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Estimación de Estados Cuánticos Puros y Transformaciones Unitarias a Través del Error Cuadrático Medio

Estimation of Pure Quantum States and Unitary Transformations Through the Mean Squared Error

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por

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Resumen

En este trabajo se propone un método para estimar un estado cuántico desconocido con alta precisión mediante la minimización del error cuadrático de las amplitudes de probabilidad complejas entre el estado desconocido y su estimador. Primero se demuestra como medir físicamente el error cuadrático usando un interferómetro, mostrándose que una realización física es posible para setups ópticos actuales. La técnica de minimización usada para obtener el estimador es una concatenación de Complex Simultaneous Perturbation Stocastic Approximation (CSPSA), un algoritmo iterativo estocástico que trabaja en el campo de los números complejos y Maximum Likelihood Estimation (MLE), un método de inferencia estadística. Haciendo uso de simulaciones numéricas se evalúa el desempeño del método propuesto, encontrando que su precisión alcanza un valor dos veces mas grande que la cota inferior de Gill-Massar, la cual expresa el mínimo valor posible de alcanzar. Más aún, esta precisión es independiente del estado desconocido, haciendo el método altamente consistente para todos los estados. La última parte de este trabajo se dedica a extender el método propuesto a la tarea de estimar transformaciones unitarias desconocidas actuando sobre un qudit y a exponer los resultados de las correspondientes simulaciones numéricas, las cuales entregan resultados similares a los obtenidos en estimación de estados

Abstract

This work proposes a method to estimate a quantum state with high accuracy through the minimization of the squared error of the complex probability amplitudes between the unknown state and its estimate. We first demonstrate how to physically measure the squared error using a multi-arm interferometer array, showing that a physical realization is plausible for actual optics setups. The minimization technique used to obtain the estimate is a concatenation of Complex Simultaneous Perturbation Stochastic Approximation (CPSA), an iterative stochastic algorithm that work within the field of complex numbers and Maximum Likelihood Estimation (MLE), an statistical inference method. By making use of numerical simulation we evaluate the performance of the proposed method, finding that its accuracy achieves twice the value of the Gill-Massar lower bound, which is the lowest attainable value. Furthermore, this accuracy is independent of the unknown state, making the method highly consistent. The remainder of this thesis is dedicated to extend the proposed method to the task of estimating unknown unitary transformations acting on a qudit, the corresponding simulations for this case yield similar results to the ones obtained in state estimation.

Introduction

Recently, the estimation of unknown quantum states has been studied from the point of view of the estimation accuracy achievable by means of an ensemble of N_T identically prepared copies of the state to be estimated [28, 40, 22, 34, 41, 18, 53]. The ultime mixed-state estimation accuracy is given by the Gill-Massar lower bound [17], which establishes the highest possible accuracy achievable by means of separable measurements on the members of the ensemble. For instance, the mean value $\bar{I}$ of the Uhlmann-Josza infidelity $I = (Tr\sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}})^2$ [24, 44] on the set of estimates $\tilde{\rho}$ of the unknown state ρ can be employed as a metric for the estimation accuracy. In this case the Gill-Massar lower bound for a density matrix of dimension d becomes $\bar{I} \geq I_{GM}^{(mixed)} = (d^2-1)(d+1)/4N_T$ [17].

On the other hand, for the case of pure states it has been shown that a much better accuracy can be obtained. In this case, the Gill-Massar lower bound for the infidelity is $I_{GM}^{(pure)} = (d-1)/N_T$. The 5-bases based quantum tomographic method [18] produces an infidelity that lays in between $I_{GM}^{(mixed)}$ and $I_{GM}^{(pure)}$ [53]. This method employs an adaptive scheme where measurements on the canonical base are employed to define four new measurement bases. The five bases determine univocally any pure state of a single qudit and allow to certify the purity assumption.

An estimation accuracy closer to $I_{GM}^{(pure)}$ can be achieved by means of formulating the problem of quantum state determination as an optimization problem [16] and solving it by means of a combination of stochastic optimization on the field of the complex numbers and maximum likelihood estimation (MLE) [45, 54]. In this approach the infidelity is considered a real function of complex arguments where the unknown state plays the role of a set of fixed and unknown complex parameters. This function is optimized by means of the Complex simultaneous stochastic approximation (CSPSA) method, which allows to handle non-holomorphic functions with unknown parameters. This optimization method requires the measurement of the infidelity at each iteration. The information provided by the sequence of measurements can be employed to enhance the rate of convergence of the optimization method when processed via maximum likelihood estimation.

Here, we study the estimation of pure quantum states using the mean-squared error (MSE) as figure of merit for the accuracy. It has been theoretically proven and experimentally demonstrated that states with a small infidelity might lead to very different physical properties [6, 10, 29]. Consequently, the infidelity might turn to be inadequate to assess the estimation of high-dimensional quantum systems. Therefore, it is advisable to explore other accuracy metrics. We resort to the mean-squared error mainly because it can be inferred from experimentally acquired data, it is inexpensive to compute, it is an excellent metric in the context of optimization, and it is a desirable measure in statistics and estimation theory [27]. We first show that the squared error (SE) between the probability amplitudes of two pure quantum states of a single qudit can be measured by means of a multi-arm interferometric array. This allows us to employ the CSPSA method to optimize SE. This iterative method and MLE are then combined to drive a sequence of measurements in such a

way that the SE rapidly decreases at each iteration. Due to the intrinsic stochasticity of CSPSA, the estimation procedure generates, for a fixed unknown state, a sample of estimates. Via Monte Carlo numerical experiments we show that the accuracy of the estimation procedure, that is, the mean of SE on the sample of estimates (or MSE), is nearly independent of the state to be estimated. Moreover, mean and median of SE agree on the sample of estimates, which indicates a symmetric distribution of estimates without outliers. Numerical simulations show that after a few iterations the estimation of unknown states enters into an asymptotic regime that follows very closely twice the Gill-Massar bound for the MSE.

We also apply our previous result to the estimation of unknown unitary transformations. This is an important application since the successful realization of quantum information protocols and quantum devices requires the use of efficient characterization tools. Among these, the most widely employed is Quantum process tomography (QPT). This is based on a selection of probe states that undergo the process to be estimated, which is followed by the estimation of the states generated by the process. QPT has been applied to multi-qubit processors [33], quantum communications channels [48], coherent transport in biological mechanisms [52], ion traps [36], nuclear magnetic resonance [12], superconducting circuits [8], nitrogen-vacancy color centers [23], and few-photon linear-optical systems [31, 14, 4].

A quantum process is described as a completely-positive, trace preserving (CPTP) map, which requires $d^4 - d^2$ real numbers to be completely characterized. If we know, however, that the process is unitary, then the number of independent parameters can be further reduced. For instance, $d^2 + d$ measurement outcomes are necessary to distinguish among unitary transformations [5]. Unitarity can be certified, for example,

through randomized benchmarking.

We can try to estimate a unitary transformation U with the help of the Uhlmann-Josza fidelity by applying U to the elements of an orthonormal base and estimating the generated states. This procedure, however, does not allow obtaining a set of d phases of the unitary transformation because the Uhlmann-Josza fidelity is insensitive to global phases. Thereby, it is necessary to increase the number of states onto which the unitary transformation acts in order to obtain the missing complex phases. Thus, the use of the Uhlmann-Josza fidelity for estimating unitary transformations becomes equivalent to the problem of estimating d pure states and d unknown phases. Alternatively, it is possible to define an infidelity-guided figure of merit to compare two unitary transformations U_1 and U_2. This is given by $I(U_1, U_2) = 1 - |Tr(U_1 U_2^\dagger)|^2/d^2$ [3]. This can be shown to be equal to $I(U_1, U_2) = 1 - |\langle\psi|(U_1^\dagger \otimes \mathcal{I})(U_2 \otimes \mathcal{I})|\psi\rangle|^2$, where $|\psi\rangle$ is the two-qudit maximally entangled state $\sum_k (1/\sqrt{d})|k\rangle \otimes |k\rangle$ [2]. Therefore, the measurement of $I(U_1, U_2)$ requires the capability of preparing maximally entangled two-qudit states and to project onto two-qudit states, which separates the estimation of states from that of unitary transformations. Instead, we apply our results on the estimation of pure states to the estimation of unitary transformations via the optimization of SE. This allows us to handle the estimation of states and unitary transformations within the same theoretical framework, avoid the use of maximally entangled two-qudit states, avoid increasing the number of measurements, and improve the estimation accuracy given a fixed number of particles interacting with the unknown unitary process. This is important, for instance, for measuring biological samples [42] and materials [50] in scenarios where the number of samples (photons) must be low to avoid sample damage Our method estimates the columns of an unknown unitary transformation

separately, which after post-processing leads to an estimation accuracy for the unitary transformations close to $2d$ times the Gill-Massar bound for the MSE of a single unknown pure state. Let us note that our estimation method for states and unitary transformations, unlike the recent proposals [55], measures all photons in the ensamble size independently, that is, no entanglement is used between photons. Also, most methods employed to estimate unitary transformations employ tomographic methods that are designed to estimate mixed states, which has an estimation accuracy limited by the Gill-Massar lower bound for mixed states.

This thesis is organized as follows: Chapter 1 contains the mathematical framework necessary to understand this work, linear algebra, probability theory, point estimation theory and optimization methods. Chapter 2 is dedicated for the principles of quantum mechanics and quantum tomography. Finally the results of our work regarding state tomography and unitary process tomography are exposed in Chapter 3 and Chapter 4 respectively.

Chapter 1

Mathematical Concepts

The following chapter consists of a review on the fundamental concepts needed to understand this work. It starts by showing the central pillar in which quantum mechanics is funded, linear algebra. The next section shows the preliminary concepts of probability theory, which allow us to work with the non-deterministic nature of quantum mechanics. The following section is dedicated to point estimation theory, the framework that studies the concepts that are necessary in the task of finding unknown parameters. Finally the chapter is closed with a section of optimization methods, introducing the algorithms used in this work.

1.1 Linear Algebra

Linear algebra is the study of vector spaces and of linear operations on those vectors [32].

1.1.1 Vector Spaces

Definition 1 *A non empty set V is called a* ***vector space over*** $\mathbb{K}$ *(where $\mathbb{K}$ is a scalar field), if there are defined two operations,*

- *A internal one: a sum of vectors $+ : V \times V \to V$, which for any $|\psi\rangle, |\phi\rangle, |\varphi\rangle \in V$ satisfies:*

  1. *Commutativity* $|\psi\rangle + |\phi\rangle = |\phi\rangle + |\psi\rangle$.

  2. *Associativity* $(|\psi\rangle + |\phi\rangle) + |\varphi\rangle = |\psi\rangle + (|\phi\rangle + |\varphi\rangle)$.

  3. *There is a unique element* $0_V \in V$ *such that* $|\psi\rangle + 0_V = 0_V + |\psi\rangle = |\psi\rangle$.

  4. *For each vector* $|\psi\rangle \in V$, *exist* $(-|\psi\rangle) \in V$ *such that* $|\psi\rangle + (-|\psi\rangle) = (-|\psi\rangle) + |\psi\rangle = 0_V s$.

- *an exterior one: the product by a scalar $\cdot : \mathbb{K} \times V \to V$. which for any $k, k' \in \mathbb{K}$ and $|\psi\rangle, |\phi\rangle \in |\psi\rangle$ satisfies:*

  1. $(k + k')|\psi\rangle = k|\psi\rangle + k'|\psi\rangle$.

  2. $k(|\psi\rangle + |\phi\rangle) = k|\psi\rangle + k|\phi\rangle$.

  3. $k(k'|\psi\rangle) = (kk')|\psi\rangle$.

  4. $1_{\mathbb{K}}|\psi\rangle = |\psi\rangle$.

For vector spaces of finite dimension d, the vectors are represented as

$$|\,\psi\,\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{pmatrix}. \tag{1.1}$$

A *basis* for a vector space V is a set of vectors $B = \{|\,e_i\,\rangle \in V\}_{i=1}^{d}$ that allows to express all vectors in V as a linear combination of the elements of the basis, that is, for any vector $|\,\psi\,\rangle \in V$ there exist a set of numbers $\{\psi_i \in \mathbb{K}\}_{i=1}^{d}$ such that

$$|\,\psi\,\rangle = \sum_{i=1}^{n} \psi_i |\,e_i\,\rangle.$$

If $\sum \alpha_i |\,i\,\rangle = 0$ implies that $\alpha_i = 0$ for all i, then we say that the basis B is *linearly independent*, otherwise it is called *linearly dependent*. The number of elements in an independent basis defines the dimension of the vector space.

Over a vector space we can define an *inner product*, which is a function whose inputs are two vectors and return a value over the scalar field $\mathbb{K}$, more specifically [21]

Definition 2 *Let $\mathbb{K}$ be the field of real or complex numbers, and V be a vector space over $\mathbb{K}$. An* inner product *on V is a function $(\cdot,\cdot) : V \times V \to \mathbb{K}$ which assigns to each ordered pair of vectors $|\,\psi\,\rangle, |\,\phi\,\rangle \in V$ a scalar $(|\,\psi\,\rangle, |\,\phi\,\rangle) \in \mathbb{K}$ in such a way that for all $|\,\psi\,\rangle, |\,\phi\,\rangle, |\,\varphi\,\rangle \in V$ and all scalar c*

- $(|\,\psi\,\rangle + |\,\phi\,\rangle, |\,\varphi\,\rangle) = (|\,\psi\,\rangle, |\,\varphi\,\rangle) + (|\,\phi\,\rangle, |\,\varphi\,\rangle)$.
- $(c|\,\psi\,\rangle, |\,\phi\,\rangle) = c(|\,\psi\,\rangle, |\,\phi\,\rangle)$.

- $(|\,\psi\,\rangle, |\,\phi\,\rangle) = (|\,\phi\,\rangle, |\,\psi\,\rangle)^*$, *where* $*$ *denotes complex conjugate.*
- $(|\,\psi\,\rangle, |\,\psi\,\rangle) \geq 0$ *with equality if and only if* $|\,\psi\,\rangle = 0$.

In a space provided with an inner product, the *norm* [1] induced by the inner product can be defined as

$$\| \, |\,\psi\,\rangle \, \| = \sqrt{(|\,\psi\,\rangle, |\,\psi\,\rangle)}.$$

Two vectors are said to be *orthogonal* if their inner product is 0, that is, $(|\,\psi\,\rangle, |\,\phi\,\rangle) = 0$. It is also said that $|\,\psi\,\rangle$ is a *unit vector* if $\| \, |\,\psi\,\rangle \, \| = 1$. A basis $B = \{|\,i\,\rangle\}_{i=1}^{n}$ of V is *orthonormal* if all the vectors on B are unitary and $(|\,i\,\rangle, |\,j\,\rangle) = \delta_{ij}$ for any i, j.

Now for any pair of vectors $|\,\psi\,\rangle, |\,\phi\,\rangle \in V$ there is an *adjoint* $\langle\,\psi\,|$ such that

$$(|\,\psi\,\rangle, |\,\phi\,\rangle) = \langle\,\psi\,|\,\phi\,\rangle. \tag{1.2}$$

The set of all adjoints vectors is a space denoted as the *dual space* V^*. Usually in quantum mechanics the operation that transforms a vector from V to the adjoint in V^* is denoted by $\langle\,\psi\,| = |\,\psi\,\rangle^\dagger$, and the operation depends on the type of space being treated. For example in a vector space of finite dimension, the adjoint vector $\langle\,\psi\,|$ correspond to the conjugate transpose of $|\,\psi\,\rangle$.

Being V a vector space provided with a inner product $(\cdot, \cdot)$, and hence an induced norm $||\cdot||$, then we can define successions $\{|\,\psi_i\,\rangle\}_{i=1}^{\infty}$ of V and the convergence of

[1] From this definition it can be seen that in every vector space with an inner product we can define a norm, but the converse is not true, that is, not every normed vector space has an inner product, but we are not going to dwell more deep into this, nor remark the differences from those two kinds of spaces in the future since it is not relevant for our works

them.

Definition 3 *A succession* $\{|\,\psi_i\,\rangle\}_{i=1}^{\infty}$ *of elements in* V *is said to* converge *(strongly) to* $|\,\psi_0\,\rangle$*, if* $\lim_{n\to\infty} \| \,|\,\psi_i\,\rangle - |\,\psi_0\,\rangle\,\| = 0$.

An important type of succession are the *Cauchy successions*, since it has been proven that every convergent succession on a set V is a Cauchy succession [38]. These successions are defined as follows.

Definition 4 *A succession* $\{|\,\psi_i\,\rangle\}_{i=1}^{\infty}$ *of elements in* V *is said to be a* Cauchy succession *if* $\lim_{n,m\to\infty} \| \,|\,\psi_n\,\rangle - |\,\psi_m\,\rangle\,\| = 0$*, that is*

$$\forall \epsilon > 0, \exists N > 0; \quad \| \,|\,\psi_n\,\rangle - |\,\psi_m\,\rangle\,\| < \epsilon, \quad \forall m, n > N.$$

If every Cauchy succession in V is also convergent in V, then we say that V is *complete*.

All these previous definitions allow us now to define a *Hilbert Space*, the one in which quantum mechanics are defined over.

Definition 5 *A* Hilbert space $\mathcal{H}$ *is a vector space* V *with an inner product* $(\cdot,\cdot)$*, which is complete under the norm induced by the inner product.*

1.1.2 Linear Operators

Definition 6 *A* linear operator *is a function* $A : V \to V'$ *that satisfies*

$$A\left(\sum_i \alpha_i |\, w_i \,\rangle\right) = \sum_i \alpha_i A(|\, w_i \,\rangle). \tag{1.3}$$

we say that A is defined on V if A is an operator from V to V. Among the operators defined on any vector space V, an important one is the identity $\mathbb{I}_V$, which satisfy $\mathbb{I}_V |\, v \,\rangle = |\, v \,\rangle$ for any $|\, v \,\rangle$. The space of all operators acting on V is denoted as $\mathcal{L}(V)$.

In the case of vector spaces of finite dimension, the operators acting on them can be represented as matrices of the form

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nm} \end{pmatrix}. \tag{1.4}$$

A convenient way to represent a linear operator is based on the *outer product*, which is an application between a pair of vectors $|\, v \,\rangle \in V$ and $|\, w \,\rangle \in W$, such that

$$(|\, w \,\rangle\langle\, v \,|)\, |\, z \,\rangle = \langle\, v \,|\, z \,\rangle |\, w \,\rangle \qquad\qquad \forall |\, z \,\rangle \in V. \tag{1.5}$$

We notice that $|\, w \,\rangle\langle\, v \,|$ is a linear operator that maps a vector in V into another one in W. Meaning that any linear operator can be written as a superposition of $|w\rangle\langle v|$. The identity $\mathbb{I}_V$ can be expressed, given any basis $\{|\, i \,\rangle\}$ of V, as $\mathbb{I}_V = \sum_i |\, i \,\rangle\langle\, i \,|$. To

prove this, let $|\,v\,\rangle = \sum_i v_i |\,i\,\rangle$ be an arbitrary vector, then

$$\mathbb{I}_V |\,v\,\rangle = \sum_i |\,i\,\rangle\langle\,i\,|\,v\,\rangle = \sum_i v_i |\,i\,\rangle = |\,v\,\rangle. \tag{1.6}$$

Which demonstrates the *completion relation* $\mathbb{I}_V = \sum_i |\,i\,\rangle\langle\,i\,|$, an equation that all complete basis should satisfy.

Definition 7 *Let V be a vector space and $A, B \in \mathcal{L}(V)$ be a pair of operators, then the* commutator *between them is defined as*

$$[A, B] = AB - BA. \tag{1.7}$$

The notion of commutator appears since the product between two different operators may not be commutative, implying the importance of the order when applying multiple operators

Definition 8 *Let $A \in \mathcal{L}(V)$ be any operator, then the sets of numbers $\lambda_i \in \mathbb{R}$ and vectors $|\,\lambda_i\,\rangle \in V$ are called* eigenvalues *and* eigenvectors *of A respectively if they satisfy*

$$A|\,\lambda_i\,\rangle = \lambda_i |\,\lambda_i\,\rangle. \tag{1.8}$$

The eigenvalues can be found by using the *characteristic equation* defined as

$$c(\lambda) = \det\left(A - \lambda \mathbb{I}_V\right) = 0, \tag{1.9}$$

This equation can be easily derived from Eq.(1.8) and it is equivalent to a polynomial with a degree equal to the dimension d of the space, meaning that there

are at most d different complex eigenvalues. It is possible that the characteristic polynomial has a root with a multiplicity m higher than one, which means that the corresponding eigenvalue is associated to m different eigenvectors. The eigenvectors are orthonormal and they form a complete basis of the space V.

Definition 9 *Let $\mathcal{H}$ be a Hilbert space and $A \in \mathcal{L}(\mathcal{H})$. The* norm *of A is defined as*

$$\| A \| = \sup_{|\psi\rangle \in V - \{0\}} \frac{\| A|\psi\rangle \|}{\| |\psi\rangle \|} \tag{1.10}$$

An operator A is said to be *bounded* if the norm $\| A \|$ does not diverge.

Definition 10 *Let A be a bounded linear operator acting on a Hilbert space $\mathcal{H}$, then there is a unique operator $A^\dagger$ defined as the* adjoint *or* Hermitian conjugate *of A, such that for any pair of vector $|v\rangle, |z\rangle \in V$,*

$$(|v\rangle, A|z\rangle) = (A^\dagger|v\rangle, |z\rangle). \tag{1.11}$$

If the operator is defined on a vector space of finite dimension, then the adjoint $A^\dagger$ is equivalent to the conjugate transpose of A.

An operator A is defined as *hermitian* or *self-adjoint*, if A is equal to its own adjoint $A^\dagger$. The eigenvalues of hermitian operators are real numbers, in effect

$$\lambda = \langle \lambda |A| \lambda \rangle = \langle \lambda |A^\dagger| \lambda \rangle = \langle \lambda |A^\dagger| \lambda \rangle^* = \lambda^*. \tag{1.12}$$

An hermitian operator A is said to be *positive definite* if all the eigenvalues of A are positive. This is commonly denoted as $A > 0$.

Let V have a vector subspace $V_1 \subset V$. An operator $P \in \mathcal{L}(V)$ is called a *projector* if $P : V \to V_1$. An important remark about projectors is that they are hermitian. Indeed, for any basis $B_1 = \{|\, w_i \,\rangle\}_{i=1}^{k}$ of V_1 the projector can be written as

$$P = \sum_{i=1}^{k} |\, w_i \,\rangle\langle\, w_i \,|, \tag{1.13}$$

and then by calculating the adjoint the expression remains the same.

Another important class of linear operators outside hermitians are the *unitary operators* $U \in \mathcal{L}(\mathcal{H})$, defined as the ones satisfying

$$U^{-1} = U^{\dagger}, \tag{1.14}$$

therefore preserving the inner product. In effect, for any pair of vectors $|\, w \,\rangle, |\, v \,\rangle \in \mathcal{H}$ the inner product between $U|\, w \,\rangle$ and $U|\, v \,\rangle$ is given by

$$(U|\, w \,\rangle, U|\, v \,\rangle) = \langle\, w \,|U^{\dagger}U|\, v \,\rangle = \langle\, w \,|\, v \,\rangle. \tag{1.15}$$

An immediate consequence is that unitary operators preserve the norm of a vector.

The eigenvalues of a unitary operator are complex numbers of modulus 1. To see this, lets suppose that $|\, \lambda \,\rangle \in \mathcal{H}$ is an eigenvector, then $U|\, \lambda \,\rangle$ has the same norm as $|\, \lambda \,\rangle$, therefore they can only differ on a phase, meaning that there exist $\phi \in \mathbb{R}$ such that

$$U|\, \lambda \,\rangle = e^{i\phi}|\, \lambda \,\rangle. \tag{1.16}$$

Unitary operators preserving the inner product implies that any unitary $U \in \mathcal{L}(\mathcal{H})$ acting on an orthonormal basis B of $\mathcal{H}$ returns a different orthonormal basis

B', if the elements of B are not the eigenvectors of B. Effectively, if $B = \{|\, v_i \,\rangle\}$ and $U|\, v_i \,\rangle = |\, w_i \,\rangle$, then the inner product between any pair $|\, w_i \,\rangle, |\, w_j \,\rangle \in \mathcal{H}$ is

$$\langle\, w_i \,|\, w_j \,\rangle = \langle\, v_i \,|U^\dagger U|\, v_j \,\rangle = \langle\, v_i \,|\, v_j \,\rangle = \delta_{ij}, \tag{1.17}$$

An operator $A \in \mathcal{L}(\mathcal{H})$ is said to be normal if $AA^\dagger = A^\dagger A$, or equivalently $[A, A^\dagger] = 0$.

Theorem 1 *(Spectral Decomposition[32]) Let $\mathcal{H}$ be a finite dimensional Hilbert space. Then any normal operator $A \in \mathcal{L}(\mathcal{H})$ with eigenvalues λ_i and eigenvectors $|\, \lambda_i \,\rangle$ can be expressed as*

$$A = \sum_{i=1}^{d} \lambda_i |\, \lambda_i \,\rangle\langle\, \lambda_i \,|. \tag{1.18}$$

This means that A is diagonal with respect to some orthonormal basis on $\mathcal{H}$.

The spectral decomposition expresses an useful and easy way of writing a normal operator. Besides, has a major importance since any function $f : \mathcal{H} \to \mathcal{H}$ that can be expanded as a Taylor series is defined to be applied as follows

$$f(A) = \sum_{i=1}^{d} f(\lambda_i) |\, \lambda_i \,\rangle\langle\, \lambda_i \,|. \tag{1.19}$$

Another consequence of the spectral decomposition theorem is that the commutator between two operators A, B with the same eigenvectors is 0, or stated in other way, any pair of operators with a non-zero conmutator do not share a common eigenbasis.

Definition 11 *Let V be a finite dimensional space and $A \in \mathcal{L}(V)$ a matrix. Then*

the trace *is a function* $\mathrm{Tr} : \mathcal{L}(V) \to \mathbb{C}$ *defined as the sum over the diagonal elements of* A*, that is*

$$\mathrm{Tr}(A) = \sum_i A_{ii} = \sum \langle\, i \,|A|\, i \,\rangle, \tag{1.20}$$

where $\{|\, i \,\rangle\}$ *can be an arbitrary basis of* V*, and is invariant of the choice.*

Some of the properties of the trace are being *linear* $\mathrm{Tr}(\gamma A + \beta B) = \gamma \mathrm{Tr}(A) + \beta \mathrm{Tr}(B)$, *cyclic* $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ and invariant under unitary *similarity transformations* $A \to UAU^\dagger$, meaning $\mathrm{Tr}(A) = \mathrm{Tr}(UAU^\dagger)$.

Since the trace $\mathrm{Tr}(A) = \sum \langle\, i \,|A|\, i \,\rangle$ is invariant of the chosen basis $\{|\, i \,\rangle\}$, then by taking the eigenvectors $\{|\, \lambda_i \,\rangle\}$ of A as the basis, it can be proven that the trace is equal to the sum of the eigenvalues, that is $\mathrm{Tr}(A) = \sum \lambda_i$.

Definition 12 *Let* $\mathcal{L}(V)$ *be the set of linear operators defined on a finite dimensional vector space. Then the* Hilbert-Schmidt *product is an inner product* $\langle \cdot, \cdot \rangle : \mathcal{L}(V) \times \mathcal{L}(V) \to \mathbb{C}$ *defined as*

$$\langle A, B \rangle = \mathrm{Tr}(A^\dagger B) \tag{1.21}$$

Since $\mathcal{L}(V)$ is a vector space on itself, and it has an inner product defined. Then the norm induced by the inner product is

$$\| A \|_{HS} = \sqrt{\langle A, A \rangle} = \sqrt{\mathrm{Tr}(A^\dagger A)} = \sqrt{\sum_{i,j} |\, A_{i,j} \,|^2} \tag{1.22}$$

and is known as the Hilbert-Schmidt norm. Furthermore, given two operators $A, B \in \mathcal{L}(V)$, the distance between them can be obtained using

$$\| A - B \|_{HS} = \sqrt{\mathrm{Tr}\left[(A - B)^\dagger (A - B)\right]}. \tag{1.23}$$

1.1.3 Direct Sum and Tensor Product

Definition 13 *Let V be a vector space and $V_1, V_2 \subset V$ the subspaces. Then V is said to be the* direct sum *of V_1 and V_2, denoted as $V = V_1 \vec{\oplus} V_2$ if any vector $|\, v \,\rangle \in V$ can be written uniquely as $|\, v \,\rangle = |\, v_1 \,\rangle + |\, v_2 \,\rangle$, meaning that there is only one vector $|\, v_1 \,\rangle \in V_1$ and only one vector $|\, v_2 \,\rangle \in V_2$ satisfying the condition.*

If the sub-spaces V_1 and V_2 are orthogonal, then the direct sum is denoted as $V_1 \oplus V_2$ and is called *orthogonal direct sum.*

In a vector space $V = V_1 \vec{\oplus} V_2$ the action of a projector $P_1 : V \to V_1$ returns the only vector $|\, v_1 \,\rangle$ of the decomposition described on definition 13, and equivalently for a projector $P_2 : V \to V_2$.

Definition 14 *Given the vector spaces V and W, the* tensor product *space $V \otimes W$ is the vector space composed of all the ordered pairs $|\, v \,\rangle \otimes |\, w \,\rangle$ where $|\, v \,\rangle \in V$ and $|\, w \,\rangle \in W$ and all the linear combination*

$$\alpha_1 |\, v_1 \,\rangle \otimes |\, w_1 \,\rangle + \alpha_2 |\, v_2 \,\rangle \otimes |\, w_2 \,\rangle + \cdots \tag{1.24}$$

Let $\{|\, v_i \,\rangle\}_{i=1}^{m}$ and $\{|\, w_j \,\rangle\}_{j=1}^{n}$ be complete bases for V and W respectively, then $\{|\, v_i \,\rangle \otimes |\, w_j \,\rangle \mid i = 1, m \ \wedge \ j = 1, n\}$ is a complete basis for the mn dimensional vector space $V \otimes W$.

The tensor product space is linear in each of the arguments, that is

$$(\alpha_1 |\, v_1 \,\rangle + \alpha_2 |\, v_2 \,\rangle) \otimes |\, w \,\rangle = \alpha_1 |\, v_1 \,\rangle \otimes |\, w \,\rangle + \alpha_2 |\, v_2 \,\rangle \otimes |\, w \,\rangle \tag{1.25}$$

$$|\, v \,\rangle \otimes (\beta_1 |\, w_1 \,\rangle + \beta_2 |\, w_2 \,\rangle) = \beta_1 |\, v \,\rangle \otimes |\, w_1 \,\rangle + \beta_2 |\, v \,\rangle \otimes |\, w_2 \,\rangle. \tag{1.26}$$

The linear operators C defined on a tensor product space $V_1 \otimes V_2$ have the form $C = A \otimes B$ with $A : V_1 \to V_1'$ and $B : V_2 \to V_2'$, or linear combinations $C = \sum \gamma_i A_i \otimes B_i$. Their action on vectors $|\, v_1 \,\rangle \otimes |\, v_2 \,\rangle$ is given by

$$(A \otimes B)(|\, v_1 \,\rangle \otimes |\, v_2 \,\rangle) = A|\, v_1 \,\rangle \otimes B|\, v_2 \,\rangle. \tag{1.27}$$

In a finite dimensional vector space, the tensor product translates to the *Kronecker product*, which for vectors is computed as

$$|\, v \,\rangle \otimes |\, w \,\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \otimes |\, w \,\rangle = \begin{pmatrix} v_1|\, w \,\rangle \\ v_2|\, w \,\rangle \\ \vdots \\ v_n|\, w \,\rangle \end{pmatrix}, \tag{1.28}$$

and for operators is

$$A \otimes B = \begin{pmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & \vdots & \vdots \\ A_{m,1} & \cdots & A_{m,n} \end{pmatrix} \otimes B = \begin{pmatrix} A_{1,1}B & \cdots & A_{1,n}B \\ \vdots & \vdots & \vdots \\ A_{m,1}B & \cdots & A_{m,n}B \end{pmatrix}. \tag{1.29}$$

1.1.4 Gram-Schmidt Orthonormalization Procedure

In a vector space V of finite dimension, several bases can be defined and all of them are complete, but there are basis that are not orthonormal, which sometimes is inconvenient. However, there is a procedure to transform any basis into an orthonormal one, this algorithm is known as the Gram-Schmidt procedure.

Given any non-orthonormal basis $B = \{|\, v_i \,\rangle\}_{i=1}^{d}$ of V, the objective is to trans-

form B into an orthonormal basis $B' = \{|\, z_i \,\rangle\}_{i=1}^{d}$ with a one-to-one map. So, first lets define $|\, w_1 \,\rangle = |\, v_1 \,\rangle$. The following step is to define $|\, w_2 \,\rangle$ as $|v_2\rangle$ minus the projection of $|\, v_2 \,\rangle$ over $|\, w_1 \,\rangle$, meaning

$$|\, w_2 \,\rangle = |\, v_2 \,\rangle - \frac{\langle\, v_2 \,|\, w_1 \,\rangle}{\langle\, w_1 \,|\, w_1 \,\rangle} |\, w_1 \,\rangle. \tag{1.30}$$

And the rest of the algorithm is to repeat this step for the following vector of the basis. Summarizing

$$\begin{aligned}
|\, w_1 \,\rangle &= |\, v_1 \,\rangle \\
|\, w_2 \,\rangle &= |\, v_2 \,\rangle - \frac{\langle\, v_2 \,|\, w_1 \,\rangle}{\langle\, w_1 \,|\, w_1 \,\rangle} |\, w_1 \,\rangle \\
|\, w_3 \,\rangle &= |\, v_3 \,\rangle - \frac{\langle\, v_3 \,|\, w_1 \,\rangle}{\langle\, w_1 \,|\, w_1 \,\rangle} |\, w_1 \,\rangle - \frac{\langle\, v_3 \,|\, w_2 \,\rangle}{\langle\, w_2 \,|\, w_2 \,\rangle} |\, w_2 \,\rangle \\
&\vdots \\
|\, w_k \,\rangle &= |\, v_k \,\rangle - \sum_{i=1}^{k-1} \frac{\langle\, v_k \,|\, w_i \,\rangle}{\langle\, w_i \,|\, w_i \,\rangle} |\, w_i \,\rangle.
\end{aligned} \tag{1.31}$$

Since the basis $\{|\, w_i \,\rangle\}$ is orthogonal by construction, and is generated as a biyect map from B, the orthonormality can be easily accomplished by defining

$$B' = \{|\, z_i \,\rangle\} = \left\{ \frac{|\, w_i \,\rangle}{\| \,|\, w_i \,\rangle\, \|} \right\}. \tag{1.32}$$

The Gram-Schmidt procedure is useful in many ways, one of them is to generate unitary matrices for any random matrix. In effect, since $UU^\dagger = \mathbb{I}_V$, it can be concluded that any column of an unitary matrix is a unitary vector and the inner product between two different columns is 0, hence a method to generate a unitary matrix from a random one would be to apply the Gram-Schmidt procedure to the

column vectors of the original matrix.

1.1.5 Nearest Unitary Matrix

In section 1.1.4 was proven that a unitary matrix $U \in \mathcal{L}(\mathcal{H})$ can be generated from any random matrix $A \in \mathcal{H}$, but not necessarily the nearest to the original operator A.

Given any invertible matrix $A \in \mathcal{L}(H)$, the problem is to find a unitary matrix U that solves the optimization problem

$$\begin{aligned} &\min \| A - U \|_{HS}^2 \\ &\text{subject to: } U^\dagger U = \mathbb{I} \end{aligned} \tag{1.33}$$

where $\| \cdot \|_{HS}$ is the Hilbert-Schmidt norm introduced in Eq. (1.22). To solve this optimization problem we use the hermitian Lagrangian multiplier Λ and search for stationary points on the Lagrangian

$$\mathcal{L}(U, \Lambda) = \mathrm{Tr}\left[(A-U)^\dagger (A-U)\right] + \mathrm{Tr}[\Lambda(U^\dagger U - \mathbb{I})]. \tag{1.34}$$

The stationary points are determined by the equation

$$\frac{d}{dU}\mathcal{L}(U, \Lambda) = 0, \tag{1.35}$$

where the derivative with respect to an operator is carried out with the Fréchet derivative [7] of a function $f : H \to H'$, defined as

$$\frac{d}{dX}f(X)(V) = \lim_{t\to 0}\frac{d}{dt}f(X+tV). \tag{1.36}$$

In order to find a solution it is useful to notice that for $A \in \mathcal{L}(\mathcal{H})$ a constant matrix

$$\frac{d}{dX}\mathrm{Tr}(AX^\dagger X)(V) = \lim_{t\to 0}\frac{d}{dt}\mathrm{Tr}\left[A(X+tV)^\dagger(X+tV)\right] \tag{1.37}$$

$$= \mathrm{Tr}\left[AV^\dagger X + AX^\dagger V\right]. \tag{1.38}$$

Now, using the result of Eq. (1.38) and replacing it into Eq. (1.35) gives the expression

$$\frac{d}{dU}\mathcal{L}(U,\lambda)(V) = \mathrm{Tr}[V^\dagger(U-A)+(U-A)^\dagger V] + \mathrm{Tr}[\Lambda V^\dagger U + \Lambda U^\dagger V] \tag{1.39}$$

$$= \mathrm{Tr}[V^\dagger(U-A+U\Lambda)] + \mathrm{Tr}[(U-A+U\Lambda)^\dagger V] = 0. \tag{1.40}$$

Remembering that $\mathrm{Tr}(A^\dagger B) = \langle A, B\rangle$ is the Hilbert-Schmidt product introduced in definition 12, and it satisfies $\mathrm{Tr}(B^\dagger A) = \langle B, A\rangle^*$, then Eq. (1.40) can be written as

$$\mathrm{Tr}[V^\dagger(U-A+U\Lambda)] + \mathrm{Tr}[V^\dagger(U-A+U\Lambda)]^* = 0. \tag{1.41}$$

It can be seen that Eq.(1.41) holds trivially for the imaginary part, but the real part does not hold. Therefore, Eq. (1.41) is true for any matrix V if $U - A + U\Lambda = 0$, or equivalently

$$A = U(\Lambda + \mathbb{I}). \tag{1.42}$$

Then the Lagrange multiplier Λ can be found by computing $A^\dagger A$, yielding

$$\Lambda = (A^\dagger A)^{\frac{1}{2}} - \mathbb{I}. \tag{1.43}$$

Replacing this into Eq.(1.42) and clearing U, using the fact that A is invertible by definition results in

$$U = A(A^{\dagger}A)^{-\frac{1}{2}}, \tag{1.44}$$

which is the nearest unitary U to the arbitrary invertible matrix A.

1.2 Probability Theory

Probability theory is the mathematical framework that studies rigorously non-deterministic or uncertain behaviors that are present in nature.

1.2.1 Axioms

Consider an experiment in which the possible outcomes are well know, but it is impossible to predict the specific outcome beforehand. The set of all possibles outcomes ω defines the *sample space* Ω, and the subsets $E \subset \Omega$ are the events of the experiment [37].

Definition 15 *Let Ω be an arbitrary nonempty space. A* class *$\mathcal{F}$ of subsets of Ω is called a* field *if [9]*

1. $\Omega \in \mathcal{F}$.

2. $E \in \mathcal{F}$ *implies* $E^{c} \in \mathcal{F}$.

3. $E_1, E_2 \in \mathcal{F}$ *implies* $E_1 \cup E_2 \in \mathcal{F}$, *or equivalently* $E_1 \cap E_2 \in \mathcal{F}$

Thus, $\mathcal{F}$ usually is the set that contains all possible events of the experiment. In order to establish a relation between an event E with its probability of occurrence, is necessary to introduce a function $P : \mathcal{F} \to [0, 1]$. Any proper probability function

or measure P has to satisfy the following axioms.

- **Axiom 1**: $0 \leq P(E) \leq 1$.
- **Axiom 2**: $P(\Omega) = 1$.
- **Axiom 3**: For any sequence of mutually exclusive events $E_1, E_2, \ldots$ (meaning, events for which $E_i \cap E_j = \phi$ when $i \neq j$),

$$P\left(\bigcup_{i=1}^{\infty} E_i\right) = \sum_{i=1}^{\infty} P(E_i), \tag{1.45}$$

By looking at the axioms, it can be noticed that if $E_1 = \Omega$ and $E_{i\geq 2} = \phi$, then by using axiom 3

$$P(\Omega) = \sum_{i=i}^{\infty} P(E_i) = P(\Omega) + \sum_{i=2}^{\infty} P(\phi), \tag{1.46}$$

implies that $P(\phi) = 0$, meaning that the empty set ϕ is a set of null probability.

1.2.2 Random Variables and Expected Values

A function $X : \Omega \to \mathbb{R}$ is called *random variable*, and is used to assign numerical values to every outcome of an experiment, if X can take at most a countable[2] number of values it is said to be *discrete*. For example, in the experiment of tossing a fair coin, the possible outcomes are $\Omega = \{H, T\}$, therefore the random variable X could be defined as 0 for heads and 1 for tails, and the probabilities $P(X = 0) = P(X = 1) = 1/2$ are the distribution of the random variable.

Definition 16 *For a discrete random variable X, the* probability mass function *of*

[2]A set is said to be countable if there is a one-to-one map with any subset I of the natural numbers $\mathbb{N}$.

X, $p : \mathbb{R} \to [0, 1]$, *is defined by*

$$p(a) = P(X = a). \tag{1.47}$$

In the discrete case, let $\{x_i\}_{i \in I \subseteq \mathbb{N}}$ be the set of values of the random variable X, then the probability mass function must satisfy

$$\sum_{i \in I} p(x_i) = 1, \tag{1.48}$$

since the experiment has to have an outcome represented by X.

The *expected value* $\mathbb{E}(X)$ of the random variable X is defined by

$$\mathbb{E}[X] = \sum_{i \in I} x_i p(x_i) = \sum_{\omega \in \Omega} X(\omega) P(\{\omega\}). \tag{1.49}$$

As it can be seen, the expected value is basically the weighted average of X, each weight being the probability of each value x_i. In the same way, any function of a random variable $g(X)$ is on itself a random variable, with an expectation value [37]

$$\mathbb{E}[g(X)] = \sum_{i \in I} g(x_i) p(x_i). \tag{1.50}$$

As it was explained before, the expected value of a random variable X is the weighted average, therefore, it defines the *mean* $\mu = \mathbb{E}[X]$ of a random variable.

The *variance* of X, is defined by

$$\mathrm{Var}(X) = \mathbb{E}[(X - \mu)^2]. \tag{1.51}$$

For a random variable X, the variance $\mathrm{Var}(X)$ represent the dispersion or spread with respect to the mean μ, and both quantities serve as a useful manner to give information about the probability function of the random variable. The variance can be computed also as

$$\begin{aligned}\mathrm{Var}(X) =& \mathbb{E}[(X-\mu)^2] && (1.52)\\ =& \mathbb{E}[X^2 - 2X\mu + \mu^2] && (1.53)\\ =& \mathbb{E}[X^2] - 2\mu\mathbb{E}[X] + \mu^2 && (1.54)\\ =& \mathbb{E}[X^2] - \mu^2. && (1.55)\end{aligned}$$

On the other hand, a random variable with an uncountable[3] set of possible values is said to be *continuous*. Let $B = \{X(\omega) \in \mathbb{R} | \omega \in E\} \subset \mathbb{R}$ be the set of values of the random variable associated with the event E, then the *probability density function* is a non-negative function $f : \mathbb{R} \to \mathbb{R}^+$ defined by

$$P(X = B) = \int_B f(x)dx, \tag{1.56}$$

and is the counterpart of the probability mass function for the discrete case. Therefore, since X must take some value after the experiment, f must satisfy

$$\int_{-\infty}^{+\infty} f(x)dx = 1. \tag{1.57}$$

In this manner, the equations defined for a discrete variable are now replaced by their equivalents with integrals. In this way, the expected value of a function g in

[3]A set A such that there does not exist a bijection between A and any subset I of the natural numbers

the continuous case is

$$\mathbb{E}[g(X)] = \int_{-\infty}^{+\infty} g(x)f(x)dx. \tag{1.58}$$

The probability of an event that has a dependency on the occurrence of another known event is defined as *conditional probability*. For example, the probability that tomorrow rains if it is known that today and yesterday has already rained. Conditional probabilities offer a more accurate description of events by using more relevant information. In the previous example, the probability of rain tomorrow obtained from a more naive calculation, as it could be the probability of rain on any given day of the year, is likely to yield a different prediction, and less accurate, than the probability of rain conditioned to the weather on the previous days, and the current season.

Therefore, the conditional probability [46] of an event A, given that an event B has occurred is equal to

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \tag{1.59}$$

provided $P(B) > 0$

1.2.3 Joint Distributions

Up to this point, the study of the probability of multiple events has been left untouched, since every definition until now has been for single events, or more formally, for probability distributions of single randoms variables.

An example of multiple events could be the experiment of throwing a pair of coins, and asking what is the probability of obtaining two tails. The function that deals with such probabilities is called *joint probability distribution* which is the main

topic of this section.

Thus, the joint probability function is defined as

$$p(x_1, \cdots, x_n) = P(X_1 = x_1, \cdots, X_n = x_n) \tag{1.60}$$

and it computes the probability that all the events labeled by x_i may happen in a given experiment altogether.

For simplicity, suppose that p is the joint probability distribution of two random variables X and Y, then, the *marginal probability distribution* of X is defined by

$$p_X(x) = \sum_y p(x, y) = \sum_y P(X = x, Y = y), \tag{1.61}$$

and it is equivalent to the probability function of X.

An especial case of multivariate distributions is when the random variables are independent between them. For example, if a dice is thrown several times, each individual result does not depend on the previous output of the dice, making each throwing independent.

By definition, a set of random variables $\{X_i\}$ are said to be independent if and only if their joint probability distribution $p(x_1, \cdots, x_n)$ satisfies

$$p(x_1, x_2, \cdots, p_n) = p_1(x_1)p_2(x_2)\cdots p_n(x_n) \tag{1.62}$$

1.3 Point Estimation

This section present the basic concepts and tools from the theory of point estimation, which is of vital importance in the task of constructing a model whose behavior resembles closely the data obtained from the experiments perform on a system, this is usually achieved by estimating a set of parameters that describe the system.

1.3.1 Estimators

In scenarios in which there is a given data-set, and our task is to find a probability density function that can originate the data, an important step is to propose a model. A *model* in this section is defined as a probability density function $p(x|\boldsymbol{\theta})$ in which $x \in \mathbb{R}$ is the random variable, and $\boldsymbol{\theta} \in \Theta$ are the parameters that characterize the density function.

Since $p(x|\boldsymbol{\theta})$ is a density function, it must satisfy the conditions specified in the section 1.2. An example of a model can be the normal distribution

$$p(x|\sigma,\mu) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{1.63}$$

where μ and σ are the parameters of the function, it can be noted that different values of μ and σ generate different density functions.

Once the model is proposed, the next step is to find a good guess of the unknown parameters through the analysis of the data. Said guess, denoted by $\tilde{\boldsymbol{\theta}}(x)$, is called *estimator* and is defined over the sample space Ω (Section 1.2.1), meaning that is a random variable, and it is used to estimate the unknown parameter $\boldsymbol{\theta}$ called *estimand*[27].

An estimator is said to be *unbiased* if it satisfy the following condition

$$\mathbb{E}\left[\tilde{\boldsymbol{\theta}}(x)\middle| x\right] = \boldsymbol{\theta}. \tag{1.64}$$

This condition ensures that the estimated value will be correct on average.

Another important quantity that can be computed from an estimator is the *mean squared error*, which quantifies the spread of the estimator $\tilde{\boldsymbol{\theta}}(x)$ around the target parameter $\boldsymbol{\theta}$ [15]. It is defined as

$$\text{MSE}\left(\tilde{\boldsymbol{\theta}}(x)\right) = \mathbb{E}\left[\left(\tilde{\boldsymbol{\theta}}(x) - \boldsymbol{\theta}\right)^2\middle| x\right], \tag{1.65}$$

which by defining $\tilde{\mu} = \mathbb{E}(\tilde{\boldsymbol{\theta}})$ can then be rewritten as

$$\begin{aligned}
\text{MSE}\left(\tilde{\boldsymbol{\theta}}(x)\right) =& \mathbb{E}\left[\left(\tilde{\boldsymbol{\theta}} - \boldsymbol{\theta}\right)^2\right] && (1.66)\\
=& \mathbb{E}\left[\left(\tilde{\boldsymbol{\theta}} + \tilde{\mu} - \tilde{\mu} - \boldsymbol{\theta}\right)^2\right] && (1.67)\\
=& \mathbb{E}\left[\left(\tilde{\boldsymbol{\theta}} - \tilde{\mu}\right)^2\right] + (\tilde{\mu} - \boldsymbol{\theta})^2 + 2\mathbb{E}\left[\tilde{\boldsymbol{\theta}} - \tilde{\mu}\right](\tilde{\mu} - \boldsymbol{\theta}) && (1.68)\\
=& \mathbb{E}\left[\left(\tilde{\boldsymbol{\theta}} - \tilde{\mu}\right)^2\right] + (\tilde{\mu} - \boldsymbol{\theta})^2 && (1.69)\\
=& \text{Var}(\tilde{\boldsymbol{\theta}}) + (\mathbb{E}(\tilde{\boldsymbol{\theta}}) - \boldsymbol{\theta})^2. && (1.70)
\end{aligned}$$

Where $\text{Var}(\tilde{\boldsymbol{\theta}})$ is the variance defined in Eq. (1.51). The term $\mathbb{E}(\tilde{\boldsymbol{\theta}}) - \boldsymbol{\theta}$ in Eq. (1.70) is defined as the *bias* of the estimator, since it is related to the expression in Eq. (1.64) when it does not hold, serving as a quantifier of the estimator biasedness.

The result of Eq.(1.70) shows that the mean squared error is the dispersion, represented in the variance, plus the bias of the estimator. Therefore an estimator

with a low mean squared error is more accurate and efficient than one with a high MSE[15].

1.3.2 Maximum Likelihood Estimation

An important tool in statistics and point estimation theory is the *Likelihood function*, as it measures in some way how well a theoretical model can adjust to a data acquired from a unknown probability distribution.

The likelihood function is defined as the model of the joint density function evaluated at the observed data [30]. That is, being $f(\boldsymbol{x}|\boldsymbol{\theta})$ the proposed model for the data, and $\boldsymbol{y} = (y_1, \cdots, y_n)$ the value which the random variable $\boldsymbol{x}$ takes at the observed data, then the likelihood function $L : \Theta \to \mathbb{R}$ is

$$L(\boldsymbol{\theta}) = f(\boldsymbol{y}|\boldsymbol{\theta}). \tag{1.71}$$

The maximum likelihood estimation method is then based on the maximum likelihood principle, which states that the estimator $\tilde{\boldsymbol{\theta}}$ of the parameter $\boldsymbol{\theta}$ should be chosen such that

$$\tilde{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}\in\Theta} L(\boldsymbol{\theta}). \tag{1.72}$$

Interestingly, in a vast amount of cases the available data $\boldsymbol{y}$ correspond to the values of a set of independent random variables $\{Y_i\}_{i=1}^n$, then according to Eq. (1.62) the likelihood can be expressed as

$$L(\boldsymbol{\theta}) = \prod_{i=1}^{n} f_1(y_1|\boldsymbol{\theta}). \tag{1.73}$$

However, the likelihood is not frequently used for calculations, instead people often recur to the *log-likelihood* defined as

$$l(\boldsymbol{\theta}) = \log L(\boldsymbol{\theta}). \tag{1.74}$$

This because of mainly two reasons; the log-likelihood and likelihood achieve their maximum at the same parameter value, and the log-likelihood is a more simple function to make calculations (and consequently easier to optimize).

To have a better understanding of the last affirmation, consider the set $\{Y_i\}_i$ of independent random variables, then $l(\boldsymbol{\theta})$ takes the form

$$l(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log f_i(y_i|\boldsymbol{\theta}), \tag{1.75}$$

which is a more simple expression to minimize than Eq.(1.73).

As a final remark, the scenarios in which maximum likelihood estimation is used, are often of independent random variables with identical distributions, therefore, the function Eq.(1.75) is frequently used. In fact since the distributions are identical, the subscript i of f is dropped, leaving the log-likelihood as

$$l(\boldsymbol{\theta}) = \sum_{i=1}^{n} f(y_i|\boldsymbol{\theta}) \tag{1.76}$$

1.3.3 Fisher Information Matrix

The fisher information matrix is used to quantify the amount of information that we have of a given data-set, which makes it a valuable tool in many applications, one

for example, being the computation of bounds for merit figures, such as the MSE[20].

Let $\tilde{\boldsymbol{\theta}} = (\tilde{\theta}_1 \cdots \tilde{\theta}_m)^t$ be an unbiased estimator of $\boldsymbol{\theta}$, and $\boldsymbol{v} = (v_1 \cdots v_n)^t$ a set of outcomes of a probability density function $p(\boldsymbol{v}|\boldsymbol{\theta})$. Since the estimators $\tilde{\boldsymbol{\theta}}(\boldsymbol{v})$ are unbiased, then we have the equality

$$\frac{\partial}{\partial\theta_k}\mathbb{E}[\tilde{\theta}_j|\boldsymbol{\theta}] = \int_{\mathbb{R}^n} \tilde{\theta}_j(\boldsymbol{v}) p_k(\boldsymbol{v}|\boldsymbol{\theta}) d^n\boldsymbol{v} = \frac{\partial}{\partial\theta_k}\theta_j = \delta_{jk}, \tag{1.77}$$

where we have defined $p_k(\boldsymbol{v}|\boldsymbol{\theta}) = \frac{\partial}{\partial\theta_k} p(\boldsymbol{v}|\boldsymbol{\theta})$. Using the fact that the probability is normalized, we can find the following relation

$$\int_{\mathbb{R}^n} (\tilde{\theta}_j(\boldsymbol{v}) - \theta_j) p_k(\boldsymbol{v}|\boldsymbol{\theta}) d^n\boldsymbol{v} = \delta_{jk}. \tag{1.78}$$

Finally, we multiply this expression by the arbitrary vectors y_j and z_k, then do the sum over both indexes, getting

$$\sum_{j,k} \int_{\mathbb{R}^n} y_j (\tilde{\theta}_j(\boldsymbol{v}) - \theta_j) z_k p_k(\boldsymbol{v}|\boldsymbol{\theta}) d^n\boldsymbol{v} = \mathbb{E}[g(\boldsymbol{v}) f(\boldsymbol{v})|\boldsymbol{\theta}] = \boldsymbol{y}^t\boldsymbol{z}.^4 \tag{1.79}$$

Where we have conveniently defined the functions

$$f(\boldsymbol{v}) = \sum_j y_j \left(\tilde{\theta}_j(\boldsymbol{v}) - \theta_j\right), \tag{1.80}$$

and

$$g(\boldsymbol{v}) = \sum_k z_k \frac{\partial}{\partial\theta_k} \ln(p(\boldsymbol{v}|\boldsymbol{\theta})). \tag{1.81}$$

[4] y^t stands for the transpose of y

If we apply the Cauchy-Schwartz inequality to Eq. (1.79), then

$$(\boldsymbol{y}^t\boldsymbol{z})^2 = \mathbb{E}[g(\boldsymbol{v})f(\boldsymbol{v})|\boldsymbol{\theta}]^2 \tag{1.82}$$

$$= \left(\int_{\mathbb{R}^n} f(\boldsymbol{v})g(\boldsymbol{v})p(\boldsymbol{v}|\boldsymbol{\theta})d^n\boldsymbol{v}\right)^2 \tag{1.83}$$

$$\leq \left(\int_{\mathbb{R}^n} f^2(\boldsymbol{v})p(\boldsymbol{v}|\boldsymbol{\theta})d^n\boldsymbol{v}\right)\left(\int_{\mathbb{R}^n} g^2(\boldsymbol{v})p(\boldsymbol{v}|\boldsymbol{\theta})d^n\boldsymbol{v}\right) \tag{1.84}$$

$$= \mathbb{E}[f^2(\boldsymbol{v})|\boldsymbol{\theta}]\mathbb{E}[g^2(\boldsymbol{v})|\boldsymbol{\theta}]. \tag{1.85}$$

Analyzing these terms separately we have

$$\mathbb{E}[f^2(\boldsymbol{v})|\boldsymbol{\theta}] = \int_{\mathbb{R}^n} \sum_j y_j(\tilde{\theta}_j(\boldsymbol{v}) - \theta_j) \sum_k y_k(\tilde{\theta}_k(\boldsymbol{v}) - \theta_k)p(\boldsymbol{v}|\boldsymbol{\theta})d^n\boldsymbol{v} \tag{1.86}$$

$$= \sum_{j,k} y_j y_k \int_{\mathbb{R}^n} [\tilde{\theta}_j(\boldsymbol{v}) - \theta_j][\tilde{\theta}_k(\boldsymbol{v}) - \theta_k]p(\boldsymbol{v}|\boldsymbol{\theta})d^n\boldsymbol{v} \tag{1.87}$$

$$= \sum_{j,k} y_j \mathbb{E}\left[(\tilde{\theta}_j - \theta_j)(\tilde{\theta}_k - \theta_k)\middle|\boldsymbol{\theta}\right] y_k \tag{1.88}$$

$$= \sum_{j,k} y_j C_{jk} y_k \tag{1.89}$$

$$= \boldsymbol{y}^t C \boldsymbol{y}, \tag{1.90}$$

where we have defined the covariance matrix

$$C_{jk} = \mathbb{E}\left[(\tilde{\theta}_j - \theta_j)(\tilde{\theta}_k - \theta_k)\middle|\boldsymbol{\theta}\right]. \tag{1.91}$$

On the other hand we have

$$\mathbb{E}[g^2(\boldsymbol{v})|\boldsymbol{\theta}] = \int_{\mathbb{R}^n} \sum_k \left[z_k \frac{\partial}{\partial \theta_k} \ln(p(\boldsymbol{v}|\boldsymbol{\theta})) \right] \sum_j \left[z_j \frac{\partial}{\partial \theta_j} \ln(p(\boldsymbol{v}|\boldsymbol{\theta})) \right] p(\boldsymbol{v}|\boldsymbol{\theta}) d^n\boldsymbol{v} \quad (1.92)$$

$$= \sum_{j,k} z_j z_k \int_{\mathbb{R}^n} \frac{\partial}{\partial \theta_k} \ln(p(\boldsymbol{v}|\boldsymbol{\theta})) \frac{\partial}{\partial \theta_j} \ln(p(\boldsymbol{v}|\boldsymbol{\theta})) p(\boldsymbol{v}|\boldsymbol{\theta}) d^n\boldsymbol{v} \quad (1.93)$$

$$= \sum_{j,k} z_j z_k \mathbb{E}\left[\frac{\partial}{\partial \theta_k} \ln p(\boldsymbol{v}|\boldsymbol{\theta}) \frac{\partial}{\partial \theta_j} \ln p(\boldsymbol{v}|\boldsymbol{\theta}) \middle| \boldsymbol{\theta} \right] \quad (1.94)$$

$$= \boldsymbol{z}^t I \boldsymbol{z}, \quad (1.95)$$

Here we have introduced the matrix I whose components are given by the expression

$$I_{jk} = \mathbb{E}\left[\frac{\partial}{\partial \theta_k} \ln p(\boldsymbol{v}|\boldsymbol{\theta}) \frac{\partial}{\partial \theta_j} \ln p(\boldsymbol{v}|\boldsymbol{\theta}) \middle| \boldsymbol{\theta} \right], \quad (1.96)$$

which is known as the *Fisher Information Matrix*, and is a function whose only dependency is on $p(\boldsymbol{v}|\boldsymbol{\theta})$.

Now by replacing Eq. (1.90) and Eq. (1.95) back into Eq. (1.85) we get the inequality

$$(\boldsymbol{z}^t \boldsymbol{y})^2 \leq \boldsymbol{y}^t C \boldsymbol{y} \boldsymbol{z}^t I \boldsymbol{z}. \quad (1.97)$$

And by occupying the particular choice $\boldsymbol{z} = I^{-1}\boldsymbol{y}$ we get

$$C - I^{-1} \geq 0, \quad (1.98)$$

which is known as the *Cramér-Rao inequality*. From here we can multiply by a weight matrix W and take the trace of the expression, which yields

$$\text{WMSE}(\tilde{\boldsymbol{\theta}}) \leq \text{Tr}[W I^{-1}]. \quad (1.99)$$

Hence, from the Cramér-Rao inequality Eq. (1.98) we can derive a fundamental bound on error measures, such as the *weighted mean squared error* (WMSE) in Eq. (1.99), or other ones by performing different operations on Eq. (1.98). Furthermore, this bound depends solely on the Fisher Information Matrix, which implies that said matrix contains the amount known information of the system, as it is a function solely of the probability function evaluated at the available data $\boldsymbol{v}$. Finally, the use of the Fisher Information Matrix is more wide than bound calculations, however it escapes the scope of this work so they will not be included.

1.4 Optimization Methods

Optimization is the branch of mathematics that focuses on finding the maximum (or minimum) value of a target function.

Formalizing the problem, let $f : \Theta \to \mathbb{R}$ be the objective function. Then the optimization problem can be formally represented [39] as finding the set

$$\Theta^* = \arg\min_{\boldsymbol{\theta}\in\Theta} f(\boldsymbol{\theta}) = \{\boldsymbol{\theta}^* \in \Theta : f(\boldsymbol{\theta}^*) \leq f(\boldsymbol{\theta}) \; \forall \; \boldsymbol{\theta} \in \Theta\}, \tag{1.100}$$

Even through the solution Θ^* is expressed as a set, it is completely plausible that the set contains only one point, or a finite amount of points or could even be a set containing infinite elements, however, no matter the case we will always restrict to finding only one solution, at least in the current work.

An important distinction between the solutions of a problem is if they are global or local, that is, if $f(\boldsymbol{\theta}^*)$ is the optimal value of f in all the domain Θ or if it is

only the optimal value in the neighborhood of $\boldsymbol{\theta}^*$. A global solution is the ideal to achieve through any optimization method, however in many cases the shape of the target function is too hard to handle and only a local solution is available. Gladly, local solutions are often more than enough.

The attempts at estimating $\boldsymbol{\theta}^*$ are done in an iterative manner, starting with an initial estimator $\tilde{\boldsymbol{\theta}}_0$ to final one $\tilde{\boldsymbol{\theta}}_k$ that is expected to be closer to $\boldsymbol{\theta}^*$ that the initial.

The remark of the section will consist on describing three optimization methods; Steepest Descent, as one of the oldest optimization techniques, from which the remaining two methods can be understood. SPSA an stochastic algorithm based on the estimation of the gradient. Finally, SPSA extension to complex field of numbers, CSPSA.

1.4.1 Steepest Descent

Steepest descent, being one of the first introduced formal methods for optimization, relies in a very simple but fundamental principle; Given a value $\boldsymbol{\theta}$, the best direction to search is the one that produces the largest local change in the target function $f : \Theta \to \mathbb{R}$ [39], said direction determined by the gradient of the function $\boldsymbol{g}(\boldsymbol{\theta}) = \boldsymbol{\nabla} f(\boldsymbol{\theta})$. Thus, the iterative algorithm to construct a guess (estimator) for the optimum parameter is given by the actualization rule

$$\tilde{\boldsymbol{\theta}}_{k+1} = \tilde{\boldsymbol{\theta}}_k - a_k \boldsymbol{g}(\tilde{\boldsymbol{\theta}}_k) \tag{1.101}$$

where k is the iteration step, $\tilde{\boldsymbol{\theta}}_k$ is a guess of $\boldsymbol{\theta}^*$ for said step and a_k is called a gain coefficient and determines the size of the step at each iteration.

In practice there is no unique way of defining the gain coefficient a_k, it could be constant or be a function of the current step, however it is more convenient to have a step that declines with each iteration. By giving bigger steps at the start we can approach faster to a neighborhood of the solution, and give small steps later to move more delicately towards the desired solution instead of getting further from it.

1.4.2 Simultaneous Perturbation Stochastic Approximation

The steepest descent method presented in Section 1.4.1 is one of the oldest and more popular algorithms for optimization, but there are a varied range of practical cases where it can not be applied or it is known to perform poorly. Specifically, if the gradient $\boldsymbol{g}(\boldsymbol{\theta})$ is not directly available. Furthermore, if the measures on the target function are noisy, then steepest descent is known to perform poorly.

Here we present a technique to work in those cases known as *Simultaneous Perturbation Stochastic Approximation* (SPSA). It only needs direct measures of the objective function, and the search direction can be computed from them by estimating the gradient. The measures performed on the target function are chosen randomly (hence Stochastic Approach). Said randomness is why Stochastic Approach methods can work even under noisy measurements and still be robust.

The algorithm is performed by the following iteration rule for the guesses

$$\tilde{\boldsymbol{\theta}}_{k+1} = \tilde{\boldsymbol{\theta}}_k - a_k \tilde{\boldsymbol{g}}_k(\tilde{\boldsymbol{\theta}}_k). \tag{1.102}$$

It is very clear that the actualization rule Eq (1.102) is almost identical to the one for steepest descent Eq (1.101), but there is a little difference of utmost importance, the quantity $\tilde{\boldsymbol{g}}_k(\tilde{\boldsymbol{\theta}}_k)$ is the *estimate of the gradient*, which can be calculated solely

from measurements of the target function, in contrast to the gradient $\boldsymbol{g}_k(\tilde{\boldsymbol{\theta}}_k)$. Thus, let $F(\tilde{\boldsymbol{\theta}}_k)$ be the target function and $f(\tilde{\boldsymbol{\theta}}_k) = F(\tilde{\boldsymbol{\theta}}_k) + \epsilon_k$ a measurement of $F(\tilde{\boldsymbol{\theta}}_k)$ with noise ϵ_k, then the estimate of the gradient is computed as

$$\tilde{g}_{k,\alpha}(\tilde{\boldsymbol{\theta}}_k) = \frac{f(\tilde{\boldsymbol{\theta}}_k + c_k\boldsymbol{\Delta}_k) - f(\tilde{\boldsymbol{\theta}}_k - c_k\boldsymbol{\Delta}_k)}{2c_k\Delta_{k,\alpha}} \tag{1.103}$$

where $\tilde{g}_{k,\alpha}$ is the α component of the vector $\tilde{\boldsymbol{g}}_k$, c_k is another gain coefficient and $\boldsymbol{\Delta}_k$ is vector whose components $\Delta_{k,\alpha}$ are independent and identically distributed random variables, with a probability distribution chosen by the user. The quantity $\boldsymbol{\theta}_{k\pm} = \tilde{\boldsymbol{\theta}}_k \pm c_k\boldsymbol{\Delta}_k$ is known as a perturbation on the parameter $\tilde{\boldsymbol{\theta}}_k$.

An important conclusion from Eq (1.103) is that in order to estimate the gradient at a given point $\tilde{\boldsymbol{\theta}}_k$ is necessary to measure two times the target function in the perturbed parameters $\tilde{\boldsymbol{\theta}}_\pm$, then for a number k of iterations of the algorithm $2k$ measurements are needed.

The standard coefficients used in the literature are

$$a_k = \frac{a}{(k+1+A)^s} \qquad\qquad c_k = \frac{b}{(k+1)^t}, \tag{1.104}$$

meanwhile the probability distribution commonly used for the components of $\boldsymbol{\Delta}_k$ is to choose uniformly from the set $\{1, -1\}$.

1.4.3 Complex Simultaneous Perturbation Stochastic Approximation

The existence of functions $f : \mathbb{C}^n \to \mathbb{R}$ that do not satisfy Cauchy-Riemann conditions is an inconvenience to SPSA, as one of the requisites for certified convergence

is that $f \in \mathcal{L}^3$ [39]. A simple example of such case is the non-holomorphic function $f(\boldsymbol{z}) = \|\boldsymbol{z}\|$. Therefore a method designed to work with complex parameters is needed.

Here we present the *Complex Simultaneous Perturbation Stochastic Approach* (CSPSA) algorithm [45] that restates SPSA within the complex numbers. This is achieved by making use of Wirtinger Calculus [49], specially the definitions of Wirtinger derivatives

$$\frac{\partial f}{\partial z} = \frac{1}{2}\left(\frac{\partial f}{\partial x} + i\frac{\partial f}{\partial y}\right) \qquad \frac{\partial f}{\partial z^*} = \frac{1}{2}\left(\frac{\partial f}{\partial x} - i\frac{\partial f}{\partial y}\right), \tag{1.105}$$

which can still exist even if the Cauchy-Riemann conditions are not satisfied, as it happens for the example $f(\boldsymbol{z}) = \|\boldsymbol{z}\|$.

The fact that Wirtinger derivatives may be well defined does not directly imply that one can look for stationary points using them. However, let $f(\boldsymbol{\mu})$ with $\boldsymbol{\mu} = (\boldsymbol{z}, \boldsymbol{z}^*)$ be a complex-valued function, and $\delta\boldsymbol{\mu} = (\delta\boldsymbol{z}, \delta\boldsymbol{z}^*)$ be a infinitesimal change, then the variation δf induced is

$$\delta f = (\partial_{\boldsymbol{\mu}} f)\delta\boldsymbol{\mu}^t. \tag{1.106}$$

If f is real-valued, we can write

$$\delta f = 2\mathrm{Re}[(\partial_{\boldsymbol{z}} f)\delta\boldsymbol{z}^t]. \tag{1.107}$$

Therefore, the stationary points are given by $\partial_{\boldsymbol{z}} f = \mathbf{0}$, or $\partial_{\boldsymbol{z}^*} f = \mathbf{0}$ [45]

To reformulate the SPSA over the complex numbers, let ζ be the space of the

complex parameters and $\tilde{\boldsymbol{z}}_k \in \zeta$ an estimator for the parameter that maximizes the target function $F(\boldsymbol{z}, \boldsymbol{z}^*)$. If we consider $f(\tilde{\boldsymbol{z}}_k, \tilde{\boldsymbol{z}}_k^*) = F(\tilde{\boldsymbol{z}}_k, \tilde{\boldsymbol{z}}_k^*) + \epsilon_k$ a measure of $F(\tilde{\boldsymbol{z}}_k, \tilde{\boldsymbol{z}}_k^*)$ with noise ϵ_k, then the update rule is given by

$$\tilde{\boldsymbol{z}}_{k+1} = \tilde{\boldsymbol{z}}_k - a_k \tilde{\boldsymbol{g}}_k(\tilde{\boldsymbol{z}}_k, \tilde{\boldsymbol{z}}_k^*) \tag{1.108}$$

where now $\tilde{\boldsymbol{g}}_k(\tilde{\boldsymbol{z}}_k, \tilde{\boldsymbol{z}}_k^*)$ is the estimate of the complex derivative $\partial_{\boldsymbol{z}^*} f(\boldsymbol{z}, \boldsymbol{z}^*)$, which is computed from

$$\tilde{g}_{k,\alpha}(\tilde{\boldsymbol{z}}_k, \tilde{\boldsymbol{z}}_k^*) = \frac{f(\tilde{\boldsymbol{z}}_{k+}, \tilde{\boldsymbol{z}}_{k+}^*) - f(\tilde{\boldsymbol{z}}_{k-}, \tilde{\boldsymbol{z}}_{k-}^*)}{2c_k \Delta_{k,\alpha}^*}, \tag{1.109}$$

with $\tilde{\boldsymbol{z}}_{k\pm} = \tilde{\boldsymbol{z}}_k \pm c_k \boldsymbol{\Delta}_k$ and $\boldsymbol{\Delta}_k$ a vector whose components $\Delta_{k,\alpha} \in \mathbb{C}$ are independent and identically distributed random variables drawn from a user defined distribution.

The standard definition for the gain coefficients are the same as the ones used for SPSA in Section 1.4.2. On the other hand, the components of the vector $\boldsymbol{\Delta}_k$ are usually drawn from the set $\{1, -1, i, -i\}$.

Chapter 2

Quantum Mechanics

Quantum mechanics is the area of physics that emerged in the XX century when trying to explain a series of phenomena (black body radiation, photoelectric effect, etc.) in which classical mechanics predicted wrong behaviors. What was found after studying those cases is that, contrary to classical mechanics and all sense of reason, considering the energy and other quantities to be discrete gave the correct predictions, therefore a new theory was necessary an the revolutionary field of quantum mechanics was born.

Henceforth quantum mechanics has given an accurate description of a plethora of phenomena that far surpasses the initial studied cases and has become fundamental in the research of microscopic system and many other areas.

In this chapter we will review the postulates of quantum mechanics, study quantum tomography which is the area that focuses on estimating accurately quantum states and finalize with the quantum fisher information matrix.

2.1 Postulates of Quantum Mechanics

The postulates of quantum mechanics as we know them today are a set of statements and together they provide a mathematical framework [32] to study any physical system within the quantum formalism. The postulates themselves are of a mathematical nature rather than a physical one, them being the result of a trial and error derivation performed in the past century.

2.1.1 State space

Postulate 1 *Associated to any isolated physical system is a complex vector space with inner product $\mathcal{H}$ (that is, a Hilbert space) known as the state space of the system. The system is completely described by its state vector, which is a unit vector in the state space of the system.*

Among all state spaces, of particular interest are physical systems with a 2-dimensional state space, called *qubit*, as they provide a counterpart for the *bit* used in classical computation and can be written as

$$|\,\psi\,\rangle = \alpha|\,0\,\rangle + \beta|\,1\,\rangle. \tag{2.1}$$

The fact that a state is a unit vector ($\|\,|\,\psi\,\rangle\,\| = 1$), implies $|\alpha|^2 + |\beta|^2 = 1$, and is usually referred as the normalization condition.

Any linear combination of states, satisfying the normalization condition, is said to be a superposition of states. Another important terminology is that d-dimensional state spaces are called *qudits*.

Quantum mechanics, up to this point, have been formulated in terms of vec-

tors, but in an scenario where the state of the system is not completely known is more convenient to use the *density matrix* or *density operator*, a formalism which is mathematically equivalent to the one already taken in postulate 1.

Let us suppose a quantum system that, with probability p_i, is in a state $|\,\psi_i\,\rangle$ belonging to an ensemble $\{p_i, |\,\psi_i\,\rangle\}_{i=1}^{n}$ of possible states with their respective probability. The system is then described by the density matrix

$$\rho = \sum_{i=1}^{n} p_i |\,\psi_i\,\rangle\langle\,\psi_i\,|. \tag{2.2}$$

The reason to introduce this formalism is that mixtures of states, called *mixed states*, can only be written in the density matrix formalism and not as a vector. On the other hand, states that can be written as a vector are defined as *pure states*.

To demonstrate that a mixed state can not be written as a vector $|\,\psi_m\,\rangle$, let us consider ρ_m and ρ_p be a mixed and pure state respectively. It can be easily seen by definition that ρ_p can be expressed as

$$\rho_p^2 = |\,\psi\,\rangle\langle\,\psi\,| = \rho_p, \tag{2.3}$$

which implies that $\rho_p^2 = \rho_p$, and $\mathrm{Tr}(\rho_p^2) = 1$.

Conversely, for a mixed state ρ_m the equality between ρ_m and ρ_m^2 does not hold, moreover, $\mathrm{Tr}[\rho_m^2] < 1$. This statement can be proven by noting that any density

matrix ρ is a positive definite operator. In effect, for any unit vector $|\,\lambda\,\rangle$

$$\langle\,\lambda\,|\rho|\,\lambda\,\rangle = \sum_{i=1}^{n} p_i \langle\,\lambda\,|\,\psi_i\,\rangle\langle\,\psi_i\,|\,\lambda\,\rangle \tag{2.4}$$

$$= \sum_{i=1}^{n} p_i |\langle\,\lambda\,|\,\psi_i\,\rangle|^2 > 0. \tag{2.5}$$

On another hand, if we suppose that ρ_m is a mixture of $n \geq 2$ different states, meaning

$$\rho_m = \sum_{i=1}^{n} p_i |\,\psi_i\,\rangle\langle\,\psi_i\,|, \tag{2.6}$$

and apply the Gram-Schmidt procedure to the set of states $\{|\,\psi_i\,\rangle\}_{i=1}^{n}$, we obtain a set of orthonormal states $\{|\,\lambda_i\,\rangle\}_{i=1}^{n}$, each of them with probability $p(\lambda_i) = \langle\,\lambda_i\,|\rho_m|\,\lambda_i\,\rangle$, where $p(\lambda_i) < 1$.

Now $\rho_i^2 = \sum_{i=1}^{n} p(\lambda_i)^2 |\,\lambda_i\,\rangle\langle\,\lambda_i\,|$, where it can be seen that

$$\mathrm{Tr}(\rho_m^2) = \sum_{i=1}^{n} p(\lambda_i)^2 < 1. \tag{2.7}$$

Thus a mixed state can not be expressed as a pure state vector $|\,\psi\,\rangle$.

2.1.2 Evolution

Postulate 2 *The evolution of a closed quantum system is described by a unitary transformation. Meaning that the state of a system at time t_f is related to the state at time t_0 by a unitary transformation $U(t_0, t_f)$ that depends only in the initial and final times t_0 and t_f respectively in the following way:*

$$|\,\psi(t_f)\,\rangle = U(t_0, t_f)|\,\psi(t_0)\,\rangle \tag{2.8}$$

The postulate as it is, does not tell how to obtain the unitary transformation U, nor the physics which the matrix represents, but only that in a closed system there is an unitary transformation such that the system in the state $|\,\psi(t_0)\,\rangle$ becomes $|\,\psi(t_f)\,\rangle$ through the application of U.

In this context, the Schrodinger equation, provides a version of this postulate with a physical interpretation and a description of the system in continuous time. Thus the postulate can be rewritten as:

Postulate 3 *The time evolution of the state of a closed system is described by the Schrodinger equation*

$$i\hbar\frac{d|\,\psi\,\rangle}{dt} = H|\,\psi\,\rangle. \tag{2.9}$$

Where H is the Hamiltonian operator of the system.

For the density matrix formalism, the evolution of ρ can be easily inferred from Eq. (2.8), yielding

$$\rho(t_f) = U\rho(t_0)U^\dagger. \tag{2.10}$$

Meanwhile the Schrödinger equation in this formalism reads

$$i\hbar\frac{d\rho}{dt} = [H,\rho], \tag{2.11}$$

where $[H,\rho]$ is the commutator Eq. (1.7) between the operators.

2.1.3 Measurements

Postulate 4 *Quantum measurements are described by a collection* $\{M_m\}_{m=1}^N$ *of measurement operators. This operators are defined on the state space of the sys-*

tem being measured. The index m refers to the possible outcome in the experiment that may occur in the process of measurement. If before the measurement the state of the system is $|\,\psi\,\rangle$*, the probability that result m occur is*

$$p(m) = \langle\,\psi\,|M_m^\dagger M_m|\,\psi\,\rangle, \tag{2.12}$$

and the state after the system is measured is given by

$$\frac{M_m|\,\psi\,\rangle}{\sqrt{\langle\,\psi\,|M_m^\dagger M_m|\,\psi\,\rangle}}. \tag{2.13}$$

The measurement operators satisfy the completeness relation

$$\sum_m M_m^\dagger M_m = \mathbb{I}. \tag{2.14}$$

One interesting thing to notice in the postulate, is that the state of the system after measurement is, in fact, not necessarily an unitary transformation of the initial state. The interaction between the system of interest, and any measuring device, makes the system no longer closed, therefore, making postulate 2 no longer applicable to the situation.

Another important remark is that in quantum mechanics any measurable quantity is called *observable*, and is represented by an hermitian operator. It is important to notice that $M_m^\dagger M_m$ is hermitian.

It can be seen from Eq (2.12) that any pair of states $|\,\psi\,\rangle$ and $|\,\phi\,\rangle$ that differ only on a phase, that is $|\,\psi\,\rangle = e^{i\alpha}|\,\phi\,\rangle$, will yield the same statistics, no matter the measurement M_m being performed. Therefore all the states that differs solely on a

phase are defined to be the same state since they are all physically indistinguishable.

A very powerful implication of this postulate is that only linear operation can be performed on quantum states, and only hermitian operators can be physically measured. This is usually a difficulty when trying to measure physical quantities that have a nonlinear dependency of the state.

Furthermore, it is relevant to say that the measurements expressed in the postulate are known as general measurements. From this point, two special cases of the general measurements are going to be explained; Projective Measurements and POVMs.

Projective measurements are described by an observable M. As observables are by definition hermitian, then the spectral decomposition of M (described in Theorem 1) is

$$M = \sum_m \lambda_m P_m, \tag{2.15}$$

where P_m are projectors (see Subsection 1.1.2). Each of this projectors is associated with an eigenvalue λ_m of M, where each λ_m represent a possible outcome of the observable M in an experiment.

By remembering that projectors are hermitian and satisfy $P_m^2 = P_m$, it can be seen that P_m is a measure operator and an observable. Therefore, the probability of measuring the outcome labeled by m is

$$p(m) = \langle \psi | P_m | \psi \rangle. \tag{2.16}$$

The POVM formalism (Positive Operator-Valued Measure), on the other hand,

does not necessarily satisfy $M_m^\dagger M_m = M_m$ in contrast to projectors. This formalism is a mathematical tool to work on scenarios where the post-measurement state is no longer relevant, or destroyed.

In this way a POVM is defined as a set of positive-definite operators $\{E_m\}$ such that

$$\sum_m E_m = I. \tag{2.17}$$

Thus, the probability of measuring the event labeled by m is $p(m) = \langle\, \psi \,| E_m |\, \psi \,\rangle$.

The measurement operators M_m described in Postulate 4 can be obtained from the POVM elements E_m by computing $M_m = \sqrt{E_m}$.

The *Expected value of an observable*, denoted by $\langle M \rangle$ can be computed by following the definition given in Eq. (1.49), yielding

$$\langle M \rangle := \mathbb{E}[M] = \sum_i x_i p(x_i) \tag{2.18}$$

$$= \sum_m \lambda_m \langle\, \psi \,| M_m |\, \psi \,\rangle \tag{2.19}$$

$$= \langle\, \psi \,| \left(\sum_m \lambda_m M_m \right) |\, \psi \,\rangle \tag{2.20}$$

$$= \langle\, \psi \,| M |\, \psi \,\rangle. \tag{2.21}$$

By looking at postulate 4 we can infer how the measurements should be on mixed states. Let $\rho = |\, \psi \,\rangle\langle\, \psi \,|$ be a pure state, then the probability of measuring M_m by

definition is

$$p(m) = \langle \psi | M_m^\dagger M_m | \psi \rangle \tag{2.22}$$

$$= \langle \psi | M_m^\dagger M_m | \psi \rangle \langle \psi | \psi \rangle \tag{2.23}$$

$$= \langle \psi | M_m^\dagger M_m \rho | \psi \rangle + \sum_{\perp} \langle \psi^\perp | M_m^\dagger M_m \rho | \psi^\perp \rangle \tag{2.24}$$

$$= \mathrm{Tr}(M_m^\dagger M_m \rho) \tag{2.25}$$

where the set of $\{| \psi^\perp \rangle\}$ is a complete basis for the Hilbert space if $| \psi \rangle$ is added, and $\langle \psi | \psi^\perp \rangle = 0$ for all $| \psi^\perp \rangle$. It can be easily checked for a mixed state ρ that the previous result also holds, since a mixed state can be written as linear combination of pure states.

The post-measurement state ρ_{pm} can be trivially computed now that the probabilities have been sorted, yielding

$$\rho_{pm} = \sum_j p_j | \psi_{pm}^j \rangle \langle \psi_{pm}^j | \tag{2.26}$$

$$= \frac{M_m \sum_j p_j | \psi^j \rangle \langle \psi^j | M_m^\dagger}{p(m)} \tag{2.27}$$

$$= \frac{M_m \rho M_m^\dagger}{tr(M_m^\dagger M_m \rho)}. \tag{2.28}$$

Finally, the expected value of an observable A over the mixed state $\rho = \sum_i p_i \rho_i =$

$\sum_i p_i |\,\psi_i\,\rangle\langle\,\psi_i\,|$ is

$$\langle A\rangle_\rho = \sum_i p_i \langle A\rangle_{\rho_i} \tag{2.29}$$

$$= \sum_i p_i \langle\,\psi_i\,|A|\,\psi_i\,\rangle \tag{2.30}$$

$$= \sum_i p_i \mathrm{Tr}(A\rho_i) \tag{2.31}$$

$$= \mathrm{Tr}(A\rho). \tag{2.32}$$

In Eq. (2.29) the fact that the expected value is a linear quantity has been used.

2.1.4 Composite systems

Postulate 5 *The state space of a composite physical system is the tensor product of the state spaces of the component physical systems.*

As the postulate enunciated, the state space of the composite system is given by

$$\mathcal{H}_{Comp} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n. \tag{2.33}$$

Thus, any operator to be performed on the system, be it a measurement or a evolution operator, must belong to the space

$$\mathcal{L}(\mathcal{H}_{Comp}) = \mathcal{L}(\mathcal{H}_1) \otimes \cdots \otimes \mathcal{L}(\mathcal{H}_n). \tag{2.34}$$

For example, let $|\,\psi_{AB}\,\rangle$ be the composite state

$$|\,\psi_{AB}\,\rangle = |\,\psi_A\,\rangle \otimes |\,\psi_B\,\rangle, \tag{2.35}$$

and let M_{iA}, M_{jB} be a pair of measurement operators acting on the systems A and B respectively. Then, the probability of measuring i on system A and j on system B at the same time is

$$p(i,j) = \langle\, \psi_{AB} \,| \left(M_{iA}^{\dagger} \otimes M_{jB}^{\dagger} \right) (M_{iA} \otimes M_{jB}) \,|\, \psi_{AB} \,\rangle \tag{2.36}$$

$$= \langle\, \psi_A \,| M_{iA}^{\dagger} M_{iA} |\, \psi_A \,\rangle \langle\, \psi_B \,| M_{iB}^{\dagger} M_{iB} |\, \psi_B \,\rangle. \tag{2.37}$$

Meanwhile the post-measurement state is

$$|\, \psi_{AB} \,\rangle \rightarrow \frac{M_{iA} \otimes M_{jB} |\, \psi_{AB} \,\rangle}{\sqrt{p(i,j)}} \tag{2.38}$$

$$= \frac{M_{iA} |\, \psi_A \,\rangle \otimes M_{jB} |\, \psi_B \,\rangle}{\sqrt{p(i,j)}}. \tag{2.39}$$

From this point is not hard to generalize how any operation previously defined should act on a composite system.

The density matrix of a composite system also belong to the space defined in Eq. (2.34). An example to a density operator could be

$$\rho = \rho_2 \otimes \rho_2 \otimes \rho_3. \tag{2.40}$$

Up to this point, it is important to remark that not every state can be expressed in a separable way like Eq.(2.40)[1] or like Eq. (2.35). States that can not be written in those ways are said to be *entangled*, which is one of the most important concepts in quantum theory, however it is not the main topic of this work and we will not dwell further into this.

[1] A density matrix is defined to be separable if it can be written as $\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B$

The reduced density operator for a subsystem is defined as the quantum state that describes said subsystem. Mathematically speaking, for a bipartite state ρ^{AB}, the reduced density matrix for system A is given by

$$\rho^A = \mathrm{Tr}_B(\rho^{AB}), \tag{2.41}$$

where Tr_B is the partial trace over B, defined as

$$\mathrm{Tr}_B(|\, a_1 \,\rangle\langle\, a_2 \,| \otimes |\, b_1 \,\rangle\langle\, b_2 \,|) = |\, a_1 \,\rangle\langle\, a_2 \,|\mathrm{Tr}(|\, b_1 \,\rangle\langle\, b_2 \,|). \tag{2.42}$$

2.2 Quantum State Tomography

Quantum state tomography is the field of study whose focus is the reconstruction of a density matrix or state vector. This is done by making measures of interest on the target state, followed by an analysis of the collected data.

2.2.1 Quantum Standard Tomography

Quantum standard tomography [43] is based on the fact that any density matrix describing a qubit can be written as

$$\rho = \frac{1}{2}\left(I + \sum_{i=1}^{3} r_i \sigma_i\right) \tag{2.43}$$

$$= \frac{1}{2}\sum_{i=0}^{4} r_i \lambda_i, \tag{2.44}$$

where $r_0 = 1$, $\boldsymbol{r} = (r_1, r_2, r_3)$ is a real valued vector satisfying $\boldsymbol{r} \cdot \boldsymbol{r} \leq 1$, $\lambda_0 = I$ and $\lambda_i = \sigma_i$ for $i = 1, 2, 3$ are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.45}$$

$$\sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.46}$$

$$\sigma_3 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}. \tag{2.47}$$

It is important to remark that this decomposition can be made since the Pauli matrices and the identity are a complete basis for hermitian matrices, and since the Pauli matrices are traceless the condition $\mathrm{Tr}(\rho) = 1$ can only be satisfied if the coefficient of the identity is equal to $1/2$.

From the parametrization given by Eq.(2.44) it can be easily deducted that the vector $\boldsymbol{r}$ fully describes a quantum state. Now if the observables σ_i are measured, the expected values obtained are

$$\langle \sigma_i \rangle = \mathrm{Tr}(\rho \sigma_i) = r_i, \tag{2.48}$$

directly suggesting that a reasonably tomography scheme is to choose as estimators $\tilde{\boldsymbol{r}}$ of $\boldsymbol{r}$ the measured values of the observables σ_i, and the estimated state resulting is

$$\tilde{\rho} = \frac{1}{2}\left(I + \sum_{i=1}^{3} \tilde{r}_i \sigma_i\right). \tag{2.49}$$

The same approach can be taken for qudits of dimension d, by using the SU(d)

generators $\{\lambda_i\}_{i=1}^{d^2-1}$ instead of the Pauli matrices. A qudit of dimension d is then written as

$$\rho = \frac{1}{d}\left(I + \sum_{i=1}^{d^2-1} r_i \lambda_i\right), \tag{2.50}$$

where now the vector $\boldsymbol{r}$ must satisfy $\sum_{i=1}^{d^2-1} r_i^2 = d(d-1)/2$.

The method previously described is known as standard tomography. However the main problem with this scheme is that in a real application, the obtained estimator $\tilde{\boldsymbol{r}}$ is not always bounded by 1, and some other times the estimated density matrix has negative eigenvalues, which in both cases yields a nonphysical state.

To sort these problems, one solution is to recur to maximum likelihood estimation (Section 1.3.2). Therefore, if the K operators $\{\lambda_i\}_{i=1}^{K}$ are measured on a unknown target state ρ with a occurrence of $\boldsymbol{n} = (n_1, \cdots, n_k)$ each, then the likelihood function defined in Eq.(1.73) for this scenario is

$$L(\tilde{\rho}|\boldsymbol{n}) = \prod_{i=1}^{K} tr(\lambda_i \tilde{\rho})^{n_i} = \left\{\prod_{i=1}^{K} tr(\lambda_i \tilde{\rho})^{n_i/N}\right\}^N, \tag{2.51}$$

where $\tilde{\rho}$ is the estimator of the unknown target state ρ and $N = \sum_i n_i$ is the number of repetitions of the experiment. The log-likelihood described in Eq.(1.76) after defining $f_i = n_i/N$ and dropping the remaining N is given by

$$l(\tilde{\rho}|\boldsymbol{n}) = \sum_{i=1}^{K} f_i \log\left[tr(\lambda_i \rho)\right]. \tag{2.52}$$

Thus the estimator state $\tilde{\rho}$ can be obtained by solving the following optimization

$$\min - l(\tilde{\rho}|\boldsymbol{n}) \tag{2.53}$$

$$\text{subject to: } \sum_{i=1}^{K^2-1} \tilde{r}_i \leq 1 \tag{2.54}$$

which solves the problems of $\boldsymbol{r}$ being unbounded and the non-physicality of the estimated state $\tilde{\rho}$.

2.2.2 Self-Guided Quantum Tomography

As the name indicates, self-guided quantum tomography is a method that provided an initial guess $|\,\tilde{\psi}_0\,\rangle$ can guide itself towards the real state of the system $|\,\psi\,\rangle$.

What the algorithm do is minimize a distance function $d(|\,\tilde{\psi}_0\,\rangle, |\,\psi\,\rangle)$ that can be directly measured in an iterative manner. For each step of the algorithm a new estimator $|\,\tilde{\psi}_k\,\rangle$ will be constructed with information of the previous step. In the original proposition SPSA was used as the optimization method (Section 1.4.2), and the infidelity was chosen as the distance function [16].

To use the tomography method, the first step is to give the estimator state a parametrization, that is

$$|\,\tilde{\psi}\,\rangle = |\,\psi(\tilde{\boldsymbol{\theta}})\,\rangle. \tag{2.55}$$

Let $|\,\psi(\tilde{\boldsymbol{\theta}}_k)\,\rangle$ be the k^{th} guess, in order to construct the next guess we compute the perturbations

$$|\,\psi(\tilde{\boldsymbol{\theta}}_{k\pm})\,\rangle = |\,\psi(\tilde{\boldsymbol{\theta}}_k \pm c_k \boldsymbol{\Delta}_k)\,\rangle \tag{2.56}$$

depicted in Section 1.4.2. Then we measure (directly from the system) the distances

$$d_{\pm} = d(|\,\psi\,\rangle, |\,\psi(\tilde{\boldsymbol{\theta}}_{k\pm})\,\rangle), \tag{2.57}$$

and use them to calculate an estimate of the gradient $\boldsymbol{g}_k$, by using the formula

$$\tilde{\boldsymbol{g}}_{k.\alpha}(\tilde{\boldsymbol{\theta}}_k) = \frac{d_+ - d_-}{2c_k\Delta_{k,\alpha}}. \tag{2.58}$$

Finally, the next estimator state is given by

$$|\,\psi(\tilde{\boldsymbol{\theta}}_{k+1})\,\rangle = |\,\psi(\tilde{\boldsymbol{\theta}}_k + a_k\tilde{\boldsymbol{g}})\,\rangle \tag{2.59}$$

The coefficients a_k, b_k are detailed in Section 1.4.2 and can be chosen as

$$a_k = \frac{a}{(k+1+A)^s} \qquad c_k = \frac{c}{(k+1)^t}. \tag{2.60}$$

The components of the vector $\boldsymbol{\Delta}_k$ (also explained in Section 1.4.2) can be drawn from the set $\{1, -1\}$ randomly, such that the choice is independent from each component and iteration.

2.3 Quantum Fisher Information

In the derivation of the Fisher information matrix in Section 1.3.3, we never used the quantum theory formalism in order to write the probabilities. Hence, the objective of this chapter is to find a new Fisher matrix, called the quantum Fisher information matrix [20, 17],by incorporating the quantum theory.

Since the value of the estimator $\tilde{\boldsymbol{\theta}}$ is obtained from the result of an experiment,

then it is an observable which quantum mechanics dictates is associated with an hermitian operator. In this way, we can think of an experiment to estimate the unknown parameters $\boldsymbol{\theta}$ of a state $\rho(\boldsymbol{\theta})$ by measuring of projectors

$$d\Pi(\tilde{\boldsymbol{\theta}}) = \Pi(\tilde{\boldsymbol{\theta}})d^n\tilde{\boldsymbol{\theta}} \tag{2.61}$$

whose outcomes are the observable quantity $d^n\tilde{\boldsymbol{\theta}}$. Thus the probability density function $p(\tilde{\boldsymbol{\theta}})$ can be written in the following form

$$p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})d^n\tilde{\theta} = \mathrm{Tr}[\rho(\boldsymbol{\theta})d\Pi(\tilde{\boldsymbol{\theta}})], \tag{2.62}$$

where

$$\int_\Theta d\Pi(\tilde{\boldsymbol{\theta}}) = \mathbb{I}. \tag{2.63}$$

The expected value of a function $f(\tilde{\boldsymbol{\theta}})$ is given by

$$\mathbb{E}[f(\tilde{\boldsymbol{\theta}})|\boldsymbol{\theta}] = \int_\Theta f(\tilde{\boldsymbol{\theta}})\mathrm{Tr}[\rho(\boldsymbol{\theta})d\Pi(\tilde{\boldsymbol{\theta}})]. \tag{2.64}$$

Assuming that the estimators are unbiased then we have

$$\frac{\partial}{\partial\theta_j}\mathbb{E}[\tilde{\theta}_k|\theta] = \int_\Theta \tilde{\theta}_k \mathrm{Tr}\left[\frac{\partial}{\partial\theta_j}\rho(\boldsymbol{\theta})d\Pi(\tilde{\boldsymbol{\theta}})\right] = \delta_{jk}, \tag{2.65}$$

and because the probability function is normalized

$$\int_\Theta \left[\frac{\partial}{\partial\theta_j}\rho(\boldsymbol{\theta})d\Pi(\tilde{\boldsymbol{\theta}})\right] = 0. \tag{2.66}$$

Then, let $\boldsymbol{z}, \boldsymbol{y}$ be some random real vectors and multiply Eq. (2.65) by y_j, z_k and

Eq. (2.66) by θ_k, y_j, z_k to finally obtain

$$\sum_{j,k} \mathrm{Tr} \int_\Theta \left\{ y_j \left[\tilde{\theta}_j - \theta_j \right] z_k \frac{\partial}{\partial \theta_k} \rho(\boldsymbol{\theta}) d\Pi(\tilde{\boldsymbol{\theta}}) \right\} = y^t z. \tag{2.67}$$

By introducing the symmetrized logarithmic derivatives (SLD) $L_k(\boldsymbol{\theta})$ defined implicitly as

$$\frac{\partial}{\partial \theta_k} \rho(\boldsymbol{\theta}) = \frac{1}{2}(L_k(\boldsymbol{\theta})\rho(\boldsymbol{\theta}) + \rho(\boldsymbol{\theta})L_k(\boldsymbol{\theta})) = \frac{1}{2}\{L_k, \rho\}. \tag{2.68}$$

It can be proven, for any hermitian operator A that the SLD's satisfies

$$\mathrm{Tr}\left[\frac{\partial \rho}{\partial \theta_k} A\right] = \frac{1}{2}\mathrm{Tr}\left[L_k \rho A + \rho L_k A\right] \tag{2.69}$$

$$= \frac{1}{2}\mathrm{Tr}\left[L_k \rho A + (A L_k^\dagger \rho)^\dagger\right] \tag{2.70}$$

$$= \frac{1}{2}\left[\mathrm{Tr}(L_k \rho A) + \mathrm{Tr}(L_k^\dagger \rho A)^*\right] \tag{2.71}$$

$$= \mathrm{Re}\left[\mathrm{Tr}(\rho L_k A)\right]. \tag{2.72}$$

Now, from Eq. (2.67) we can obtain

$$(\boldsymbol{y}^t \boldsymbol{z})^2 = \mathrm{Re}\left(\mathrm{Tr}\left\{\sum_{j,k} \int_\Theta y_j \left[\tilde{\theta}_j - \theta_j\right] \rho z_k L_k d\Pi\right\}\right)^2 \tag{2.73}$$

$$= \mathrm{Re}\left(\mathrm{Tr}\int_\Theta T_\theta \rho T_L d\Pi\right)^2 \tag{2.74}$$

$$\leq \left|\mathrm{Tr}\int_\Theta T_\theta \rho T_L d\Pi\right|^2 \tag{2.75}$$

where we have defined $T_\theta = \mathbb{I}\sum_j y_j \left[\tilde{\theta}_j - \theta_j\right]$, and $T_L = \sum_k z_k L_k$. By applying inequality [19]

$$\mathrm{Tr}\left[\rho\int_\Theta T_\theta^\dagger d\Pi T_\theta\right]\mathrm{Tr}\left[\rho\int_\Theta T_L^\dagger d\Pi T_L\right]\geq\left|\mathrm{Tr}\left[\rho\int_\Theta T_L^\dagger d\Pi T_\theta\right]\right|^2 \tag{2.76}$$

to Eq (2.75) and taking into account that T_θ and T_L are both hermitian, we can compute the traces on the left side of Eq (2.76), obtaining

$$\mathrm{Tr}\left[\rho\int_\Theta T_\theta d\Pi T_\theta\right]=\sum_{j,k}y_j y_k\mathrm{Tr}\left[\rho\int_\Theta\left(\tilde{\theta}_j-\theta_j\right)\left(\tilde{\theta}_k-\theta_k\right)d\Pi\right] \tag{2.77}$$

$$=\sum_{j,k}y_j y_k\left[\int_\Theta\left(\tilde{\theta}_j-\theta_j\right)\left(\tilde{\theta}_k-\theta_k\right)p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})d^n\tilde{\boldsymbol{\theta}}\right] \tag{2.78}$$

$$=\sum_{j,k}y_j C_{jk}y_k \tag{2.79}$$

$$=\boldsymbol{y}^t C\boldsymbol{y}. \tag{2.80}$$

And

$$\mathrm{Tr}\left[\rho\int_\Theta T_L d\Pi T_L\right]=\sum_{j,k}z_j z_k\mathrm{Tr}\left[\rho\int_\Theta L_j L_k d\Pi\right] \tag{2.81}$$

$$=\sum_{j,k}z_j z_k\mathrm{Tr}[\rho L_j L_k] \tag{2.82}$$

$$=\sum_{j,k}z_j z_k H_{jk} \tag{2.83}$$

$$=\boldsymbol{z}^t H\boldsymbol{z}. \tag{2.84}$$

In these calculations we have left out of the integral the logarithmic derivatives L because they only depend on $\boldsymbol{\theta}$ and not in the random variable $\tilde{\boldsymbol{\theta}}$. Also we have introduced the matrix

$$H_{jk}=\mathrm{Tr}[\rho L_j L_k]=\frac{1}{2}(\mathrm{Tr}[\rho L_j L_k]+\mathrm{Tr}[\rho L_k L_j]), \tag{2.85}$$

which is known as the quantum Fisher information matrix.

Finally we get the inequality between the covariance matrix and the quantum Fisher matrix

$$(\boldsymbol{y}^t\boldsymbol{z})^2 \leq \boldsymbol{y}^t C \boldsymbol{y} \boldsymbol{z}^t H \boldsymbol{z} \tag{2.86}$$

from where we can derive the quantum Cramér-Rao inequality

$$c - H^{-1} \geq 0. \tag{2.87}$$

Now, in order to estimate the parameters $\boldsymbol{\theta}$, we have N quantum system prepared equally in the state $\rho(\boldsymbol{\theta})$, then the state of the whole system is given by

$$\rho^{\otimes N}(\boldsymbol{\theta}) = \rho(\boldsymbol{\theta}) \otimes \rho(\boldsymbol{\theta}) \cdots \otimes \rho(\boldsymbol{\theta}). \tag{2.88}$$

Thus, the symmetrized logarithmic derivative is defined implicitly by the equation

$$\frac{\partial}{\partial \theta_k}\rho^{\otimes N}(\boldsymbol{\theta}) = \frac{1}{2}\left(L_k^{(N)}(\boldsymbol{\theta})\rho^{\otimes N}(\boldsymbol{\theta}) + \rho^{\otimes N}(\boldsymbol{\theta})L_k^{(N)}(\boldsymbol{\theta})\right), \tag{2.89}$$

where the derivative of the density matrix can be calculated by using the Leibniz rule, obtaining

$$\frac{\partial}{\partial \theta_k}\rho^{\otimes N}(\boldsymbol{\theta}) = \frac{\partial \rho}{\partial \theta_k} \otimes \rho \cdots \otimes \rho + \cdots + \rho \otimes \cdots \otimes \frac{\partial \rho}{\partial \theta_k}, \tag{2.90}$$

hence the SLD of the entire system can be written as a superposition of the SLD's of each individual subsystem as follows

$$L_k^{(N)}(\boldsymbol{\theta}) = L_k \otimes \mathbb{I} \cdots \otimes \mathbb{I} + \cdots + \mathbb{I} \otimes \cdots \otimes L_k. \tag{2.91}$$

Now the Helstrom matrix can be easily computed

$$H_{lm}^{(N)} = \mathrm{Tr}\left[\frac{\partial \rho^{\otimes N}}{\partial \theta_l} L_m^{(N)}\right] \tag{2.92}$$

$$= \sum_{i=1}^{N} \mathrm{Tr}\left[\frac{\partial \rho}{\partial \theta_l} L_m\right] \tag{2.93}$$

$$= N\mathrm{Tr}\left[\frac{\partial \rho}{\partial \theta_l} L_m\right] \tag{2.94}$$

$$= N H_{lm}. \tag{2.95}$$

Here we point out that the Fisher and Helstrom matrices are not equals, in fact they are related as follows (see Apendix A)

$$C^{(N)} \geq \frac{1}{I^{(N)}} \geq \frac{1}{H^{(N)}} = \frac{H^{-1}}{N}. \tag{2.96}$$

This result is rather confusing, since it gives the wrong idea that quantum mechanics allows for more precision. The correct interpretation is that the inequality can be saturated, that is $I^{(N)} = NH$, if the performed measures happens to be optimal ones.

To understand the last affirmation we remember that the Fisher information matrix is explicitly dependent on the projectors to be measured, contrary to the quantum version. Thus the classical information matrix achieves its maximum just for a few (or one) set of projectors, meaning

$$\max_{\Pi} I^{(N)} = NH. \tag{2.97}$$

This means that the quantum matrix gives the optimum bound for any distance

function, but does not tell us what is the set of projectors that achieve the optimum. However, it has been proven that the Fisher information matrix has to satisfy another bound, implying that reaching the quantum Cramér-Rao bound is in general not possible. This constrain is shown in the following theorem.

Theorem 2 *(Gill-Massar) [17] When $\rho(\boldsymbol{\theta}) = |\Psi(\boldsymbol{\theta})\rangle\langle\Psi(\boldsymbol{\theta})|$ is a pure d-dimensional state, then the Fisher and Helstrom information matrices satisfy the relation.*

$$\mathrm{Tr}[H^{-1}I^{N}] \leq N(d-1). \tag{2.98}$$

Given this new limitation, in order to obtain a correct bound for the WMSE we must solve the following optimization problem

$$\begin{aligned} \min_{\boldsymbol{\theta}\in\Theta} \ & \mathrm{Tr}(WC^{(N)}(\boldsymbol{\theta})), \\ & \mathrm{Tr}(I^{(N)}(\boldsymbol{\theta})H^{-1}(\boldsymbol{\theta})) = N(d-1). \end{aligned} \tag{2.99}$$

Which has the following solution

$$\mathrm{Tr}[WC^{(N)}(\boldsymbol{\theta})] = \frac{\left(\mathrm{Tr}\left[\sqrt{H^{-1/2}WH^{-1/2}}\right]\right)^2}{N(d-1)}. \tag{2.100}$$

In the particular case of our work, we are interested in the bound for the Mean Squared Error, hence we choose the weight matrix as the identity. Thus, for pure states the bound yields (See Appendix B)

$$MSE(\tilde{\boldsymbol{\theta}}) = \frac{d-1}{N}. \tag{2.101}$$

Chapter 3

State Estimation Via Squared Error Minimization

Our main aim is to obtain an estimate $|\tilde{\psi}\rangle = \sum_i \tilde{z}_i|i\rangle$ of an unknown quantum state $|\psi\rangle = \sum_i z_i|i\rangle$, where $\{z_i\}$ and $\{\tilde{z}_i\}$ are properly normalized. In order to do this we consider the squared error

$$SE(\boldsymbol{z}, \tilde{\boldsymbol{z}}) = \sum_{i=1}^{d} |z_i - \tilde{z}_i|^2, \tag{3.1}$$

which is a function of the probability amplitudes $\tilde{z}_i$ of $|\tilde{\psi}\rangle$. The probability amplitudes z_i of $|\psi\rangle$ play the role of unknown fixed parameters. The unknown state $|\psi\rangle$ can be characterized as

$$\boldsymbol{z} = \text{Arg}\{\min_{\tilde{\boldsymbol{z}}} SE(\boldsymbol{z}, \tilde{\boldsymbol{z}})\}, \tag{3.2}$$

that is, SE achieves a global minimum when $\tilde{\boldsymbol{z}} = \boldsymbol{z}$.

To solve the minimization of $SE(\boldsymbol{z}, \tilde{\boldsymbol{z}})$ we employ a concatenation between the CSPSA (Section 1.4.3) and MLE (Section 1.3.2) methods, in order to accelerate convergence. This requires the capability to obtain the value of $SE(\boldsymbol{z}, \tilde{\boldsymbol{z}})$ for all $\tilde{\boldsymbol{z}}$. In the simplest case of estimating the polarization state of a single photon, a Mach-Zehnder interferometer whose arms are supplemented with unitary transformations acting on the polarization degree of freedom allows us to infer the value of $SE(\boldsymbol{z}, \tilde{\boldsymbol{z}})$. In this setup, the initial state $|\psi\rangle_{in}$ of a single photon before entering the interferometer is given by $|\psi\rangle_{in} = |h\rangle_1$, where $|h\rangle_1$ describes a horizontally polarized single photon. After the interaction of the photon with the first beam splitter, the quantum state of the photon becomes $(|h\rangle_a + |h\rangle_b)/\sqrt{2}$, which corresponds to an equally weighted coherent superposition of the two possible propagation paths a and b for the photon inside the interferometer. The polarization state of the photon changes conditional on the path, that is,

$$U_a|h\rangle_a = z_h|h\rangle_a + z_v|v\rangle_a = |\psi\rangle, \tag{3.3}$$

which is the unknown state to be estimated, and

$$U_b|h\rangle_b = \tilde{z}_h|h\rangle_b + \tilde{z}_v|v\rangle_b = |\tilde{\psi}\rangle, \tag{3.4}$$

which is the estimate of $|\psi\rangle$. Thereby, the state of the photon before the second beam splitter becomes $[(z_h|h\rangle_a + z_v|v\rangle_a) + (\tilde{z}_h|h\rangle_b + \tilde{z}_v|v\rangle_b)]/\sqrt{2}$. After the second beam splitter, the state is given by

$$\begin{aligned} |\psi\rangle_{out} &= \frac{1}{2}[(z_h + \tilde{z}_h)|h\rangle_1 + (z_v + \tilde{z}_v)|v\rangle_1] \\ &+ \frac{1}{2}[(z_h - \tilde{z}_h)|h\rangle_2 + (z_v - \tilde{z}_v)|v\rangle_2], \end{aligned} \tag{3.5}$$

where the sub-indexes 1 and 2 indicates the output ports of the interferometer. The probability P_2 of detecting a photon at output port 2 is

$$P_2 = \frac{1}{4}(|z_h - \tilde{z}_h|^2 + |z_v - \tilde{z}_v|^2), \tag{3.6}$$

which can be identified with the squared error of the complex probability amplitudes as

$$SE(\boldsymbol{z}, \tilde{\boldsymbol{z}}) = 4P_2. \tag{3.7}$$

Thus, in the setup above described the unitary transformation U_a is employed to create the unknown polarization state $|\psi\rangle$ defined by the pair of complex probability amplitudes (z_h, z_v). The unitary transformation U_b is employed to generate an estimate $|\tilde{\psi}\rangle$, which is defined by the pair of complex probability amplitudes $(\tilde{z}_h, \tilde{z}_v)$. Equation (3.7) indicates that the transformation U_b has to be changed in such a way that no photon is detected at output port 2, in which case $|\tilde{\psi}\rangle = |\psi\rangle$. We employ CSPSA and MLE to drive the sequence of choices of U_b toward the unknown state. Let us note that if the output ports of the interferometer are supplemented with polarizing beam splitters and single-photon detectors it is possible to measure independently the four combinations of coefficients $|z_h - \tilde{z}_h|^2$, $|z_v - \tilde{z}_v|^2$, $|z_h + \tilde{z}_h|^2$, and $|z_v + \tilde{z}_v|^2$.

The case of higher dimensions can be realized by considering a spatial qudit, that is, a qudit encoded in the propagation paths of a single photon. The initial state of the qudit is given by $|k\rangle$, where the state $|k\rangle$ describes a single photon propagating along one of several distinguishable paths $k = 1, \ldots, d$. On path k a beam splitter transforms the state $|k\rangle$ into the superposition $(1/\sqrt{2})(|k_1\rangle + |k_2\rangle)$,

where the subindexes $i = 1, 2$ distinguish the propagations paths at the exit ports of the beam splitter. Thereafter, on paths k_1 and k_2 the unitary transformations U and $\tilde{U}$ are applied, respectively. These transformations create a superposition of path states, that is, $U|k_1\rangle = \sum_k z_k|k_1\rangle$ and $\tilde{U}|k_2\rangle = \sum_k \tilde{z}_k|k_2\rangle$. This leads to the state $(1/\sqrt{2})(U|k_1\rangle + \tilde{U}|k_2\rangle)$. Finally, paths k_1 and k_2 for each $k = 1, \ldots, d$ are merged together by beam splitters, which leads to the state $(1/2)[\sum_k (z_k + \tilde{z}_k)|k_{1'}\rangle + \sum_k (z_k - \tilde{z}_k)|k_{2'}\rangle)]$ with $i = 1', 2'$ the output ports of each beam splitter. The probability of detecting a photon on any path $k_{2'}$ is given by

$$P_2 = \frac{1}{4}\sum_{k=1}^{d} |z_k - \tilde{z}_k|^2. \tag{3.8}$$

Thereby, we have that

$$SE(\boldsymbol{z}, \tilde{\boldsymbol{z}}) = 4P_2, \tag{3.9}$$

which generalizes Eq. (3.7) to the case $d > 2$.

We have formulated our proposal to measure the SE in terms of bulk optics based setup. However, this proposal can easily be translated to other experimental platforms, such as, for instance, integrated quantum photonics [47] and space-division multiplexing optical fibres [51, 11]. On this platforms unitary transformations can be implemented by means of sequences composed of beam splitters and controlled phase transformations [35, 13].

Our estimation method is based on the optimization of the SE with the help of CSPSA concatenated to MLE. The concatenation is motivated by the hope of achieving the Gill-Massar bound or at least approach as much as possible, since it is impossible to get near the bound without exploiting all the information accumulated

through the measurements. Alternatively, we can reinterpret the method considering SE optimization through CSPSA to accelerate the MLE convergence rate. That is, MLE is calculated with the data obtained through SE measurements. These are chosen with the help of CSPSA in such a way that they increase the convergence of MLE towards the estimate. In this scenario, the existence of a linear regime is consistent with the efficiency and asymptotic normality of MLE estimators [26].

The main steps of the MSE-based method for estimating pure quantum states are summarized as pseudocode in Algorithm 1, where we have considered the proposals to estimate the SE with the help of a multi-arm interferometer. An implementation of the pseudocode in the Julia programming language can be found in the GitHub repository [1].

The minimization of SE via CSPSA requires an initial guess (or estimate) of the unknown state. Since no a priori information about the unknown state is available, the initial guess is also generated according to a uniform distribution. At each iteration, CSPSA generates the $\mathbf{\Delta}$ vector whose components are randomly chosen. Also, at each iteration CSPSA uses the value of SE on the states $\boldsymbol{z}_{k\pm}$. According to Eq. (3.7), the value of the SE can be inferred from a probability, which requires an ensemble of N independently and identically prepared copies. Thereby, the total number of copies employed after k iterations of CSPSA is given by $N_T = 2Nk$. Since this ensemble is finite, the value of SE will be affected by finite statistics effects. Thus, the estimation process for a fixed unknown state has three sources of randomness: the choice of the initial guess, the choice of the $\mathbf{\Delta}$ vector, and the measurement process of SE. Thereby, each time that CSPSA is employed to obtain an estimate of a fixed unknown state $\boldsymbol{z}$, a different estimate $\tilde{\boldsymbol{z}}$ is generated. In this

Algorithm 1 MSE-based estimation of pure states

1: Consider a known pure state $|\psi\rangle$, which is prepared on the upper arm of the interferometer by means of the transformation U.
2: Choose an initial guess $|\tilde{\psi}_0\rangle$ and define $\tilde{z}_{0,i} = \langle i|\tilde{\psi}_0\rangle$.
3: Set gain coefficients a, A, s, b and r.
4: **for** $k = 1, \ldots, k_{max}$ **do**
5: Set

$$a_k = \frac{a}{(k+1+A)^s}, \quad c_k = \frac{b}{(k+1)^r}.$$

6: Choose $\Delta_{k,i}$ randomly in the set $\{\pm 1, \pm i\}$.
7: Calculate $|\psi_{k\pm}\rangle = \sum_i \tilde{z}_{k\pm,i}|i\rangle/|\tilde{\boldsymbol{z}}_{k\pm}|$, with $\tilde{\boldsymbol{z}}_{k\pm} = \tilde{\boldsymbol{z}}_k \pm c_k \boldsymbol{\Delta}_k$.
8: Prepare the states $|\psi_{k\pm}\rangle$ on the lower arm of the interferometer by means of the transformation U'
9: Estimate experimentally the square errors $SE(\boldsymbol{z}, \tilde{\boldsymbol{z}}_{k\pm})$ with a sample of size N.
10: Estimate the gradient as

$$\tilde{g}_{k,i} = \frac{SE(\boldsymbol{z}, \tilde{\boldsymbol{z}}_{k+}) - SE(\boldsymbol{z}, \tilde{\boldsymbol{z}}_{k-})}{2c_k \Delta^*_{k,i}}.$$

11: Actualize the guess $\tilde{\boldsymbol{z}}_{k+1} = \tilde{\boldsymbol{z}}_k - a_k \tilde{\boldsymbol{g}}_k$.
12: Maximize the cumulative logarithmic likelihood function using $|\phi\rangle = \sum_i \tilde{z}_{k+1,i}|i\rangle/|\tilde{\boldsymbol{z}}_{k+1}|$ as starting point,

$$|\tilde{\psi}_{k+1}\rangle = \arg\max_{|\phi\rangle} \log P(D_k; |\psi\rangle, S), \quad \text{s. t.} \quad \langle\phi|\phi\rangle = 1,$$

and update the estimate as $\tilde{z}_{k+1,i} = \langle i|\tilde{\psi}_{k+1}\rangle$.
13: **end for**

scenario the estimation accuracy for a fixed state $\boldsymbol{z}$ is given by

$$MSE(\boldsymbol{z}) = \mathbb{E}[SE(\boldsymbol{z}, \tilde{\boldsymbol{z}})|\tilde{\boldsymbol{z}}], \tag{3.10}$$

where the expectation is calculated over the set of all possible estimates $\tilde{\boldsymbol{z}}$ of $\boldsymbol{z}$. The mean-squared error can also be cast as

$$MSE(\boldsymbol{z}) = \int \tilde{p}(\tilde{\boldsymbol{z}}) SE(\boldsymbol{z}, \tilde{\boldsymbol{z}}) \boldsymbol{d}\tilde{\boldsymbol{z}}, \tag{3.11}$$

where $\tilde{p}(\tilde{\boldsymbol{z}})$ probability density function of obtaining the estimate $\tilde{\boldsymbol{z}}$ that characterizes the estimation procedure.

In order to study the properties of the estimation procedure we create the set $\Omega_d = \{\boldsymbol{z}_i\}$ (with $i = 1, \ldots, m$) containing m unknown pure quantum states in dimension d. The states in Ω_d are independently generated according to a uniform distribution. Each state in Ω_d is estimated by minimizing SE by means of CSPSA concatenated to MLE. This creates the set $\tilde{\Omega}_i = \{\tilde{\boldsymbol{z}}_{i,j}\}$ (with $j = 1, \ldots, n$) for each $\boldsymbol{z}_i$, which is formed by n estimates $\tilde{\boldsymbol{z}}_{i,j}$ of $\boldsymbol{z}_i$. The estimation accuracy of $\boldsymbol{z}_i$ is given by the expectation value of $SE(\boldsymbol{z}_i, \tilde{\boldsymbol{z}})$ over the set of all estimates $\tilde{\boldsymbol{z}}$ of $\boldsymbol{z}_i$, which is approximated by the expression

$$MSE(\boldsymbol{z}_i) = \frac{1}{n} \sum_{j=1}^{n} SE(\boldsymbol{z}_i, \tilde{\boldsymbol{z}}_{i,j}). \tag{3.12}$$

On the other hand the expectation of $MSE(\boldsymbol{z})$ over the Hilbert space of unknown states is given by

$$\overline{MSE} = \mathbb{E}[MSE(\boldsymbol{z})|\boldsymbol{z}], \tag{3.13}$$

which can also be approximated as the average of the $MSE(\boldsymbol{z})$ over Ω_d, meaning

$$\overline{MSE} = \frac{1}{m} \sum_{i=1}^{m} MSE(\boldsymbol{z}_i). \tag{3.14}$$

Insets 3.1(a), 3.1(b), 3.1(c), and 3.1(d) show the behavior of $\overline{MSE}$ as a function of the number k of iterations for dimension d =2, 4, 8, and 16, respectively, and for several ensemble sizes. As is apparent from these figures, the expectation of $MSE(\boldsymbol{z})$ over the Hilbert space of unknown states exhibits a rapid estimation accuracy gain

followed by a linear regime. The latter arises after a number of iterations that depends on the particular dimension. In particular, the higher the dimension the more iterations are needed for the emergence of the linear regimen. The insets also depict the lower bound $MSE_{GM}(2d, N_T)$ as a function of the iteration number k and the ensemble size N, for various dimensions. As the insets show, the estimation accuracy characteristic of our method becomes very close to $MSE_{GM}(2d, N_T)$ as N increases. In fact, the accuracy of the estimates seems to be asymptotically close to $MSE_{GM}(2d, N_T)$. Insets 3.1(e), 3.1(f), 3.1(g), and 3.1(h) illustrate the median of $MSE(\boldsymbol{z_i})$ over Ω_d. This exhibits a behavior similar to that of $\overline{MSE}$, but the linear regime emerges earlier. Once the optimization method enters into the linear regime, the mean and the median of $MSE(\boldsymbol{z}_i)$ reach values that cannot be distinguished. Furthermore, the interquartile range becomes extremely narrow. This indicates that in the linear regime the minimization of SE via the concatenation of CSPSA and MLE leads to an estimation procedure characterized by a state-independent MSE. Insets 3.1(e), 3.1(f), 3.1(g), and 3.1(h) also show twice the Gill-Massar lower bound for the MSE. As is apparent in all insets, in the linear regime the median of the estimation accuracy is also very close to $MSE_{GM}(2d, N_T)$.

To study the linear regime we fitted the numerical data obtained from the Monte Carlo simulations to the function p/N_T^a, as suggested by the observation that behavior of $\overline{MSE}$ is close to $MSE_{GM}(2d, N_T) = (2d-1)/N_T$, where $N_T = 2kN$, $p = 2d-1$ and $a = 1$. The best fits for the values of p and a are shown in Table 3.1, where two sets of p and a values are indicated for each dimension d and ensemble size N. The first set of values is obtained fitting data from iteration $k = 10$ until $k = 20$. The second set of values is obtained fitting data from iteration $k = 21$ until $k = 30$. With the exception of the first dataset for $d = 16$, Table 3.1 indicates that the value of a

	$N = 10^3$		$N = 10^4$		$N = 10^5$	
d=2	p=6.34	a=1.03	p=9.97	a=1.03	p=6.52	a=1.02
	p=7.41	a=1.04	p=4.21	a=0.99	p=3.57	a=0.99
d=4	p=10.56	a=1.00	p=9.12	a=0.99	p=8.77	a=0.99
	p=10.18	a=1.00	p=8.12	a=0.99	p=8.50	a=0.99
d=8	p=56.69	a=1.09	p=25.76	a=1.02	p=19.66	a=0.99
	p=21.30	a=1.00	p=20.16	a=1.00	p=17.41	a=0.99
d=16	p=4.80	a=2.21	p=1.18	a=2.09	p=8.84	a=2.93
	p=147.62	a=1.10	p=39.13	a=0.99	p=33.87	a=0.99

Table 3.1: Fit $\overline{MSE} = p/(2kN)^a$ in asymptotic regime. $MSE_{GM}(2d, 2kN)$ is obtained with $p = 2d-1$ and $a = 1$. For d and N fixed, the first pair (p, a) is obtained fitting iterations from $k = 10$ until $k = 45$. The second pair is obtained fitting iterations from $k = 46$ until $k = 100$.

are in the range $[0.99, 1.1]$ with an average value $\bar{a}$ to 1.01. The anomalous behavior of the first dataset for $d = 16$ can be attributed to the fact that for $d = 16$ more than 10 iterations are required for the onset of the linear asymptotic regime. The first dataset exhibits values of p that are larger than the values of p of the second dataset. In both datasets, the values of p decrease with an increase in the ensemble size N. This indicates an increase in the rate at which the algorithm approaches the minimizer. Finally, the values of p for $N = 10^4$ and 10^5 in the second dataset are close to the value of $2d$, specially the latter. Thus, for larger values of N and k, we can approximate $\overline{MSE}$ as

$$\overline{MSE} = \frac{2d + \alpha}{2kN}, \tag{3.15}$$

where α is a small quantity in comparison to $2d$.

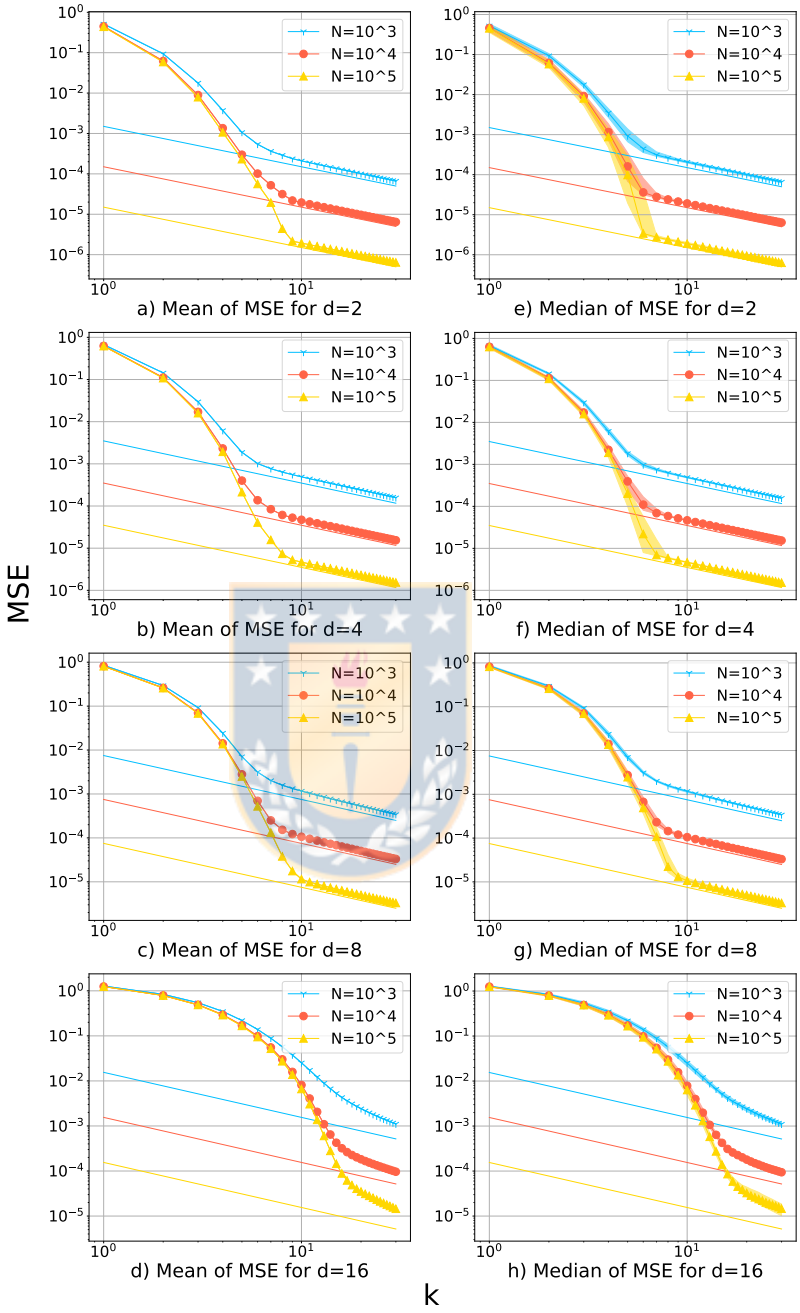

Figure 3.1: Mean (upper row) and median (lower row) of $MSE(\boldsymbol{z}_i)$ on Ω_d as a function of the iteration number k, for dimension d=2, 4, 8, and 16 (from left to right) and ensemble size $N = 10^3$ (light blue down threes), 10^4 (solid red triangles), and 10^5 (solid yellow circles) per iteration. Straight lines depict the Gill-Massar lower bound $MSE_{GM}(2d, N_T)$ for the respective total ensemble size $N_T = 2Nk$. Shaded areas represent interquartile range.

Chapter 4

Estimation of Unitary Transformations Via Squarred Error Minimization

The estimation of processes acting on quantum states is a much more demanding problem than the estimation of quantum states. For instance, the estimation of an unknown process acting onto a single qudit requires the characterization of $d^4 - d^2$ real parameters [32]. In the case of a unitary transformation, only d^2 parameters must be determined.

In general, the estimation of a quantum process is carried out by carefully choosing a set of states, letting the process act on them, and reconstructing the output states by means of a quantum tomographic method [5]. We will employ this strategy to estimate an unknown unitary transformation U. This is suggested by Eq. (3.8),

which can be cast in the form

$$P_2 = \frac{1}{4}\sum_{j=1}^{d} |U_{j,k} - \tilde{U}_{j,k}|^2. \tag{4.1}$$

Thus, the probability P_2 is proportional to the squared error between the k-th columns of the matrices U and $\tilde{U}$, where k is controlled by the initial path state $|k\rangle$ followed by the single photon. Clearly, we can reconstruct each column of U by minimizing the squared error by CSPSA and MLE. After estimating all columns of U independently, we obtain an estimate $\tilde{U}$ of U.

However, the present estimation method cannot guarantee that the estimate $\tilde{U}$ is really unitary. We consider two transformations to be implemented at each iterations in order to convert any estimate into a unitary one. One of those methods is given by the expression [25]

$$\tilde{U}_c = \tilde{U}(\tilde{U}\tilde{U}^\dagger)^{-1/2}, \tag{4.2}$$

which is the closest unitary operator (Section 1.1.5) to the transformation $\tilde{U}$. In order to quantify how close $\tilde{U}_c$ is from U we employ the Hilbert-Schmidt distance $D(U, \tilde{U}_c) = Tr[(U - \tilde{U}_c)(U - \tilde{U}_c)^\dagger]$. Another method to generate a unitary estimate $\tilde{U}_{gs}$ consists in the application of the Gramm-Schmidt orthogonalization procedure to the columns $\tilde{U}_{j,k}$.

Figure 4.1 shows the mean and median mean-squared error achieved in process of estimating unknown unitary transformations acting onto a 2-dimensional quantum system. The left (right) column exhibits the mean (median) achieved with the estimates $\tilde{U}$, $\tilde{U}_c$, and $\tilde{U}_{gs}$ from top to bottom, respectively. The typical behavior of a rapidly increasing estimation accuracy followed by a linear regimen is clearly present.

This exhibits in the linear regime a mean and a median that cannot be distinguished from each other and an extremely narrow interquartile range, which indicates that after 10 iterations all unitary transformations are estimated with the same accuracy. This is almost twice the accuracy obtained in estimating a 2-dimensional pure state, as expected. The three estimates lead to very similar accuracies, but the estimate $\tilde{U}_c$ generates a marginally better performance. Figure 4.2 exhibits similar results in the case $d = 4$.

In Algorithm 2 we present a basic pseudocode for implementing the MSE-based estimation of unitary transformations. An implementation of the pseudocode in the Python programming language can be found in the GitHub repository [1]. We consider the different choices for the post-processing of the estimates. According to option 1 we project the possibly non-unitary estimate onto the set of unitary transformations and evaluate the infidelity. These projections are used in option 2 to provide a better update of the estimate.

Since each of the d columns of U is estimated with an accuracy close to $(2d + \alpha)/N_T$, where N_T is the total ensamble size used in the estimation of each column, we have that the unitary transformations are estimated with an accuracy $MSE(U)$ given approximately by

$$MSE(U) \approx \frac{d(2d + \alpha)}{N_T}. \tag{4.3}$$

Thereby, the estimation accuracy of our procedure becomes

$$MSE(U) \approx \frac{d^2(2d + \alpha)}{N_T^*}, \tag{4.4}$$

where $N_T^* = dN_T$ is the total number of copies used in the estimation of all d columns

of U.

Algorithm 2 MSE-based estimation of unitary transformations

Consider a known unitary transformation U on the upper arm of the interferometer.

Choose initial estimate $\tilde{U}_0$ and define $\tilde{z}^j_{0,i} = \tilde{U}_{0,ij}$.

Set gain coefficients a, A, s, b and r.

for $k = 1, \ldots, k_{max}$ **do**

Set

$$a_k = \frac{a}{(k+1+A)^s}, \quad c_k = \frac{b}{(k+1)^r}.$$

for $j = 1, \ldots, d$ **do**

Choose $\Delta^j_{k,i}$ randomly in the set $\{\pm 1, \pm i\}$.

Calculate $|\psi^j_{k\pm}\rangle = \sum_i \tilde{z}^j_{k\pm,i}|i\rangle / |\tilde{\boldsymbol{z}}^j_{k\pm}|$, with $\tilde{\boldsymbol{z}}^j_{k\pm} = \tilde{\boldsymbol{z}}_k \pm c_k \boldsymbol{\Delta}_k$.

Feed the interferometer in the mode $|j\rangle$.

Prepare the states $|\psi^j_{k\pm}\rangle$ on the lower arm of the interferometer with the transformation U'.

Estimate experimentally the square errors $SE(\boldsymbol{z}^j, \tilde{\boldsymbol{z}}^j_{k\pm})$ of the j-column of U with a sample of size N.

Estimate the gradient as

$$\tilde{g}^j_{k,i} = \frac{SE(\boldsymbol{z}^j, \tilde{\boldsymbol{z}}^j_{k+}) - SE(\boldsymbol{z}^j, \tilde{\boldsymbol{z}}^j_{k-})}{2c_k \Delta^*_{k,i}}.$$

Actualize the guess $\tilde{\boldsymbol{z}}^j_{k+1} = \tilde{\boldsymbol{z}}^j_k - a_k \tilde{\boldsymbol{g}}^j_k$.

Maximize the cumulative Likelihood function using $|\phi^j\rangle = \sum_i \tilde{z}^j_{k+1,i}|i\rangle / |\tilde{\boldsymbol{z}}^j_{k+1}|$ as starting point,

$$|\tilde{\psi}^j_{k+1}\rangle = \arg\max_{|\phi\rangle} \log P(D^j_k; |U|j\rangle, S), \quad \text{s. t.} \quad \langle\phi|\phi\rangle = 1,$$

and update the estimate as $\tilde{z}^j_{k+1,i} = \langle i|\tilde{\psi}^j_{k+1}\rangle$.

end for

Option 1: In order to guarantee the unitarity of the estimator, we consider two postprocessing methods:

- $\tilde{U}_c$: Project $\tilde{U}$ into its closest unitary matrix.
- $\tilde{U}_{gs}$: Apply the Gram-Schmidt procedure to the columns of $\tilde{U}_{k+1}$.

Option 2: Re-update the estimates $\{\tilde{\boldsymbol{z}}^j_{k+1}\}$ with the postprocessed unitary matrix,

$$\tilde{z}^j_{k+1,i} = (\tilde{U}_c)_{k+1,ij} \qquad \text{or} \qquad \tilde{z}^j_{k+1,i} = (\tilde{U}_{gs})_{k+1,ij}.$$

end for

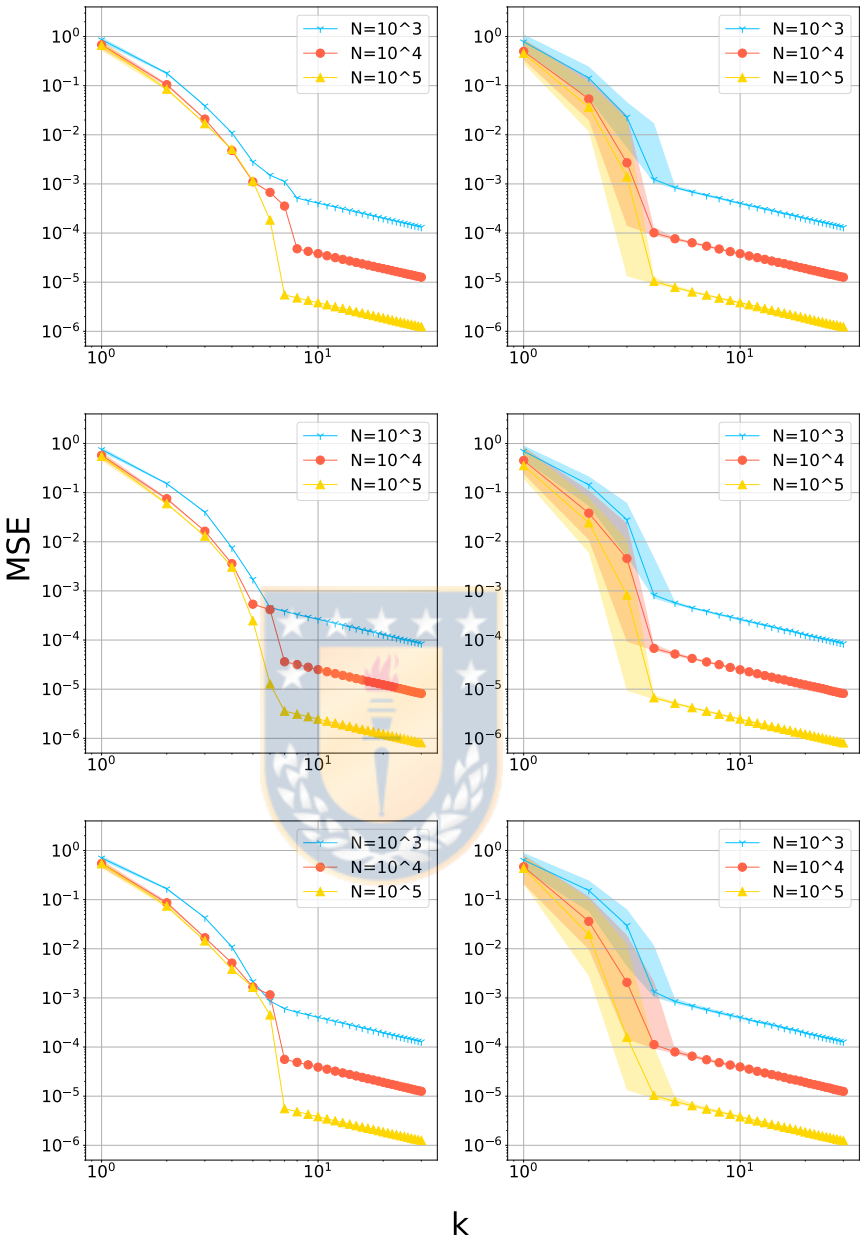

Figure 4.1: Mean (left column) and median (right column) of MSE for randomly generated unitary transformations as a function of the iteration number k for dimension d=2 and ensemble size $N = 10^3$ (light blue down threes), 10^4 (solid red triangles), and 10^5 (solid yellow circles) per iteration. Shaded areas represent interquartile range. From the top row to the bottom row: estimates provided by CSPSA, estimates provided by CSPSA updated at each iteration by projection to the closest unitary transformation, and estimates provided by CSPSA updated at each iteration with the Gramm-Schmidt orthogonalization procedure.

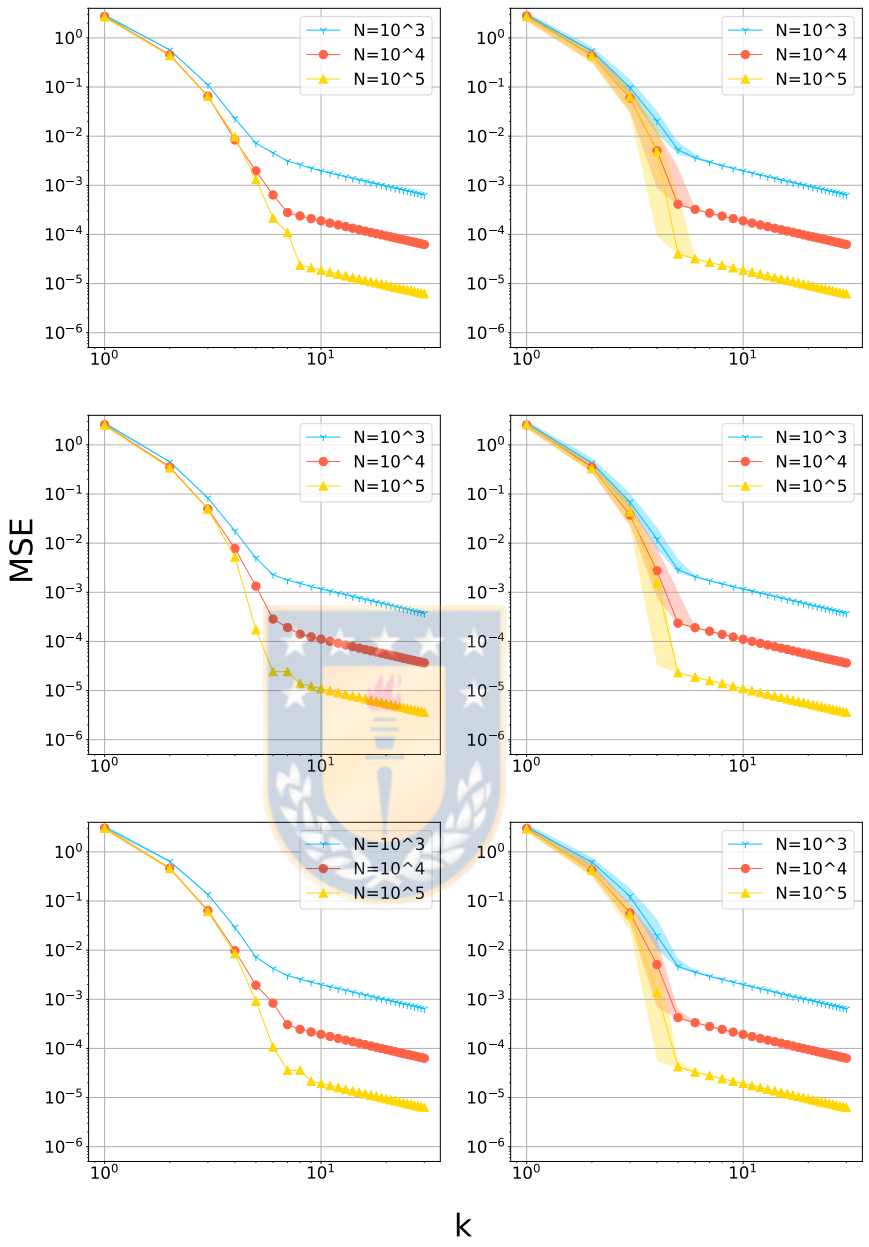

Figure 4.2: Mean (left column) and median (right column) of MSE for randomly generated unitary transformations as a function of the iteration number k for dimension d=4 and ensemble size $N = 10^3$ (light blue down threes), 10^4 (solid red triangles), and 10^5 (solid yellow circles) per iteration. Shaded areas represent interquartile range. Estimates are updated after each iteration. From the top row to the bottom row: estimates provided by CSPSA, estimates provided by CSPSA updated at each iteration by projection to the closest unitary transformation, and estimates provided by CSPSA updated at each iteration with the Gramm-Schmidt orthogonalization procedure.

Chapter 5

Conclusions

In this work we have presented the tomography of quantum states based on the minimization of the squared error, along with a plausible manner to measure this quantity in polarization qubits and path-encoded qudits. The used optimization methods were the CSPSA algorithm, which was concatenated with MLE in order to drastically increase the convergence rate and make use of all the available information. We study the behavior of the algorithm by making Monte-Carlo numerical simulations in states of dimension $d = 2, 4, 8$ and 16.

The simulations display a fast decrease of the metric in the early iterations followed by a seemingly linear regime. In the later regime, for all the treated dimensions, both mean and median become indistinguishable from one another and the interquartile range becomes extremely narrow, implying that one can expect in average a uniform performance of the algorithm in all the states, meaning, that there are no special states with a different demeanor. Furthermore, from the numerical results it seems that the linear regime approaches the Gill-Massar bound for states

of a dimension twice as large. This can be attributed to the fact that in order to measure the squared error between two states we need to work on a bigger space, of size two times larger than the original target state, however we do not have proof for this claim.

The mixing of CSPSA and MLE is introduced in order to exploit all the information available and it is known that this concoction achieves the Gill-Massar bound for tomographic schemes based on the minimization of the infidelity [54], which is why it was hoped that this work could accomplish the same feat. However, the rate of convergence being twice the bound is still a good result, as standard tomography has a convergence rate of the order $\mathcal{O}(1/\sqrt{N})$ for dimensions higher than that of a qubit, and adaptative tomography has been proven to yield a convergence rate on the order of $\mathcal{O}(1/N)$ [34] which is the standard for high accurate methods and where we currently stand.

We also extended our method to the case of the estimation of unitary transformations. The approach taken is to estimate the unitary matrix column by column and enforce the unitarity by applying the Gramm-Schmidt procedure or project onto the closest unitary at each iteration. What was found on the numerical simulations performed for dimensions $d = 2, 4$ is a demeanor similar to the state estimation case, to no surprise since the extension relies heavily on the proposed method to estimate states. The likeliness can also be appreciated in the narrow interquartile range and the similarity between mean and median, and hence, the independence of the unitary to be estimated. On the other hand, closest unitary projection proved to reach a higher accuracy between the two tried methods, but it is also drastically more computational demanding than Gramm-Schmidt ortogonalization, and

for larger dimensions the projection could become infeasible.

Finally we would like to point out that the tomography of unitary processes is the area where this work has more prospect, as the studies of self-guided process tomography are still new. Which is why in the future we will focus on minimizing the amount of input states to make implementations on high dimensional systems more plausible, and research a way to extend the method to process tomography of CPTP transformations.

Appendix A

Relationship Between the Quantum and Classical Fisher Matrices

The classical Fisher matrix can be written as

$$I_{ij} = \int_{\Theta} d^n\tilde{\boldsymbol{\theta}} \frac{1}{p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})} \frac{\partial p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})}{\partial \theta_i} \frac{\partial p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})}{\partial \theta_j}. \tag{A.1}$$

On the other hand the probability function can be expressed in terms of measure operators as

$$p(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta}) d^n\tilde{\boldsymbol{\theta}} = \mathrm{tr}(\rho(\boldsymbol{\theta}) d\Pi(\tilde{\boldsymbol{\theta}})) = \mathrm{tr}(\rho(\boldsymbol{\theta})\Pi(\tilde{\boldsymbol{\theta}})) d^n\tilde{\boldsymbol{\theta}}. \tag{A.2}$$

Let $\boldsymbol{v}$ be any real non-null vector, then

$$\boldsymbol{v}^t I \boldsymbol{v} = \sum_{i,j} \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{p} v_i \partial_{\theta_i} p v_j \partial_{\theta_j} p \tag{A.3}$$

$$= \sum_{i,j} \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{4p} v_i v_j \mathrm{tr}(\rho L_i \Pi + L_i \rho \Pi)\mathrm{tr}(\rho L_j \Pi + L_j \rho \Pi) \tag{A.4}$$

$$= \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{p} \sum_{i,j} \mathrm{Re}(\mathrm{tr}(v_i \rho L_i \Pi))\mathrm{Re}(\mathrm{tr}(v_j \rho L_i \Pi)) \tag{A.5}$$

$$\leq \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{p} |\mathrm{tr}(\rho L \Pi)|^2, \tag{A.6}$$

where $L = \sum v_i L_i$ has been defined. Since the density matrix ρ and the projector Π are positive defined, then

$$\boldsymbol{v}^t I \boldsymbol{v} \leq \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{p} |\mathrm{tr}(\sqrt{\Pi\rho}^\dagger \sqrt{\rho\Pi} L)|^2 \tag{A.7}$$

$$= \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{p} |\langle \sqrt{\rho\Pi}, \sqrt{\rho\Pi} L \rangle_{HS}|^2, \tag{A.8}$$

where $\langle , \rangle_{HS}$ is the Hilbert-Schmidt inner product. By applying the Cauchy-Schwartz inequality to Eq (A.8) we get

$$\boldsymbol{v}^t I \boldsymbol{v} \leq \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{p} ||\sqrt{\rho\Pi}||^2_{HS} ||\sqrt{\rho\Pi} L||^2_{HS} \tag{A.9}$$

$$= \int_\Theta d^n\tilde{\boldsymbol{\theta}} \frac{1}{p} \mathrm{tr}(\rho\Pi)\mathrm{tr}(L\rho\Pi L) \tag{A.10}$$

$$= \int_\Theta d^n\tilde{\boldsymbol{\theta}} \sum_{i,j} v_i v_j \mathrm{tr}(L_i L_j \rho \Pi) \tag{A.11}$$

$$= \boldsymbol{v}^t H \boldsymbol{v}. \tag{A.12}$$

Thus, it has been proven that

$$I \leq H \tag{A.13}$$

Appendix B

Gill Massar Bound Derivation

The objective problem is given by

$$\min \ \mathrm{Tr}(WC^N) \tag{B.1}$$

$$\text{subject to: } \mathrm{Tr}(I^N H^{-1}) = N(d-1) \tag{B.2}$$

which we are going to solve by using Lagrange multipliers. Therefore we use the Frechet directional derivative defined as

$$Df(A)(B) = \frac{d}{dt} f(A+tB)\Big|_{t=0}. \tag{B.3}$$

On the other hand, since our task is to find the minimum value of $\mathrm{Tr}(WC^N)$ we can suppose that C^N saturates the Cramér-Rao bound, that is $C = \frac{1}{I^N}$, where we have dropped the N index in order to make the notation more easier. Thus, the

objective Lagrangian to minimize is

$$\mathcal{L}(C) = \mathrm{Tr}(WC) + \lambda \mathrm{Tr}(CH^{-1}) = f(C) + \lambda g(C), \tag{B.4}$$

where $f(C) = \mathrm{Tr}(WC)$, $g(C) = \mathrm{Tr}(CH^{-1})$ and λ is the Lagrange multiplier. The minimum value will then be given by

$$Df(C)(B) + \lambda Dg(C)(B) = 0. \tag{B.5}$$

Now we compute the Frechet derivatives of each function

$$Df(C)(B) = \frac{d}{dt}\mathrm{Tr}[WC + WBt]\Big|_{t=0} \tag{B.6}$$

$$= \mathrm{Tr}[WB], \tag{B.7}$$

and

$$Dg(C)(B) = \frac{d}{dt}\mathrm{Tr}[(C + Bt)^{-1}H^{-1}]\Big|_{t=0} \tag{B.8}$$

$$= \mathrm{Tr}[D(C^{-1})(B)H^{-1}]. \tag{B.9}$$

To calculate $D(C^{-1})(B)$ we use the fact that $CC^{-1} = \mathbb{I}$, thus

$$D(C^{-1})(B)C + C^{-1}D(C)(B) = 0, \tag{B.10}$$

which implies that $D(C^{-1})(B) = -C^{-1}D(C)(B)C^{-1}$, from here is not hard to see that $D(C)(B) = B$. Now we replace this results into the Lagrange equation (B.5),

getting

$$\mathrm{Tr}[WB] - \lambda \mathrm{Tr}[C^{-1}BC^{-1}H^{-1}] = 0. \tag{B.11}$$

What we have to do now is find some relation between C, λ and the other operators, assuming that (B.11) holds for any operator B, and finally find the value of λ. So, we see that we can rewrite eq. (B.11) in the following form

$$\mathrm{Tr}[WB - \lambda C^{-1}H^{-1}C^{-1}B] = 0, \tag{B.12}$$

since this has to be satisfied for any matrix B, then we get the condition for the Lagrange multiplicators

$$W = \lambda C^{-1}H^{-1}C^{-1}, \tag{B.13}$$

amplifying by $H^{-1/2}$ from left and right we get

$$H^{-1/2}WH^{-1/2} = \lambda H^{-1/2}C^{-1}H^{-1}C^{-1}H^{-1/2} \tag{B.14}$$

$$= \lambda (H^{-1/2}C^{-1}H^{-1/2})^2, \tag{B.15}$$

from here is easy to find

$$C^{-1} = \frac{1}{\sqrt{\lambda}} H^{1/2}\sqrt{H^{-1/2}WH^{-1/2}}H^{1/2}. \tag{B.16}$$

And now we find λ from the condition $g(C) = 0$, getting

$$0 = \mathrm{Tr}[C^{-1}H^{-1}] - N(d-1) \tag{B.17}$$

$$= \frac{1}{\sqrt{\lambda}} \mathrm{Tr}\left[H^{1/2}\sqrt{H^{-1/2}WH^{-1/2}}H^{1/2}H^{-1}\right] - N(d-1) \tag{B.18}$$

$$= \frac{1}{\sqrt{\lambda}} \mathrm{Tr}\left[\sqrt{H^{-1/2}WH^{-1/2}}\right] - N(d-1), \tag{B.19}$$

from here we find

$$\lambda = \left(\frac{\mathrm{Tr}\left[\sqrt{H^{-1/2} W H^{-1/2}}\right]}{N(d-1)} \right)^2 . \tag{B.20}$$

Now we can calculate the bound by replacing this into the function f, getting

$$\mathrm{Tr}[WC] = \frac{\mathrm{Tr}\left[\sqrt{H^{-1/2} W H^{-1/2}}\right]}{N(d-1)} \mathrm{Tr}\left[W H^{-1/2} (H^{-1/2} W H^{-1/2})^{-1/2} H^{-1/2}\right] \tag{B.21}$$

$$= \frac{\mathrm{Tr}\left[\sqrt{H^{-1/2} W H^{-1/2}}\right]}{N(d-1)} \mathrm{Tr}\left[\sqrt{H^{-1/2} W H^{-1/2}}\right] \tag{B.22}$$

$$= \frac{\left(\mathrm{Tr}\left[\sqrt{H^{-1/2} W H^{-1/2}}\right]\right)^2}{N(d-1)}. \tag{B.23}$$

Since our work is estimating states through MSE optimization, we choose W as the identity, then the bound becomes

$$MSE(\hat{\theta}) = \frac{\mathrm{Tr}[\sqrt{H^{-1}}]^2}{N(d-1)}. \tag{B.24}$$

In order to compute the calculate the explicit bound for a pure state we need to compute the elements of the Helmstrom matrix H. Therefore lets consider a fixed point θ^0 in the parameter space. At this point we choose a basis such that

$$\rho_0 = \rho(\theta^0) = |1\rangle\langle 1| \tag{B.25}$$

$$\rho^N = \rho_0 \otimes \rho_0 \otimes \cdots \otimes \rho_0. \tag{B.26}$$

On the other hand, let's consider another point θ in the neighborhood of θ^0, such that a density matrix $\rho(\theta)$ at this point may be expressed as a first order approximation

of ρ_0, that is,

$$\rho = \rho(\theta) = \rho_0 + \sum_{k,\pm}(\theta_{k\pm} - \theta^0_{k\pm})\rho_{k\pm}. \tag{B.27}$$

where $\theta_{k\pm}$ are the parameters that we wish to estimate and $\rho_{k\pm}$ are $2(d-1)$ traceless hermitian matrices for $2 \leq k \leq d$ defined by

$$\rho_{k\pm} = i^{(1\mp 1)/2}(|1\rangle\langle k| \pm |k\rangle\langle 1|). \tag{B.28}$$

The reason for choosing this parametrization can be seen from the fact that a state $|\psi\rangle$ in the neighborhood of $|1\rangle$ can be written as

$$|\psi\rangle = |1\rangle + \sum_{k=1}^{d}\alpha_k|k\rangle + i\sum_{k=1}^{d}\beta_k|k\rangle, \tag{B.29}$$

then the density matrix of the state at first order in α and β is

$$\rho = |1\rangle\langle 1| + \sum \alpha_k(|1\rangle\langle k| + |k\rangle\langle 1|) + \sum \beta_k i(|1\rangle\langle k| - |k\rangle\langle 1|) \tag{B.30}$$

$$= \rho_0 + \sum_{k,\pm}\gamma_{k\pm}\rho_{k\pm} \tag{B.31}$$

from where we can identify $\gamma_{k\pm}$ with $(\theta_{k\pm} - \theta^0_{k\pm})$. Now it is easy to see that $\frac{\partial\rho}{\partial\theta_{k\pm}} = \rho_{k\pm}$, hence we have $L_{k\pm} = 2\rho_{k\pm}$. No we can calculate the quantum fisher information

$$H_{k\pm k'\pm'} = \mathrm{Tr}[\rho_{j\pm}L_{k\pm'}] \tag{B.32}$$

$$= 2(i)^{(1\mp 1)/2}(i)^{(1\mp' 1)/2}\mathrm{Tr}[(|1\rangle\langle k| \pm |k\rangle\langle 1|)(|1\rangle\langle k'| \pm' |k'\rangle\langle 1|)] \tag{B.33}$$

$$= 2(i)^{(1\mp)/2}(i)^{(1\mp' 1)/2}\mathrm{Tr}[\pm|k\rangle\langle k'| \pm' |1\rangle\langle 1|\delta_{kk'}] \tag{B.34}$$

$$= 2(i)^{(1\mp 1)/2}(i)^{(1\mp' 1)/2}(\pm\delta_{kk'} \pm' \delta_{kk'}) \tag{B.35}$$

$$= 4\delta_{kk'}\delta_{\pm\pm'}. \tag{B.36}$$

By replacing this into (B.24) we finally get

$$MSE(\hat{\theta}) = \frac{(2d-2)^2}{4N(d-1)} \tag{B.37}$$

$$= \frac{d-1}{N}. \tag{B.38}$$

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[1] A Julia programming language version of the pseudocode in Algorithm 1 can be found in the GitHub repository.

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