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Classification of Quantum Correlations via Quantum inspired Machine Learning

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The *Pretty Good Measurement* (PGM) classifier

Given an ensemble of possible quantum states with their respective a-priori probabilities $R = \{(p_1, \rho_1), \ldots, (p_\ell, \rho_\ell)\}_\ell$ no known analytical description exists for the exact optimal measurement for discriminating the states in R. However, the so-called PGM [1] performs well in several situations. The average state of R is given by: $\sigma = \sum_{i=1}^{\ell} p_i \rho_i$ and for any $i : 1 \leq i \leq \ell$, operators $E_i = (\sigma^\dagger)^{1/2} p_i \rho_i (\sigma^\dagger)^{1/2}$ $\sigma^\dagger$ is the pseudoinverse (or Moore-Penrose inverse) of σ. Now, let us consider that each object ρ_i is the quantum centroid, obtained as $\sum_{j=1}^{n} \rho_i^j$, where ρ_i^j represents the *quantum encoding* of classical objects belonging to class i (and n is the cardinality of class i). Given an *unknown* object ρ from the test set, the quantity $Tr(E_i \rho)$ represents the *probability* that ρ *belongs* to class i. By applying a majority rule over all $i \in [1, \ell]$, we classify ρ [3,5,6].

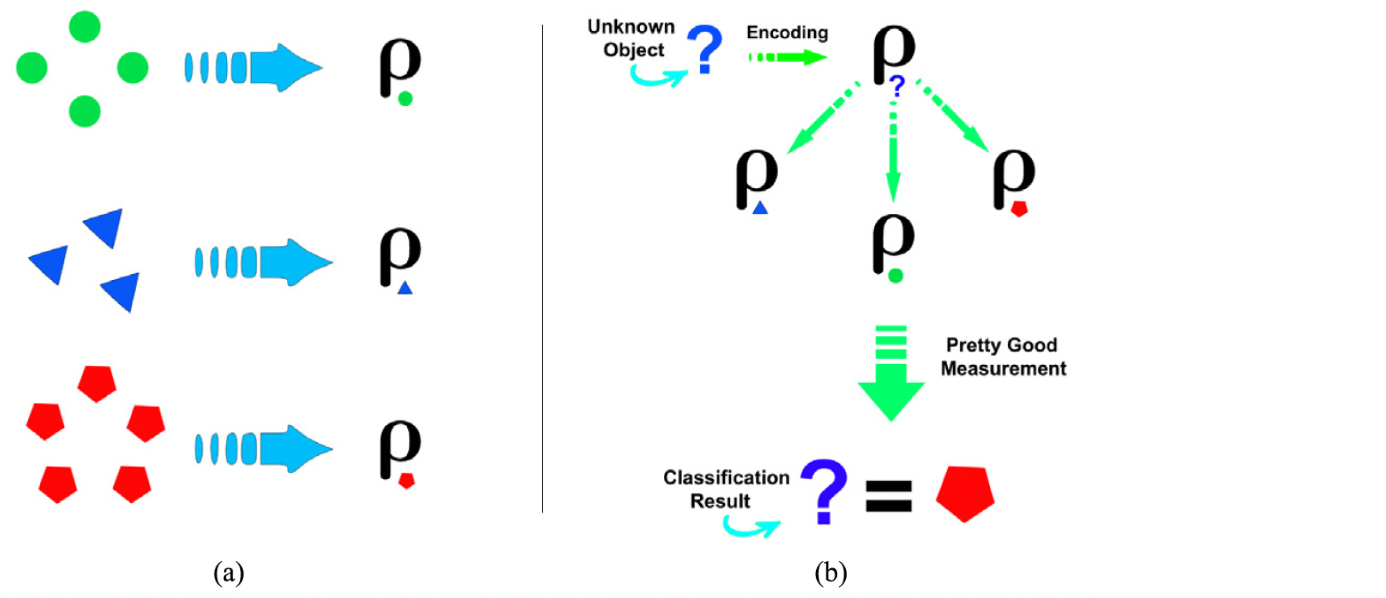


Figure 1. Illustration of the QI classification procedure. (a) Construction of quantum centroids using the feature map. The three classes of objects (classical data) are represented as three different types of geometric figures (red balls, blue triangles, and red pentagons). Under the action of the encoding map (blue arrows), the different classes are transformed into quantum states (centroids), in the form of density operators. In principle, the number of classes and the number of elements in each class can be arbitrary. (b) An unknown object is compared with the quantum centroids. Classification is performed using the PGM classifier: an unknown object (represented by a blue question mark) is identified by a red pentagon.

Performances of PGM classifiers

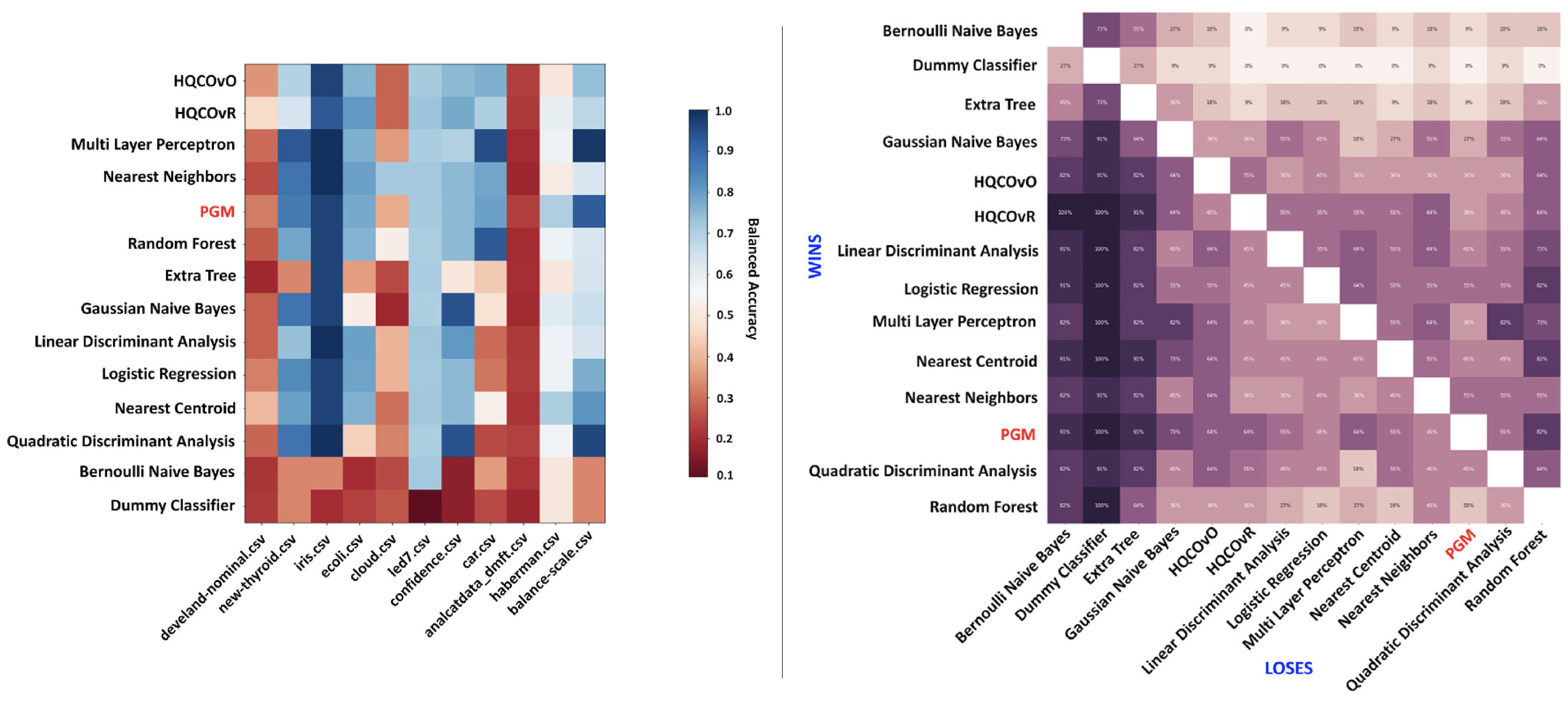


Figure 2. Heatmap of the values of each classifier applied to each dataset. Biclastering map: percentage of datasets for which the balanced accuracy of classifier A (in the column) outperforms that of classifier B (in the row). Darker (lighter) color indicates higher (lower) percentage.

Average value of Balanced Accuracy for each classifier over all datasets.

Classifier	Average Balanced Accuracy
Multi Layer Perceptron	0.679 ± 0.276
PGM	$\mathbf{0.675 \pm 0.238}$
Nearest Neighbors	0.657 ± 0.238
Random Forest	0.646 ± 0.231
Nearest Centroid	0.633 ± 0.227
HQC OvR	0.621 ± 0.208
HQC OvO	0.614 ± 0.225
Logistic Regression	0.606 ± 0.24
Quadratic Discriminant Analysis	0.6 ± 0.294
Linear Discriminant Analysis	0.589 ± 0.243
Gaussian Naive Bayes	0.586 ± 0.269
Extra Tree	0.463 ± 0.226
Bernoulli Naive Bayes	0.329 ± 0.153
Dummy Classifier	0.255 ± 0.1

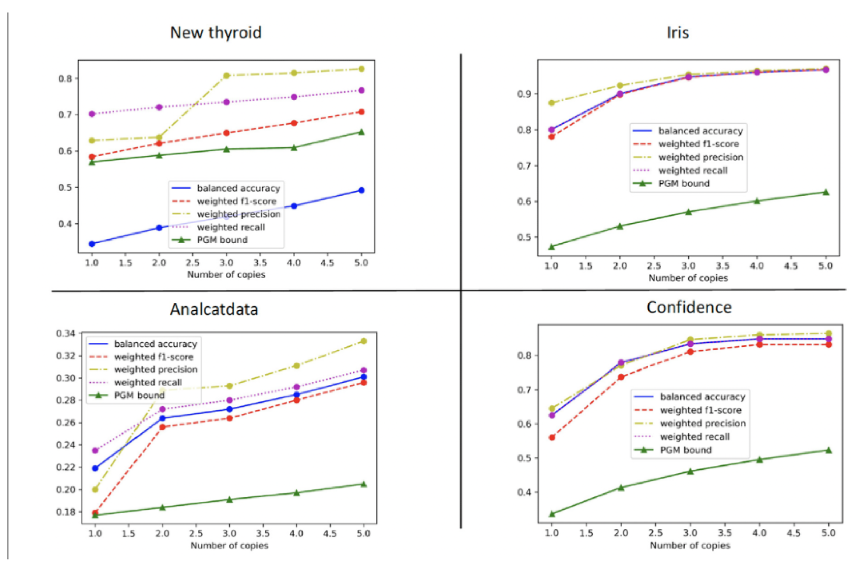


Figure 3. After the encoding of each real object into a density operator ρ, we apply the tensor copy of ρ, i.e. $\rho \otimes \ldots \rho$. This strategy turns out to produce an increasing of the performances of the PGM classifier.

Representing PGM classifier in IBM-Q

We use Neumark's dilation theorem, which allows us to transform any POVM into the composition of unitary operators. In particular, the PGM can be represented as a suitable combination of quantum gates that can be implemented in a quantum circuit.

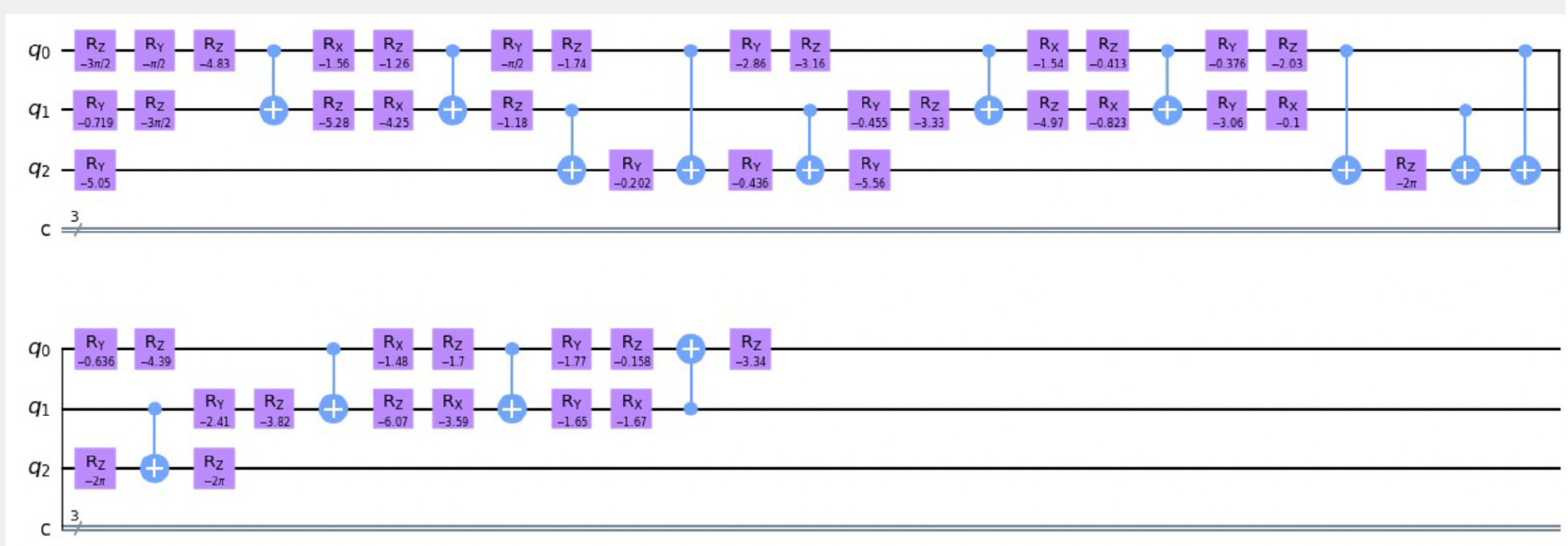


Figure 4. The circuit that implements the PGM in IBM-Q simulator. This circuit only contains C-Not gates (indicated by the usual representation) and rotations $R_i(n)$ along a given direction $i(x, y \text{ or } z)$ of a given angle n.

Applying PGM classifier for Clonogenic Essay evaluation

A clonogenic assay is a quantification technique of the survival degree of in vitro cell cultures, which is based on the ability of a single cell to grow and form a colony of cells after a given treatment. The purpose is to count the number of the colonies. Actually, many strategies to count the number of the colonies are by hands. Recent results show how by a classification between "pixel x belongs to the colony" and "pixel x belongs to the background" it is possible to have information about the number of the colonies. It allows us to move to a standard classification problem [2,4]. Each cell line is given by 30 different pictures (30 different datasets), each picture is given by 90601 pixels (301 x 301 square picture). In total we deal with more than 10 millions of data (large dataset). Further, each pixel is featured not only by its position in the image but also by important biological features: *homogeneity, correlation, energy, contrast, RGB, LUV*.

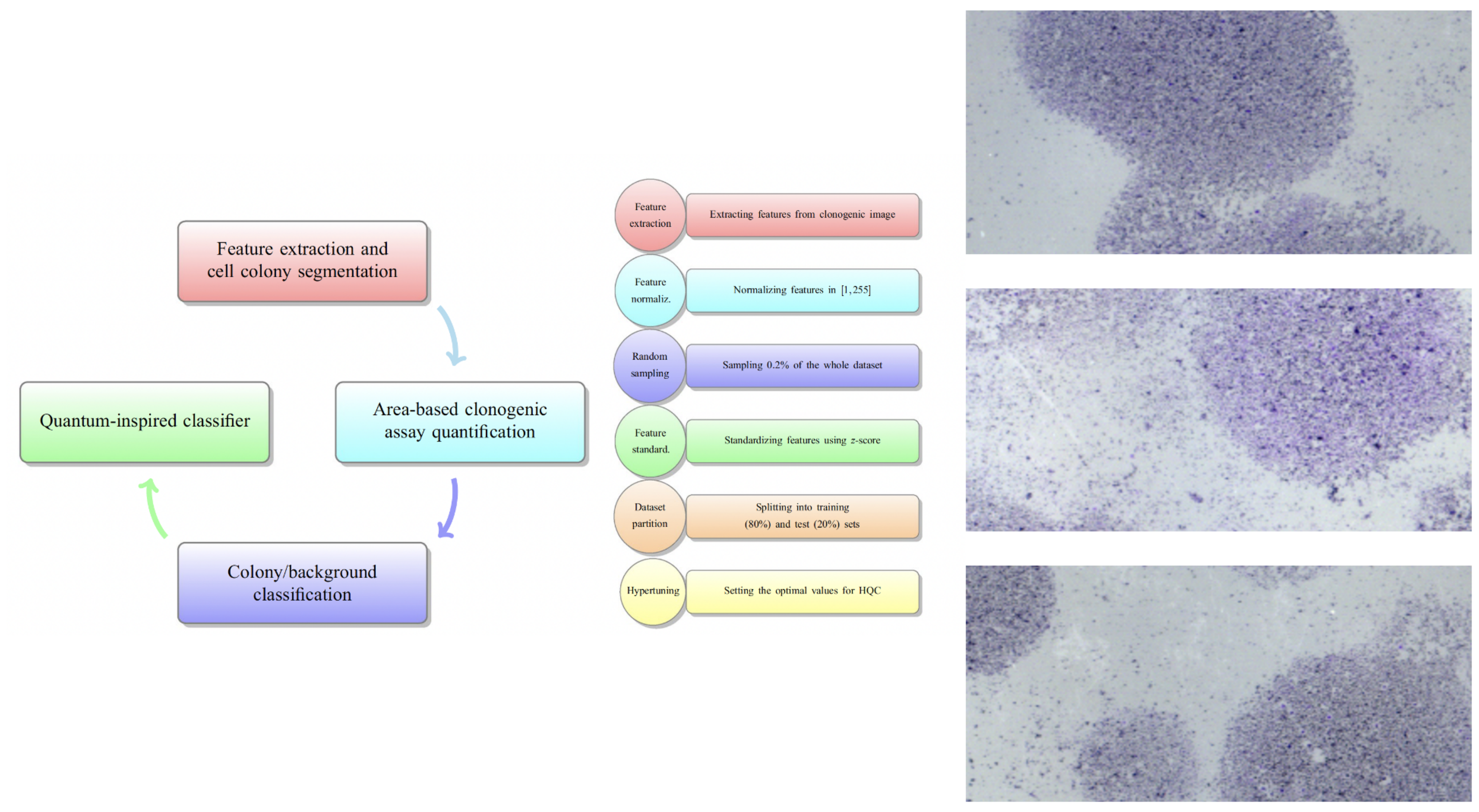


Figure 5. The conceptual scheme of the process together with some example of cell colony.

Classifying Quantum Correlations

Factorized	Entangled
$a\ b$	$A\ A$

Table1: Possible configuration for each case of a 2-qubit system

Factorized	Separable	Entangled
abc	AAb	AAA
	AbA	
	bAA	

Table2: Possible configuration for each case of a 3-qubit system

Factorized	Separable type I	Separable type II	Separable type III	Entangled
$abcd$	$AAAb$	$AABB$	$AAbc$	$AAAA$
	$AAbA$	$ABAB$	$AbAc$	
	$AbAA$	$ABBA$	$AbcA$	
	$bAAA$		$bAcA$	
			$bcAA$	
			$bAAc$	

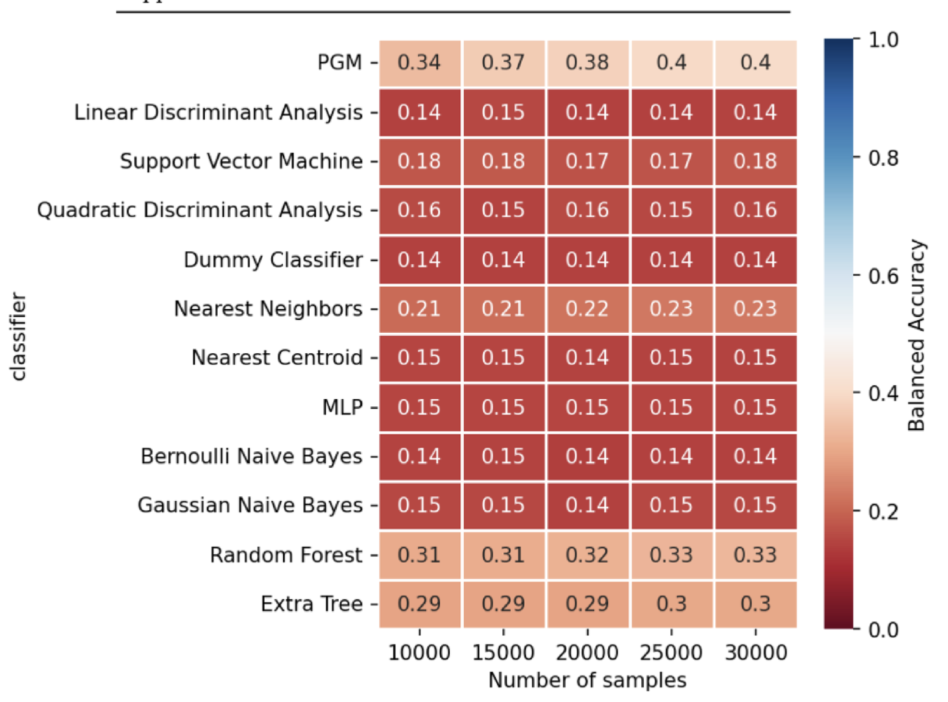
Table3: Possible configuration for each case of a 3-qubit system

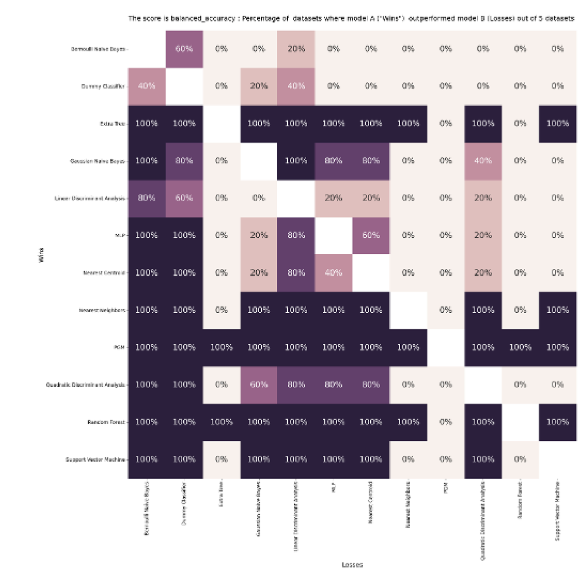
Factorized	Sep. t. I	Sep. t. II	Sep. t. III	Sep. t. IV	Sep. t. V	Entangled
$abcde$	$AAAAb$	$AAAbc$	$AAbcd$	$AABBc$	$AABBB$	$AAAAA$
	$AAAbA$	$AAbAc$	$AbAcd$	$ABABc$	$ABAAB$	
	$AAbAA$	$AAbcA$	$bAAcd$	$ABBAc$	$ABABA$	
	$AbAAA$	$AbAAc$	$AbcAd$	$AABcB$	$ABBAA$	
	$bAAAA$	$AbAcA$	$bAcAd$	$ABAcB$	$AABBA$	
		$AbcAA$	$bcAAd$	$ABBcA$	$AAABB$	
		$bAAAc$	$AbcdA$	$AAcBB$	$BAAAB$	
		$bAAcA$	$bAcdA$	$ABcAB$		
		$bAcAA$	$bcAdA$	$ABcBA$		
		$bcAAA$	$bcdAA$	$AcABB$		
				$AcBAB$		
				$AcBBA$		
				$cAABB$		
				$cABAB$		
				$cABBA$		

Table4: Possible configuration for each case of a 4-qubit system

We apply the PGM Classifier to discriminate between factorized states, separable states, and entangled states. We analyze from the simplest case (**2** qubits) up to a system of **5** qubits and offer a comparison between our quantum-inspired classifier and other classical classifiers.

Classifier	Average Balanced Accuracy
Bernoulli Naive Bayes	0.143 ± 0.003
Dummy Classifier	0.143 ± 0.000
Extra Tree	0.298 ± 0.004
Gaussian Naive Bayes	0.152 ± 0.005
Linear Discriminant Analysis	0.146 ± 0.004
MLP	0.149 ± 0.000
Nearest Centroid	0.149 ± 0.003
Nearest Neighbors	0.220 ± 0.008
PGM	0.377 ± 0.023
Quadratic Discriminant Analysis	0.154 ± 0.003
Random Forest	0.319 ± 0.008
Support Vector Machine	0.176 ± 0.004





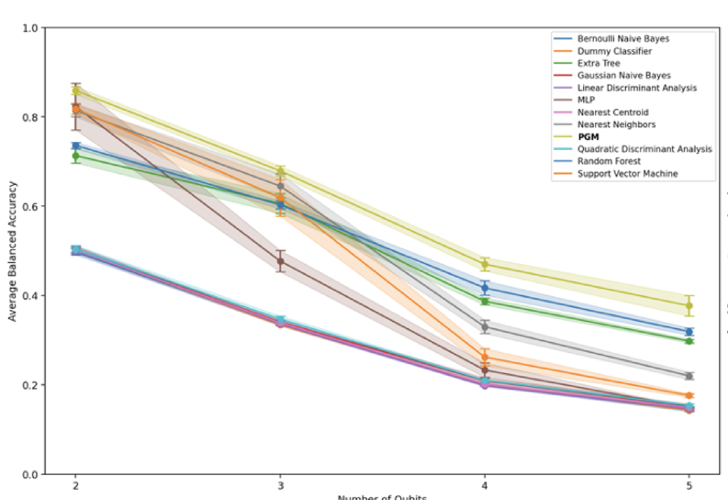


Figure 6. 5-qubit case. (i) Average Balanced Accuracy for each classifier, (ii) Heatmap of the Balanced Accuracy for different sam- ples, (iii) Biclustering map, when a classifier A outperforms a classifier B according to the Balanced Accuracy (lighter color indicates lower percentage), (iv) comparison of classifier per- formance for different numbers of qubits. The graph shows the average balanced accuracy of various classifiers. Error bars represent the standard deviation, and shaded regions indicate confidence intervals for each classifier.

References

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