Kernel Density Estimation for Totally Positive Random Vectors

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Abstract

We study the estimation of the density of a totally positive random vector. Total positivity of the distribution of a vector implies a strong form of positive dependence between its coordinates, and in particular, it implies positive association. We take on a modified kernel density estimation approach for estimating such a totally positive density. Our main result is that the sum of scaled standard Gaussian bumps centered at a min-max closed set provably yields a totally positive distribution. Hence, our strategy for producing a totally positive estimator is to form the min-max closure of the set of samples, and output a sum of Gaussian bumps centered at the points in this set. We provide experimental results to demonstrate the improved convergence of our modified kernel density estimator over the regular kernel density estimator, conjecturing that augmenting our sample with all points from its min-max closure relieves the curse of dimensionality.

Keywords: Total Positivity, Kernel Density Estimation, MTP\(_2\)

1. Introduction

Let \(X_1, \ldots, X_n \in \mathbb{R}^d\) be independent and identically distributed (i.i.d.) samples from a distribution with density function \(f_0\). Nonparametric methods are attractive for computing an estimate for \(f_0\) since they do not impose any parametric assumptions. Popular such methods include kernel density estimation (KDE), adaptive smoothing, neighbor-based techniques, and nonparametric shape constraint estimation. For details we refer to the surveys [Ize91, Tur93, Sco15, Sil18, WJ94, Che17, Was16, GJ14] and references therein. We restrict our attention to the kernel density estimation approach. The general kernel density estimate \(\hat{f}(x)\) of the density at a point \(x \in \mathbb{R}^d\) is given by

\[
\hat{f}(x) = \frac{1}{nh^d} \sum_{i=1}^{n} K \left( \frac{x - X_i}{h} \right)
\]
where $K$ is a kernel function and $h$ is the smoothing parameter. The choice of $h$ is important and there exist many rules and heuristics to chose an appropriate $h$ [Tur93]. The kernel density estimator is thus the normalized sum of kernel functions centered at the points in the sample $X = \{X_1, \ldots, X_n\}$. Motivations for this estimator can be found, for example, in [Sco15, pp. 138-142].

In this paper we study density estimation under the assumption that the original density fulfills the condition of total positivity, a specific, strong form of positive dependence. A distribution defined by a density function $f$ over $\mathcal{X} = \prod_{i=1}^{d} X_i$, where each set $X_i$ is totally ordered, is multivariate totally positive of order 2 (MTP2) if

$$f(x)f(y) \leq f(x \wedge y)f(x \vee y) \quad \text{for all } x, y \in \mathcal{X},$$

where $x \wedge y$ and $x \vee y$ are the coordinate-wise minimum and maximum. We restrict our attention to densities on $\mathcal{X} = \mathbb{R}^d$. If $f$ is strictly positive, then $f$ is MTP2 if and only if $f$ is log-supermodular, i.e., $\log(f)$ is supermodular:

$$\log(f(x)) + \log(f(y)) \leq \log(f(x \vee y)) + \log(f(x \wedge y)).$$

MTP2 was introduced in [FKG71] and it implies positive association, an important property in probability theory and statistical physics, which is usually difficult to verify. In fact, most notions of positive dependence are implied by MTP2: see for example [CSS05, CSS06] for an overview. Furthermore, the class of MTP2 distributions has desirable properties [MS00], for example, it is closed under marginalization and conditioning [KR80] (in particular, Yule-Simpson’s Paradox cannot happen for an MTP2 distribution), and independence models generated by MTP2 distributions are compositional semigraphoids [FLS+17].

The special case of Gaussian MTP2 distributions was studied by Karlin and Rinott [KR83] and also in [SH15, LUZ17] from the perspective of MLE and optimization.

Even though the MTP2 condition is quite strong (recall that it implies all other forms of positive dependence), a variety of distributions are intrinsically MTP2. For example, order statistics of i.i.d. variables [KR80], ferromagnetic Ising models [Leb72], Brownian motion tree models, and Gaussian and binary latent tree models [Zwi16].

2. Our contribution and related work

With regards to density estimation, the MTP2 assumption is a shape constraint on $f_0$, the true density at hand. Estimation under MTP2 has been studied in the recent past. In [RSTU18], the authors study maximum likelihood estimation under MTP2; since the likelihood function is unbounded over the set of MTP2 distributions, they impose the additional restriction of log-concavity on the unknown density. In another paper, [HMRR19], the authors study the minimax rates of estimating 2-dimensional MTP2 densities with bounded domain.

In the present paper, we take a kernel density estimation approach for estimating general MTP2 densities. The standard kernel density estimator
would, in general, not be MTP. Instead, we augment our sample set to produce a new estimator which is MTP. We exploit the assumption that the true density is MTP by substituting the sample $X = \{X_1, \ldots, X_n\}$ with its min-max closure $\text{MM}(X)$. By definition of the MTP property, we know that any two points $a$ and $b$ in the sample $X$, satisfy $f_0(a)f_0(b) \leq f_0(a \wedge b)f_0(a \vee b)$ under the true density $f_0$. Thus, intuitively, the points $a \wedge b$ and $a \vee b$ could serve as even better representatives for the unknown distribution $f_0$ than $a$ and $b$ themselves, motivating us to add them to our sample. Performing this process repeatedly, we arrive at the min-max closure $\text{MM}(X)$ of the original sample $X$. We then convolve the indicator function of $\text{MM}(X)$ with a scaled standard Gaussian kernel. In other words, our estimator is a sum of scaled standard Gaussian bumps at the points in the min-max closure of the sample as opposed to the points in the original sample itself, which is the case in standard kernel density estimation. It is in general not true that convolving two MTP functions yields an MTP function. However, our main result (cf. Theorem 5) shows that the convolution is MTP in the specific case of our estimator — convolving (the indicator of) a min-max closed set with any scaled standard Gaussian kernel yields an MTP density. In the process of proving this result we provide a general condition on when the convolution of an MTP function and a standard Gaussian is MTP (cf. Theorem 7) and we prove that the indicator function of a min-max closed set satisfies this condition (cf. Proposition 9). Finally, we provide experimental evidence that our estimator has a lower error than the standard kernel density estimator (for MTP densities we tested), and we supply conjectures on the convergence rates.

The rest of the paper is organized as follows. In Section 3 we define and describe our estimator, the Totally Positive Kernel Density Estimator (TPKDE), in detail. In Section 4 we discuss convolutions and compositions of totally positive functions in a general setting and introduce Theorem 7 and Proposition 9. In Theorem 7 we provide a sufficient condition for the convolution of two MTP functions to be MTP. In Proposition 9 we show that this condition is satisfied by our estimator (and actually any min-max closed set), meaning that it yields an MTP density. This is a combinatorial result of independent mathematical interest, and its proof is located in Section 5. In Section 6 we discuss the algorithmic implementations we devised and used to compute the min-max closure of a set of points. In Section 7 we provide experimental evidence that our estimator outperforms the standard kernel density estimator with lower approximate expected errors in case of an MTP true density. We conclude our study in Section 8 where we raise a multitude of questions for future work.

3. The Totally Positive Kernel Density Estimator (TPKDE)

Instead of using standard kernel density estimation, in which one sums up, say, Gaussian bumps centered at the points in our sample set $X = \{X_1, \ldots, X_n\}$, we propose to exploit the MTP condition in order to obtain a better estimator.
Recall that given two points $X_i$ and $X_j$, under the true density, $f_0$, we have
\[
f_0(X_i) f_0(X_j) \leq f_0(X_i \land X_j) f_0(X_i \lor X_j).
\]
Therefore, intuitively the (coordinate-wise) minimum $X_i \land X_j$ and the maximum $X_i \lor X_j$ have a higher likelihood of occurring than $X_i$ and $X_j$ themselves. This is why we add $X_i \land X_j$ and $X_i \lor X_j$ to $X$. Continuing this process recursively, we arrive at the \textit{min-max closure} of $X$, denoted $\text{MM}(X)$.

**Definition 1.** The \textit{min-max closure} of a finite set of points $X = \{X_1, \ldots, X_n\} \subset \mathbb{R}^d$ is the smallest set $S$ such that $X \subseteq S$, and $S$ is \textit{min-max closed}, i.e., for every $a, b \in S$, their minimum $a \land b$ and maximum $a \lor b$ are also in $S$.

Note that the process described above terminates since MM$(X)$ is contained in the finite set of points $Z$ such that for each $i$, the $i$-th coordinate of $Z$ equals the $i$-th coordinate of one of $X_1, \ldots, X_n$. We sometimes call this finite set the \textit{grid generated by} $X_1, \ldots, X_n$.

In our setting it is assumed that the true density is MTP$_2$. Thus, intuitively, we can see that using MM$(X)$ instead of $X$ would give us a “more representative” set of points than $X$ and, therefore, would yield a better estimator.

Accordingly, in our modified version of the kernel density estimator, we replace the role of $X$ by its min-max closure MM$(X)$. Without this modification, we would in general \textit{not} get an MTP$_2$ density. We can see why this is the case by a simple counterexample.

**Counterexample 2.** Consider the average of two 2-dimensional standard Gaussians centered at $(0, 1)$ and $(1, 0)$ (i.e. $X = \{(0, 1), (1, 0)\}$ is our sample) and let us call this density $\hat{f}$. To see that it is not MTP$_2$, consider the points $p_1 = (0, 1)$ and $p_2 = (1, 0)$. Then $p_1 \land p_2 = (0, 0), p_1 \lor p_2 = (1, 1), \hat{f}(p_1) \hat{f}(p_2) = \hat{f}(0, 1) \hat{f}(1, 0) \approx 0.012$, and $\hat{f}(p_1 \land p_2) \hat{f}(p_1 \lor p_2) = \hat{f}(0, 0) \hat{f}(1, 1) \approx 0.009$. So $\hat{f}(p_1) \hat{f}(p_2) > \hat{f}(p_1 \land p_2) \hat{f}(p_1 \lor p_2)$ which shows that the MTP$_2$ condition is not satisfied.

We wish to remark that we need to use the multivariate scaled \textit{standard} Gaussian kernel in $d$-coordinates for our kernel (see Section 4 for why we need this kernel as a opposed to, for example, a general (MTP$_2$) Gaussian kernel). We now define our estimator.

**Definition 3.** [Totally Positive Kernel Density Estimator] Given $n$ i.i.d. samples in the sample set $X = \{X_1, \ldots, X_n\}$, each $X_i \in \mathbb{R}^d$ drawn from a true density $f_0$, denote the min-max closure by MM$(X)$ and the size of MM$(X)$ by $m$. We can then write MM$(X)$ as MM$(X) = \{X_1, \ldots, X_n, \ldots, X_m\}$, where $m - n \geq 0$ is the number of additional points we added to $X$ to transform it into MM$(X)$. The \textit{Totally Positive Kernel Density Estimator} (or TPKDE) $\hat{f}(x)$ at a point $x \in \mathbb{R}^d$ is then
\[
\hat{f}(x) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{h^d} N_d \left( \frac{x - X_i}{h} \right)
\]
where $h \in \mathbb{R}, h > 0$ and $N_d$ is the standard Gaussian kernel (with identity covariance matrix) in $d$-coordinates.

**Remark 4.** Note that we can also write the TPKDE equivalently as

\[
\hat{f}(x) = \frac{1}{m} \sum_{i=1}^{m} N_d^h(x - X_i) \tag{1}
\]

where $N_d^h$ is a multivariate Gaussian density in $d$-coordinates with covariance matrix, $\Sigma = h^2 I$, where $I$ is the $d \times d$ identity matrix. This is because for \( y_1, \ldots, y_d \in \mathbb{R} \), we have

\[
N_d^h(y_1, \ldots, y_d) = \frac{1}{\sqrt{2\pi \det(h^2 I)}} e^{-\frac{1}{2} \left( \frac{1}{h^2}(y_1)^2 + \cdots + \frac{1}{h^2}(y_d)^2 \right)} = \frac{1}{h^d} N_d(y_1/h, \ldots, y_d/h).
\]

We will often use this equivalent form due to ease of manipulation. We saw above that the unmodified kernel density estimator need not be MTP\(^2\). One of our results is that the TPKDE is, in fact, MTP\(^2\) as stated in the following theorem.

**Theorem 5.** The totally positive kernel density estimator is an MTP\(^2\) density.

This result is a consequence of Theorem 7 and Proposition 9 and its proof is stated at the end of Section 4. The result is interesting not only because of its use for kernel density estimation, but also because typically convolutions of MTP\(^2\) functions are not MTP\(^2\); i.e., the set of MTP\(^2\) functions is not closed under convolution. We devote Section 4 to a discussion of this matter.

Also note that for our estimator to be MTP\(^2\) we need to use a scaled standard Gaussian kernel, i.e., with covariance matrix $\Sigma = hI$, a multiple of the identity matrix. In Section 4 we provide Counterexample 6, which shows that using an MTP\(^2\) Gaussian kernel with different covariance could give rise to a non-MTP\(^2\) density.

### 4. Convolutions of MTP\(^2\) Functions

The Totally Positive Kernel Density estimator for a sample set $X = \{X_1, \ldots, X_n\}$ with min-max closure $\text{MM}(X) = \{X_1, \ldots, X_m\}$ given in (1) can actually be stated as an instance of a general class of convolutions involving MTP\(^2\) functions. For functions $g : \mathbb{R}^d \to \mathbb{R}$ and $\alpha : \mathbb{R}^d \to \mathbb{R}$, we define their convolution $C(a) : \mathbb{R}^d \to \mathbb{R}$ at $(a_1, \ldots, a_d) = a \in \mathbb{R}^d$ as

\[
C(a_1, \ldots, a_d) \triangleq \int_{x_1 \in \mathbb{R}} \cdots \int_{x_d \in \mathbb{R}} \alpha(x_1, \ldots, x_d) g(a_1 - x_1, \ldots, a_d - x_d) dx_1, \ldots, dx_d,
\]

or more compactly as

\[
C(a) \triangleq \int_{x \in \mathbb{R}^d} \alpha(x) g(a - x) dx. \tag{2}
\]
Note that the totally positive kernel density estimator is
\[ \hat{f}(a) = C(a) \]  
(3)
with
\[ g = N^h_d, \]
and
\[ \alpha(x) = U_{MM(X)}(x) \]
where \( U_{MM(X)}(x) \) is the uniform density over \( MM(X) \), or more precisely, \( \frac{1}{m} \) if \( x \in X \) and 0 otherwise. So our estimator is just an instance of convolution where \( g \) is a scaled standard multivariate Gaussian density and \( \alpha \) is the uniform distribution over the min-max closure of our sample set.

This convolution is similar to other types used in many composition theorems of MTP_2 kernels that have been proved and discussed in great detail by Karlin, for example, in [Kar68]. However, the type of convolution we have defined above is generally omitted from any such previous discussion. This is because it, in general, does not satisfy the MTP_2 condition. Specifically, despite both of \( g \) and \( \alpha \) being MTP_2 functions, it is generally not true that \( C \) is MTP_2.

One such counterexample is given by Karlin and Rinott in [KR80, pp. 486]. They use the result from [KR83] that a multivariate Gaussian density is MTP_2 if and only if the inverse of its covariance matrix has only non-positive off-diagonal entries (i.e. is an \( M \)-matrix). They provide two 3-dimensional positive definite matrices \( A \) and \( B \) whose inverses are \( M \)-matrices, but the inverse \((A + B)^{-1}\) of \( A + B \) is not an \( M \)-matrix. (Note that the convolution of the two Gaussians with covariances \( A \) and \( B \) is another Gaussian distribution with covariance \( A + B \).) Therefore, the convolution of two MTP_2 Gaussians need not be MTP_2 and, accordingly, two general MTP_2 functions need not convolve to produce an MTP_2 function.

We provide another counterexample in 2-dimensions, that is also relevant to our setting. We show that convolving the uniform distribution of a min-max closed set with a non-standard MTP_2 Gaussian need not be MTP_2. We also discuss this counterexample in [Appendix B]

**Counterexample 6.** Consider the set of points \( X = \{(2, 0), (0, 1)\} \). Its min-max closure is \( MM(X) = \{(2, 0), (0, 1), (2, 1), (0, 0)\} \). Then the uniform distribution on this set \( \alpha(x) = U_{MM(X)}(x) \) is obviously MTP_2 due to the definition of a min-max closed set. However, if we convolve \( \alpha \) with an MTP_2 Gaussian \( g \) whose inverse covariance matrix is the \( M \)-matrix
\[ \Sigma^{-1} = \begin{pmatrix} 5 & -2 \\ -2 & 1 \end{pmatrix} \]
the result is not MTP_2. For example, if \( p_1 = (0.98, 0.43) \) and \( p_2 = (0.49, 0.7) \), and if \( C \) denotes the convolution of \( g \) and \( \alpha \) we get that
\[ C(p_1 \wedge p_2)C(p_1 \vee p_2) < C(p_1)C(p_2). \]
This is a violation of the MTP_2 condition.
This shows that not all MTP₂ Gaussian densities can be used as the kernel in our estimator. We now show (cf. Theorem 7) that choosing a covariance of \( \Sigma = hI \) and imposing a further restriction on \( \alpha \) (cf. Constraint A) yields an MTP₂ convolution. Then in Proposition 9 we show that if \( \alpha \) is the uniform distribution on a min-max closed set (which is what our estimator uses) it satisfies the sufficient Constraint A, and therefore, our proposed totally positive kernel density estimator from Definition 3 is an MTP₂ density.

**Theorem 7.** Let \( N^h_d(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R} \) be a \( d \)-dimensional multivariate Gaussian density function with covariance matrix \( \Sigma = hI \), i.e., with independent coordinates and a common variance \( h \). Let \( \alpha \) be either a probability density on \( \mathbb{R}^d \) or the distribution over a finite subset in \( \mathbb{R}^d \). Suppose further that \( \alpha \) satisfies the constraint

**Constraint A.** Let \( x_{10} < x_{11}, x_{20} < x_{21}, \ldots, x_{d0} < x_{d1} \), where \( x_{ij} \in \mathbb{R} \) for all \( 1 \leq i \leq d \) and \( 0 \leq j \leq 1 \). For each binary string \( b \in \{0, 1\}^d \), denote \( x_b := (x_{b1}, x_{2b}, \ldots, x_{db}) \in \mathbb{R}^d \), and let \( \overline{b} := (1 - b_1, \ldots, 1 - b_d) \) be the complementary binary string. Then for any permutation \( \pi \) of \( \{1, \ldots, d\} \) we have

\[
\sum_{a \in \{0, 1\}^{d-2}} \left( \alpha(x_{\pi(1)a})\alpha(x_{\pi(00\overline{a})}) - \alpha(x_{\pi(0a)})\alpha(x_{\pi(01\overline{a})}) \right) \geq 0. \tag{4}
\]

Then the \( d \)-dimensional convolution of \( N^h_d(\cdot) \) with \( \alpha(\cdot) \) is an MTP₂ function. In other words, the function

\[
C(a_1, \ldots, a_d) = \int_{(x_1, \ldots, x_d) \in \mathbb{R}^d} \alpha(x_1, \ldots, x_d) N^h_d(a_1 - x_1, \ldots, a_d - x_d) dx_1 \ldots dx_d,
\]

is MTP₂.

**Remark 8.** Note that Constraint A gives a restriction on the values of \( \alpha \) at the vertices of the hypercube \( \prod_{i=1}^d \{x_{i0}, x_{i1}\} \). For example, when \( d = 2 \), it is equivalent to the MTP₂ condition. When \( d = 3 \), the constraint simply says

\[
\alpha(x_{(111)})\alpha(x_{(000)}) - \alpha(x_{(101)})\alpha(x_{(010)}) + \alpha(x_{(110)})\alpha(x_{(001)}) - \alpha(x_{(100)})\alpha(x_{(011)}) \geq 0,
\]

a condition involving all of the vertices of the hypercube \( \{x_{10}, x_{11}\} \times \{x_{20}, x_{21}\} \times \{x_{30}, x_{31}\} \) in \( \mathbb{R}^3 \).

We provide the proof of this theorem (Theorem 7) in Appendix A. Our next result (Proposition 9) is the final ingredient to showing Theorem 5. It is an interesting combinatorial result on its own and we provide its proof in Section 5.

**Proposition 9.** Let \( \alpha(x) : \mathbb{R}^d \rightarrow \{0, c\} \) be the uniform distribution over a min-maxed closed set \( M \subseteq \mathbb{R}^d \) (which is potentially a finite set), then \( \alpha \) satisfies Constraint A.

Note that the set we use in the TPKDE is a min-max closed set (it is just the min-max closure of the set of sample points). Thus we can now state the simple proof that the TPKDE yields an MTP₂ density.
Proof of Theorem 5 The TPKDE uses a min-max closed set $MM(X)$ where $X$ is the original sample set. Now, from Proposition 9 we know that the uniform distribution over $MM(X)$, say $\alpha$, satisfies Constraint A. Since the TPKDE can be framed as a convolution of $\alpha$ and a scaled standard Gaussian as shown in 3, we can use Theorem 7 to immediately conclude that the totally positive kernel density estimator is MTP$_2$. \hfill $\Box$

5. Proof of Proposition 9

Proposition 9 is much more general than its use here in the TPKDE setting. It states that if we take any min-max closed set, then the uniform distribution over it (or the set’s indicator function) will satisfy Constraint A, which is also a general constraint. This result is of independent mathematical interest as well.

We first introduce a lemma that will be used in the proof of Proposition 9.

Lemma 10. For a binary string $b$ of arbitrary length $d$, i.e., $b \in \{0, 1\}^d$, we use $\bar{b} := (1 - b_1, \ldots, 1 - b_d)$ to denote the complementary binary string. For any two binary strings, $a, b \in \{0, 1\}^d$, we have that

$$(\pi \land b) = \overline{(a \lor \bar{b})}.$$  

Proof. Let $A \subseteq [d]$ be the set of indices where the string $a$ has 1s. And similarly, let $B \subseteq [d]$ be the set of indices where the string $b$ has 1s. Then $(\pi \land b)$ has 1s in the index set $(A') \cap B$. But if we look at $(a \lor \bar{b})$, it has 1s in the set $A \cup B$. So then its complement, $(a \lor \bar{b})$, would have 1s in the remaining indices i.e. $(A \cup B)^c = A^c \cap B$. But this is exactly the set of indices in which $(\pi \land b)$ had 1s, thus proving this lemma. \hfill $\Box$

Now, we can start proving Proposition 9.

Proof of Proposition 9 Let $x_{10} < x_{11}, x_{20} < x_{21}, \ldots, x_{d0} < x_{d1}$, where $x_{ij} \in \mathbb{R}$ for all $1 \leq i \leq d$ and $0 \leq j \leq 1$. For each binary string $b \in \{0, 1\}^d$, denote $x_b := (x_{b1}, \ldots, x_{bd}) \in \mathbb{R}^d$, and let $\bar{b} := (1 - b_1, \ldots, 1 - b_d)$ be the complementary binary string. By symmetry, let $\pi$ be the identity permutation on $\{1, 2, \ldots, d\}$. We will show that

$$\sum_{a \in \{0, 1\}^{d-2}} (\alpha(x_{11a})\alpha(00\pi) - \alpha(x_{10a})\alpha(01\pi)) \geq 0,$$

where $\alpha(x) : \mathbb{R}^d \to \{0, c\}$ is the uniform distribution over a min-maxed closed set $M \subseteq \mathbb{R}^d$.

If $M$ is a finite set, then $\alpha(x) = c := 1/|M|$ when $x \in M$, and 0 when $x \notin M$. Otherwise $\alpha$ is the density of the uniform probability measure on $M$, and $\alpha(x) = c$ for the appropriate $c \in \mathbb{R}$ for $x \in M$ and 0 otherwise.

Let $B_1 = \{a \in \{0, 1\}^{d-2} : \alpha(x_{10a}) = c > 0\}$. Note that $x_a \land x_b = x_{a \land b}$ and $x_a \lor x_b = x_{a \lor b}$. Now since $M$ is min-max closed, so is $B_1$. This is because if $a, b \in B_1$, then $\alpha(x_{10a}) = \alpha(x_{10b}) = c$ which means $x_{10a}, x_{10b} \in M$ so...
$$x_{10a} \lor x_{10b} = x_{10a \lor b} \in M$$ (due to its min-max closure). This means \(\alpha(x_{10a \lor b}) = c\), hence \(a \lor b \in B_1\), and similarly for the minimum \(a \land b\).

Let \(B_2 := \{a \in \{0, 1\}^{d-2} : \alpha(x_{10a}) > 0\}\). Similarly, since \(M\) is min-max closed, so is \(B_2\). We use the notation \(\overline{B}_2\) to denote the set of complementary strings of \(B_2\), and we can see that \(\overline{B}_2\) is also min-max closed. This is because when we take the complementary strings, coordinate-wise minima become coordinate-wise maxima and vice-versa, as shown in Lemma 10—precisely,

\[
a, b \in \overline{B}_2 \implies \pi, \overline{b} \in B_2 \implies \pi \lor \overline{b} \in B_2 \implies \overline{\pi \lor \overline{b}} = a \land b \in \overline{B}_2,
\]

and similarly for \(a \lor b\).

Now, let \(A = B_1 \cap \overline{B}_2\). This is precisely the set of \(a \in \{0, 1\}^{d-2}\) such that \(\alpha(x_{10a}) = c\) and \(\alpha(x_{01}) = c\), i.e. \(\alpha(x_{10a})\alpha(x_{01}) = c^2\). Moreover, \(A\) is min-max closed (intersection of two min-max closed sets).

We now let \(a^*\) be the minimum of \(A\) (i.e. the indices where \(a^*\) has 1s are common to all \(a \in A\)). Therefore, since \(\overline{A} = B_1 \cap B_2\) (i.e. the set of \(\pi \in \{0, 1\}^{d-2}\) such that \(\alpha(x_{10a})\alpha(x_{01}) > 0\)), necessarily \(\overline{a^*}\) is the maximum of \(A\). To see this, let \(O(x)\) be the set of indices where the binary string \(x\) has ones. Then

\[
\forall b \in A, O(a^*) \subseteq O(b) \quad \text{(since } a^* \text{ is minimum of } A) \\
\implies \forall b \in A, O(a^*) \supseteq O(b) \\
\implies \forall b \in A, O(\overline{a^*}) \supseteq O(\overline{b}) \\
\implies \forall b \in \overline{A}, O(\overline{a^*}) \supseteq O(\overline{b}) \quad \text{i.e. } \overline{a^*} \text{ is maximum of } \overline{A}.
\]

So now, for every \(a \in A\), we have that \(\pi \in B_2\), thus, \(\alpha(x_{01}) > 0\). Therefore, since \(M\) is min-max closed, \(\alpha(x_{10a} \lor x_{01}) = c > 0\) and \(\alpha(x_{10a} \land x_{01}) = c > 0\).

But note that \(x_{10a} \lor x_{01} = x_{11(a^* \lor \pi)}\) and \(x_{10a} \land x_{01} = x_{00(\overline{a^*} \land \pi)}\). Moreover, by Lemma 10, \(\overline{a^*} \land a = a^* \lor \pi\). Finally, since \(a^*\) is the minimum over all \(a \in A\), and \(\overline{a^*}\) is the maximum over all \(\pi\) for \(a \in A\), then, for all \(a \neq b \in A\), \(a^* \lor \pi \neq a^* \lor \overline{b}\) (as in the indices where \(a^*\) has 1s, \(\pi\) and \(\overline{b}\) will both have 0s anyways), and similarly, \(\overline{a^*} \land a \neq \overline{a^*} \land b\).

Now let \(C = \{a^* \lor \pi : a \in A\}\). Then, finally,

\[
\sum_{a \in \{0, 1\}^{d-2}} (\alpha(x_{11a})\alpha(x_{00}) - \alpha(x_{10a})\alpha(x_{01})) \\
= \sum_{a \in \{0, 1\}^{d-2}} \alpha(x_{11a})\alpha(x_{00}) - \sum_{a \in \{0, 1\}^{d-2}} \alpha(x_{10a})\alpha(x_{01}) \\
= \sum_{a \in \{0, 1\}^{d-2}} \alpha(x_{11a})\alpha(x_{00}) - \sum_{a \in A} \alpha(x_{10a})\alpha(x_{01}) \\
= \sum_{a \in \{0, 1\}^{d-2} \setminus C} \alpha(x_{11a})\alpha(x_{00}) + \sum_{a \in A} \left(\alpha(x_{11(a^* \lor \pi)})\alpha(x_{00(\overline{a^*} \land \pi)}) - \alpha(x_{10a})\alpha(x_{01})\right).
\]

The first summation is nonnegative. Each of the terms in the second summation equals \(c^2 - c^2 = 0\). Thus, the whole expression is nonnegative, which completes the proof of the Proposition 9. \(\Box\)
6. Algorithms

The most intensive task for computing our estimator is finding the min-max closure of the set of samples. The cardinality of $MM(X)$ appears to be on the order of (and is certainly upper bounded by) $n^d$, where $n$ is the cardinality of the original set $X$. Therefore computing this set is possibly exponentially hard. Due to the upper bound $n^d$, however, the algorithms are guaranteed to terminate.

We designed and implemented several different algorithms for finding $MM(X)$.

The Naive method, Algorithm 1 simply goes through each pair of points in the set and adds their element-wise minima and maxima to $MM(X)$. It then iterates over the points in the current $MM(X)$ and repeats the procedure. It is guaranteed to converge when the min-max closure is found, which is bounded in size by $n^d$. However, it the worse case run-time is $\Omega(n^{2d})$ since we may have to iterate over all $n^d \times n^d$ pairs of points before termination.

Algorithm 1 Naive Algorithm for $MM(X)$

1: $n \leftarrow |X|
2: M \leftarrow X
3: \text{while True do}
4: \hspace{1em} oldSize $\leftarrow |M|
5: \hspace{1em} \text{for } (i < j \leq n) \text{ do}
6: \hspace{2em} \text{add } X_i \land X_j \text{ to } M
7: \hspace{2em} \text{add } X_i \lor X_j \text{ to } M
8: \hspace{1em} \text{end for}
9: \hspace{1em} \text{if } |M| = oldSize \text{ then}
10: \hspace{2em} \text{break}
11: \hspace{1em} \text{end if}
12: \text{end while}
13: \text{return } M

As a more efficient strategy, we utilized the parallel compute capabilities of GPUs by modifying the naive method and got Algorithm 2 - note that the for loop in lines 6-9 of Algorithm 2 is a parallel for loop over the set of all points currently in the set. The $\text{MakeGrid}$ method takes the set $X$ and generates a $d$-dimensional grid with $n^d$ entries. This is possible when $X$ has a fixed order - we simply sort it to maintain this order. Then the coordinates of each point in the set can be mapped to $\{0, \ldots, n\}$ i.e. their position in the ordered set - so for a point in the set we simply put a 1 in the $d$-dimensional grid which is filled with zeros otherwise. We can represent the whole set in the $n^d$ grid. The $\text{GetPts}$ method simply returns the $d$-dimensional indices of all the entries in the set which are 1 i.e. a list of all the points currently in the $MM(X)$.

We further modified Algorithm 2 to be parallel over all the possible points in the grid i.e. all the $n^{2d}$ pairs of indices in the grid. This allows us to avoid copying the grid back to the CPU and calling $\text{GetPts}$ on the grid to get the list of the points that we are iterating over. Instead we can just keep running on the
GPU and modifying the grid in-place. After some set number, \( K \), of iterations, we can just check if the algorithm has converged and terminate accordingly. Note that the for loop in lines 8-14 of Algorithm 3 is a parallel for loop.

Algorithm 2 Parallel Algorithm 1 for \( MM(X) \)

1: \( n \leftarrow |X| \)
2: \( G \leftarrow \text{MakeGrid}(X) \)
3: \( P \leftarrow \text{getPts}(G) \)
4: while True do
5:     \( \text{oldSize} \leftarrow |P| \)
6:     for \( pt_1, pt_2 \) in \( P \) do  \( \triangleright \) This for loop is parallel
7:         \( G.\text{SetOne}(pt_1 \lor pt_2) \)
8:         \( G.\text{SetOne}(pt_1 \land pt_2) \)
9:     end for
10:    \( P \leftarrow \text{getPts}(G) \)
11:   if \( |P| = \text{oldSize} \) then
12:     break
13:   end if
14: end while

Algorithm 3 Parallel Algorithm 2 for \( MM(X) \), \( K \) is an integer parameter

1: \( n \leftarrow |X| \)
2: \( G \leftarrow \text{MakeGrid}(X) \)
3: \( P \leftarrow \text{getPts}(G) \)
4: \( \text{count} \leftarrow 0 \)
5: while True do
6:     \( \text{count} \leftarrow \text{count} + 1 \)
7:     \( \text{oldSize} \leftarrow |P| \)
8:     for \( idx_i, idx_j \) in \( G \) do  \( \triangleright \) This for loop is parallel
9:         \( \text{if} \ (G[\text{idx}_i] == 0 \text{ or } G[\text{idx}_j] == 0) \) then
10:         \( \text{continue} \)
11:     end if
12:     \( G.\text{SetOneIdx}(\text{idx}_j \lor \text{idx}_i) \)
13:     \( G.\text{SetOneIdx}(\text{idx}_j \land \text{idx}_i) \)
14: end for
15: if \( \text{count} \% K == 0 \) then
16:     \( P \leftarrow \text{getPts}(G) \)
17: if \( |P| = \text{oldSize} \) then
18:     break
19: end if
20: end if
21: end while

The worst-case run-time for all algorithms is \( \Omega(n^d) \) since in the worst case we do have to return \( n^d \) points. However Algorithm 3 has parallel run-time \( O(n^d) \)
assuming there are enough cores since the time spent outside copying the set will just be a function of the number of iterations. In our evaluation, we achieved a 15x speedup using Algorithm 3 on GPU compared to Algorithm 1.

7. Experiments

In this section we include our experimental results. We observe that our estimator has a smaller error than the standard kernel density estimator. We leave the provable analysis of this error to a future study. For the true densities we use and sample from MTP$_2$ Gaussian densities due to ease of specifying and sampling from these densities - these are just multivariate Gaussian densities with covariance matrices whose inverses are $M$-matrices. Throughout we use Silvermann’s Rule \cite{Silverman86} for selection of the bandwidth.

Figures 1 and 2 show the estimated expected absolute error of our estimator and the unmodified kernel density estimator. We calculate the error using a Monte Carlo approach, i.e. by sampling from the true distribution and calculating the sample average of

$$|f_0(x) - \hat{f}(x)|,$$

where $\hat{f}(x)$ is the estimated density. Figure 1 shows the error of the regular kernel density estimator, as well as our modified Totally Positive Kernel Density Estimator for different values of $n$. The $\text{iter}$ variable refers to the number of iterations we ran the min-max closure algorithm for, and we can see that the error decreases with more iterations i.e. as we get closer to the complete min-max closure. The error at $\text{iter} = 2$ and $\text{iter} = 3$ is the same since the algorithm has converged, hence we don’t add to the min-max closure further. Figure 2 shows the error for complete iterations and we can see our modified estimator does increasingly better for large values of $n$.

![Figure 1: Absolute Error, $d = 2$, $\text{iter} = 1, 2, 3$](image-url)
Figure 2: Absolute Error, $d = 2$

Figure 3: Error Ratio, $d = 2$

Figure 4: Error Ratio, $d = 3$, $iter = 1$
We can see this increasingly better performance in Figures 3, 4 and 5, where we plot the ratio of the estimated absolute error of regular kernel density estimation to the error of our estimator. We observe that this ratio is an increasing function, although we do not have enough computation power to speculate the limiting behavior of this function.

8. Conclusion

In this paper we considered estimating a density under the constraint that it is MTP$_2$. We proposed augmenting the set of i.i.d. samples and then convolving with a standard Gaussian kernel, thus, yielding our totally positive kernel density estimator. In particular, because of the nature of the MTP$_2$ condition, instead of considering the original sample of points $X$, we consider the min-max closure, MM($X$). Then, our estimator is the convolution of the indicator of MM($X$) with the standard Gaussian kernel. One of our main results, Theorem 5, shows that this convolution does in deed yield an MTP$_2$ function, and therefore, our estimator is proper. It is not in general true that convolutions of MTP$_2$ functions are MTP$_2$. In Theorem 7 we give a sufficient condition for when the convolution of a function with a standard Gaussian yields an MTP$_2$ function. This raises an interesting general theoretical question.

**Question 11.** What are necessary conditions on $\alpha : \mathbb{R}^d \rightarrow \mathbb{R}$ so that the convolution $\int_{x \in \mathbb{R}^d} \alpha(x)N^h_d(x-a)dx$ is an MTP$_2$ function?

We provide experimental evidence that our estimator converges to the true density at a rate much faster than the standard kernel density estimator. Since our sample is far from independent, even proving consistency of our estimator would require tools outside of the standard set of tools one usually uses to show such a result.

**Problem 12.** Develop the necessary mathematical tools to show consistency of the totally positive kernel density estimator, as well as, of other estimators which rely on a highly dependent set of samples.
Problem 13. Compute the statistical rate of convergence of the TPKDE to the original true density.

We expect the statistical rate of convergence to be highly dependant on $h$, the choice of bandwidth, which raises the question

Question 14. What is the optimal choice of bandwidth, $h^*$, of the TPKDE?

We conjecture that due to the large size of $\text{MM}(X)$, this statistical rate will not suffer from the curse of dimensionality. The size of $\text{MM}(X)$ appears to be on the order of $n^d$, although this is also an interesting mathematical question that needs a proof.

Problem 15. Compute the expected size of $\text{MM}(X)$ when $X$ is drawn i.i.d. from a distribution $f_0$. How do different types of distributions $f_0$ influence this expected size?

Finally, perhaps we could use a different MTP$_2$ density on $\text{MM}(X)$ instead of the uniform one. For this we would have to prove a new version of Proposition 9

Problem 16. Show that if $\alpha$ is an MTP$_2$ distribution over a min-max closed set $M \subset \mathbb{R}^d$, then it satisfies Constraint A.

We are hopeful that the resolution of the above mentioned problems would lead to interesting practical and theoretical advances.

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Appendix A. Proof of Theorem 7

Proof of Theorem 7. We want to show that $C(\cdot)$, which is the convolution of a scaled standard multivariate Gaussian $N^h_d(\cdot)$ and $\alpha(\cdot)$ satisfying Constraint A is MTP2. We know that $C(\cdot): \mathbb{R}^d \to \mathbb{R}^+$ is strictly positive everywhere since it is a convolution involving a Gaussian kernel. The result by Karlin and Rinott in [KRS80] states a $d$-dimensional strictly positive function is MTP2 if and only if it is MTP2 in 2 coordinates, with the rest held constant (i.e. pairwise MTP2 property implies the global MTP2 property for strictly positive measures). Thus it is sufficient to show that $C(\cdot)$ is MTP2 in the first two coordinates as that would imply pairwise MTP2 since the multivariate Gaussian kernel is symmetric in all coordinates.

Specifically we need that for all $a_1, a_2, b_1, b_2 \in \mathbb{R}$ with $a_1 > a_2$ and $b_1 > b_2$, and some fixed $c^d_3 \in \mathbb{R}^{d-2}$, where use the notation $(x - c)^d_3$ to denote $(x_3 - c_3, \ldots, x_d - c_d)$, the condition

$$C(a_1, b_1, c^d_3)C(a_2, b_2, c^d_3) \geq C(a_1, b_2, c^d_3)C(a_2, b_1, c^d_3)$$

is satisfied. Note that we can replace integrals with summations throughout our analysis.

First, we expand $C(\cdot)$ using the definition of convolution in (2) to get the condition that

$$\left( \int_{x_1, \ldots, x_d} \alpha(x) N^h_d (a_1 - x_1, b_1 - x_2, (c - x)^d_3) \right) \left( \int_{x_1, \ldots, x_d} \alpha(x) N^h_d (a_2 - x_1, b_2 - x_2, (c - x)^d_3) \right) \geq \left( \int_{x_1, \ldots, x_d} \alpha(x) N^h_d (a_1 - x_1, b_2 - x_2, (c - x)^d_3) \right) \left( \int_{x_1, \ldots, x_d} \alpha(x) N^h_d (a_2 - x_1, b_1 - x_2, (c - x)^d_3) \right)$$

where we use the notation $(x - c)^d_3$ to denote $(x_3 - c_3, \ldots, x_d - c_d)$, and $x$ for $(x_1, \ldots, x_n)$. We also drop $dx_1 \ldots dx_d$ throughout the proof to ease notation and since the domain of integration is clearly stated throughout.

We can multiply both sides by $\frac{1}{2\pi h^d}$ and use vector norm notation, where we use $\| \cdot \|$ to denote the $L_2$ norm. We also use the simple integral $\int$ notation instead.
of $\int \cdots \int$ for simpler notation since the domain is clearly stated. We get

$$
\left( \int_{\mathbb{R}^d} \alpha(x) e^{\frac{-1}{2} \|x\|^2} \right)^{\alpha} \left( \int_{\mathbb{R}^d} \alpha(x) e^{\frac{-1}{2} \|x\|^2} \right)^{2 - \alpha} \geq \left( \int_{\mathbb{R}^d} \alpha(x) e^{\frac{-1}{2} \|x\|^2} \right)^{\alpha} \left( \int_{\mathbb{R}^d} \alpha(x) e^{\frac{-1}{2} \|x\|^2} \right)^{2 - \alpha}.
$$

(A.1)

We denote $c^d_i$ by $c \in \mathbb{R}^{d-2}$. We now rename $x_1, x_2,$ and $x_3$ to $x_i, x_j,$ and $x_k$ respectively for the factors on the left and also rename $x_1, x_2,$ and $x_3$ to $x_i, x_j, x_k$ respectively for the factors on the right. Splitting the factors in the integrals we get

$$
\left( \int_{m \in \mathbb{R}^{d-2}} e^{\frac{-1}{2} \|c - m\|^2} \alpha(x, x_j, m) e^{\frac{-1}{2} \|x - x_i\|^2} \right) \left( \int_{n \in \mathbb{R}^{d-2}} e^{\frac{-1}{2} \|c - n\|^2} \alpha(x, x_i, n) e^{\frac{-1}{2} \|x - x_j\|^2} \right) \geq \left( \int_{m \in \mathbb{R}^{d-2}} e^{\frac{-1}{2} \|c - m\|^2} \alpha(x, x_j, m) e^{\frac{-1}{2} \|x - x_i\|^2} \right) \left( \int_{n \in \mathbb{R}^{d-2}} e^{\frac{-1}{2} \|c - n\|^2} \alpha(x, x_i, n) e^{\frac{-1}{2} \|x - x_j\|^2} \right).
$$

Combining the factors into one integral and using the notation $\alpha_{ijm}$ for $\alpha(x, x_j, m)$, we get

$$
\left( \int_{m, n \in \mathbb{R}^{d-2}} e^{\frac{-1}{2} \|c - m\|^2} \alpha_{ijm} e^{\frac{-1}{2} \|x - x_i\|^2} + e^{\frac{-1}{2} \|x - x_j\|^2} \right) \geq 0.
$$

(A.2)

Let us now examine the inner integrals in (A.2) in more detail by dividing into the regions of integration. We can divide the region of $\int x_i, x_j, x_k, x_l \in \mathbb{R}$ into 7 cases corresponding to each of

Case 1: $x_i > x_k$, Case 2: $x_i > x_k$, Case 3: $x_i < x_k$, Case 4: $x_i < x_k$, Case 5: $x_i = x_k$.
Case 6: $\int_{x_i = x_k, \ x_j \neq x_l}$, and Case 7: $\int_{x_i \neq x_k, \ x_j = x_l}$

We will look at the different cases separately. For Case 5 ($\int_{x_i = x_k, \ x_j = x_l}$) we have

$$
\int_{m, n \in \mathbb{R}^{d-2}} e^{-\frac{1}{2} \|c - m\|^2} \left[ \int_{x_j = x_l} \alpha_{ijm} \alpha_{kln} e^{-\frac{1}{2} \left( \|a_1 - x_i\| + \|a_2 - x_k\| \right)} \right]
$$

$$
\int_{x_i = x_k} \alpha_{ijm} \alpha_{kln} e^{-\frac{1}{2} \left( \|b_1 - x_j\| + \|b_2 - x_l\| \right)} = 0
$$

and this vanishes since the inner terms are the same. For Case 7 ($\int_{x_i \neq x_k, \ x_j = x_l}$) we can see that

$$
\int_{m, n \in \mathbb{R}^{d-2}} e^{-\frac{1}{2} \|c - m\|^2} \left[ \int_{x_j = x_l} \alpha_{ijm} \alpha_{kln} e^{-\frac{1}{2} \left( \|a_1 - x_i\| + \|a_2 - x_k\| \right)} \right]
$$

$$
\int_{x_i = x_k} \alpha_{ijm} \alpha_{kln} e^{-\frac{1}{2} \left( \|b_1 - x_j\| + \|b_2 - x_l\| \right)} = 0
$$
And for Case 6 \((f_i=r_k)\) we can simplify the inner terms as

\[
\int_{x_i=r_k, x_j \neq x_l} \alpha_{ijm} \alpha_{kln} e^{-\frac{1}{2} h \left( \|a_1-x_i\| + \|b_2-x_l\| \right)} - \int_{x_i=r_k, x_j \neq x_l} \alpha_{ijm} \alpha_{kln} e^{-\frac{1}{2} h \left( \|a_1-x_j\| + \|b_2-x_l\| \right)}
\]

\[
= \int_{x_j \neq x_l} \alpha_{ijm} \alpha_{iln} e^{-\frac{1}{2} h \left( \|a_1-x_i\| + \|a_2-x_j\| \right)} - \int_{x_j \neq x_l} \alpha_{ilm} \alpha_{ijn} e^{-\frac{1}{2} h \left( \|a_1-x_i\| + \|a_2-x_j\| \right)}
\]

\[
= \int_{x_j \neq x_l} (\alpha_{ijm} \alpha_{iln} - \alpha_{ijn} \alpha_{ilm}) e^{-\frac{1}{2} h \left( \|a_1-x_i\| + \|a_2-x_j\| \right)}.
\]

So for this case we get

\[
\int_{m,n \in \mathbb{R}^{d-2}} e^{-\frac{1}{2} (\|c-m\| + \|c-n\|)} \left[ \int_{x_j \neq x_l} (\alpha_{ijm} \alpha_{iln} - \alpha_{ijn} \alpha_{ilm}) e^{-\frac{1}{2} h \left( \|a_1-x_i\| + \|a_2-x_j\| \right)} \right] = 0
\]

\[(A.3)\]

This is because the outer integral \(\int_{m,n \in \mathbb{R}^{d-2}} \) over \(m,n \in \mathbb{R}^{d-2}\) is symmetric in \(m,n\), and so we can switch \(m\) and \(n\) in one of the terms. Hence, \(\int_{m,n \in \mathbb{R}^{d-2}} (\alpha_{ijm} \alpha_{iln} - \alpha_{ijn} \alpha_{ilm}) = 0\), and this implies (A.3).
Now for the remaining cases i.e. Case 1, 2, 3, and 4, we have

\[ \int_{m,n \in \mathbb{R}^{d-2}} e^{-\frac{1}{2} \| \mathbf{c} - \mathbf{m} \|} \left[ \int_{x_i > x_k \atop x_j < x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} \right] - \int_{x_i > x_k \atop x_j > x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} + \int_{x_i < x_k \atop x_j < x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} - \int_{x_i < x_k \atop x_j > x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} \right] \]

Now with renaming indices and manipulation of terms, we get

\[ \int_{m,n \in \mathbb{R}^{d-2}} e^{-\frac{1}{2} \| \mathbf{c} - \mathbf{m} \|} \left[ \int_{x_i > x_k \atop x_j > x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} \right] - \int_{x_i > x_k \atop x_j > x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} + \int_{x_i > x_k \atop x_j > x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} - \int_{x_i > x_k \atop x_j > x_l} \alpha_{ijm} \alpha_{klm} e^{-\frac{1}{2} \left( \| x_i - x_k \| \right)} \right] \]
We now collect terms and write the whole expression as

\[
\int_{m,n \in \mathbb{R}^{d-2}} \int_{x_i > x_k \atop x_j > x_l} \left\{ \frac{\pi}{e} \| c - m \| \right\} \left[ \alpha_{ijmn} \alpha_{klm} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \right. \\
- \left. \alpha_{ilm} \alpha_{kjm} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \right] \\
+ \alpha_{ijn} \alpha_{klm} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \\
- \alpha_{km} \alpha_{ijn} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \right] \\
\]

Now here the integral in \( m, n \) is symmetric and we can switch the names of \( m \) and \( n \) in the last two terms to get

\[
\int_{m,n \in \mathbb{R}^{d-2}} \int_{x_i > x_k \atop x_j > x_l} \left\{ \frac{\pi}{e} \| c - n \| \right\} \left[ \alpha_{ijmn} \alpha_{klm} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \right. \\
- \left. \alpha_{ilm} \alpha_{kjm} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \right] \\
+ \alpha_{ijn} \alpha_{klm} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \\
- \alpha_{km} \alpha_{ijn} \left( \frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right) - e^{\frac{1}{\pi} \left( \left\| \frac{a_1 - x_i}{b_1 - x_j} \right\| + \frac{a_2 - x_k}{b_2 - x_l} \right)} \right) \right].
\]
We can switch order of integrals to get
\[
\int_{x_i > x_k \atop x_j > x_l} \left( e^{-\frac{1}{2}h \left( \|a_1 - x_i\| + \|b_2 - x_l\| \right)} - e^{-\frac{1}{2}h \left( \|a_1 - x_i\| + \|b_2 - x_j\| \right)} \right) \frac{1}{2} e^{\frac{1}{2}h \left( \|a_1 - x_k\| + \|b_2 - x_l\| \right)} - \frac{1}{2} e^{\frac{1}{2}h \left( \|a_1 - x_k\| + \|b_2 - x_j\| \right)} \right) \int_{m, n \in \mathbb{R}^{d-2}} (\alpha_{ijm} \alpha_{kln} - \alpha_{ilm} \alpha_{kjn}).
\]

Now the inner integral in \((A.4)\),
\[
\int_{m, n \in \mathbb{R}^{d-2}} (\alpha_{ijm} \alpha_{kln} - \alpha_{ilm} \alpha_{kjn}), \tag{A.5}
\]
is non-negative due to Constraint A. To see this let \(x_{11} = x_i, x_{21} = x_j, x_{10} = x_k, \) and \(x_{20} = x_l\). And let \((x_3, \ldots, x_d) = m \lor n\); similarly let \((x_0, \ldots, x_d) = m \land n\). So we have \(x_{10} < x_{11}, x_{20} < x_{21}, \ldots, x_{d0} < x_{d1}\). Now we can write \((A.5)\) as
\[
\int_{x_{30} < x_{31} \atop x_{00} < x_{d1}} \sum_{a \in \{0, 1\}^{d-2}} (\alpha(x_{1(1a)}) \alpha(x_{00}) - \alpha(x_{10a}) \alpha(x_{01}))\]
which can easily be seen as true due to Constraint A. Note that if we considered the above analysis for any other pair of coordinates (above we only considered the first two coordinates), we will use that \(\alpha_{ijk} = \alpha(m_1, \ldots, x_i, \ldots, x_j, \ldots, m_d)\), where \(x_i\) and \(x_j\) could be any two of the \(d\) coordinates. Thus in Constraint A we require that
\[
\sum_{a \in \{0, 1\}^{d-2}} (\alpha(x_{\pi(1a)}) \alpha(x_{\pi(00)}) - \alpha(x_{\pi(10a)}) \alpha(x_{\pi(01)})) \geq 0
\]
for any permutation \(\pi\) of \(\{1, \ldots, d\}\).

Now we have shown the inner summation in \((A.4)\) is non-negative. We can further say that its factor in \((A.4)\) is also non-negative due to Lemma 17. Thus the whole summation is positive, proving Theorem 7.

\[\square\]

\[1\] This is done by splitting the integral into the \(2^{d-2}\) orderings of the coordinates of \(m\) and \(n\) and renaming so that our sum/integral is over only one orthant.
Lemma 17. For any $a_1, b_1, a_2, b_2 \in \mathbb{R}$ such that $a_1 > a_2, b_1 > b_2$, and any $x_i, x_j, x_k, x_l \in \mathbb{R}$ such that $x_i > x_k, x_j > x_l$, we have

$$\frac{1}{e} \frac{1}{n} \left( \frac{a_1 - x_i}{b_1 - x_j} + \frac{a_2 - x_i}{b_2 - x_j} \right) - e \frac{1}{n} \left( \frac{a_1 - x_k}{b_1 - x_l} + \frac{a_2 - x_k}{b_2 - x_l} \right) + e \frac{1}{n} \left( \frac{a_1 - x_k}{b_1 - x_l} + \frac{a_2 - x_i}{b_2 - x_j} \right) - e \frac{1}{n} \left( \frac{a_1 - x_i}{b_1 - x_j} + \frac{a_2 - x_i}{b_2 - x_j} \right) \geq 0$$

where $\| \cdot \|$ is used denote the $L_2$ norm.

Proof. We can write the expression as

$$e^{-\frac{1}{n} \left( a_i^2 + a_j^2 + b_i^2 + b_j^2 + x_i^2 + x_j^2 + x_k^2 + x_l^2 \right)} \left( e^{\frac{1}{n} \left( a_i x_i + b_j x_j + a_j x_j + b_i x_i \right)} - e^{\frac{1}{n} \left( a_i x_k + b_j x_l + a_j x_l + b_i x_k \right)} + e^{\frac{1}{n} \left( a_i x_i + b_j x_j + a_j x_j + b_i x_i \right)} - e^{\frac{1}{n} \left( a_i x_k + b_j x_l + a_j x_l + b_i x_k \right)} \right)$$

The common factor $e^{-\frac{1}{n} \left( a_i^2 + a_j^2 + b_i^2 + b_j^2 + x_i^2 + x_j^2 + x_k^2 + x_l^2 \right)} > 0$ so we only need to show that the sum of the inner terms are non-negative to show that the whole expression is negative. So looking at the inner expression, we have

$$\left( e^{\frac{1}{n} \left( a_i x_i + b_j x_j + a_j x_j + b_i x_i \right)} - e^{\frac{1}{n} \left( a_i x_k + b_j x_l + a_j x_l + b_i x_k \right)} + e^{\frac{1}{n} \left( a_i x_i + b_j x_j + a_j x_j + b_i x_i \right)} - e^{\frac{1}{n} \left( a_i x_k + b_j x_l + a_j x_l + b_i x_k \right)} \right)$$

The inequality at the end follows from the fact that both factors in the expression are non-negative. This is because in both factors, the exponent of the positive term is larger than the exponent of the negative term. Precisely

$$a_1 x_i + a_2 x_j - a_1 x_k - a_2 x_i = (a_1 - a_2) (x_i - x_k) \geq 0,$$

and

$$b_1 x_j + b_2 x_j - b_2 x_j - b_1 x_i = (b_1 - b_2) (x_j - x_i) \geq 0,$$

where the inequalities here are due to our predicate that $a_1 > a_2, b_1 > b_2$ and $x_i > x_k, x_j > x_l$.

Appendix B. Discussion of Counterexample 6

The Totally Positive Kernel Density estimator (TPKDE) can be interpreted as the convolution of the uniform distribution over a min-max closed set with a scaled standard multivariate Gaussian kernel, that is, with covariance matrix.
\( hI \), where \( h \) is scalar. We show this in [3]. We also show in Theorem 5 (using Theorem 7 and Proposition 9) that this convolution yields an MTP \( 2 \) density. A natural question to ask is whether we can relax the condition on the Gaussian kernel to also include Gaussian kernels with general covariance matrices, that is, Gaussian kernels with covariance matrices that are not the product of a scalar and the identity matrix. Counterexample 9 shows that, in fact, such a relaxation is not possible. Since we use an M-matrix in Counterexample 9 it also shows that we cannot even relax the condition to MTP \( 2 \) Gaussians, that is, Gaussians whose inverse covariance matrix is an M-matrix, which is already a less general class of Gaussians.

In order to derive this counterexample, we can look at Appendix A for the proof of Theorem 7 for the two-dimensional Gaussian cases (since Counterexample 6 is for the two-dimensional case). The proof would proceed exactly the same as in Appendix A with the \( L_2 \) norm being replaced by \( \| \cdot \|_\Sigma \) where for any vector \( x \), we have \( \| x \|_\Sigma = x^T \Sigma^{-1} x \). For the purpose of deriving a counterexample, we ignore equality cases when decomposing the integral into regions (i.e. we ignore Cases 5, 6, and 7 - they do not vanish as in Appendix A). We end up with a version of (A.4) which says

\[
\int_{x_i > x_j, x_i > x_l} e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_i}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_k}{b_2 - x_l} \right\| \Sigma \right)} - e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_i}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_k}{b_2 - x_l} \right\| \Sigma \right)}

+ e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_k}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_l}{b_2 - x_l} \right\| \Sigma \right)} - e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_k}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_l}{b_2 - x_l} \right\| \Sigma \right)} (\alpha_{ij} \alpha_{kl} - \alpha_{ij} \alpha_{kj}).
\]

Now in (B.1), the factor \((\alpha_{ij} \alpha_{kl} - \alpha_{ij} \alpha_{kj})\) is non-negative due to Constraint A (which is the same as the MTP \( 2 \) condition in 2-dimensions as shown in Remark 5). For the whole expression to be non-negative, it would be sufficient for

\[
\int e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_i}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_k}{b_2 - x_l} \right\| \Sigma \right)} - e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_i}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_k}{b_2 - x_l} \right\| \Sigma \right)}

+ e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_k}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_l}{b_2 - x_l} \right\| \Sigma \right)} - e^{-\frac{1}{2} \left( \left\| \frac{a_1 - x_k}{b_1 - x_l} \right\| \Sigma + \left\| \frac{a_2 - x_l}{b_2 - x_l} \right\| \Sigma \right)} (\alpha_{ij} \alpha_{kl} - \alpha_{ij} \alpha_{kj}).
\]

to be non-negative for the whole region of the integral. In Appendix A this ends up being the case due to [17] However, here this is not necessarily true. For covariance matrix \( \Sigma \) such that

\[
\Sigma^{-1} = \begin{bmatrix} a & c \\ c & d \end{bmatrix}
\]

with \( a > 0, d > 0, c < 0 \in \mathbb{R} \) chosen such that \( \Sigma^{-1} \) is a positive-definite M-matrix, we can compare the coefficients of the exponents and get the sufficient condition
that
\[(a(x_i - x_k) + c(x_j - x_l))(d(x_j - x_l) + c(x_i - x_k)) \geq 0.\]

This is not satisfied when \((x_i - x_k) > (x_j - x_l)\) and \(a > |c| > d\). We can now try out different values of \(\Sigma\) and the sample set that violate the sufficient condition. Indeed the set \(\text{MM}(X) = \{(2, 0), (0, 1), (2, 1), (0, 0)\}\) has \((x_i - x_k) > (x_j - x_l)\) for the points \((2, 1)\) and \((0, 0)\) (i.e. \(x_i = 2, x_j = 1, x_k = 0, x_j = 0\)). And
\[
\Sigma^{-1} = \begin{pmatrix} 5 & -2 \\ -2 & 1 \end{pmatrix}
\]

has \(5 = a > 2 = |c| > d = 1\). This is exactly the inverse covariance matrix and set used in Counterexample 6.