A new class of binning-free, multivariate goodness-of-fit tests: the energy tests

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Abstract

We present a new class of multivariate binning-free and nonparametric goodness-of-fit tests. The test quantity energy is a function of the distances of observed and simulated observations in the variate space. The simulation follows the probability distribution function $f_0$ of the null hypothesis. The distances are weighted with a weighting function which can be adjusted to the variations of $f_0$. We have investigated the power of the test for a uniform and a Gaussian distribution of one or two variates, respectively and compared it to that of conventional tests. The energy test with a Gaussian weighting function is closely related to the Pearson $\chi^2$ test but is more powerful in most applications and avoids arbitrary bin boundaries. The test is especially powerful in the multivariate case.

1 Introduction

There exist a large number of binning-free goodness-of-fit tests for univariate distributions. The extension to the multivariate case is difficult, because there a natural ordering system is missing. The popular $\chi^2$ test on the other hand suffers from the arbitrariness of the binning and from lack of power for small samples.

The test proposed in this article avoids both, ordering and binning. It is especially powerful in the multivariate case. It is called energy test, because the definition of the test statistic is closely related to the energy of electric charge distributions. To facilitate the computation of the test statistic, we approximate the probability distribution function (p.d.f.) $f_0$ of the null hypothesis by simulated observations. The statistic “energy” can also be used to test whether two samples belong to the same parent distribution.

In Section 2 we define the test and study its properties. Section 3 contains a comparison of the power of the energy test with that of other popular tests in one dimension. In Section

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4 we apply the energy test to two-dimensional problems. We discuss possible modifications and extensions of the test in Section 5 and conclude with a summary in Section 6.

2 The test statistic

2.1 The energy function

We define a quantity \( \phi \), the energy, which measures the difference between two p.d.f.'s \( f_0(x) \) and \( f(x), x \in \mathbb{R}^n \), by

\[
\phi = \frac{1}{2} \int \int [f(x) - f_0(x)] [f(x') - f_0(x')] R(x, x') dx dx'. \tag{1}
\]

The integrals extend over the full variate space. The weight function \( R \) is a monotonically decreasing function of the Euclidean distance \(|x - x'|\). Relation (1) with \( R = 1/|x - x'| \) is the electrostatic energy of two charge distributions of opposite sign which is minimum if the charges neutralize each other. Setting the function \( R = \delta(x - x') \), where \( \delta(x - x') \) is the Dirac Delta function, \( \phi \) reduces to the integrated quadratic difference of the two p.d.f.s

\[
\phi_\delta = \frac{1}{2} \int [f(x) - f_0(x)]^2 dx.
\]

Since we want to generalize (1) in such a way that we can apply it to a comparison of a sample with a distribution or of two samples with each other, \( \phi_\delta \) is not suitable. Functions like Gaussians which correlate different locations have to be used.

The test which we will introduce is based on the fact that for fixed \( f_0(x) \), \( \phi \) is minimum for the null hypothesis \( f(x) \equiv f_0(x) \) for all \( x \in \mathbb{R}^n \). We sketch a prove of this assertion in the Appendix.

Expanding (1)

\[
\phi = \frac{1}{2} \int \int [f(x)f(x') + f_0(x)f_0(x') - 2f(x)f_0(x')R(|x - x'|)] dx dx',
\]

we obtain three terms which have the form of expectation values of \( R \). They can be estimated from two samples \( X_1, X_2, ..., X_N \) and \( Y_1, Y_2, ..., Y_M \) drawn from \( f \) and \( f_0 \), respectively. Since in the first and the second term a product of identical distributions occurs, there it is not necessary to draw two different samples of the same p.d.f.. The expectation value of \( R \) in these expressions is given by the mean value of \( R \) computed from all combinations of the sample observations

\[
\phi_{NM} = \frac{1}{N(N-1)} \sum_{j>i} R(|x_i - x_j|) + \frac{1}{M(M-1)} \sum_{j>i} R(|y_i - y_j|) - \frac{1}{NM} \sum_{i,j} R(|x_i - y_j|).
\]
Throughout this article unless specified differently, all sums run from 1 to the maximum value of the index. For the energy statistic $\phi_N$ of a sample $X_1, X_2, ..., X_N$ relative to the p.d.f. $f_0$ is given by:

$$\phi_N = \frac{1}{N(N-1)} \sum_{j>i} R(|x_i - x_j|) + \int \int f_0(x)f_0(x')R(|x - x'|)dx'dx' + \frac{-1}{N} \sum_i \int f_0(x')R(|x_i - x'|)dx'.$$

To test whether a statistical sample $X_1, X_2, ..., X_N$ of size $N$ is compatible with the null hypothesis $H_0$, we could in principle use the test statistic $\phi_N$ of the sample with respect to the associated p.d.f. $f_0$ but since the evaluation of $\phi_N$ usually requires a sum over difficult integrals, we prefer to represent $f_0$ by a sample $Y_1, Y_2, ..., Y_M$, usually generated through a Monte Carlo simulation. We drop in $\phi_{NM}$ the term depending only on $f_0$ which is independent from the sample observations and obtain:

$$\phi_{NM} = \frac{1}{N^2} \sum_{j>i} R(|x_i - x_j|) - \frac{1}{NM} \sum_{i,j} R(|x_i - y_j|)$$  \hspace{1cm} (2)

Furthermore, we have replaced the denominator of the first term $1/N(N-1)$ by $1/N^2$ which has superior small sample properties (see Appendix). Statistical fluctuations of the simulation are negligible if $M$ is large compared to $N$, typically $M \geq 10N$.

### 2.2 The weight function

We have investigated three different types of weight functions, power laws, a logarithmic dependence and Gaussians.

$$R_{\text{pow}}(r) = \begin{cases} \frac{1}{d_{\text{min}}} & \text{for } r > d_{\text{min}} \\ \frac{1}{d_{\text{min}}} & \text{for } r \leq d_{\text{min}} \end{cases}$$  \hspace{1cm} (3)

$$R_{\log}(r) = \begin{cases} -\ln r & \text{for } r > d_{\text{min}} \\ -\ln d_{\text{min}} & \text{for } r \leq d_{\text{min}} \end{cases}$$  \hspace{1cm} (4)

$$R_G(r) = \exp \left( -r^2/(2s^2) \right)$$  \hspace{1cm} (5)

The first type is motivated by the analogy to electrostatics, the second is long range and the third emphasizes a limited range for the correlation between different observations. The power $\kappa$ of the denominator in (3) and the parameter $s$ in (5) may be chosen differently for different dimensions of the sample space and different applications. For slowly varying $f_0$ a small value of $\kappa$ around 0.1 is recommended. For short range variations the test quantity with larger values around 0.3 is more sensitive.

Also the logarithmic function $R_{\log}$ is well adapted to slowly varying $f_0$. The corresponding test quantiles are invariant under the transformation $r \rightarrow ar$. For more rapidly varying $f_0$, the Gaussian weight function $R_G$ is recommended. It permits to adjust the range of the smearing to the shape of $f_0$. 

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The inverse power law and the logarithm exhibit a pole at $r$ equal to zero which could produce infinities in the double discrete version of the energy function $\phi_{NM}$. Very small distances, however, should not be weighted too strongly since deviations from $f_0$ with sharp peaks are not expected and usually inhibited by the finite experimental resolution. We eliminate the poles by introducing a lower cutoff $d_{\text{min}}$ for the distances $r$. Distances less than $d_{\text{min}}$ are replaced by $d_{\text{min}}$. The value of this parameter is not critical at all, it should be of the order of the average distance of the simulation points in the region where $f_0$ is maximum.

2.3 The distribution of the test statistic

![Energy distributions for a Gaussian weighting function (left) and a logarithmic weighting function (right) and their approximation by extended extreme value distributions.](image)

Figure 1: Energy distributions for a Gaussian weighting function (left) and a logarithmic weighting function (right) and their approximation by extended extreme value distributions.

The distribution of $\phi$ depends on the distribution function $f_0$ and on the weight function $R$. Figure 1 shows the distributions for uniform $f_0$ with Gaussian and logarithmic weight functions. The distributions are well described by a generalized extreme value distribution

$$f(x) = \frac{1}{\sigma} \left(1 + \frac{x - \mu}{\sigma} \right)^{-1/\xi - 1} \exp \left\{- \left(1 + \frac{x - \mu}{\sigma} \right)^{-1/\xi} \right\}$$

depending on three parameters, a scale parameter $\sigma$, a location parameter $\mu$, and a shape parameter $\xi$. Rather than computing these parameters from the moments of the specific $\phi$ distributions, we propose to generate the distribution of the test statistic and the quantiles
by a Monte Carlo simulation. As a consequence of the dramatic increase of computing power during the last decade, it has become possible to perform the calculations on a simple PC within minutes. There is no need to publish tables of percentage points, to distinguish between simple and composite hypotheses and also censoring can be incorporated into the simulation.

### 2.4 Relation to the Pearson $\chi^2$ test

Let us assume that we have in a certain $\chi^2$-bin $n_i$ experimental observations and $m_i$ Monte Carlo observations and $\beta = M/N \gg 1$. Then the $\chi^2$ contribution of that bin is

$$\chi_i^2 = \frac{(n_i - m_i/\beta)^2}{m_i/\beta}$$

$$= \frac{n_i^2 - 2n_im_i/\beta + m_i^2/\beta^2}{m_i/\beta}$$

For a goodness-of-fit test, an additive constant is irrelevant. Thus we can drop $m_i^2$ in the last relation. If in addition the theoretical distribution is uniform and the bins have constant size, we can also ignore the denominator.

$$\chi_i^{2'} = \frac{n_i^2}{2} - \frac{n_im_i}{\beta}$$

Up to a constant factor this last relation corresponds nearly to the energy defined in (2) for a weight function which is constant inside the bin and zero outside:

$$\phi_{NM} = \frac{n_i(n_i - 1)}{2N^2} - \frac{n_im_i}{NM} \approx \frac{1}{N^2} \chi_i^{2'}$$

The $\chi^2$ test applied to a uniform distribution $f_0$ is equivalent to an energy test with a box shaped weight function and fixed box locations.

Replacing the box function by the Gaussian weight function, the sharp cut at the bin boundaries and the arbitrary location of the boundary for fixed binning are avoided but the idea underlying the $\chi^2$ test is retained.

### 2.5 Optimization of the test parameters in a simple case

To study the dependence of the power of the test on the choice of the weight function and its parameters, we have chosen for $H_0$ a uniform, univariate p.d.f. $f_0$ restricted to the unit interval $[0, 1]$. We determined the rejection power with respect to contaminations of $f_0$ with a linear and two different Gaussian distributions which represent a wide and a more local distortion.

$$f_0 = 1$$

$$f_1(X) = 2X$$

$$f_2(X) = c_2 \exp \left( -64(X - 0.5)^2 \right)$$

$$f_3(X) = c_3 \exp \left( -256(X - 0.5)^2 \right)$$
We required 5% significance level and computed the rejection power which is equal to one minus the probability for an error of the second kind.

As a reference, we also computed the power of a $\chi^2$ test with bins of fixed width. The number of bins $B \approx 2N^{2/5}$ was chosen according to the prescription proposed in [3].

The cut-off parameter $d_{\text{min}}$ for $R_\kappa$ (power law) and $R_l$ (logarithmic) was set equal to $1/(4N)$.

In Figure 2 we show the results for samples of 100 observations for 70% contamination with $f_1$, 30% contamination with $f_2$, and 20% contamination with $f_3$. Five different values of the Gaussian width parameter $s$, four different power laws and the logarithmic weight function have been studied.

As expected, the linear distribution is best discriminated by slowly varying weight functions like the logarithm, low power laws and the wide Gaussians.

The contamination with the narrow Gaussian $f_3$ is better recognized by the narrow weight functions ($s = 1/8, \kappa = 0.3$). Here the two wide Gaussian weight functions fail completely.

Figure 3 illustrates the dependence of the rejection power on the sample size for the three different distortions (6), (7), (8) of the uniform distribution. The amount of contamination was reduced with increasing sample size.

We applied the energy tests with power law $\kappa = 0.3$, the logarithmic and two Gaussian weight functions with fixed width $s = 1/8$ (Gfix) and variable width (Gvar). The variable width was chosen such that the full width at half maximum is equal to the $\chi^2$ bin width, chosen according to the $2N^{2/5}$ law. This allows for a fair comparison between the two methods.

As expected the linear distribution is best discriminated by the energy test with logarithmic weight function. The power of the $\chi^2$ test is considerably worse. The energy test with variable Gaussian weight function follows the trend of the $\chi^2$ test but performs better in 14 out of the 15 cases.

Comparing the samples with sizes 50 and 100, respectively, we realize one of the caveats of the $\chi^2$ test: For the sample of size 50 there are 9 bins. The central bin coincides favorably with the location of the distortion peak of the background sample and consequently leads to a high rejection power. For the sample of size 100, however, there are 12 bins, thus two bins share the narrow peak and the power is reduced. The Gaussian energy test is insensitive to the location of the distortion.

3 Comparison with alternative univariate tests

We have investigated the following goodness-of-fit tests, some of which have been designed for special applications and can be found in [2]: $\chi^2$ test, Kolmogorov test, Kuiper test, Anderson-Darling test, Watson test, Neyman smooth test, Region test, Energy tests with logarithmic and Gaussian weight functions. The region test has been developed to detect localized bumps by partitioning the variate range of the order statistic into three regions.
Figure 2: Rejection power of different energy tests for a uniform distribution $f_0$ with respect to a linear distribution and two Gaussian contaminations, $exp[-64(x-0.5)^2]$ and $exp[-256(x-0.5)^2]$. 

\[ \chi^2, \text{ 12 bins} \]
Figure 3: Power of tests for 3 different contaminations to uniform distribution and 5 different sample sizes ranging from 10 to 200. The shape of the contamination is displayed on top of the columns. The type of test is indicated in the lowest left hand plot.
with expected probabilities $p_i, p_j, 1 - p_i - p_j$. For $N_i$ and $N_j$ observations observed in the first two regions, the test statistic is

$$R = \sup_{i,j} \{(N_i - Np_i)^2 + (N_j - Np_j)^2 + [N_i + N_j - N(p_i + p_j)]^2\}$$

where $N_i$ is the number of observations with $x \leq x_i$.

Samples contaminated by different background sources were tested against $H_0$, corresponding to the uniform distribution. The power of each test for a 5 % significance limit was evaluated from $10^5$ Monte Carlo simulations containing 100 observations each.

Samples with background contamination by a linear distribution, Gaussians and the following distributions displayed in Figure 4 were generated by

$$b_A(x) \propto (1 - x)^3$$

$$b_B(x) \propto \begin{cases} 
   x^2 & \text{for } 0 \leq x < 0.5 \\
   (1 - x)^2 & \text{for } 0.5 \leq x < 1 
\end{cases}$$

$$b_C(x) \propto (x - 0.5)^2$$

The power of the different tests is presented in Figure 5. As expected, none of the tests is optimum for all kind of distortions. The energy tests are quite powerful independent of the background function.

4 The energy test for two or more variates

While numerous goodness-of-fit tests exist for univariate distributions in higher dimensions only tests of the $\chi^2$ type have become popular.
Figure 5: Rejection power of tests with respect to different contaminations to the uniform distribution. The contaminations correspond to the distributions shown in the previous figure.
The extension of binning-free tests based on linear rank statistics to the multivariate case is difficult because no obvious ordering scheme of the observations exist. Sequential ordering in the different variates depends on the sequence in which the variates are chosen. In addition to this logical difficulty there is a more fundamental problem: The re-shuffling of the observations destroys the natural metric used to display the data. The situation in goodness-of-fit problems is very similar to that in pattern recognition. The possibility to detect distortions of the expected distribution by background or resolution effects depends on an appropriate selection of the random variables. The natural choice is usually given by the experiment. By mapping a multivariate space onto a space defined by the ordering recipe much of the information contained in the original distribution may be lost.

4.1 Test for bivariate Gaussian distribution

It is rather common to deal with samples of observations which are drawn from a multivariate normality. Multivariate goodness-of-fit tests have been developed mostly for multinormality. An overview can be found in [1]. An extension of the moment tests introduced by K. Pearson to two variates is Mardia’s test [2]. Skewness $\beta_1$ and kurtosis $\beta_2$ are compared to the nominal values for the normal distribution, $\beta_1 = 0$ and $\beta_2 = 3$ respectively. We compared the logarithmic and the Gaussian energy tests to Mardia’s tests and to the two-dimensional Neyman smooth test [7].

We chose a standard Gaussian

$$f_0 = \frac{1}{2\pi} \exp\left(-\frac{x^2 + y^2}{2}\right)$$

to represent the null hypothesis.

Background samples added to $f_0$ are shown in Figure 6. In addition, a uniform background in the region $(0 < X, Y < 1)$ and variations of the Gaussian background were investigated. All Gaussians have the same width in both coordinates $X$ and $Y$, but differ in the value of the width and the correlation coefficient.

Figure 7 displays the results. We were astonished how well the energy test competes with alternatives especially designed to test normality. We attribute the excellent performance of the energy test to the fact that it is sensitive to all deviations of two distributions whereas the Mardia tests are based only on two specific moments.

4.2 Example from particle physics

Figure 8 is a scatter plot of data obtained in the particle physics experiment HERA-B at DESY. The positions of tracks from $\psi$ decays are plotted against the momentum of the $\psi$ meson. The 20 square entries represent the experimental data, the black dots correspond to a Monte Carlo simulation.

We have computed the energy statistic $\phi$ with the logarithmic weighting function for the experimental data relative to the Monte Carlo prediction. Separately, the energy was determined for 100 independent Monte Carlo samples of 20 events each to estimate the
distribution of $\phi$ under $H_0$. The experimental value is larger than all Monte Carlo values (see Figure 8), indicating that the data do not follow the prediction.

5 Extensions and variations of the energy test

5.1 Normalization to probability density

The Gaussian energy test has proven to be similar but superior to the $\chi^2$ test for the uniform distribution. For non-uniform p.d.f.s the similarity can be retained by effectively dividing the elements of the sums in (2) by the p.d.f. $f_0$.

$$R(|x_i - x_j|) \to R'(|x_i - x_j|) = \frac{R(|x_i - x_j|)}{\sqrt{f_0(x_i)f_0(x_j)}}$$

If the density is only given by a Monte Carlo simulation, the density can be estimated from the volume of a multidimensional sphere in the variate space containing a fixed number of Monte Carlo observations. In the example of Figure 8 the density at $x$ could be estimated from the area $A(x)$ of the smallest circle centered at $x$ containing 10 Monte Carlo points: $f_0(x) \approx 10/A(x)$.

5.2 Width of the weighting function $R$ and metric

Some statisticians recommend to use equal probability bins for the $\chi^2$ test in one dimension. An equivalent procedure for the Gaussian energy test would be to adjust the width of the Gaussian weighting function to the p.d.f.

$$R_s(r_{ij}) \to R'_s(r_{ij}) = \exp\left(-r^2/(2s_is_j)\right)$$

$$s_i \propto 1/f_0(x_i)$$
Figure 7: Rejection power of tests with respect to different contaminations of a two-dimensional Gaussian. The uniform background is denoted by $U$, the Gaussian contamination by $N(\text{mean, st.dev.})$.

Such an adjustment can be applied independent of the dimension of the variate space while an equal probability binning is rather difficult in two or higher dimensions.

The resolution of $R$ should be adjusted to the expected deviations. The constants $s$ can be chosen differently for the different coordinates. Alternatively, a variate transformation may be performed before the test is applied.

The multi-dimensional logarithmic energy test requires a sensible choice of the metric. The distances of the observations should be about equal numerically in all directions of the variate space. This can be achieved by normalizing the variates to the square root of their variance.

### 5.3 Clustering of observations

For very large samples, the computation of $\phi$ may become excessively long even with powerful computers. A possible solution to this problem is to combine observations to clusters. The
cluster weight is equal to the sum of the observations included in the cluster and its location is their center of gravity. The details of the clustering are not important. The simplest method consists in combining points in bins formed by a simple grid. Another possibility could be the following: Observations and clusters (once clusters have been formed) are chosen randomly and combined with all points and clusters which are within a fixed maximum distance. The process is terminated when the number of clusters is below an acceptable limit.

5.4 Are two samples drawn from the same distribution?

A frequently occurring problem is to check whether two random samples belong to the same unknown parent distribution. In the framework of the “energy” concept we can use bootstrap or permutation methods to deduce a reference energy distribution. The energy computed according to (2) is then compared to this distribution. Quantiles can be used to measure the compatibility of the samples.

6 Summary and conclusions

Energy tests represent a powerful alternative to conventional tests. To our knowledge the energy test is the first multi-variate binning-free test which is independent of a subjective
ordering system. With a logarithmic weighting function it is very sensitive to long range distortions of the distribution to be tested, a situation which is frequent in physics applications. With a Gaussian weighting function the energy test has similar properties as tests of the $\chi^2$ type, but avoids arbitrary bin boundaries. It is more powerful than the $\chi^2$ test in almost all cases which we have considered. It can cope with arbitrarily small sample sizes. It is astonishing how well the energy test can compete with the Mardia test for testing normality in two dimensions.

The necessity to determine the distribution function of the test statistic for the specific application is not a serious restriction with today’s computing power.

The energy statistic can be used to test whether different samples belong to the same parent distribution. A corresponding study will be presented in a forthcoming article.

## 7 Appendix

### 7.1 Continuous case

We conjecture that $f(x) \equiv f_0(x)$ corresponds to a minimum of $\phi$ in (11). Substituting $g(x) = f(x) - f_0(x)$ we obtain

$$ \phi = \frac{1}{2} \int \int g(x)g(x')R(|x - x'|)dx dx' \geq 0 $$

where $g$ fulfills the condition $\int g(x)dx = 0$. We conjecture that $\phi$ is minimum for $g(x) \equiv 0$ for weight functions $R$ which decrease continuously with $|x - x'|$.

In the following, we sketch a prove of this conjecture without full mathematical rigor and generality.

The property (9) is invariant under a linear transformation

$$ R \rightarrow R' = \alpha R + \text{const} $$

where $\alpha$ is a positive scaling factor. Assuming that $R$ is finite, we can restrict its values to the range $-1 \leq R \leq 1$ with $R(0) = 1$. We approximate the function $g$ by a histogram with function value $g_i$ in bin $i$. The size of each bin is $\Delta^n$.

$$ \phi_h = \Delta^{2n} \sum_{i,j} g_i g_j R_{ij} $$

with self-explaining notation. The weights can be substituted by cosines, $\cos \theta_{ij} = R_{ij}$ with $\cos \theta_{ii} = 1$ in our approximation. The sum then can be written as a sum of vectors $g_i$ in $\mathbb{R}^n$:

$$ \phi_h = \Delta^{2n} \sum_{i,j} g_i g_j \cos \theta_{ij} $$

$$ \phi_h = \Delta^{2n} \left( \sum_i g_i \right)^2 \geq 0 $$

The minimum of $\phi_h$ is realized only if all $g_i$ are equal to zero.
7.2 Discrete case

When we approximate both densities \( f \) and \( f_0 \) by distributions of \( N \) points each, with weights equal \( 1/N \), we require that the energy be minimum if the two samples coincide, \( x_j = y_j \) \( \forall j \). To fulfil this condition, we have to replace the factors \( 1/(N - 1) \) and \( 1/(M - 1) \) by \( 1/N \) in \( \phi_{NM} \).

\[
\phi_{NN} = \frac{1}{N^2} \sum_{j>i} R(|x_i - x_j|) + \frac{1}{N^2} \sum_{j>i} R(|y_i - y_j|) +
- \frac{1}{N^2} \sum_{i,j} R(|x_i - y_j|)
\]

To demonstrate the minimum condition which leads to \( \phi_{NN} = 0 \), we apply an infinitesimal shift to one observation. For \( x_j = y_j \) for \( j \neq k \) and \( x_k - y_k = \delta x_k \), only the pair \( x_k, y_k \) contributes to the energy, all other terms cancel.

\[
\phi_{NN} = -\frac{1}{N^2} [R(|\delta x_k|) - R(0)]
\]

Since \( R \) decreases with its argument, \( R(0) - R(|\delta x_k|) > 0 \), we have found a local minimum of the energy.

For the special choice where \( R \) is the distance function, i.e. increasing with the distance, it has been demonstrated by [6] that \( \phi \)

\[
\phi = \frac{1}{N^2} \sum_{j>i} [|x_i - x_j| + |y_i - y_j|] - \frac{1}{N^2} \sum_i \sum_j |x_i - y_j| \leq 0
\]
is maximum for \( x_j = y_j \) for all \( j \). Since \( \phi \) is constant for constant \( R \), it is plausible that for discrete distributions \( \phi \) is minimum for \( x_j = y_j \) for all decreasing functions of the distance, and maximum for all increasing functions of the distance, however, we did not succeed in finding a general prove of this conjecture.

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