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Quantum Foundations, Probability and Information

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Quantum Foundations, Probability and Information

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Preface

The last 20 years were characterized by tremendous development of the fields of quantum probability and information. The *quantum information revolution* has also renewed the interest in the foundations of quantum theory (philosophical and mathematical), to the extent that fundamental concepts are now reconsidered in terms of a new information-theoretical perspective [1–9]. This recent revolutionary transformation of quantum physics toward information physics also stimulated the development of novel mathematical models and methods.

This book is composed of contributions by leading experts in quantum foundations, especially from informational, probabilistic, and mathematical perspectives, and it presents their expert viewpoints on a number of foundational problems as well as novel mathematical models of quantum and subquantum phenomena. The mathematical content of the book is very rich and multidisciplinary: theory of partial differential equations of quantum field theory (derivation, modification, properties of solutions), differential geometry (including Riemann and Weyl geometries), oscillatory processes and vibrations, probability theory and its interpretations (especially the subjective one), classical versus quantum Bayesian inference, update of probabilities, Turing machines and random generators, action–reaction models, Feynman integrals for quickly growing potential functions, theory of open quantum systems, quantum master equation, quantum Markovian processes, mathematical modeling of decoherence in quantum and classical frameworks, Bell's inequality and its probabilistic structure, mathematical models of theories of hidden variables, theory of cellular automata, quantum versus classical entropy, measures of quantum information, theory of complexity and optimization, quantum theory of classification, clustering based on the Hilbert space framework, and representation of information by density operators. Some of these chapters are quite speculative, but the complexity (physical, mathematical, and philosophical) of the problems under study justifies such speculative considerations. Some of them depart far from the mainstream of quantum physical studies. This is up to the reader whether to accept or to reject such novel but sometimes controversial arguments and mathematical models of the authors. Other chapters are devoted to the fundamental problems of the conventional quantum theory including its mathematical formalism. We trust

that these contributions would be useful for experts in the corresponding areas of quantum theory. In this preface a few such contributions will be discussed in more detail.

One cluster of related chapters in this book concerns quantum and classical field theory and oscillatory processes. These are the contributions of A. Akhmeteli, "The Dirac Equation as One Fourth-Order Equation for One Function: A General, Manifestly Covariant Form"; B.R. La Cour, C.I. Ostrove, M.J. Starkey, and G.E. Ott, "Quantum Decoherence Emulated in a Classical Device"; S.A. Rashkovskiy, "Classical-Field Theory of the Photoelectric Effect"; and H. Yau, "Temporal Vibrations in a Quantized Field."

Some of these studies go beyond the conventional quantum theory. For example, Rashkovskiy claims that he can show that all properties of the photoelectric effect can be completely described within the framework of classical field theory without any quantization; in particular, three well-known laws of the photoelectric effect are derived without quantization of light and atom.

The chapter of C. Lopez, "The Action Reaction Principle in Quantum Mechanics," reminds the reader that the action–reaction principle is not automatically fulfilled in the standard formulation of quantum mechanics. An extended phase space can be considered where the formulation is consistent. In an extended spin phase space, there is a new quantum state, isotropic. Using this new state the composite singlet becomes separable instead of entangled. The perfect anticorrelation between both particles of the singlet appears in the subquantum states.

The chapter of C. Baladrón and A. Khrennikov, "At the Crossroads of Three Seemingly Divergent Approaches to Quantum Mechanics," considers quantum mechanics from the Darwinian evolutionary perspective. Several concepts stemming from three apparently divergent approaches to quantum mechanics, i.e., Bohmian mechanics, QBism, and time-symmetric quantum mechanics, are interwoven in an information-theoretic Darwinian scheme applied to fundamental physical systems that might shed light on some long-standing quantum mechanical conundrums. Here quantum systems are treated as endowed with individual Turing machines and random generators. Such systems have predictive power explaining nonlocal correlations and violation of Bell's inequality. The problem of nonlocality, probabilistic structure of quantum correlation functions, and violation of Bell's inequality is also studied in the chapters of H. Geurdes, "A Computational Proof of Locality in Entanglement," and G.N. Mardari, "Local Realism Without Hidden Variables." Closely related problems are discussed in the chapter of D.J. Ben Daniel, "Implications of Einstein-Weyl Causality on Quantum Mechanics."

The chapter of A. Baumeler, J. Degorre, and S. Wolf, "Bell Correlations and the Common Future," starts with the reminder that Reichenbach's principle states that in a causal structure, correlations of classical information can stem from a common cause in the common past or a direct influence from one of the events in correlation to the other. The difficulty of explaining Bell correlations through a mechanism in that spirit can be read as questioning either the principle or even its basis: causality. In the former case, the principle can be replaced by its quantum version, accepting as a common cause an entangled state, leaving the phenomenon as mysterious as

ever on the classical level (on which, after all, it occurs). If, more radically, the causal structure is questioned in principle, closed space–time curves may become possible that, as is argued in the present note, can give rise to nonlocal correlations if to-be-correlated pieces of classical information meet in the common future—which they need to if the correlation is to be detected in the first place. The result is a view resembling Brassard and Raymond-Robichaud's parallel-lives variant of Hermann's and Everett's relative state formalism, avoiding "multiple realities."

The chapter of E.N. Dzhafarov, "Replacing Nothing with Something Special: Contextuality-by-Default and Dummy Measurements," presents quantum contextuality (playing the fundamental role in modern quantum information theory) in the rigorous probabilistic framework. This approach is also closely related to aforementioned problems: violation of the Bell-type inequalities and theories of hidden variables. The object of contextuality analysis is a set of random variables, each of which is uniquely labeled by a content and a context. In the measurement terminology, the content is that which the random variable measures, whereas the context describes the conditions under which this content is measured (in particular, the set of other contents being measured together with this one). Such a set of random variables is deemed noncontextual or contextual depending on whether the distributions of the context-sharing random variables are or are not compatible with certain distributions imposed on the content-sharing random variables. In the traditional approaches, contextuality is either restricted to only consistently connected systems (those in which any two content-sharing random variables have the same distribution) or else all inconsistently connected systems (those not having this property) are considered contextual. In the Contextuality by Default theory, an inconsistently connected system may or may not be contextual.

An important biological application of quantum theory is presented in the chapter of Y. Mitome, S. Iriyama, K. Sato, and I.V. Volivich, "Efficient Energy Transfer in Network Model of Photosynthesis." G. Jaeger critically analyzes computer-like models of nature in his contribution "Clockwork Rebooted: Is the Universe a Computer?" A. Khrennikov in his chapter "External Observer Reflections on QBism, Its Possible Modifications, and Novel Applications" critically discusses development of QBism from its early days and the first sound presentations at the Växjö conferences early this century to the flourishing modern theory. This is the collection of very personal recollections of the author about his long-term debates with the creator of the subjective probability approach to quantum mechanics, Christopher Fuchs. The chapter of S. Kak, "Epistemic View of Quantum Communication," is devoted to the foundational problems of quantum information theory and especially quantum communications.

The team of researchers (theoreticians and experimenters), J. Marton, S. Bartalucci, A. Bassi, M. Bazzi, S. Bertolucci, C. Berucci, M. Bragadireanu, M. Cargnelli, A. Clozza, C. Curceanu, L. De Paolis, S. Di Matteo, S. Donadi, J.-P. Egger, C. Guaraldo, M. Iliescu, M. Laubenstein, E. Milotti, A. Pichler, D. Pietreanu, K. Piscicchia, A. Scordo, H. Shi, D. Sirghi, F. Sirghi, L. Sperandio, O. Vazquez-Doce, E. Widmann, and J. Zmeskal, present the recent experimental study, "Underground Test of Quantum Mechanics: The VIP2 Experiment," where

they investigate possible violations of standard quantum mechanics predictions. They tested with high precision the *Pauli Exclusion Principle (PEP) and the collapse of the wave function (collapse models)*. Included here is the novel method of searching for possible small violations of PEP for electrons, through the search for anomalous X-ray transitions in copper atoms, produced by fresh electrons (brought inside the copper bar by circulating current) which can have the probability to undergo Pauli-forbidden transition to the level already occupied by two electrons. Also therein is described the VIP2 (VIolation of PEP) experiment taking data at the Gran Sasso underground laboratories. From the mathematical side, this study is based on advanced statistical analysis for occurrence of events having very small probabilities.

H. Mohameden and H. Ouerdiane have written the chapter, "Feynman Integrals for a New Class of Time-Dependent Exponentially Growing Potentials," devoted to the rigorous mathematical study about justification of the method of the path integral. This is a complex mathematical problem which has been studied by many authors, mathematicians, and physicists. And this chapter is the important contribution to this area of research on the boundary between pure mathematics and quantum physics.

The chapter of E. Santucci and G. Sergioli, "Classification Problem in a Quantum Framework," is devoted to application of the methods of quantum theory to classification problems. One of the important outputs of this study is the design of the novel method of presentation of information by density matrices. The main aim of this study is to provide a quantum counterpart of the well-known minimum-distance classifier named nearest mean classifier (NMC). In particular, this chapter contains the review about previous works in this area.

The chapter of N. Watanabe, "On Complexity for Open System Dynamics," represents in detail measures of quantum entropy and information, especially the achievements of the school of M. Ohya at Tokyo University of Science.

We hope that the reader will enjoy this book, which will be useful to experts working in quantum physics and quantum probability and information theory, ranging from theoreticians, experimenters, and mathematicians to philosophers.

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Classification Problem in a Quantum Framework

Enrica Santucci and Giuseppe Sergioli

1 Introduction

In recent years there has been an increasing interest toward the use of the quantum mechanical formalism in non-microscopic contexts. The idea is that the powerful predictive properties of quantum mechanics, used for describing the behavior of microscopic phenomena, turn out to be particularly beneficial also in non-microscopic domains. At this purpose, several nonstandard applications involving the formalism of quantum theory have been proposed in research fields, such as game theory [7, 16], economics [10], cognitive sciences [1, 2], signal processing [8], and so on. Further, particular applications, interesting for the specific topics of the present paper, concern the areas of machine learning and pattern recognition. About this, some attempts which connect quantum information to pattern recognition can be found in [18], while an exhaustive survey and bibliography of the developments concerning the use of quantum computing techniques in artificial intelligence are provided in [14, 26].

In pattern recognition area, one of the main aspects is focused on the application of quantum information processing methods to solve classification and clustering problems [4, 23].

The use of quantum states for representing patterns has a twofold motivation: firstly, it gives the possibility of exploiting quantum algorithms to boost the computational efficiency of the classification process [25]. Secondly, it is possible to use quantum-inspired models in order to reach some benefit with respect to classical problems [22].

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Even if the state-of-art approaches suggest possible computational advantages of this sort [3, 12, 13], the main problem to find a *more convenient* encoding from classical to quantum object is nowadays an open and interesting matter of debate [14, 18]. In this context, our contribution consists in constructing a quantum-inspired version of a classical classifier in order to reach some convenience, in terms of the error in pattern classification, with respect to the corresponding classical model. We have already proposed this kind of approach in two previous works [19, 20], where a "quantum counterpart" of a well-known minimum-distance classifier, called *Nearest Mean Classifier* (NMC), has been introduced.

In both cases, the model is based on the introduction of two main ingredients: first, an appropriate encoding of arbitrary patterns into density operators, and, second, a distance measure between density operators, representing the quantum counterpart of the Euclidean distance in the "classical" NMC. The main differences between the two previous works are as follows: (1) in the first case [20], we tested our quantum classifier on two-dimensional datasets, and we proposed a generalization to arbitrary dimension from a theoretical point of view only; (2) in the second case [19], a new encoding for arbitrary n-dimensional patterns into quantum states has been proposed, and it was tested on different real-world and artificial datasets. Anyway, in both cases, we have observed a significant improvement of the accuracy in the classification process. In addition, we found that, by using the encoding proposed in [19] and for two-dimensional problems only, the classification accuracy of our quantum classifier can be further improved, by performing a uniform rescaling of the original dataset.

In this work we propose a new encoding of arbitrary n-dimensional patterns into quantum objects, which preserves information about the norm of the original pattern. This idea has been inspired by recent debates on quantum machine learning [18], according to which it is crucial to avoid loss of information when a particular encoding of real vectors into quantum states is considered. Such an approach turns out to be very promising in terms of classification performances with respect to the classical version of the NMC. Further, differently from the NMC, our quantum classifier is invariant under uniform rescaling. More precisely, the accuracy of the quantum classifier changes by rescaling (of an arbitrary real number) the coordinates of the dataset. Consequently, we have observed that, for several datasets, the new encoding exhibits a further advantage that can be gained by exploiting the non-invariance under rescaling, also for n-dimensional problems (conversely to the previous works). At this purpose, some experimental results have been presented.

The paper is organized as follows: in Sect. 2 we briefly describe the classification process and, in particular, the formal structure of the NMC. Section 3 is devoted to the definition of a new encoding of real patterns into quantum states. In Sect. 4 we introduce the quantum version of the NMC, called *Quantum Nearest Mean Classifier* (QNMC) based on the new encoding previously described. In Sect. 5 we compare the NMC and the QNMC on different datasets showing that, in general, the QNMC exhibits better performances (in terms of accuracy and other significant statistical quantities) with respect to the NMC. Further, starting from the fact that, differently from the NMC, the QNMC is not invariant under rescaling, we also show

that, for some dataset, it is possible to provide a benefit from this non-invariance property. Some conclusions and possible further developments are proposed at the end of the paper.

2 On the Classification Process

Here, we address the classification problem, which is an instance of supervised learning, i.e., learning from a training set of correctly labeled objects. More precisely, each object can be characterized by its features; hence, a d-feature object can be naturally represented by a d-dimensional real vector, i.e., $\mathbf{x} = [x^{(1)}, \ldots, x^{(d)}] \in \mathscr{X}$, where $\mathscr{X} \subseteq \mathbb{R}^d$ is generally a subset of the d-dimensional real space representing the *feature space*. Hence, any arbitrary object is represented by a vector $\mathbf{x}$ associated to a given class of objects (but, in principle, we do not know which one). Let $\mathscr{Y} = \{1, \ldots, L\}$ be the class label set. A *pattern* is represented by a pair $(\mathbf{x}, y)$, where $\mathbf{x}$ is the *feature vector* representing an object and $y \in \mathscr{Y}$ is the *label* of the class which $\mathbf{x}$ is associated to. The aim of the classification process is to design a function (*classifier*) that attributes (in the most accurate way) to any unlabeled object the corresponding label (where the label attached to an object represents the class which the object belongs to), by learning about the set of objects whose class is known. The *training set* is given by $\mathscr{S}_{\text{tr}} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$, where $\mathbf{x}_n \in \mathscr{X}$, $y_n \in \mathscr{Y}$ (for $n = 1, \ldots, N$) and N is the number of patterns belonging to $\mathscr{S}_{\text{tr}}$. Finally, let N_l be the cardinality of the training set associated to the l-th class (for $l = 1, 2, \ldots, L$) such that $\sum_{l=1}^{L} N_l = N$.

We now introduce the well-known *Nearest Mean Classifier* (NMC) [6], which is a particular kind of minimum-distance classifier widely used in pattern recognition. The strategy consists in computing the distances between an object $\mathbf{x}$ (to classify) and patterns chosen as prototypes of each class (called *centroids*). Finally, the classifier associates to $\mathbf{x}$ the label of the closest centroid. So, we can resume the NMC algorithm as follows:

1. the computation of the *centroid* (i.e., the sample mean [11]) associated to each class, whose corresponding feature vector is given by

$$\boldsymbol{\mu}_l = \frac{1}{N_l} \sum_{n=1}^{N_l} \mathbf{x}_n, \quad l = 1, 2, \ldots, L, \tag{1}$$

   where l is the label of the class;
2. the classification of the object $\mathbf{x}$, provided by

$$\underset{l=1,\ldots L}{\operatorname{argmin}}\, d_E(\mathbf{x}, \boldsymbol{\mu}_l), \quad \text{with} \quad d_E(\mathbf{x}, \boldsymbol{\mu}_l) = \|\mathbf{x} - \boldsymbol{\mu}_l\| \tag{2}$$

where d_E is the standard Euclidean distance.[1]

Depending on the particular distribution of the dataset patterns, it is possible that a pattern belonging to a given class is closest to the centroid of another class. In this case, if the algorithm would be applied to this pattern, it would fail. Hence, for an arbitrary object $\mathbf{x}$, whose class is a priori unknown, the output of the above classification process has the following four possibilities [9]: (1) *true positive* (TP), pattern belonging to the l-th class and correctly classified as l; (2) *true negative* (TN), pattern belonging to a class different than l and correctly classified as not l; (3) *false positive* (FP), pattern belonging to a class different than l and incorrectly classified as l; and (4) *false negative* (FN), pattern belonging to the l-th class and incorrectly classified as not l.

In order to evaluate the performance of a certain classification algorithm, the standard procedure consists in dividing the original labeled dataset $\mathscr{S}$ of N' patterns, into a training set $\mathscr{S}_{\text{tr}}$ of N patterns and a set $\mathscr{S}_{\text{ts}}$ of $(N' - N)$ patterns (i.e., $\mathscr{S} = \mathscr{S}_{\text{tr}} \cup \mathscr{S}_{\text{ts}}$). This set $\mathscr{S}_{\text{ts}}$ of patterns is called *test set* [6], and it is defined as $\mathscr{S}_{\text{ts}} = \{(\mathbf{x}_n, y_n)\}_{n=N+1}^{N'}$.

Then, by applying the NMC to the test set, it is possible to evaluate the classification algorithm performance by considering the following statistical measures associated to each class l depending on the quantities listed above:

- *True Positive Rate* (TPR): $\text{TPR} = \frac{\text{TP}}{\text{TP+FN}}$;
- *True Negative Rate* (TNR): $\text{TNR} = \frac{\text{TN}}{\text{TN+FP}}$;
- *False Positive Rate* (FPR): $\text{FPR} = \frac{\text{FP}}{\text{FP+TN}} = 1 - \text{TPN}$;
- *False Negative Rate* (FNR): $\text{FNR} = \frac{\text{FN}}{\text{FN+TP}} = 1 - \text{TPR}$.

Further, other standard statistical coefficients [9] used to establish the reliability of a classification algorithm are:

- *Classification error* (E): $\text{E} = 1 - \frac{\text{TP}}{\text{N}'-\text{N}}$;
- *Precision* (P): $\text{P} = \frac{\text{TP}}{\text{TP+FP}}$;
- *Cohen's Kappa* (K): $\text{K} = \frac{\text{Pr(a)}-\text{Pr(e)}}{1-\text{Pr(e)}}$, where
  $\text{Pr(a)} = \frac{\text{TP+TN}}{\text{N}'-\text{N}}$, $\text{Pr(e)} = \frac{(\text{TP+FP})(\text{TP+FN})+(\text{FP+TN})(\text{TN+FN})}{(\text{N}'-\text{N})^2}$.

In particular, the classification error represents the percentage of misclassified patterns, the precision is a measure of the statistical variability of the considered model, and the Cohen's kappa represents the degree of reliability and accuracy of a statistical classification, and it can assume values ranging from -1 to $+1$ ($K = +1$ corresponds to a perfect classification procedure, while $K = -1$ corresponds to a completely wrong classification). Let us note that these statistical

[1] We remind that, given a function $f : X \to Y$, the *argmin* (i.e., the argument of the minimum) over some subset S of X is defined as: $\text{argmin}_{x \in S \subseteq X} f(x) = \{x | x \in S \wedge \forall y \in S : f(y) \geq f(x)\}$. In this framework, the argmin plays the role of the classifier, i.e., a function that associates to any unlabeled object the correspondent label.

coefficients have to be computed for each class. Then, the final value of each statistical coefficient related to the classification algorithm is the weighted sum of the statistical coefficients of each class.

3 Correspondence Between Pattern and Density Operator

In order to introduce a quantum version of the NMC, the first step is to find an appropriate quantum encoding for a real pattern.

Generally, given a d-dimensional feature vector, there exist different ways to encode it into a density operator [18]. In [20], the proposed encoding was based on the use of the stereographic projection [5]. In particular, it allows to unequivocally map any point $r = (r_1, r_2, r_3)$ on the surface of a radius-one sphere $\mathbb{S}^2$ (except for the north pole) onto an arbitrary point $\mathbf{x} = [x^{(1)}, x^{(2)}]$ in $\mathbb{R}^2$, i.e.,

$$SP : (r_1, r_2, r_3) \mapsto \left(\frac{r_1}{1 - r_3}, \frac{r_2}{1 - r_3}\right). \tag{3}$$

The inverse of the stereographic projection is given by

$$SP^{-1} : [x^{(1)}, x^{(2)}] \mapsto \left[\frac{2x^{(1)}}{||\mathbf{x}||^2 + 1}, \frac{2x^{(2)}}{||\mathbf{x}||^2 + 1}, \frac{||\mathbf{x}||^2 - 1}{||\mathbf{x}||^2 + 1}\right], \tag{4}$$

where $||\mathbf{x}||^2 = [x^{(1)}]^2 + [x^{(2)}]^2$. Then, by imposing that $r_1 = \frac{2x^{(1)}}{||\mathbf{x}||^2+1}$, $r_2 = \frac{2x^{(2)}}{||\mathbf{x}||^2+1}$, $r_3 = \frac{||\mathbf{x}||^2-1}{||\mathbf{x}||^2+1}$, if we consider r_1, r_2, r_3 as Pauli components[2] of a density operator $\rho_{\mathbf{x}} \in \mathbb{C}^2$, the density operator associated to the pattern $\mathbf{x} = [x^{(1)}, x^{(2)}]$ can be written as

$$\frac{1}{2}\begin{pmatrix} 1 + r_3 & r_1 - ir_2 \\ r_1 + ir_2 & 1 - r_3 \end{pmatrix} = \frac{1}{||\mathbf{x}||^2 + 1}\begin{pmatrix} ||\mathbf{x}||^2 & x^{(1)} - ix^{(2)} \\ x^{(1)} + ix^{(2)} & 1 \end{pmatrix}. \tag{5}$$

The advantage in using this encoding consists in the fact that it provides an easy visualization of an arbitrary two-feature vector on the Bloch sphere [20]. However, the main problem concerns the generalization of this encoding to d-feature vectors with $d > 2$. Although in [20] a generalization to the d-feature case was introduced, it exhibits some difficulties to be implemented for general cases.

[2]We consider the representation of an arbitrary density operator as linear combination of Pauli matrices.

An alternative encoding of a d-feature vector $\mathbf{x} = [x^{(1)}, \ldots, x^{(d)}]$ into a density operator was proposed in [19]. It is obtained (1) by mapping $\mathbf{x} \in \mathbb{R}^d$ into a $(d+1)$-dimensional vector $\mathbf{x}' \in \mathbb{R}^{d+1}$ according to the generalized version of Eq. (4), i.e.,

$$\mathbf{x}' = SP^{-1}(\mathbf{x}) = \frac{1}{||\mathbf{x}||^2 + 1}\left[2x^{(1)}, \ldots, 2x^{(d)}, ||\mathbf{x}||^2 - 1\right] \tag{6}$$

where $||\mathbf{x}||^2 = \sum_{i=1}^{d}[x^{(i)}]^2$ and then (2) by considering the projector $\rho_{\mathbf{x}} = \mathbf{x}' \cdot (\mathbf{x}')^T$.

In this work we propose a different version of the QNMC based on a new encoding again, and we show that this exhibits interesting improvements mostly by exploiting the non-invariance under rescaling of the features.

Accordingly with [12, 17, 18], when a real vector is encoded into a quantum state, in order to avoid a loss of information, it is important that the quantum state keeps some information about the norm of the original real vector. In light of this fact, we introduce the following alternative encoding.

Let $\mathbf{x} = [x^{(1)}, \ldots, x^{(d)}] \in \mathbb{R}^d$ be an arbitrary d-feature vector.

1. We map the vector $\mathbf{x} \in \mathbb{R}^d$ into a vector $\mathbf{x}' \in \mathbb{R}^{d+1}$, whose first d features are the components of the vector $\mathbf{x}$ and the $(d+1)$-th feature is the norm of $\mathbf{x}$. Formally:

$$\mathbf{x} = [x^{(1)}, \ldots, x^{(d)}] \;\mapsto\; \mathbf{x}' = [x^{(1)}, \ldots, x^{(d)}, ||\mathbf{x}||]. \tag{7}$$

2. Finally, we obtain the vector $\mathbf{x}'$ by dividing the first d components of the vector $\mathbf{x}'$ for $||\mathbf{x}||$:

$$\mathbf{x}' \;\mapsto\; \mathbf{x}'' = \left[\frac{x^{(1)}}{||\mathbf{x}||}, \ldots, \frac{x^{(d)}}{||\mathbf{x}||}, ||\mathbf{x}||\right]. \tag{8}$$

3. We consider the norm of the vector $\mathbf{x}''$, i.e., $||\mathbf{x}''|| = \sqrt{||\mathbf{x}||^2 + 1}$ and we map the vector $\mathbf{x}''$ into the normalized vector $\mathbf{x}'''$ as follows:

$$\mathbf{x}'' \;\mapsto\; \mathbf{x}''' = \frac{\mathbf{x}''}{||\mathbf{x}''||} = \left[\frac{x^{(1)}}{||\mathbf{x}||\sqrt{||\mathbf{x}||^2 + 1}}, \ldots, \frac{x^{(d)}}{||\mathbf{x}||\sqrt{||\mathbf{x}||^2 + 1}}, \frac{||\mathbf{x}||}{\sqrt{||\mathbf{x}||^2 + 1}}\right]. \tag{9}$$

Now, we provide the following definition.

Definition 1 (Density Pattern)
Let $\mathbf{x} = [x^{(1)}, \ldots, x^{(d)}]$ be an arbitrary d-feature vector and $(\mathbf{x}, y)$ the corresponding pattern. Then, the *density pattern* associated to $(\mathbf{x}, y)$ is represented by the pair $(\rho_{\mathbf{x}}, y)$, where the matrix $\rho_{\mathbf{x}}$, corresponding to the feature vector $\mathbf{x}$, is defined as

$$\rho_{\mathbf{x}} \doteq \mathbf{x}''' \cdot (\mathbf{x}''')^{\dagger}, \tag{10}$$

where the vector $\mathbf{x}'''$ is defined according to Eq. (9) and y is the label of the original pattern.

Hence, this encoding maps real d-dimensional vectors $\mathbf{x}$ into $(d+1)$-dimensional pure states $\rho_{\mathbf{x}}$. In this way, we obtain an encoding that takes into account the information about the initial real vector norm and, at the same time, allows to easily encode also arbitrary real d-dimensional vectors.

4 Quantum Classification

In this section we introduce a quantum-inspired version of the NMC, named *Quantum Nearest Mean Classifier* (QNMC). It can be seen as a particular kind of minimum-distance classifier between quantum objects (i.e., density patterns). The use of this new formalism could lead not only to achieve the well-known advantages related to the quantum computation with respect to the classical one (mostly related to the speedup of the computational process) but also to make a full comparison between NMC and QNMC performance by using a classical computer only.

In order to provide a quantum counterpart of the NMC, we need (1) an encoding from real patterns to quantum objects (already defined in the previous section), (2) a quantum counterpart of the classical centroid (i.e., a sort of class quantum prototype) that will be named *quantum centroid*, and (3) a suitable definition of *quantum distance* between density patterns that plays the same role as the Euclidean distance for the NMC. In this quantum framework, the quantum version $\mathscr{S}^q$ of the dataset $\mathscr{S}$ is given by

$$\mathscr{S}^q = \mathscr{S}^q_{\text{tr}} \cup \mathscr{S}^q_{\text{ts}}, \quad \mathscr{S}^q_{\text{tr}} = \{(\rho_{\mathbf{x}_n}, y_n)\}_{n=1}^{N}, \quad \mathscr{S}^q_{\text{ts}} = \{(\rho_{\mathbf{x}_n}, y_n)\}_{n=N+1}^{N'},$$

where $(\rho_{\mathbf{x}_n}, y_n)$ is the density pattern associated to the pattern $(\mathbf{x}_n, y_n)$. Consequently, $\mathscr{S}^q_{\text{tr}}$ and $\mathscr{S}^q_{\text{ts}}$ represent the quantum versions of training and test set, respectively, i.e., the sets of all the density patterns obtained by encoding all the elements of $\mathscr{S}_{\text{tr}}$ and $\mathscr{S}_{\text{ts}}$. Now, we naturally introduce the quantum version of the classical centroid $\boldsymbol{\mu}_l$, given in Eq. (1), as follows.

Definition 2 (Quantum Centroid) Let $\mathscr{S}^q$ be a labeled dataset of N' density patterns such that $\mathscr{S}^q_{\text{tr}} \subseteq \mathscr{S}^q$ is a training set composed of N density patterns. Further, let $\mathscr{Y} = \{1, 2, \ldots, L\}$ be the class label set. The *quantum centroid* of the l-th class is given by

$$\rho_l = \frac{1}{N_l} \sum_{n=1}^{N_l} \rho_{\mathbf{x}_n}, \quad l = 1, \ldots, L \tag{11}$$

where N_l is the number of density patterns of the l-th class belonging to $\mathscr{S}^q_{\text{tr}}$, such that $\sum_{l=1}^{L} N_l = N$.

Notice that the quantum centroids are generally mixed states, and they are not obtained by encoding the classical centroids $\boldsymbol{\mu}_l$, i.e.,

$$\rho_l \neq \rho_{\boldsymbol{\mu}_l},\ \forall l \in \{1, \ldots, L\}. \tag{12}$$

Accordingly, the definition of the quantum centroid leads to a new object that is no longer a pure state and does not have any classical counterpart. This is the main reason that establishes, even in a fundamental level, the difference between NMC and QNMC. In particular, it is easy to verify [20] that, unlike the classical case, the expression of the quantum centroid is sensitive to the dataset dispersion.

In order to consider a suitable definition of distance between density patterns, we recall the well-known definition of trace distance between quantum states (see, *e.g.,* [15]).

Definition 3 (Trace Distance) Let ρ and ρ' be two quantum density operators belonging to the same dimensional Hilbert space. The *trace distance* between them is given by

$$d_T(\rho, \rho') = \frac{1}{2} \operatorname{Tr} |\rho - \rho'|, \tag{13}$$

where $|A| = \sqrt{A^\dagger A}$.

Notice that the trace distance is a true metric for density operators, that is, it satisfies (1) $d_T(\rho, \rho') \geq 0$ with equality iff $\rho = \rho'$ (*positivity*), (2) $d_T(\rho, \rho') = d_T(\rho', \rho)$ (*symmetry*), and (3) $d_T(\rho, \rho') + d_T(\rho', \rho'') \geq d_T(\rho, \rho'')$ (*triangle inequality*).

We have introduced all the ingredients we need to describe the QNMC process that, similarly to the classical case, consists in the following steps:

- constructing the quantum training and test sets $\mathscr{S}^q_{\text{tr}}, \mathscr{S}^q_{\text{ts}}$ by applying the encoding introduced in Definition 1 to each pattern of the classical training and test sets $\mathscr{S}_{\text{tr}}, \mathscr{S}_{\text{ts}}$;
- calculating the quantum centroids ρ_l ($\forall l \in \{1, \ldots L\}$), by using the quantum training set $\mathscr{S}^q_{\text{tr}}$, according to Definition 2;
- classifying an arbitrary density pattern $\rho_{\mathbf{x}} \in S^q_{\text{ts}}$ accordingly with the following minimization problem

$$\underset{l=1,\ldots,L}{\operatorname{argmin}}\, d_T(\rho_{\mathbf{x}}, \rho_l), \tag{14}$$

  where d_T is the Trace distance introduced in Definition 3.

5 Experimental Results

This section is devoted to show a comparison between the NMC and the QNMC performances in terms of the statistical coefficients introduced in Sect. 2. We use both classifiers to analyze 14 datasets. In particular, two different kinds of datasets have been studied: five of them (*Gaussian (I), Gaussian (II), Gaussian (III), Moon,*

Banana) are artificial datasets, while the others (*Balance, Bands, Breast Cancer (I), Breast Cancer (II), Ilpd, Ionosphere, Liver, Pima, Tic Tac*) are real-world datasets, extracted from the UCI repository,[3] which follow unknown distributions. Let us note that, in real situations, we usually deal with data whose distribution is unknown, then the most interesting case is the one in which we use real-world datasets. However, the use of artificial datasets following known distribution, and in particular Gaussian distributions with specific parameters, can help to catch precious information, as we will see in the next section.

5.1 Comparison Between QNMC and NMC

In Table 1 we summarize the characteristics of the datasets involved in our experiments. In particular, for each dataset, we list the total number of patterns, the number of patterns belonging to each class, and the number of features. Let us note that, although we mostly confine our investigation to two-class datasets, our model can be easily extended to multiclass problems (as we show for the three-class datasets *Balance* and *Gaussian (III)*).

In order to make our results statistically significant, we apply the standard procedure which consists in randomly splitting each dataset into two parts, the training set (representing the 80% of the original dataset) and the test set (representing the 20% of the original dataset). Finally, we perform ten experiments for each dataset, where the splitting is every time randomly taken.

In Table 2, we report QNMC and NMC performance for each dataset, evaluated in terms of mean value and standard deviation (computed on ten runs) of the statistical coefficients, discussed in the previous section. For the sake of simplicity, we omit the values of FPR and FNR because they can be easily obtained by TPR and TNR values (i.e., FPR = 1 − TNR, FNR = 1 − TPR).

We observe, by comparing QNMC and NMC performances (see Table 2), that the first provides a significant improvement with respect to the standard NMC in terms of all the statistical parameters we have considered. Further, the new encoding, for two-feature datasets, provides better performance than the one considered in [20] (where the QNMC error with related standard deviation was 0.174 ± 0.047 for *Moon* and 0.419 ± 0.015 for *Banana*), and it generally exhibits quite similar performance with respect to the one in [19] for multidimensional datasets, except in the case of *Breast Cancer (II)* and *Gaussian (I)* datasets, for which the new encoding provides a classification improvement of about 3% and 5%, respectively.

The artificial Gaussian datasets may deserve a brief comment. Let us discuss the way in which the three Gaussian datasets have been created. *Gaussian (I)* [21] is a perfectly balanced dataset (i.e., both classes have the same number of patterns); patterns have the same dispersion in both classes, and only some features

[3] http://archive.ics.uci.edu/ml.

Table 1 Characteristics of the datasets used in our experiments

Data set	Instances	Features (d)
Balance	625 (49 + 288 + 288)	4
Banana	5300 (2376 + 2924)	2
Bands	365 (135 + 230)	19
Breast Cancer (I)	683 (444 + 239)	10
Breast Cancer (II)	699 (458 + 241)	9
Ilpd	583 (416 + 167)	9
Ionosphere	351 (225 + 126)	34
Liver	578 (413 + 165)	10
Moon	200 (100 + 100)	2
Pima	768 (500 + 268)	8
TicTac	958 (626 + 332)	9
Gaussian (I)	400 (200 + 200)	30
Gaussian (II)	1000 (100 + 900)	8
Gaussian (III)	2050 (50 + 500 + 1500)	8

The number of instances in each class is shown between brackets

are correlated [24]. *Gaussian (II)* is an unbalanced dataset (i.e., classes have a very different number of patterns), patterns do not exhibit the same dispersion in both classes, and features are not correlated. *Gaussian (III)* is composed of three classes, and it is an unbalanced dataset with different pattern dispersion in all the classes, where all the features are correlated.

For these Gaussian datasets, the NMC is not the best classifier [6] because of the particular characteristics of the class dispersion. Indeed, the NMC does not take into account data dispersion. Conversely, by looking at Table 2, the improvements of the QNMC seem to exhibit some kind of sensitivity of the classifier with respect to the data dispersion. A detailed description of this problem will be addressed in a future work.

As a remark, it is important to remind that, even if it is possible to establish whether a classifier is "good" or "bad" for a given dataset by the evaluation of some a priori data characteristics, generally it is not possible to establish an absolute superiority of a given classifier for any dataset, according to the well-known *No Free Lunch Theorem* [6]. Anyway, the QNMC seems to be particularly convenient when the data distribution is difficult to treat with the standard NMC.

5.2 Non-invariance Under Rescaling

The final experimental results that we present in this paper regard a significant difference between NMC and QNMC. Let us suppose that all the components of the feature vectors $\mathbf{x}_n$ ($\forall n = 1, \ldots, N'$) belonging to the original dataset $\mathscr{S}$ are multiplied by the same parameter $t \in \mathbb{R}$, i.e., $\mathbf{x}_n \mapsto t\mathbf{x}_n$. Then, the whole dataset

Table 2 Comparison between QNMC and NMC performance

Dataset	E	TPR	TNR	P	K
QNMC					
Balance	0.148 ± 0.018	0.852 ± 0.018	0.915 ± 0.014	0.862 ± 0.022	0.767 ± 0.029
Banana	0.316 ± 0.017	0.684 ± 0.017	0.660 ± 0.017	0.684 ± 0.018	0.350 ± 0.034
Bands	0.394 ± 0.053	0.606 ± 0.053	0.528 ± 0.071	0.606 ± 0.058	0.133 ± 0.112
Breast Cancer (I)	0.386 ± 0.038	0.614 ± 0.038	0.444 ± 0.045	0.583 ± 0.044	0.062 ± 0.069
Breast Cancer (II)	0.040 ± 0.015	0.946 ± 0.023	0.986 ± 0.016	0.993 ± 0.009	0.912 ± 0.033
Ilpd	0.351 ± 0.037	0.649 ± 0.037	0.705 ± 0.056	0.734 ± 0.041	0.292 ± 0.073
Ionosphere	0.165 ± 0.049	0.835 ± 0.049	0.764 ± 0.059	0.842 ± 0.051	0.624 ± 0.105
Liver	0.342 ± 0.037	0.607 ± 0.057	0.783 ± 0.059	0.870 ± 0.039	0.318 ± 0.061
Moon	0.156 ± 0.042	0.857 ± 0.063	0.831 ± 0.066	0.841 ± 0.066	0.683 ± 0.085
Pima	0.304 ± 0.030	0.696 ± 0.030	0.690 ± 0.044	0.720 ± 0.030	0.365 ± 0.066
Tic Tac	0.410 ± 0.032	0.590 ± 0.032	0.597 ± 0.039	0.629 ± 0.036	0.172 ± 0.061
Gaussian (I)	0.274 ± 0.051	0.726 ± 0.051	0.728 ± 0.049	0.745 ± 0.048	0.452 ± 0.099
Gaussian (II)	0.210 ± 0.025	0.790 ± 0.025	0.744 ± 0.061	0.900 ± 0.019	0.308 ± 0.058
Gaussian (III)	0.401 ± 0.036	0.599 ± 0.036	0.558 ± 0.026	0.654 ± 0.041	0152 ± 0.043
NMC					
Balance	0.267 ± 0.038	0.733 ± 0.038	0.969 ± 0.014	0.925 ± 0.025	0.686 ± 0.034
Banana	0.453 ± 0.019	0.548 ± 0.019	0.552 ± 0.020	0.556 ± 0.020	0.098 ± 0.038
Bands	0.435 ± 0.048	0.565 ± 0.048	0.582 ± 0.055	0.605 ± 0.054	0.135 ± 0.092
Breast Cancer (I)	0.442 ± 0.037	0.558 ± 0.037	0.464 ± 0.046	0.551 ± 0.039	0.022 ± 0.076
Breast Cancer (II)	0.042 ± 0.015	0.973 ± 0.015	0.931 ± 0.032	0.963 ± 0.017	0.908 ± 0.033
Ilpd	0.470 ± 0.037	0.530 ± 0.037	0.757 ± 0.041	0.761 ± 0.037	0.193 ± 0.051
Ionosphere	0.323 ± 0.051	0.677 ± 0.051	0.676 ± 0.051	0.680 ± 0.051	0.351 ± 0.102
Liver	0.472 ± 0.048	0.388 ± 0.057	0.891 ± 0.055	0.905 ± 0.045	0.193 ± 0.060
Moon	0.234 ± 0.065	0.772 ± 0.089	0.762 ± 0.085	0.771 ± 0.091	0.528 ± 0.130
Pima	0.375 ± 0.033	0.625 ± 0.033	0.546 ± 0.045	0.622 ± 0.037	0.173 ± 0.075
Tic Tac	0.439 ± 0.031	0.561 ± 0.031	0.571 ± 0.042	0.606 ± 0.036	0.119 ± 0.063
Gaussian (I)	0.322 ± 0.042	0.679 ± 0.042	0.680 ± 0.043	0.685 ± 0.042	0.355 ± 0.085
Gaussian (II)	0.320 ± 0.032	0.680 ± 0.032	0.588 ± 0.102	0.860 ± 0.032	0.129 ± 0.055
Gaussian (III)	0.530 ± 0.029	0.470 ± 0.029	0.625 ± 0.030	0.620 ± 0.036	0.066 ± 0.044

is subjected to an increasing dispersion (for $|t| > 1$) or a decreasing dispersion (for $|t| < 1$), and the classical centroids change according to $\boldsymbol{\mu}_l \mapsto t\boldsymbol{\mu}_l$ ($\forall l = 1, \ldots, L$). Consequently, the classification problem for each pattern of the rescaled test set can be written as

$$\underset{l=1,\ldots,L}{\operatorname{argmin}} d_E(t\mathbf{x}_n, t\boldsymbol{\mu}_l) = t \underset{l=1,\ldots,L}{\operatorname{argmin}} d_E(\mathbf{x}_n, \boldsymbol{\mu}_l), \ \forall n = N+1, \ldots, N'.$$

For any value of the parameter t it can be proved [19] that, while the NMC is invariant under rescaling, for the QNMC this invariance fails. Interestingly enough, it is possible to consider the failure of the invariance under rescaling as a resource

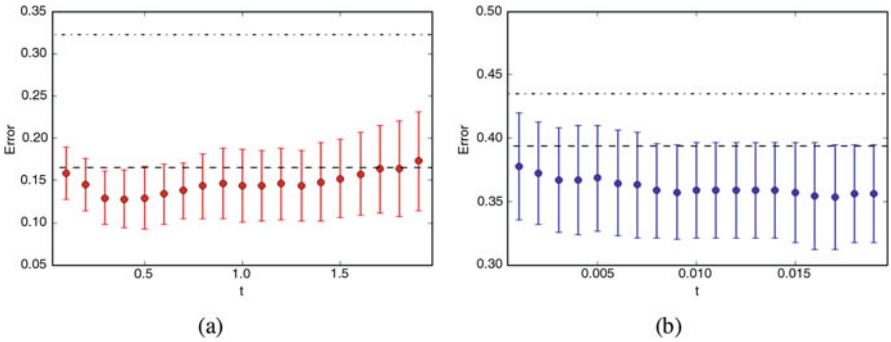

Fig. 1 Comparison between NMC and QNMC performance in terms of the classification error for the datasets (**a**) *Ionosphere* and (**b**) *Bands*. In both cases, the simple dashed line represents the QNMC classification error without rescaling, the dashed line with points represents the NMC classification error (which does not depend on the rescaling parameter), and points with related error bars (red in (**a**) and blue in (**b**)) represent the QNMC classification error for increasing values of the parameter t. In (a) $t \in [0.1, 1.9]$ and it increases with step 10^{-1}. In (b), $t \in [0.001, 0.019]$ and it increases with step 10^{-3}

for the classification problem. In other words, a suitable choice of the rescaling factor is possible, in principle, to get a decreasing of the classification error. At this purpose, we have studied the variation of the QNMC performance (in particular of the classification error) in terms of the *free* parameter t, and in Fig. 1 the results for the datasets *Ionosphere* and *Bands* are shown. In the figure, each point represents the mean value (with corresponding standard deviation represented by the vertical bar) over ten runs of the experiments. We can observe that, for the considered datasets, the QNMC performance for most of t values is better than the NMC, but for some particular value of t the error gets a further significant reduction (with respect the unrescaled case).

Let us note that the range of the rescaling parameter t, for which the QNMC performance improves, is generally not unique and depends on the dataset. For instance, in Fig. 1, we observe that the classification error provided by the QNMC decreases for t ranging from 0.1 to 1.9 in the *Ionosphere* case and from 0.001 to 0.019 in the *Bands* case. As a consequence, we do not generally get an improvement in the classification process for any t ranges. On the contrary, there exist some intervals of the parameter t where the QNMC classification performance is worse than the case without rescaling. Then, each dataset has specific and unique characteristics (in accord to the No Free Lunch Theorem), and the incidence of the non-invariance under rescaling in the decreasing of the error, in general, should be determined by empirical evidences.

6 Conclusions and Future Work

In this work a quantum counterpart of the well-known Nearest Mean Classifier was proposed. We introduced a quantum minimum-distance classifier, called Quantum Nearest Mean Classifier, obtained by defining a suitable encoding of real patterns, i.e., *density patterns*, and by recovering the trace distance between density operators.

We proposed a new encoding of a real pattern into a quantum object that was suggested by recent debates on quantum machine learning according to which, in order to avoid a loss of information caused by encoding a real vector into a quantum state, we need to normalize the real vector maintaining some information about its norm. Secondly, we defined the *quantum centroid*, i.e., the pattern chosen as the prototype of each class, which is not invariant under uniform rescaling of the original dataset (unlike the NMC) and seems to exhibit a kind of sensitivity to the data dispersion.

The experiments were organized as follows: both classifiers were compared in terms of significant statistical coefficients. In particular, we considered 14 different datasets having different nature (real-world and artificial). Further, the non-invariance under rescaling of the QNMC suggested to study the variation of the classification error in terms of a free parameter t, whose variation produces a modification of the data dispersion and, consequently, of the classifier performance. In particular we showed as, in the most of cases, the QNMC exhibits a significant decreasing of the classification error (and of the other statistical coefficients) with respect to the NMC and, for some case, the non-invariance under rescaling can provide a significant positive incidence in the classification process.

Let us remark that, even if there is not an absolute superiority of QNMC with respect to the NMC, the method we introduced allows to get some relevant improvements of the classification when we have an a priori knowledge about the distribution of the dataset we have to deal with.

In light of such considerations, further developments of the present work will be focused on (1) finding out the encoding (from real vectors to density operators) that guarantees the *optimal* improvement (at least for a finite class of datasets) in terms of the classification process accuracy, (2) obtaining a general method to find the suitable rescaling parameter range to apply to a given dataset in order to get further improvement of the accuracy, and (3) understanding for which kind of distribution the QNMC performs better than the NMC. At this purpose, it will be useful to compare the *optimal* QNMC also with other standard classical classifiers.

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