Topological mixture estimation

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(Dated: December 14, 2017)

Density functions that represent sample data are often multimodal, i.e. they exhibit more than one maximum. Typically this behavior is taken to indicate that the underlying data deserves a more detailed representation as a mixture of densities with individually simpler structure. The usual specification of a component density is quite restrictive, with log-concave the most general case considered in the literature, and Gaussian the overwhelmingly typical case. It is also necessary to determine the number of mixture components a priori, and much art is devoted to this. Here, we introduce topological mixture estimation, a completely nonparametric and computationally efficient solution to the one-dimensional problem where mixture components need only be unimodal. We repeatedly perturb the unimodal decomposition of Baryshnikov and Ghrist to produce a topologically and information-theoretically optimal unimodal mixture. We also detail a smoothing process that optimally exploits topological persistence of the unimodal category in a natural way when working directly with sample data. Finally, we illustrate these techniques through examples.

I. INTRODUCTION

Let \( D(\mathbb{R}^d) \) denote a suitable space of continuous probability densities (henceforth merely called densities) on \( \mathbb{R}^d \). A mixture on \( \mathbb{R}^d \) with \( M \) components is a pair \( (\pi, p) \in \Delta_M^d \times D(\mathbb{R}^d)^M \), where \( \Delta_M := \{ \pi \in (0,1]^M : \sum_m \pi_m = 1 \} \); we write \( |(\pi, p)| := M \), and note that \( \pi \) cannot have any components equal to zero. The corresponding mixture density is \( f_{\pi,p} := \sum_{m=1}^M \pi_m p_m \). The Jensen-Shannon divergence of \( (\pi, p) \) is

\[
J(\pi, p) := H\langle (\pi, p) \rangle - \langle \pi, H(p) \rangle
\]

where \( H(p)_m := H(p_m) \) and \( H(f) := -\int f \log f \, dx \) is the entropy of \( f \).

Now \( J(\pi, p) \) is the mutual information between the random variables \( \Xi \sim \pi \) and \( X \sim (\pi, p) \). Since mutual information is always nonnegative, the same is true of \( J \). The concavity of \( H \) gives the same result, i.e. \( H\langle (\pi, p) \rangle \geq \langle \pi, H(p) \rangle \). If \( M := |(\pi, p)| > 1 \) and

\[
(\hat{\pi}, \hat{p}) := \left( (\pi_1, \ldots, \pi_{M-2}, \pi_{M-1} + \pi_M), \left( p_1, \ldots, p_{M-2}, \frac{\pi_{M-1} p_{M-1} + \pi_M p_M}{\pi_{M-1} + \pi_M} \right) \right)
\]

then is easy to show that \( J(\hat{\pi}, \hat{p}) \leq J(\pi, p) \).

We say that a density \( f \in D(\mathbb{R}^d) \) is unimodal if \( f^{-1}(\{y, \infty]\}) \) is either empty or contractible (within itself, or equivalently, has the homotopy type of a point) for all \( y \); for \( d = 1 \), this simply means that any nonempty sets \( f^{-1}(\{y, \infty]\}) \) are intervals. We call a mixture \( (\pi, p) \) unimodal if each of the component densities \( p_m \) is unimodal. The unimodal category \( \text{ucat}(f) \) is the least integer such that there exists a unimodal mixture \( (\pi, p) \) with \( \text{ucat}(f) \) components satisfying \( f = (\pi, p) \); in this event we write \( (\pi, p) \equiv f \). The unimodal category is a topological invariant that generalizes the geometric category and is related to the Lusternik-Schnirelmann category \[4\] \[12\].

The preceding constructions naturally lead us to consider the unimodal Jensen-Shannon divergence

\[
J_\gamma(f) := \sup_{(\pi, p) = f} J(\pi, p) \tag{2}
\]

as a simultaneous measure of both the topological and information-theoretical complexity of \( f \), and

\[
(\pi_\gamma, p_\gamma) := \arg \max_{(\pi, p) = f} J(\pi, p) \tag{3}
\]

as an information-theoretically optimal topological mixture estimate (TME). The natural questions are if such an estimate exists (is the supremum attained?), is unique, and if so, how to perform TME in practice. In this paper we address these questions for the case \( d = 1 \), and we demonstrate the utility of TME in examples (see Figures \[4\] and \[5\].

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II. RELATED WORK

While density estimation enables various clustering techniques [2, 20], mixture estimation is altogether more powerful than clustering; e.g., it is possible to have mixture components that significantly and meaningfully overlap. For example, a cluster with a bimodal density will usually be considered as arising from two unimodal mixture components that are of interest in their own right. In this light and in view of its totally nonparametric nature, our approach can be seen as particularly powerful, particularly when coupled with topological density estimation and deblurring/reblurring (see §VII and §VIII).

Still, even for clustering (even in one dimension, where an optimal solution to k-means can be computed efficiently [13, 28, 37]), determining the number of clusters in data [26] is as much an art as a science. All of the techniques we are aware of either require some ad hoc determination to be made, require auxiliary information (e.g., 33) or are parametric in at least a limited sense (e.g., [34]). While a parametric approach allows likelihoods and thus various information criteria [7] or their ilk to be computed for automatically determining the number of clusters, this comes at the cost of a very strong modeling assumption, and the criteria values themselves are difficult to compare meaningfully [24].

These shortcomings—including determining the number of mixture components—carry over to the more difficult problem of mixture estimation. [22, 24] As an example, an ad hoc and empirically derived unimodal mixture estimation technique that requires one of a few common functional forms for the mixture components has been recently employed in [25]. Univariate model-based mixtures of skew distributions admit EM-type algorithms and can outperform Gaussian mixture models [5, 21]; though these generalize to the multivariate case quite effectively (see, e.g., [19]), the EM-type algorithms are generically vulnerable to becoming trapped in local minima without good initial parameter values, and they require some model selection criterion to determine the number of mixture components (though the parameter learning and model selection steps can be integrated as in [10]). A Bayesian nonparametric mixture model that incorporates many—but not arbitrary—unimodal distributions is considered in [32]. Principled work has been done on estimating mixtures of log-concave distributions [36]; [8] describes how densities of discrete unimodal mixtures can be estimated. However, actually estimating generic unimodal mixtures themselves appears to be unaddressed in the literature, even in one dimension. Indeed, even estimating individual modes and their associated uncertainties or significances has only been addressed recently [11, 27].

III. OUTLINE

Given \( f \), the “sweep” algorithm of [4] yields \( (\pi, p) \models f \). We will show how to repeatedly perturb \( (\pi, p) \) to obtain \[ \] using two key lemmas. The first lemma, that \( J \) is convex under perturbations of \( (\pi, p) \) that preserve \( \langle \pi, p \rangle \), is the subject of §IV. The second lemma, a characterization of perturbations of two components of a piecewise affine and continuous (or piecewise constant) mixture that preserve the predicate \( (\pi, p) \models f \) (i.e., that preserve unimodality and the mixture density), is the subject of §V. Together, these results entail that greedy unimodality- and density-preserving local perturbations of pairs of mixture components converge to \[ \]. The proof in §VI is scarcely more involved than the preceding statement once the lemmas are in hand. Next, in §VII we review the related technique of topological density estimation (TDE) before showing in §VIII how blurring and deblurring mixture estimates can usefully couple TDE and TME. Finally, in §IX we produce examples of TME in action.

IV. CONVEXITY

The following lemma shows that \( J \) is convex as we gradually shift part of one mixture component to another.

**Lemma.** Let \( |(\pi, p)| = 3 \). The function \( g_{\pi, p} : [0, 1] \to [0, \infty) \) defined by

\[
g_{\pi, p}(t) := J \left( (\pi_1 + (1 - t)\pi_2, t\pi_2 + \pi_3), \left( \frac{\pi_1p_1 + (1 - t)\pi_2p_2}{\pi_1 + (1 - t)\pi_2}, \frac{tp_2 + \pi_3p_3}{t\pi_2 + \pi_3} \right) \right)
\]

satisfies

\[
g_{\pi, p}(t) \leq t \cdot g_{\pi, p}(1) + (1 - t) \cdot g_{\pi, p}(0).
\]

December 14, 2017
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PROOF. The statement as well as the proof of the lemma can be simplified with a bit of extra notation. Define

\[
\pi_{12,t} := \pi_1 + (1-t)\pi_2; \\
\pi_{23,t} := t\pi_2 + \pi_3; \\
p_{12,t} := \frac{\pi_1 p_1 + (1-t)\pi_2 p_2}{\pi_{12,t}}; \\
p_{23,t} := \frac{t\pi_2 p_2 + \pi_3 p_3}{\pi_{23,t}}.
\]

Now \(\langle (\pi_{12,t}, \pi_{23,t}), (p_{12,t}, p_{23,t}) \rangle = \langle \pi, p \rangle\), so

\[
g_{\pi,p}(t) = J((\pi_{12,t}, \pi_{23,t}), (p_{12,t}, p_{23,t})) = H((\langle (\pi_{12,t}, \pi_{23,t}), (p_{12,t}, p_{23,t}) \rangle) - \langle (\pi_{12,t}, \pi_{23,t}), (H(p_{12,t}), H(p_{23,t})) \rangle = H(\langle \pi, p \rangle) - \langle (\pi_{12,t}, \pi_{23,t}), (H(p_{12,t}), H(p_{23,t})) \rangle \). \tag{6}
\]

Furthermore, if we write \(\pi_{12} := \pi_1 + \pi_2\), \(\pi_{23} := \pi_2 + \pi_3\), \(p_{12} := \frac{\pi_1 p_1 + \pi_2 p_2}{\pi_{12}}\), and \(p_{23} := \frac{\pi_2 p_2 + \pi_3 p_3}{\pi_{23}}\), then

\[
\pi_{12,t} = t\pi_1 + (1-t)\pi_{12}; \\
\pi_{23,t} = t\pi_{23} + (1-t)\pi_3; \\
p_{12,t} = \frac{t\pi_1 p_1 + (1-t)\pi_{12} p_{12}}{\pi_{12,t}}; \\
p_{23,t} = \frac{t\pi_{23} p_{23} + (1-t)\pi_{23} p_{3}}{\pi_{23,t}}.
\]

It is well known that \(H\) is a concave functional: from this it follows that

\[
H(p_{12,t}) \geq \frac{t\pi_1}{\pi_{12,t}} H(p_1) + \frac{(1-t)\pi_{12}}{\pi_{12,t}} H(p_{12}); \\
H(p_{23,t}) \geq \frac{t\pi_{23}}{\pi_{23,t}} H(p_{23}) + \frac{(1-t)\pi_3}{\pi_{23,t}} H(p_3).
\]

Therefore

\[
g_{\pi,p}(t) = H(\langle \pi, p \rangle) - \langle (\pi_{12,t}, \pi_{23,t}), (H(p_{12,t}), H(p_{23,t})) \rangle \\
\leq H(\langle \pi, p \rangle) - t\pi_1 H(p_1) - (1-t)\pi_{12} H(p_{12}) - t\pi_{23} H(p_{23}) - (1-t)\pi_3 H(p_3) \\
= t [H(\langle \pi, p \rangle) - \langle (\pi_{12}, \pi_{23}), (H(p_1), H(p_{23})) \rangle] + (1-t) [H(\langle \pi, p \rangle) - \langle (\pi_{12}, \pi_3), (H(p_{12}), H(p_3)) \rangle] \\
= t \cdot g_{\pi,p}(1) + (1-t) \cdot g_{\pi,p}(0)
\]

as claimed. \(\square\)

V. PRESERVING UNIMODALITY

Suppose that \((\pi, p)\) is a unimodal mixture on \(\mathbb{R}\) with \(|\langle \pi, p \rangle| > 1\). We would like to determine how we can perturb two components of this mixture so that the result is still unimodal and yields the same density. In the event that the mixture is piecewise affine and continuous (or piecewise constant) the space of permissible perturbations can be characterized by the following

**LEMMA.** For \(0 \leq k \leq N\), let \(y_k \in [0, \infty)\) be such that there are integers \(\ell, u\) satisfying \(0 < \ell \leq u < N\) and

\[
0 = y_0 \leq \cdots \leq y_{r-1} < y_r = \cdots = y_u > y_{u+1} \geq \cdots \geq y_N = 0. \tag{7}
\]

(That is, \(y_1, \ldots, y_{N-1}\) is a nonnegative, nontrivial unimodal sequence.) Then for \(1 \leq r \leq N - 1\) and \(\varepsilon_r^- \geq 0\),

\[
y_k - \delta_k r \varepsilon_r^- \text{ is nonnegative and unimodal } \iff \varepsilon_r^- \leq y_r - (y_{r-1} \wedge y_{r+1}). \tag{8}
\]
Similarly, for $\varepsilon_r^+ \geq 0$,
\[ y_k + \delta_{kr} \varepsilon_r^+ \text{ is nonnegative and unimodal } \iff \varepsilon_r^+ \leq \begin{cases} \infty & \text{if } \ell - 1 \leq k \leq u + 1 \\ (y_{r-1} \lor y_{r+1}) - y_r & \text{otherwise.} \end{cases} \tag{9} \]

**Proof (sketch).** We first sketch $(\ref{eq:nonnegativity}).$ Nonnegativity follows from $0 \leq y_{r-1} \lor y_{r+1} \leq y_r - \varepsilon_r^-$. Unimodality follows from a series of trivial checks for the cases $1 \leq r < \ell - 1$, $r = \ell - 1$, $r = \ell$, and $\ell < r < u$: the remaining cases $r = u$, $r = u + 1$, and $u + 1 < r \leq N - 1$ follow from symmetry. For example, in the case $1 \leq r < \ell - 1$, we only need to show that $y_{r-1} \leq y_r - \varepsilon_r^- \leq y_{r+1}$.

A sketch of $(\ref{eq:unimodality}), \implies$ amounts to using the same cases and symmetry argument to perform equally trivial checks. For example, in the case $1 \leq r < \ell - 1$, we have $\varepsilon_r^- \leq y_r - y_{r-1} \leq y_r - (y_{r-1} \lor y_{r+1})$.

The proof of $(\ref{eq:unimodality})$ is mostly similar to that of $(\ref{eq:nonnegativity})$: the key difference here is that any argument adjacent to or at a point where the maximum is attained can have its value increased arbitrarily without affecting unimodality (or nonnegativity). □

The example in figure 1 is probably more illuminating than filling in the details of the proof sketch above.

![A unimodal sequence $y$ with unimodality-saturating perturbations $\varepsilon^\pm$ respectively indicated above and below.](image)

**VI. ALGORITHM**

**Theorem.** Let $-\infty = x_{-1} < x_0 < \cdots < x_N < x_{N+1} = \infty$ and $f$ be piecewise constant (or affine) over each $[x_k, x_{k+1}]$. Then there is an efficient algorithm to compute $(\ref{eq:objectivesimplification}).$

**Proof.** First, compute $(\pi, p) \models f$ via the “sweep” algorithm of \cite{[4]}. Then, for each $k \in [N]$ and pair of mixture components, compute the largest possible local perturbation of the mixture according to the lemma in \S \ref{sec:lemma}. By the lemma in \S \ref{sec:lemma}, choosing a resulting maximal value of $J$ and repeating the perturbation-evaluation procedure gives the desired result in $O(MN)$ iterations. This result is unique by convexity. □

**VII. TOPOLOGICAL DENSITY ESTIMATION**

The obvious situation of practical interest for TME is that a density has been obtained from a preliminary estimation process involving some sample data. There is a natural approach to this preliminary estimation process called topological density estimation (TDE) \cite{[16]} that naturally dovetails with (and as it happens, inspired) TME.

We recall the basic idea here. Given a kernel $K$ and sample data $X_j$ for $1 \leq j \leq n$, and for each proposed bandwidth $h$, we compute the kernel density estimate \cite{[9, 33]}
\[ \hat{f}_{h,X}(x) := \frac{1}{n} \sum_{j=1}^{n} K_{X_j,h} \] (10)
where $K_{\mu,\sigma}(x) := \frac{1}{\sigma}K(\frac{x-\mu}{\sigma})$. Next, we compute

$$u_X(h) := \text{ucat}(\hat{f}_{h,X})$$

and estimate the unimodal category of the PDF that $X$ is sampled from via

$$\hat{m}_X := \arg \max_m \mu(u_X^{-1}(m))$$

where $\mu$ denotes an appropriate measure (nominally counting measure or the pushforward of Lebesgue measure under the transformation $h \mapsto 1/h$).

That is, (12) gives the most prevalent (and usually in practice, also topologically persistent \cite{12,31}) value of the unimodal category, i.e., this is a topologically robust estimate of the number of components required to produce the PDF that $X$ is sampled from as a mixture. While any element of $u_X^{-1}(\hat{m}_X)$ is a bandwidth consistent with the estimate (12), we typically make the more detailed nominal specification

$$\hat{h}_X := \text{median}_\mu(u_X^{-1}(\hat{m}_X)).$$

TDE turns out to be very computationally efficient relative to the traditional technique of cross-validation (CV). On highly multimodal densities, TDE is competitive or at least reasonably performing relative to CV and other nonparametric density estimation approaches with respect to traditional statistical evaluation criteria. Moreover, TDE outperforms other approaches when qualitative criteria such as the number of local maxima and the unimodal category itself are considered (see Figures 2 and 3). In practice, such qualitative criteria are generally of paramount importance. For example, precisely estimating the shape of a density is generally less important than determining if it has two or more clearly separable modes.

As an illustration, consider $\mu(j,m) := \frac{j}{m+1}$, $\sigma(k,m) := 2^{-(k+2)}(m+1)^{-2}$ and the family of distributions

$$f_{km} := \frac{1}{m} \sum_{j=1}^{m} K_{\mu(j,m),\sigma(k,m)}$$

for $1 \leq k \leq 3$ and $1 \leq m \leq 10$, and where here $K$ is the standard Gaussian density: see Figure 2. Exhaustive details relating to the evaluation of TDE on this family and other densities are presented in the software package and test suite \cite{3}: here, we content ourselves with the performance data for (14) shown in Figure 3.

![Figure 2](image-url)

FIG. 2: The densities $f_{km}$ in (14) for $1 \leq k \leq 3$ and $1 \leq m \leq 6$ over the interval $[-0.5, 1.5]$. Rows are indexed by $k$ and columns are indexed by $m$; the upper left panel shows $f_{11}$ and the lower right panel shows $f_{36}$.

TDE has the very useful feature (shared by essentially no high-performing density estimation technique other than CV) that it requires no free parameters or assumptions. Indeed, TDE can be used to evaluate its own suitability: for unimodal distributions, it is clearly not an ideal choice— but it is good at detecting this situation in the first place. Furthermore, TDE is very efficient computationally.

In situations of practical interest, it is tempting to couple TDE and TME in the obvious way: i.e., perform them sequentially and independently. This yields a completely nonparametric estimate of a mixture from sample data alone. However, there is a better way to couple these techniques, as we shall see in the sequel.

VIII. BLURRING AND DEBLURRING

A. Blurring

Recall that a log-concave function is unimodal, and moreover that a function is log-concave iff its convolutions with unimodal functions are identically unimodal. \cite{6,17,18} This observation naturally leads to the following question:
The persistence of the unimodal category under blurring) that we proceed to illustrate in light of TDE. This question of how much blurring a minimal unimodal mixture model can sustain defines a topological scale (viz., if \((\pi,p) \models f\), how good of an approximation to the \(\delta\) distribution must a log-concave density \(g\) be in order to have \((\pi,p \ast g) = f \ast g^2\)? In particular, suppose that \(g\) is a Gaussian density: what bandwidth must it have? An answer to this question of how much blurring a minimal unimodal mixture model can sustain defines a topological scale (viz., the persistence of the unimodal category under blurring) that we proceed to illustrate in light of TDE.

In this paragraph we assume that \(K\) is the standard Gaussian density, so that \(K_{\mu,h} \ast K_{\mu',h'} = K_{\mu+\mu',(h^2+\sigma^2)^{1/2}}\) and \(\hat{f}_{X;\pi} \ast K_{0,h'} = \hat{f}_{X;\pi} + K_{0,h'}\). Write \(\hat{h}_X\) for the bandwidth obtained via TDE, whether via the nominal specification \([13]\) or any other: by construction we have that \(\inf u_X^{-1}(\hat{m}_X) \leq \hat{h} \leq \sup u_X^{-1}(\hat{m}_X)\). Now if \((\pi,p) \models f_{X;\pi}\), then \(\hat{m}_X = u_X(\hat{h}_X) = |(\pi,p)|\). In order to have \((\pi,p \ast K_{0,h'}) \models f \ast K_{0,h'}\), it must be that \(\hat{m}_X = u_X(\hat{h}_X) = |(\pi,p)| = |(\pi,p \ast K_{0,h'})| = u_X((\hat{h}_X^2 + \sigma^2)^{1/2}),\) i.e.,

\[
\hat{h}' \leq \left(\sup u_X^{-1}(\hat{m}_X)^2 - \hat{h}_X^2\right)^{1/2}.
\]

In particular, we have the weaker inequality involving a purely topological scale:

\[
\hat{h}' \leq \left(\sup u_X^{-1}(\hat{m}_X)^2 - \inf u_X^{-1}(\hat{m}_X)^2\right)^{1/2}.
\]

The preceding considerations generalize straightforwardly if we define \(u_f(h) := ucat(f \ast K_{0,h})\), where once again \(K\) is a generic kernel. This generalizes \([11]\) so long as we associate sample data with a uniform average of \(\delta\) distributions. Under reasonable conditions, we can write \(u_f(0) = ucat(f)\), and it is easy to see that the analogous bound is

\[
h' \leq \sup u_f^{-1}(u_f(0)).
\]

Of course, \([17]\) merely restates the triviality that the blurred mixture ceases to be minimal precisely when the number of mixture components exceeds the unimodal category of the mixture density. Meanwhile, the special case furnished by TDE with the standard Gaussian kernel affords sufficient structure for a slightly less trivial statement.

**B. Deblurring/reblurring**

The considerations of \([18]\) suggest how to couple TDE and TME in a much more effective way than performing them sequentially and independently. The idea is to use a Gaussian kernel and instead of \([13]\), pick the bandwidth

\[
\hat{h}_X^{(-)} := \inf u_X^{-1}(\hat{m}_X)
\]

In Figure 2 for \(n = 500\) sample points using a Gaussian kernel. Data for CV is shown in red, while data for TDE is shown in blue. Each panel represents data on a particular performance measure (left, ucat for TDE alone; middle, ucat for CV alone; right, the empirical probability that the estimate of ucat is correct) and value of \(k\) (top, \(k = 1\); middle, \(k = 2\); bottom, \(k = 3\)), with \(m\) varying from 1 to 10. (R) As in the left panel, but for the number of local maxima instead of the unimodal category.
and then perform TME; finally, convolve the results with $K_{0,\Delta h}$ where

$$\Delta h := \left( \hat{h}_{X}^{2} - \left[ \hat{h}_{X}^{\ast} \right]^{2} \right)^{1/2}. \quad (19)$$

This preserves the result of TDE while giving a smoother, less artificial, and more practically useful mixture estimate than the information theoretically optimal result.

Of course, a similar tactic can be performed directly on a density $f$ by considering its Fourier deconvolution $F^{-1}(Ff/FK_{0,h'})$, where $F$ denotes the Fourier transform and $h'$ is as in (17); however, any a priori justification for such a tactic is necessarily context-dependent in general, and our experience suggests that its implementation would be delicate and/or prone to aliasing. Nevertheless, this would be particularly desirable in the context of heavy-tailed distributions, where kernel density estimation requires much larger sample sizes in order to achieve acceptable results. In this context it would also be worth considering the use of a symmetric stable density [29, 38] (e.g., a Cauchy density) as a kernel with the aim of recapturing the essence of (19).

**IX. EXAMPLES**

We present two phenomenologically illustrative examples. First, in Figure 4 we consider the $n = 272$ waiting times between eruptions of the Old Faithful geyser from the data set in [14]. Then, in Figure 5 we consider the $n = 2107$ Sloan Digital Sky Survey $g - r$ color indices accessed from the VizieR database [30] at http://cdsarc.u-strasbg.fr/viz-bin/Cat?J/ApJ/700/523 and discussed in [1].

![Figure 4](image-url)

**FIG. 4:** TME applied to $n = 272$ waiting times between eruptions of the Old Faithful geyser. Left panels, from top to bottom: area plots of unimodal decompositions obtained by (top) the “sweep algorithm” of [4] on a topological density estimate with bandwidth given by (13); (second from top) the result of (3) on a topological density estimate with bandwidth given by (13); (second from bottom) the result of (3) on a topological density estimate with bandwidth given by (18); (bottom) the convolution of the mixture in the preceding panel with a Gaussian kernel with bandwidth given by (19). Note that three of the four mixture estimates have the same density, but that the deblurred density is different (this is why we have used the "*" annotation for this case). Right panels: line plots of the same decompositions.

As suggested, several phenomena are readily apparent from these examples. First, mixtures obtained via the sweep algorithm are manifestly parity-dependent, i.e., the direction of sweeping matters; second, mixtures obtained via TME alone exhibit artificial anti-overlapping behavior; third, deblurring followed by reburring preserves unimodality, the overall density, a topologically persistent invariant (viz., the unimodal category) and the spirit of information-theoretical optimality while producing an obviously better behaved mixture; fourth and finally, the various techniques involved here can significantly shift classification/decision boundaries based on the dominance of various mixture components.

While the data in Figure 4 is at least qualitatively approximated by a two-component Gaussian mixture, it is clear that a three-component Gaussian mixture cannot capture the highly oscillatory behavior of the density in Figure 5. Indeed, this example illustrates how such oscillatory behavior can actually arise from a unimodal mixture with many fewer components than might naively appear to be required.
Figure 6 shows that there are strong and independent grounds to conclude that the color index data of Figure 5 is produced by a unimodal mixture of three components, with componentwise modes as suggested by TME, and furthermore that CV undersmooths this data. For each density estimate shown, each componentwise extremum of the corresponding mixture (3) is virtually identical to one of the local extrema of the density estimate itself: this is a consequence of the anti-overlapping tendency described above.

In particular, the fourth panel of Figure 6 illustrates that it is possible and potentially advantageous to use TME as an alternative mode identification technique in the LPMode algorithm of [27]. Furthermore, while we have not implemented a reliable Fourier deconvolution/reblurring algorithm of the sort hinted at in § VIII B, the fifth and sixth panels of Figure 6 suggest that this is not particularly important for the narrow task of mode finding/bump hunting.

Acknowledgments

The author thanks Adelchi Azzalini, Robert Ghrist, Subhadeep Mukhopadhyay, and John Nolan for their helpful and patient discussions. This material is based upon work supported by the Defense Advanced Research Projects Agency (DARPA) and the Air Force Research Laboratory (AFRL). Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of DARPA or AFRL.

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FIG. 6: Structural analyses of the color index data from Figure 5. Top panel: density estimates obtained via CV, the default LPMode algorithm of [27] (kindly provided by its author), and TDE. Second panel from top: the local extrema of the density estimates above. Third through fifth panels from top: the result of (3) on the CV, LPMode, and topological density estimates, respectively, with extrema of components indicated. Bottom panel: the reblurred mixture from the bottom left panel of Figure 5 with extrema of components additionally indicated.

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