

Schoenberg-Rao Distances: Entropy-based and Geometry-aware Statistical Hilbert Distances

Gaëtan Haderes^{*†1} and Frank Nielsen^{*2}

¹Sony Computer Science Laboratories, Paris

²Sony Computer Science Laboratories, Tokyo

Abstract

Distances between probability distributions that take into account the geometry of their sample space, like the Wasserstein or the Maximum Mean Discrepancy (MMD) distances have received a lot of attention in machine learning as they can, for instance, be used to compare probability distributions with disjoint supports. In this paper, we study a class of statistical Hilbert distances that we term the Schoenberg-Rao distances, a generalization of the MMD that allows one to consider a broader class of kernels, namely conditionally negative semi-definite kernels. In particular, we introduce a principled way to construct such kernels and derive novel closed-form distances between mixtures of Gaussian distributions, among others. These distances, derived from the concave Rao’s quadratic entropy, enjoy nice theoretical properties and possess interpretable hyperparameters which can be tuned for specific applications. Our method constitutes a practical alternative to Wasserstein distances and we illustrate its efficiency on a broad range of machine learning tasks such as density estimation, generative modeling and mixture simplification.

1 Introduction

Choosing a suitable statistical distance [11, 2] based on first principles is essential to ensure the relevancy and effectiveness of tasks in machine learning. Various statistical distances have been proposed in the literature, starting with the early days of Mahalanobis [22]. Later, these statistical distances have been studied under the umbrella of families of statistical distances called divergences: The Csiszár f -divergences [9] $I_f(p||q) = \int p(x)f(q(x)/p(x))dP(x) = I_{f^*}(q||p)$ defined for a convex generator $f(u)$ with $f(1) = 0$ (including the total variation metric for

^{*}Equal contribution

[†]gaetan.haderes@sony.com

$f(u) = |u - 1|$ and the Kullback-Leibler (KL) divergence for $f(u) = -\log u$ with conjugate generator $f^*(u) = uf(1/u)$, the Bregman divergences [6], the Jensen divergences (also called Burbea-Rao divergences [7]), etc. From the viewpoint of statistical invariances, f -divergences are the only invariant separable divergences in information geometry [1]: They are kept unchanged under a diffeomorphism of the sample space (and sufficient statistics) and under a smooth one-to-one mapping of the parameter space of parametric families of distributions [24]. However, those entropy-based distances do not take into account the geometry of the sample space, and are infinite when the distribution supports are disjoint except for bounded f -divergences with $f(0) + f^*(0) < \infty$ like the Jensen-Shannon divergence used in GANs [16].

Many algorithms in machine learning are based on dot product similarities or squared Euclidean dissimilarities. Those algorithms can be easily extended to reproducing kernel Hilbert spaces using the kernel trick [23, 33] of positive-definite kernels. However, although the induced Hilbert distances $D(x, y) = \|x - y\|_H$ for a Hilbert norm are translation-invariant, this is not the case of the dot-product which depends on a reference point. Thus, [32, 5] proposed to use the broader class of conditionally positive-definite (CPD) kernels l which include the positive-definite (PD) kernels and for which can define an associated dissimilarity $D_l(x, y) = l(x, x) + l(x, y) - 2l(x, y)$. When $l(x, x) = 0$, we have $D_l(x, y) = -l(x, y)$ and $\sqrt{D_l}$ yields a metric. In order to use the geometry of the sample space via a ground distance, Integral Probability Metrics [34] (IPMs) have been broadly used in ML: Wasserstein distances and its fast Sinkhorn divergences [15], Maximum Mean Discrepancy [17] (MMD), etc. Recently, geometry-aware information-theoretic (GAIT) divergences which rely on Bregman or Jensen divergences for geometry-aware strictly concave entropic generators [20] have been convincingly demonstrated for many ML tasks [14]. However, GAIT divergences relies on a crucial conjecture about the convexity of a kernelized Rényi divergence. Except for the trivial identity kernel, it is an open (hard) problem to prove the concavity of this entropy and the well-formedness of the induced Bregman/KL divergences. In contrast, we choose the Rao quadratic entropy [25, 26, 27, 19] which is geometry-aware and proven concave for Euclidean metric kernels (isometrically Hilbert-embeddable distances) to build a generalization of both the Mahalanobis and the MMD distances. These geometry-aware statistical distances are particularly useful in GANs [16] as the data being modeled is often considered to be lying on a low-dimensional manifold, a framework in which the KL divergence proved to be ill-adapted.

Our contribution is the following: we propose to focus on an existing class of statistical distances which we term the Schoenberg-Rao distances. They are entropy-based, theoretically sound and take into account the geometry of the sample space. We first introduce the Conditionally Negative Semi-Definite kernels (CNSD) and show that they are a natural relaxation of positive-definite (PD) kernels when working with normalized probability distributions. As a by-product, we obtain a principled way to construct novel CSND kernels for families of probability distributions and, in particular, we obtain a new closed-form distance between mixtures of univariate Normal distributions. We conclude

by showcasing a wide range of applications in which these distances play an interesting role¹.

2 Schoenberg-Rao distances

In the following, we denote by \mathcal{X} the sample space which can be either discrete or continuous, and $P(\mathcal{X})$ the set of probability distributions over \mathcal{X} .

2.1 Conditionally negative semi-definite kernels

We start with the following definition:

Definition 2.1 (Conditionally negative semi-definite kernel). *Let $d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a symmetric kernel (i.e. $d(x, y) = d(y, x)$) for all $x, y \in \mathcal{X}$). We call the function d a conditionally negative semi-definite kernel (CNSD) if*

$$\sum_{i=1}^n \sum_{j=1}^n c_i c_j d(x_i, x_j) \leq 0, \quad (1)$$

for all $n \geq 2$ and all $x_i \in \mathcal{X}$ and $c_i \in \mathbb{R}$ with $i \in [1, n]$ such that

$$\sum_{i=1}^n c_i = 0. \quad (2)$$

The difference with the usual definition of negative semi-definite kernel (NSD) is that Eq. 1 needs only be verified for the c_i 's verifying Eq. 2. With this definition, it is immediate that a negative semi-definite kernel is also conditionally negative semi-definite and so CNSD kernels generalize NSD kernels. In the following, we use the notational shortcut $d_{ij} := d(x_i, x_j)$. The difference between CNSD and NSD kernels can be appreciated with the following simple example:

Example 2.1. *Any constant function $d(x, y) = a$ with $a \in \mathbb{R}$ defines a CNSD kernel since*

$$\sum_{i=1}^n \sum_{j=1}^n c_i c_j a = a \left(\sum_{i=1}^n c_i \right)^2 = 0,$$

due to Eq. 2. This function is NSD iff $a \leq 0$.

We chose the unusual notation d for a CNSD kernel due to the following proposition:

Proposition 2.1 (The squared Euclidean norm is CNSD). *For $\mathcal{X} = \mathbb{R}^d$ for some $d \geq 1$, let $d(x, y) = \|x - y\|^2$ be the squared Euclidean norm. The kernel d is CNSD since*

$$\sum_{i=1}^n \sum_{j=1}^n c_i c_j \|x_i - x_j\|^2 = 2 \left(\sum_{i=1}^n c_i \right) \sum_{j=1}^n c_j \|x_j\|^2 - 2 \left(\sum_{i=1}^n c_i x_i \right)^2 \leq 0 \quad (3)$$

¹Our code is available at <https://github.com/Ghadjeres/schoenberg-rao>

The squared Euclidean norm consists of the prototypical example of CNSD kernels. We shall see in Sect. 2.7 composition rules to create new CSND kernels from existing ones and derive new CNSD kernels. In the following, we will always consider kernels that embody a notion of distance so that we always have $d(x, x) = 0$ and $d \geq 0$.

The next propositions show important links between CNSD kernels and NSD kernels:

Proposition 2.2 (Connection between CNSD and NSD kernels [3]). *For any base point $x_0 \in \mathcal{X}$, the kernel \tilde{d} defined by*

$$\frac{\tilde{d}(x, y)}{2} := d(x, y) - d(x, x_0) - d(y, x_0) + d(x_0, x_0) \quad (4)$$

is NSD iff d is CNSD.

Proposition 2.3 (Characterisation of CNSD [3]). *The kernel $\exp(td)$ is positive semi-definite for all $t > 0$ iff d is CNSD.*

Using Prop. 2.1 and Prop. 2.3, we readily obtain that the RBF kernel is positive semi-definite.

CNSD kernels naturally appeared in the context of Euclidean distance geometry [21] when studying the following problem: given a collection of distances $d_{ij} = d_{ji} \geq 0$ for $i, j \in [1, n]$ with $d_{ii} = 0$, does there exist points $x_i \in \mathbb{R}^m$ for some fixed dimension m such that $d_{ij} = \|x_i - x_j\|^2$? The answer to this problem is given by Schoenberg's theorem [30]:

Theorem 2.1 (Schoenberg's embedding theorem [31]). *Let $d_{ij} = d_{ji} \geq 0$ for $i, j \in [1, n]$ with $d_{ii} = 0$. There exists a Euclidean embedding, i.e. $m > 0$ and $x_i \in \mathbb{R}^m$ such that $d_{ij} = \|x_i - x_j\|^2$ iff the matrix $d = [d_{ij}]$ is CNSD.*

This result is the converse of Prop. 2.1.

2.2 Schoenberg-Rao distances from Rao's quadratic entropies

A NSD matrix \tilde{d} naturally defines a *concave* function \tilde{H} via

$$\tilde{H}(p) = \tilde{H}(p_1, \dots, p_n) := \sum_{i=1}^n \sum_{j=1}^n p_i p_j \tilde{d}_{ij}, \quad (5)$$

for the p_i 's in \mathbb{R} . Using Prop. 2.2, we obtain a concave function \tilde{H} from a CNSD kernel d by considering its associated NSD kernel \tilde{d} given by Eq. 4. Using the symmetry of d and the fact that $d_{ii} = 0$ this can be written as

$$\tilde{H}(p) := 2 \sum_{i=1}^n \sum_{j=1}^n p_i p_j d_{ij} - 4 \left(\sum_{j=1}^n p_j \right) \sum_{i=1}^n p_i d_{i0}. \quad (6)$$

Finally, we can define a divergence based on the concave function \tilde{H} by considering the Jensen difference:

$$\begin{aligned} J(p, q) &:= \tilde{H}\left(\frac{p+q}{2}\right) - \frac{1}{2}\tilde{H}(p) - \frac{1}{2}\tilde{H}(q) \\ &= \sum_{i,j=1}^n p_i q_j d_{ij} - \frac{1}{2} \sum_{i,j=1}^n p_i p_j d_{ij} - \frac{1}{2} \sum_{i,j=1}^n q_i q_j d_{ij} \\ &\quad - \left(\sum_{i=1}^n p_i - \sum_{i=1}^n q_i \right) \left(\sum_{i=1}^n (p_i - q_i) d_{i0} \right) \geq 0. \end{aligned} \quad (7)$$

By definition, we have $J(p, p) = 0$ for all p . However, since the function \tilde{H} is only concave (and not strictly concave), the divergence defined above is not guaranteed to be a proper divergence (i.e. that $J(p, q) = 0$ implies $p = q$). We will see in Sect. 3 examples where such a construction leads to an improper divergence.

An important observation in Eq. 7 is that if $\sum_{i=1}^n p_i = \sum_{i=1}^n q_i$, the last term cancels and removes the dependence on the base point $x_0 \in \mathcal{X}$. A CNSD kernel d thus defines a unique divergence denoted by SR_d on the space of probability distributions over $\mathcal{X} = \{x_1, \dots, x_n\}$:

$$\text{SR}_d(p, q) := \sum_{i,j=1}^n p_i q_j d_{ij} - \frac{1}{2} \sum_{i,j=1}^n p_i p_j d_{ij} - \frac{1}{2} \sum_{i,j=1}^n q_i q_j d_{ij}. \quad (8)$$

In fact, we just proved the following:

Proposition 2.4 (Equivalence between d CNSD and SR_d positive). *On the space of probability distributions over $\mathcal{X} = \{x_1, \dots, x_n\}$, there is equivalence between*

1. *Eq. 8 is positive for all $p, q \in P(\mathcal{X})$,*
2. *the kernel d is CNSD.*

If the distance SR appeared in some works in ecology [8], it was never named as it was not used directly as a distance on probability measures. We propose to term it *Schoenberg-Rao distance* due to its relation with Schoenberg's embedding theorem and Rao's quadratic entropy which is defined as follows:

Definition 2.2 (Rao's quadratic entropy [25, 26, 19]). *The Rao's quadratic entropy H_d of a probability measure $p \in P(\mathcal{X})$ is defined as*

$$H_d(p) := \sum_{i=1}^n \sum_{j=1}^n p_i p_j d_{ij}, \quad (9)$$

where d is a CNSD matrix. We also note

$$H_d(p, q) = \sum_{i=1}^n \sum_{j=1}^n p_i q_j d_{ij}, \quad (10)$$

so that $\text{SR}_d(p, q) := H_d(p, q) - \frac{1}{2}H_d(p) - \frac{1}{2}H_d(q) \geq 0$.

This entropy was mainly studied in the context of diversity measures in ecology [4, 28] where a distance between species is to be taken into account. It possesses an intrinsic meaning for probability distributions and we could have used it directly, instead of \tilde{H} , to compute the Jensen difference of Eq. 7.

The Schoenberg-Rao distance possesses interesting properties: it is always *bounded* and can be used to compare distributions with *disjoint supports*. This contrasts with the Kullback-Leibler divergence which is unbounded and infinite when the supports do not match. In particular, for p defined on n atoms and q defined on m disjoint atoms, the complexity of computing Eq. 8 is $O(\max(n^2, m^2))$. This distance can also be used to optimize the location of the atoms x_i in some applications. It is geometry-aware, in the sense that the geometry of the sample space is used to create a distance over probability distributions. For instance, the SR distance between two Dirac distributions over two distinct atoms x_i and x_j is simply d_{ij} . Such properties make it close to the Wasserstein distances, but the SR distance has always a *simple formulation* which does not require optimization procedures to be run (i.e. optimal transport).

We note that all sums in Sect. 2.2 can be replaced by integrals and the discrete distributions by continuous ones. In particular, the definition of the Schoenberg-Rao distances becomes

Definition 2.3 (Schoenberg-Rao distance). *When p and q are probability density functions, The Schoenberg-Rao distance SR_d with base CNSD kernel d can be written as*

$$\begin{aligned} \text{SR}_d(p, q) &= \int \int p(x)q(y)d_{xy}dx dy \\ &\quad - \frac{1}{2} \int \int p(x)p(y)d_{xy}dx dy - \frac{1}{2} \int \int q(x)q(y)d_{xy}dx dy. \end{aligned} \quad (11)$$

The above equation is also valid for any probability distribution P , by replacing the $p(x)dx$ terms in the integrals by $dP(x)$.

2.3 Properties of Rao's quadratic entropy

We now discuss some properties of Rao's quadratic entropy. We first show that we can fuse atoms that are identical with the following propositions:

Proposition 2.5 (Grouping of atoms). *Let d be a CNSD kernel over n atoms x_i . We denote by $C = (C_1, \dots, C_L)$ a partition of the atoms x_i such that for all $l \in [1, L]$, we have $x_i = x_j$ for all $x_i, x_j \in C_l$. Then $H_d(p) = H_d(p')$, where $p'(C_l) = \sum_{x_i \in C_l} p_i$ and $d(C_l, C_{l'}) := d(x_i, x_j)$ for any $x_i \in C_l$ and $x_j \in C_{l'}$.*

Next, we mention that the Rao's quadratic entropy of independent variables is a sum of the Rao's quadratic entropies.

Proposition 2.6 (Rao's quadratic entropy for independent variables). *Let \mathcal{X}, \mathcal{Y} be two sample spaces and consider $p(x, y) = p(x)p(y)$ a joint distribution of*

independent variables. Then the Rao's quadratic entropy H_d of $p(x, y)$ is a sum of the Rao's quadratic entropies for $p(x)$ and $p(y)$ if the CNSD kernel d is separable, i.e. if we have

$$d((x, y), (x', y')) := d_x(x, x') + d_y(y, y'),$$

for some CNSD kernels d_x and d_y for all $x, x' \in \mathcal{X}$ and $y, y' \in \mathcal{Y}$.

2.4 Constructing CNSD kernels

Up so far, the only non trivial example of CNSD kernel we mentioned was the squared Euclidean distance. In this section, we mention classical results on how to create novel CNSD kernels. We then demonstrate a novel way to create CNSD kernels using the SR distances.

Proposition 2.7 (Composition rules for CNSD kernels [3]). *Let $d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$ be CNSD. Then, for all $\alpha \in [0, 1[$, d^α and $\log(1 + d)$ are CNSD kernels. Also, the sum of CNSD kernels is CNSD and so is the multiplication by a positive constant of a CNSD kernel.*

In particular, using Prop. 2.1 and 2.7, we readily obtain that the (non-squared) Euclidean metric is CNSD.

We now prove a principled method to obtain symmetric distances over the parameter space of a family of parametrized distributions.

Theorem 2.2 (The Schoenberg-Rao distance defines a CNSD kernel). *Let \mathcal{F} be a family of probability distributions over \mathcal{X} and let d be a CNSD kernel defined on \mathcal{X} . Then $\text{SR}_d : \mathcal{F} \times \mathcal{F} \rightarrow \mathbb{R}^+$ defined in Eq. 8 is a CNSD kernel over \mathcal{F} .*

Proof. For all $n, n' > 1$, let $g_i, g'_j \in \mathcal{F}$ for $i \in [1, n]$, $j \in [1, n']$ and π, π' be probability distributions over $[1, n]$ and $[1, n']$ respectively. We then note that

$$\text{SR}_{\text{SR}_d}(\pi, \pi') = \text{SR}_d \left(\sum_{i=1}^n \pi_i g_i, \sum_{j=1}^{n'} \pi'_j g'_j \right) \geq 0, \quad (12)$$

which is positive by Eq. 7 since the two mixture distributions $\sum_{i=1}^n \pi_i g_i$ and $\sum_{j=1}^{n'} \pi'_j g'_j$ have equal mass. Using Prop. 2.4, we obtain that SR_d defines a CNSD kernel over \mathcal{F} . \square

Corollary 2.2.1 (The square root of SR is a metric). *In particular, using Thm. 2.1 we obtain that $\sqrt{\text{SR}_d}$ is a metric distance over \mathcal{F} when SR_d verifies the discernability axiom. In particular, it verifies the triangle inequality.*

Theorem 2.2 thus provides a simple method to leverage a metric distance over a sample space into a metric distance over probability distributions. We investigate in Sect. 3 how the choice of the base CNSD kernel d influences the resulting metric $\sqrt{\text{SR}_d}$ over the probability distributions. Combined with the different composition rules of Prop. 2.7, this theorem allows us to construct a wide variety of metrics over mixture distributions for instance. We still note that if the divergence is not proper, the law of the indiscernible may not be verified.

3 Examples

We now illustrate some examples for which the SR_d of Eq. 11 can be computed in closed-form. This includes the case of Gaussian distributions with d being the squared and non-squared Euclidean metric, the case of the Laplace distributions and the case of the SR distance between discrete and continuous distributions. All proofs can be found in the appendix. In the following, we note $\mathcal{N}(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ the density of the univariate Normal distribution with mean μ and variance σ^2 .

Example 3.1 (Gaussian distributions, d squared Euclidean distance). *When $d(x, y) = (x - y)^2$, the SR_d distance between two Normal distributions is*

$$\text{SR}_d(\mathcal{N}(x; \mu_1, \sigma_1), \mathcal{N}(x; \mu_2, \sigma_2)) = (\mu_1 - \mu_2)^2. \quad (13)$$

The Rao's quadratic entropy of a Gaussian distribution is

$$H_d(\mathcal{N}(x; \mu, \sigma)) = 2\sigma^2. \quad (14)$$

We see that this is not a proper divergence since $\text{SR}_d(\mathcal{N}(x; \mu_1, \sigma_1), \mathcal{N}(x; \mu_2, \sigma_2)) = 0$ only implies the equality only between the means. We note that this is not in contradiction with Schoenberg's theorem Thm. 2.1 since $\sqrt{|\mu_1 - \mu_2|^2}$ is indeed a distance over \mathbb{R} . In this particular case, the Euclidean embedding Φ is explicit, non injective, and given by $\Phi(\mathcal{N}(x; \mu, \sigma)) = \mu$.

In fact, we can write the explicit formula for $\text{SR}_d(p, q)$ for the squared Euclidean kernel for any distributions p and q :

Example 3.2 (d squared Euclidean distance for general distributions). *When $d(x, y) = (x - y)^2$, the SR_d distance between two distributions only depend on the first moments:*

$$\text{SR}_d(p, q) = (\mathbb{E}_p[X] - \mathbb{E}_q[X])^2, \quad (15)$$

and Rao's quadratic entropy equals twice the variance:

$$H_d(p) = 2\mathbb{E}_p[X^2] - 2(\mathbb{E}_p[X])^2 = 2\mathbb{V}_p(X). \quad (16)$$

We shall see that considering the squared Euclidean distance as the base CNSD kernel appears to lead to degenerate cases for the SR_d distance. Indeed it can be proved that, for d the squared Euclidean metric, d^α is CNSD iff $\alpha \in [0, 1]$ [3]. We conjecture that for all other cases considered, SR defines a proper divergence.

In particular, we now look at the case where d is the Euclidean distance. By Prop. 2.7 it defines a CNSD as well.

Example 3.3 (Gaussian distributions, d euclidean distance). *When $d(x, y) = |x - y|$, the SR_d distance between two Normal distributions $p(x) = \mathcal{N}(x; \mu_1, \sigma_1)$*

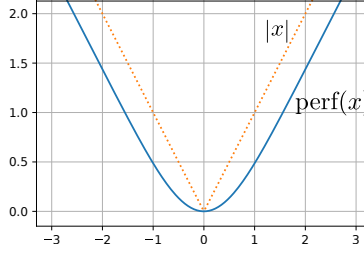


Figure 1: Graphs of the perf function Eq. 62 (full line) and of the absolute value (dotted line).

and $q(x) = \mathcal{N}(x; \mu_2, \sigma_2)$ is:

$$\begin{aligned} \text{SR}_d(p, q) = & \sqrt{2} \sqrt{\sigma_1^2 + \sigma_2^2} \text{perf} \left(\frac{\mu_2 - \mu_1}{\sqrt{2} \sqrt{\sigma_1^2 + \sigma_2^2}} \right) \\ & + \sqrt{\frac{2}{\pi}} \sqrt{\sigma_1^2 + \sigma_2^2} - \frac{\sigma_1 + \sigma_2}{\sqrt{\pi}}, \end{aligned} \quad (17)$$

where we denoted by perf (for primitive of the error function) the integral of the error function erf which equals zero in 0:

$$\text{perf}(x) = x \text{erf}(x) + \frac{e^{-x^2} - 1}{\sqrt{\pi}}. \quad (18)$$

The Rao's quadratic entropy in this case is given by:

$$H_d(\mathcal{N}(x; \mu, \sigma)) = \frac{2\sigma}{\sqrt{\pi}}. \quad (19)$$

Considering the Euclidean distance as the base kernel provides more interesting results since we obtain a *proper divergence* satisfying the law of indiscernibles so that $\sqrt{\text{SR}_d(p, q)}$ is a metric distance on the family of 1D Gaussian distributions. The perf function which appears in Eq. 17 has interesting properties: it is an even function with a linear growth, since $\lim_{x \rightarrow \infty} \text{erf}(x) = 1$. We plot its graph in Fig. 1 and compare it with the absolute value function.

It is also worth noting that the second line in the SR_d expression of Eq. 17 is itself a CNSD kernel acting solely on the σ parameters. It can be interpreted as $\frac{2}{\sqrt{\pi}}(Q(\sigma_1, \sigma_2) - A(\sigma_1, \sigma_2))$, where $Q(a, b) = \sqrt{\frac{a^2 + b^2}{2}}$ stands for the quadratic mean and $A(a, b) = \frac{a+b}{2}$ stands for the arithmetic mean (with $Q(a, b) \geq A(a, b)$). To the best of our knowledge, we think that this distance between Normal distributions is novel and provides an interesting alternative to usual distances over Normal distributions (like the Wasserstein distance or the Hellinger distance).

Example 3.4 (Mixture of Gaussian distributions). *The proof of Thm. 2.2 provides a way to construct a distance over the space of mixtures of Normal*

distributions: for two mixtures $p(x) = \sum_{i=1}^n \pi_i g_i(x)$ and $q(x) = \sum_{i=1}^n \pi_i g_i(x)$, where the mixture components g_i are Gaussian distributions, we have (by linearity of the integrals)

$$\begin{aligned} \text{SR}_d(p, q) &= \sum_{i=1}^n \sum_{j=1}^n \pi_i \pi_j' \text{SR}_d(g_i, g_j) \\ &- \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \pi_i \pi_j \text{SR}_d(g_i, g_j) - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \pi_i' \pi_j' \text{SR}_d(g_i, g_j). \end{aligned} \quad (20)$$

This yields a closed-form formula in the case where d is the squared Euclidean distance (Eq. 3.1) or the Euclidean distance (Eq. 3.3). This expression includes the case where the two mixtures have different components since some of the π_i 's can be zero. Note that it is also possible to consider other CNSD kernels in the r.h.s. of Eq. 20 like SR_d^α for $0 < \alpha < 1$ due to Prop. 2.7. Finding closed-form formulae for statistical mixture distances have been considered in many applications but the SR distance is geometric-aware while the Jensen-Rényi divergence [36] is not.

Example 3.5 (Discrete v.s. Normal distribution, d Euclidean distance). *When considering the Euclidean distance d as the base metric, we can take the limiting case $\sigma_1 \rightarrow 0$ in Eq. 17 to obtain the SR_d between a Gaussian distribution and a Dirac distribution δ_{μ_1} at μ_1 . This writes as:*

$$\begin{aligned} \text{SR}_d(\mathcal{N}(\mu, \sigma), \delta_x) &= \sqrt{2}\sigma \text{erf}\left(\frac{\mu - x}{\sqrt{2}\sigma}\right) + \sigma \frac{\sqrt{2} - 1}{\sqrt{\pi}} \\ &= (\mu - x) \text{erf}\left(\frac{\mu - x}{\sqrt{2}\sigma}\right) + \frac{\sigma}{\sqrt{\pi}} \left(\sqrt{2} e^{-\frac{(\mu - x)^2}{2\sigma^2}} - 1 \right). \end{aligned} \quad (21)$$

By injecting Eq. 21 in Eq. 20, we obtain closed-form formulae for the SR_d distance between empirical distributions and mixtures of Normal distributions (also called Gaussian Mixture Models, GMMs).

We now investigate how to deal with multivariate normal distributions $\mathcal{N}(x; \mu, \Sigma) := \frac{1}{(2\pi)^{d/2} \det(\Sigma)^{1/2}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right)$ in dimension $d > 1$, with Σ a PD matrix. However, computing the Schoenberg-Rao distance as in Ex. 3.3 proved to be challenging. We propose the following workarounds:

Example 3.6 (Diagonal Gaussian distributions). *Since the sum of two CNSD kernels is CNSD (Prop. 2.7), the ℓ^1 distance over \mathbb{R}^n is CNSD. In the case of diagonal Gaussian distributions, the SR_{ℓ^1} distance Eq. 11 is separable and can be written as the sum of Eq. 17 over all dimensions.*

However, the resulting SR distance from Ex. 3.6 is not proper. Since we have a closed-form distance between mixture of Gaussian distributions, we propose to use the fact that a projection over a 1D line of a mixture of multivariate Gaussian distributions is a mixture of univariate Gaussian distributions. This motivates us to introduce the following *sliced Schoenberg-Rao distance* between mixtures of multivariate Gaussian distributions:

Example 3.7 (Sliced Schoenberg-Rao distance). *Let X be a random variable whose probability distribution $m(x) = \sum_{i=1}^N \pi_i \mathcal{N}(x; \mu_i, \Sigma_i)$ is a mixture of multivariate normal distributions with parameters π_i, μ_i, Σ_i , such that π is a discrete probability distribution over $[1, N]$. For any $b \in \mathbb{R}^d$, $b \cdot X$ is a univariate random variable with probability distribution*

$$m^b(x) := \sum_{i=1}^N \pi_i \mathcal{N}(x; b \cdot \mu_i, b^T \Sigma_i b). \quad (22)$$

We can use this to introduce the sliced Schoenberg-Rao distance (SSR) between mixtures of multivariate normal distributions as:

$$\text{SSR}(m_1, m_2) = \frac{1}{|S|} \int_S \text{SR}(m_1^b, m_2^b) dS(b), \quad (23)$$

where $S := \{x \in \mathbb{R}^d; \|x\|^2 = 1\}$ denotes the unit d -dimensional sphere and $|S|$ its surface area.

In practice, we compute Monte Carlo estimates of the integral of Eq. 23.

4 Experiments

In this section, we illustrate some usages of the Schoenberg-Rao distances computed in Sect. 3. Our aim is to showcase the versatility of our method and the wide range of applications it covers, from the computation of barycenters of probability distributions to its use as a regularizer in generative modeling².

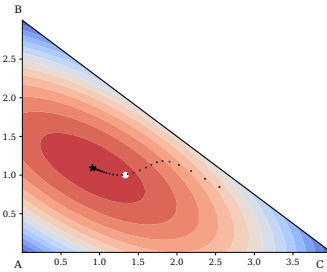


Figure 2: Maximum entropy distribution over 3 atoms (black star). The distance between the atoms reflects the Euclidean distance d . The white dot (better seen in color) represents the maximum entropy distribution for the Shannon entropy. The minimization path is depicted using small black dots. Level sets for the H_d function are displayed.

We first start by emphasizing the geometry-aware property of the Rao’s quadratic entropy.

²Some of these examples are adapted from the code provided by the authors of [14].

4.1 Maximum Entropy

Given a CNSD kernel d over n atoms x_i , we can compute the maximum Rao's quadratic entropy distribution $p^* = \operatorname{argmax}_p H_d(p)$. We plot in Fig. 2 the maximum entropy distribution for distributions over three atoms embedded in a Euclidean space. Taking into account the geometry of the sample space gives us a maximum entropy distribution which is different from the usual maximum entropy distribution for the Shannon entropy (uniform distribution). These two distributions coincide only when all atoms are at an equal distance with respect to one another.

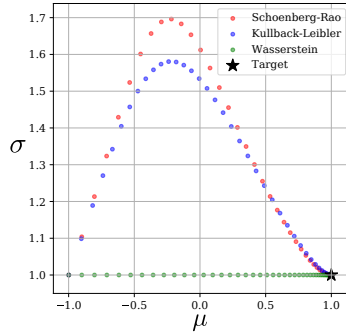


Figure 3: Minimization trajectories when minimizing $D(p : \mathcal{N}(1, 1))$ starting from $p := \mathcal{N}(-1, 1)$, for different divergences: SR_d with d Euclidean, Kullback-Leibler divergence and the 2-Wasserstein distance. Each point correspond to a Normal distribution in the (μ, σ) plane.

4.2 Minimizing distances between two Gaussian distributions

We now investigate the behaviour of the SR_d distances when performing minimization in the space of 1D Normal distributions. An example of such minimization is shown in Fig. 3 together with a comparison of other known distances over Normal distributions like the 2-Wasserstein distance and the Kullback-Leibler divergence. It is interesting to note that the behaviour of the trajectories is much more similar to the one obtained using the Kullback-Leibler divergence than the 2-Wasserstein distance. In other words, when "moving" a Normal distribution to another one with the same variance, the Gaussian distributions at the intermediate steps tend to be more spread than the ones at the start and end points.

The explicit form of the Schoenberg-Rao for Gaussian mixtures makes the computation of barycenters between Gaussian mixtures simple. In Fig. 4a, we display the α -barycenters for varying α between two Gaussian mixtures with two components. More precisely, given two Gaussian mixtures p and q the

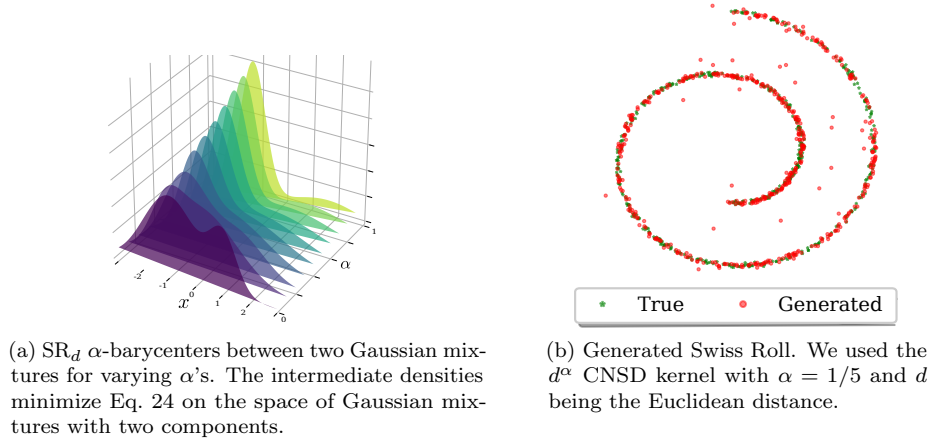


Figure 4: Barycenters and density fitting examples.

α -barycenter between these two distributions is the solution of the following minimization problem:

$$\operatorname{argmin}_{m \in \mathcal{F}} \alpha SR_d(p, m) + (1 - \alpha) SR_d(m, q), \quad (24)$$

where we chose the family \mathcal{F} to be the space of Gaussian mixtures with two components. In fact, Eq. 24 is equivalent to

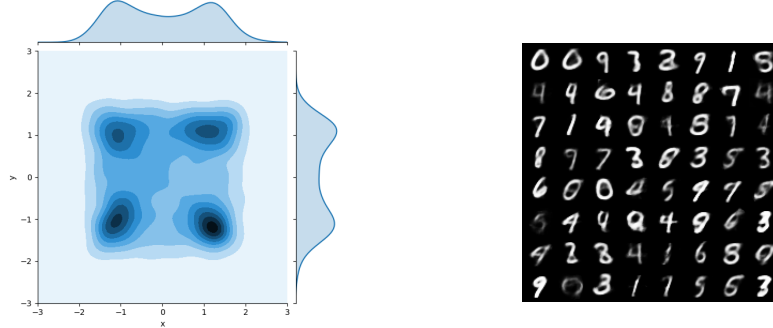
$$\operatorname{argmin}_{m \in \mathcal{F}} SR_d(\alpha p + (1 - \alpha)q, m), \quad (25)$$

since the two equations are equal up to a constant depending only on p and q by Eq. 20. Therefore, computing the α -barycenter amounts to computing the projection over \mathcal{F} of the mixture $\alpha p + (1 - \alpha)q$. In particular, when the two mixtures p and q are defined on the same components, the α -barycenter is exactly $\alpha p + (1 - \alpha)q$.



Figure 5: SR_d barycenter for each MNIST digit class, computed on discrete probability distributions supported over 28×16 atoms. The probabilities of the atoms are either learnt (up) or fixed (bottom). For display, we aggregated the probabilities of all atoms representing the same pixel.

We can use SR_d to compute barycenters between n discrete probability distributions. We run the same experiments as in [14, 10] and address the problem of computing the barycenters of MNIST digits, considered as probability



(a) Joint plot of the aggregated distribution for two latent dimensions. The four modes are identifiable. (b) Uncurated MNIST samples.

Figure 6: Schoenberg-Rao auto-encoders with an SR_d penalty obtained by sampling the prior and using a deterministic encoder. The prior is a mixture of Gaussian distributions with standard deviation of 0.4 whose means are located on the 6-dimensional hypercube.

distributions over pixels. We can then consider the Euclidean distance between pixels as our base CNSD kernel d . However, given our previous remark, doing so on the space of all discrete probability distributions supported over all pixels would result in the computation of the averaged distribution. Instead, we compute the barycenters over a trainable set of pixels. The resulting cluster centers are displayed in Fig. 5.

4.3 Fitting discrete parameterized densities

Following [14], we show that the Schoenberg-Rao distance can be used effectively to fit discrete densities parameterized by a neural network. More precisely, given f a neural network and $p(z)$ a noise distribution, $f_{\#}^n(p) := \frac{1}{n} \sum_{i=1}^n f(z_i)$ is the pushforward by f of the empirical noise distribution, where z_i are samples from p . We can then use the SR_d distance to fit this distribution to an empirical target distribution. Figure. 4b displays results of this minimization on the Swiss roll toy dataset.

4.4 Schoenberg-Rao auto-encoders

A particularly useful case in machine learning is to compute the distance between a unit Gaussian distribution and an empirical distribution. This is for instance the case in the Wasserstein Auto-Encoders (WAE) with MMD loss [35]. We show that SR_d can be used as a drop-in replacement of the MMD loss between samples from the prior and samples from the aggregated distribution. We reproduced the experiments from [14] and [15] by training a simple two-layer multilayer perceptron on the MNIST dataset. Using Eq. 8, we are able to consider both deterministic and stochastic encoders. In particular, we show that we are able to

fit complex prior distributions even in this restricted setting. Figure 6a displays the fitted aggregated distribution for an auto-encoder with deterministic encoder networks and Fig. 6b some samples from a standard auto-encoder with SR regularization. We believe that the SR regularization can be particularly useful in this context due to its behaviour regarding outliers. Indeed, [29] mentions that the RBF kernel used in WAE suffers from outlier insensitivity due to its exponential decay. This is the reason why kernels with slower tail decays (such as the inverse multiquadric kernel) often tend to be used in practice as in [35]. This is not the case with the SR distance: suppose that we have two empirical distributions centered at the origin and that one atom x_i on which p is supported is far away from the origin denoted by 0 (so that d_{ij} is large for all $j \neq i$). Then, the dominating term in the SR distance from Eq. 8 is loosely equal to $p_i d_{i0}(1 - \frac{1}{2} \sum_{j \neq i} p_j)$, which is large for all CNSD kernels we mentioned. During a minimization procedure, the outlier x_i would be heavily penalized. This is a noticeable difference compared to many isotropic kernels used in machine learning.

Recently, in the context of WAE with MMD loss it proved to be efficient to compute closed-form formulae between the aggregated distribution and the prior instead of sampling from the unit Gaussian prior [29] since this reduces the variance of the MMD estimator. In our setting, we can use the sliced Schoenberg-Rao distance Eq. 23 to compute a distance between the empirical aggregated posterior (which is a GMM) and the prior (which can also be a GMM). Note that our framework includes the case where the encoder is deterministic since the empirical aggregated posterior can be a degenerated GMM, in which case we would use the sliced Schoenberg-Rao distance with Eq. 21.

In our case, we approximate the integral of Eq. 23 using only one sample per batch. In practice, this proved to be highly efficient and stable, provided that we initialize the variance of the approximate posterior distributions to a small value. By using SSR, the stochasticity introduced by the sampling of the prior and of the approximate posterior can be removed and put instead into the estimator of Eq. 23.

5 Related works

The Schoenberg-Rao distance can be seen as a generalization of MMD [17]. Indeed, let p and q be two distributions, x_i and y_j be m (resp. n) samples from p (resp. q). The V-estimator (biased estimator) of the MMD using a positive semi definite (PSD) kernel k is

$$\begin{aligned} \text{MMD}_b^{m,n}(p, q) := & -\frac{2}{mn} \sum_{i=1}^m \sum_{j=1}^n k(x_i, y_j) \\ & + \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m k(x_i, x_j) + \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(y_i, y_j). \end{aligned} \quad (26)$$

Since k is PSD, $-k$ is CNSD since NSD kernels are also CNSD kernels by definition. Dividing Eq. 26 by 2, we obtain the SR_{-k} distance from Eq. 11 on empirical distributions from p and q . The Schoenberg-Rao distance is thus a way to consider a more general class of kernels in the MMD framework. Especially, the major difference for us is that we can have $d(x, x) = 0$. Also, the SR distances are based on the notion of distance on the sample space while the MMD kernels account for a notion of similarity over the sample space. In particular, positive isotropic kernels $k(x, y) = f(|x - y|)$ often requires $f(0) = 1$ and $\lim_{x \rightarrow \infty} f(x) = 0$ and their rate of decay at infinity proved to be important in applications [29].

Also related to our work is the recent GAIT entropy [14] from which the authors construct a Bregman divergence. As Rao's quadratic entropy, it is a geometry-aware entropy that first appeared in ecological studies. However, this framework relies on a conjecture about the concavity of the GAIT entropy. This entropy, which was tested experimentally to be concave is written as:

$$H^{\text{GAIT}}(p) = - \sum_{i=1}^n p_i \log \left(\sum_{j=1}^n k_{ij} p_j \right), \quad (27)$$

where $k := e^{-d}$ is a PSD kernel by Prop. 2.3. It was first introduced in [20] with an additional parameter α , the GAIT Rényi entropy writes as:

$$H_{\alpha}^{\text{GAIT}}(p) = \frac{1}{1 - \alpha} \log \left(\sum_{i=1}^n \frac{p_i}{(\sum_{j=1}^n k_{ij} p_j)^{1 - \alpha}} \right), \quad (28)$$

Eq. 27 being the limit $\alpha \rightarrow 1$ of $H_{\alpha}^{\text{GAIT}}(p)$. We want to highlight the following observation: the case $\alpha = 2$ seems linked to SR since

$$\exp(-H_2^{\text{GAIT}}(p)) = \sum_{i=1}^n \sum_{j=1}^n p_i p_j k_{ij}. \quad (29)$$

This would suggest that the choice of k in [14] might be too restrictive since Eq. 29 forces $0 \leq k \leq 1$. We also saw that it is more natural to consider a positive CNSD kernel in the r.h.s. 29 than a positive PSD kernel, since it makes the Rao's entropy concave over the probability simplex.

Although geometry-aware, the SR distance possesses properties clearly distinct from Wasserstein distances as can be seen in Fig. 3. In particular, the computation of barycenters differs drastically as discussed in Sect. 4.2. We believe it should not be considered to be interchangeable with Wasserstein distances in all applications.

The use of CNSD kernels in machine learning was mainly considered in the literature on Support Vector Machines [32, 5, 18]. In these works, the authors study how to use CNSD kernels instead of CPD kernels but did not introduce the associated Schoenberg-Rao distance. These works report improved results through the use of this more general class of kernels.

Finally, we mention the works of [13, 12, 36] which also study closed-form entropy-based divergences for mixture of Gaussians and their relation to Schoenberg's theorem.

As future work, we hope to find a general way to compute closed-form solutions of SR for multivariate distributions: this would allow one to impose regularizers with nice properties in WAEs without the need to sample the prior distribution or without relying on the sliced Schoenberg-Rao distance.

6 Conclusion

We introduced the Schoenberg-Rao distances, a Hilbert distance on probability distributions based on Rao’s quadratic entropy. We were able to provide new closed-form solutions for Gaussian mixtures and also demonstrated its versatility on a variety of machine learning tasks, due to its geometry-aware property. Through the discussion of the related work and experiments, we highlighted the connections and differences between MMD, GAIT and Wasserstein distances. We hope these insights will spur the interest of researchers in these areas as well as practitioners.

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A Proof of example 3.1

In the case $d(x_1, x_2) = |x_1 - x_2|^2$,

$$H_d(p, q) = \int \int p(x)q(y)|x - y|^2 dx dy \quad (30)$$

$$= \int x^2 p(x) dx + \int p(y)y^2 dy \quad (31)$$

$$- 2 \left(\int xp(x) dx \right) \left(\int yq(y) dy \right) \quad (32)$$

$$= \mu_1^2 + \sigma_1^2 + \mu_2^2 + \sigma_2^2 - 2\mu_1\mu_2 \quad (33)$$

$$= (\mu_1 - \mu_2)^2 + \sigma_1^2 + \sigma_2^2. \quad (34)$$

For this, we readily obtain

$$H_d(\mathcal{N}(\mu, \sigma)) = 2\sigma^2, \quad (35)$$

and

$$J(p, q) = (\mu_1 - \mu_2)^2 + \sigma_1^2 + \sigma_2^2 - \sigma_1^2 - \sigma_2^2 = (\mu_1 - \mu_2)^2. \quad (36)$$

B Proof of example 3.3

We now consider the case $d(x_1, x_2) = |x_1 - x_2|$ and write $H_d(p, q)$ as:

$$H_d(p, q) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(x)q(y)|x - y| dx dy = \int_{-\infty}^{\infty} q(y) dy \int_y^{+\infty} xp(x) dx \quad (37)$$

$$- \int_{-\infty}^{\infty} yq(y) dy \int_y^{+\infty} p(x) dx - \int_{-\infty}^{\infty} q(y) dy \int_{-\infty}^y xp(x) dx \quad (38)$$

$$+ \int_{-\infty}^{\infty} yq(y) dy \int_{-\infty}^y p(x) dx, \quad (39)$$

and compute all the terms separately. We now write $\Phi^p(y) := \int_{-\infty}^y p(x) dx$ the cdf of p and use the notation $\mu^p(y) := \int_{-\infty}^y xp(x) dx$. We note that $\mu^p(\infty) = \mu_1$.

Then, the first term of Eq. 37 becomes:

$$\int_{-\infty}^{\infty} q(y)(\mu_1 - \mu^p(y)) dy = \mu_1 - \int_{-\infty}^{\infty} q(y)\mu^p(y) dy \quad (40)$$

$$= \mu_1 - \mathbb{E}_q(\mu^p(.)). \quad (41)$$

The second one becomes

$$- \int_{-\infty}^{\infty} yq(y)(1 - \Phi^p(y)) dy = -\mu_2 + \int_{-\infty}^{\infty} yq(y)\Phi^p(y) dy \quad (42)$$

$$= -\mu_2 + [\mu^q(.)\Phi^p(.)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \mu^q(y)p(y) dy \quad (43)$$

$$= -\mu_2 + \mu_2 - \mathbb{E}_p(\mu^q(.)) = -\mathbb{E}_p(\mu^q(.)), \quad (44)$$

since $\Phi^p(\infty) = 1$ and $\Phi^p(-\infty) = 0$.

The third one becomes

$$-\int_{-\infty}^{\infty} q(y)\mu^p(y) dy = -\mathbb{E}_q(\mu^p(.)), \quad (45)$$

and the last one becomes

$$\int_{-\infty}^{\infty} yq(y)\Phi^p(y) dy = [\mu^q(.)\Phi^p(.)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \mu^q(y)p(y) dy \quad (46)$$

$$= \mu_2 - \mathbb{E}_p(\mu^q(.)). \quad (47)$$

Putting everything together we obtain:

$$H_d(p, q) = \mu_1 + \mu_2 - 2\mathbb{E}_p\mu^q - 2\mathbb{E}_q\mu^p. \quad (48)$$

We note that up so far we have not used any property of the Gaussian distributions so Eq. 48 is valid for all pdf provided that all the integrals above exist.

We now compute simplify (48) when p and q are Normal distributions.

The integrals $\mathbb{E}_q\mu^p$ can be rewritten as:

$$\mathbb{E}_q\mu^p = \int_{-\infty}^{\infty} q(y) dy \int_{-\infty}^y xp(x) dx \quad (49)$$

$$= \int_{-\infty}^{\infty} q(y) dy \int_{-\infty}^y (\mu_1 p(x) - \sigma_1^2 p'(x)) dx \quad (50)$$

$$= \mu_1 \int_{-\infty}^{\infty} q(y)\Phi^p(y) dy - \sigma_1^2 \int_{-\infty}^{\infty} q(y)p(y) dy, \quad (51)$$

where we note $\Phi^p(x) := \Phi(\frac{x-\mu_1}{\sigma_1})$ the cdf of p .

Using Eq. 49 in Eq. (48) we obtain:

$$H(p, q) = \mu_1 \int_{-\infty}^{\infty} q(y)(1 - 2\Phi^p(y)) dy \quad (52)$$

$$+ \mu_2 \int_{-\infty}^{\infty} p(y)(1 - 2\Phi^q(y)) dy \quad (53)$$

$$+ 2(\sigma_1^2 + \sigma_2^2) \int_{-\infty}^{\infty} q(y)p(y) dy. \quad (54)$$

The integral in the first term in the r.h.s. of Eq. 52 can be further simplified as:

$$\int_{-\infty}^{\infty} q(y)(1 - 2\Phi^p(y)) dy = \int_{-\infty}^{\infty} q(y)(1 - 2\Phi(\frac{y-\mu_1}{\sigma_1})) dy \quad (55)$$

$$= \int_{-\infty}^{\infty} q(y) \operatorname{erf}\left(\frac{y-\mu_1}{\sqrt{2}\sigma_1}\right) dy \quad (56)$$

$$= \operatorname{erf}\left(\frac{\mu_2 - \mu_1}{\sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2}}\right), \quad (57)$$

by denoting $\text{erf}(x) := \frac{1}{\sqrt{\pi}} \int_{-x}^x e^{-y^2} dy$ the standard error function and using the fact that

$$\int_{-\infty}^{\infty} \mathcal{N}(x; \mu, \sigma) \text{erf}(ax + b) dx = \text{erf}\left(\frac{a\mu + b}{\sqrt{1 + 2a^2\sigma^2}}\right). \quad (58)$$

The last term in Eq. 52 is

$$\int_{-\infty}^{\infty} q(y)p(y) dy = \mathcal{N}(\mu_2; \mu_1, \sqrt{\sigma_1^2 + \sigma_2^2}) = \frac{1}{\sqrt{2\pi}\sqrt{\sigma_1^2 + \sigma_2^2}} e^{-\frac{(\mu_2 - \mu_1)^2}{2(\sigma_1^2 + \sigma_2^2)}}. \quad (59)$$

Injecting Eq. (58) and (59) in Eq. (52) we finally get:

$$\begin{aligned} H(p, q) &= (\mu_2 - \mu_1) \text{erf}\left(\frac{\mu_2 - \mu_1}{\sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2}}\right) + \frac{2(\sigma_1^2 + \sigma_2^2)}{\sqrt{2\pi}\sqrt{\sigma_1^2 + \sigma_2^2}} e^{-\frac{(\mu_2 - \mu_1)^2}{2(\sigma_1^2 + \sigma_2^2)}} \\ &= \sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2} \left[\frac{(\mu_2 - \mu_1)}{\sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2}} \text{erf}\left(\frac{\mu_2 - \mu_1}{\sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2}}\right) + \frac{1}{\sqrt{\pi}} e^{-\left(\frac{\mu_2 - \mu_1}{\sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2}}\right)^2} \right]. \end{aligned} \quad (60)$$

$$(61)$$

We observe that the term in brackets is a primitive of the error function erf , namely $x \mapsto x \text{erf}(x) + \frac{1}{\sqrt{\pi}} e^{-x^2}$. We denote by perf (for *primitive of the error function*) the integral which equals zero in 0:

$$\text{perf}(x) = x \text{erf}(x) + \frac{e^{-x^2} - 1}{\sqrt{\pi}}. \quad (62)$$

We finally get the following nice expression:

$$H_d(p, q) = \sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2} \text{perf}\left(\frac{\mu_2 - \mu_1}{\sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2}}\right) + \sqrt{\frac{2}{\pi}}\sqrt{\sigma_1^2 + \sigma_2^2}. \quad (63)$$