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Kernelized Infomax Clustering

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Abstract. We propose a simple information-theoretic clustering approach based on maximizing the mutual information $I(\mathsf{x}, y)$ between the unknown cluster labels y and the training patterns x with respect to parameters of specifically constrained encoding distributions. The constraints are chosen such that patterns are likely to be clustered similarly if they lie close to specific (unknown) vectors in the feature space. The method may be conveniently applied to learning the optimal affinity matrix, which corresponds to learning parameters of the kernelized encoder. The procedure does not require computations of eigenvalues or inverses of the Gram matrices, which makes it potentially attractive for clustering large data sets.

1 Introduction

Let $\mathsf{x} \in \mathbb{R}^{|\mathsf{x}|}$ be a visible pattern, and $y \in \{y_1, \ldots, y_{|y|}\}$ its discrete unknown cluster label. Rather than learning a density model of the observations, our goal here will be to learn a mapping $\mathsf{x} \rightarrow y$ from the observations to the latent codes (cluster labels) by optimizing a formal measure of coding efficiency. Good codes y should be in some way informative about the underlying high-dimensional source vectors x, so that the useful information contained in the sources is not lost. The fundamental measure in this context is the mutual information

$$I(\mathsf{x}, y) \overset{\text{def}}{=} H(\mathsf{x}) - H(\mathsf{x}|y) \equiv H(y) - H(y|\mathsf{x}), \tag{1}$$

which indicates the decrease in uncertainty about the pattern x due to the knowledge of the underlying cluster label y (e.g. [Cover and Thomas, 1991]). Here $H(y) \equiv -\langle \log p(y) \rangle_{p(y)}$ and $H(y|\mathsf{x}) \equiv -\langle \log p(y|\mathsf{x}) \rangle_{p(\mathsf{x},y)}$ are marginal and conditional entropies respectively, and the brackets $\langle \ldots \rangle_p$ represent averages over p. In our case the *encoder* model is defined as $p(\mathsf{x}, y) \propto \sum_{m=1}^{M} \delta(\mathsf{x} - \mathsf{x}^{(m)}) p(y|\mathsf{x})$, where $\{\mathsf{x}^{(m)} | m = 1, \ldots, M\}$ is a set of training patterns.

Our goal is to maximize (1) with respect to parameters of a constrained encoding distribution $p(y|\mathsf{x})$. In contrast to most applications of the *infomax* principle ([Linsker, 1988]) in stochastic channels (e.g. [Brunel and Nadal, 1998, Fisher and Principe, 1998, Torkkola and Campbell, 2000]), optimization of the objective (1) is computationally tractable since the cardinality of the code space $|y|$ (the number of clusters) will typically be low. Indeed, had the code space been high-dimensional, computation of $I(\mathsf{x}, y)$ would have required evaluation of the generally intractable entropy of the mixture $H(\mathsf{y})$, and approximations would need to be considered (e.g. [Barber and Agakov, 2003, Agakov and Barber, 2005]).

Maximization of the mutual information with respect to parameters of the encoder model effectively defines a *discriminative unsupervised* optimization framework, where the model is parameterized similarly to a conditionally trained classifier, but where the cluster allocations are generally unknown. Training such models $p(y|\mathsf{x})$ by maximizing the likelihood $p(\mathsf{x})$ would be meaningless, as the cluster variables would marginalize out, which motivates also our information theoretic approach. In this way we may extract soft cluster allocations directly from the training set, with no additional information about class labels, relevance patterns, etc. required. This is an important difference from other clustering techniques making a recourse to information theory, which consider different channels and generally require additional information about relevance or irrelevance variables (*cf* [Tishby et al., 1999, Chechik and Tishby, 2002, Dhillon and Guan, 2003]).

Our infomax approach is in contrast with probabilistic clustering approaches based on likelihood maximization. There the task of finding an optimal cluster allocation y for an observed pattern x may be viewed as an inference problem in *generative* models $y \rightarrow \mathsf{x}$, where the probability of the data $p(\mathsf{x}) = \sum_y p(y) p(\mathsf{x}|y)$ is defined as a mixture of $|y|$ processes. The key idea of fitting such models to data is to find a constrained probability distribution $p(\mathsf{x})$ which would be likely to generate the visible patterns $\{\mathsf{x}^{(1)}, \ldots, \mathsf{x}^{(M)}\}$ (this is commonly achieved by maximizing the marginal likelihood with respect to deterministic parameters of the constrained distribution). The unknown clusters y corresponding to each pattern x may then be assigned according to the posterior $p(y|\mathsf{x}) \propto p(y) p(\mathsf{x}|y)$. Such generative approaches are well-known but suffer from the constraint that $p(\mathsf{x}|y)$ is a correctly normalised distribution in x. In high dimensions $|\mathsf{x}|$ this restricts the class of generative distributions usually to (mixtures of) Gaussians whose mean is dependent (in a linear or non-linear way) on the latent cluster y. Typically data will lie on low dimensional curved manifolds embedded in the high dimensional x-space. If we are restricted to using mixtures of Gaussians to model this curved manifold, typically a very large number of mixture components will be required. No such restrictions apply in the infomax case so that the mappings $p(y|\mathsf{x})$ may be very complex, subject only to sensible clustering constraints.

2 Clustering in Nonlinear Encoder Models

Arguably, there are at least two requirements which a meaningful cluster allocation procedure should satisfy. Firstly, clusters should be, in some sense, locally smooth. For example, each pair of source vectors should have a high probability of being assigned to the same cluster if the vectors satisfy specific geometric constraints. Secondly, we may wish to avoid assigning unique cluster labels to outliers (or other constrained regions in the data space), so that under-represented regions in the data space are not over-represented in the code space. Note that degenerate cluster allocations are generally suboptimal under the objective (1), as they would lead to a reduction in the marginal entropy $H(y)$. On the other hand, it is intuitive that maximization of the mutual information $I(\mathsf{x}, y)$ favors hard assignments of cluster labels to equiprobable data regions, as this would result in the growth in $H(y)$ and reduction in $H(y|\mathsf{x})$.

2.1 Learning Optimal Parameters

Local smoothness and "softness" of the clusters may be enforced by imposing appropriate constraints on $p(y|\mathsf{x})$. A simple choice of the encoder is

$$p(y_j|\mathsf{x}^{(i)}) \propto \exp\{-\|\mathsf{x}^{(i)} - \mathsf{w}_j\|^2/s_j + b_j\}, \tag{2}$$

where the cluster centers $\mathsf{w}_j \in \mathbb{R}^{|\mathsf{x}|}$, the dispersions s_j, and the biases b_j are the encoder parameters to be learned. Clearly, under the encoding distribution (2) patterns x lying close to specific centers w_j in the *data* space will tend to be clustered similarly. In principle, we could consider other choices of $p(y|\mathsf{x})$; however (2) will prove to be particularly convenient for the kernelized extensions.

Learning the optimal cluster allocations corresponds to maximizing (1) with respect to the encoder parameters (2). The gradients are given by

$$\frac{\partial I(\mathsf{x}, y)}{\partial \mathsf{w}_j} = \frac{1}{M}\sum_{m=1}^{M} p(y_j|\mathsf{x}^{(m)})\frac{(\mathsf{x}^{(m)} - \mathsf{w}_j)}{s_j}\alpha_j^{(m)} \tag{3}$$

$$\frac{\partial I(\mathsf{x}, y)}{\partial s_j} = \frac{1}{M}\sum_{m=1}^{M} p(y_j|\mathsf{x}^{(m)})\frac{\|\mathsf{x}^{(m)} - \mathsf{w}_j\|^2}{2s_j^2}\alpha_j^{(m)}. \tag{4}$$

Analogously, we get $\partial I(\mathsf{x}, y)/\partial b_j = \sum_{m=1}^{M} p(y_j|\mathsf{x}^{(m)})\alpha_j^{(m)}/M$.

Expressions (3) and (4) have the form of the weighted EM updates for isotropic Gaussian mixtures, with the weighting coefficients $\alpha_j^{(m)}$ defined as

$$\alpha_j^{(m)} \overset{\text{def}}{=} \alpha_j(\mathsf{x}^{(m)}) \overset{\text{def}}{=} \log\frac{p(\mathsf{x}^{(m)}|y_j)}{p(\mathsf{x}^{(m)})} - KL\left(p(y|\mathsf{x}^{(m)})\|\langle p(y|\mathsf{x})\rangle_{\tilde{p}(\mathsf{x})}\right), \tag{5}$$

where KL defines the Kullback-Leibler divergence (e.g. [Cover and Thomas, 1991]). Clearly, if $\alpha_j^{(m)}$ is kept fixed for all $m = 1, \ldots, M$ and $j = 1, \ldots, |y|$, the gradients (3) are identical to those obtained by maximizing the log-likelihood of a Gaussian mixture model (up to irrelevant constant pre-factors). Generally, however, the coefficients $\alpha_j^{(m)}$ will be functions of w_l, s_l, and b_l for all cluster labels $l = 1, \ldots, |y|$.

In practice, we may impose a simple construction ensuring that $s_j > 0$, for example by assuming that $s_j = \exp\{\tilde{s}_j\}$ where $\tilde{s}_j \in \mathbb{R}$. For this case, we may re-express the gradients for the variances as $\partial I(\mathsf{x}, y)/\partial\tilde{s}_j = s_j\partial I(\mathsf{x}, y)/\partial s_j$. Expressions (3) and (4) may then be used to perform gradient ascent on $I(\mathsf{x}, y)$ for w_j, $\tilde{s}_j$, and b_j, where $j = 1, \ldots, |y|$. After training, the optimal cluster allocations may be assigned according to the encoding distribution $p(y|\mathsf{x})$.

2.2 Infomax Clustering with Kernelized Encoder Models

We now extend (2) by considering a kernelized parameterization of a nonlinear encoder. Let us assume that the source patterns $\mathsf{x}^{(i)}$, $\mathsf{x}^{(j)}$ have a high probability of being assigned to the same cluster if they lie close to a specific cluster center in some *feature* space. One choice of the encoder distribution for this case is

$$p(y_j|\mathsf{x}^{(i)}) \propto \exp\{-\|\boldsymbol{\phi}(\mathsf{x}^{(i)}) - \mathsf{w}_j\|^2/s_j + b_j\}, \tag{6}$$

where $\boldsymbol{\phi}(\mathsf{x}^{(i)}) \in \mathbb{R}^{|\boldsymbol{\phi}|}$ is the feature vector corresponding to the source pattern $\mathsf{x}^{(i)}$, and $\mathsf{w}_j \in \mathbb{R}^{|\boldsymbol{\phi}|}$ is the (unknown) cluster center in the feature space. The feature space may be very high- or even infinite-dimensional.

Since each cluster center $\mathsf{w}_i \in \mathbb{R}^{|\boldsymbol{\phi}|}$ lives in the same space as the projected sources $\boldsymbol{\phi}(\mathsf{x}^{(i)})$, it is representable in the basis of the projections as

$$\mathsf{w}_j = \sum_{m=1}^{M} \alpha_{mj}\boldsymbol{\phi}(\mathsf{x}^{(m)}) + \mathsf{w}_j^{\perp}, \tag{7}$$

where $\tilde{\mathsf{w}}_i^{\perp} \in \mathbb{R}^{|\boldsymbol{\phi}|}$ is orthogonal to the span of $\boldsymbol{\phi}(\mathsf{x}_1), \ldots, \boldsymbol{\phi}(\mathsf{x}_M)$, and $\{\alpha_{mj}\}$ is a set of coefficients (here j and m index $|y|$ codes and M patterns respectively). Then we may transform the encoder distribution (6) to

$$\begin{aligned} p(y_j|\mathsf{x}^{(m)}) &\propto \exp\left\{-\left(K_{mm} - 2\mathsf{k}^T(\mathsf{x}^{(m)})\mathsf{a}_j + \mathsf{a}_j^T\mathsf{K}\mathsf{a}_j + c_j\right)/s_j\right\} \\ &\stackrel{\text{def}}{=} \exp\{-f_j(\mathsf{x}^{(m)})\}, \end{aligned} \tag{8}$$

where $\mathsf{k}(\mathsf{x}^{(m)})$ corresponds to the m^{th} column (or row) of the Gram matrix $\mathsf{K} \stackrel{\text{def}}{=} \{K_{ij}\} \stackrel{\text{def}}{=} \{\boldsymbol{\phi}(\mathsf{x}^{(i)})^T\boldsymbol{\phi}(\mathsf{x}^{(j)})\} \in \mathbb{R}^{M\times M}$, $\mathsf{a}_j \in \mathbb{R}^M$ is the j^{th} column of the matrix of the coefficients $\mathsf{A} \stackrel{\text{def}}{=} \{a_{mj}\} \in \mathbb{R}^{M\times|y|}$, and $c_j = (\mathsf{w}_j^{\perp})^T\mathsf{w}_j^{\perp} - s_jb_j$. Without loss of generality, we may assume that $\mathsf{c} = \{c_j\} \in \mathbb{R}^{|y|}$ is a free unconstrained parameter. Additionally, we will ensure positivity of the dispersions s_j by considering a construction constraint $s_j = \exp\{\tilde{s}_j\}$, where $\tilde{s}_j \in \mathbb{R}$.

Learning Optimal Parameters

First we will assume that the Gram matrix $\mathsf{K} \in \mathbb{R}^{M\times M}$ is *fixed* and *known* (which effectively corresponds to considering a fixed affinity matrix, see e.g. [Dhillon et al., 2004]). Objective (1) should be optimized with respect to the log-dispersions $\tilde{s}_j \equiv \log(s_j)$, biases c_j, and coordinates $\mathsf{A} \in \mathbb{R}^{M\times|y|}$ in the space spanned by the feature vectors $\{\boldsymbol{\phi}(\mathsf{x}^{(i)})|i = 1, \ldots, M\}$. From (8) we get

$$\frac{\partial I(\mathsf{x}, y)}{\partial \mathsf{a}_j} = \frac{1}{s_j}\left\langle p(y_j|\mathsf{x})\left(\mathsf{k}(\mathsf{x}) - \mathsf{K}\mathsf{a}_j\right)\alpha_j(\mathsf{x})\right\rangle_{\tilde{p}(\mathsf{x})} \in \mathbb{R}^M, \tag{9}$$

$$\frac{\partial I(\mathsf{x}, y)}{\partial \tilde{s}_j} = \frac{1}{2s_j}\left\langle p(y_j|\mathsf{x})f_j(\mathsf{x})\alpha_j(\mathsf{x})\right\rangle_{\tilde{p}(\mathsf{x})}, \tag{10}$$

where $\tilde{p}(\mathsf{x}) \propto \sum_{m-1}^{M} \delta(\mathsf{x} - \mathsf{x}^{(m)})$ is the empirical distribution. Analogously, we obtain

$$\partial I(\mathsf{x}, y)/\partial c_j = \langle \alpha_j(\mathsf{x})\rangle_{\tilde{p}(\mathsf{x})}, \tag{11}$$

where the coefficients $\alpha_j(\mathsf{x})$ are given by (5). For a known Gram matrix $\mathsf{K} \in \mathbb{R}^{M\times M}$, the gradients $\partial I/\partial \mathsf{a}_j$, $\partial I/\partial \tilde{s}_j$, and $\partial I/\partial c_j$ given by expressions (9) – (11) may be used in numerical optimization for the model parameters. (Note that in order to optimize the objective (1) one could potentially apply the iterative Arimoto-Blahut algorithm for maximizing channel capacity (see e.g. [Cover and Thomas, 1991]). However, for the considered encoder distribution it is generally difficult to derive closed-form updates for parameters of $p(y|\mathsf{x})$, which stipulates numerical optimization).

Learning Optimal Kernels

Since we presume that explicit computations in $\mathbb{R}^{|\boldsymbol{\phi}|}$ are expensive, we cannot compute the Gram matrix by trivially applying its definition $\mathsf{K} = \{\boldsymbol{\phi}(\mathsf{x}_i)^T\boldsymbol{\phi}(\mathsf{x}_j)\}$. Instead, we may interpret scalar products in feature spaces as *kernel functions*

$$\boldsymbol{\phi}(\mathsf{x}^{(i)})^T\boldsymbol{\phi}(\mathsf{x}^{(j)}) = \mathcal{K}_{\boldsymbol{\Theta}}(\mathsf{x}^{(i)},\mathsf{x}^{(j)};\boldsymbol{\Theta}),\ \ \forall \mathsf{x}^{(i)},\mathsf{x}^{(j)} \in \mathcal{R}_{\mathsf{x}}, \tag{12}$$

where $\mathcal{K}_{\boldsymbol{\Theta}} : \mathcal{R}_{\mathsf{x}} \times \mathcal{R}_{\mathsf{x}} \to \mathbb{R}$ satisfies Mercer's kernel properties (e.g. [Scholkopf and Smola, 2002]). We may now apply our *unsupervised* framework to implicitly learn the optimal nonlinear features by optimizing $I(\mathsf{x}, y)$ with respect to the parameters $\boldsymbol{\Theta}$ of the kernel function $\mathcal{K}_{\boldsymbol{\Theta}}$. After some algebraic manipulations, we get

$$M\frac{\partial I(\mathsf{x},y)}{\partial \boldsymbol{\Theta}} = \sum_{m=1}^{M} KL(p(y|\mathsf{x}^{(m)})\|p(y)) \sum_{k=1}^{|y|} \frac{\partial f_k(\mathsf{x}^{(m)})}{\partial \boldsymbol{\Theta}} p(y_k|\mathsf{x}^{(m)}) \\ - \sum_{m=1}^{M}\sum_{j=1}^{|y|} \frac{\partial f_j(\mathsf{x}^{(m)})}{\partial \boldsymbol{\Theta}} p(y_j|\mathsf{x}^{(m)}) \log\frac{p(y_j|\mathsf{x}^{(m)})}{p(y_j)} \tag{13}$$

where $f_k(\mathsf{x}^{(m)})$ is given by (8). The computational complexity of computing the updates for $\boldsymbol{\Theta}$ is $O(M|y|^2)$, where M is the number of training patterns and $|y|$ is the number of clusters (which is assumed to be small). In contrast to spectral methods (see e.g. [Shi and Malik, 2000], [Ng et al., 2001]) neither the objective (1) nor its gradients require inversion of the Gram matrix $\mathsf{K} \in \mathbb{R}^{M\times M}$ or computations of its eigenvalue decomposition. Hence, provided that the objective function is well behaved, we may hope that the method is computationally relatively cheap.

In the special case of the radial basis function (RBF) kernels

$$\mathcal{K}_{\beta}(\mathsf{x}^{(i)},\mathsf{x}^{(j)}) = \exp\{-\beta\|\mathsf{x}^{(i)} - \mathsf{x}^{(j)}\|^2\}, \tag{14}$$

the gradients of the encoder potentials are simply given by

$$\frac{\partial f_j(\mathsf{x}^{(m)})}{\partial \beta} = \frac{1}{s_j}\left(\mathsf{a}_j^T\tilde{\mathsf{K}}\mathsf{a}_j - 2\tilde{\mathsf{k}}^T(\mathsf{x}^{(m)})\mathsf{a}_j\right), \tag{15}$$

where $\tilde{\mathsf{K}} \overset{\text{def}}{=} \{\tilde{K}_{ij}\} \overset{\text{def}}{=} K(\mathsf{x}^{(i)},\mathsf{x}^{(j)})(1-\delta(\mathsf{x}^{(i)}-\mathsf{x}^{(j)}))$, and δ is the Kronecker delta. By substituting (15) into the general expression (13), we obtain the gradient of the mutual information with respect to the RBF kernel parameters.

3 Demonstrations

We have empirically compared our kernelized information-theoretic clustering approach with Gaussian mixture, k-means, feature-space k-means, non-kernelized information-theoretic clustering (see Section 2.1), and a multi-class spectral clustering method optimizing the *normalized cuts*. We illustrate the methods on datasets that are particularly easy to visualize. Figure 1 shows a typical application of the methods to the spiral data, where $x_1(t) = t\cos(t)/4$, $x_2(t) = t\sin(t)/4$ correspond to different coordinates of $\mathsf{x} \in \mathbb{R}^{|\mathsf{x}|}, |\mathsf{x}| = 2$, and $t \in [0, 3.(3)\pi]$. The kernel parameters β of the RBF-kernelized encoding distribution were initialized at $\beta_0 = 2.5$ and learned according to (15). The initial settings of the coefficients $\mathsf{A} \in \mathbb{R}^{M\times|\mathsf{y}|}$ in the feature space were sampled from $\mathcal{N}_{A_{ij}}(0, 0.1)$. The log-variances $\tilde{s}_1, \ldots, \tilde{s}_{|y|}$ were initialized at zeros. The encoder parameters A and $\{\tilde{s}_j|j = 1, \ldots, |y|\}$ (along with the RBF kernel parameter β) were optimized by applying the scaled conjugate gradients. We found that Gaussian mixtures trained by maximizing the likelihood usually resulted in highly stochastic cluster allocations; additionally, they led to a large variation in cluster sizes. The Gaussian mixtures

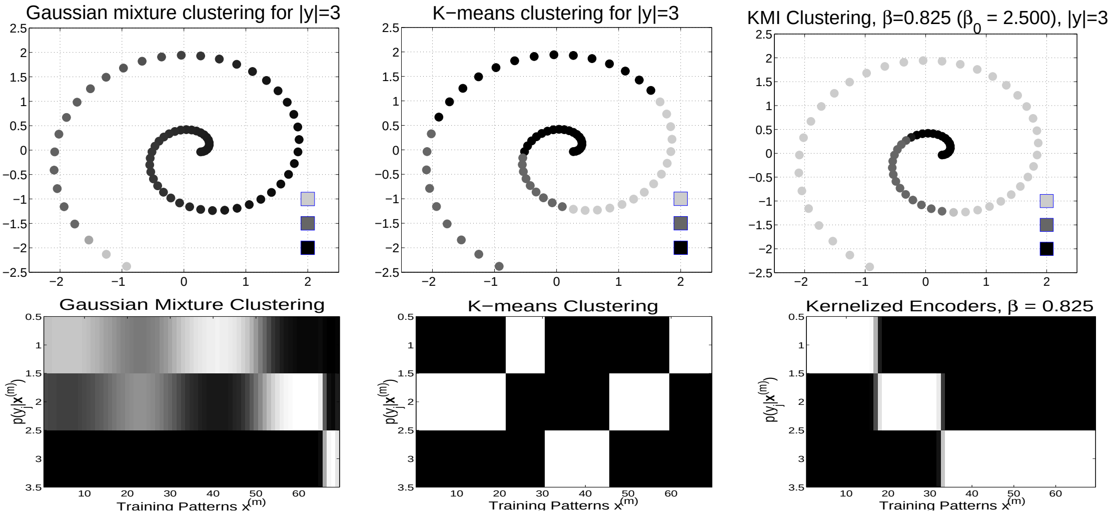
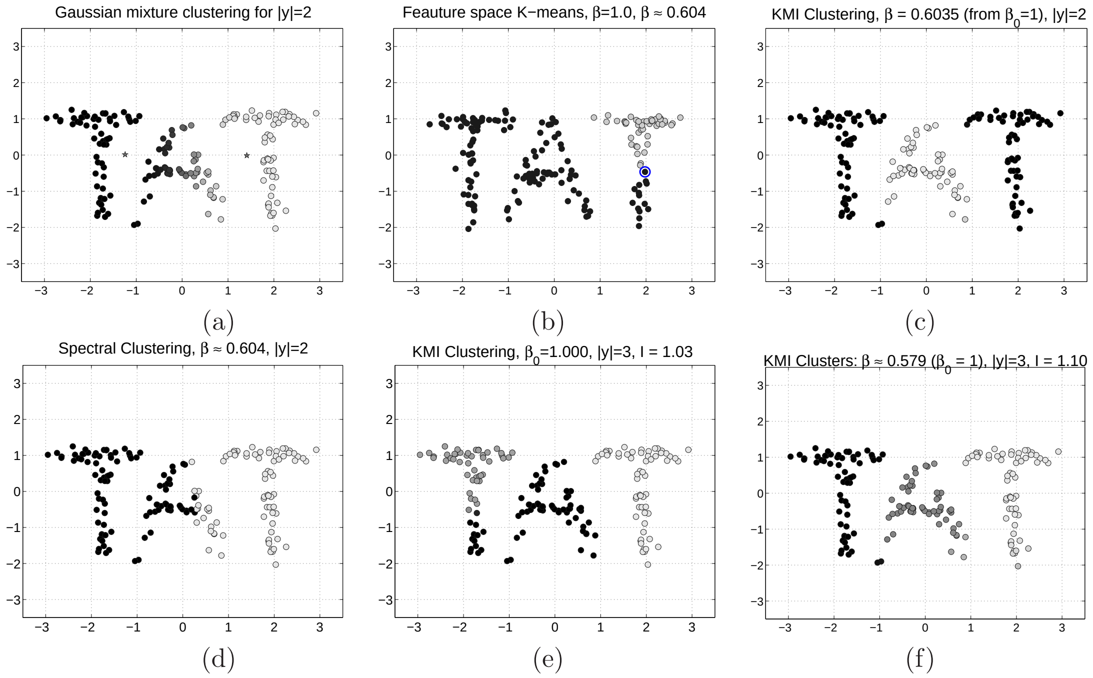


Figure 1: Cluster allocations (*top*) and the corresponding responsibilities (*bottom*) $p(y_j|\mathsf{x}^{(m)})$ for $|\mathsf{x}| = 2$, $|y| = 3$, $M = 70$ (the patterns are sorted to indicate local smoothness in the phase parameter). *Left:* Gaussian mixtures; *middle:* K-means; *right:* information-maximization for the (RBF-)kernelized encoder (the learned parameter $\beta \approx 0.825$). Light, medium, and dark-gray squares show the cluster colors corresponding to deterministic cluster allocations. The color intensity of each training point $\mathsf{x}^{(m)}$ is the average of the pure cluster intensities, weighted by the responsibilities $p(y_j|\mathsf{x}^{(m)})$. Nearly indistinguishable dark colors of the Gaussian mixture clustering indicate soft cluster assignments.

were initialized using k-means – other choices usually led to worse performance. We also see that the k-means effectively breaks, as the similarly clustered points lie close to each other in $\mathbb{R}^2$ (according to the L_2-norm), but the allocated clusters are *not* locally smooth in t. On the other hand, our method with the RBF-kernelized encoders typically led to locally smooth cluster allocations.

Figure 2 shows typical results for spatially translated letters with $|\mathsf{x}| = 2$, $M = 150$, and $|y| = 2$ (or $|y| = 3$), where we compare Gaussian mixture, feature-space k-means, the spectral method of [Ng et al., 2001], and our information-theoretic clustering method. The initializations followed the same procedure as the previous experiment. The results produced by our kernelized infomax method were generally stable under different initializations, provided that β_0 was not too large or too small. In contrast to Gaussian mixture, spectral, and feature-space k-means clustering, the clusters produced by kernelized infomax for the cases considered are arguably more anthropomorphically appealing. Note that feature-space k-means, as well as the spectral method, presume that the kernel matrix $\mathsf{K} \in \mathbb{R}^{M \times M}$ is fixed and known (in the latter case, the Gram matrix defines the edge weights of the graph). For illustration purposes, we show the results for the fixed Gram matrices with kernel parameters β set to the initial values $\beta_0 = 1$ or the learned values $\beta \approx 0.604$ of the kernelized infomax method for $|y| = 2$. One may potentially improve the performance of these methods by running the algorithms several times (with different kernel parameters β), and choosing β which results in tightest clusters ([Ng et al., 2001]). We were indeed able to apply the spectral method to obtain clusters for TA and T (for $\beta \approx 1.1$). While being useful in some situations, the procedure generally requires multiple runs. In contrast, the kernelized infomax method typically resulted in meaningful cluster allocations (TT and A) after a single run of the algorithm (see Figure 2 (c)), with the results qualitatively consistent under a variety of initializations.

Additionally, we note that in situations when we used simpler encoder models (see expression (2)) or did not adapt parameters of the kernel functions, the extracted clusters were often more intuitive than those produced by rival methods, but inferior to the ones produced by (6) with the optimal



(a) (b) (c)

(d) (e) (f)

Figure 2: Learning cluster allocations for $|y| = 2$ and $|y| = 3$. Where appropriate, the stars show the cluster centers. *(a)* two-component Gaussian mixture trained by the EM algorithm; *(b)* feature-space k-means with $\beta = 1.0$ and $\beta \approx 0.604$ (the only pattern clustered differently is shown by ⊚); *(c)* kernelized infomax clustering for $|y| = 2$ (the inverse variance β of the RBF kernel varied from $\beta_0 = 1$ (at the initialization) to $\beta \approx 0.604$ after convergence); *(d)* spectral clustering for $|y| = 2$ and $\beta \approx 0.604$; *(e)* kernelized infomax clustering for $|y| = 3$ with a *fixed* Gram matrix; *(f)* kernelized infomax clustering for $|y| = 3$ started at $\beta_0 = 1$ and reaching $\beta \approx 0.579$ after convergence.

learned β. Our results suggest that by learning kernel parameters we may often obtain higher values of the objective $I(\mathsf{x}, y)$, as well as more appealing cluster labeling (see Figure 2 (*e*), (*f*)). Undoubtedly, a careful choice of the kernel function could potentially lead to an even better visualization of the locally smooth, non-degenerate structure.

4 Discussion

The proposed information-theoretic clustering framework is fundamentally different from the generative latent variable clustering approaches. Instead of explicitly parameterizing the data-generating process, we impose constraints on the *encoder* distributions, transforming the clustering problem to learning optimal discrete encodings of the unlabeled data. Many possible parameterizations of such distributions may potentially be considered. Here we discussed one such choice, which implicitly utilizes projections of the data to high-dimensional feature spaces.

Our method suggests a formal information-theoretic procedure for learning optimal cluster allocations. One potential disadvantage of the method is a potentially large number of local optima; however, our empirical results suggest that the method is stable under different initializations. Moreover, the results suggest that in the cases considered the method favorably compares with the common generative clustering techniques, k-means, feature-space k-means, and the variants of the method which do not use nonlinearities or do not learn parameters of kernel functions.

A number of interesting interpretations of clustering approaches in feature spaces are possible.

Recently, it has been shown ([Dhillon et al., 2004]) that spectral clustering methods optimizing normalized cuts ([Shi and Malik, 2000, Ng et al., 2001]) may be viewed as a specific form of weighted feature-space k-means, for a specific fixed similarity matrix. We are currently working on relating our method to the common spectral clustering approaches and a form of annealed weighted feature-space k-means. We stress, however, that our information-maximizing framework suggests a principled way of learning optimal similarity matrices by adapting parameters of the kernel functions. Additionally, our method does not require computations of eigenvalues of the similarity matrix, which may be particularly beneficial for large datasets. Finally, we expect that the proper information-theoretic interpretation of the encoder framework may facilitate extensions of the information-theoretic clustering method to richer families of encoder distributions.

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