UNIMODAL DECOMPOSITIONS OF PROBABILITY DISTRIBUTIONS AND MAXWELL'S CONJECTURE

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Abstract. We discuss several problems related to representation of a probability distribution as a positive linear combination (mixture) of unimodal probability distributions.

1. Introduction

In statistics one often considers mixtures of standard distributions for modelling of various sets of empirical data, see e.g. [**?**]. Gaussian mixtures are of special importance and frequently used. In particular, in recent years several papers discussing the possible number of modes, i.e. the number of local maxima of the density function for Gaussian mixtures appeared, see [**?**, **?**, **?**, **?**]. One of the observations made about 2 decades ago is that although a Gaussian distribution is a unimodal function, already in two dimensions the mixture of ℓ Gaussians can have substantially more maxima than ℓ. If we consider other classes of unimodal distributions the question about of the maximal possible number of modes of their mixture becomes non-trivial already in dimension one. In particular, for any positive integer N there exist pairs of positive unimodal functions in one variable whose sum has N local maxima.

Below we formulate two natural problems (direct and inverse) in this area closely related to factor analysis. Both of them seem quite difficult, but having substantial interest for applications.

Consider a collection $\mathcal{F}_\alpha(x_1, \dots, x_n)$ of unimodal continuous densities of probability distributions depending on parameter α and supported on some open contractible domain $\Omega \subset \mathbb{R}^n$. (The parameter α can be discrete or continuous, one- or multidimensional.)

1.1. **Direct problem.**

Problem 1.1. Given a collection $\mathcal{F}_\alpha(x_1, \dots, x_n)$ of probability densities as above and a positive integer ℓ, find/estimate the maximal number of local minima which can occur in non-negative combinations of ℓ densities from $\mathcal{F}_\alpha(x_1, \dots, x_n)$.

An interesting modification of Problem **??** is as follows.

Definition 1.2. A collection $\mathcal{F}_\alpha(x_1, \dots, x_n)$ of probability densities as above is called *strongly unimodal* if for any positive integer ℓ, any positive linear combination of ℓ densities from this collection has at most ℓ modes (i.e. local maxima) in Ω.

Problem 1.3. Find interesting examples of strongly unimodal collections $\mathcal{F}_\alpha(x_1, \dots, x_n)$.

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Examples of strongly unimodal collections include Gaussian distribution with fixed ... in every dimension $\mathbb{R}^n$. Interestingly, in the 1-dimensional case, the proof of the fact that the positive linear combination of ℓ Gaussian densities has at most ℓ modes goes back to Joseph Fourier, see [**?**, **?**].

Our interest in Problem **??** comes from the following (rather unexpected) source. In Section 113 of [**?**] J. C. Maxwell claims that any configuration of ℓ point charges in $\mathbb{R}^3$ such that all critical points of its electrostatic potential are non-degenerate has at most $(\ell-1)^2$ such points (i.e. points of equilibrium of its electrostatic field. He provides it with an incomplete proof which contains a serious gap.

In [**?**] and some further publications including a recent advance [**?**] one can find several weaker upper bounds of the number of points of equilibrium than in the original Maxwell claim and its generalizations. In particular, in [**?**] (based on a more general claim of [**?**]) the following 1-dimensional version of (relative) Maxwell's conjecture has been formulated.

Conjecture 1.4. *Let $(x_1,y_1),(x_2,y_2),\dots,(x_\ell,y_\ell)$ be any collection of points in $\mathbb{R}^2$, $\xi_1,\xi_2,\dots,\xi_\ell$ be arbitrary real charges, and $\alpha\geq 1/2$. Then the real rational function*

$$\Psi(x)=\sum_{j}^{\ell}\frac{\xi_j}{((x-x_j)^2+y_j^2)^\alpha},\quad x\in\mathbb{R}$$

has at most $2\ell-1$ real critical points. (If all ξ_j's are positive then $\Psi(x)$ has at most ℓ local maxima on $\mathbb{R}$).

Remark 1.5. Notice that for positive ξ_j's, Conjecture **??** is equivalent to the claim that the 2-dimensional family of functions

$$\Phi_\alpha(x)=\frac{1}{((x-x_0)^2+y_0^2)^\alpha} \tag{1.1}$$

is strongly unimodal for every fixed $\alpha\geq 1/2$ with (x_0,y_0) being parameters of the family. (If $\alpha>\frac{1}{2}$, the positive function $\Phi_\alpha(x)$ is integrable over $\mathbb{R}$ and its scaled version is a probability density.)

In [**?**] Conjecture **??** is proven for fixed ξ_j's, x_j's and y_j's and all sufficiently large α. But unfortunately, it is still open already in the simplest case when $\ell=3,\alpha=1$, and unit charges.

1.2. **Inverse problem.** A natural inverse problem originally suggested by Y. Baryshnikov and R. Ghrist can be stated as follows, see [**?**, **?**] and also [**?**].

Problem 1.6. Given a smooth probability density function f in $\mathbb{R}^k$ (or an open contractible domain $\Omega\subset\mathbb{R}^k$), find/estimate the minimal number ℓ such that f can be represented as

$$f=\sum_{i=1}^{\ell}f_i, \tag{1.2}$$

where each f_i is a smooth, non-negative and unimodal function. The minimal number ℓ (if finite) will be called the *unimodal category* of f and denoted by $ucat(f)$.

We will call expression (**??**) *positive unimodal decomposition* of f. Problem **??** asks to find a *minimal* positive unimodal decomposition. In [**?**] Y. Baryshnikov and R. Ghrist provided an algorithm for finding a minimal positive unimodal decomposition in one-dimensional case, see Fig. **??** which they later extended to the case when the support of densities is a tree, see [**?**]. Some related results can be found in the writings of G. Govc, see [**?**, **?**]. However already for densities on $\mathbb{R}^2$, Problem **??** seems to be widely open.

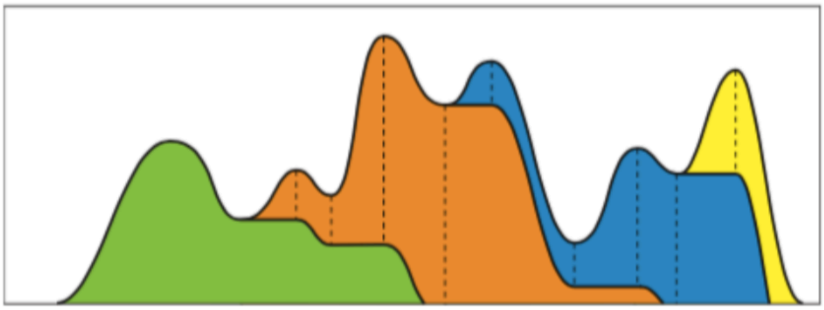

FIGURE 1. Algorithm of finding *ucat* for smooth univariate densities.

Remark 1.7. Observe that the unimodality property of a function is preserved under the action of diffeomorphisms on its (contractible) domain of definition. The orbit of a function under the action of the group of diffeomorphisms of the domain of definition can be often identified with functions Reeb graph (which contains finite topological information) whose vertices correspond to the critical points of f and each vertex is labelled by the respective critical value. In other words, Problem **??** is (more or less) topological.

We this note we present some results related to Problems **??** and **??**.

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2. RESULTS

2.1. **Around direct problem.** Below we provide necessary condition for a collection of univariate probability distributions to be strongly unimodal.

Definition 2.1. A positive continuous integrable unimodal function $f(x)$ defined in some interval $I \subseteq \mathbb{R}$ is called *cusp-like* if it is (non-strictly) convex everywhere outside its (unique) maximum $x^{max} \in I$.

Remark 2.2. Obviously any cusp-like function is not differentiable at its maximum.

Theorem 2.3. *Any collection of cusp-like functions is strongly unimodal.*

Proof. Indeed, consider a mixture

$$F(x) = \alpha_1 f_1(x) + \alpha_2 f_2(x) + \cdots + \alpha_\ell f_\ell(x),$$

where each $f_j(x)$ is cusp-like and $\alpha_j > 0$. The second derivative $F''(x)$ is non-negative except at the finite number of points $x_1^{max}, x_2^{max}, \ldots, x_\ell^{max}$ where x_j^{max} is the maximum of $f_j(x)$. (At these points F'' is typically a scaled δ-function.) Thus the first derivative is (non-strictly) increasing everywhere except at at most ℓ points where it drops and can intersect the real axis. Thus at such points $F(x)$ might have a local maximum and their number its at most ℓ. □

Remark 2.4. Observe that a strongly unimodal collection does not necessarily consist of cusp-like functions. In particular, for univariate Gaussians the second derivative is negative on an interval.

Lemma 2.5 (Guess 7)**.** *If the intervals of negativity for the second derivatives of potentials of individual (positive) charges are disjoint then Maxwell's conjecture is true.*

Proof. Similar to the proof of Theorem **??**. □

However in the case known to us the k-th derivative of functions in a strongly unimodal family seems to have at most k real roots for each k. One wonders if this property is relevant for the strong unimodality. Is there criterion/representation of such densities? (Something like totally-positive functions? Lieb?)

IS THERE A SIMILAR NOTION IN SEVERAL DIMENSIONS?

2.2. **Around inverse problem.** Let us give a crude upper bound for the number ℓ of summands in a minimal positive unimodal decomposition of a given positive smooth function.

Theorem 2.6. *Any positive smooth density with finitely many isolated local maxima has a positive unimodal decomposition into K unimodal density functions where K is the number of latter local maxima.*

Remark 2.7. Proof of Theorem **??** will be a consequence of the following statement.

In this case, associate to any local maximum $m \in S^n$ of $\tilde{f}$ the subset $\mathcal{C}_m \subseteq S^n$. Take a small disk around m and consider the union $\mathcal{C}_m^o$ of all trajectories of $-grad(\tilde{f})$ on S^n starting in the latter disk. Set $\mathcal{C}_m$ be the closure of $\mathcal{C}_m^o$.

Lemma 2.8. *In the above notation, $\mathcal{C}_m^o$ is contractible. The union of $\mathcal{C}_m$ for m running over the set of all local maxima of $\tilde{f}$ coincides with S^n.*

Proof. (Should be trivial from the classical Morse theory.) □

Extension 1. The same should hold a) under the assumption that all local maxima are non-degenerate but the rest of critical points are only finitely many; b) local maxima can be degenerate but there are finite many critical points all together;

Proof of Theorem **??**. Sketch for a restricted class of functions. Assume first that the probability density f is a Morse function which vanishes at the boundary of its domain Ω. Introduce $\tilde{f}$ which is a function on the 1-point compactification of Ω which is an n-dimensional sphere S^n. Assume that $\tilde{f}$ is a Morse non-negative function on S^n.

From the above claim we can produce the decomposition of $\tilde{f}$ into the following unimodal functions. Associate to each local maximum m the following function

$$\tilde{f}_m(p) := \begin{cases} \tilde{f}(p), \text{ for } p \in \mathcal{C}_m \\ 0, \text{ otherwise} \end{cases}. \tag{2.1}$$

Claim: $\tilde{f} = \sum_m \tilde{f}_m$ almost everywhere.

HOW TO SMOOTHEN AT THE EDGES?

— Boris

□

Extension 2. It would be good to extend the above to certain continuous functions.

Corollary 2.9. *For any smooth density f with $K > 1$ isolated local maxima, its unimodal category $ucat(f)$ satisfies the condition*

$$2 \leq ucat(f) \leq K$$

both bounds being sharp in some examples.

Let us now present a construction which deforms a given smooth density f into a positive function ϕ such that $ucat(\phi) = 2$. Indeed assume that a density f is given in some bounded contractible domain $\Omega \subset \mathbb{R}^n$ with a smooth boundary $\partial\Omega$. Denote by $\partial\Omega_\epsilon \subset \mathbb{R}^n$ the ϵ-neighborhood of $\partial\Omega$ in some fixed Euclidean metric in $\mathbb{R}^n$. Let χ_Ω be the characteristic function of Ω. We say that a non-negative smooth function $\widetilde{\chi}$ is a *boundary ϵ-deformation* of χ_Ω if $\widetilde{\chi} \neq \chi_\Omega$ only in $\partial\Omega_\epsilon$. Given f in Ω consider the family of positive functions $f_t := f + t \cdot \widetilde{\chi}$ where $t \geq 0$ and ϵ is sufficiently small positive number.

Theorem 2.10. *In the above notation, $ucat(f_t) = 2$ for all sufficiently large positive t.*

Proof. BLA □

3. Different guesses

Lemma 3.1 (Guess 1)**.** *Fix $x_1 < x_2 < \dots, x_\ell$ and $\xi_1 > 0, \xi_2 > 0, \dots, \xi_\ell > 0$. Then there exists $\epsilon > 0$ such that if each $0 < y_j < \epsilon$, $j = 1, 2, \dots, \ell$ then the potential $\Psi(x)$ has exactly ℓ local maxima.*

Conjecture 3.2 (Guess 2)**.** *Assume that $x_1 \leq x_2 \leq \dots \leq x_\ell$. Fix $x_1 < x_\ell$ and the values of the charges $\xi_1 > 0, \xi_2 > 0, \dots, \xi_\ell > 0$. Then there exists $\delta > 0$ such that Maxwell's 1D-conjecture holds, i.e. $\Psi(x)$ has at most ℓ local maxima.*

Lemma 3.3 (Guess 3)**.** *Fix a charge configuration $(x_1, y_1), \dots (x_\ell, y_\ell)$ with positive y_j's and the charges $\xi_1 > 0, \xi_2 > 0, \dots, \xi_\ell > 0$. Then there exists $A > 0$ such that if we shift our configuration by a number $\geq A$ up then $\Psi(x)$ will become unimodal.*

Lemma 3.4 (Guess 4)**.** *If $\xi_1 = \xi_2 = \dots = \xi_\ell$ and $y_1 = y_2 = \dots = y_\ell$ Maxwell's 1D-conjecture holds.*

Lemma 3.5 (Guess 5)**.** *If all charges are positive and one moves up then charge at the maximal height then the number of real critical points can only decrease.*

Consider the second derivative of $\Phi(x) = \frac{\xi}{((x-x_0)^2+y_0^2)^\alpha}$. One has

$$\Phi'(x) = -\xi \frac{2\alpha(x - x_0)}{((x - x_0)^2 + y_0^2)^{\alpha+1}}$$

$$\Phi''(x) = -2\alpha\xi \frac{((x - x_0)^2 + y_0^2) - 2(x - x_0)^2(\alpha + 1)}{((x - x_0)^2 + y_0^2)^{\alpha+2}} = -2\alpha\xi \frac{y_0^2 - (2\alpha + 1)(x - x_0)^2}{((x - x_0)^2 + y_0^2)^{\alpha+2}}.$$

Thus $\Phi''(x)$ vanishes at exactly two points $x = x_0 \pm y_0/\sqrt{2\alpha + 1}$. We call $I = [x_0 - y_0/\sqrt{2\alpha + 1}, x_0 + y_0/\sqrt{2\alpha + 1}]$ the *interval of negativity* of the 2-nd derivative.

Lemma 3.6 (Guess 6)**.** *If we scale the real part x as tx, $t \geq 1$, then the number of critical points can only increase.*

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