

---

# Measuring statistical dependencies via maximum norm and characteristic functions

---

Anonymous Author(s)

Affiliation

Address

email

## Abstract

In this paper we focus on the problem of statistical dependence estimation. We propose statistical dependence measure based on the maximum-norm of the absolute value of difference between joint and product-marginal characteristic functions, and its iterative estimation algorithm. The proposed measure is differentiable, can be efficiently applied to high-dimensional data, and integrated into modern machine learning pipelines. We also conduct experiments both with simulated and real data, which reveal that the proposed measure can exploit statistical dependence in non-linear data sets more efficiently, comparing to the previous work in this line of research, and that it can improve real-data classification accuracy, when applied for different tasks.

## 1 Introduction

The measurement of statistical dependence plays important role in various empirical learning methods (e.g. hypothesis testing [1], feature selection and extraction [2, 3], information bottleneck methods [4], causal inference [5], self-supervised learning [6], representation learning [7], among others). Historically, earliest statistical dependence estimation ideas (e.g. conditional probability) share nearly-common origin with the beginning of formal statistical reasoning itself. During last two centuries ideas of correlation and (relative) entropy (including various generalizations) were proposed and became very popular in numerous applications and theoretical developments. In recent years, various other approaches (e.g. [1], [9, 10], [11]) induced several lines of research of different popularity. However, with the increasing growth of machine and deep learning, new statistical dependence estimation methods, that are robust, applicable to noisy, high-dimensional, structured data, and which can be efficiently integrated with modern machine learning and deep learning methods are helpful for the development both of the theory and application.

In this article we focus on quantitative estimation of statistical dependencies, using characteristic functions. We begin with the short review of some important previous approaches (Section 2), devoting special attention to ones based on characteristic functions (Section 2.1). Afterwards, in (Section 3), we formulate the proposed measure, its empirical estimator, and conduct preliminary theoretical analysis, which are the main theoretical contribution of our paper. Section 4 is devoted to the empirical investigation of the proposed measure. Therein we conduct experiments both with simulated and real-world data sets, in order to empirically investigate its properties and applicability in various empirical inference scenarios. Finalizing Section 5 discusses and concludes this article.

## 2 Previous Work

During recent years, various approaches have been used in order to construct statistical dependence estimation methods. For example, information theory (mutual information [8], and generalisations),

reproducing kernel Hilbert spaces (Hilbert-Schmidt independence criterion [1]), characteristic functions (distance correlation [9, 10]), and other (e.g. [11] copula-based kernel dependence measures, integral-probability-metric-reliant Sobolev independence criterion [12]). Further we will focus on characteristic-function-based methods.

## 2.1 Characteristic-function-based methods

Characteristic function (CF) of  $d_X$ -dimensional random vector  $X$  defined in some probability space  $(\Omega_X, \mathcal{F}_X, \mathbb{P}_X)$  is defined as:

$$\phi_X(\alpha) := \mathbb{E}_X e^{i\alpha^T X}, \quad (1)$$

where  $i = \sqrt{-1}$ ,  $\alpha \in \mathbb{R}^{d_X}$ . Having  $n$  i.i.d. realisations of  $X$ , corresponding empirical characteristic function (ECF) is defined as:

$$\widehat{\phi}_X(\alpha) := \frac{1}{n} \sum_{j=1}^n e^{i\langle \alpha, x_j \rangle}. \quad (2)$$

Having pair of two random vectors  $(X, Y)$  defined in another probability space  $(\Omega_{X,Y}, \mathcal{F}_{X,Y}, \mathbb{P}_{X,Y})$  joint CF is defined as:

$$\phi_{X,Y}(\alpha, \beta) := \mathbb{E}_{X,Y} e^{i(\alpha^T X + \beta^T Y)}, \quad (3)$$

where  $\alpha \in \mathbb{R}^{d_X}$  and  $\beta \in \mathbb{R}^{d_Y}$ . Similarly, having  $n$  i.i.d. realisations of  $(X, Y)$ , joint ECF is defined as:

$$\widehat{\phi}_{X,Y}(\alpha, \beta) := \frac{1}{n} \sum_{j=1}^n e^{i(\langle \alpha, x_j \rangle + \langle \beta, y_j \rangle)}. \quad (4)$$

Uniqueness theorem states that two random variables  $X$  and  $Y$  have the same distribution if and only if their CF's are identical [?]. Therefore, CF's can be regarded as an alternative description of distribution. Roughly speaking, CF can be regarded as Fourier transform of probability density function (PDF).

If for all  $x \in \mathbb{R}^{d_X}$  and  $y \in \mathbb{R}^{d_Y}$  cumulative distribution function (CDF)  $F_{X,Y}(x, y)$  of  $(X, Y)$  factorises as,

$$F_{X,Y}(x, y) = F_X(x)F_Y(y), \quad (5)$$

where  $F_X(x)$  and  $F_Y(y)$  are marginal CDF's,  $X$  and  $Y$  are called independent (the same holds for probability density function, PDF). However, this criterion is impractical due to need of evaluation of potentially high-dimensional CDF or PDF, and often alternative independence criteria are more useful. Let us define

$$\Delta_{X,Y}(\alpha, \beta) := \phi_{X,Y}(\alpha, \beta) - \phi_X(\alpha)\phi_Y(\beta), \quad (6)$$

an its empirical counterpart:

$$\widehat{\Delta}_{X^n, Y^n}(\alpha, \beta) := \widehat{\phi}_{X^n, Y^n}(\alpha, \beta) - \widehat{\phi}_{X^n}(\alpha)\widehat{\phi}_{Y^n}(\beta), \quad (7)$$

where  $(X^n, Y^n) := (x_j, y_j)_{j=1}^n$ .

In terms of CF's, statistical independence of  $X$  and  $Y$  is equivalent to  $\forall \alpha \in \mathbb{R}^{d_X}, \forall \beta \in \mathbb{R}^{d_Y}, \Delta_{X,Y}(\alpha, \beta) = 0$  [18].

Previously,  $\Delta_{X,Y}(\alpha, \beta)$  was used as the basis (first in [9] for one-dimensional case, and afterwards extended and developed by [10] for bivariate multidimensional random vectors) for construction of statistical independence tests and measures. Distance covariance and distance correlation, proposed by [10] relies on weighted  $L^2$ -norm analysis of (6). They select weighting function in such a way, that dependence measure can be expressed in terms of corelection of data-dependent distances. Recent result of [13] generalises [10] to multivariable case. [14] proposed computationally efficient algorithm for estimation of distance correlation measure, reducing computational complexity from  $O(n^2)$  to  $O(n \cdot \log n)$ , where  $n$  is sample size.

**Motivation and Connection To Previous Work** Taking  $\Delta_{X,Y}(\alpha, \beta) = 0$  (6) as the criterion of statistical independence we view the work [10] from the perspective of weighted  $L^p$  spaces, measuring statistical dependence by the corresponding  $L^p$ -norms of  $|\Delta_{X,Y}(\alpha, \beta)|$  (6) (i.e.  $\|\Delta_{X,Y}(\alpha, \beta)\|_{L^p} = \int |\Delta_{X,Y}(\alpha, \beta)|^p d\alpha d\beta)^{\frac{1}{p}}$ ).

74 Taking into account that [10] in high dimensions is affected with the curse of dimensionality [15], we  
 75 focus on the limit case  $p \rightarrow \infty$  ( $L^\infty$  space), which is associated to the supremum norm. This norm  
 76 has several potential advantages.

77 We hypothesise, that its locality could be exploited to detect statistical independence more efficiently,  
 78 comparing to case  $p = 2$ . In addition, numerically calculation of  $L^\infty$  norm would not require to  
 79 directly calculate norm integral, since norm of  $L^p$  converges to supremum norm when  $p \rightarrow \infty$ . Also,  
 80 from practical point of view maximization is convenient, because it is efficiently implemented in  
 81 modern deep learning frameworks (e.g. Pytorch [16]). In addition, in our opinion it is worth to note,  
 82 that applications of characteristic functions in machine learning are quite scarce, despite that they  
 83 provide quite convenient theoretical proxy to access distributions.

### 84 3 Proposed Measure

85 The above considerations serves as the basis for constructing of a novel dependence measure, which  
 86 we further refer to as Kac independence measure (KacIM). Having two random vectors  $X$  and  $Y$ ,  
 87 KacIM is defined as

$$\kappa(X, Y) := \max_{\alpha \in \mathbb{R}^{d_X}, \beta \in \mathbb{R}^{d_Y}} |\Delta_{X,Y}(\alpha, \beta)|. \quad (8)$$

#### 88 3.1 Basic Properties

89 **Theorem 1.** *KacIM (8) has the following properties:*

- 90 1.  $\kappa(X, Y) = \kappa(Y, X)$ ,
- 91 2.  $0 \leq \kappa(X, Y) \leq 1$ ,
- 92 3.  $\kappa(X, Y) = 0$  iff  $X \perp Y$ .

93 *Proof.* Property 1. is obvious from definition (8) (commutativity of addition and multiplication), and  
 94 property 2. directly follows from Cauchy inequality and that absolute value of CF is bounded by 1:

$$\begin{aligned} |\phi_{X,Y}(\alpha, \beta) - \phi_X(\alpha)\phi_Y(\beta)|^2 &= \mathbb{E}_{X,Y} |(e^{i\alpha^T X} - \phi_X(\alpha))(e^{i\beta^T Y} - \phi_Y(\beta))|^2 \leq \\ &\mathbb{E}_{X,Y} |(e^{i\alpha^T X} - \phi_X(\alpha))|^2 |(e^{i\beta^T Y} - \phi_Y(\beta))|^2 = (1 - |\phi_X(\alpha)|^2)(1 - |\phi_Y(\beta)|^2). \end{aligned}$$

95 Property 3. directly follows from properties of CF's (see e.g. [17], Corollary 14.1)<sup>1</sup>.  $\square$

96 Although (8) is not scale invariant in general, scale invariance can be achieved by assuming standarti-  
 97 zation of  $X$  and  $Y$ .

#### 98 3.2 Estimation

99 Having i.i.d. observations  $(X^n, Y^n) := (x_j, y_j)$ ,  $j = 1, 2, \dots, n$ , an empirical estimator of (8) is  
 100 defined via corresponding ECF's (4) and (2):

$$\hat{\kappa}(X^n, Y^n) := \max_{\alpha, \beta} |\hat{\Delta}_{X^n, Y^n}(\alpha, \beta)| = \max_{\alpha, \beta} |\hat{\phi}_{X^n, Y^n}(\alpha, \beta) - \hat{\phi}_{X^n}(\alpha)\hat{\phi}_{Y^n}(\beta)|. \quad (9)$$

101 By *Levy continuity theorem* [18] ECF pointwise converges to CF. Therefore empirical estimator (9)  
 102 almost surely converges into KacIM (8). In practice, KacIM (8) can be estimated iteratively by  
 103 Algorithm 1<sup>2</sup>.

104 Algorithm 1 requires to initialise  $\alpha$  and  $\beta$ , and gradient-based (local) optimiser. In our implementation  
 105 we use uniform initialisation of parameters, and decoupled weight decay regularization optimizer [19].  
 106 We also empirically observed that normalisation of parameters  $\alpha$  and  $\beta$  on to unit sphere increases  
 107 estimation stability. After the estimation of KacIM via Algorithm 1, the evaluation the estimator has  
 108 computation complexity  $O(n)$ , where  $n$  is sample size.

<sup>1</sup>This property also is known as Kac's theorem [18]. Although it is quite simple mathematical fact, this provides the basis of the proposed measure's name.

<sup>2</sup>Pytorch [16] implementation can be accessed from [https://github.com/povidanius/kac\\_independence\\_measure](https://github.com/povidanius/kac_independence_measure)

---

**Algorithm 1** KacIM estimation

---

**Require:** Number of iterations  $N$ , batch size  $n_b$ , gradient-based optimiser  $\text{GradOpt}([parameters], \cdot)$ , initial  $\alpha \in \mathbb{R}^{d_x}, \beta \in \mathbb{R}^{d_y}$ .  
**for** iteration=1 to  $N$  **do**  
    Sample data batch  $(X^n, Y^n) := (x_i, y_i)_{i=1}^{n_b}$ .  
    Normalize  $(X^n, Y^n)$  to zero mean and unit variance (scale invariance).  
    Calculate  $\hat{\Delta}_{\alpha, \beta}((X^n, Y^n))$ .  
    Perform one maximization iteration of  $\hat{\Delta}_{\alpha, \beta}(X^n, Y^n)$ :  $\hat{\Delta}_{\alpha, \beta}(X^n, Y^n)$  via  $\alpha, \beta \rightarrow \text{GradOpt}([\alpha, \beta], \hat{\Delta}_{\alpha, \beta}(X^n, Y^n))$ .  
**end for**

---

### 109 3.3 Interpretation and connection to the related approaches

110 **Interpretation as maximum covariance.** Since (8) can be reformulated as

$$\kappa(X, Y) = \max_{\alpha, \beta} |\text{cov}(e^{i\alpha^T X}, e^{i\beta^T Y})|, \quad (10)$$

111 by Euler's formula, it corresponds to the maximum pseudocovariance between complex exponents  
112  $e^{i\alpha^T X} = \cos(\alpha^T X) + i \cdot \sin(\alpha^T X)$  and  $e^{i\beta^T Y} = \cos(\beta^T Y) + i \cdot \sin(\beta^T Y)$ . Since  $\text{var}(e^{i\alpha^T X}) =$   
113  $\phi(2\alpha) - \phi(\alpha)^2$ , one can also define the normalised version of KacIM (refine or remove this):

$$\kappa_{\text{norm}}(X, Y) = \max_{\alpha, \beta} |\text{corr}(e^{i\alpha^T X}, e^{i\beta^T Y})| = \max_{\alpha, \beta} \frac{|\text{cov}(e^{i\alpha^T X}, e^{i\beta^T Y})|}{\sqrt{|\phi_X(2\alpha) - \phi_X(\alpha)^2| |\phi_Y(2\beta) - \phi_Y(\beta)^2|}}. \quad (11)$$

114 **Interpretation in Gaussian case.** In special case when both  $X$  and  $Y$  are zero mean Gaussian  
115 random vectors we have:

$$\kappa(X, Y) = \max_{\alpha, \beta} |e^{-\frac{1}{2}(\alpha^T \Sigma_x \alpha + \beta^T \Sigma_y \beta)} (e^{-\alpha^T \Sigma_{x,y} \beta} - 1)|. \quad (12)$$

116 Assuming constant  $\alpha^T \Sigma_x \alpha$  and  $\beta^T \Sigma_y \beta$ , the maximization corresponds to the maximization of  
117  $\alpha^T \Sigma_{x,y} \beta$ , which coincides with canonical correlation analysis [21]. Here  $\Sigma_x$ ,  $\Sigma_y$ , and  $\Sigma_{x,y}$  are  
118 covariance matrices of  $X$ ,  $Y$ , and cross-covariance matrix between  $X$  and  $Y$ , respectively.

119 **Mutual information** For the neural estimation of mutual information its variational (Donsker-  
120 Varadhan) representation  $I(X, Y) = \max_{\theta} \mathbb{E}_{X,Y} f(x, y|\theta) - \log \mathbb{E}_X \mathbb{E}_Y e^{f(x,y|\theta)}$  [20] is often used,  
121 since it allows to avoid density estimation (here  $f(x, y|\theta)$  is neural network with parameters  $\theta$ ). The  
122 estimation is also iterative process, similar to Algorithm 1. In this case, optimisation is conducted  
123 over the space of neural network parameters, which often is substantially larger than the number of  
124 parameters needed to estimate KacIM (i.e.  $d_x + d_y$  parameters).

## 125 4 Experiments

126 Further we will conduct empirical investigation of KacIM in order to investigate its behaviour in  
127 simulations and practical applications.

### 128 4.1 Generated data

129 **Non-linear statistical dependence detection.** We begin with simulated multivariate data with  
130 additive and multiplicative noise.

131 Figure 1 reflects KacIM values during iterative adaptation (200 iterations). In the case of independent  
132 data, both  $x_i$  and  $y_i$  ( $d_x = 512, d_y = 4$ ) are sampled from gaussian distribution, independently. In the  
133 case of dependent data, an additive noise and multiplicative noise, the dependent variable is generated  
134 according to  $y_i = \sin(Px_i) + \cos(Px_i) + \lambda \epsilon_i$  ( $\lambda = 1.00$ ) and  $y_i = (\sin(Px_i) + \cos(Px_i))\epsilon_i$ ,  
135 respectively, where  $P$  is  $d_x \times d_y$  random projection matrix,  $\epsilon_i \sim N(0, 1)$  and  $\epsilon_i \perp x_i$ .

136 When data is independent, both in additive and multiplicative cases, due to independence, estimator (9)  
137 is resistant to maximisation, and oscillates near zero. On the other hand, when the data is not  
138 independent, the condition (6) is violated and maximization of estimator (9) is possible.

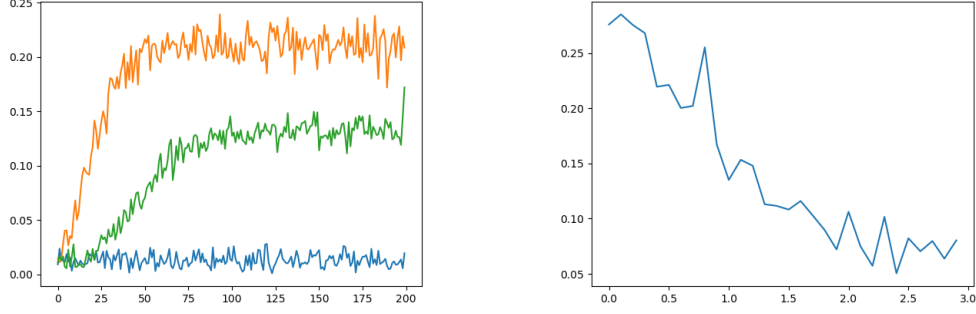


Figure 1: Left figure: KacIM evaluation for independent data (blue), additive (orange) and multiplicative (green) noise scenarios ( $x$  axis - iteration, and  $y$  - corresponding value of KacIM). Right figure: noise level ( $x$  axis) vs final iteration KacIM value ( $y$  axis). KacIM values for larger noise levels saturates as in tail of graph

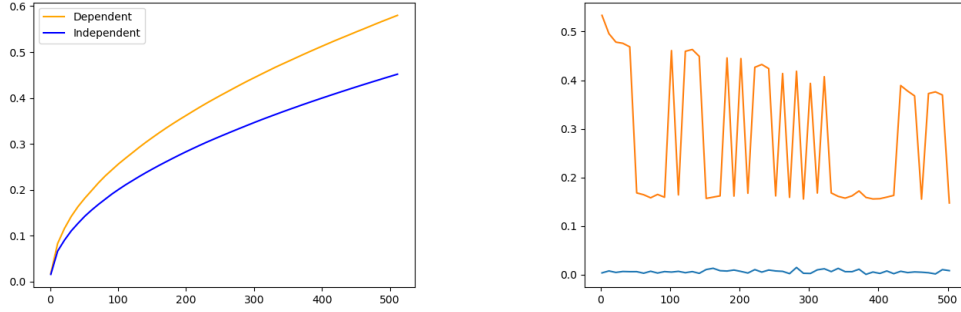


Figure 2: The dimension of data is on the  $x$  axis, and on  $y$  axis is evaluation of distance correlation (left) and KacIM (right). Blue graph corresponds of independent data of dimension, indicated by  $x$  axis, and orange one corresponds to dependent data.

139 **Noise variance effect** In this simulation we use the same additive noise setting as in previous  
 140 paragraph, but evaluate all noise levels  $\lambda \in [0.1, 3.0]$ , with step 0.1. Figure 1 empirically shows that  
 141 value of KacIM negatively correlates with noise level, and therefore the proposed measure is able not  
 142 only to detect whether independence is present, but also to quantitatively evaluate it.

143 **Comparison with distance correlation** We also evaluated distance correlation [10] on the same  
 144 generated samples of data, comparing it with KacIM. From Figure. 2 we see that as data dimensionality  
 145 grows, for independent data, the values of measure not only is significantly larger than zero, but it  
 146 also grows like values of measure of dependent data. This empirically demonstrates that distance  
 147 correlation is affected by the curse of dimensionality. On the other side, KacIM even for larger  
 148 dimensions oscillates near zero for independent data, and significantly deviates from zero for dependent  
 149 data case, as indicated in right component of Figure. 2.

## 150 4.2 Feature extraction

151 Previous work in the field of supervised feature extraction, which rely on dependency-based cost  
 152 functions, include [2, 3, 22] (HSIC),....().

153 Let us denote by  $T := (x_i, y_i)_{i=1}^N$  a supervised-learning dataset of  $N$  pairs of  $d_x$ -dimensional inputs  
 154  $x_i$ , and  $d_y$ -dimensional one-hot-encoded outputs  $y_i$ .

Dataset	$N/d_x/n_c$	Raw	KacIMFE	NCA
isolet	(7797,617,26)	0.9261	0.9437	<b>0.9477</b>
madelon	(2600,500,2)	<b>0.6015</b>	0.5484	0.5685
prnn-viruses	(61,18,4)	0.6452	0.9265	0.9355
ionosphere	(351,34,2)	0.8807	0.9278	<b>0.9375</b>
micro-mass	(360,1300,10)	0.8778	<b>0.9282</b>	0.8944
clean1	(476,168,2)	0.7689	<b>0.9888</b>	0.9790
robot-failures-lp2	(47,90,5)	0.4583	0.6067	0.5833
waveform-5000	(5000,40,3)	<b>0.8692</b>	0.8017	0.8516
spambase	(4601,57,2)	0.6906	0.8285	<b>0.8705</b>
gina-agnostic	(3468,970,2)	<b>0.8512</b>	0.7894	0.8080
scene	(2407,299,2)	0.8895	<b>0.9707</b>	0.9336
tokyo1	(959,44,2)	0.7250	0.8995	<b>0.9062</b>
one-hundred-plants-shape	(1600,64,100)	0.1013	<b>0.4913</b>	0.4688

Table 1: Classification accuracies.  $N$  denotes full data set size,  $d_x$  - input dimensionality, and  $n_c$  - number of classes. In this table feature dimension is equal to a half of original input dimension. Best accuracies that are also statistically significant (Wilcoxon’s signed rank test [25], 25 runs,  $p$ -value threshold 0.01) are indicated in bold text.

In feature extraction experiments we will use a set of classification data sets from OpenML [23], which cover different domains. We use KacIM in order to conduct supervised linear feature extraction by seeking

$$W^* = \arg \max_W \kappa(Wx, y) - \lambda \text{Tr}\{(W^T W - I)^T (W^T W - I)\}, \quad (13)$$

where the regularisation term, controlled by multiplier  $\lambda \geq 0$ , enforces semi-orthogonality of projection matrix  $W^*$ , and  $\text{Tr}\{\cdot\}$  denotes matrix trace operator.

In all the experiments (13) the cost function is optimised iteratively (250 iterations), learning rate was set to 0.007, simultaneously optimising parameters of KacIM ( $\alpha$  and  $\beta$ ) and projection matrix  $W$ . After the optimisation, the feature extraction is conducted by  $f(x) = W^*x$ , where  $x$  is original input vector, and  $f$  are corresponding feature vector.

In each experiment, we randomly split all the datasets in training and testing sets of equal size, and report accuracy, measured on the testing set as the performance measure. We set  $\lambda$  to 1.0 to quickly ensure orthogonal projection matrices, and further proceed to dependence maximization stage. In order to quantitatively evaluate features, we use logistic regression classifier accuracy, measured on the testing set. The logistic regression classifier is trained using the data from the training set.

We compare our approach with the two baselines: raw features (RAW column in Table 1) and neighborhood component analysis [24] (NCA column in Table 1).

The classification accuracies, reported in Table 1 demonstrate that KacIM-based feature extraction procedure (KacIMFE column) indeed allows to increase classification accuracy when applied to real data sets from different domains, including high-dimensional and ill-defined ones (e.g. *micro-mass* dataset). In contrast to our feature extraction approach, NCA explicitly optimises for classification accuracy, rather than more abstract dependency of features  $f(x)$  with the dependent variable  $y$ .

### 4.3 Ensemble Redundancy Regularisation

We investigate lung x-ray classification task. It is a binary classification data set, consisting of 5856 images, which should be classified as healthy or pneumonia (e.g. Figure 3). For classification we train Resnet18 with 3 classification heads, and majority voting output.

As a baseline we minimize average cross-entropy loss, on all three heads. We compare it with the same model, but which loss includes additive redundancy regularization term,  $\kappa(z_1, z_2) + \kappa(z_1, z_3) + \kappa(z_2, z_3)$ , where  $z_i$  are internal output of  $i$ -th classification head. We expect that this regularization term will make classification heads rely on independent features, thereby redundancy of (bias-variance).

Mode	Average accuracy (%)
Without regularisation	93.01
With regularisation	<b>93.34</b>

Table 2: Melanoma classification accuracy comparison of regularised and not regularised model. Bold text indicates that model with regulariser was more accurate (Wilcoxon’s signed rank test [25], 30 runs,  $p$ -value threshold 0.04))

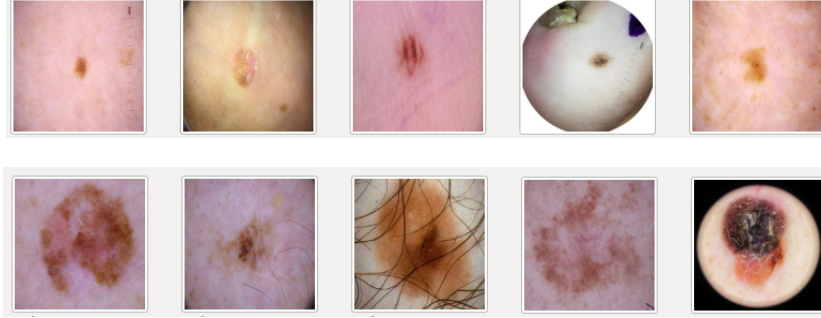


Figure 3: Top figure - benign moles, bottom figure - malignant tumors.

185 We will follow the same protocol as previously, in each experiment splitting the data into random  
186 training and testing set (in 80%/20% proportion), training both models on the first one, and testing on  
187 the second one. We compare average accuracies of both models, and evaluate statistical significance  
188 via Wilcoxon signed rank test.

#### 189 4.4 Regularisation

190 In regularisation experiments we investigate skin lesion classification task. It is a binary classification  
191 data set, consisting of 10605 images, which should be classified as benign or malignant (e.g. Figure 3).

192 We use ResNet18 backbone model (pretrained on ImageNet) with added classification head. Fur-  
193 ther we train this model with batches of 128 elements. We denote our classification network as  
194  $f(\phi(x|\theta_0)|\theta_1)$ , where  $\theta_0$  are parameters of ResNet18,  $\theta_1$  are classification head parameters, and  $x$  is  
195  $224 \times 224$  input image. For optimisation we use decoupled weight decay regularization optimizer [19]  
196 with learning rate set to 0.0002, and weight decay parameter set to 0.00001 (3 epochs). The internal  
197 learning rate of estimator (seeñefalگو) was set to 0.07 and weight decay parameters to 0.01.

198 We will investigate additive regularizer, which maximises dependency of bottleneck the feature  $\phi(x|\theta_0)$   
199 and target variable  $y$  (one-hot encoding):

$$Cost(\theta_0, \theta_1, W) := (1 - \rho)CE(f(\phi(x|\theta_0)|\theta_1), y) - \rho\kappa(\phi(x|\theta_0), y), \quad (14)$$

200 where  $CE(., .)$  is cross-entropy loss,  $\rho \geq 0$  is regularisation parameter (in our experiments  $\rho = 0.2$ ).  
201 During backward pass, this regularizer is designed to directly transfer information from  $y$  to the  
202 output ResNet18  $\phi(.\theta_0)$ , and we hypothesise that this could provide possibility to learn more  
203 discriminative features.

Mode	Average accuracy (%)
Without regularisation	93.01
With regularisation	<b>93.34</b>

Table 3: Melanoma classification accuracy comparison of regularised and not regularised model. Bold text indicates that model with regulariser was more accurate (Wilcoxon’s signed rank test [25], 30 runs,  $p$ -value threshold 0.04))

204 In each experiment we train classifier 30 times with randomly splitted training and testing data  
 205 (9000 images for training, and 1605 for testing). The average accuracies reported in Table 3, that  
 206 application (14) slightly (but with statistical significance) increased classification accuracy.

## 207 5 Conclusion

208 In this article we propose statistical dependence measure, KacIM, which corresponds to the  $L^\infty$  norm  
 209 of the absolute value of difference between joint characteristic function and the product of marginal  
 210 ones. The proposed measure, in theory can detect non-linear statistical dependence between a pairs  
 211 of random variables of possibly different dimension, extended to various directions (e.g. kernels,  
 212 multiple variables), applied to several machine learning tasks (e.g. feature extraction, regularisation,  
 213 among others). On the other side, it raises a corresponding set of unanswered questions, both  
 214 theoretical and empirical.

215 For example, although it converges, the variance of the estimator sometimes is high and it is still  
 216 remains unclear how to control it, also the interpretability when it approaches its maximal value  
 217 remains insufficiently clear. However empirical experiments with simulated data reveals, that  
 218 increasing independence between two random variables is reflected in a decreasing trend on the  
 219 estimated values of the proposed dependence measure(e.g. Figure 1).

220 Therefore, parameter initialization, meta-parameter (e.g. stopping criteria, batch size) selection are  
 221 needed in order to evaluate it efficiently.

222 Beside demonstrated applications in Section 4, the proposed measure is differentiable and thereby can  
 223 be integrated with various modern deep-learning methods, applied to high-dimensional and structured  
 224 data. We see exploration and comparative analysis of KacIM in causality, information bottleneck  
 225 theory, self-supervised learning, and other modern problems, where dependence measures define a  
 226 criterion of optimisation, as future work.

## 227 6 Acknowledgements

228 We sincerely thank Dr. Pranas Vaitkus, Dr. Linas Petkevičius, Dr. Aleksandras Voicikas, and  
 229 colleagues from Neurotechnology for discussions. We also thank Neurotechnology for supporting  
 230 this research.

## 231 References

## 232 References

- 233 [1] Arthur Gretton, Olivier Bousquet, Alex Smola, and Bernhard Schölkopf. Measuring Statistical Dependence  
 234 with Hilbert-Schmidt Norms. In *ALT*, 2005.
- 235 [2] Daniušis, P. and Vaitkus, P. Supervised Feature Extraction Using Hilbert-Schmidt Norms. In Corchado,  
 236 Emilio and Yin, Hujun, editor, *Intelligent Data Engineering and Automated Learning - IDEAL 2009*, pages  
 237 25–33, Berlin, Heidelberg, 2009. Springer Berlin Heidelberg.
- 238 [3] P. Daniušis, Pr. Vaitkus, and L. Petkevičius. Hilbert–Schmidt component analysis. *Lithuanian mathematical*  
 239 *journal*, 57(A):7–11, Dec. 2016.
- 240 [4] Kurt Wan-Duo Ma, J. P. Lewis, and W. Kleijn. The hsc bottleneck: Deep learning without back-propagation.  
 241 *ArXiv*, abs/1908.01580, 2020.
- 242 [5] Patrik Hoyer, Dominik Janzing, Joris M Mooij, Jonas Peters, and Bernhard Schölkopf. Nonlinear causal  
 243 discovery with additive noise models. In D. Koller, D. Schuurmans, Y. Bengio, and L. Bottou, editors,  
 244 *Advances in Neural Information Processing Systems*, volume 21. Curran Associates, Inc., 2009.
- 245 [6] Yazhe Li, Roman Pogodin, Danica J. Sutherland, and Arthur Gretton. Self-supervised learning with kernel  
 246 dependence maximization. In *Thirty-Fifth Conference on Neural Information Processing Systems*, 2021.
- 247 [7] Ruggero Ragonesi, Riccardo Volpi, Jacopo Cavazza, and Vittorio Murino. Learning Unbiased Representations via Mutual Information Backpropagation. *2021 IEEE/CVF Conference on Computer Vision and Pattern Recognition Workshops (CVPRW)*, pages 2723–2732, 2021.



- [8] Thomas M. Cover and Joy A. Thomas. *Elements of Information Theory 2nd Edition (Wiley Series in Telecommunications and Signal Processing)*. Wiley-Interscience, July 2006.
- [9] Andrey Feuerverger. A Consistent Test for Bivariate Dependence. *International Statistical Review / Revue Internationale de Statistique*, 61(3):419–433, 1993.
- [10] Gábor J. Székely, Maria L. Rizzo, and Nail K. Bakirov. Measuring and testing dependence by correlation of distances. *The Annals of Statistics*, 35(6):2769 – 2794, 2007.
- [11] Barnabás Póczos, Zoubin Ghahramani, and Jeff G. Schneider. Copula-based Kernel Dependency Measures. *ArXiv*, abs/1206.4682, 2012.
- [12] Mroueh, Youssef and Sercu, Tom and Rigotti, Mattia and Padhi, Inkit and Nogueira dos Santos, Cicero. Sobolev Independence Criterion. In *Advances in Neural Information Processing Systems 32*, editor = H. Wallach and H. Larochelle and A. Beygelzimer and F. d'Alché-Buc and E. Fox and R. Garnett, pages 9505–9515. Curran Associates, Inc., 2019.
- [13] Björn Böttcher, Martin Keller-Ressel, and René Schilling. Distance multivariate: New dependence measures for random vectors, 10 2018.
- [14] Arin Chaudhuri and Wenhao Hu. A fast algorithm for computing distance correlation. *Computational Statistics and Data Analysis*, 135:15–24, 2019.
- [15] Dominic Edelmann, Konstantinos Fokianos, and Maria Pitsillou. An Updated Literature Review of Distance Correlation and Its Applications to Time Series. *International Statistical Review*, 87(2):237–262, August 2019.
- [16] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems 32*, pages 8024–8035. Curran Associates, Inc., 2019.
- [17] Jacod Jean. *Probability essentials / Jean Jacod, Philip Protter*. Universitext. Springer, Berlin Heidelberg New York, 2nd edition edition, 2003.
- [18] Johan Kustermans J. Martin Lindsay Michael Schuermann Uwe Franz David Applebaum, B.V. Rajarama Bhat. Quantum Independent Increment Processes I: From Classical Probability to Quantum Stochastic Calculus. 2005.
- [19] Ilya Loshchilov and Frank Hutter. Decoupled Weight Decay Regularization. In *ICLR*, 2019.
- [20] Mohamed Ishmael Belghazi, Aristide Baratin, Sai Rajeshwar, Sherjil Ozair, Yoshua Bengio, Aaron Courville, and Devon Hjelm. Mutual Information Neural Estimation. In Jennifer Dy and Andreas Krause, editors, *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 531–540. PMLR, 10–15 Jul 2018.
- [21] Bernhard Schölkopf, Alexander J. Smola, and Francis Bach. *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*. The MIT Press, 2018.
- [22] Yin Zhang and Zhi-Hua Zhou. Multilabel dimensionality reduction via dependence maximization. *ACM Trans. Knowl. Discov. Data*, 4(3), oct 2010.
- [23] Joaquin Vanschoren, Jan N. van Rijn, Bernd Bischl, and Luis Torgo. Openml: Networked science in machine learning. *SIGKDD Explorations*, 15(2):49–60, 2013.
- [24] Jacob Goldberger, Geoffrey E Hinton, Sam Roweis, and Russ R Salakhutdinov. Neighbourhood Components Analysis. In L. Saul, Y. Weiss, and L. Bottou, editors, *Advances in Neural Information Processing Systems*, volume 17. MIT Press, 2004.
- [25] Wilcoxon, Frank. *Individual Comparisons by Ranking Methods*, pages 196–202. Springer New York, New York, NY, 1992.

## A Appendix

Optionally include extra information (complete proofs, additional experiments and plots) in the appendix. This section will often be part of the supplemental material.