Scoring Functions for Multivariate Distributions and Level Sets

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Abstract

Interest in predicting multivariate probability distributions is growing due to the increasing availability of rich datasets and computational developments. Scoring functions enable the comparison of forecast accuracy, and can potentially be used for estimation. A scoring function for multivariate distributions that has gained some popularity is the energy score. This is a generalization of the continuous ranked probability score (CRPS), which is widely used for univariate distributions. A little-known, alternative generalization is the multivariate CRPS (MCRPS). We propose a theoretical framework for scoring functions for multivariate distributions, which encompasses the energy score and MCRPS, as well as the quadratic score, which has also received little attention. We demonstrate how this framework can be used to generate new scores. For univariate distributions, it is well-established that the CRPS can be expressed as the integral over a quantile score. We show that, in a similar way, scoring functions for multivariate distributions can be “disintegrated” to obtain scoring functions for level sets. Using this, we present scoring functions for different types of level set, including those for densities and cumulative distributions. To compute the scoring functions, we propose a simple numerical algorithm. We illustrate our proposals using simulated and stock returns data.

Keywords: Probabilistic Forecasts; Scoring Functions; Multivariate Probability Distributions; Quantiles; Level Sets.
1 Introduction

Forecasts of uncertain future outcomes should be probabilistic (Gneiting and Katzfuss 2014). In many applications, it is a forecast for a multivariate probability distribution that is needed, for example, to manage the impact of extreme weather (Berrocal et al. 2010), financial risk (Diks et al. 2014), or uncertain energy generation (Jeon and Taylor 2012).

Distributional forecast accuracy should be evaluated by maximizing sharpness subject to calibration (Gneiting and Katzfuss 2014). Sharpness relates to the concentration of the probabilistic forecast, while calibration concerns its statistical consistency with the data. A scoring function (or score) summarizes both calibration and sharpness, and can be used to compare forecasts from competing methods, or as the objective function in model estimation.

The continuous ranked probability score (CRPS) is well-established for univariate distributions. For multivariate distributions, the energy score has been proposed as a generalization of the CRPS (Gneiting and Raftery 2007), and used in a number of studies (see, for example, Sloughter et al. 2013; Schefzik 2017). An alternative generalization is the multivariate CRPS (MCRPS), which is briefly introduced by Gneiting and Raftery (2007), and has seemingly received no further attention in the literature, except for Yuen and Stoew (2014), who use the MCRPS for estimation in extreme value theory. Gneiting and Raftery (2007) also introduce the quadratic score, which can be used for multivariate densities, but is notably distinct from the popular log score. We are not aware of any further studies that have considered the quadratic score.

Often the object of interest is some functional of the distribution, such as the level sets of a distribution. A typical example is the quantile of a univariate distribution (see, for example, Komunjer 2005; Gneiting 2011; Ehm et al. 2016). For multivariate distributions, various types of level sets have been considered. These include different forms of multivariate quantiles, such as level sets for cumulative distribution functions (see, for example, Cousin and Di Bernardino 2013) and projection quantiles (see, for example, Kong and Mizera 2012).
Another example of a level set associated with a distribution is the density level set (see, for example, Hallin et al. 2010; Hartigan 1987; Cadre 2006; Singh et al. 2009; Chen et al. 2017). As with the univariate case, estimates of level sets for multivariate distributions can be used to summarize regions of the distribution, enabling, for example, outlier detection (Rinaldo et al. 2012) or clustering (Hartigan 1987). In spite of this, to the best of our knowledge, scoring functions have not been properly studied for these types of multivariate level sets, with the only exception to this being the excess mass for density level sets (see, for example, Hartigan 1987; Müller and Sawitzki 1991; Polonik 1995; Tsybakov 1997).

For a univariate distribution, the CRPS can be expressed as an integral over a quantile score (Laio and Tamea 2007). In this paper, we generalize this to the multivariate context. In doing so, we make a number of contributions regarding scores for multivariate distributions and their level sets. First, we propose a natural theoretical framework that links the quadratic score, MCRPS and energy score. Finding more scoring functions is an interesting question in its own right in the forecasting literature, and our framework can be used to generate new scores for multivariate distributions. We demonstrate this by developing a score that is based on lower partial moments. Second, we show that by “disintegrating” the quadratic score, MCRPS, and our new score, we obtain, in a simple and intuitive manner, new scores for level sets of densities, cumulative distributions, and lower partial moments, respectively. The proposed scores encompass the excess mass, and the full class of quantile scores considered in Komunjer (2005) and Gneiting (2011). Finally, to calculate the various scores, we propose a simulation-based numerical approach, which can be used for high-dimensional distributions, without posing any restriction on the geometry of these level sets.

Section 2 describes notation and conventions used in this paper. Section 3 reviews existing scores for distributions and level sets. Section 4 presents our framework for scores for multivariate distributions. Section 5 shows that the scores of Section 4 can be disintegrated to obtain scores for different types of level set. Section 6 describes how we calculate the scores, and presents empirical analysis. Section 7 summarizes the paper.
2 Preliminaries

In this section, we explain some notation and conventions used in the subsequent parts of the paper. Let \( \mathbb{R}^d \) be the \( d \)-dimensional Euclidean space. We identify a vector in \( \mathbb{R}^d \) with a \( d \times 1 \) (column) matrix; thus, the Euclidean inner product of \( z, s \in \mathbb{R}^d \) is written as \( z^T s \), with superscript \(^T\) denoting matrix transpose. The boldface lower-case letters \( z, s, t, \ldots \) designate points in \( \mathbb{R}^d \); and \( \| \bullet \| \) is the Euclidean modulus. For \( z \in \mathbb{R} \) or \( \mathbb{C} \) we write \( \| z \| \equiv |z| \). Given any set \( A \subset \mathbb{R}^d \), \( \partial A \) denotes its topological boundary.

For integers \( d, n \geq 1 \) and \( p \in [1, \infty) \), we define the Lebesgue spaces

\[ L^p(\mathbb{R}^d, \mathbb{R}^n) := \{ g : \mathbb{R}^d \to \mathbb{R}^n \text{ Lebesgue measurable}: \| g \|_{L^p(\mathbb{R}^d)} < \infty \}, \]

where \( \| g \|_{L^p(\mathbb{R}^d)} := \left( \int_{\mathbb{R}^d} \| g(z) \|^p \, dz \right)^{\frac{1}{p}} \). A function with finite \( L^1 \) norm is said to be integrable, and a Radon measure \( \mu \) on \( \mathbb{R}^d \) with \( \int_{\mathbb{R}^d} d\mu < \infty \) is said to be of finite mass. The Lebesgue measure on \( \mathbb{R}^d \) is denoted by \( \mathcal{L}^d \). A measure \( \lambda \) is said to be absolutely continuous with respect to \( \mathcal{L}^d \) if for each Borel set \( A \subset \mathbb{R}^d \) with \( \mathcal{L}^d(A) = 0 \), we have \( \lambda(A) = 0 \). For every such \( \lambda \), we can define its Radon–Nikodym derivative via

\[ \int_{\mathbb{R}^d} g(z) \, d\lambda(z) = \int_{\mathbb{R}^d} g(z) \frac{d\lambda}{d\mathcal{L}^d}(z) \, dz, \]

where \( g \) is an arbitrary \( \lambda \)-integrable function.

Let \((\Omega, \mathcal{B}, P)\) be a probability space. A random variable on \((\Omega, \mathcal{B}, P)\) is a function \( X : \Omega \to \mathbb{R}^d \) measurable with respect to \( \mathcal{B} \) and the Borel \( \sigma \)-algebra on \( \mathbb{R}^d \). We use capital letters \( X, Y, Z, \ldots \) for univariate random variables, and boldface capital letters \( \mathbf{X}, \mathbf{Y}, \mathbf{Z}, \ldots \) for multivariate random variables. Denote by \( \mathcal{V}^d \) the space of integrable random variables:

\[ \mathcal{V}^d := \left\{ X : \Omega \to \mathbb{R}^d : X \in L^1(\Omega, \mathbb{R}^d) \right\}. \]

A natural equivalence relation \( \sim \) can be defined on \( \mathcal{V}^d \): for \( X, Y \in \mathcal{V}^d \), \( X \sim Y \) if and only if \( X \) and \( Y \) have the same distribution. It induces the quotient space

\[ \mathcal{V}^d/\sim := \left\{ [X] : Y \in \mathcal{V}^d, Y \sim X \right\}, \]

viewed as the space of \( d \)-dimensional distributions. To be consistent with the notation in the
literature (see, for example, Gneiting and Raftery [2007], we use \( P_X, P_Y, P_Z, \ldots \) to denote the equivalence classes \([X], [Y], [Z], \ldots \in \mathcal{V}/\sim\).

For distributions \( P_X, P_Y, P_Z, \ldots \), denote by \( f_X, f_Y, f_Z, \ldots \) their probability density functions (PDFs), and by \( F_X, F_Y, F_Z, \ldots \) their cumulative distribution functions (CDFs), respectively. We also write \( q_Y(\alpha) \) for the \( \alpha \) quantile of random variable \( Y \) for \( \alpha \in [0, 1] \).

The \( k \)th Lower Partial Moment (LPM) of a random variable \( Y \) with respect to a reference point \( z \) is defined as

\[
\text{LPM}_{Y,k}(z) := \int_{-\infty}^{z_1} \cdots \int_{-\infty}^{z_d} \prod_{j=1}^{d} (z_j - s_j)^k f_Y(s_1, s_2, \ldots, s_d) \, ds_1 \, ds_2 \cdots ds_d.
\] (2)

For a function \( g : \mathbb{R}^d \rightarrow \mathbb{C} \), its Fourier transform \( \hat{g} \equiv \mathcal{F}(g) : \mathbb{R}^d \rightarrow \mathbb{C} \) is given by

\[
\hat{g}(t) := \int_{\mathbb{R}^d} e^{2\pi i z^T t} g(z) \, dz,
\] (3)

where \( t \in \mathbb{R}^d \) and \( i \) is the imaginary unit. When \( g \) is a PDF of a distribution, \( \hat{g} \) is called the characteristic function of the distribution.\(^1\) Whenever \( g \in L^1(\mathbb{R}^d, \mathbb{C}) \), \( \hat{g} \) is a continuous function decaying to zero at infinity (cf. the Riemann–Lebesgue lemma). If moreover \( g \in L^2(\mathbb{R}^d, \mathbb{C}) \), then \( \hat{g} \in L^2(\mathbb{R}^d, \mathbb{C}) \); in fact, \( \mathcal{F} \) is an \( L^2 \)-isometry:

\[
\|g\|_{L^2(\mathbb{R}^d)} = \|\hat{g}\|_{L^2(\mathbb{R}^d)}.
\] (4)

This relation (4) is known as Plancherel’s identity. We also comment that the definition of Fourier transform can be extended to certain generalized functions and measures, including the Dirac delta masses. The inverse Fourier transform is denoted by \( \mathcal{F}^{-1} \). As is customary, the function before taking Fourier transform (or, after taking the inverse Fourier transform) \( g(z) \) is said to be “on the physical side”, and the Fourier transform \( \hat{g}(t) \) of \( g(z) \) is said to be “on the Fourier side”. We adhere to the convention of writing \( z \in \mathbb{R}^d \) for the variable on the physical side, and \( t \in \mathbb{R}^d \) for that on the Fourier side.

\(^1\)There are other widely adopted definitions of the Fourier transform, which are off by a sign or a factor of \( 2\pi i \) compared to expression (3). The results of this paper remain unchanged when we use any such variant.
3 Review of Scoring Functions for Distributions and Level Sets

In the rest of the paper, let $P_Y$ be the distribution that we want to study. In practice, typically, $P_Y$ is unknown and we can only observe a finite collection of realizations of $Y$, labeled as $\{y^t\}_{t=1,2,...,T}$. Let $P_X$ be an estimate of $P_Y$. Naturally, a key problem is to evaluate the quality of the probabilistic estimate $P_X$, given the realizations $\{y^t\}_{t=1,2,...,T}$ of $Y$. A central tool developed for this purpose is the scoring function

$$S(P_X, y) : (\mathcal{Y}^d / \sim) \times \mathbb{R}^d \to [-\infty, \infty].$$

It is said to be consistent if $\mathbb{E}_{P_Y} [S(P_X, \cdot)]$, the expectation of $S(P_X, \cdot)$ with respect to $P_Y$, is minimized when $P_X = P_Y$, and strictly consistent if furthermore $P_X$ is the unique minimizer.

The object of interest is often a certain functional of the distribution $\Psi_Y$, such as a quantile of a univariate distribution, rather than the entire distribution. Analogously, $S(\Psi_X, y)$ is said to be consistent if $\mathbb{E}_{P_Y} [S(\Psi_X, \cdot)]$ is minimized by $\Psi_Y$, and strictly consistent if, additionally, no other $\Psi_X$ minimizes $\mathbb{E}_{P_Y} [S(\Psi_X, \cdot)]$.

Sections 3.1 and 3.2 review scoring functions that have been presented in the literature for distributions and their associated levels sets, respectively. In Section 3.3, we focus on the energy score, and show how it can be used to derive the scoring function for projection quantiles. We treat projection quantiles separately from our consideration of level sets because, as we discuss in Section 3.3, a projection quantile is not a form of level set.

### 3.1 Review of Scoring Functions for Distributions

The best known scoring function for a distribution is the log score, $\log(f_X(y))$. It is proposed by Good (1952) and has been widely studied in various applications, such as model estimation, evaluation, and selection. Another PDF-based score is the quadratic score (Gneiting and Raftery 2007), which has the following expression:

$$\text{DQS} (P_X, y) := \left( \int_{\mathbb{R}^d} f_X^2(z) \, dz \right) - 2f_X(y).$$  (5)
Both the log and quadratic scores can be used for multivariate distributions. In comparison with the log score, the quadratic score has the advantage of allowing zero values for PDFs.

A natural limitation of both the log and quadratic scores is that neither is applicable to discrete distributions. As a consequence, for applications involving discrete distributions, such as weather ensemble predictions (see, for example, Gneiting et al. 2005; Schefzik 2017), scoring functions based on CDFs have been considered instead. For univariate distributions, a well-established CDF-based scoring function is the CRPS, which has the following expression:

$$\text{CRPS}(P_X, y) := \int_{-\infty}^{+\infty} \left( F_X(z) - 1 \{ z \geq y \} \right)^2 dz$$

$$= 2 \int_{0}^{1} \left( \alpha - 1 \{ y < q_X(\alpha) \} \right) \left( y - q_X(\alpha) \right) d\alpha$$

$$= \mathbb{E}_{P_X} |X - y| - \frac{1}{2} \mathbb{E}_{P_X} |X - X'|,$$

where $X'$ denotes an independent copy of the random variable $X$. In expression (6), $(F_X(z) - 1 \{ z \geq y \})^2$ is the Brier Score for the binary event $\{ z \geq Y \}$. The integrand in expression (7) is the widely used score for quantile of a univariate distribution, defined as

$$\text{QS}(q_X(\alpha), y; \alpha) := \left( \alpha - 1 \{ y < q_X(\alpha) \} \right) \left( y - q_X(\alpha) \right),$$

where $q_X(\alpha)$ is the $\alpha$ quantile of the random variable $X$. It is sometimes referred to as the check-loss function, but we refer to it as the quantile score. The CRPS has been widely applied in finance and meteorology (see, for example, Gneiting and Ranjan 2011).

There is no unique, canonical way to generalize the CRPS to multivariate distributions. One generalization that has been proposed is the energy score (Gneiting and Raftery 2007; Ziel and Berk 2019):

$$\text{ES}(P_X, y) := \mathbb{E}_{P_X} \| X - y \| - \frac{1}{2} \mathbb{E}_{P_X} \| X - X' \|,$$

where $X'$ is an independent copy of the random variable $X$. It can be viewed as the direct generalization of the CRPS via expression (8) Baringhaus and Franz (2004) and Székely and
Rizzo (2013) show that the energy score can also be expressed as follows:

\[
\begin{align*}
\text{ES}(P_X, y) &= \int_{\mathbb{R}^d} \frac{|\hat{f}_X(t) - \hat{\delta}_y(t)|^2}{\|t\|^{d+1}} \, dt \\
&= \gamma_d \int_{S^{d-1}} \int_{-\infty}^{\infty} |F_{a^T X}(t) - \mathbb{1}\{t > a^T y\}|^2 \, dt \, d\text{can}(a),
\end{align*}
\]

where \(\delta_y\) is the Dirac delta mass supported at \(y\), \(a\) is a unit vector on \(S^{d-1}\), \(\gamma_d\) is the volume of the \(d\)-dimensional unit ball, and \(\text{can}\) is the canonical volume measure of the unit round sphere. In fact, we can view the last line \(\int_{-\infty}^{\infty} |F_{a^T X}(t) - \mathbb{1}\{t > a^T y\}|^2 \, dt\) as the CRPS for the univariate random variable \(a^T X\) and the realization \(a^T y\). Therefore, the energy score can be viewed “projectively” as the integral over the unit sphere of the CRPS computed for \(X\) and \(y\) projected onto each 1-dimensional subspace.

Gneiting and Raftery (2007) propose an alternative generalization of the CRPS, presented in expression (13). We term this the \textit{multivariate CRPS} (MCRPS).

\[
\begin{align*}
\text{MCRPS}(P_X, y) := \int_{\mathbb{R}^d} \left(F_X(z) - \mathbb{1}\{z \geq y\}\right)^2 \, d\lambda(z),
\end{align*}
\]

where the multi-dimensional indicator function is defined by

\[
\mathbb{1}\{z \geq y\} := \prod_{i=1}^{d} \mathbb{1}\{z_i \geq y_i\} = \begin{cases} 
1 & \text{if} \quad z_i \geq y_i, \forall i = 1, 2, \ldots, d, \\
0 & \text{otherwise},
\end{cases}
\]

and \(\lambda\) is a generic positive Borel measure on \(\mathbb{R}^d\) that ensures the convergence of relevant integrals. The definition of the MCRPS in (13) directly extends expression (6) to higher dimensions. While the energy score has become reasonably popular (see, for example, Sloughter et al. 2013; Schefzik 2017), the MCRPS has seemingly only been considered by Yuen and Stoev (2014) for estimation in the context of extreme value theory.

The scoring functions that we have discussed so far are all defined on the physical side. We now present a scoring function based on the characteristic functions (Example 12 in
Gneiting and Raftery (2007):

\[ \text{CFS}(P_X, y) = \int_{\mathbb{R}^d} \left| \hat{f}_X(t) - \hat{\delta}_y(t) \right|^2 d\lambda(t). \]  

(14)

As CFS is based on the characteristic functions \( \hat{f}_X \) and \( \hat{\delta}_y \), we call it the characteristic function score. This score serves as the prototypical example of a more general framework, which enables us to construct scoring functions for level sets of distributions.

### 3.2 Review of Scoring Functions for Level Sets

Before we consider scoring functions, let us first formally define a level set. For any function \( g(z) \) and any \( \alpha \in \mathbb{R} \), define the \( \alpha \) level set by

\[ L(g; \alpha) := \{ z \in \mathbb{R}^d : g(z) \geq \alpha \} \equiv \{ g \geq \alpha \}. \]  

(15)

In the literature sometimes \( L(g; \alpha) \) is referred to as the upper level set, and \( \partial \{ L(g; \alpha) \} \) as the level set (see, for example, Chen et al. 2017). Our notation is consistent with Cadre (2006); Singh et al. (2009); Di Bernardino et al. (2013). Three examples of level sets in the context of probability distributions are given below:

**Density Level Sets.** Consider \( g = f_Y \), the PDF of the distribution \( P_Y \). The \( \alpha \) density level set is defined as

\[ D(P_Y; \alpha) = \{ z \in \mathbb{R}^d : f_Y(z) \geq \alpha \} \equiv \{ f_Y \geq \alpha \}. \]  

(16)

Density level sets have been applied in areas such as anomaly detection, binary classification and clustering (see, for example, Cadre 2006; Rinaldo et al. 2012; Chen et al. 2017).

**CDF Level Sets.** Now we take \( g = F_Y \), the CDF of the distribution \( P_Y \). The \( \alpha \) CDF level set is defined as

\[ C(P_Y; \alpha) = \{ z \in \mathbb{R}^d : F_Y(z) \geq \alpha \} \equiv \{ F_Y \geq \alpha \}. \]  

(17)

CDF level sets have been used in financial risk analysis (Cousin and Di Bernardino 2013; Di Bernardino et al. 2013), judgemental forecasting (Abbas et al. 2010), and hydrology (Salvadori et al. 2016). In the bivariate case, CDF level sets are sometimes termed
“isoprobability contours” (Abbas et al. 2010). Note that if $P_Y$ is a univariate distribution, then the boundary of the $\alpha$ CDF level set is simply the $\alpha$ quantile.

**LPM Level Sets.** If $g = \text{LPM}_{Y,k}$, i.e. the $k$-th lower partial moment function of the distribution $P_Y$, then the $\alpha$ LPM level set can be defined by

$$M(P_Y; \alpha, k) = \{ z \in \mathbb{R}^d : \text{LPM}_{Y,k}(z) \geq \alpha \} \equiv \{ \text{LPM}_{Y,k} \geq \alpha \}.$$  

(18)

The LPM for univariate distributions has been widely considered for systemic risk (Price et al. 1982), asset pricing (Anthonisz 2012), and portfolio management (Briec and Kerstens 2010; Brogan and Stidham Jr 2008). However, to the knowledge of the authors, the level sets of lower partial moments have not been studied in the literature.

In Figure 1, we illustrate density level sets, CDF level sets, and LPM level sets, for the bivariate Gaussian distribution with zero means, unit variances, and covariance $0.5$.

Figure 1: Plots for (a) density level sets, (b) CDF level sets, and (c) LPM level sets ($k = 1$) for the bivariate Gaussian distribution with zero means, unit variances, and covariance 0.5. The numerical values in each plot indicate the value of $\alpha$ for each level set.
functions for quantiles is presented in expression (19), where $H$ is a non-decreasing function:

$$QS(q_X(\alpha), y) = \left( \alpha - 1 \left\{ y < q_X(\alpha) \right\} \right) \left( H(y) - H(q_X(\alpha)) \right).$$  \hspace{1cm} (19)$$

For density level sets, the *excess mass scoring function* has been widely utilized as a loss function for estimation (see, for example, [Hartigan 1987; Müller and Sawitzki 1991; Cheng and Hall 1998; Polonik 1995]:

$$EMS(D(P_X; \alpha), y) = \alpha L^d \left\{ f_X \geq \alpha \right\} - 1 \left\{ f_X(y) \geq \alpha \right\},$$  \hspace{1cm} (20)$$

where $L^d \{ \cdot \}$ denotes the $d$-dimensional Lebesgue measure of a set, and $D(P_X; \alpha)$ is the $\alpha$ density level set defined in expression (16). When this score is used for estimation, the density level set is typically specified as a piecewise polynomial function. Despite the fact that the score has been studied in the density level set literature, it has not been fully recognized as a scoring function. In this paper, we show that the excess mass in expression (20) is not the only consistent scoring function for density level sets; in fact, we construct a family of scoring functions encompassing the excess mass.

### 3.3 Energy Score and Projection Quantiles

It is well-known that the CRPS in expression (6) can be disintegrated as the integral of the scoring functions for quantiles in expression (7). Using this result, we can disintegrate the energy score as follows.

Recall that expression (12) shows the energy score can be viewed “projectively” as the integral over the unit sphere of the CRPS computed for $X$ and $y$ projected onto each 1-dimensional subspace. If we replace the CRPS in expression (12) by the integral of the quantile score along that direction using expression (7), and apply Fubini’s theorem, we obtain

$$ES(P_X, y) = \gamma_d \int_{S^{d-1}} \left( \alpha - 1 \left\{ a^T y < q_{a^T X}(\alpha) \right\} \right) \left( a^T y - q_{a^T X}(\alpha) \right) d\gamma(a) d\alpha.$$  \hspace{1cm} (21)$$
The inner integrand
\[
PQS(P_Y; \alpha) = \int_{S^{d-1}} \left( \alpha - 1 \left\{ a^T y < q_{a^T X}^{\alpha} \right\} \right) \left( a^T y - q_{a^T X}^{\alpha} \right) d\mathbf{can}(a)
\]
can be viewed as a scoring function for the \( \alpha \)-projection quantile, which is defined as the totality of the \( \alpha \)-univariate quantiles associated with the projection of \( Y \in V^d \) onto each direction, \( i.e., \) along each vector \( a \in S^{d-1} \):
\[
PQ(P_Y; \alpha) := \left\{ r_a(\alpha) : r_a(\alpha) = q_{a^T Y}^{\alpha} \in \mathbb{R}, \ a \in S^{d-1} \right\},
\]
(22)
where \( \alpha \in [0, 1] \). The projection quantile has been briefly studied in the context of halfspace depth (see, for example, [Hallin et al. 2010; Kong and Mizera 2012]), but has seemingly not been considered by others.

In passing, we remark that the projection quantile is not a form of level set as defined in Section 3.2. To see this, notice that \( PQ(P_Y; \alpha) = PQ(P_Y; 1 - \alpha) \). But in expression (15), \( L(g; \alpha) \neq L(g; 1 - \alpha) \) as this would imply that \( g \) has two different values at any point on \( \partial L(g; \alpha) \), which immediately shows that \( g \) is not a well-defined function.

The above disintegration of the energy score is essentially straightforward, as it only relies on the decomposition of the CRPS for univariate distributions. In this paper, we will show that the quadratic score and the MCRPS can also be disintegrated into the scoring functions for their level sets, however, the procedure will be more complex.

4 A New Framework for Scoring Functions of Distributions

In the previous section, for distributions, we discussed the quadratic score, the CRPS, as well as two multivariate generalizations of the CRPS: the energy score and the MCRPS. Although it is established that these are all consistent scoring functions, little is known about the linkages between them. In this section, we propose a new theoretical framework for scoring functions that unify the existing quadratic score, CRPS, energy score and MCRPS. This framework will serve as the foundation to develop the scoring functions for level sets in

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Section 5

In Section 4.1, we propose a class of $L^2$ scoring functions for distributions by generalizing the characteristic function score of expression (14). In Section 4.2, we derive some useful alternative expressions for the $L^2$ scoring function for distributions. In Section 4.3, we show that the new class of scoring functions encompasses the quadratic score, CRPS, and MCRPS. We also show that this framework can easily be used to generate other scoring functions, and we demonstrate this by proposing a scoring function based on lower partial moments.

4.1 $L^2$ Scoring Function for Distributions

Consider

$$S(P_X, y; \hat{w}, \hat{h}) = \int_{\mathbb{R}^d} \left| (\hat{f}_X \hat{w} - \delta_y \hat{w}) \ast \hat{h} \right|^2(t) \, dt \quad \text{for each } P_X \in V^d/\sim \text{ and } y \in \mathbb{R}^d,$$

where $\ast$ is the convolution and $\hat{w}, \hat{h} : \mathbb{R}^d \to \mathbb{C}$ are measurable functions to be specified. We will show that $S(P_X, y; \hat{w}, \hat{h})$ is a consistent scoring function for distributions in Theorem 1. As $S(P_X, y; \hat{w}, \hat{h})$ is the squared $L^2$ distance between $\hat{f}_X \hat{w} \ast \hat{h}$ and $\delta_y \hat{w} \ast \hat{h}$, we call $S(P_X, y; \hat{w}, \hat{h})$ the $L^2$ scoring function for distributions. For simplicity, in the rest of the paper, we drop “for distribution” and simply refer to $S(P_X, y; \hat{w}, \hat{h})$ as the $L^2$ scoring function. Next, we specify our assumptions for $\hat{w}$ and $\hat{h}$ as follows:

**Assumption 1.** (1) $\hat{f}_X \hat{w}, \delta_y \hat{w},$ and $\hat{h}$ are locally finite Borel measures on $\mathbb{R}^d$ with inverse Fourier transforms $\mathcal{F}^{-1}(\hat{f}_X \hat{w}), \mathcal{F}^{-1}(\delta_y \hat{w})$ and $h$, respectively;

(2) $(\hat{f}_X \hat{w} - \delta_y \hat{w}) \ast \hat{h} \in L^2(\mathbb{R}^d; \mathbb{C})$;

(3) $|\hat{w}|$ and $|h|$ are non-zero $\mathcal{L}^d$-a.e.

In the above, a signed Borel measure on $\mathbb{R}^d$ is said to be locally finite if every point $z \in \mathbb{R}^d$ has a neighborhood of finite measure. Here, by a slight abuse of notations, we identify a locally integrable function $g$ on $\mathbb{R}^d$ with the measure $gd\mathcal{L}^d$. Notice that if we let $\hat{h}(t) \equiv \delta_y(t)$ and let $\hat{w}$ be such that $|\hat{w}(t)|^2 = d\lambda/d\mathcal{L}^d$, then the proposed $L^2$ scoring function $S(P_X, y; \hat{w}, \hat{h})$ reduces to the characteristic function score in expression (14).
Theorem 1. \( S(P_X, y; \hat{w}, \hat{h}) \) in expression (23) is a strictly consistent scoring function.

Recall that Plancherel’s identity yields an \( L^2 \) isometry between the Fourier and physical sides. Also, the inverse Fourier transform intertwines convolution and multiplication, namely that \( \mathcal{F}^{-1}(a \ast b) = (\mathcal{F}^{-1}a) \cdot (\mathcal{F}^{-1}b) \); thus,

\[
S(P_X, y; \hat{w}, \hat{h}) = \int_{\mathbb{R}^d} \left( \mathcal{F}^{-1}(\hat{f}_X \hat{w})(z) - \mathcal{F}^{-1}(\hat{\delta}_y \hat{w})(z) \right)^2 h(z)^2 \, dz. \tag{24}
\]

The proof of Theorem 1 is given in the appendix. It immediately implies the following Corollary.

Corollary 1. \( S(P_X, y; \hat{w}, \hat{h}) \) in expression (24) is a strictly consistent scoring function.

We refer to expressions (23) and (24) as the “physical” and the “Fourier” versions of the \( L^2 \) scoring function \( S(P_X, y; \hat{w}, \hat{h}) \), respectively. In practice, one may choose whichever version is computationally more convenient.

Several remarks are in order regarding the roles of the terms in expression (24). Roughly speaking, \( \hat{w} \) is key to the structure of relevant scoring functions, and \( h \) can be considered as a weight function, which assigns different weights to different regions. In the literature, for a particular \( \hat{w} \), scoring functions with different \( h \) are usually considered to belong to the same family (see, for example, Gneiting and Ranjan 2011). The term \( \mathcal{F}^{-1}(\hat{\delta}_y \hat{w})(z) \) can be viewed as the proxy of \( \mathcal{F}^{-1}(\hat{f}_Y \hat{w})(z) \) for a single observation \( y \). In addition, the weight function \( h \) has other roles that seemingly have not been considered: it can be used to warrant the convergence of the integral defining \( S(P_X, y; \hat{w}, \hat{h}) \); and it can be used to facilitate the numerical computation of \( S(P_X, y; \hat{w}, \hat{h}) \). The latter will be discussed in Section 6.

### 4.2 Alternative Expressions for the \( L^2 \) Scoring Function

In this section, we present useful alternatives to expressions (23) and (24) for the \( L^2 \) scoring function. For scoring functions, we are more concerned with the relative performance, \( i.e., \) the difference \( S(P_X, y; \hat{w}, \hat{h}) - S(P_Y, y; \hat{w}, \hat{h}) \) between the scoring
functions of two probabilistic estimates $P_X$ and $P_V$, rather than the actual values of the scoring function [Nolde and Ziegel 2017]. Therefore, any $S'(\bullet, \bullet; \hat{w}, \hat{h})$ satisfying

$$S(P_X, y; \hat{w}, \hat{h}) - S(P_V, y; \hat{w}, \hat{h}) = S'(P_X, y; \hat{w}, \hat{h}) - S'(P_V, y; \hat{w}, \hat{h}),$$

for every pair $(P_X, P_V)$ and every $y$, shall be viewed as equivalent to $S(\bullet, \bullet; \hat{w}, \hat{h})$.

Expanding the integrand in expression (24) and ignoring the term $\int_{\mathbb{R}^d} (F^{-1}(\delta_y \hat{w})(z))^2 \, dz$, we arrive at the following expression:

$$S'(P_X, y; \hat{w}, \hat{h}) = \int_{\mathbb{R}^d} \left( F^{-1}(\hat{f}_X \hat{w})(z) \right)^2 h(z)^2 \, dz$$

$$- 2 \int_{\mathbb{R}^d} F^{-1}(\hat{f}_X \hat{w})(z) F^{-1}(\delta_y \hat{w})(z) h(z)^2 \, dz.$$  \hspace{1cm} (26)

The term we omitted, $\int_{\mathbb{R}^d} (F^{-1}(\delta_y \hat{w})(z))^2 \, dz$, is purely dependent on $y$. Thus, this term has the same value regardless of $P_X$, which immediately shows that $S'$ in expression (26) satisfies the equality in expression (25). Therefore, we have obtained an equivalent scoring function $S'(\bullet, \bullet; \hat{w}, \hat{h})$ to that in expression (24). We can apply the same argument to the physical form version of the $L^2$ scoring function $S(P_X, y; \hat{w}, \hat{h})$ in expression (23) to obtain the following equivalent expression ($\Re(z)$ denotes the real part of $z \in \mathbb{C}$):

$$S''(P_X, y; \hat{w}, \hat{h}) = \int_{\mathbb{R}^d} \left| \hat{f}_X \hat{w} * \hat{h} \right|^2 \, dt - 2 \int_{\mathbb{R}^d} \Re\left\{ (\hat{f}_X \hat{w} * \hat{h})(\delta_y \hat{w} * \hat{h}) \right\} \, |dt|.$$  \hspace{1cm} (27)

In the sequel, we mainly focus on the physical version of the $L^2$ scoring function in expression (26). We develop our scoring functions for level sets in Section 5 based on expression (26). Next, several key examples will be studied, for which the term $F^{-1}(\hat{f}_X \hat{w})(z)$ has natural statistical interpretations.

### 4.3 Examples of $L^2$ Scoring Functions

When $\hat{w}(t) = (\|t\|^{d+1})^{-1}/2$ and $\hat{h}(t) = \delta_0(t)$, the $L^2$ scoring function of expression (23) leads to the energy score in expression (11). In the remainder of this section, we present three additional concrete examples, all of which are based on the version of the $L^2$ scoring
function of expression (26). We first show that the quadratic score and the MCRPS emerge as special instances of the general framework laid down in Sections 4.1 and 4.2. We then demonstrate how our framework naturally generates other scoring functions, which are of both statistical importance and mathematical interest.

4.3.1 Quadratic Score

For \( \hat{w} \equiv 1 \) and \( \hat{h}(t) = \delta_0(t) \), using the identity \( \hat{f}_X \ast \hat{h} \equiv \hat{f}_X \) and expression (26), we get

\[
S'(P_X, y; \hat{w}, \hat{h}) = \left( \int_{\mathbb{R}^d} f^2_X(z) dz \right) - 2f_X(y),
\]

which is precisely the quadratic score of expression (5). This shows that the quadratic score is equivalent to the characteristic function score in expression (14), when \( \lambda \) is the Lebesgue measure on \( \mathbb{R}^d \). This connection, to the best of our knowledge, has not been identified previously in the literature. We remark that for this example, \( S(P_X, y; \hat{w}, \hat{h}) \) in expression (24) is not well-defined, because the square of the Dirac delta mass function \( \delta_0(t) \) is not well-defined.

More generally, we can consider a weight function \( \hat{h} \) satisfying Assumption 1, which induces the following expression:

\[
DQS'(P_X, y; h) = \left( \int_{\mathbb{R}^d} f^2_X(z) h^2(z) dz \right) - 2f_X(y)h^2(y). \tag{28}
\]

This expression generalizes the quadratic score of expression (5). Expression (28) is particularly useful because it enables us in Section 5 to develop the scoring functions of the density level sets. In view of this, from now on, we refer to expression (28) as the quadratic score.

4.3.2 MCRPS

For \( \hat{w}(t) = \frac{1}{(2\pi)^d} \frac{1}{t_1 t_2 \ldots t_d} \) with \( t = (t_1, \ldots, t_d)^T \), \( w := \mathcal{F}^{-1}(\hat{w}) \) can be computed via

\[
w(z) = \prod_{j=1}^d \frac{1}{2\pi} \int_{\mathbb{R}} e^{-2\pi it_j z_j} dt_j = \prod_{j=1}^d 1\{z_j \geq 0\} = 1\{z \geq 0\},
\]

16
where we use the fact that the Fourier transform of the Heaviside function, 
\( H(z_j) := 1 \{ z_j \geq 0 \} \) for \( x \in \mathbb{R} \), is \( \hat{H}(t_j) = (-2\pi i t_j)^{-1} \). Notice that the convolution of a PDF \( f_x \) and \( w \) gives the CDF \( F_X \):

\[
(f_x \ast w)(z) = \int_{\{z \geq s\}} f_X(s) \, ds
\]

\[
= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_X(s_1, \ldots, s_d) \prod_{j=1}^{d} 1 \{ z_j \geq s_j \} \, ds_1 \cdots ds_d =: F_X(z_1, \ldots, z_d).
\]

Thus, we can use expression (24) to obtain the following scoring function:

\[
S(P_X, y; \hat{w}, \hat{h}) = \int_{\mathbb{R}^d} \left| F_X(z) - 1 \{ z \geq y \} \right|^2 h^2(z) \, dz. \tag{29}
\]

This is precisely the MCRPS, if we identify \( h^2(z) \) with the Radon–Nikodym derivative \( d\lambda/dL \) in expression (13). When \( d = 1 \), the MCRPS reduces to the threshold weighted CRPS studied in Gneiting and Ranjan (2011). Following the discussion in Section 4.2, we obtain an equivalent expression for the MCRPS by expression (26):

\[
\text{MCRPS}'(P_X, y; h) = \int_{\mathbb{R}^d} F_X^2(z) h^2(z) \, dz - 2 \int_{\mathbb{R}^d} F_X(z) 1 \{ z \geq y \} h^2(z) \, dz. \tag{30}
\]

In Section 5, we will use this expression as the basis for developing the scoring functions of the CDF level sets.

### 4.3.3 A New Scoring Function Based on Lower Partial Moments

We can consider \( \hat{w}(t) = \frac{1}{(2\pi)^\frac{k}{d} (t_1 t_2 \cdots t_d)^k} \), where \( k = 1, 2, 3, \ldots \). In this case, \( w(z) \) is simply the \( k \)-th convolution power of the Heaviside function \( H(x) \),

\[
w(z) = H^k(z) \equiv H * H * \cdots * H(z) = \prod_{j=1}^{d} \frac{1}{k!} z_j^k 1 \{ z_j \geq 0 \}.
\]

It implies that

\[
f_X \ast H^k(z) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_X(s_1, \ldots, s_d) \prod_{j=1}^{d} \frac{1}{k!} (z_j - s_j)^k 1 \{ z_j \geq s_j \} \, ds_1 \cdots ds_d, \tag{31}
\]

\[
\delta_y \ast w(z) = \int_{-\infty}^{z_1} \cdots \int_{-\infty}^{z_d} \delta_y(s_1, \ldots, s_d) \prod_{j=1}^{d} \frac{1}{k!} (z_j - s_j)^k 1 \{ z_j \geq s_j \} \, ds_1 \cdots ds_d
\]
\[ f_X \ast H^{*k} = f_X \ast w \text{ in expression (31) is the lower partial moment of order } k \text{ in expression (2).} \]

Hence, we arrive at a new scoring function for a distribution:

\[
\text{LPMS}(P_X, y; k, h) = \int_{\mathbb{R}^d} \left| \text{LPM}_{X,k}(z) - \prod_{j=1}^{d} \frac{1}{k!} (z_j - y_j)^k \mathbbm{1}\{z_j \geq y_j\} \right|^2 h^2(z) \, dz.
\]

The term \( \prod_{j=1}^{d} \frac{1}{k!} (z_j - y_j)^k \mathbbm{1}\{z_j \geq y_j\} \) can be viewed as the proxy of \( \text{LPM}_{Y,k}(z) \) for a single observation \( y \). When \( k = 0 \), the above expression reduces to the MCRPS. By expression (26) in Section 4.2 we obtain the following equivalent expression for the LPMS:

\[
\text{LPMS}'(P_X, y; k, h) = \int_{\mathbb{R}^d} \text{LPM}^2_{X,k}(z) h^2(z) \, dz
- 2 \int_{\mathbb{R}^d} \text{LPM}_{X,k}(z) \prod_{j=1}^{d} \frac{1}{k!} (z_j - y_j)^k \mathbbm{1}\{z_j \geq y_j\} h^2(z) \, dz. \tag{33}
\]

In Section 5 we will develop the scoring functions of the LPM level sets based on this expression.

5 New Scoring Functions for Level Sets

Recall that in Section 3.1, we discussed the well-known result that the CRPS can be expressed as the integral of the quantile score, and in Section 3.3 we also showed that the energy score can be expressed as the integral of the scoring function for the projection quantiles. These disintegrating procedures are essentially based on the equivalence between expressions (6) and (7), which can be easily established via a change of variables (see, for example, Laio and Tamea 2007). Although these manipulations do not extend in a straightforward way to scoring functions for the other multivariate distributions, we show how the results of Section 4 enable us to use these scoring functions to obtain scoring functions for level sets.

More specifically, we show that each \( L^2 \) scoring function can be expressed as the integral
of the scoring functions for certain level sets. We describe our approach in Section 5.1. It is based on the “layer cake representation”, which enables us to decompose the scoring functions $S'(P_X, y; \hat{w}, \hat{h})$ in expression (26) into an integral of scoring functions for the level sets of $F^{-1}(\hat{f}_X \hat{w})$. This provides a unified approach for constructing scoring functions for different types of level sets, including density level sets, CDF level sets, and LPM level sets, and we show this in Section 5.2. Furthermore, using this approach one can generate, in the univariate context, the full class of quantile scores studied in Komunjer (2005) and Gneiting (2011). Finally, one can also derive the excess mass scoring function for density level sets.

5.1 Scoring Functions for Level Sets

Before we disintegrate the scoring functions $S'(P_X, y; \hat{w}, \hat{h})$ in expression (26), we make a further assumption:

**Assumption 2.** $F^{-1}(\hat{\delta}_y \hat{w})$ is non-negative $\mathcal{L}^d$-a.e.. It is integrable with respect to both $\lambda$, $\mathcal{L}^d$, and the PDF of $P_Y$. Also, $\lambda$ is an absolutely continuous measure on $\mathbb{R}^d$ with $\mathcal{L}^d$-a.e. positive Radon–Nikodym derivative $d\lambda / d\mathcal{L}^d \equiv h^2$.

This setup covers all the examples of level sets in Section 3.2. The key tool for our construction is the following:

**Lemma 1** ("Layer Cake Representation"). Let $\lambda$ be a Borel measure on $\mathbb{R}^d$, and let $g : \mathbb{R}^d \to [0, \infty]$ be a $\lambda$-measurable function. For any $p \in [1, \infty)$ we have

$$\int_{\mathbb{R}^d} g(z)^p d\lambda(z) = \int_0^\infty p \alpha^{p-1} \lambda\left(\{z \in \mathbb{R}^d : g(z) \geq \alpha\}\right) d\alpha. \quad (34)$$

A proof of this lemma can be found in (Lieb and Loss 2001); “layer cake” refers to the level sets of $g$. This elementary result has numerous applications in real and harmonic analysis (Stein 1970). We apply Lemma 1 to $S'(P_X, y; \hat{w}, \hat{h})$ in expression (26). Then the first term therein can be written as

$$\int_{\mathbb{R}^d} \left(F^{-1}(\hat{f}_X \hat{w})(z)h(z)\right)^2 dz = 2 \int_0^\infty \alpha \lambda\left\{z \in \mathbb{R}^d : F^{-1}(\hat{f}_X \hat{w})(z) \geq \alpha\right\} d\alpha,$$
where $\lambda\{\bullet\}$ denotes the measure of a set under $\lambda$. For the second term, as $F^{-1}(\hat{\delta}_y \hat{w})$ is integrable and $L^d$-a.e. non-negative, define a Radon measure $\mu_{y,\hat{w}}$ on $\mathbb{R}^d$ by

$$\frac{d\mu_{y,\hat{w}}}{d\lambda} := F^{-1}(\hat{\delta}_y \hat{w}) \quad \text{for each } y \in \mathbb{R}^d. \quad (35)$$

It follows that the second term in expression (26) is given by

$$2 \int_{\mathbb{R}^d} F^{-1}(\hat{f}_X \hat{w})(z) F^{-1}(\hat{\delta}_y \hat{w})(z) h^2(z) \, dz = 2 \int_0^\infty \mu_{y,\hat{w}} \left\{ z \in \mathbb{R}^d : F^{-1}(\hat{f}_X \hat{w})(z) \geq \alpha \right\} \, d\alpha. \quad (36)$$

Therefore, we can rewrite expression (26) as

$$\frac{1}{2} S'(P_X, y; \hat{w}, \hat{h}) = \int_0^\infty \left( \alpha \lambda \left\{ z \in \mathbb{R}^d : F^{-1}(\hat{f}_X \hat{w})(z) \geq \alpha \right\} \right. \left. - \mu_{y,\hat{w}} \left\{ z \in \mathbb{R}^d : F^{-1}(\hat{f}_X \hat{w})(z) \geq \alpha \right\} \right) \, d\alpha. \quad (37)$$

The ensuing theorem states that the integrand on the right-hand side of expression (36) is a consistent scoring function for the $\alpha$ level set $L(P_X; \hat{w}, \alpha) = \{ z \in \mathbb{R}^d : F^{-1}(\hat{f}_X \hat{w})(z) \geq \alpha \}$ for every $\alpha > 0$. Its proof is postponed to the appendix.

**Theorem 2.** For each $\alpha > 0$, under Assumptions 1 and 2, the following defines a scoring function for the $\alpha$ level set $L(P_X; \hat{w}, \alpha)$ of $F^{-1}(\hat{f}_X \hat{w})(z)$:

$$(S')^\Gamma(L(P_X; \hat{w}, \alpha), y; \hat{w}, \hat{h}) := \alpha \lambda \{ L(P_X; \hat{w}, \alpha) \} - \mu_{y,\hat{w}} \{ L(P_X; \hat{w}, \alpha) \}, \text{ where } y \in \mathbb{R}^d. \quad (37)$$

Similar to a remark that we made in Section 4.1, we note that we can choose the weight function $h(z)$ to warrant the convergence of the scoring function in expression (37). We use the notation $\Gamma$ to denote a scoring function for a level set. We use the notation $(S')^\Gamma(L(P_X; \hat{w}, \alpha), y; \hat{w}, \hat{h})$ for the level set scoring function that is derived from the $L^2$ scoring function $S'(P_X, y; \hat{w}, \hat{h})$ in expression (26).

### 5.2 Examples of Scoring Functions for Level Sets

We now present scoring functions for the density level set, CDF level set, and LPM level sets, discussed in Section 3.2.
5.2.1 Density Level Sets

Applying Theorem 2 to the quadratic score $DQS'(P_X, y; h)$ in expression (28) of Section 4.3.1, we get

$$(DQS')_\Gamma(D(P_X; \alpha), y; \alpha) = \alpha \lambda \left\{ D(P_X; \alpha) \right\} - \mu_{y, \hat{w}} \left\{ D(P_X; \alpha) \right\},$$  

where $D(P_X; \alpha)$ is the $\alpha$ density level set defined in expression (16). We can simplify the second term on the right hand side of the above expression,

$$\mu_{y, \hat{w}} \left\{ D(P_X; \alpha) \right\} = \mathbb{1} \left\{ y \in D(P_X; \alpha) \right\} h^2(z).$$

Thus, we obtain the following scoring function for the $\alpha$-density level set:

$$(DQS')_\Gamma(D(P_X; \alpha), y; \alpha) := \alpha \lambda \left\{ D(P_X; \alpha) \right\} - \mathbb{1} \left\{ y \in D(P_X; \alpha) \right\} h^2(z).$$  

When $h \equiv 1$, the above expression reduces to the excess mass scoring function in expression (20) (see, for example, Hartigan 1987, Müller and Sawitzki 1991, Polonik 1995, Tsybakov 1997).

5.2.2 CDF Level Sets

Applying Theorem 2 to the MCRPS $'P(P_X, y; h)$ in expression (30) of Section 4.3.2, we get

$$(MCRPS')_\Gamma(C(P_X; \alpha), y; \alpha) = \alpha \lambda \left\{ C(P_X; \alpha) \right\} - \mu_{y, \hat{w}} \left\{ C(P_X; \alpha) \right\},$$

where $C(P_X; \alpha)$ is the $\alpha$ CDF level set given by expression (17). Notice that

$$\mu_{y, \hat{w}} \left\{ C(P_X; \alpha) \right\} = \int_{\{F_X > \alpha\}} h^2(z) \mathbb{1} \left\{ z \geq y \right\} dz = \lambda \left\{ C(P_X; \alpha) \cap \{ z \geq y \} \right\}.$$  

This yields the following scoring function for the $\alpha$ CDF level set:

$$(MCRPS')_\Gamma(C(P_X; \alpha), y; \alpha) := \alpha \lambda \left\{ C(P_X; \alpha) \right\} - \lambda \left\{ C(P_X; \alpha) \cap \{ z \geq y \} \right\}.$$  

In order to gain more insights into the scoring function for the CDF level set, let us consider an equivalent expression. We can apply Theorem 2 to the MCRPS in expression (13), which essentially amounts to adding the term $(1 - \alpha) \lambda \left\{ z \in \mathbb{R}^d : z \geq y \right\}$
purely dependent on $y$ to expression (40) to obtain the following equivalent scoring function,

$$
\alpha \lambda \left\{ C(P_X; \alpha)^c \cap \{z \geq y\} \right\} + (1 - \alpha) \lambda \left\{ C(P_X; \alpha) \cap \{z \geq y\} \right\},
$$

(41)

where $C$ denotes the set complement.

When $d = 1$, expression (41) is the full class of quantile scores (see, for example, Komunjer 2005; Gneiting 2011). To see this, we can expand the integrals in expression (41) as follows,

$$
\alpha \lambda \left\{ C(P_X; \alpha)^c \cap \{z \geq y\} \right\} + (1 - \alpha) \lambda \left\{ C(P_X; \alpha) \cap \{z \geq y\} \right\}
$$

$$
= \alpha \left( H(y) - H(q_X(\alpha)) \right) 1 \{ y > q_X(\alpha) \} + (1 - \alpha) \left( H(q_X(\alpha)) - H(y) \right) 1 \{ y < q_X(\alpha) \}
$$

$$
= \left( \alpha - 1 \{ y < q_X(\alpha) \} \right) \left( H(y) - H(q_X(\alpha)) \right),
$$

where $H$ is an anti-derivative of $h^2$, and hence is clearly non-decreasing. The final line is simply expression (19), which is the full class of quantile scoring functions.

### 5.2.3 Lower Partial Moment Level Sets

Applying Theorem 2 to the LPMS' $(P_X, y; k)$ in expression (33) of Section 4.3.3, we get

$$
\text{LPMS}' \Gamma \left( M(P_X; \alpha, k), y; \alpha, k \right) = \alpha \lambda \left\{ M(P_X; \alpha, k) \right\} - \mu_{y, \hat{w}} \left\{ M(P_X; \alpha, k) \right\},
$$

(42)

where $M$ is the LPM level set, defined in expression (18). We can simplify the second term on the right hand side of the above expression,

$$
\mu_{y, \hat{w}} \left\{ M(P_X; \alpha, k) \right\} = \int_{\mathbb{R}^d} 1 \{ z \in M(P_X; \alpha, k) \} 1 \{ z \geq y \} \prod_{j=1}^d \frac{1}{k!} (z_j - y_j)^k h^2(z) \, dz.
$$

Thus, we obtain the following scoring function for the $\alpha$ LPM level set,

$$
\text{LPMS}' \Gamma \left( M(P_X; \alpha, k), y; \alpha \right) := \alpha \lambda \left\{ M(P_X; \alpha, k) \right\}
$$

$$
- \int_{\mathbb{R}^d} 1 \{ z \in M(P_X; \alpha, k) \} 1 \{ z \geq y \} \prod_{j=1}^d \frac{1}{k!} (z_j - y_j)^k h^2(z) \, dz.
$$

(43)
6 Empirical Analysis

In this section, we first describe the novel simulation-based method that we use to compute the scoring functions. We then present studies of simulated and real data to demonstrate the use of the scores. We implement our proposed new scoring functions, developed in Section 5: the $(DQS')^\Gamma$ for density level sets in expression (39), the $(MCRPS')^\Gamma$ for CDF level sets in expression (40), and the $(LPMS')^\Gamma$ for LPM level sets in expression (43). To save space, for the LPM level sets, we consider only the case of $k = 1$. For each type of level set, we also implement the corresponding $L^2$ scoring function for distributions, which we presented in Section 4. These are the $DQS'$ in expression (28), the $MCRPS'$ in expression (30) and our new scoring function, the $LPMS'$, in expression (33). We note that these three $L^2$ scoring functions are related to the physical version $S'(P_X, y; \hat{w}, \hat{h})$ in expression (26). Other versions of the $L^2$ scoring functions in Section 4 will lead to the same ranking of the model performance because they are equivalent to $S'(P_X, y; \hat{w}, \hat{h})$.

6.1 Computation of the Scoring Functions

The computation of the $L^2$ scoring functions and the scoring functions for level sets is a highly nontrivial problem, due to the multidimensional integration involved. For example, let us write the scoring functions for level sets in expression (37) as an integration as follows,

\[
(S')^\Gamma(L(P_X; \hat{w}, \alpha), y; \hat{w}, \hat{h}) = \alpha \lambda \{ L(P_X; \hat{w}, \alpha) \} - \mu_{y, \hat{w}} \{ L(P_X; \hat{w}, \alpha) \}
\]

\[
= \alpha \int_{\mathbb{R}^d} \mathbb{1} \{ z \in L(P_X; \hat{w}, \alpha) \} h^2(z) dz - \int_{\mathbb{R}^d} \mathbb{1} \{ z \in L(P_X; \hat{w}, \alpha) \} \mathcal{F}^{-1}(\delta_y \hat{w})(z) h^2(z) dz. \tag{44}
\]

This expression shows that the computation of $(S')^\Gamma(L(P_X; \hat{w}, \alpha), y; \hat{w}, \hat{h})$ is complex as it involves the term $\mathbb{1} \{ z \in L(P_X; \hat{w}, \alpha) \}$, which is dependent on the geometry of $L(P_X; \hat{w}, \alpha)$.

The computation of this type of scoring function has received little attention in the literature, with the studies of Hartigan (1987) and Yuen and Stoev (2014) being the only ones...
that we have found. The former considers a polygon-based approach for discrete distributions $P_X$, and the latter considers an approximation of the MCRPS integral in expression (13) for a specific type of measure $\lambda$, and with $P_X$ having compact support.

In this paper, we propose a simple simulation-based numerical approach, which can be applied to a wide class of distributions $P_X$. The idea is to compute the integrals of the scoring function expressions, such as expression (44), with the weight function $h^2 = \frac{d\lambda}{dL}$ chosen to be the PDF of a known distribution. With this choice, $\lambda$ can be viewed as a probability measure on $\mathbb{R}^d$. Hence, all the terms involved in the $L^2$ scoring functions and the scoring functions for level sets can be viewed simply as the expectation of functions under the probability measure $\lambda$. In practice, we simply simulate a random sample from the probability measure $\lambda$, and replace the integrals in the scoring functions by sample expectations. The method is easy to implement even for high-dimensional multivariate distributions.

We remark that our motivation for using a weight function $h^2$ in a scoring function differs from those who have been interested in putting more weight on regions of interest, such as tails of univariate distributions (see, for example, Gneiting and Ranjan 2011; Diks et al. 2011). We acknowledge that different choices for $h^2$ in general lead to different scoring functions, and that it would interesting to study the difference between them. However, a detailed consideration of this is essentially beyond the scope of this paper.

6.2 Simulation Study

In this study, we used the various scoring functions to compare the fit of candidate distributions and their level sets to simulated data. The data consisted of 200000 observations generated from a bivariate Gaussian distribution with zero means, unit variances, and covariance 0.5.

For CDF level sets, $\alpha$ has range $[0, 1]$, regardless of the distribution that is considered. For density level sets, however, $\alpha$ does not have a universal range for all distributions. For LPM level sets, $\alpha$ is unbounded. To select a set of values of $\alpha$ for each type of level set,
we first recorded the value of $\alpha$ for the level set on which each of the 200000 simulated observations was located. We then chose $\alpha$ to be the 0.1, 0.2, ..., 0.9 quantiles of these values. The resultant values of $\alpha$ for each type of level set are presented in the second rows of Tables 1-3.

We compared five candidate distributions in terms of their fit to the simulated observations. We considered the bivariate Gaussian distributions that had zero means, unit variances, and the following five different covariances: 0.1, 0.3, 0.5, 0.7, and 0.9. We calculated the scoring functions using the method described in Section 6.1, with $h^2$ chosen to be the PDF of a standard bivariate normal distribution, and 20000 values sampled from this distribution. For each of the 200000 observations, we computed the scoring function for each type of level set and the corresponding $L^2$ scoring function. Our results tables report the mean of the 200000 scores, with a lower value indicating better fit.

Table 1 presents the density level set score $(DQS')^\Gamma$ and its corresponding $L^2$ scoring function $DQS'$; Table 2 presents the CDF level set score $(MCRPS')^\Gamma$ and its corresponding $L^2$ scoring function $MCRPS'$; and Table 3 presents the LPM level set score $(LPMS')^\Gamma$ and its corresponding $L^2$ scoring function $LPMS'$. For each column in each table, the third row of results has the lowest values, indicating that the scores are correctly able to identify the distribution that was used to generate the data. This supports our assertion that our proposed new scores are consistent scoring functions; namely that the $LPMS'$ is a consistent scoring function for distributions, and $(DQS)^\Gamma$, $(MCRPS')^\Gamma$, and $(LPMS')^\Gamma$ are consistent scoring functions for density level sets, CDF level sets, and LPM level sets, respectively. It also supports the more general theoretical result that the $L^2$ scoring function $S'$ in expression (26) is a consistent scoring function for distributions, and $(S')^\Gamma$ in expression (37) is a consistent scoring function for level sets.
Table 1: For the simulated data, comparison of the fit of five candidate distributions using the density level set score \((\text{DQS}')^\Gamma\), and \(L^2\) scoring function \(\text{DQS}'\) \((\times 10^{-5})\). Lower values are better. Each covariance value corresponds to a different candidate distribution. The distribution with covariance of 0.5 is identical to the distribution used to simulate the data.

| \(\alpha\)   | 0.0184 | 0.0365 | 0.0551 | 0.0736 | 0.0921 | 0.1104 | 0.1287 | 0.1472 | 0.1654 |
|-------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| Covariance  | \(-6530\) | \(-5094\) | \(-3852\) | \(-2761\) | \(-1864\) | \(-1151\) | \(-621\) | \(-186\) | \(0\) | \(-958\) |
| 0.3         | \(-6568\) | \(-5162\) | \(-3920\) | \(-2856\) | \(-1952\) | \(-1209\) | \(-655\) | \(-225\) | \(-22\) | \(-976\) |
| 0.5         | \(-6592\) | \(-5185\) | \(-3939\) | \(-2871\) | \(-1999\) | \(-1237\) | \(-681\) | \(-284\) | \(-34\) | \(-985\) |
| 0.7         | \(-6593\) | \(-5097\) | \(-3865\) | \(-2815\) | \(-1924\) | \(-1221\) | \(-629\) | \(-195\) | \(102\) | \(-942\) |
| 0.9         | \(-5639\) | \(-4359\) | \(-3308\) | \(-2416\) | \(-1659\) | \(-993\) | \(-442\) | \(58\) | \(448\) | \(-449\) |

Table 2: For the simulated data, comparison of the fit of five candidate distributions using the CDF level set score \((\text{MCRPS}')^\Gamma\), and \(L^2\) scoring function \(\text{MCRPS}'\) \((\times 10^{-5})\). Lower values are better. Each covariance value corresponds to a different candidate distribution. The distribution with covariance of 0.5 is identical to the distribution used to simulate the data.

| \(\alpha\)   | 0.0352 | 0.0824 | 0.1378 | 0.2033 | 0.2772 | 0.3620 | 0.4606 | 0.5787 | 0.7293 |
|-------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| Covariance  | \(-25667\) | \(-21593\) | \(-17438\) | \(-13369\) | \(-9695\) | \(-6459\) | \(-3783\) | \(-1748\) | \(-438\) | \(-13348\) |
| 0.3         | \(-25714\) | \(-21683\) | \(-17575\) | \(-13506\) | \(-9815\) | \(-6556\) | \(-3840\) | \(-1777\) | \(-445\) | \(-13455\) |
| 0.5         | \(-25724\) | \(-21709\) | \(-17616\) | \(-13552\) | \(-9858\) | \(-6595\) | \(-3863\) | \(-1789\) | \(-448\) | \(-13494\) |
| 0.7         | \(-25719\) | \(-21690\) | \(-17582\) | \(-13505\) | \(-9810\) | \(-6551\) | \(-3828\) | \(-1771\) | \(-443\) | \(-13451\) |
| 0.9         | \(-25709\) | \(-21645\) | \(-17501\) | \(-13371\) | \(-9641\) | \(-6393\) | \(-3675\) | \(-1684\) | \(-406\) | \(-13291\) |

Table 3: For the simulated data, comparison of the fit of five candidate distributions using the LPM level set score \((\text{LPMS}')^\Gamma\), and \(L^2\) scoring function \(\text{LPMS}'\) \((\times 10^{-4})\). Lower values are better. Each covariance value corresponds to a different candidate distribution. The distribution with covariance of 0.5 is identical to the distribution used to simulate the data.

| \(\alpha\)   | 0.0158 | 0.0472 | 0.0943 | 0.1632 | 0.2605 | 0.3998 | 0.6086 | 0.9510 | 1.6284 |
|-------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| Covariance  | \(-4398\) | \(-4107\) | \(-3730\) | \(-3273\) | \(-2758\) | \(-2193\) | \(-1601\) | \(-990\) | \(-409\) | \(-5779\) |
| 0.3         | \(-4405\) | \(-4129\) | \(-3766\) | \(-3319\) | \(-2811\) | \(-2247\) | \(-1649\) | \(-1027\) | \(-428\) | \(-5934\) |
| 0.5         | \(-4408\) | \(-4135\) | \(-3779\) | \(-3337\) | \(-2832\) | \(-2270\) | \(-1669\) | \(-1043\) | \(-437\) | \(-6002\) |
| 0.7         | \(-4407\) | \(-4134\) | \(-3775\) | \(-3330\) | \(-2822\) | \(-2259\) | \(-1657\) | \(-1032\) | \(-432\) | \(-5963\) |
| 0.9         | \(-4406\) | \(-4129\) | \(-3762\) | \(-3305\) | \(-2785\) | \(-2213\) | \(-1606\) | \(-991\) | \(-408\) | \(-5798\) |
6.3 Real Data Study

We used the scoring functions to evaluate forecasts of trivariate distributions and their level sets for daily log returns on the following three stocks listed on the NYSE: Alcoa, MacDonald’s, and Merck. These were the three stocks considered by Diks et al. (2014). We considered the 5000 daily returns, recorded between 8 May 1996 and 1 July 2018. Using a rolling window of 2000 observations, we repeatedly re-estimated model parameters and generated day-ahead forecasts for the conditional joint distribution. This delivered 3000 out-of-sample forecasts.

We considered six parametric methods to estimate the joint distribution. For the marginal distributions, we used the GARCH(1,1) model with Gaussian or Student-t distribution. To capture the dependence structure between the returns, we used either a Gaussian or t copula fitted between the marginal distributions (see, for example, Patton 2012), or an assumption of independence. In our results tables, N-NoCop is our abbreviation for the model with Gaussian marginals and no copula; t-NoCop is the model with Student-t marginals and no copula; N-GCop and t-GCop are the models using the Gaussian copula; and N-tCop and G-tCop are the models using the t copula.

For the weight function \( h^2 \), we felt it would be sensible to use a function that puts a reasonable weighting across the main body of the trivariate Gaussian distribution. This led us to set \( h^2 \) as the trivariate Gaussian PDF, with zero means and covariance matrix equal to the empirical covariance matrix of the three in-sample series of returns.

For the density level sets and LPM level sets, the range of \( \alpha \) is time-varying and unknown, as the conditional distribution is time-varying and unknown. To select values of \( \alpha \), we first applied kernel density estimation to all 5000 daily returns to obtain an estimate of the unconditional trivariate distribution, where the bandwidths were selected following Silverman’s “rule of thumb” (Silverman 1986). To select a set of values of \( \alpha \) for each type of level set, we then followed a similar approach to the one we used in Section 6.2, with the estimated unconditional distribution treated as the data generating process. Using this
distribution, we recorded the value of $\alpha$ for the level set on which each of the 5000 observations was located. We then chose $\alpha$ to be the $0.1, 0.2, \ldots, 0.9$ quantiles of these values. The resultant values of $\alpha$ are presented in the second rows of Tables 4-6.

Table 4 presents the results for the density level set score $(DQS')^\Gamma$ and its corresponding $L^2$ scoring function $DQS'$; Table 5 presents the results for the CDF level set score $(MCRPS')^\Gamma$ and its corresponding $L^2$ scoring function $MCRPS'$; and Table 6 presents the results for the LPM level sets $(LPMS')^\Gamma$ and its corresponding $L^2$ scoring function $LPMS'$. In these results tables, we report the mean of these 200000 scores, with a lower value indicating better fit. Our first comment is that using Student-t marginals was more accurate than Gaussian marginals. Secondly, we note that using the Gaussian or t copula was more accurate than no copula. Thirdly, there is no clear superiority between using the Gaussian and t copula. This was not surprising to us as we had noted that our estimates for the degrees of freedom of the t copula were consistently over 25, which makes the t copula similar to a Gaussian copula. These findings are broadly consistent with the literature (see, for example, Patton 2012), which provides support for our proposed $L^2$ scoring functions and the scoring functions for level sets.

Table 4: For the stock returns data, forecasting methods compared using the density level set score $(DQS')^\Gamma$ and its corresponding $L^2$ scoring function $DQS'$ ($\times 10^{-5}$). Lower values are better.

| $\alpha$ | 0.0003 | 0.0010 | 0.0021 | 0.0036 | 0.0056 | 0.0080 | 0.0110 | 0.0148 | 0.0192 |
|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| N-NoCop  | -5120  | -4636  | -4009  | -3423  | -2789  | -2267  | -1734  | -1180  | -624   | -95    |
| t-NoCop  | -5118  | -4643  | -4031  | -3454  | -2877  | -2335  | -1894  | -1438  | -1070  | -119   |
| N-GCop   | -5131  | -4657  | -4056  | -3501  | -2895  | -2350  | -1817  | -1314  | -784   | -103   |
| t-GCop   | -5136  | -4681  | -4118  | -3557  | -2993  | -2453  | -1962  | -1512  | -1148  | -128   |
| N-tCop   | -5128  | -4653  | -4064  | -3507  | -2915  | -2362  | -1849  | -1422  | -866   | -108   |
| t-tCop   | -5134  | -4675  | -4123  | -3546  | -3013  | -2469  | -1959  | -1521  | -1141  | -130   |
Table 5: For the stock returns data, forecasting methods compared using the CDF level set score \((\text{MCRPS}'^\Gamma)\) and its corresponding \(L^2\) scoring function \(\text{MCRPS}'\) \((\times 10^{-5})\). Lower values are better.

| \(\alpha\)   | 0.0150 | 0.0350 | 0.0612 | 0.0938 | 0.1327 | 0.1787 | 0.2397 | 0.3206 | 0.4654 |
|--------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| N-NoCop      | -18136 | -16690 | -15058 | -13313 | -11533 | -9731  | -7771  | -5721  | -3115  | -9328  |
| t-NoCop      | -18080 | -16618 | -14995 | -13278 | -11528 | -9763  | -7830  | -5804  | -3224  | -9430  |
| N-GCop       | -18198 | -16771 | -15157 | -13426 | -11648 | -9854  | -7893  | -5838  | -3219  | -9470  |
| t-GCop       | -18201 | -16792 | -15200 | -13481 | -11709 | -9913  | -7936  | -5860  | -3250  | -9543  |
| N-tCop       | -18194 | -16755 | -15136 | -13403 | -11624 | -9833  | -7890  | -5838  | -3225  | -9458  |
| t-tCop       | -18205 | -16797 | -15206 | -13486 | -11710 | -9911  | -7934  | -5860  | -3251  | -9541  |

Table 6: For the stock returns data, forecasting methods compared using the LPM level set score \((\text{LPMS}'^\Gamma)\) and its corresponding \(L^2\) scoring function \(\text{LPMS}'\) \((\times 10^{-2})\). Lower values are better.

| \(\alpha\)   | 0.4430 | 0.7366 | 1.0525 | 1.3734 | 1.7807 | 2.3016 | 3.0298 | 4.3036 | 7.4149 |
|--------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| N-NoCop      | -417   | -397   | -377   | -360   | -341   | -319   | -292   | -254   | -188   | -9707  |
| t-NoCop      | -416   | -396   | -376   | -359   | -340   | -318   | -292   | -255   | -190   | -9819  |
| N-GCop       | -429   | -414   | -397   | -383   | -365   | -347   | -329   | -293   | -230   | -12450 |
| t-GCop       | -430   | -414   | -402   | -387   | -372   | -353   | -331   | -297   | -244   | -13359 |
| N-tCop       | -430   | -414   | -399   | -385   | -369   | -352   | -329   | -294   | -234   | -12987 |
| t-tCop       | -431   | -413   | -402   | -387   | -374   | -355   | -336   | -303   | -243   | -13476 |

7 Conclusion

In this paper, we have studied the scoring functions for multivariate distributions and level sets. The paper has several novel contributions. Firstly, we propose the class of \(L^2\) scoring functions for multivariate distributions, for which the existing quadratic score and MCRPS are specific examples. The \(L^2\) scoring functions can easily generate new scoring functions for multivariate distributions, and we demonstrate this with the introduction of the LPMS, a new scoring function based on the lower partial moments. Secondly, by disintegrating the \(L^2\) scoring functions, we obtain a unified approach for generating scoring functions for level sets,
including the scoring functions for density level sets, CDF level sets, and LPM level sets. Thirdly, we propose a simple numerical algorithm for computing the $L^2$ scoring functions and the scoring functions for level sets. Finally, the theoretical properties of our new scoring functions are supported by a simulation study and an analysis of stock returns data.

**Appendix**

In the appendix, we present the technical proofs of Theorem 1 and Theorem 2.

**Proof of Theorem 1.** We need to show that

$$\Delta := E_{P_Y} \left[ S(P_X, Y; \hat{w}, \hat{h}) - S(P_Y, Y; \hat{w}, \hat{h}) \right] \geq 0$$

for arbitrary $P_X \in \mathcal{V}^d / \sim$, and that the equality holds if and only if $P_X$ and $P_Y$ are identically distributed. Indeed, by Funini’s theorem we have

$$\Delta = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left\{ \left| (\hat{f}_X \hat{w} - \hat{\delta}_Y \hat{w}) * \hat{h} \right|^2 (t) - \left| (\hat{f}_Y \hat{w} - \hat{\delta}_Y \hat{w}) * \hat{h} \right|^2 (t) \right\} f_Y(z) \, dz \, dt.$$

For complex numbers $a, b, c$ one has the identity

$$|a - b|^2 - |c - b|^2 = |a|^2 - |c|^2 + 2 \Re \{b \bar{c} - a\},$$

where $\Re(z)$ denotes the real part and $\bar{z}$ the complex conjugate of $z \in \mathbb{C}$. Thus

$$\Delta = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left\{ \left| (\hat{f}_X \hat{w} - \hat{\delta}_Y \hat{w}) \right|^2 (t) - \left| (\hat{f}_Y \hat{w} - \hat{\delta}_Y \hat{w}) \right|^2 (t) \right\} f_Y(z) \, dz \, dt$$

$$+ 2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \Re \left\{ \left( \hat{\delta}_Y \hat{w} \right) (t) \cdot \left[ \left( \hat{f}_Y \hat{w} - \hat{f}_X \hat{w} \right) * \hat{h} \right] (t) \right\} f_Y(z) \, dz \, dt.$$

Observing that $\int_{\mathbb{R}^d} f_Y(z) \, dz = 1$ and $\int_{\mathbb{R}^d} \hat{\delta}_Y(t) f_Y(z) \, dz = \hat{f}_Y(t)$ for each $t \in \mathbb{R}^d$, and using Fubini’s theorem once more, we can rewrite

$$\Delta = \int_{\mathbb{R}^d} \left\{ \left| \hat{f}_X \hat{w} * \hat{h} \right|^2 (t) - \left| \hat{f}_Y \hat{w} * \hat{h} \right|^2 (t) \right\} dt$$

$$+ 2 \int_{\mathbb{R}^d} \Re \left\{ \left( \hat{f}_Y \hat{w} \right) (t) \cdot \left[ \left( \hat{f}_Y \hat{w} - \hat{f}_X \hat{w} \right) * \hat{h} \right] (t) \right\} dt.$$
A simple rearrangement gives us
\[
\Delta = \int_{\mathbb{R}^d} \left\{ |\hat{f}_X \hat{w} \ast \hat{h}|^2(t) + |\hat{f}_Y \hat{w} \ast \hat{h}|^2(t) - 2R \left\{ \left[ (\hat{f}_Y \hat{w}) \ast \hat{h} \right](t) \cdot \left[ (\hat{f}_X \hat{w}) \ast \hat{h} \right](t) \right\} \right\} dt.
\]
Therefore, the non-negativity of \( \Delta \) follows directly from the Cauchy–Schwarz inequality.

Finally, notice that \(|a|^2 + |b|^2 - 2R(ab) = 0\) if and only if \(a = b\) for \(a, b \in \mathbb{C}\); in our case it means that \(\Delta = 0\) if and only if \((\hat{f}_X \hat{w}) \ast \hat{h} = (\hat{f}_Y \hat{w}) \ast \hat{h}\) \(\mathcal{L}^d\)-a.e. on \(\mathbb{R}^d\). By the Plancherel’s identity and Fubini’s theorem, one may infer the following:
\[
\mathcal{F}^{-1}(\hat{f}_X \hat{w})(z)h(z) = \mathcal{F}^{-1}(\hat{f}_Y \hat{w})(z)h(z) \quad \text{for } z \in \mathbb{R}^d.
\]
As \(|h(z)| > 0\) for \(\mathcal{L}^d\)-a.e. \(z \in \mathbb{R}^d\) by Assumption 1 (3), this implies \(\mathcal{F}^{-1}(\hat{f}_X \hat{w}) = \mathcal{F}^{-1}(\hat{f}_Y \hat{w})\) \(\mathcal{L}^d\)-a.e.. By the uniqueness of locally finite Borel measures (see Assumption 1 (2)), we have
\[
\hat{f}_X(t) \hat{w}(t) = \hat{f}_Y(t) \hat{w}(t) \quad \text{for } \mathcal{L}^d - a.e. \ t \in \mathbb{R}^d.
\]
But \(|\hat{w}(t)| > 0\) for \(\mathcal{L}^d\)-a.e. \(t \in \mathbb{R}^d\) by Assumption 1 (3), so \(\hat{f}_X = \hat{f}_Y\) \(\mathcal{L}^d\)-a.e.. As before, it follows that \(f_X = f_Y\) \(\mathcal{L}^d\)-a.e., namely that \(P_X = P_Y\) in \(\mathcal{V}^d/\sim\). \(\square\)

**Proof of Theorem 2** We need to prove that
\[
\Delta' := \mathbb{E}_{P_Y}\left[ S(L(P_X; \hat{\omega}, \alpha), y; \hat{w}, \hat{h}) - S(L(P_Y; \hat{\omega}, \alpha), y; \hat{w}, \hat{h}) \right] \geq 0, \quad \text{for each } \alpha \geq 0. \ (45)
\]
For notational convenience, for any \(X \in \mathcal{V}^d\) we write \(\Xi[X](z) := \mathcal{F}^{-1}(\hat{f}_X \hat{w})(z)\) and \(\hat{\omega}(y, z) := \mathcal{F}^{-1}(\hat{f}_Y \hat{w})(z)\). We can express (45) by \(\Delta' = \mathbb{E}_{P_Y}[\Delta'']\), where
\[
\Delta'' = \alpha \left( \lambda \{ \Xi[X] > \alpha \} - \lambda \{ \Xi[Y] > \alpha \} \right) + \mu_y \{ \Xi[Y] > \alpha \} - \mu_y \{ \Xi[X] > \alpha \} =: A_1 + A_2.
\]

Partition \(\mathbb{R}^d = \Sigma_{++} \sqcup \Sigma_{+-} \sqcup \Sigma_{-+} \sqcup \Sigma_{--}\) where \(\sqcup\) is the disjoint union:
\[
\begin{align*}
\Sigma_{++} & := \{ \Xi[X] > \alpha \} \cap \{ \Xi[Y] > \alpha \}, \quad \Sigma_{+-} := \{ \Xi[X] > \alpha \} \cap \{ \Xi[Y] \leq \alpha \}, \\
\Sigma_{-+} & := \{ \Xi[X] \leq \alpha \} \cap \{ \Xi[Y] > \alpha \}, \quad \Sigma_{--} := \{ \Xi[X] \leq \alpha \} \cap \{ \Xi[Y] \leq \alpha \}.
\end{align*}
\]
By construction, each of these four sets is Borel measurable. Using \(d\mu_{X,Y}/d\lambda = \mathcal{F}^{-1}(\hat{f}_Y \hat{w})\),
\[\frac{d\lambda}{d\mathcal{L}^d} = h^2,\] and Fubini’s theorem, we get

\[A_2 = \int_{\mathbb{R}^d} \vartheta(y, z) h^2(z) \left[ \mathbb{1}_{\Sigma_{++}}(z) - \mathbb{1}_{\Sigma_{++}}(z) \right] dz\]

\[A_1 = \alpha \int_{\mathbb{R}^d} \left[ \mathbb{1}_{\Sigma_{++}}(z) - \mathbb{1}_{\Sigma_{++}}(z) \right] h^2(z) dz,\]

\[\Delta'' = \int_{\mathbb{R}^d} \left\{ \left( \alpha - \vartheta(y, z) \right) \left[ \mathbb{1}_{\Sigma_{++}} - \mathbb{1}_{\Sigma_{++}} \right] \right\} h^2(z) d\mathcal{L}^d.\]

Now we notice that \( \mathbb{E}_{P_Y} [\vartheta(\bullet, z)] = \Xi[Y](z) \) for each \( z \in \mathbb{R}^d \). Indeed, we have

\[\mathbb{E}_{P_Y} [\vartheta(\bullet, z)] = \int_{\mathbb{R}^d} \mathcal{F}^{-1} \left( \hat{\vartheta}_Y \right)(z) f_Y(y) dy\]

\[= \iint_{\mathbb{R}^d \times \mathbb{R}^d} \hat{w}(t) \hat{\vartheta}_Y(t) f_Y(y) e^{-2\pi i t \cdot z} dt dy\]

\[= \int_{\mathbb{R}^d} \hat{f}_Y(t) \hat{w}(t) e^{-2\pi i t \cdot z} dt = \Xi[Y](z),\]

by Fubini’s and dominant convergence theorems. It follows that

\[\Delta' = \mathbb{E}_{P_Y} [\Delta''] = \int_{\mathbb{R}^d} \left\{ \left( \alpha - \Xi[Y](z) \right) \left[ \mathbb{1}_{\Sigma_{++}}(z) - \mathbb{1}_{\Sigma_{++}}(z) \right] \right\} h^2(z) dz.\]

On \( \Sigma_{++} \) one has \( \mathbb{1}_{\Sigma_{++}} - \mathbb{1}_{\Sigma_{++}} = 1 \) and \( \alpha - \Xi[Y] \geq 0 \), and on \( \Sigma_{++}, \mathbb{1}_{\Sigma_{++}} - \mathbb{1}_{\Sigma_{++}} = 1 \) and \( \alpha - \Xi[Y] \leq 0 \). Therefore, the integrand of \( \Delta' \) is pointwise non-negative, hence \( \Delta' \geq 0 \). □

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