma_y) \end{cases} \quad \begin{cases} \alpha_k = \Sigma_k^{-1/2}(\Sigma_k^{1/2} \Sigma_y^{1/2} \Sigma_k^{1/2})^{1/2} \Sigma_k^{-1/2} \\ \beta_k = \bar{y} - \alpha_k x_k \end{cases}$$

This definition extends naturally to a data-based formulation. Assume that we are given a sample \( \{x_i\}_{i=1}^m \) with a partition plan \( \{S_1, \ldots, S_K\} \) which serves as an assignment of the samples to the classes 1, \ldots, K. Then the means and covariances can be determined empirically, the proportion \( P_k = |S_k|/m \) becomes the weight of \( \rho_k \), and \( \bar{y} \) coincides with the mean of the sample.
4 Factor discovery with affine maps

In the context of unsupervised learning, we are given an unlabeled sample \( \{x_i\} \) and a proposed number \( K \) of latent classes. The factor discovery problem seeks the assignment of class labels \( k_i \in \{1, \ldots, K\} \) to the \( x_i \), so that \( k_i \) has maximal explanatory power \([22]\), which can be interpreted as minimizing the variance remaining once we remove the influence of \( k_i \) from \( x_i \) using transport maps \( Y_k \):

\[
\min_{\{k_i\}} Var(\{Y_k(x_i)\}). \tag{10}
\]

For both intuitive and implementational purposes, we extend the factor discovery problem to include soft assignments. Each \( x_i \) is assigned a probability vector \( P_i \) on the \( K \)-dimensional simplex \( \Delta^K \), where \( P_k \) is the estimated probability that \( x_i \) belongs to cluster \( k \). Let \( P = (P_k) \in \prod \Delta^K \) be a stochastic matrix. The hard assignment \( k_i = k \) corresponds to the case \( P^i = \text{unit vector} \ e_k \), and its domain is the set of extremal points of \( \prod \Delta^K \) \([5]\).

A probabilistic formulation of \([10]\) is, given \( \rho \in \mathcal{P}_{2, ac}(\mathbb{R}^d) \) and class number \( K \),

\[
\min_{\text{partition } \rho = \sum_{k=1}^K P_k \rho_k} Var(Y) \text{ where } Y \sim \mu, \text{ the weighted barycenter of } \rho_1, \ldots, \rho_K \in \mathcal{P}_{2, ac}.
\]

By the alternative characterization (6) of the barycenter, this problem is equivalent to

\[
\min_{\rho = \sum P_k \rho_k} \max_{\pi \in \Pi(\rho_1, \ldots, \rho_K)} Var(\tilde{X}) \text{ where } \tilde{X} = \sum_k P_k X_k, \ X_k \sim \rho_k
\]

which by Theorem 3.1 is further equivalent to

\[
\min_{\rho = \sum P_k \rho_k} Tr[\Sigma_y] \text{ where } \Sigma_y = F(\Sigma_y). \tag{11}
\]

Then it is straightforward to shift to a data-based formulation using empirical means and covariances:

\[
\bar{x}_k = \frac{1}{i} P_k^i x_i / \sum_i P_k^i \text{ and } \Sigma_k = \frac{1}{i} P_k^i (x_i - \bar{x}_k) \cdot (x_i - \bar{x}_k)^T / \sum_i P_k^i
\]

It has been demonstrated in \([22]\) that if we further restrict the transport maps \( Y_k \) to rigid translations, \( Y_k(x) = x + \beta_k \), then the factor discovery problem becomes the minimization of the sum of within-class variances (equivalently, sum of squared errors)

\[
Var(\{Y_k(x_i)\}) = \sum_{k=1}^K \sum_{i \in S_k} ||x_i - \bar{x}_k||^2 \text{ or } \sum_{k=1}^K \sum_{i=1}^m P_k^i ||x_i - \bar{x}_k||^2 \tag{12}
\]

which agrees with the objective function of the \( k \)-means algorithm. Intuitively, adopting the more general affine maps, which by Remark 3.1 are optimal for the clustering problem \([11]\), one can obtain more robust algorithms.

4.1 Exact solution via gradient descent

The implicit nonlinear matrix equation \( \Sigma_y = F(\Sigma_y) \) prevents \([11]\) from being solved straightforwardly. Instead, we apply gradient descent to move each \( P^i \in \Delta^K \) to minimize \( Tr[\Sigma_y] \). In Appendix \([\mathbf{B}]\) we prove that \( \partial \Sigma_y / \partial P_k^i \), the partial derivative of the barycenter’s covariance with respect to each membership probability, always exists, and in Appendix \([\mathbf{C}]\) we derive the explicit formulae for these derivatives that we use below.

The gradient of our objective function \( Tr[\Sigma_y] \) with respect to each sample point \( x_i \)’s probability vector \( P^i \) is given by

\[
\nabla_{P^i} Tr[\Sigma_y] = \sum_{k=1}^K vec(I)^T X_k vec[(x_i - \bar{x}_k) \cdot (x_i - \bar{x}_k)^T + \Sigma_k] e_k \tag{13}
\]
where \( \text{vec} \) is vectorization, \( \otimes \) is Kronecker product and

\[
X_k := \left( \Sigma_y^{1/2} \otimes \Sigma_y^{1/2} \right) \left[ \sum_{h=1}^{K} P_h (U_h \otimes U_h) (D_h^{1/2} \otimes I + I \otimes D_h^{1/2})^{-1} (D_h^{1/2} \otimes D_h^{1/2}) (U_h^T \otimes U_h^T) \right]^{-1} \\
\left[ (U_k \otimes U_k) (D_k^{1/2} \otimes I + I \otimes D_k^{1/2})^{-1} (U_k^T \otimes U_k^T) \right] (\Sigma_y^{1/2} \otimes \Sigma_y^{1/2})
\]

is a \( d^2 \times d^2 \) matrix that contains the eigendecompositions

\[
\Sigma_y^{1/2} \Sigma_y^{1/2} = U_k D_k U_k^T \quad \text{and} \quad \Sigma_y = U_y D_y U_y^T
\]

To implement gradient descent on \( (11) \), the update rule at each time step \( t \)

\[
P(t + 1) = \text{Proj}_{\Pi_k \Delta_k} \left( P(t) - \lambda \cdot \nabla P \text{Tr}[\Sigma_y] \right),
\]

where \( \lambda \) is the step’s length and \( \text{Proj}_{\Pi_k \Delta_k} (v) \) is the closest point in \( P \)'s domain to \( v \), which can be computed efficiently \( [25] \). The step’s length \( \lambda \) is determined at each step by backtracking line search \( [6] \), with threshold \( \alpha \in (0, 1/2) \) and shortening rate \( \beta \in (0, 1) \). We shorten \( \lambda \) into \( \beta \lambda \) if the amount of descent is not enough:

\[
\text{Tr}[\Sigma_y] (P(t + 1)) - \text{Tr}[\Sigma_y](P(t)) > \alpha \text{vec}(\nabla P \text{Tr}[\Sigma_y])^T \cdot \text{vec}(P(t + 1) - P(t)).
\]

The gradient descent algorithm is summarized below. An advantage of this solution is that \( X_1, \ldots, X_K \) do not depend on the sample index \( i \), so that they only need to be computed once during each iteration of the algorithm.

**Data:** sample \( \{x_i\} \) and number of classes \( K \)

Initialize the means \( \{\bar{x}_k\} \) randomly and stochastic matrix \( P \) (by the closest \( \bar{x}_k \));

while not converging do

- compute \( \Sigma_y \) by \( [9] \) and \( X_1, \ldots, X_K \) by \( [14] \);
- compute and normalize the gradient \( \nabla P \text{Tr}[\Sigma_y] = (\nabla P \text{Tr}[\Sigma_y])_i = \sum_{i,k} \text{vec}(I)^T X_k \text{vec}[(x_i - \bar{x}_k) \cdot (x_i - \bar{x}_k)^T + \Sigma_k] e_{ik} \);
- find an optimal step length \( \lambda \) by backtracking;
- update \( P \leftarrow \text{Proj}_{\Pi_k \Delta_k} \left( P - \lambda \cdot \nabla P \text{Tr}[\Sigma_y] \right) \);
- update centers \( \{\bar{x}_k\} \) and covariances \( \{\Sigma_k\} \);
end

**Algorithm 1:** Soft Exact Clustering, or gradient-descent soft assignment that utilizes the exact solution.

The following is a hard assignment version that simplifies Algorithm \([1] \). Instead of moving \( P^i \) by small steps backward along the gradient, we directly set all entries of \( P^i \) to zero except the entry corresponding to the minimum \( \partial P^i \text{Tr}[\Sigma_y] \). An equivalent derivation is that, if we optimize a step length \( \lambda_i \) for each individual \( P^i \), then Algorithm \([1] \) will move each \( P^i \) toward an extremal point in \( \Delta^K_i \), eventually yielding a hard assignment.

Initialize the means \( \{\bar{x}_k\} \) (randomly) and labels \( k_i \) (by the closest mean);

while not converging do

- compute the gradient \( \nabla P \text{Tr}[\Sigma_y] \);
- for \( x_i \) in sample do
  \( k_i \leftarrow \text{argmin}_k (\partial P^i_k \text{Tr}[\Sigma_y]) \);
- end
- update centers and covariances;
- (possibly apply an update rate \( c \) to smooth the process: \( \bar{x}_k \leftarrow c \text{ new} + (1 - c) \text{ old} \))
end

**Algorithm 2:** Hard Exact Clustering

### 4.2 Relation to \( k \)-means

Now we show that our solution reduces to \( k \)-means in the latter’s setting. The “standard data” \( [20] \) for the \( k \)-mean’s algorithm consist of spherical clusters with identical radii and proportions, which implies that
\( P_1 = \cdots = P_K = 1/K \) and \( \Sigma_1 = \cdots = \Sigma_K = \lambda I \) for some positive constant \( \lambda \). The entries of the gradient (13) become
\[
\partial_{P_k} \text{Tr}[\Sigma_y] = \text{Tr}\left[ (x_i - \overline{x}_k) \cdot (x_i - \overline{x}_k)^T + \Sigma_k \right] = ||x_i - \overline{x}_k||^2 + \lambda d.
\]
Since each \( P^k \) lies in the simplex \( \Delta^K \), the direction of any gradient descent must be parallel to \( \Delta^K \), and thus the term \( \lambda d \) shared by all entries of \( \nabla_{P^k} \text{Tr}[\Sigma_y] \) is eliminated by the projection map \( \text{Proj}_{\Pi, \Delta^K} \) of Algorithm 1 (for Algorithm 2 it is eliminated by the argmin step). The resulting gradient
\[
\nabla_{P^k} \text{Tr}[\Sigma_y] = \sum_{k=1}^{K} ||x_i - \overline{x}_k||^2 e_k
\]
is precisely the gradient of the sum of square errors (12), the objective function of \( k \)-means. It is straightforward to check that Algorithm 2 reduces to \( k \)-means.

An intuition into the solution (13) can be obtained from the partial derivatives of the barycenter’s covariance matrix (derived in Appendix C)
\[\partial_{P_k} \Sigma_y = \text{vec}^{-1}(X_k \text{vec}[(x_i - \overline{x}_k) \cdot (x_i - \overline{x}_k)^T + \Sigma_k]).\]
The conjugation by \( \text{vec} \) and \( \text{vec}^{-1} \) pulls out each term of the “perturbation” \( (x_i - \overline{x}_k) \cdot (x_i - \overline{x}_k)^T + \Sigma_k \), which depends on both the influence of tweaking \( P_k \) and the current shape of cluster \( k \). Then the multiplicative factor \( X_k \), which depends on the shapes of all clusters \( 14 \), weighs the contribution of each term of the “perturbation”. In effect, the non-isotropy of the existing clusters distorts the Euclidean metric of \( \mathbb{R}^d \) by the factor \( X_k \), whereas for the “standard data” of \( k \)-means, the conjugation and weighing collapse and \( \Sigma_y \) is influenced equally by perturbations from all directions.

### 4.3 Approximate solution using isotropy

In Section 5, we will demonstrate that Algorithms 1 and 2 can recognize clusters that deviate from the “standard data”, for which \( k \)-means and fuzzy \( k \)-means would fail. It is natural to expect that by incorporating certain assumption weaker than the “standard data”, we can obtain solutions that are more robust than \( k \)-means and at the same time simpler than the exact solutions (13) and easier to interpret.

Since the complexity of (13) results mostly from the non-commutativity of matrix product, we can impose the assumption that all covariances \( \Sigma_k \) are of the form \( \lambda_k I \) (whereas \( P_k \) and \( \lambda_k \) may vary). In particular, it holds when all measures \( \rho_k \) are isotropic, that is, their distribution functions are radial. Thus, our assumption generalizes the “standard data” requirement that all clusters be spherical.

Insert \( \{ \Sigma_k = \lambda_k I \} \) into the solution (13). By Theorem 3.1 \( \Sigma_y = \lambda_y I \) where \( \sqrt{\lambda_y} = \sum_{k=1}^{K} P_k \sqrt{\lambda_k} \).
\[
\partial_{P_k} \text{Tr}[\Sigma_y] = \sigma_y \left( \frac{||x_i - \overline{x}_k||^2}{\sigma_k} + \sigma_k \right)
\]
where \( \sigma_k = \sqrt{\lambda_k d} \) is the standard deviation of each cluster. Since our algorithms only involve the ratio of the gradient’s entries, the gradient is effectively
\[
\nabla_{P^k} \text{Tr}[\Sigma_y] = \sum_{k} \left( \frac{||x_i - \overline{x}_k||^2}{\sigma_k} + \sigma_k \right) e_k
\]
This term is not only simpler to compute, but also admits an intuitive explanation: it is the gradient of the weighted sum of standard deviations
\[
\nabla P \sum_{k} P_k \sigma_k \propto \nabla P \left( \sum_{k} P_k \sigma_k \right)^2 \propto \nabla P^2 \lambda_y \propto \nabla P \text{Tr}[\Sigma_y]. \tag{15}
\]
Then, in the isotropic setting, decreasing the barycenter’s variance is equivalent to decreasing the variance of each cluster.
Algorithms 1 and 2 can be slightly modified by the above approximate solution into the following:

Initialize the means \( \{ \mu_k \} \) randomly and the stochastic matrix \( P \) (by the closest \( \mu_k \));

while not converging do
    compute and normalize the gradient \( \nabla_P \text{Tr}[\Sigma_y] = \sum_{i,k} (\sigma_k + \frac{||x_i - \mu_k||^2}{\sigma_k}) e_{ik} \);
    find an optimal step length \( \lambda \) by backtracking;
    update \( P \leftarrow \text{Proj}_\{\Pi, \Delta, \cdots\} (P - \lambda \cdot \nabla_P \text{Tr}[\Sigma_y]) \);
    update centers and standard deviations
end

Algorithm 3: Soft Approximate Clustering, or gradient-descent soft assignment using the approximate solution.

Initialize the means \( \{ \mu_k \} \) (randomly) and labels \( k_i \) (by the closest \( \mu_k \));

while not converging do
    for \( x_i \) in sample do
        \( k_i \leftarrow \text{argmin}_k (\frac{||x_i - \mu_k||^2}{\sigma_k} + \sigma_k) \);
    end
    update centers and standard deviations
end

Algorithm 4: Hard Approximate Clustering

Section 5 will confirm the expectation that these algorithms are more robust than \( k \)-means under varying proportions and radii (\( P_k \) and \( \lambda_k \)), but are more vulnerable to non-isotropy (\( \Sigma_k \) not of the form \( \lambda_k I \)) than Algorithms 1 and 2.

5 Performance

In sections 5.1 and 5.2 we compare \( k \)-means and our algorithms on two parametrized families of test cases that deviate from the “standard data” of \( k \)-means, and in section 5.3 they are tested on real-world classification data sets.

Our first test family, the “expansion test”, is a collection of three spherical normal distributions:

- 100 samples from \( \mathcal{N}((0,0), (1/10, 0, 0/10)) \)
- 100\((1 + t)\) samples from \( \mathcal{N}(\left(0, \frac{(1 + t)^2/10}{2^{1/2}}, 0\right), (1 + t)^2/10, 0, (1 + t)^2/10) \)
- 100\((1 + 2t)\) samples from \( \mathcal{N}(\left(t^{1/2}, \frac{(1 + 2t)^2/10}{2^{1/2}}, 0\right), (1 + 2t)^2/10, 0, (1 + 2t)^2/10) \)

The means and standard deviations are designed so that, for all \( t \geq 0 \), the three samples are roughly contained in three pairwise adjacent balls of radii \( 1, 1 + t, 1 + 2t \). As \( t \) increases, the sample sizes and radii grow in distinct rates.

Our second test family, the “dilation test”, is given by

- 100 samples from \( \mathcal{N}(\left(0, (1 + t)^2/25, 0\right), \left(0, 0, 1/25\right) \)
- 100 samples from \( \mathcal{N}(\left(0, 0, 1/25\right), \left(1/25, 0, 1/25\right) \)
- 100 samples from \( \mathcal{N}(\left(-1, (1 + t)^2/25, 0\right), \left(0, 0, 1/25\right) \)

which are unit normals stretched horizontally at different rates.

The expansion test challenges the “standard data” in its first two assumptions: similar radii and similar proportions, while the dilation test challenges the last assumption of isotropy or spherical clusters. In both cases, the amount of deviation from the standard data is parametrized by \( t \). Nevertheless, a reasonable \( t \) should be bounded above, since for very large \( t \) the Gaussians become so disparate that the true labeling no longer minimizes \( \text{Tr}[\Sigma_y] \) or yields clusters from a human’s perception viewpoint.
The performance of each algorithm is measured by its correct rate, the percentage of overlap between
the true labeling and the labeling produced by the algorithm, maximized over all identifications between
the proposed clusters and the true clusters: given the true labeling \( \{z_i\} \) and the labeling \( \{k_i\} \) or stochastic
matrix \( P \) produced by algorithm, define the correct rate as

\[
\max_{\sigma \in S_K} \sum_{z_i = \sigma(k_i)} \text{ for hard assignment and } \max_{\sigma \in S_K} \sum_{i} P_{\sigma(z_i)}^i \text{ for soft assignment}
\]

where \( \sigma \) ranges over all permutations.

5.1 Comparison of soft assignments

We first compare the soft assignment algorithms: fuzzy \( k \)-means, Soft Exact Clustering (Algorithm 1),
and Soft Approximate Clustering (Algorithm 3). The fuzzy \( k \)-means algorithm [5] is a soft assignment
generalization of \( k \)-means that minimizes the following generalized sum of squared errors,

\[
J_c(P, \{x_k\}) = \sum_i \sum_k (P_{i}^{k})^c ||x_i - \tau_k||^2
\]

where the exponent \( c > 1 \) makes \( J_c \) strictly convex in \( P_{i}^{k} \), unlike the sum of squared errors (12) with \( c = 1 \),
which yields only hard assignments. Here we adopt the common choice \( c = 2 \).

**Data:** sample \( \{x_i\} \), exponent \( c = 2 \\
Initialize the means \( \tau_k \) and stochastic matrix \( P = (P^k_i) \) randomly;
while not converging do
    for \( x_i \) in sample and \( k = 1 \) to \( K \) do
        \( P_{i}^{k} \leftarrow (||x_i - \tau_k||^2)^{1-c} / \sum_j (||x_j - \tau_k||^2)^{1-c} \)
    end
    for \( k = 1 \) to \( K \) do
        \( \tau_k \leftarrow \sum_k (P_{i}^{k})^c x_i / \sum_k (P_{i}^{k})^c \)
    end
end

**Algorithm 5:** Fuzzy \( k \)-means

Since each algorithm starts with a random initialization, to stabilize performance each algorithm is run
100 times over the same sample set and the result that minimizes the objective function (sum of squared
errors [12] for \( k \)-means, \( Tr[\Sigma_y] \) for Soft Exact, and the weighted sum of standard deviations [15] for Soft
Approximate) is selected.

The experimental results on the expansion test \( t = 2.2 \) are plotted below. The class assignment displayed
is given by the maximum probability, \( k_i \leftarrow \arg\max_k P_{i}^{k}. \)

![Figure 1: Left: Clusters produced by fuzzy \( k \)-means. Middle: Soft Approximate. Right: Soft Exact. The
black arrows are the clusters’ means. Fuzzy \( k \)-means merged the two smaller clusters and split the largest
cluster. Soft Approximate and Soft Exact only made a few errors on the periphery.](image)

Below is the plot of correct rates for \( t \in [0, 4] \). Fuzzy \( k \)-means with a steady decline is dominated by Soft
Approximate and Soft Exact, while the difference between the latter two is negligible. Eventually, for large \( t \),
Soft Approximate and Soft Exact become unstable and often require more than 100 trials to find the optimal and correct clustering plans.

The results on the dilation test ($t = 3.0$) are plotted below. Again, the objective-minimizing solution among 100 trials over the same sample set is selected, and class assignments are determined by maximum probability. It is not surprising that Soft Exact performs better than $k$-means and Soft Approximate on non-isotropic test cases, as section 4.2 has demonstrated that the latter are the isotropic approximations of the former.

Figure 2: Left: Fuzzy $k$-means. Middle: Soft Approximate. Right: Soft Exact. The correct clusters are produced by Soft Exact, whereas fuzzy $k$-means and Soft Approximate split the clusters.

In fact, the contrast can be seen long before $t = 3.0$. The following is the result for $t = 1.6$, and the shaded regions are the convex hulls containing the “core points” of each class, defined as $C_k = \{x_i, P^i_k > 1/3\}$. The soft clusters produced by $k$-means have significant overlap, even though such error is often hidden by the labeling $k_i \leftarrow \arg\min_k P^i_k$. 
This performance gap is more pronounced in the comparison of correct rates below. Fuzzy $k$-means showed a steady decline in correct rate, indicating that many sample points are assigned highly ambiguous probability vectors $P^i$, containing more than one $P^i_k$ with large value. In contrast, the over 90% correct rates of Soft Exact and Soft Approximate indicate that most of its probability vectors $P^i$ are almost “hard”, that is, approximately a unit vector $\vec{c}_k$ corresponding to the true label. Eventually, Soft Exact and Soft Approximate become unstable for large $t$ and require more than 100 trials to find the optimal clustering.

5.2 Comparison of hard assignments

We compare next the hard assignment algorithms: $k$-means [2], Hard Exact Clustering (Algorithm [2]), and Hard Approximate Clustering (Algorithm [4]). The results on the expansion test and dilation test are plotted below. Again, for each algorithm on each sample set, the objective-minimizing result over 100 trials is selected. The performance comparison is analogous to that of soft assignment.
Clustering via optimal transport

Nevertheless, Hard Exact is a simplified version of Soft Exact and replaces the latter’s gradient descent, which moves only by small steps, by class reassignment, which hops among the extremal points of soft assignment’s domain. The correct rate curves of dilation test indicate that, whereas Hard Approximate has similar performance as Soft Approximate, Hard Exact is more unstable than Soft Exact.

Figure 4: Hard assignment on expansion test ($t = 3.2$). Left: $k$-means. Middle: Hard Approximate. Right: Hard Exact.

Figure 5: Hard assignment on dilation test ($t = 2$). Left: $k$-means. Middle: Hard Approximate. Right: Hard Exact.

Figure 6: For the expansion test, we have the ranking: $k$-means < Hard Exact < Hard Approximate, and for the dilation test: $k$-means < Hard Approximate < Hard Exact.
5.3 Performance on real-world data

In order to compare the performance of $k$-means and our algorithms on real-world problems, we use data sets from the online UCI Machine Learning Repository [9]. These data sets, intended for the task of classification, are provided with the true labeling, which we use to calculate the correct rates (16). The “Wine” [1] data set classifies wines based on chemical compositions. “Seeds” [7] classifies wheats by the shapes of wheat kernels. “Breast cancer (original)” [27] classifies benign/malign cancers by the shapes of cell nuclei, while “Breast cancer (diagnostic)” [21] classifies them by other cell statistics. “Parkinson’s” [10] diagnoses the disease by the patients’ voice and speech. “E.coli” [12] classifies proteins by their sequences and structures.

Since the proper setting for our clustering problem requires all attributes to be real valued, all categorical attributes, as well as entries with missing data, are removed. The samples are normalized in each dimension before clustering, since their attributes are often on disparate scales. Again, each algorithm is run 100 times on each sample set, and the objective-minimizing result is selected.

In the following table, for each sample set, the marked entries are the ones with maximum correct rates among the hard and soft assignment groups. The second table records the ratios of running times to those of $k$-means.

| Wine | Seeds | Breast cancer (original) | Breast cancer (diagnostic) | Parkinson’s | E.coli |
|------|-------|--------------------------|---------------------------|-------------|-------|
| Number of classes $K$ | 3 | 3 | 2 | 2 | 2 | 8 |
| Dimension $d$ | 13 | 7 | 9 | 30 | 22 | 6 |
| Sample size | 178 | 210 | 683 | 569 | 197 | 336 |
| Correct rates % |
| $k$-means | 96.63 | 91.90 | 95.75 | 91.04 | 54.36 | 55.65 |
| Hard Approximate | 97.19 | 91.90 | 96.34 | 89.46 | 53.33 | 59.82 |
| Hard Exact | 97.19 | 92.86 | 96.49 | 90.69 | 60.00 | 59.82 |
| Fuzzy $k$-means | 60.92 | 74.76 | 87.19 | 73.79 | 54.21 | 34.01 |
| Soft Approximate | 94.34 | 89.56 | 96.51 | 88.78 | 53.25 | 57.41 |
| Soft Exact | 91.71 | 88.73 | 96.29 | 89.94 | 50.91 | 52.67 |
| Relative runtime |
| $k$-means | 1 | 1 | 1 | 1 | 1 | 1 |
| Hard Approximate | 1.4 | 1.5 | 1.1 | 0.7 | 0.9 | 1.2 |
| Hard Exact | 3.0 | 1.2 | 3.1 | 5.5 | 1.9 | 5.2 |
| Fuzzy $k$-means | 1 | 1 | 1 | 1 | 1 | 1 |
| Soft Approximate | 2.0 | 3.1 | 1.5 | 0.9 | 0.6 | 1.1 |
| Soft Exact | 6.5 | 17.0 | 2.4 | 2.5 | 4.3 | 6.2 |

Our algorithms outperformed (fuzzy) $k$-means on the majority of data sets. For hard assignment, we have the ranking, $k$-means < hard approximate < hard exact, and for soft assignment we have fuzzy $k$-means < hard exact < hard approximate, though the performance gap between the exact and approximate solutions is minuscule.

One notable difference between our test family and these real-world data is that the latter have higher dimensions, which negatively influence fuzzy $k$-means’ performance. Previous studies [26] have shown that, as dimension increases, the pairwise distances of the sample points become homogeneous, and fuzzy $k$-means tends to assign $P^*_k$ that are close to $1/K$. Nevertheless, Soft Exact and Soft Approximate remain robust in the dimensions of these data sets, as shown in the following plots.
Figure 7: Soft assignment on the “Wine” data set. The sample is projected onto its principal 2-plane, with the true labeling given in the first panel. The following three panels correspond to fuzzy $k$-means, Soft Approximate and Soft Exact. The shaded polygons depict the convex hulls spanned by the “core points” of each cluster, $C_k = \{x_i, P_{ik} > 1/4\}$. Fuzzy $k$-means assigned each $x_i$ very ambiguous probabilities ($P_{ik}$ close to 1/3), so many sample points belong to the “cores” of two or more clusters, whereas the assignments produced by Soft Approximate and Soft Exact are relatively “hard”.

6 Conclusions

This article develops a conceptualization of clustering in terms of maximal explanation of variability by class assignment first proposed in [22]. When class assignments are known, the Wasserstein barycenter problem of optimal transport provides a natural framework to remove variability: moving the distributions underlying the various classes to a common one eliminates the component of variability attributable to class, while minimizing a transportation cost corresponds to minimizing data deformation, so that no class-independent variability is added or subtracted from the data. Then it is natural to characterize the optimal class assignment (i.e. the output of the clustering procedure) as the one that minimizes the amount of variability remaining in the barycenter.

The transportation cost proposed to characterize deformation is the squared Euclidean distance, while the variability left in the barycenter is quantified by the trace of its covariance matrix. It was shown in [22] that, in this scenario, restricting the transportation maps from each class to the barycenter to rigid translations yields the same optimal answer as $k$-means. This article broadens the family of transportations allowed to affine maps, showing that

1. Affine maps are in fact optimal in this setting: no further extension of the family of maps allowed would yield a smaller variance in the barycenter,

2. Including this larger class of maps extends the range of applicability of the methodology to distributions which are not mere translations of each other, not isotropic and not equally weighted, and
3. An effective procedure can be devised to solve the resulting constrained optimization problem.

The problem is most naturally posed and solved in its soft-assignment version, where the output is the probability that each sample belongs to each of the classes. Then the procedure can be simplified in two independent directions: making all assignments hard ab initio and treating all classes as if their underlying distributions were isotropic. The resulting algorithms are simpler but less robust that the more general one. All these procedures are tested and compared to the more standard $k$-means and fuzzy $k$-means on simple synthetic data built to illustrate the effects of relaxing the various hypotheses underlying the “standard data” for $k$-means, and on real-world data. In nearly all cases, the new procedure in its most general version shows better and more robust performance than its peers.

The methodology developed in this article, in addition to its value as a practical tool for clustering, opens the way to further inquiry into various directions:

1. Moving from the standard Euclidean distance to others possibly better suited for the problem at hand. In particular, one can still use a squared distance, but one defined along geodesics of the manifold underlying the data, such as the Fermat distance introduced in [19]. An interesting question here is whether an analogue of our proof that affine maps suffice to reach optimality applies to this scenario, once one extends both the concept of affine maps and the quantification of the variability via variance to manifolds.

2. Quantifying the variability remaining in the barycenter more thoroughly than through its variance, and developing the corresponding clustering methodology.

3. Extending the explanation of variability from the discrete factor underlying clustering (i.e. the class) to continuous and vectorial ones, providing a novel conceptualization and generalization of principal curves and surfaces.

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A Proof of Theorem 3.1

Proof. Denote by $\text{Dom}(\Sigma_y)$ the set of all possible barycenter’s covariances $\Sigma_y$ produced by couplings $\pi \in \Pi(\rho_1, \ldots, \rho_K)$. Denote by $\mathcal{D} \subseteq \text{Dom}(\Sigma_y)$ the subset where $Tr[\Sigma_y]$ is maximized. The goal is to show that the matrix function $F$ defined by (8) has a fixed point in $\mathcal{D}$.

First of all, $\mathcal{D}$ is compact in the space of matrices: Represent any vector $x \in \mathbb{R}^{Kd}$ by $(x_1, \ldots, x_K)$ with all $x_k \in \mathbb{R}^d$. Given any coupling $\pi$, the following multidimensional random variable (with $X_k \sim \rho_k$) has covariance:

$$
\text{Cov} \begin{bmatrix} X_1 \\ \vdots \\ X_K \end{bmatrix} = \begin{pmatrix} \Sigma_1 & Cov_{12} & \cdots & Cov_{1K} \\ Cov_{21} & \Sigma_2 & \cdots & Cov_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ Cov_{K1} & Cov_{K2} & \cdots & \Sigma_K \end{pmatrix}
$$
where

\[ \text{Cov}_{kh} = \text{Cov}_{kh}^T = \int_{\mathbb{R}^{K_d \times K_d}} x_k \cdot y_h^T d\pi(x,y) \]

Then

\[ \Sigma_y = \sum_{k,h=1}^{K} P_k P_h E[X_k \cdot X_h^T] = \sum_{k,h=1}^{K} P_k P_h \text{Cov}_{kh} \]

Since the marginals of all \( \pi \in \Pi(\rho_1, ... \rho_K) \) are fixed to be \( \rho_1, ... \rho_K \), the family \( \Pi(\rho_1, ... \rho_K) \) is closed in the weak topology of \( \mathcal{P}(\mathbb{R}^{K}) \) and tight (e.g. Theorem 4.4 of [24]), so by Prokhorov’s theorem, it is compact. Given any sequence \( \{\text{Cov}_n\}_{n=1}^\infty \subseteq \text{Cov}(\Pi(\rho_1, ... \rho_K)) \), let \( \{\pi_n\} \) be its preimage. Selecting a subsequence if necessary, we can assume that \( \{\pi_n\} \) converges weakly to some \( \pi \in \Pi(\rho_1, ... \rho_K) \). Let the covariance of \( \pi \) be \( \text{Cov} = (\text{Cov}_n) \), and we show that \( \{\text{Cov}_n\} \) converges to \( \text{Cov} \).

For all \( 1 \leq k < h \leq K \), define a sequence of compactly-supported functions \( \{f_{m}^{kh}\}_{m=1}^\infty \) on \( \mathbb{R}^{K_d \times K_d} \) that converges pointwise to \( x_k \cdot y_h^T \), e.g.

\[ f_{m}^{kh} := \mathbb{1}_m(x^k) \mathbb{1}_m(y^h) x_k \cdot y_h^T \]

where \( \mathbb{1}_m \in C^\infty_c(\mathbb{R}^d) \) is a bump function equal to 1 in \([-m, m]^d\) and vanishing outside \([-m - 1, m + 1]^d\). For all \( n \), the sequence \( \{f_{m}^{kh} \pi_n\}_{m=1}^\infty \) converges to the entry \( (\text{Cov}_n)_{kh} \) by the dominated convergence theorem, and this convergence is uniform in \( n \) because all \( \pi_n \) share the same marginals. Meanwhile,

\[ ||(\text{Cov}_{nh} - \text{Cov}_{nh})|| \leq ||(\text{Cov}_{nh}) - f_{m}^{kh} d\pi_n|| + ||f_{m}^{kh} d\pi_n - f_{m}^{kh} d\pi|| + ||\text{Cov}_{nh} - f_{m}^{kh} d\pi|| \]

for all \( \epsilon > 0 \), and \( m \) can be chosen large enough such that the first and third terms drop below \( \epsilon / 3 \). By weak convergence, \( N \) can be chosen so that for all \( n > N \), the second term is bounded by \( \epsilon / 3 \) for all \( m \). We conclude that \( \text{Cov} \) is a limit point of \( \{\text{Cov}_n\} \) and thus \( \text{Cov}(\Pi(\rho_1, ... \rho_K)) \) is compact.

It follows that

\[ \text{Dom}(\Sigma_y) = \{ \Sigma_y \mid \Sigma_y = \sum_{k,h=1}^{K} P_k P_h \text{Cov}_{kh}, \text{ for some } \text{Cov} \in \text{Cov}(\Pi(\rho_1, ... \rho_K)) \} \]

is compact as well, and our continuous objective function \( Tr[\Sigma_y] \) attains its maximum in \( \text{Dom}(\Sigma_y) \). Then, \( \mathcal{D} \), as the preimage of the maximum, is a non-empty compact subset of \( \text{Dom}(\Sigma_y) \).

Next, \( \mathcal{D} \) is convex. Given any \( \Sigma_y, \Sigma_y' \in \mathcal{D} \) and \( \lambda \in [0, 1] \), let \( \pi, \pi' \) and \( \text{Cov}, \text{Cov}' \) be the corresponding couplings and covariances. Then

\[ \lambda \Sigma_y + (1 - \lambda) \Sigma_y' = \sum_{k,h=1}^{K} P_k P_h [\lambda \text{Cov}_{kh} + (1 - \lambda) \text{Cov}'_{kh}] = \sum_{k,h=1}^{K} P_k P_h \int_{\mathbb{R}^{K_d \times K_d}} x_k \cdot y_h^T d(\lambda \pi + (1 - \lambda) \pi')(x,y) \]

So the convex combination is given by the coupling \( \lambda \pi + (1 - \lambda) \pi' \), which belongs to the convex set \( \Pi(\rho_1, ... \rho_K) \), and thus the combination belongs to \( \text{Dom}(\Sigma_y) \). Meanwhile, since the objective function \( Tr[\Sigma_y] \) is linear, convex combination preserves maximality. Therefore, \( \lambda \Sigma_y + (1 - \lambda) \Sigma_y' \in \mathcal{D} \) and \( \mathcal{D} \) is convex.

Finally, \( F \) is a continuous function on the positive-semidefinite matrices, and by inequality (7), it maps \( \mathcal{D} \) into itself. Since \( \mathcal{D} \) is compact and convex, Brouwer’s fixed point theorem implies that \( F \) must have a fixed point \( \Sigma_y \) in \( \mathcal{D} \). It follows that the coupling \( \pi \) that yields \( \Sigma_y \) maximizes (4) and produces a barycenter.

Given that some \( \rho_k \) is absolutely continuous, the covariance \( \Sigma_k \) is positive-definite, and by Theorem 4.2 of [4], the equation \( \Sigma_y = F(\Sigma_y) \) has a unique positive-definite solution \( \Sigma_y \). Absolute continuity of at least one \( \rho_k \) also implies that the barycenter \( \mu \) is unique [10] and absolutely continuous [13], and thus has a positive-definite covariance. Hence, the coupling \( \pi \) corresponding to \( \Sigma_y \) produces the unique \( \mu \), and the covariance of \( \mu \) is exactly \( \Sigma_y \). \[\square\]

**B Existence of derivative**

Here we establish that the partial derivatives \( \partial \Sigma_y / \partial P_k \) of our objective function (10) with respect to each membership probability always exist. Theorem 1.1 from [8] will be useful and we restate it below. Denote by \( \mathcal{S}_d, \mathcal{S}_d^+ \subseteq \mathcal{M}_d \) the linear subspace of symmetric matrices and the cone of positive-definite matrices.
Theorem B.1. The principal matrix square root function \( S \in \mathcal{S}_d^+ \rightarrow S^{1/2} \in \mathcal{S}_d^+ \) is Fréchet differentiable to any order, and the first order derivative is given by the operator
\[
(\nabla S^{1/2})(H) := \nabla S^{1/2}|_H = \int_0^\infty e^{-S^{1/2}t} H e^{-S^{1/2}t} \, dt
\]
so that for any \( H \in \mathcal{S}_d \) and \( S + hH \in \mathcal{S}_d^+ \)
\[
\lim_{h \to 0} \frac{1}{h} [(S + hH)^{1/2} - S^{1/2} - h(\nabla S^{1/2})(H)] = 0.
\]

Now we can apply the implicit function theorem to prove the existence of the partial derivatives.

Theorem B.2. For \( \{\Sigma_1, \ldots, \Sigma_K\} \subseteq \mathcal{S}_d^+ \), the solution \( \Sigma_y \) to
\[
\Sigma_y = F(\Sigma_y) = \sum_{k=1}^K P_k(\Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2})^{1/2}
\]
depends differentiably on \( \Sigma_1, \ldots, \Sigma_K \).

Proof. For convenience, let us slightly modify the function \( F(\Sigma_y) \) into
\[
F(\Sigma_y, \Sigma_1, \ldots, \Sigma_K) = \sum_{k=1}^K P_k(\Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2})^{1/2} - \Sigma_y
\]
which is a composition of \( C^1 \) functions on \( \prod_{i=1}^{K+1} S_d^+ \) and thus is \( C^1 \). To confirm that the gradient \( \nabla_{\Sigma_y} F \) is non-singular, perturb \( \Sigma_y \) along an arbitrary direction \( S \in \mathcal{S}_d \)
\[
(\nabla_{\Sigma_y} F)(S) = \sum_{k=1}^K P_k \left( \nabla \left( \Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2} \right)^{1/2} \right) \left( \left( \nabla \Sigma_y^{1/2} \right)(S) \Sigma_k \Sigma_y^{1/2} + \Sigma_y^{1/2} \Sigma_k \left( \nabla \Sigma_y^{1/2} \right)(S) \right) - S
\]
\[
= \sum_{k=1}^K \int_0^\infty e^{-\Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2}/2} t \left[ \left( \int_0^\infty e^{-\Sigma_y^{1/2} u} S e^{-\Sigma_y^{1/2} u} \, du \right) \Sigma_k \Sigma_y^{1/2}
\right.
\]
\[
+ \Sigma_y^{1/2} \Sigma_k \left( \int_0^\infty e^{-\Sigma_y^{1/2} u} S e^{-\Sigma_y^{1/2} u} \, du \right) \left( e^{-\Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2} t/2} - S \right)
\]
To evaluate \( \int_0^\infty e^{-\Sigma_y^{1/2} u} S e^{-\Sigma_y^{1/2} u} \, du \), we apply the eigendecomposition \( \Sigma = U D U^T \)
\[
\int_0^\infty e^{-t(DU^T)^{1/2} u} (DU^T)^{1/2} \, dt = U \left( \int_0^\infty e^{-t(DU^T)^{1/2} u} U^T e^{-t(DU^T)^{1/2} t} \, dt \right) U^T = U (T \circ U^T SU) U^T
\]
where \( \circ \) is Hadamard product and \( T_{ij} = \frac{1}{\sqrt{x_i} + \sqrt{x_j}} \). Thus, using \( \Sigma_y^{1/2} \Sigma_k \Sigma_y^{1/2} = U_k D_k U_k^T \), \( \Sigma_y = U_y D_y U_y^T \) and the corresponding \( T_k, T_y \), we obtain
\[
(\nabla_{\Sigma_y} F)(S) = \sum_{k=1}^K P_k U_k \left[ T_k \circ U_k^T \left[ U_y \left( T_y \circ U_y^T SU_y \right) U_y^T \Sigma_k \Sigma_y^{1/2} + \Sigma_y^{1/2} \Sigma_k U_y \left( T_y \circ U_y^T SU_y \right) U_y^T \right] U_k \right] U_k^T - S
\]
To check non-singularity, we set \( (\nabla_{\Sigma_y} F)(S) = 0 \) and vectorize the equation to disentangle \( S \). We utilize the property that \( \text{vec}(AXB) = (B^T \otimes A) \text{vec}(X) \) where \( \otimes \) is the Kronecker product [11]. Meanwhile, vectorizing the Hadamard product yields
\[
\text{vec}(T \circ X) = \text{diag} \left( \text{vec}(T) \right) \text{vec}(X) = (D^{1/2} \otimes I + I \otimes D^{1/2})^{-1} \text{vec}(X).
\]
The original equation \( (\nabla_{\Sigma_y} F)(S) = 0 \) becomes,
\[
\text{vec}(S) = \text{vec} \left\{ \sum_{k=1}^K P_k U_k \left[ T_k \circ U_k^T \left[ U_y \left( T_y \circ U_y^T SU_y \right) U_y^T \Sigma_k \Sigma_y^{1/2} + \Sigma_y^{1/2} \Sigma_k U_y \left( T_y \circ U_y^T SU_y \right) U_y^T \right] U_k \right] U_k^T \right\}
\]
\[
= \sum_{k=1}^{K} P_k(U_k \otimes U_k)(D_{1/2}^{1/2} \otimes I + I \otimes D_{1/2}^{1/2})^{-1}(U_k^T \otimes U_k^T)(\Sigma^{1/2} \Sigma_k \otimes I + I \otimes \Sigma_k \Sigma^{1/2})
\]

\[
(U_y \otimes U_y)(D_{y}^{1/2} \otimes I + I \otimes D_{y}^{1/2})^{-1}(U_y^T \otimes U_y^T) \text{vec}(S)
\]

Splitting the term \(\Sigma^{1/2} \Sigma_k \otimes I = (\Sigma^{1/2} \Sigma_k \Sigma^{1/2} \otimes I) \cdot (\Sigma^{-1/2} \otimes I)\), we obtain

\[
\text{vec}(S) = \left\{ \left[ \sum_{k=1}^{K} P_k(U_k \otimes U_k)(D_{1/2}^{1/2} \otimes I + I \otimes D_{1/2}^{1/2})^{-1}(D_k \otimes I)(U_k^T \otimes U_k^T) \right] - (U_y \otimes U_y)(D_{y}^{-1/2} \otimes I)(D_{y}^{1/2} \otimes I + I \otimes D_{y}^{1/2})^{-1}(U_y^T \otimes U_y^T) \right\} \text{vec}(S).
\]

Applying the three identities

\[
D_k \otimes I = (D_{1/2}^{1/2} \otimes I + I \otimes D_{1/2}^{1/2})(D_{1/2}^{1/2} \otimes I - I \otimes D_{1/2}^{1/2}) + I \otimes D_k,
\]

\[
I \otimes D_k = (D_{1/2}^{1/2} \otimes I + I \otimes D_{1/2}^{1/2})^2 - D_{1/2}^{1/2} \otimes I - 2D_{1/2}^{1/2} \otimes D_{1/2}^{1/2},
\]

\[
D_{y}^{-1/2} \otimes D_{y}^{-1/2} = (D_{y}^{1/2} \otimes I + I \otimes D_{y}^{1/2})^{-1}(D_{y}^{-1/2} \otimes I + I \otimes D_{y}^{-1/2}),
\]

we obtain

\[
\text{vec}(S) = \left\{ \left[ \sum_{k=1}^{K} P_k(U_k \otimes U_k)(D_{1/2}^{1/2} \otimes I - I \otimes D_{1/2}^{1/2})(U_k^T \otimes U_k^T) \right] - (U_y \otimes U_y)(D_{y}^{-1/2} \otimes D_{y}^{-1/2})(U_y^T \otimes U_y^T) \right\} \text{vec}(S).
\]
\[
- \left[ \sum_{k=1}^{K} P_k(U_k \otimes U_k)(D_k^{1/2} \otimes I + I \otimes D_k^{1/2})^{-1}(D_k^{1/2} \otimes D_k^{1/2})(U_k^T \otimes U_k^T) \right].
\]
\[
\left[ (U_y \otimes U_y)(D_y^{-1/2} \otimes D_y^{-1/2})(U_y^T \otimes U_y^T) \right] vec(S)
\]
\[
= \left\{ I - \left[ \sum_{k=1}^{K} P_k(U_k \otimes U_k)(D_k^{1/2} \otimes I + I \otimes D_k^{1/2})^{-1}(D_k^{1/2} \otimes D_k^{1/2})(U_k^T \otimes U_k^T) \right] \cdot \left( \Sigma_y^{-1/2} \otimes \Sigma_y^{-1/2} \right) \right\} vec(S)
\]

Hence, it follows that
\[
\left[ \sum_{k=1}^{K} P_k(U_k \otimes U_k)(D_k^{1/2} \otimes I + I \otimes D_k^{1/2})^{-1}(D_k^{1/2} \otimes D_k^{1/2})(U_k^T \otimes U_k^T) \right] \cdot \left( \Sigma_y^{-1/2} \otimes \Sigma_y^{-1/2} \right) vec(S) = O
\]

Denote the lengthy matrix by \( \left[ \sum_{k=1}^{K} P_kY_k \right] Y \). Since each \( Y_k \) and \( Y \) is positive-definite, the entire matrix is positive-definite and the equation holds if and only if \( S = O \). We can conclude that the gradient \( (\nabla \Sigma_y F) \) is always non-singular, and the implicit function theorem implies that \( \Sigma_y \) depends differentiably on \( \{ \Sigma_1, \ldots, \Sigma_K \} \subseteq \prod_{i=1}^{K} S_d^+ \). \( \square \)

It follows that since \( \Sigma_k \) depends differentiably on \( P_k^i \), the derivatives \( \partial \Sigma_y / \partial P_k^i \) exist.

## C Computation of derivative

To solve for the gradient \( \nabla \Sigma_y Tr[\Sigma_y] \), set \( \Lambda_k^i = \frac{\partial \Sigma_y}{\partial P_k} \in S_d \) as an unknown variable, and rather artificially, define
\[
\Omega_k^i := \frac{1}{P_k} \frac{\partial (P_k)^2 \Sigma_k}{\partial P_k} = (x_i - \bar{x_k}) \cdot (x_i - \bar{x_k})^T + \Sigma_k
\]

Taking partial derivative \( \partial P_k^i \) on both sides of the equation
\[
\Sigma_y = \sum_{k=1}^{K} \left[ \Sigma_y^{1/2}((P_k)^2 \Sigma_k) \Sigma_y^{1/2} \right]^{1/2}
\]

which is rewritten from \( \Sigma_y = F(\Sigma_y) \), we obtain
\[
\Lambda_k^i = \sum_{h \neq k} \left( \nabla \left( \Sigma_y^{1/2}((P_k)^2 \Sigma_h) \Sigma_y^{1/2} \right) \right) \cdot \left( \nabla \Sigma_y^{1/2}((P_k)^2 \Sigma_h) \right) \cdot \left( \Sigma_y^{1/2}((P_k)^2 \Sigma_h) \right) \cdot \left( \nabla \Sigma_y^{1/2}((P_k)^2 \Sigma_h) \right)
\]
\[
+ \left( \nabla \left( \Sigma_y^{1/2}((P_k)^2 \Sigma_k) \Sigma_y^{1/2} \right) \right) \cdot \left( \nabla \Sigma_y^{1/2}((P_k)^2 \Sigma_k) \right) \cdot \left( \Sigma_y^{1/2}((P_k)^2 \Sigma_k) \right) \cdot \left( \nabla \Sigma_y^{1/2}((P_k)^2 \Sigma_k) \right)
\]
\[
= \sum_{h=1}^{K} U_h \left[ (P_h)^{-1}T_h \odot U_h^T \right] U_h \left[ T_y \odot U_y \Lambda_k U_y \right] U_y^T \left( P_h \right)^2 \Sigma_h \Sigma_y^{1/2} + \Sigma_y^{1/2} \Sigma_h \left( T_y \odot U_y \Lambda_k U_y \right) U_y^T U_h^T
\]
\[
+ U_k \left[ (P_k)^{-1}T_k \odot U_k^T \right] \left( \Sigma_y^{1/2}P_k \Sigma_k \right) \Sigma_y^{1/2} + \Sigma_y^{1/2} U_k \right] U_k^T
\]
\[
= \sum_{h=1}^{K} U_h \left[ T_h \odot U_h^T \right] U_h \left[ T_y \odot U_y \Lambda_k U_y \right] U_y^T \left( \Sigma_y^{1/2} \Sigma_h \right) + \Sigma_y^{1/2} \Sigma_h U_y \left( T_y \odot U_y \Lambda_k U_y \right) U_y^T U_h^T
\]
\[
+ U_k \left[ T_k \odot U_k^T \right] \left( \Sigma_y^{1/2} \Sigma_k \right) + \Sigma_y^{1/2} U_k \right] U_k^T
\]

Vectorize and simplify it by the previous computations,
\[
vec(\Lambda_k^i) = \left\{ I - \left[ \sum_{h=1}^{K} P_h(U_h \otimes U_h)(D_h^{1/2} \otimes I + I \otimes D_h^{1/2})^{-1}(D_h^{1/2} \otimes D_h^{1/2})(U_h^T \otimes U_h^T) \right] \cdot \left( \Sigma_y^{-1/2} \otimes \Sigma_y^{-1/2} \right) \right\}
\]
\[
\cdot vec(\Lambda_i^k) + (U_k \otimes U_k)(D_{1/2}^k \otimes I + I \otimes D_{1/2}^k)^{-1}(U_k^T \otimes U_k^T)(\Sigma_{y/2}^1 \otimes \Sigma_{y/2}^1) vec(\Omega_i^k)
\]

Therefore,

\[
vec(\Lambda_i^k) = (\Sigma_{y/2}^1 \otimes \Sigma_{y/2}^1)
\]

\[
\left[ \sum_{h=1}^{K} Pb(U_h \otimes U_h)(D_{1/2}^h \otimes I + I \otimes D_{1/2}^h)^{-1}(D_{1/2}^h \otimes D_{1/2}^h)(U_h^T \otimes U_h^T) \right]^{-1}
\]

\[
\left[ (U_k \otimes U_k)(D_{1/2}^k \otimes I + I \otimes D_{1/2}^k)^{-1}(U_k^T \otimes U_k^T) \right] (\Sigma_{y/2}^1 \otimes \Sigma_{y/2}^1) \cdot vec(\Omega_k^i)
\]

Denote the solution by \( \Lambda_i^k = vec^{-1}(X_k vec(\Omega_i^k)) \), we obtain an expression for the gradient of the objective function

\[
\nabla_{\rho_i} Tr[\Sigma_y] = \sum_{k=1}^{K} Tr[\Lambda_i^k] e_k^i = \sum_{k=1}^{K} vec(I)^T X_k vec(\Omega_k^i) e_k^i
\]