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MODEL SELECTION FOR QUANTUM HOMODYNE TOMOGRAPHY

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Abstract. This paper deals with a non-parametric problem coming from physics, namely quantum tomography. That consists in determining the quantum state of a mode of light through a homodyne measurement. We apply several model selection procedures: penalized projection estimators, where we may use pattern functions or wavelets, and penalized maximum likelihood estimators. In all these cases, we get oracle inequalities. In the former we also have a polynomial rate of convergence for the non-parametric problem. We finish the paper with applications of similar ideas to the calibration of a photocounter, a measurement apparatus counting the number of photons in a beam. Here the mathematical problem reduces similarly to a non-parametric missing data problem. We again get oracle inequalities, and better speed if the photocounter is good.

Résumé. Nous nous intéressons à un problème de statistique non-paramétrique issu de la physique, et plus précisément à la tomographie quantique, c'est-à-dire la détermination de l'état quantique d'un mode de la lumière *via* une mesure homodyne. Nous appliquons plusieurs procédures de sélection de modèles : des estimateurs par projection pénalisés, où on peut utiliser soit des fonctions motif, soit des ondelettes, et l'estimateur du maximum de vraisemblance pénalisé. Dans chaque cas, nous obtenons une inégalité oracle. Nous prouvons également une vitesse de convergence polynomiale pour ce problème non-paramétrique, pour les estimateurs par projection. Nous appliquons ensuite des idées à la calibration d'un photocompteur, l'appareil dénombrant le nombre de photons dans un rayon lumineux. Le problème mathématique se réduit dans ce cas à un problème non-paramétrique à données manquantes. Nous obtenons à nouveau des inégalités oracle, qui nous assurent des vitesses de convergence d'autant meilleures que le photocompteur est bon.

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1. Introduction

Quantum mechanics introduce intrinsic randomness in physics: the result of a measurement, or any macroscopic interaction, on a physical system is not deterministic. Therefore, a host of statistical problems can stem from it. Some are (almost) specifically quantum, notably any question about which measurement yields the maximum information, or whether simultaneously measuring n samples is more efficient than measuring them sequentially [12]. However, once we have chosen the measurement we carry out on our physical system, we are left with an entirely classical statistical problem. This paper aims at applying model selection methods

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à la Birgé-Massart to one such instance, which is of interest both practical, as physicists use this measurement quite often (the underlying physical system is elementary; it is the particle with one degree of freedom), and mathematical, as it yields a non-parametric inverse problem with uncommon features.

Moreover, as this classical problem stemming from quantum mechanics could be seen as an easy introduction to the subject to classical statisticians, we have added more general notions on quantum statistics at the beginning of the appendix. The interested reader can get further acquaintance with these concepts through the textbooks [13] and [15] or the review article [3].

More precisely, the problem we are interested in is quantum homodyne tomography. As an aside, we apply the results we get to the calibration of a photocounter, using a quantum tomographer as a tool. The word "Homodyne" refers to the experimental technique used for this measurement, first implemented in [20], where the state of one mode of electromagnetic radiation, that is a pulse of laser light at a given frequency, is probed using a reference laser beam at the same ("homo") frequency. Respectively, "Tomography" is used because one of the physicists' favourite representations of the state, the Wigner function, can be recovered from the data by inverting a Radon transform.

Mathematically, our data are samples from a probability distribution p_ρ on $\mathbb{R}\times[0,\pi]$. From this data, we want to recover the "density operator" ρ of the system. This is the most common representation of the state, that is a mathematical object which encodes all the information about the system. Perfect knowledge of the state means knowing how the system will evolve and the probability distribution of the result of any measurement we might carry out on the system. These laws of evolution and measurement can be expressed naturally enough within the density operator framework (see Appendix). The density operator is a non-negative trace-one self-adjoint operator ρ on $L^2(\mathbb{R})$ (in our particular case). We know the linear transform $\mathcal{T}$ which takes ρ to p_ρ and can make it explicit in particular bases such as the Fock basis. We may also settle for the Wigner function W, another representation of the state. That is a two-dimensional real function with integral one, and p_ρ is the Radon transform of W.

The first reconstruction methods used the Wigner function as an intermediate representation: after collecting the data in histograms and smoothing, one inverted the Radon transform to get an estimate of W. This smoothing, however, introduces hard-to-control bias. Pattern functions (bidual bases) for the entries of the density operator ρ were introduced in [7], yielding an unbiased estimator of those individual entries. They were later extended to allow for low noise in the measurement. Maximum likelihood procedures are used since [2]. For both these estimators, we need an arbitrary cut-off of the density operator, so that the model is finite-dimensional. Consistency of these two estimators used with a sieve was established in [1]. Then, a sharp adaptive kernel estimator for the Wigner function was devised in [5], and this even if there is noise in the measurement (see Sect. 3.6).

In this paper, we devise penalized estimators that fulfill oracle-type inequalities among the L^2 projections on submodels, analyze the penalized maximum likelihood estimator and apply these estimators to the calibration of a photocounter. Hence, we provide automatic cut-offs for the estimators formerly mentioned. We can also cast in the L^2 projection framework wavelets estimators used for inverting the Radon transform on classical probability densities, to whom the Wigner function does not belong. We also have finer granularity for pattern functions, since we threshold them one by one, instead of keeping a whole submatrix. We get an explicit polynomial rate of convergence for this estimator. Notice that all our results are derived for finite samples (all the previous works considered only the asymptotic regime). We have mainly worked under the idealized hypothesis where there is no noise, however.

The appendix is not logically necessary for the article. We have inserted it for background and as an invitation to this field. It first features a general introduction to quantum statistics with a public of classical statisticians in mind. We then describe what quantum homodyne tomography precisely is. This latter subsection is largely based on [5].

Section 2 formalizes the statistical problem at hand, with no need of the appendix, except the equations explicitly referred to therein.

Section 3 aims at devising a model selection procedure to choose between L^2 projection estimators. We first give general theorems (Th. 3.2 and Th. 3.4) leading to oracle-type inequalities for hard-thresholding estimators. We then apply them to two bases. One is the Fock basis and the corresponding pattern functions physicists have used for a while. For it we also prove a polynomial convergence rate for any state with finite energy. The other is a wavelet basis for the Wigner function. We finish with a short subsection describing what changes are entailed by the presence of noise. Especially, we do not need to adapt our theorems if the noise is low enough, as long as we change the dual basis.

Section 4 similarly applies a classical theorem (Th. 4.2) to solve the question of which (size of) model is best to use a maximum likelihood estimator on.

Section 5 switches to the determination of a kind of measurement apparatus (and not any more on the state that is sent in) using a known state and this same tomographer that was studied in the previous sections. The law of our samples are then very similar and we apply the same type of techniques (penalized projection and maximum likelihood estimators). The fact that the POVM (mathematical modelling of a measurement) is a projective measurement (see Appendix) enables us to work with L^1 operator norm, however.

2. The mathematical problem

We now describe the mathematical problem at hand.

We are given n independent identically distributed random variables $Y_i = (X_i, \Phi_i)$ with density p_ρ on $[0, \pi) \times \mathbb{R}$.

This data is the result of a measurement on a physical system. Now the "state" of a system is described by a mathematical object, and there are two favourites for physical reasons: one is the *density operator* ρ, the other is the *Wigner function* W_ρ. We describe them below.

Therefore we are not actually interested in p_ρ, but rather in W_ρ or (maybe preferably) ρ. The probability distribution p_ρ of our samples can be retrieved if we know either ρ or W_ρ.

In other words we aim at estimating as precisely as possible ρ or W_ρ from the data $\{Y_i\}$. By "as precisely as possible", we mean that with a suitable notion of distance, we shall minimize $\mathbb{E}\left[d(\rho, \hat{\rho})\right]$. Our choice of distance will be partly dictated by mathematical tractability.

We now briefly explain what W_ρ and ρ stand for.

The Wigner function $W_\rho : \mathbb{R}^2 \to \mathbb{R}$ is the inverse Radon transform of p_ρ. In fact we would rather say that p_ρ is the Radon transform of W_ρ. Explicitly:

$$p_\rho(x, \phi) = \int_{-\infty}^{\infty} W(x\cos\phi + y\sin\phi, x\sin\phi - y\cos\phi)\mathrm{d}y.$$

Figure 1 might be of some help. An important remark is that the Wigner function is not a probability density, but only a quasi-probability density: a function with integral 1, but that may be negative at places. However its Radon transform is a true probability density, since it is p_ρ.

Retrieving W_ρ from P_ρ then amounts to inverting the Radon transform, hence the name of tomography: that is the same mathematical problem as with the brain imagery technique called Positron Emission Tomography.

As for ρ, this is a density operator on the Hilbert space $L^2(\mathbb{R})$, that is a *self-adjoint positive* operator with *trace* 1. We denote the set of such operators by $\mathcal{S}(L^2(\mathbb{R}))$. There is a linear transform $\mathbf{T}$ that takes ρ to p_ρ. We give it explicitly using a basis of $L^2(\mathbb{R})$ known as the *Fock basis*. This orthonormal basis, which has many nice physical properties, is defined by:

$$\psi_k(x) \quad = \quad H_k(x)\mathrm{e}^{-x^2/2} \tag{2.1}$$

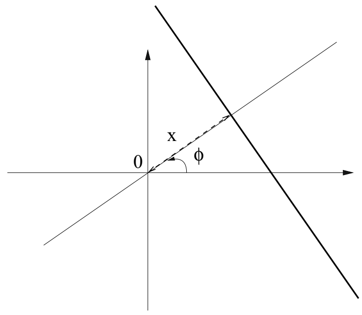

FIGURE 1. The value of p_ρ at (x,ϕ) is the integral of the Wigner function over the bold line.

where H_k is the kth Hermite polynomial normalized such that $\|\psi_k\|_2 = 1$. The matrix entries of ρ in this basis are $\rho_{j,k} = \langle \psi_j, \rho\psi_k\rangle$. Then $\mathbf{T}$ can be written:

$$\begin{array}{rcl} \mathbf{T}:\mathcal{S}(L^2(\mathbb{R})) & \longrightarrow & L^1(\mathbb{R}\times[0,\pi]) \\ \rho & \mapsto & \left(p_\rho : (x,\phi) \mapsto \displaystyle\sum_{j,k=0}^{\infty} \rho_{j,k}\psi_j(x)\psi_k(x)e^{-i(j-k)\phi}\right). \end{array}$$

Notice that as we have defined precisely the set of possible ρ, this mapping yields the set of possible p_ρ and W_ρ.

The relations between ρ, W_ρ and p_ρ are further detailed in Section A.2.

Anyhow we may now state our problem as consisting in inverting either the Radon transform or $\mathbf{T}$ from empirical data.

This is a classical problem of non-parametric statistics, that we want to treat non-asymptotically. We then take estimators based on a *model*, that is a subset of the operators on $L^2(\mathbb{R})$, or equivalently of the two-dimensional real functions. These models are usually vector spaces, which may not be the domain of the object to be estimated. To choose a candidate within a given model, there are different methods, two of which we study, projection estimators and maximum likelihood estimators. Once we have a candidate within each model, we then use model selection methods to choose (almost) the best.

We first study projection estimators, for which the most convenient distance comes from the L^2 norm

$$\|\tau\|_2 = \sqrt{\sum|\lambda_i(\tau)|^2} = \sqrt{\sum_{j,k}|\tau_{j,k}|^2},$$

where the λ_i are the eigenvalues of τ, and the second equality holds for τ written in any orthonormal basis. Notice that there is an isometry (up to a constant) between the space of density operators with L^2 operator norm and the space of Wigner functions with L^2 Lebesgue norm, that is:

$$\|W_\rho - W_\tau\|_2^2 = \iint |W_\rho(q,p) - W_\tau(q,p)|^2 \,\mathrm{d}p\,\mathrm{d}q = \frac{1}{2\pi}\|\rho-\tau\|_2^2.$$

For maximum likelihood estimators, we have to make do with the weaker Hellinger distance (see later (4.2)) on $L^1\big(\mathbb{R}\times[0,\pi]\big)$, to which p_ρ belongs.

3. Projection estimators

In this section, which owes much to [19], we apply penalization procedures to projection estimators. The first subsection explains that we want to obtain oracle-type inequalities. In the second we obtain a general inequality where the left-hand side corresponds to an oracle inequality, and where the remainder term in the right-hand side depends on the penalty and on the large deviations of empirical coefficients. The two following subsections give two ways to choose the penalty term large enough for this remainder term to be small enough. In Section 3.3 this penalty is deterministic. We design it and prove that it is a "good choice" by keeping Hoeffding's inequality in mind. In Section 3.4, the penalty is random, and designed by taking Bernstein's inequality into account.

We next express these theorems in terms of two specific bases. For the Fock basis, we obtain polynomial worst-case convergence rates, using the structure of states. For a wavelet basis, we notice we obtain a usual estimator in classical tomography. We finish by saying what can be done if there is noise, that is (mainly) convolution of the law of the sample by a Gaussian. We multiply the Fourier transform of the dual basis with the inverse of the Fourier transform of the Gaussian, and as long as we still have well-defined functions, and we can re-use our theorems without changes.

3.1. **Aim of model selection**

Let's assume we are given a (countable) L^2 basis $(e_i)_{i\in\mathcal{I}}$ of a space in which $\mathcal{S}(L^2(\mathbb{R}))$ is included (typically $\mathcal{T}(L^2(\mathbb{R}))$, the trace-class operators on $L^2(\mathbb{R})$). We may then try and find the coefficients of ρ in this basis. The natural way to do so is to find a dual basis $(f_i)_{i\in\mathcal{I}}$ such that $\langle \mathbf{T}(e_i), f_j\rangle = \delta_{i,j}$ for all i and j. Then, if $\rho = \sum_i \rho_i e_i$ we get $\langle p_\rho, f_i\rangle = \rho_i$ for all i. And if the f_i are well enough behaved, then $\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k) = \hat{\rho}_i$ tends to ρ_i by the law of large numbers.

Now if we took $\sum_i \hat{\rho}_i e_i$ as an estimator of ρ, we would have an infinite risk as the variance would be infinite. We must therefore restrict ourselves to models $m \in \mathcal{M}$, that is $\operatorname{Vect}(e_i, i\in m)$, where m is a finite set, and $\mathcal{M}$ is a set of models (we might take $\mathcal{M}$ smaller than the set of all finite sets of $\mathbb{N}$).

We may then write the loss as

$$\|\hat{\rho}_m - \rho\|^2 = \sum_{i\notin m} |\rho_i|^2 + \sum_{i\in m} |\rho_i - \hat{\rho}_i|^2$$

where the first term is a bias (modelling error) and the second term is an estimation error. The risk would have this expression:

$$\mathbb{E}\left[\|\hat{\rho}_m - \rho\|^2\right] = \sum_{i\notin m} |\rho_i|^2 + \sum_{i\in m} \mathbb{E}\left[|\rho_i - \hat{\rho}_i|^2\right]$$

where the expectation is taken with respect to p_ρ, since $\hat{\rho}_i$ depends on the (X_k,Φ_k).

If we use an arbitrary model m, we probably do not strike a good balance between the bias term and the variance term. The whole point of penalization is to have a data-driven procedure to choose the "best" model. We are aiming at choosing a model with (almost) the lowest error. We would dream of obtaining:

$$\hat{m} = \arg \inf_{m\in\mathcal{M}} \|\hat{\rho}_m - \rho\|^2 .$$

That is of course too ambitious. Instead, we shall obtain the following kind of bound, called an oracle inequality:

$$\mathbb{E}\left[\left\{\|\hat{\rho}_{\hat{m}} - \rho\|^2 - \left(C \inf_{m\in\mathcal{M}} \left(d^2(\rho,m) + \operatorname{pen}(m)\right)\right)\right\} \vee 0\right] \leq \epsilon_n \tag{3.1}$$

where $d^2(\rho,m)$ is the bias of the model m, C is some constant, independent of ρ, $\operatorname{pen}(m)$ is a *penalty* associated to the model m (the bigger the model, the bigger the penalty) and ϵ_n depends only on n the number of observations, and goes to 0 when n is going to infinity. We shall try to take the penalty of the order of the variance of the model.

Notice that we have given in (3.1) an unusual form of oracle inequality. These inequalities are more often written as

$$\mathbb{E}\left[\|\hat{\rho}_{\hat{m}} - \rho\|^2\right] \quad \leq \quad \left(C \inf_{m \in \mathcal{M}} \left(d^2(\rho, m) + \mathbb{E}\left[\text{pen}(m)\right]\right)\right) + \epsilon_n.$$

Our form implies the latter.

The strategy is the following:

- First, rewrite the projection estimators as *minimum contrast estimators*, that is minimizers of a function (called the *empirical contrast* function, and written γ_n), which is the same for all models. We also demand that, for any m, this empirical contrast function converges to a *contrast* function γ, the minimizer in m of which is the projection of ρ on m.
- Second, find a penalty function that overestimates with high enough probability $(\gamma - \gamma_n)(\hat{\rho}_m)$ for all m simultaneously. Use of concentration inequalities is pivotal at this point.

Next section makes all this more explicit.

3.2. Risk bounds and choice of the penalty function

First we notice that the minimum of

$$\begin{aligned}\gamma(\tau) &= \|\tau\|^2 - 2\langle \tau, \rho \rangle \\ &= \|\rho - \tau\|^2 - \|\rho\|^2\end{aligned}$$

over a model m is attained at the projection of ρ on m. Moreover

$$\gamma_n(\tau) = \|\tau\|^2 - 2 \sum_i \frac{1}{n} \sum_{k=1}^{n} \tau_i f_i(X_k, \Phi_k)$$

converges in probability to γ for any m (and all τ such that $\|\tau\| = 1$ simultaneously), as there is only a finite set of i such that $\tau_i \neq 0$ for $\tau \in m$.

Now the minimum of γ_n over m is attained by

$$\tau = \sum_{i \in m} \frac{1}{n} \sum_{k=1}^{n} f_i(X_k, \Phi_k) e_i.$$

So we have succeeded in writing projection estimators as minimum contrast estimators. We then define our final estimator by:

$$\hat{\rho}^{(n)} = \hat{\rho}_{\hat{m}}$$

with

$$\hat{m} = \arg\min_{m \in \mathcal{M}} \gamma_n(\hat{\rho}_m) + \text{pen}_n(m)$$

where pen_n is a suitably chosen function depending on n, m and possibly the data.

We then get, for any m, for any $\tau_m \in m$,

$$\gamma_n(\hat{\rho}^{(n)}) + \text{pen}_n(\hat{m}) \leq \gamma_n(\hat{\rho}_m) + \text{pen}_n(m) \leq \gamma_n(\tau_m) + \text{pen}_n(m). \tag{3.2}$$

What's more, for any m, for any $\tau_m \in m$,

$$\gamma_n(\tau_m) \quad = \quad \|\rho - \tau_m\|^2 - \|\rho\|^2 - 2\nu_n(\tau_m) \tag{3.3}$$

with

$$\begin{aligned}\nu_n(\tau) &= \langle \tau, \rho\rangle - \sum_i \sum_{k=1}^n \tau_i f_i(X_k, \Phi_k) \\ &= \sum_{i\in m} \tau_i(\rho_i - \hat{\rho}_i) + \sum_{i\notin m} \tau_i \rho_i.\end{aligned}$$

Putting together (3.2) and (3.3), we get, for all m and $\tau_m \in m$:

$$\left\|\hat{\rho}^{(n)} - \rho\right\|^2 \leq \|\tau_m - \rho\|^2 + 2\nu_n(\hat{\rho}^{(n)} - \tau_m) + \mathrm{pen}_n(m) - \mathrm{pen}_n(\hat{m}).$$

We then want to take penalties big enough to dominate the fluctuations ν_n. Some manipulations will make this expression more tractable. First we bound $\nu_n(\hat{\rho}^{(n)} - \tau_m)$ by $\left\|\hat{\rho}^{(n)} - \tau_m\right\| \chi_n(m \cup \hat{m})$, with

$$\chi_n(m) = \sup_{\substack{\tau\in m \\ \|\tau\|=1}} \nu_n(\tau).$$

Now the triangle inequality gives $\left\|\hat{\rho}^{(n)} - \tau_m\right\| \leq \left\|\hat{\rho}^{(n)} - \rho\right\| + \|\rho - \tau_m\|$, so that:

$$\left\|\hat{\rho}^{(n)} - \rho\right\|^2 \leq \|\rho - \tau_m\|^2 + 2\chi_n(m\cup\hat{m}) \left\|\rho - \hat{\rho}^{(n)}\right\| + 2\chi_n(m\cup\hat{m}) \|\rho - \tau_m\| - \mathrm{pen}_n(\hat{m}) + \mathrm{pen}_n(m).$$

For all $\alpha > 0$, the following holds:

$$2ab \leq \alpha a^2 + \alpha^{-1} b^2. \tag{3.4}$$

Using this twice, we get, for all $\epsilon > 0$:

$$\frac{\epsilon}{2+\epsilon}\left\|\rho - \hat{\rho}^{(n)}\right\|^2 \leq \left(1 + \frac{2}{\epsilon}\right)\|\rho - \tau_m\|^2 + (1+\epsilon)\chi_n^2(m\cup\hat{m}) - \mathrm{pen}_n(\hat{m}) + \mathrm{pen}_n(m).$$

Noticing that $\chi_n(m\cup\hat{m}) \leq \chi_n(m) + \chi_n(\hat{m})$ and putting our estimate of the error in the left-hand side:

$$\frac{\epsilon}{2+\epsilon}\left\|\rho - \hat{\rho}^{(n)}\right\|^2 - \left\{\left(1+\frac{2}{\epsilon}\right)\|\rho - \tau_m\|^2 + 2\,\mathrm{pen}(m)\right\} \leq (1+\epsilon)(\chi_n^2(\hat{m}) + \chi_n^2(m)) - \mathrm{pen}_n(\hat{m}) - \mathrm{pen}_n(m).$$

Now what we want to avoid is that our penalty is less than the fluctuations, so we separate this event and take its expectation:

$$\begin{aligned}\mathbb{E}\left[\left\{\frac{\epsilon}{2+\epsilon}\left\|\rho - \hat{\rho}^{(n)}\right\|^2 - \left(\left(1+\frac{2}{\epsilon}\right)\|\rho - \tau_m\|^2 + 2\,\mathrm{pen}_n(m)\right)\right\} \vee 0\right] \leq \\ \mathbb{E}\left[\left\{(1+\epsilon)(\chi_n^2(\hat{m}) + \chi_n^2(m)) - \mathrm{pen}(\hat{m}) - \mathrm{pen}(m)\right\} \vee 0\right] \\ \leq 2\mathbb{E}\left[\sup_m \left\{(1+\epsilon)\chi_n^2(m) - \mathrm{pen}(m)\right\} \vee 0\right].\end{aligned} \tag{3.5}$$

Thus stated, our problem is to take a penalty large enough to make the right-hand side negligible, that is vanishing like $1/n$.

We shall use this form of $\chi_n(m)$:

$$\chi_n(m) \;=\; \sup_{\substack{(\tau_i)_{i\in m}\\ \sum \tau_i^2=1}} \sum_{i\in m} \tau_i(\rho_i - \hat{\rho}_i) \;=\; \sqrt{\sum_{i\in m} |\rho_i - \hat{\rho}_i|^2}$$

so that

$$\chi_n(m)^2 \;=\; \sum_{i\in m} |\rho_i - \hat{\rho}_i|^2 \;=\; \sum_{i\in m} \left| \rho_i - \frac{1}{n}\sum_{k=1}^{n} f_i(X_k, \Phi_k) \right|^2. \tag{3.6}$$

3.3. **Deterministic penalty**

First we may try to craft a deterministic penalty.

We plan to use Hoeffding's inequality, recalling that $\hat{\rho}_i$ is a sum of independent variables:

Lemma 3.1. Hoeffding's inequality [14]. *Let $X_1, \ldots, X_n$ be independent random variables, such that X_i takes his values in $[a_i, b_i]$ almost surely for all $i \le n$. Then for any positive x,*

$$\mathbb{P}\left[\sum_{i=1}^{n} \Big(X_i - \mathbb{E}\left[X_i\right] \Big) \ge x \right] \le \exp\left(- \frac{2x^2}{\sum_{i=1}^{n} (b_i - a_i)^2} \right)\cdot$$

We may also apply this inequality to $-X_i$ so as to get a very probable lower bound on the sum of X_i.

This is enough to prove:

Theorem 3.2. *Let ρ be a density operator. Assume that each f_i is bounded, where $(f_i)_{i\in\mathcal{I}}$ is the dual basis of $(e_i)_{i\in\mathcal{I}}$, as defined at the beginning of this section. Let $M_i = \sup_{(x,\phi)\in\mathbb{R}\times[0,\pi]} f_i(x,\phi) - \inf_{(x,\phi)\in\mathbb{R}\times[0,\pi]} f_i(x,\phi)$. Let $(x_i)_{i\in\mathcal{I}}$ be a family of positive real numbers such that $\sum_{i\in\mathcal{I}} \exp(-x_i) = \Sigma < \infty$. Let*

$$\mathrm{pen}_n(m) \;=\; \sum_{i\in\mathcal{I}_m} (1+\epsilon) \left(\ln(M_i) + \frac{x_i}{2} \right) \frac{M_i^2}{n}\cdot \tag{3.7}$$

Then the penalized projection estimator satisfies:

$$\mathbb{E}\left[\frac{\epsilon}{2+\epsilon} \left\| \hat{\rho}^{(n)} - \rho \right\|^2 \right] \;\le\; \inf_{m\in\mathcal{M}} \left(1 + \frac{2}{\epsilon} \right) d^2(\rho, m) + 2\,\mathrm{pen}_n(m) + \frac{(1+\epsilon)\Sigma}{n}\cdot \tag{3.8}$$

Remark. Here the penalty depends only on the subspace spanned by the model m. So it is the same whether $\mathcal{M}$ is small or large. The best we can do is then to take $\mathcal{M} = \mathcal{P}(\mathcal{I})$, that is to choose for every vector e_i whether to keep the estimated coordinate $\hat{\rho}_i$ or to put it to zero. In other words we get a hard-thresholding estimator:

$$\hat{\rho}^{(n)} = \sum_{i\in\mathcal{I}} \hat{\rho}_i \mathbf{1}_{|\hat{\rho}_\mathbf{i}| > \alpha_\mathbf{i}} \mathbf{e_i}$$

with

$$\alpha_i = \sqrt{(1+\epsilon)\left(\ln(M_i) + \frac{x_i}{2} \right)} \frac{M_i}{\sqrt{n}}\cdot \tag{3.9}$$

Proof. Considering (3.5), we have only to bound appropriately $\mathbb{E}\left[\sup_m \big((1+\epsilon)\chi_n^2(m) - \mathrm{pen}(m) \big) \vee 0 \right]$.

Now, by (3.6) and (3.7), both $\chi_n^2(m)$ and pen_m are a sum of terms over m. As the positive part of a sum is smaller than the sum of the positive parts, we obtain:

$$\mathbb{E}\left[\sup_m \left\{(1+\epsilon)\chi_n^2(m) - \mathrm{pen}(m)\right\} \vee 0\right] \leq$$
$$\mathbb{E}\left[\sup_m \left\{\sum_{i\in m} \left((1+\epsilon)\left(\hat{\rho}_i - \rho_i\right)^2 - \alpha_i^2\right\} \vee 0\right)\right]$$
$$= \sum_{i\in\mathcal{I}} \mathbb{E}\left[\left\{(1+\epsilon)\left(\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k) - \rho_i\right)^2 - (1+\epsilon)\left(\ln(M_i) + \frac{x_i}{2}\right)\frac{M_i^2}{n}\right\} \vee 0\right].$$

Each of the expectations is evaluated using the following formula, valid for any positive function f:

$$\mathbb{E}\left[f\right] = \int_0^\infty \mathbb{P}\left[f(x) \geq y\right] \mathrm{d}y. \tag{3.10}$$

Remembering (3.9) we notice that the inequality

$$\left\{(1+\epsilon)\left(\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k) - \rho_i\right)^2 - (1+\epsilon)\left(\ln(M_i) + \frac{x_i}{2}\right)\frac{M_i^2}{n}\right\} \vee 0 \quad \geq \quad y$$

is equivalent to

$$\left|\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k) - \rho_i\right| \geq \sqrt{\frac{\alpha_i^2 + y}{1+\epsilon}}.$$

We may then conclude, using Hoeffding's inequality on the second line and the value (3.9) of α_i on the fourth line:

$$\begin{aligned}
\mathbb{E}\left[\sup_m \left\{(1+\epsilon)\chi_n^2(m) - \mathrm{pen}(m)\right\} \vee 0\right] &\leq \sum_{i\in\mathcal{I}} \int_0^\infty \mathbb{P}\left[\left|\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k) - \rho_i\right| \geq \sqrt{\frac{\alpha_i^2 + y}{1+\epsilon}}\right] \mathrm{d}y \\
&= \sum_{i\in\mathcal{I}} \int_0^\infty 2\exp\left(-\frac{2n(\alpha_i^2 + y)}{(1+\epsilon)M_i^2}\right) \mathrm{d}y \\
&= \sum_{i\in\mathcal{I}} 2\exp\left(-\frac{2n\alpha_i^2}{(1+\epsilon)M_i^2}\right) \frac{(1+\epsilon)M_i^2}{2n} \\
&= \frac{1+\epsilon}{n} \sum_{i\in\mathcal{I}} \exp(-x_i) \\
&= \frac{(1+\epsilon)\Sigma}{n}.
\end{aligned}$$

□

3.4. **Random penalty**

The most obvious way to improve on Theorem 3.2 is to use sharper inequalities than Hoeffding's. Indeed the range of f_i might be much larger than its standard deviation, so that we gain much by using Bernstein's inequality:

Lemma 3.3. Bernstein's inequality [4]. *Let $X_1, \dots, X_n$ be independent, bounded, random variables. Then with*

$$M = \sup_i \|X_i\|_\infty, \qquad v = \sum_{i=1}^n \mathbb{E}\left[X_i^2\right],$$

for any positive x

$$\mathbb{P}\left[\sum_{i=1}^n (X_i - \mathbb{E}[X_i]) \geq \sqrt{2vx} + \frac{M}{3}x\right] \quad \leq \quad \exp(-x).$$

With this tool, we may devise a hard-thresholding estimator where the thresholds are data-dependent:

Theorem 3.4. *Let $(y_i)_{i\in\mathcal{I}}$ be positive numbers such that $\sum_{i\in\mathcal{I}} \mathrm{e}^{-y_i} = \Sigma < \infty$. Let then*

$$x_i \quad = \quad 2\ln(\|f_i\|_\infty) + y_i.$$

Let the penalty be a sum of penalties over the vectors we admit in the model. That is, for any $\delta \in (0,1)$, for any $i \in \mathcal{I}$, define

$$\mathrm{pen}_n^i \quad = \quad \frac{1+\epsilon}{n}\left(\sqrt{\frac{2}{1-\delta}x_i\left(\mathbb{P}_n\left[f_i^2\right] + \frac{1}{n}\|f_i\|_\infty^2\,(\frac{1}{3}+\frac{1}{\delta})x_i\right)} + \frac{\|f_i\|_\infty}{3\sqrt{n}}x_i\right)^2 \tag{3.11}$$

and the penalty of the model m:

$$\mathrm{pen}_n(m) \quad = \quad \sum_{i\in m} \mathrm{pen}_n^i\,.$$

Then there is a constant C such that:

$$\mathbb{E}\left[\left(\frac{\epsilon}{2+\epsilon}\left\|\hat{\rho}^{(n)} - \rho\right\|^2 - \left(\inf_{m\in\mathcal{M}_n}\left(1+\frac{2}{\epsilon}\right)d^2(\rho,m) + 2\,\mathrm{pen}_n(m)\right)\right)\vee 0\right] \quad \leq \quad \frac{C\Sigma}{n}$$

where $\mathcal{M}_n$ is the set of models m for which $i \in m \to x_i \leq n$.

Remark. As with the deterministic penalty, we end up with a hard-thresholding estimator. Morally, that is, forgetting all the small δ whose origin is technical, the threshold is

$$\sqrt{\frac{2\mathbb{P}_n\left[f_i^2\right]\ln\|f_i\|_\infty^2}{n}}.$$

Proof. Once again we have to dominate the right-hand side of (3.5). We first subtract and add, inside that expression, what could be seen as a target for the penalty. Writing

$$M_i = \|f_i\|_\infty, \qquad v_i = n\mathbb{E}\left[f_i^2\right], \qquad \alpha_i = \sqrt{2v_ix_i} + \frac{M_i}{3}x_i \tag{3.12}$$

we have

$$\mathbb{E}\left[\sup_m \left((1+\epsilon)\chi_n^2(m) - \mathrm{pen}(m)\right)\vee 0\right] \leq \\ \mathbb{E}\left[\sup_m (1+\epsilon)\left(\chi_n^2(m) - \sum_{i\in m}\frac{1}{n^2}\alpha_i^2\right)\vee 0\right] + \mathbb{E}\left[\left(\sum_{i\in m}\frac{1+\epsilon}{n^2}\alpha_i^2 - \mathrm{pen}(m)\right)\vee 0\right]. \tag{3.13}$$

Using (3.6), we bound the first term as a sum of expectations.

$$\mathbb{E}\left[\sup_m(1+\epsilon)\left(\chi_n^2(m)-\sum_{i\in m}\frac{1}{n^2}\alpha_i^2\right)\vee 0\right] \le (1+\epsilon)\sum_{i\in m}\mathbb{E}\left[\left(\left|\rho_i-\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k)\right|^2-\frac{1}{n^2}\alpha_i^2\right)\vee 0\right].$$

We now bound each of these expectations using (3.10).

$$\mathbb{E}\left[\left(\left|\rho_i-\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k)\right|^2-\frac{1}{n^2}\alpha_i^2\right)\vee 0\right] = \int_0^\infty \mathbb{P}\left[\left|\rho_i-\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k)\right|\ge\sqrt{y+\frac{\alpha_i^2}{n^2}}\right]\mathrm{d}y. \quad (3.14)$$

We change variables in the integral, choosing ξ defined by:

$$\sqrt{y+\frac{\alpha_i^2}{n^2}} = \frac{\sqrt{2v_i\xi}+\frac{M_i}{3}\xi}{n^2}. \quad (3.15)$$

Using Bernstein's inequality, the integrand in (3.14) is upper bounded by $2\exp(-\xi)$. Given the value of α_i (3.12), the range of the integral is now from x_i to ∞. Finally, taking the square on both sides of (3.15), then using (3.4), we get:

$$\begin{aligned}\mathrm{d}y &= 2\frac{\sqrt{2v_i\xi}+\frac{M_i}{3}\xi}{n^2}\left(\frac{M_i}{3}+\frac{\sqrt{2v_i}}{2\sqrt{\xi}}\right)\mathrm{d}\xi\\ &= \frac{2}{n^2}\left(v_i+\frac{M_i^2}{9}\xi+\frac{M_i}{2}\sqrt{2v_i}\sqrt{x}\right)\mathrm{d}\xi\\ &\le \frac{2}{n^2}\left(2v_i+\frac{11M_i^2}{18}\xi\right)\mathrm{d}\xi.\end{aligned}$$

Hence

$$\begin{aligned}\mathbb{E}\left[\left(\left|\rho_i-\frac{1}{n}\sum_{k=1}^n f_i(X_k,\Phi_k)\right|^2-\frac{1}{n^2}\alpha_i^2\right)\vee 0\right] &\le \frac{4}{n^2}\int_{x_i}^\infty\exp(-\xi)\left(2v_i+\frac{11M_i^2}{18}\xi\right)\mathrm{d}\xi\\ &= \frac{4}{n^2}\left(2v_i+\frac{11M_i^2}{18}(1+x_i)\right)\exp(-x_i). \quad (3.16)\end{aligned}$$

Let us now look over the second term of (3.13). We notice, through (3.11) and (3.12), that this term is of the form:

$$\frac{1+\epsilon}{n^2}\sum_{i\in m}\mathbb{E}\left[\left(\left(a_i+\frac{M_ix_i}{3}\right)^2-\left(b_i+\frac{M_ix_i}{3}\right)^2\right)\vee 0\right]\le\frac{1+\epsilon}{n^2}\sum_{i\in m}\mathbb{E}\left[2\left(a_i^2-b_i^2\right)\vee 0\right],$$

with

$$a_i^2-b_i^2=2v_ix_i-\frac{2}{1-\delta}\left(n\mathbb{P}_n\left[f_i^2\right]x_i+M_i^2\left(\frac{1}{3}+\frac{1}{\delta}\right)x_i^2\right).$$

Using again (3.10), we end up with:

$$\mathbb{E}\left[\left(\sum_{i\in m}\frac{1+\epsilon}{n^2}\alpha_i^2-\mathrm{pen}(m)\right)\vee 0\right]\le$$

$$\frac{1+\epsilon}{n^2}\sum_{i\in m}\frac{2}{1-\delta}x_i\int_0^\infty\mathbb{P}\left[(1-\delta)v_i-\left(n\mathbb{P}_n\left[f_i^2\right]+M_i^2\left(\frac{1}{3}+\frac{1}{\delta}\right)x_i\right)\ge y\right]\mathrm{d}y. \quad (3.17)$$

We can again make use of Bernstein's inequality:

$$\mathbb{P}\left[v_i - \sum_{k=1}^{n} f_i^2(X_k,\Phi_k) \geq \sqrt{2n\mathbb{E}\left[f_i^4\right]\xi} + \frac{\left\|f_i^2\right\|_\infty \xi}{3}\right] \leq \exp(-\xi).$$

Noticing that f_i^2 is non-negative everywhere, so that $\mathbb{E}\left[f_i^4\right] \leq \mathbb{E}\left[f_i^2\right]\left\|f_i^2\right\|_\infty$, and using (3.4), we get:

$$\mathbb{P}\left[(1-\delta)v_i \geq n\mathbb{P}_n\left[f_i^2\right] + M_i^2\left(\frac{1}{3}+\frac{1}{\delta}\right)\xi\right] \leq \exp(-\xi).$$

Recalling (3.17), we get

$$\begin{aligned}
\int_0^\infty \mathbb{P}\left[(1-\delta)v_i - \left(n\mathbb{P}_n\left[f_i^2\right] + M_i^2\left(\frac{1}{3}+\frac{1}{\delta}\right)x_i\right) \geq y\right]\mathrm{d}y &= \int_0^\infty \exp\left(-x_i - \frac{y}{M_i^2\left(\frac{1}{3}+\frac{1}{\delta}\right)}\right)\mathrm{d}y \\
&= \exp(-x_i)M_i^2\left(\frac{1}{3}+\frac{1}{\delta}\right)\exp\left(-\frac{x_i}{M_i^2\left(\frac{1}{3}+\frac{1}{\delta}\right)}\right) \\
&\leq \exp(-y_i)\left(\frac{1}{3}+\frac{1}{\delta}\right).
\end{aligned}$$

With that and (3.16), we are left with:

$$\mathbb{E}\left[\sup_m \left\{(1+\epsilon)\chi_n^2(m) - \mathrm{pen}(m)\right\} \vee 0\right] \leq \frac{C}{n^2}\sum_{i\in\mathcal{I}} \mathrm{e}^{-x_i}(v_i + M_i^2(1+x_i)) + x_i\mathrm{e}^{-y_i}.$$

Replacing x_i with its value, and overestimating v_i by nM_i^2 we obtain (under the condition that $2\ln M_i + y_i \leq n$):

$$\mathbb{E}\left[\sup_m \left\{(1+\epsilon)\chi_n^2(m) - \mathrm{pen}(m)\right\} \vee 0\right] \leq C\left(\frac{\Sigma}{n} + \frac{\Sigma}{n^2}\right). \qquad \square$$

Remark. The logarithmic factor in the penalty (that would not be here if we took only the variance) comes from the multitude of models allowed by a hard-thresholding estimator. By selecting fewer models (for example the square matrices obtained by truncating the density operator) and using a random penalty, we can get rid of this term. However, crafting the penalty requires much more work and more powerful inequalities (Talagrand's). An interested reader may have a look at Section 3.4 of [16].

3.5. Applications with two bases

We now give two bases that are reasonable when applying these theorems. As can be seen from (3.1), a good basis should approximate well any density operator (so that the bias term gets low fast when m is big), with dual vectors having a low variance. With the first of the two bases, we have this interesting phenomenon that we obtain a polynomial convergence rate under the mere physical hypothesis that the state has finite energy.

3.5.1. *Photon basis*

Here we shall take as our $(e_i)_{i\in\mathcal{I}}$ a slight variation of the matrix entries of our density operator with respect to the Fock basis (2.1).

More precisely, we worked in the previous subsections with real coefficients. To apply Theorems 3.4 and 3.2, we then need to parametrize ρ with real coefficients. The matrix entries are *a priori* complex. However, using the fact that ρ is self-adjoint, we may separate the real and imaginary parts.

We use a double index for i and define the orthonormal basis, denoting by $E_{j,k}$ the null matrix except for a 1 in case (j,k):

$$e_{j,k} \quad = \quad \begin{cases} \frac{1}{\sqrt{2}}(E_{j,k}+E_{k,j}) & \text{if } j<k \\ \frac{i}{\sqrt{2}}(E_{k,j}-E_{j,k}) & \text{if } k<j \\ E_{j,j} & \text{if } j=k. \end{cases}$$

Then, using a tilde to distinguish it from the matrix entries, with $\tilde{\rho}_{j,k} = \langle \rho, e_{j,k}\rangle$, we have

$$\langle \psi_j, \rho\psi_k\rangle = \begin{cases} \frac{1}{\sqrt{2}}(\tilde{\rho}_{j,k}+i\tilde{\rho}_{k,j}) & \text{if } j<k \\ \frac{1}{\sqrt{2}}(\tilde{\rho}_{k,j}-i\tilde{\rho}_{j,k}) & \text{if } j>k \\ \tilde{\rho}_{j,j} & \text{if } j=k. \end{cases}$$

The associated $\tilde{f}_{j,k}$ are well-known. They are a slight variation of the usual "pattern functions" (see App. A.2, and (A.8) therein), the behaviour of which may be found in [1]. Notably, we know that:

$$\sum_{j,k=0}^{N} \|f_{j,k}\|_\infty^2 \le CN^{7/3}. \tag{3.18}$$

As the upper bounds on the supremum of $\tilde{f}_{j,k}$ may not be sharp, the best way to apply the above theorems (especially Th. (3.2)) would probably be to tabulate these maxima for the (j,k) we plan to use.

The interest of this basis is that it is *a priori* adapted to the structure of our problem: if we have a bound on the energy (let's say it is lower than $H+\frac{1}{2}$), we get worst-case estimates on the convergence speed with the deterministic penalty: indeed, the energy of a state ρ may be written $\frac{1}{2}+\sum_j j\rho_{j,j}$, so that

$$\sum_{j\ge N} \tilde{\rho}_{j,j} \quad \le \quad \frac{H}{N}.$$

Moreover, by positivity of the operator,

$$\tilde{\rho}_{j,k}^2 + \tilde{\rho}_{k,j}^2 \quad \le \quad \tilde{\rho}_{j,j}\tilde{\rho}_{k,k}.$$

If we look at the models N such that $\mathcal{I}_N = \{(j,k) : j<N, k<N\}$, we can get:

$$\begin{aligned} d^2(\rho,N) &\le \sum_{j,k=0}^{\infty} \tilde{\rho}_{j,k}^2 - \sum_{j,k=0}^{N} \tilde{\rho}_{j,k}^2 \\ &\le (\sum_{j\ge 0} \tilde{\rho}_{j,j})^2 - (\sum_{j=0}^{N} \tilde{\rho}_{j,j})^2 \\ &\le 1-(1-\frac{H}{N})^2 \\ &\le \frac{2H}{N} \end{aligned}$$

where we have used that the density operator has trace one.

We substitute in (3.8) and get:

$$\mathbb{E}\left[\left\|\hat{\rho}^{(n)}-\rho\right\|^2\right] \le C\left(\frac{H}{N}+\mathrm{pen}_n(N)+\frac{1}{n}\right).$$

Now, using the bounds on infinite norms (3.18), the penalty is less than:

$$\mathrm{pen}_n(N) = C\frac{N^{7/3}\ln(N)}{n}\cdot$$

Optimizing in N ($N = C(Hn)^{3/10}$), we get

$$\mathbb{E}\left[\left\|\hat{\rho}^{(n)} - \rho\right\|^2\right] \leq CH^{7/10}\ln(H)n^{-3/10}\ln(n). \tag{3.19}$$

This estimate holds true for any state and is non-asymptotic. It is generally rather pessimistic, though. For many classical states, such as squeezed states or thermal states, $\rho_{j,j} \equiv A\exp(-B/n)$, the same calculation yields a rate for the square of the L^2 distance as $n^{-1}\ln(n)^\beta$ for some β. In such a case, the penalized estimator automatically converges at this latter rate.

3.5.2. *Wavelets*

Another try could be to use functions known for their good approximations properties. To this end we look at the Wigner function and write it in a wavelet basis.

Recall that wavelets on $\mathbb{R}$ are an orthonormal basis such that all functions are scaled translations of a same function, the mother wavelet. In multiscale analysis, we use a countable basis $\psi_{j,k} : x \mapsto 2^{j/2}\psi_{0,0}(2^j x + k)$, for j and k integers. Let $\mathcal{V}_i = \{\psi_{j,k} : j \leq i\}$. There is a ϕ, called father wavelet, such that the $\phi_k(x) = \phi(x + k)$ for $k \in \mathbb{Z}$ are a basis of the vector space generated by all the wavelets of larger or equal scale, that is $\mathcal{V}_0$. We may choose them with compact support, or localized both in frequency and position. So they harvest local information and can fetch this whatever the regularity of the function to be approximated, as they exist at several scales.

From a one-dimensional wavelet basis $\psi_{j,k} : x \mapsto 2^{j/2}\psi_{0,0}(2^j x + k)$, C^3 and zero mean, with a father wavelet $\phi_{j,k}$, also C^3, we shall make a tensor product basis on $L^2(\mathbb{R}^2)$: let $I = (j, k, \epsilon)$ be indices, with j integer (scale), $k = (k_x, k_y) \in \mathbb{Z}^2$ (position), and $\epsilon \in 0, 1, 2, 3$. Let

$$\Psi_I(x,y) = \begin{cases} \phi_{j,k}(x)\phi_{j,k}(y) & \text{if } \epsilon = 0 \\ \phi_{j,k}(x)\psi_{j,k}(y) & \text{if } \epsilon = 1 \\ \psi_{j,k}(x)\phi_{j,k}(y) & \text{if } \epsilon = 2 \\ \psi_{j,k}(x)\psi_{j,k}(y) & \text{if } \epsilon = 3. \end{cases}$$

We may then define a multiscale analysis from the one-dimensional one (written $\mathcal{V}, \mathcal{W}$): $V_0 = \overline{\mathcal{V}_0 \otimes \mathcal{V}_0}$ and for all $j \in \mathbb{Z}$, $V_{j+1} = V_j \oplus W_j$, so that $W_{j+1} = \overline{\mathcal{V}_j \otimes \mathcal{W}_j} \oplus \overline{\mathcal{W}_j \otimes \mathcal{V}_j} \oplus \overline{\mathcal{V}_j \otimes \mathcal{W}_j}$.

For any j, $V_j \cup \bigcup_{k\geq j} W_k$ is then an orthonormal basis of $L^2(\mathbb{R}^2)$. We hereafter choose our models as subspaces spanned by finite subsets of the basis vectors for well-chosen j.

It can be shown that:

$$\gamma_I(x,\phi) = \frac{1}{4\pi}\int_{-\infty}^{\infty} |u|\, \hat{\Psi}_I(u\cos\phi, u\sin\phi)\mathrm{e}^{ixu}\mathrm{d}u$$

fulfills this property:

$$[\gamma_I, Kf] = \langle \Psi_I, f\rangle.$$

Noticing that

$$\gamma_I(x,\phi) = 2^j\gamma_{0,0,\epsilon}(2^j x - k_x\cos\phi - k_y\sin\phi, \phi),$$

we see that these functions have the same dilation properties as wavelets, and they are "translated" in a way that depends on ϕ, through sinusoids. Their normalizations, though, explode with j; this derives from inverting the Radon transform being an ill-posed problem.

We can now apply Theorem 3.4. Before doing so, though, we restrict ourselves to a finite subdomain of $\mathbb{R}^2$, which we denote $\mathcal{D}$, and put the Wigner function to zero outside this domain, that we should choose big enough to ensure this does not cost too much.

Then, $\mathcal{M}$ is the set of all models characterized by

$$m = \big\{(j_1,k,0) : 2^{j_1}k \in \mathcal{D}\big\} \cup \big\{(j,k,\epsilon) : (j,k,\epsilon) \in \mathcal{I}'_m \subset \{(j,k,\epsilon) : \epsilon = 1;2;3, j_1 < j < j_0, 2^j k \in \mathcal{D}\}\big\}.$$

To have good approximating properties, we choose $2^{j_1} \equiv n^{1/7}$ and $2^{j_0} \equiv \frac{n}{(\ln n)^2}$. The projection estimator within a model is then:

$$\hat{f} = \sum_{I\in m} \alpha_I \Psi_I$$

with

$$\alpha_I = \frac{1}{n}\sum_{i=1}^{n} \gamma_I(X_i,\Phi_i).$$

Denoting $B_\epsilon = \|\gamma_{0,0,\epsilon}\|_\infty$, the translation of Theorem 3.4 gives (notice that applying (3.2) would be awkward, as the variance of γ_I is like 2^j whereas its maximum is like 2^{2j}):

Theorem 3.5. *Let y_I be such that $\sum_I \exp(-y_I) = \Sigma \leq \infty$. For example $y_I = j$. Let then:*

$$x_I \quad = \quad 2(j + \ln(B_\epsilon)) + y_I.$$

We choose an $\alpha \in (0,1)$ and the penalty (and restraining ourselves to the m such that $I \in m \to x_I \leq n$):

$$\mathrm{pen}(m) \quad = \quad \frac{1+\epsilon'}{n}\sum_{I\in\mathcal{M}} 2\left(\sqrt{\frac{2}{1-\alpha}x_I\left(\mathbb{P}_n\left[\gamma_I^2\right] + \frac{1}{n}2^{2j}B_\epsilon^2\Big(\frac{1}{3}+\frac{1}{\alpha}\Big)x_I\right)} + \frac{2^j B_\epsilon}{3\sqrt{n}}x_I\right)^2.$$

Then there is a constant C such that:

$$\mathbb{E}\left[\left\{\frac{\epsilon}{2+\epsilon}\left\|\rho - \hat{\rho}^{(n)}\right\|^2 - \left(\inf_{m\in\mathcal{M}}\left(1+\frac{2}{\epsilon}\right)d^2(\rho,m) + 2\,\mathrm{pen}_n(m)\right)\right\}\vee 0\right] \quad \leq \quad \frac{C\Sigma}{n} + C\frac{1}{n}2^{2j_1}. \tag{3.20}$$

Proof. First it's easily checked that $x_I = 2\ln(\|\gamma_I\|_\infty) + y_I$. Second $\sum_I \exp(-j) = C\sum_j 2^j \exp(-j) < \infty$ implies that $y_I = j$ does indeed the work, as there are at most $C2^j$ wavelets at scale j whose support meet $\mathcal{D}$.

The last term is the variance of $\hat{a}_{j_1,k,0}$, corresponding to the vectors that are in every model:

$$\begin{aligned}
\frac{1}{n}\mathbb{V}\left[\sum_{2^{j_1}k\in\mathcal{D}}\gamma_{j_1,k,0}\right] &\leq \frac{1}{n}\mathbb{E}\left[\sum_{2^{j_1}k\in\mathcal{D}}\gamma_{j_1,k,0}^2\right] \\
&\leq \frac{1}{n}\sum_{2^{j_1}k\in\mathcal{D}}\int_{\mathbb{R}\times[0,\pi]}\gamma_{j_1,k,0}^2(x,\phi)\mathrm{d}x\frac{\mathrm{d}\phi}{\pi}p_\rho(x,\phi) \\
&= \frac{1}{n}\sum_{2^{j_1}k\in\mathcal{D}}\int_{\mathbb{R}}\gamma_{j_1,k,0}^2(x,0)\int_0^\pi p_\rho(x - k_x\cos\phi - k_y\sin\phi,\phi)\mathrm{d}x\frac{\mathrm{d}\phi}{\pi} \\
&= C\frac{1}{n}2^{2j_1}
\end{aligned}$$

where we have used that for all x and k, $\int_0^\pi p_\rho(x - k_x\cos\phi - k_y\sin\phi,\phi)\frac{\mathrm{d}\phi}{\pi}$ is less than a constant about 1.086. Indeed, the translation of a Wigner function is still the Wigner function of a state, so that we may take $k = 0$. Then

$$\int_0^\pi p_\rho(x - k_x\cos\phi - k_y\sin\phi,\phi)\frac{\mathrm{d}\phi}{\pi} \leq \sup_{i,x}|\psi_i(x)|^2$$

and the upper bound on this supremum is due to Cramér (10.18.19 in [11]). □

Remarks. As the variance of γ_I goes like 2^j the threshold might be seen as $C2^{j/2}\sqrt{\frac{j}{n}}$. This yields the wavelets estimator studied in [6], for a general Radon transform on usual (non-negative) probability densities (*i.e.* not on Wigner functions).

The role of the approximation speed is apparent in (3.20). Articles like [6] show that this strategy is asymptotically (quasi)-optimal for approximating a function in a Besov ball. However, this is no proof of the efficiency in our case, as the set of Wigner functions is not a Besov ball. There is still some work in approximation theory needed there. In particular, we do not know if a statement similar to (3.19) can be proven.

Finally, notice that we may combine projection estimators: as the contrast function is the same for any basis we are working with, keeping the same penalizations, we could find an estimator that is almost the best among those built with the photon basis and those with the wavelet basis simultaneously (just add a $\ln(2)$ to Σ). In other words, we do not have to choose beforehand which basis we use. Moreover an estimator allowing for the two bases would satisfy (3.19).

3.6. Noisy observations

The situation we have studied was very idealized: we did not take any noise into account. In practice, a number of photons fail to be detected. These losses may be quantified by one single coefficient η between 0 (no detection) and 1 (ideal case). We suppose it to be known.

There are several methods to recover the state from noisy observations. One consists in calculating the density matrix as if there was no noise, and then apply the Bernoulli transformation with factor η^{-1}. We can also use modified pattern functions [8]. Or we can approximate the Wigner function with a kernel estimator that performs both the inverse Radon transform and the deconvolution [5]. The former two methods fail if the observations are too noisy ($\eta \leq \frac{1}{2}$), but the latter is asymptotically optimal for all η over wide classes of Wigner functions.

This noise can be seen as a convolution of the result (X, Φ) with a Gaussian of variance depending on η:

$$p^{\eta}_{\rho}(y,\phi) = \frac{1}{\sqrt{\pi(1-\eta)}}\int_{-\infty}^{\infty} p_{\rho}(x,\phi)\exp\left(-\frac{\eta}{1-\eta}\left(x-\eta^{-1/2}y\right)^2\right)\mathrm{d}x$$

or equivalently in terms of generating functions

$$\int p^{\eta}_{\rho}(x,\phi)\mathrm{e}^{irx}\mathrm{d}x = \mathrm{e}^{-\frac{1-\eta}{4\eta}r^2}\int p_{\rho}(x,\phi)\mathrm{e}^{irx}\mathrm{d}x.$$

We can use the methods described above and then use the Bernoulli transform. For free, we may also use the modified pattern functions $f^{\eta}_{j,k}$ knowing $f_{j,k}$. Explicitly we see that the dual basis of the matrix entry $\rho_{j,k}$ becomes:

$$f^{\eta}_{j,k}(x,\phi) = \frac{1}{2\pi}\int \mathrm{d}r\mathrm{e}^{\frac{1-\eta}{4\eta}r^2}\int \mathrm{d}y f_{j,k}(y,\phi)\mathrm{e}^{iry}.$$

The reason why one needs $\eta > \frac{1}{2}$ is for this Fourier transform to be well defined.

And we can again apply Theorems 3.2 and 3.4 with the dual basis $\tilde{f}^{\eta}_{j,k}$.

Obtaining results with high noise $\eta \leq \frac{1}{2}$ is harder. We would need to introduce a cut-off h within the inverse Fourier transform (and therefore a bias). Using the same h as in [5] would ensure this bias $b(\rho, h)$ is asymptotically reasonable. We could then reuse Theorems 3.2 and 3.4 to have an "almost best" approximation of $\rho + b(\rho, h)$ within a set of models, for finite samples. Careful examination would then be required to check the variance (or the penalties) go to 0 as n and $h(n)$ go to infinity. Moreover, we would need to translate conditions on the Wigner function into conditions on the density operator to see whether we can reproduce the asymptotic optimality results of Butucea *et al.* with model selection in the Fock basis (or any other basis chosen and studied *a priori*).

4. Maximum likelihood estimator

Projection estimators are not devoid of defects. Notably, the variance of empirical coefficients might be high, the convergence therefore rather slow, and the estimator is not a true density matrix. Especially, the trace is probably not one, though this could be fixed easily enough. We can diagonalize the estimated density matrix, replace the negative eigenvalues with 0, and divide by the trace.

Anyhow, there are other types of estimator that automatically yield density matrices. One such estimator is the maximum likelihood estimator, which selects the nearest point of the empirical probability measure in a given model for the Kullback-Leibler distance (which is not a true distance as it is not symmetric). Recall that the Kullback-Leibler distance between two probability measures is:

$$K(p,q) = \int \ln\left(\frac{p(x)}{q(x)}\right) p(x)\mathrm{d}x.$$

In other words, the maximum likelihood estimator is

$$\arg\min_{\tau\in\mathcal{Q}} \sum_{l=1}^{n} -\ln p_\tau(X_l,\Phi_l)$$

where $\mathcal{Q}$ is any set of density operators (such that the minimum exists). This way, it is automatically a true density operator. A practical drawback is that calculating it is very power-consuming.

As $\gamma_n(\cdot) \to -\int \ln(p.)d_{p_\rho}$, we have defined a minimum contrast estimator in the sense of Section 3.1. Much like for projection estimators, the Kullback distance thus estimated might be overly optimistic, and all the more when $\mathcal{Q}$ is big. Indeed, if $\mathcal{Q}$ is the set of all density operators, then there is no minimizer of the distance with the empirical distribution; however when we take only finite-dimensional models, such as

$$\mathcal{Q}(N) = \left\{\tau \in \mathcal{S}(L^2(\mathbb{R})) : \tau_{j,k} = 0 \text{ for all } j > N \text{ or } k > N\right\}, \tag{4.1}$$

then the minimum is attained by compactness. Here the matrix entries $\tau_{j,k}$ are taken in the Fock basis (2.1).

We then have to define a penalty for choosing (almost) the best model. To do so, we make use of a (slightly simplified but sufficient for our needs) version of a theorem from [19], but we need a few definitions before stating it.

First we need a distance with which to express our results, and it is not the Kullback-Leibler, but the Hellinger distance. The Hellinger distance between two probability densities is defined in relation with the L^2 distance of the square roots of these densities:

$$h^2(p,q) = \frac{1}{2}\int \left(\sqrt{p}-\sqrt{q}\right)^2. \tag{4.2}$$

This distance does not depend on the underlying measure. The following relations are well-known:

$$\begin{aligned} \frac{1}{8}\|p-q\|_1^2 &\leq h^2(p,q) \leq \frac{1}{2}\|p-q\|_1 \\ h^2(p,q) &\leq \frac{1}{2}K(p,q). \end{aligned} \tag{4.3}$$

The penalty to be defined shall depend on the size of the model, that we have to estimate. The right tool is the metric entropy, and more precisely the metric entropy with bracketing of the model.

Definition 4.1. Let $\mathcal{G}$ a function class. Let $N_{B,2}(\delta, \mathcal{G})$ be the smallest p such that there are couples of functions $[f_i^L, f_i^U]$ for i from 1 to p that fulfill $\left\|f_i^L - f_i^U\right\|_2 \leq \delta$ for every j, and for any $f \in \mathcal{G}$, there is an $i \in [1, p]$ such that:

$$f_i^L \leq f \leq f_i^U.$$

Then $H_{B,2}(\delta, \mathcal{G}) = \ln N_{B,2}(\delta, \mathcal{G})$ is called the δ-bracketing entropy of $\mathcal{G}$

Remarks.

- Notice that the f_i^U and f_i^L need not be in $\mathcal{G}$.
- The 2 in $H_{B,2}$ stands for L^2 distance.

Looking closely at Definition 4.1, we see that the concept of entropy depends only on those of positivity and norms. We may then define a similar bracketing entropy for any space with a norm and a partial order, such as the L^1 δ-bracketing entropy of $\mathcal{Q}(N)$: we must find couples of Hermitian operators $[\tau_i^L, \tau_i^U]$ such that $\left\|\tau_i^U - \tau_i^L\right\|_1 \leq \delta$ and such that for any $\tau \in \mathcal{Q}(N)$, there is an i such that $\tau_i^L \leq \tau \leq \tau_i^U$.

We are chiefly interested in the L^2 entropy of square roots of density (denoted by $H_{B,2}(\delta, \mathcal{P}^{\frac{1}{2}})$):

$$\mathcal{P}^{1/2}(N) = \left\{\sqrt{p_\rho} : p_\rho \in \mathcal{P}(N)\right\}.$$

Now the Theorem from [19]:

Theorem 4.2. *Let $X_1, \ldots, X_n$ be independent, identically distributed variables with unknown density s with respect to some measure μ. Let $(S_m)_{m\in\mathcal{M}}$ be an at most countable collection of models, where for each $m \in \mathcal{M}$, the elements of S_m are assumed to be densities with respect to μ. We consider the corresponding collection of maximum likelihood estimators $\hat{s}_m$. Let* $\mathrm{pen} : \mathcal{M} \longrightarrow \mathbb{R}$ *and consider the random variable $\hat{m}$ such that:*

$$\mathbb{P}_n\left[-\ln(\hat{s}_{\hat{m}})\right] + \mathrm{pen}(\hat{m}) = \inf_{m\in\mathcal{M}} \mathbb{P}_n\left[-\ln(\hat{s}_m)\right] + \mathrm{pen}(m).$$

Let $(x_m)_{m\in\mathcal{M}}$ a collection of numbers such that

$$\sum_{m\in\mathcal{M}} e^{-x_m} = \Sigma \leq \infty.$$

For each m, we consider a function ϕ_m of $\mathbb{R}^{+*}$, nondecreasing, and such that $x \mapsto \frac{\phi_m(x)}{x}$ is nonincreasing, and:

$$\phi_m(\sigma) \geq \int_0^\sigma \sqrt{H_{B,2}(\epsilon, S_m^{\frac{1}{2}})}d\epsilon.$$

We then define each σ_m as the one positive solution of

$$\phi_m(\sigma) = \sqrt{n}\sigma^2.$$

Then there are absolute constants κ and C such that if for all $m \in \mathcal{M}$,

$$\mathrm{pen}(m) \geq \kappa\left(\sigma_m^2 + \frac{x_m}{n}\right),$$

then

$$\mathbb{E}\left[h^2(s, \hat{s}_{\hat{m}})\right] \leq C\left(K(s, S_m) + \mathrm{pen}(m) + \frac{\Sigma}{n}\right)$$

where, for every $m \in \mathcal{M}$, $K(s, S_m) = \inf_{t\in S_m} K(s,t)$.

We notice that what is bounded *in fine* is the Hellinger distance and not the Kullback. Indeed our evaluation of the estimation error, which depends upon the size of the model (its bracketing entropy), dominates the Hellinger distance but maybe not the Kullback-Leibler distance.

In our case, we have parametrized the models m by N, through definition (4.1).

To apply Theorem 4.2, we need to find suitable ϕ_m, and this calls for dominating the entropy integral. We reproduce here [1].

By (4.3), it is sufficient to control $H_{B,1}(\delta, \mathcal{P}(N))$. Moreover, the linear extension of the morphism $\mathbf{T}$ sends a positive matrix to a positive function, and is contractive. So any covering of $\mathcal{Q}(N)$ by δ-brackets is sent upon a covering of $\mathcal{P}(N)$ by L^1 δ-brackets, that is $[p_j^L, p_j^U] = [p_{\tau_j^L}, p_{\tau_j^U}]$. Thus

$$H_{B,1}(\delta, \mathcal{P}(N)) \leq H_{B_1}(\delta, \mathcal{Q}(N)),$$

so that

$$H_{B,2}(\delta, \mathcal{P}^{\frac{1}{2}}(N)) \leq C H_{B,1}(\delta^2, \mathcal{Q}(N)).$$

Moreover:

Lemma 4.3.

$$H_{B,1}(\delta, \mathcal{Q}(N)) \leq C N^2 \ln \frac{N}{\delta}$$

where C is a constant not depending on δ or N, and can be put to $1 + \ln(5)$.

Proof. Let $\{\rho_j : j = 1, \ldots, c(\delta, N)\}$ a maximal set of density matrices in $\mathcal{Q}(N)$ such that for all $j \neq k$, $\|\rho_j - \rho_k\|_1 \geq \frac{\delta}{2N}$. Define the brackets $[\rho_j^L, \rho_j^U]$ as

$$\rho_j^L = \rho_j - \frac{\delta}{2N}\mathbf{1} \qquad \rho_j^U = \rho_j + \frac{\delta}{2N}\mathbf{1}.$$

Then $\|\rho_j^L - \rho_j^U\|_1 = \delta$. Moreover for any ρ in the ball $B_1(\rho_j, \frac{\delta}{2N})$, as $\|\rho - \rho_j\|_1 \leq \frac{\delta}{2N}\mathbf{1}$, we have

$$\rho_j^L \leq \rho \leq \rho_j^U$$

and as $\{\rho_j\}$ was a maximal set, this set of brackets cover $\mathcal{Q}(N)$.

So $H_{B,1}(\delta, \mathcal{Q}(N)) \leq c(\delta, N)$.

Notice that $B_1(\rho_j, \frac{\delta}{4N})$ are disjoint and included in the shell $B_1(0, 1 + \frac{\delta}{4N}) - B_1(0, 1 - \frac{\delta}{4N})$, so that

$$\begin{aligned} c(\delta, N) &\leq \left(\frac{4N}{\delta}\right)^{N^2} \left(\left(1 + \frac{\delta}{4N}\right)^{N^2} - \left(1 - \frac{\delta}{4N}\right)^{N^2}\right) \\ &\leq \left(1 + \frac{4N}{\delta}\right)^{N^2} \\ &\leq \left(\frac{5N}{\delta}\right)^{N^2}, \end{aligned} \tag{4.4}$$

concluding the demonstration. □

From this, we can obtain:

Corollary 4.4. *There is a constant C such that:*

$$H_{B,2}(\delta, \mathcal{P}^{\frac{1}{2}}(N)) \leq C N^2 \ln \frac{N}{\delta^2}.$$

Writing

$$\phi_N(\sigma) = \int_0^\sigma \sqrt{H_{B,2}(\epsilon, \mathcal{P}^{\frac{1}{2}}(N))}\mathrm{d}\epsilon$$

and $\sigma_N(n)$ the only σ such that

$$\phi_N(\sigma) = \sqrt{n}\sigma^2$$

we get

$$\sigma_N(n) \leq \sqrt{\frac{C}{n}} N \left(1 + \sqrt{0 \vee \ln \frac{n}{N}}\right)\cdot \tag{4.5}$$

Indeed

$$\begin{aligned}
\phi_N(\sigma) &\leq CN \int_0^\sigma \sqrt{\ln\left(\frac{N}{\epsilon^2}\right)}\mathrm{d}\epsilon \\
&= CN^{\frac{3}{2}} \int_{\sqrt{\ln \frac{N}{\sigma^2}}}^{\infty} x\mathrm{e}^{-\frac{x^2}{2}}\mathrm{d}x \\
&= CN^{\frac{3}{2}} \left(\int_{\sqrt{\ln \frac{N}{\sigma^2}}}^{\infty} \mathrm{e}^{-\frac{x^2}{2}}\mathrm{d}x - \left[x\mathrm{e}^{-\frac{x^2}{2}}\right]_{\sqrt{\ln \frac{N}{\sigma^2}}}^{\infty}\right) \\
&\leq CN\sigma\left(1 + \sqrt{\ln \frac{N}{\sigma^2}}\right)
\end{aligned}$$

where we have made use of, in each line in turn,

- Corollary 4.4;
- the change of variables $x = \sqrt{\ln(N\epsilon^{-2})^2}$, with $\frac{\mathrm{d}\epsilon}{\mathrm{d}x} = -\sqrt{N}x\mathrm{e}^{-\frac{x^2}{2}}$;
- integration by parts, with x seen as a primitive and $x\mathrm{e}^{-\frac{x^2}{2}}$ as a derivative;
- the upper bound $C\mathrm{e}^{-\frac{x^2}{2}}$ of $\int_x^\infty \mathrm{e}^{-x^2/2}\mathrm{d}x$ for x positive when evaluating the first term.

We are looking for an upper bound on σ_N, solution of the equation

$$\sqrt{n}\sigma_N^2 = CN\sigma\left(1 + \sqrt{\ln \frac{N}{\sigma_N^2}}\right)\cdot$$

We lower bound the second term by 0, and get

$$\sigma_N \geq C\frac{N}{\sqrt{n}} \equiv \sigma_m.$$

Hence the upper bound

$$\begin{aligned}
\sigma_N &= CNn^{-\frac{1}{2}}\left(1 + \sqrt{\ln \frac{N}{\sigma_N^2}}\right) \\
&\leq CNn^{-\frac{1}{2}}\left(1 + \sqrt{\ln \frac{N}{\sigma_m^2}}\right) \\
&= C\frac{N}{\sqrt{n}}\left(1 + \sqrt{\ln \frac{n}{C^2N}}\right)\cdot
\end{aligned}$$

We may absorb the C^2 in the first multiplicative constant to find (4.5). Of course we take only the positive part of the logarithm. This will always be the case hereafter.

Applying Theorem 4.2 we get:

Theorem 4.5. *Consider the collection of maximum likelihood estimators $(\hat{\rho}_N)_{N\in\mathbb{N}}$, that is for any integer N,*

$$\mathbb{P}_n\left[-\ln(p_{\hat{\rho}_N})\right] = \inf_{\rho\in\mathcal{Q}(N)} \mathbb{P}_n\left[-\ln(p_{\hat{\rho}})\right].$$

Let $\mathrm{pen}: \mathbb{N} \mapsto \mathbb{R}_+$ and consider a random variable $\hat{N}$ such that

$$\mathbb{P}_n\left[-\ln(p_{\hat{\rho}_{\hat{N}}})\right] + \mathrm{pen}(\hat{N}) = \inf_{N\in\mathbb{N}}(\mathbb{P}_n\left[-\ln(p_{\hat{\rho}_N})\right] + \mathrm{pen}(N)).$$

Let $(x_N)_{N\in\mathbb{N}}$ a family of positive numbers such that

$$\sum_{N\in\mathbb{N}} e^{-x_N} = \Sigma \;<\; \infty.$$

Then there are absolute constants κ and C such that if

$$\mathrm{pen}(N) \geq \kappa\left(\frac{N^2}{n}\left(1+\left(0\vee\ln\frac{n}{N}\right)\right)+\frac{x_N}{n}\right)$$

then

$$\mathbb{E}[h^2(p_\rho, p_{\hat{\rho}_{\hat{N}}})] \leq C\left(\inf_{N\in\mathbb{N}}(\mathbb{E}[K(\rho,\mathcal{Q}(N))] + \mathrm{pen}(N)) + \frac{\Sigma}{n}\right)$$

with $K(\rho,\mathcal{Q}(N)) = \inf_{\tau\in\mathcal{Q}(N)} K(p_\rho, p_\tau)$.

Remarks.

- When designing the penalty, what stands out in this theorem is the general form of the penalty. Now the constant κ that can be explicitly computed would be very pessimistic. The best thing to do is therefore to keep the general formula for the penalty and calibrate κ using cross-validation, the slope heuristic [19] or any other appropriate method.
- If we wanted an explicit convergence rate for a given state, as for the photon basis in Section 3.5.1, we would first need to know how the Kullback-Leibler distance $K(\rho,\mathcal{Q}(N))$ is decreasing with N. One thing that is obvious, however, is that if we add noise we convolve with the same function p_ρ and p_σ for all σ in $\mathcal{Q}(N)$, so the Kullback-Leibler distance is decreasing with the noise, so convergence is faster when there is noise... The reason for this is that we are looking at convergence in Hellinger distance, that is a distance between the law of the result of the measurement p_ρ and p_σ. This does not tell us directly anything about what we are really interested in, that is the distance between ρ and σ (as operators). Indeed we may bound the L^2 or L^1 norm between elements of $\mathcal{Q}(N)$ by the Hellinger distance, times something depending on the sum of the L^2 or L^∞ norms of the $f^\eta_{j,k}$. And these norms are going very fast to infinity when there is noise, so that low Hellinger distance gives no indication on the operator norms.

5. Quantum calibration of a photocounter

This section features a scheme to calibrate an apparatus M measuring the number of photons in a beam with the help of a photocounter.

The physical motivation is given in Appendix A.3.

The first subsection states the mathematical problem. In the two others, projection estimators and maximum likelihood estimators are respectively studied.

5.1. **Statistical problem**

The practical problem of calibration of a photocounter turns out to be mathematically speaking an entirely classical missing data problem. However, to the best of our knowledge, it has never been studied. We now describe this missing data problem.

We are given samples (I, X) in $\mathbb{N} \times \mathbb{R}$ from a probability density of the form

$$p(i, x) = \sum_{k=0}^{\infty} b_k^2 P_i^k \psi_k(x)^2. \tag{5.1}$$

In this expression, the real numbers b_k^2 satisfy $\sum_k b_k^2 = 1$. The ψ_k are the Fock basis functions given in equation (2.1). For any k, the P_i^k are a probability measure, that is they are non-negative and $\sum_{i=0}^{\infty} P_i^k = 1$.

We know the b_k^2, and we want to retrieve the P_i^k, which we do not know. We write $P = (P_i^k)_{i,k}$.

To make clearer that this is a missing data problem, we give the following way to obtain this experiment. First we choose $K \in \mathbb{N}$ with probability given by b_k^2. We forget K, which is the missing data. Our data consists in (I, X), with i having law given by P_i^k and x with law $\psi_k(x)$.

Notice that the experimentalist has some control on the b_k^2, but usual techniques will yield b_k^2 proportional to ξ^k. This means that the low k are probed faster.

We propose below two types of estimators $\hat{P}$ for P. To get results on their efficiency, we must first find meaningful distance $d(P, \hat{P})$. Since $\sum_i P_i^k = 1$ for all $k \in \mathbb{N}$, distances like $d_2^2(P, Q) = \sum_{i,k} (P_i^k - Q_i^k)^2$ are bound to yield infinite errors on our estimators. We then must weight them, using $(a_k)_{k \in \mathbb{N}}$ of our choice. We shall use, depending on the estimator, either $d_2^2(P, Q) = \sum_{i,k} a_k^2 (P_i^k - Q_i^k)^2$ with $\sum a_k^2 = 1$, or $d_1(P, Q) = \sum_{i,k} a_k |P_i^k - Q_i^k|$, with $\sum_k a_k = 1$. Then these distances are bounded by 2 on the set of all P such that $\{P_i^k\}_{i \in \mathbb{N}}$ is a probability measure for every k.

Varying the choice of a_k corresponds to putting the emphasis on different k, that is deciding which P_i^k we demand to know with the most precision. If we take the a_k decreasing, it means physically that we are more interested in the behaviour of our photocounter for a low number of photons. This is usually the case for a physicist. A possible choice is to take a_k or a_k^2 equal to b_k^2.

In the next subsection, we use projection estimators, and in the following, maximum likelihood estimators.

5.2. **Using projection estimators**

As in the tomography problem, the parameter space is contained in an infinite-dimensional vector space, and a natural type of estimators are projections of the empirical law on finite-dimensional subspaces. The problem we are left with is then again finding the best subspace.

Concretely, we consider the distance $d_2^2(P, Q) = \sum_{i,k} a_k^2 (P_i^k - Q_i^k)^2$ and write $E_i^k = a_k P_i^k$. Similarly we shall write $\hat{E}_i^k = a_k \hat{P}_i^k$ for our estimator. Then

$$d_2^2(P, \hat{P}) = \sum_{i,k} (E_i^k - \hat{E}_i^k)^2,$$

and the law of our samples can be rewritten as

$$p(i, x) = \sum_k E_i^k \frac{b_k^2}{a_k} \psi_k(x)^2. \tag{5.2}$$

We may then consider $\{(b_k^2/a_k)\psi_k \mathbf{1}_{i=l}\}_{k,i}$ as a basis of our functions on $\mathbb{N} \times \mathbb{R}$. We want to use the general constructions of Section 3. We first need a dual basis $\{g_{i,k}\}$. Now, the dual basis of $\{\psi_k^2\}$ as functions on $\mathbb{R}$ is well-known. Those are the "pattern functions" $f_{k,k}$ introduced in [7] (see (A.8)). From this, we deduce:

$$g_{i,k}(l,x) = \frac{a_k}{b_k^2} f_{k,k}(x) \mathbf{1}_{i=l}.$$

With these dual functions, we can define the minimum contrast function:

$$\gamma_n(Q) = d_2^2(Q,0) - 2\left(\sum_{\alpha=1}^{n} \frac{g_{i,k}(L_\alpha, X_\alpha)}{a_k}\right)\left(\sum_{i,k} a_k^2 Q_i^k\right),$$

where the (L_α, X_α) are our data, that is n independent samples with law p.

Our models $m \in \mathcal{M}$ consist in the subsets of $\mathbb{N}^2$. If $(i,k) \notin m$, then $\hat{P}_i^k = 0$. In a model m, the estimator $\hat{P}^{(m)}$ given by minimizing the contrast function is then

$$\hat{P}_i^k = \frac{1}{n} \sum_{\alpha=1}^{n} \frac{g_{i,k}(L_\alpha, X_\alpha)}{a_k} \quad \text{for} \quad (i,k) \in m.$$

The penalized estimator is as always the projection estimator of the model $\hat{m}$ such that:

$$\hat{m} = \arg\min_{m \in \mathcal{M}} \gamma_n(\hat{P}^{(m)}) + \operatorname{pen}_n(m).$$

We also use the usual notation for the distance to a model:

$$d_2(P,m) = \inf_{Q \in m} d_2(P,Q).$$

We then obtain from the general theorems in Section 3:

Theorem 5.1. *Let P be a photocounter and (a_k) and (b_k) with $\sum_k a_k^2 = \sum_k b_k^2 = 1$. Let $(x_{i,k})_{(i,k)\in\mathbb{N}^2}$ such that $\sum_{i,k} e^{-x_{i,k}} = \Sigma < \infty$. We define a penalty as*

$$\operatorname{pen}_n(m) = \sum_{(i,k)\in m} (1+\epsilon)\left(\ln(M_{i,k}) + \frac{x_{i,k}}{2}\right)\frac{M_{i,k}^2}{n}$$

with

$$M_{i,k} = \frac{a_k}{b_k^2}(\sup_x f_{k,k}(x) - \inf_x f_{k,k}(x)).$$

Then the penalized estimator fulfills

$$\mathbb{E}\left[\frac{\epsilon}{2+\epsilon} d_2^2(P,\hat{P})\right] \leq \inf_{m\in\mathcal{M}} \left(1+\frac{2}{\epsilon}\right) d_2^2(P,m) + 2\operatorname{pen}_n(m) + \frac{(1+\epsilon)\Sigma}{n}.$$

Theorem 5.2. *Let P be a photocounter and (a_k) and (b_k) with $\sum_k a_k^2 = \sum_k b_k^2 = 1$. Let $(y_{i,k})_{(i,k)\in\mathbb{N}^2}$ such that $\sum_{i,m} e^{-y_{i,m}} = \Sigma < \infty$. Let then*

$$x_{i,k} \quad = \quad 2\ln\left(\frac{a_k}{b_k^2}\|f_{k,k}\|_\infty\right) + y_{i,k}.$$

For any $\delta \in (0,1)$, with

$$
\begin{aligned}
\mathrm{pen}_n(m) &= \sum_{(i,k)\in m} \mathrm{pen}_n^{(i,k)} \\
\mathrm{pen}_n^{(i,k)} &= 2\frac{1+\epsilon}{n}\left(\sqrt{\frac{2}{1-\delta}x_{i,k}\left(\mathbb{P}_n[g_{i,k}^2] + \frac{1}{n}\frac{a_k^2}{b_k^4}\left\|f_{k,k}\right\|_\infty^2\left(\frac{1}{3}+\frac{1}{\delta}\right)x_{i,k}\right)} + \frac{a_k\left\|f_{k,k}\right\|_\infty}{3b_k^2\sqrt{n}}x_{i,k}\right)^2,
\end{aligned}
$$

there is a constant C such that:

$$
\mathbb{E}\left[\left(\frac{\epsilon}{2+\epsilon}d_2^2(P,\hat{P}) - \left(\left(1+\frac{2}{\epsilon}\right)\inf_{m\in\mathcal{M}_n} d_2^2(P,m) + 2\,\mathrm{pen}_n(m)\right)\right)\vee 0\right] \leq \frac{C\Sigma}{n}
$$

where $\mathcal{M}_n$ is the set of models m for which $(i,k)\in m$ implies $x_{i,k} < n$.

Remarks.

- As with the estimation of states with tomography in Section 3, we choose with high efficiency the best subspace. It should be noticed that convergence is fast if the photocounter is good, and could be slower if it is bad. In the latter case, we know it is bad, though. Indeed, the dependence of the convergence rate on the photocounter P lies in the approximation properties of the models – subspaces – m, that is on how fast $d_2^2(P,m)$ decrease when m gets bigger. Now for an ideal photocounter, we need only the (i,i) to be in m. The penalty would be as low as possible when neglecting what happens to beams with more than a given number k of photons. For a worse photocounter, to have a good approximation of how a k-photons beam is read, we might need many i, and the penalty would include all the $\mathrm{pen}^{i,k}$.
- The estimator depends only weakly on (a_k) (unlike the distance), which is good news as it is somewhat arbitrary. Indeed, the empirical $\hat{P}_i^k$ does not depend of this sequence at all, nor do the main terms in the threshold on $\hat{P}_i^k$ of both theorems. For Theorem 5.1, this main term is $a_k^{-1}\sqrt{(1+\epsilon)\ln(B_{i,k})B_{i,k}/\sqrt{n}}$. Now $B_{i,k}$ depends linearly on a_k, so the only a_k left in this expression is in the logarithm which can be developed as $\ln(B_{i,k}/a_k) + \ln(a_k)$. In this way, we see that we only get another term in the penalty. For Theorem 5.2, the threshold is essentially $a_k^{-1}\sqrt{8(1+\epsilon)\mathbb{P}_n\left[g_{i,k}^2\right]\ln(\|g_{i,k}\|_\infty)/((1-\delta)n)}$; and as $g_{i,k}$ is proportional to a_k, the situation is the same.
- The process by which we get our data includes a tomographer and the laws $p(i,x)$ were given in the ideal case when there is no noise. If there is noise, as briefly sketched in Section 3.6, these laws are different. However we may characterize the noise with a single $0 < \eta < 1$. We then have for free the same theorems for $\eta > \frac{1}{2}$: we only need to replace $f_{k,k}$ with $f_{k,k}^\eta$.

5.3. Maximum likelihood procedure

In this case, our results are easier expressed with the distance

$$
\begin{aligned}
d_1(P,\hat{P}) &= \sum_{i,k} a_k\left|P_i^m - \hat{P}_i^k\right| \\
&= \sum_{i,k}\left|E_i^k - \hat{E}_i^k\right|
\end{aligned}
$$

with $E_i^k = a_k P_i^k$ and $\sum_k a_k = 1$. We denote $w_i = \sum_k E_i^k$. Notice that $\sum_i w_i = 1$.

Recall that our data consists in n independent samples (L_α, X_α) with law p given by equation (5.1).

The main difficulty with applying here Theorem 4.2 lies in that the Kullback distance to the models is usually infinite (if we have $\hat{E}_i^k = 0$ for all k for some i, then $\hat{p}(i,\mathbb{R}) = 0$ and this is generally not the case for $p(i,\mathbb{R})$). The easiest way around is to keep independence and restrict attention to some set of i.

Explicitly, we take an ordering on the possible results i of the photocounter (typically, if we expect that one result corresponds roughly to a given number of photons, we can order them in increasing order. The idea is that the results that interest us most should come first). We then choose, still beforehand, $I_{max} \in \mathbb{N}$, and we restrict our attention to the first $i \in [0, I_{max}]$. We just throw away the part of the data where the photocounter gave a result more than I_{max}. We are left with data size $n_{I_{max}}$, with law $p_{I_{max}}$ on $[0, I_{max}] \times \mathbb{R}$:

$$p_{I_{max}} = \frac{p_{|[0,I_{max}]\times\mathbb{R}}}{\int_{[0,I_{max}]\times\mathbb{R}} p}.$$

This law is the probability measure associated to the apparatus $\tilde{P}$ for which $\tilde{P}_i^k = \frac{1}{\sum_{l \le I_{max}} w_l} P_i^k \mathbf{1}_{i \le I_{max}}$.

The models $m_{I,K}$ we work with are indexed by $K \in \mathbb{N}$ and $I \le I_{max}$. They are given by the constraints:

$$\begin{aligned}
\hat{E}_i^k &= 0 && \text{if } i > I_{max} \\
\hat{E}_i^k &= 0 && \text{if } i > I_{max} \text{ and } k \le K \\
\sum_{i \le I} \hat{E}_i^k &= a_k && \text{for } k \le K \\
\hat{E}_i^k &= \frac{a_k}{I_{max} + 1} && \text{for } k > K \text{ and } i \le I_{max}.
\end{aligned} \tag{5.3}$$

Any such element gives a probability measure on $([0, I_{max}] \times \mathbb{R})$. Similarly to equation (5.2), the corresponding probability law reads $\hat{p}(l, x) = \sum_{i,k} b_k^2 a_k^{-1} \hat{E}_i^k \psi_k(x)^2 \mathbf{1}_{i=l}$. The fourth condition (5.3) does not increase the complexity of the model and ensures that the Kullback distance remains finite.

We can now use an empirical maximum likelihood procedure to select within each model an estimator. It minimizes on each $m_{I,K}$ the contrast function

$$\gamma_n(Q) = \sum_{\alpha=1}^{n} - \ln q(L_\alpha, X_\alpha),$$

where Q is an element of the model $m_{I,K}$ and q the associated probability law.

We then use Theorem 4.2 to select the model of which we keep the estimator, through a penalization procedure. We obtain the following theorem.

Theorem 5.3. *Consider the collection of maximum likelihood estimators $(\hat{P}_{I,K})_{I \le I_{max}, K \in \mathbb{N}}$, defined as minimizers of*

$$\gamma_n(\hat{P}_{I,K}) = \inf_{P \in m_{I,K}} \gamma_n(P).$$

Let $\mathrm{pen} : [0, I_{max}] \times \mathbb{N} \to \mathbb{R}$ *be a penalty function and define $(\hat{I}, \hat{K})$ by*

$$\gamma_n(\hat{P}_{(\hat{I},\hat{K})}) + \mathrm{pen}(\hat{I}, \hat{K}) = \inf_{I \le I_{max}, K \in \mathbb{N}} \gamma_n(\hat{P}_{I,K}) + \mathrm{pen}(I, K).$$

Let $(x_{I,K})$ be a family of numbers such that

$$\sum_{I \le I_{max}, K \in \mathbb{N}} e^{-x_{I,K}} = \Sigma \ < \ \infty.$$

Then there are absolute constants κ and C such that if

$$\mathrm{pen}(I, K) \ge \kappa \left((I+1)(K+1) \frac{\ln(n_{I_{max}})}{n_{I_{max}}} + \frac{x_{I,K}}{n_{I_{max}}} \right),$$

then

$$\mathbb{E}\left[d_1(P, \hat{P}_{(\hat{I},\hat{K})})\right] \leq$$

$$\sum_{i>I_{max}} w_i + \sum_{k\in\mathbb{N}} \left(2a_k \wedge \left(C\frac{a_k}{b_k^2}\|f_{k,k}\|_\infty \sqrt{\inf_{I\leq I_{max},K\in\mathbb{N}} K(p_{I_{max}}, m_{I,K}) + \mathrm{pen}(I,K) + \frac{\Sigma}{n_{I_{max}}}}\right)\right),$$

where $K(p_{I_{max}}, m_{I,K}) = \inf_{Q\in m_{I,K}} K(p_{I_{max}}, q)$, *intended as the Kullback distance on* $[0, I_{max}] \times \mathbb{R}$.

Remarks.

- As with projection estimators, we can expect fairly quick approximation if the photocounter is good. Indeed, for $K = I_{max}$ and the ideal photocounter, the distance $K(p_{I_{max}}, m_{I_{max},K}) = 0$.
- Like projection estimators, the maximum likelihood strategy can also be used with noise. If $\eta > \frac{1}{2}$, we get the same theorem changing $f_{k,k}$ in $f^\eta_{k,k}$. Just notice that the infinite norm $\|f_{k,k}\|_\infty$ is exploding.
- As in Section 4, an explicit computation of κ would be over-pessimistic and it is best to estimate it with a data-driven procedure.

Proof. First we rewrite and bound the distance d_1 in a way that suits our purpose. We separate the entries corresponding to measurement results bigger than I_{max}, and we recall at the third line that $\sum_{i\in\mathbb{N}} E_i^k = a_k$. Then

$$\begin{aligned}
d_1(P,\hat{P}) &= \sum_{i,k} \left|E_i^k - \hat{E}_i^k\right| \\
&= \sum_{i>I_{max}} \sum_k E_i^k + \sum_k \sum_{i\leq I_{max}} \left|\hat{E}_i^k - E_i^k\right| \\
&\leq \sum_{i>I_{max}} \sum_k E_i^k + \sum_k \left(2a_k \wedge \left(\sum_{i\leq I_{max}} \left|\hat{E}_i^k - \frac{1}{\sum_{i\leq I_{max}} w_i} E_i^k\right| + \left(\frac{1}{\sum_{i\leq I_{max}} w_i} - 1\right) E_i^k\right)\right) \\
&= \sum_{i>I_{max}} w_i + \sum_{i\leq I_{max}} \frac{\sum_{i>I_{max}} w_i}{\sum_{i\leq I_{max}} w_i} \sum_k E_i^k + \sum_k \left(2a_k \wedge \sum_{i\leq I_{max}} \left|\hat{E}_i^k - \frac{1}{\sum_{i\leq I_{max}} w_i} E_i^k\right|\right) \\
&= 2\sum_{i>I_{max}} w_i + \sum_k \left(2a_k \wedge \sum_{i\leq I_{max}} \left|\hat{E}_i^k - \frac{1}{\sum_{i\leq I_{max}} w_i} E_i^k\right|\right).
\end{aligned}$$

Let us now work a little on the last term:

$$\begin{aligned}
\frac{1}{\sum_{i\leq I_{max}} w_i} E_i^k &= \int \frac{a_k}{b_k^2} f_{k,k}(x) \mathbf{1}_{i=l} \mathrm{d}p_{I_{max}}(l,x), \\
\hat{E}_i^k &= \int \frac{a_k}{b_k^2} f_{k,k}(x) \mathbf{1}_{i=l} \mathrm{d}\hat{p}(l,x).
\end{aligned}$$

So that

$$\begin{aligned}
\left|\frac{1}{\sum_{i\leq I_{max}} w_i} E_i^k - \hat{E}_i^k\right| &= \left|\int f_{k,k}(x) \mathbf{1}_{i=l} d(p_{I_{max}} - \hat{p})(l,x)\right| \\
&\leq \frac{a_k}{b_k^2} \|f_{k,k}\|_\infty \int \mathbf{1}_{i=l} \mathrm{d}|p_{I_{max}} - \hat{p}|(l,x).
\end{aligned}$$

Summing over i, we get:

$$\sum_{i\leq I_{max}}\left|\frac{1}{\sum_{i\in I_{max}} w_i}E_i^k-\hat{E}_i^k\right|\leq\frac{a_k}{b_k^2}\left\|f_{k,k}\right\|_\infty\int \mathrm{d}|p_{I_{max}}-\hat{p}|(l,x).$$

We may then bound the distance between the POVM we calibrate and our estimator by

$$d_1(P,\hat{P})=2\sum_{i>I_{max}}w_i+\sum_{k\in\mathbb{N}}\left(2a_k\wedge\left(\frac{a_k}{b_k^2}\left\|f_{k,k}\right\|_\infty\int \mathrm{d}|p_{I_{max}}-\hat{p}|(l,x)\right)\right).$$

Finishing the proof of our theorem amounts to controlling $\int \mathrm{d}|p_{I_{max}}-\hat{p}|(l,x)$. We first apply Theorem 4.2 (assuming that our penalty is big enough, which we check below). We get:

$$\mathbb{E}\left[h^2(p_{I_{max}},\hat{p}_{(\hat{I},\hat{K})})\right]\leq C\left(\inf_{I\leq I_{max},K\in\mathbb{N}}K(p_{I_{max}},m_{I,K})+\mathrm{pen}(I,K)+\frac{\Sigma}{n_{I_{max}}}\right)\cdot$$

We then use the bound (4.3) of the square of the L^1 distance in the Hellinger distance, and finish with Jensen, using the concavity of both the function $x\mapsto(C\wedge x)$ and the square root.

$$\begin{aligned}
\mathbb{E}\left[d_1(P,\hat{P}_{(\hat{I},\hat{K})})\right] &\leq \mathbb{E}\left[\sum_{i>I_{max}}w_i+\sum_{k\in\mathbb{N}}\left(2a_k\wedge\left(C\frac{a_k}{b_k^2}\left\|f_{k,k}\right\|_\infty\int \mathrm{d}|p_{I_{max}}-\hat{p}_{(\hat{I},\hat{K})}|(l,x)\right)\right)\right]\\
&\leq \sum_{i>I_{max}}w_i+\sum_{k\in\mathbb{N}}\mathbb{E}\left[\left(2a_k\wedge\left(C\frac{a_k}{b_k^2}\left\|f_{k,k}\right\|_\infty\sqrt{h^2\left(p_{I_{max}}-\hat{p}_{\hat{I},\hat{K}}\right)}\right)\right)\right]\\
&\leq \sum_{i>I_{max}}w_i+\sum_{k\in\mathbb{N}}\left(2a_k\wedge\left(C\frac{a_k}{b_k^2}\left\|f_{k,k}\right\|_\infty\sqrt{\mathbb{E}\left[h^2\left(p_{I_{max}}-\hat{p}_{\hat{I},\hat{K}}\right)\right]}\right)\right)\\
&\leq \sum_{i>I_{max}}w_i+\sum_{k\in\mathbb{N}}\left(2a_k\wedge\left(C\frac{a_k}{b_k^2}\left\|f_{k,k}\right\|_\infty\right.\right.\\
&\qquad\left.\left.\times\sqrt{\inf_{I\leq I_{max},K\in\mathbb{N}}K(p_{I_{max}},m_{I,K})+\mathrm{pen}(I,K)+\frac{\Sigma}{n_{I_{max}}}}\right)\right)\cdot
\end{aligned}$$

The only thing we still have to check is our penalty. We must dominate $H_{B,2}(\delta,\mathcal{P}^{1/2}(I,\mathcal{M}))$ where

$$\mathcal{P}^{1/2}(I,K)=\{\sqrt{q},Q\in m_{I,K}\}.$$

With the same reasoning as in Section 4, it is sufficient to dominate $H_{B,1}(\delta^2,m_{I,K})$. We then mimic Lemma 4.3. All the elements of $m_{I,K}$ are on the L^1 sphere of radius $\sum_{k\leq K}a_k$ of a vector space of dimension $(K+1)(I+1)$. We can then associate a maximal collection of brackets to a maximal collection (P_j) of $P\in m_{I,K}$ separated by $\delta^2/(2(K+1)(I+1))$. The balls $B_1(P_j,\frac{\delta^2}{(K+1)(I+1)})$ are disjoint and in the shell $B_1(0,\sum_{k\leq K}a_k+\frac{\delta^2}{(K+1)(I+1)})-B_1(0,\sum_{k\leq K}a_k-\frac{\delta^2}{(K+1)(I+1)})$. And as with equation (4.4), we obtain

$$H_{B,1}(\delta^2,m_{I,K})\leq C(K+1)(I+1)\ln\left(\frac{(K+1)(I+1)}{\delta^2}\right)\cdot$$

Imitating the calculation in the proof of Corollary 4.4, we find that the solution $\sigma_{I,K}$ of the equation

$$\sqrt{n_{I_{max}}}\sigma_{I,K}^2=\int_0^{\sigma_{I,K}}\sqrt{H_{B,2}(\delta,\mathcal{P}^{1/2}(I,K))}$$

admits this upper bound:

$$\sigma_{I,K} \le C\sqrt{\frac{(K+1)(I+1)}{n_{I_{max}}}}(1+\sqrt{\ln n_{I_{max}}})$$

We may absorb the latter 1 in the constant, as long as $n_{I_{max}} \geq 2$...

This ends the proof. □

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Appendix. Background in quantum mechanics

Section A.1 gives parallel developments of classical statistics and quantum statistics, so that any quantum notion is linked with a classical equivalent.

Section A.2 describes both the experimental setup of quantum homodyne tomography and some basic mathematics playing a role in it. More precisely, it highlights several different representations of the state to be recovered (our unknown) and the links between them.

Section A.3 is background for Section 5. Notably, it explains where the formulas such as (5.2) come from.

A.1. Statistics: classical and quantum

We have here three different parts. The aim is to highlight the equivalences in classical and quantum formalism. The first part lies then upon the classical world, the second part recast this construction as a special case of what will be our quantum formalism, and the third part describes these quantum statistics. Bold numbers refer to the same number in the other sections. They might be repeated inside a section if the same object is introduced under different forms.

In this short introduction to the subject, we shall restrict ourselves more or less to describing what physical measurements can be done and how they can be encoded mathematically. In other words, we characterize what information can be retrieved from a system.

A.1.1. Classical

In the classical setting of statistics, we are working with probability measures p **{1}** on a probability space $(\mathcal{X},\mathcal{A})$ **{2}**. For comparison, we recall that probability measures are normalized **{3}** real **{4}** non-negative **{5}** measures. Similarly measures are elements of $\mathcal{M}(\mathcal{X},\mathcal{A})$ **{6}**, the dual of $L^{\infty}(\mathcal{X},\mathcal{A})$ **{7}**.

Notice that the probability measures form a convex set, the extremal points of which are the Dirac measures **{8}** on x for $x \in (\mathcal{X},\mathcal{A})$. They may then be described by x **{9}**. If we want to draw on the analogy with physics $(\mathcal{X},\mathcal{A})$ may be viewed as a phase space, and the x would be the pure states. A general probability measure would describe a mixed state. These are systems that have a probability to be in this or that pure state. Any mixed state (probability measure) can be decomposed in a unique way over pure states (Dirac).

A statistical *model* **{10}** consists in a set of probability measures p_θ on a probability space $(\mathcal{X},\mathcal{A})$ indexed by a parameter θ, for $\theta \in \Theta$ **{11}** the *parameter space*. A statistical problem consists in determining as precisely as possible, with a meaning depending on the instance, a function of θ.

Now we must gain access at information on these θ in some way. What we have access at are random variables.

The aforementioned space $L^{\infty}(\mathcal{X},\mathcal{A})$ is the space of real bounded random variables f **{12}**. By analogy with the quantum case, we call these f *observables*. They correspond to the set of physical measurements that can be carried out on the system, to what can be "observed".

"Measuring" an observable f yields a result $f(x)$ **{13}**, with law:

$$\mathbb{P}_p\left[f \in B\right] = \int_{\mathcal{X}} \mathbf{1}_{f(x)\in B}\mathrm{d}p(x) \qquad \text{for } B \in \mathcal{B}\ \mathbf{\{14\}} \tag{A.1}$$

where $\mathcal{B}$ is the Borelian σ-algebra of $\mathbb{R}$. Notice that this result is not random for a pure state.

Notice also that the way we could see the probability measures p as elements of the dual of $L^\infty(\mathcal{X}, \mathcal{A})$ was by writing $p(f) = \int_{\mathcal{X}} f(x)\mathrm{d}p(x)$ **{15}**.

The most general type of statistic or estimator we can extract from data, including random strategies, is obtained by associating to each x a probability measure on an auxiliary space $(\mathcal{X}_a, \mathcal{A}, a)$ **{16}** and draw a final result according to this probability measure. This is equivalent (at the price of changing the auxiliary space) to measuring a function f **{17}** on a space $(\mathcal{X} \otimes \mathcal{X}_a, \mathcal{A} \otimes \mathcal{A}_a)$ **{18}** according to a probability measure $p_\theta \otimes s$ **{19}** with s independent of θ.

If we write (A.1) in this case, we get

$$\mathbb{P}_\theta\left[f \in B\right] = \int_{\mathcal{X}}\int_{\mathcal{X}_a} \mathbf{1}_{f(x,x_a)\in B}\mathrm{d}p_\theta(x)\mathrm{d}s(x_a) \qquad \text{for } B \in \mathcal{B}.$$

If we integrate out $\mathcal{X}_a$, this yields

$$\mathbb{P}_\theta\left[f \in B\right] = \int_{\mathcal{X}} f_B(x)\mathrm{d}p_\theta(x) \qquad \text{for } B \in \mathcal{B}\ \mathbf{\{20\}}$$

where

- $f_{\mathbb{R}} = \mathbf{1}$ **{21}**;
- $0 \leq f_B \leq 1$ **{22}**;
- for countable disjoint B_i, $\sum_i f_{B_i} = f_{\bigcup_i B_i}$ **{23}**.

As a remark, the result $f(x)$ is essentially a label. We could write the same formula for functions with values in other measure spaces $(\mathcal{Y}, \mathcal{B})$ than $\mathbb{R}$. Just let $\mathcal{B}$ be the σ-algebra on this space. In this way, we retrieve in particular estimators in $\mathbb{R}^d$.

Another very important remark is that if we have access to two statistics f and g, we have access to both **{24}**. Indeed suppose that f was taking its values in $(\mathcal{Y}, \mathcal{B})$ and g in $(\mathcal{Z}, \mathcal{C})$. Then take a new statistic with values in the product space $(\mathcal{Y} \otimes \mathcal{Z}, \mathcal{B} \otimes \mathcal{C})$, characterized by $h_{B\otimes C} = f_B * g_C$ as real functions on $(\mathcal{X}, \mathcal{A})$. We see that the three conditions are satisfied, and that the marginals of h are f and g.

A.1.2. From classical to quantum

The above description was already somewhat non-conventional, with the parallel with quantum formalism in mind. In this subsection, we take one further step, by setting classical probability as a special case of what will be our quantum probability theory.

To have something easy to understand, we start from a finite probability space $(\mathcal{X}, \mathcal{A}) = \{1, \ldots, d\}$ **{2}**. We associate to it the Hilbert space of complex valued functions on this space, that is $\mathcal{H} = \mathbb{C}^d$ **{2}**. We are here endowed with a distinguished orthonormal basis $\{|e_i\rangle\}_{1\leq i\leq d}$ with $|e_i\rangle$ the function whose value is one on i and zero elsewhere.

Notice by the way the notation $|\psi\rangle$: this is a physicist's notation for vectors, elements of $\mathcal{H}$. They call this a "ket". The associated linear form, that is, the adjoint of the vector, is called a "bra" and denoted $\langle\psi|$. Thus $\langle\phi|\psi\rangle$ is the scalar product of $|\phi\rangle$ and $|\psi\rangle$ (a "bracket").

Now to the probability measure $p = (p_1, \ldots, p_d)$ **{1}** on $\{1, \ldots, d\}$, we associate the matrix ρ **{1}** diagonal in our special orthonormal basis **{6}**, with diagonal entries $(p_1, \ldots, p_d)$. As this is a diagonal matrix in an orthonormal basis, with non-negative elements, this is a self-adjoint **{4}** non-negative **{5}** matrix. Moreover, as $\sum_i p_i = 1$ **{3}**, it has trace 1 **{3}**.

We see that the extremal points of our set of matrices are the orthogonal projectors on the lines spanned by our special eigenvectors, that is $|e_i\rangle\langle e_i|$ **{8}**. They correspond to the Dirac measures on i. We may represent any of these *pure states* by the eigenvector $|e_i\rangle$ **{9}**. We may also rewrite $\rho = \sum_i p_i |e_i\rangle\langle e_i|$.

A statistical *model* **{10}** consists in a set of non-negative matrices ρ_θ with trace 1, on a Hilbert space $\mathcal{H}$, diagonal in the $\{|e_i\rangle\}_i$ basis, indexed by a parameter θ, for $\theta \in \Theta$ **{11}** the *parameter space*. A statistical problem consists in determining as precisely as possible, with a meaning depending on the instance, a function of θ.

As we have done for probability measures, we identify $f \in L^\infty(\{1,\dots,d\})$ **{12,7}** with the diagonal matrix $O \in M(\mathbb{C}^d)$ **{12,7}** whose diagonal elements are the $O_{i,i} = f(i)$. This is still the dual of the set of matrices diagonal on our special basis. We view the action of ρ by taking the trace of the product with ρ. That is $p(f) = \mathrm{tr}\,(\rho O)$ **{15}**. One can see that we have only rewritten the classical formula for the expectation.

Equivalently, measuring an observable O yields as a result an eigenvalue of O **{13}**. The law of the result is given by:

$$\mathbb{P}_\rho\,[O \in B] = \mathrm{tr}\,(\rho P_{O,B}) \qquad\qquad \text{for } B \in \mathcal{B}\ \textbf{\{14\}}$$

where $P_{O,B}$ is the projection upon the space spanned by the eigenspaces of O corresponding to those eigenvalues λ of O such that $\lambda \in B$. In other words, in our case, $O = \sum_i f(i)|e_i\rangle\langle e_i|$. Then $P_{O,B} = \sum_{i|f(i)\in B} |e_i\rangle\langle e_i|$. This $P_{O,B}$ is playing the role of $\mathbf{1}_{f(x)\in B}$ in the classical setting. And we take note that $\mathrm{tr}\,(\rho P_{O,B}) = \sum_{i|f(i)\in B} p_i$, as we should obtain from the classical formula.

We can encode in the same framework the general strategies for estimators, provided that $\mathcal{X}_a$ is also finite **{16}**. The auxiliary space is then identified to $\mathcal{H}_a = \mathbb{C}^{d_a}$. We have matrices $\rho_\theta \otimes \sigma$ **{19}**, with σ independent of θ. We are allowed to use as observable O **{17}** any matrix diagonal in the same basis as these $\rho_\theta \otimes \sigma$. The procedure equivalent to the partial integration on $\mathcal{X}_a$ is then taking partial trace on $\mathcal{H}_a$ in $\mathbb{P}_\theta[O \in B] = \mathrm{tr}\,((\rho_\theta \otimes \sigma)P_{O,B})$. And this yields $\mathrm{tr}\,(\rho_\theta M(B))$ **{20}** with

- $M(\mathbb{R}) = \mathbf{1}_\mathcal{H}$ **{21}**;
- $M(B)$ is non-negative and diagonal in the $\{|e_i\rangle\}$ basis **{22}**;
- For countable disjoint B_i, $\sum_i M(B_i) = M(\bigcup_i B_i)$ **{23}**.

Here again, we see that if we have access to O_1 and O_2 characterized by the families $M_1(B)$ and $M_2(C)$, we have access to both **{24}**. Our new measurement would be characterized by $N(B \otimes C) = M_1(B)M_2(C)$ as multiplication of matrices. Notice that this set of matrices still satisfies the three above conditions. Especially, the fact that they are still non-negative stems from that they are diagonal in the same eigenbasis.

Going from classical to quantum now means throwing away our special eigenbasis $\{|e_i\rangle\}$. The immediate consequence will be that we shall deal with objects that do not commute. And of course, we did not restrain to finite probability spaces in the classical case. Likewise, we do not restrain to finite-dimensional Hilbert spaces in the quantum case. We shall therefore deal with operators rather than matrices. Keeping the finite-dimensional example firmly in mind should be a guide to the intuition of those less proficient in operator theory.

A.1.3. Quantum

A quantum system is described by a *density operator* ρ **{1}** over a Hilbert space $\mathcal{H}$ **{2}**, that is:

Definition A.1. Density operator
A density operator, usually denoted by ρ, is a trace-class linear operator on a (complex, separable) Hilbert space $\mathcal{H}$ that satisfies:

- ρ is self-adjoint **{4}**.
- ρ is non-negative (notice that this implies self-adjointness) **{5}**.
- $\mathrm{tr}\ \rho = 1$ **{3}**.

If $\mathcal{H}$ is finite-dimensional, those are just the (self-adjoint) non-negative matrices with trace 1.

We denote by $\mathcal{S}(\mathcal{H})$ the set of density operators on $\mathcal{H}$.

Density operators are a convex set, too. The extremal points are called "pure states". They are the orthogonal projectors on 1-dimensional spaces **{8}**. Thus we can represent them by a norm 1 element of $\mathcal{H}$, denoted by $|\psi\rangle$ **{9}**. The corresponding density matrix is then $\rho = |\psi\rangle\langle\psi|$. Notice that it would be more precise to speak of $|\psi\rangle$ as an element of the projective space $\mathcal{PH}$, but we conform here to the usage of physicists. Notice also that there are infinitely many pure states even in the finite-dimensional case, unlike in the classical framework. Let us finally signal that the decomposition of a mixed state on pure states is *not* unique. It is essentially unique if we further impose that the pure states of the decomposition are all orthogonal, though.

A quantum statistical *model* **{10}** consists in a set of density operators ρ_θ on a Hilbert space $\mathcal{H}$ indexed by a parameter θ, for $\theta \in \Theta$ **{11}** the *parameter space*. A statistical problem consists in determining as precisely as possible, with a meaning depending on the instance, a function of θ.

Now the role of random variables is played by observables. Those are the elements O **{12}** of $\mathcal{B}_{sa}(\mathcal{H})$ **{7}**, the bounded self-adjoint operators upon $\mathcal{H}$. If we are dealing with finite-dimensional $\mathcal{H}$, those are the self-adjoint matrices.

As a remark, the dual of $\mathcal{B}_{sa}(\mathcal{H})$ is the set of self-adjoint trace-class operators, which ρ is in. This duality is given by the formula of the expectation of measuring O on ρ, also called *Born's rule*:

$$\mathbb{E}_\rho[O] = \operatorname{tr}(\rho O) \quad \textbf{\{15\}} \tag{A.2}$$

when measuring O, the result is an element of the spectrum of O **{13}**, that is in the finite-dimensional picture, an eigenvalue of O. The law of the result when measuring O on ρ is:

$$\mathbb{P}_\rho\left[O \in B\right] = \operatorname{tr}\left(\rho P_{O,B}\right) \qquad \text{for } B \in \mathcal{B} \ \textbf{\{14\}} \tag{A.3}$$

where $P_{O,B}$ is coming from the spectral measure of O. This is an object associated to self-adjoint operators through the spectral theorem, whose main property is that the expectation of the law above is given by the Born's rule for any density operator ρ. We only give the derivation for finite-dimensional $\mathcal{H}$. Then, as O is self-adjoint, we can diagonalize it in an orthonormal basis, and write $O = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$. Then $P_{O,B} = \sum_{i|\lambda_i \in B} |\psi_i\rangle\langle\psi_i|$. We see that in this case the law of the measurement is coherent with the expectation given by Born's rule (A.2).

Generally $\{P_{O,B}\}_B$ is a projector valued measure, the definition of which we give below. To each projector valued measure corresponds an observable, and to each observable corresponds a projector valued measure. We may then consider that this concept is also a definition of an observable.

Definition A.2. Projector valued measure {12}
A projector operator valued measure $\{P(B)\}_{B\in\mathcal{B}}$ is a set of operators on $\mathcal{H}$ such that:

- $P(B)$ is an orthogonal projector.
- $P(\mathbb{R}) = \mathbf{1}_{\mathcal{H}}$.
- For disjoint countable B_i, $\sum_i P(B_i) = P(\bigcup_i B_i)$.

Notice that these are the axioms of a probability measure, except that we do not deal with real numbers but with projection operators.

Combining this definition with the definition of a density operator, we can check that formula (A.3) yields a true probability measure. Indeed, as both ρ and $P_{O,B}$ are non-negative, the probability of any event is non-negative. With the countable additivity property of projector valued measure and linearity of product and trace, we get the countable additivity of a probability measure. Finally, the probability of the universe is $\operatorname{tr}(\rho P_{O,\mathbb{R}}) = \operatorname{tr}(\rho \mathbf{1}_{\mathcal{H}}) = 1$.

Remark. Even for a pure state, the result of the measurement is random, unless the pure state is an eigenvector of O.

Now what is the most general estimation strategy, or measurement? The right analogy is that of the auxiliary space. We measure observables O **{17}** on a Hilbert space $\mathcal{H} \otimes \mathcal{H}_a$ **{18}** under the density operator $\rho_\theta \otimes \sigma$ **{19}**, with σ independent of θ. Now we may take partial trace in (A.3) along $\mathcal{H}_a$, and we obtain equivalence of this scheme with measuring a *positive operator valued measure* (POVM).

Definition A.3. Measurement (POVM) {17}

A measurement M on a quantum system, taking values x in a measurable space $(\mathcal{X}, \mathcal{A})$ is specified by a *positive operator valued probability measure* or *POVM* for short, that is a collection of self-adjoint matrices $M(A) : A \in \mathcal{A}$ such that:

- $M(\mathcal{X}) = \mathbf{1}$, the identity matrix **{21}**.
- Each $M(A)$ is non-negative **{22}**.
- For disjoint countable A_i, $\sum_i M(A_i) = M(\bigcup A_i)$ **{23}**.

The $M(A)$ are called the *POVM elements.*

The law of measuring M on ρ is given by

$$\mathbb{P}_\rho [O \in A] = \mathrm{tr}\,(\rho M(A)) \qquad \text{for } A \in \mathcal{A} \ \mathbf{\{20\}}. \tag{A.4}$$

With the same reasoning as for projector valued measure (which are a special case of these POVMs), this is a genuine probability measure.

A special case of POVM is that of a POVM dominated by σ-finite measure ν on $(\mathcal{X}, \mathcal{A})$, that is

$$M(A) = \int_A m(x) \mathrm{d}\nu(x) \text{ for all } A \in \mathcal{A} \tag{A.5}$$

where $m(x)$ is positive for all x and $\int_{\mathcal{X}} m(x)\mathrm{d}\nu(x) = \mathbf{1}_{\mathcal{H}}$. The POVM associated to homodyne tomography is dominated by the Lebesgue measure.

The very important difference with the classical world is that if we can have access to M_1 or M_2, in general, we cannot have access to both simultaneously **{24}**. We cannot copy what we have done in the former paragraph, since $M_1(A)M_2(B) + M_2(B)M_1(A)$ might not be non-negative if $M_1(A)$ and $M_2(B)$ do not commute. More generally, there is usually no way to create a new POVM N with values in $(\mathcal{X} \otimes \mathcal{Y}, \mathcal{A} \otimes \mathcal{B})$ such that the marginals are M_1 and M_2. Notably, two observables that do not commute can never be measured simultaneously. As an example, consider that M_1 and M_2 are two projector valued measures on $\mathbb{C}^2$, each with values in $\{0, 1\}$, corresponding to observables diagonal in different bases $\{e_0, e_1\}$ and $\{f_0, f_1\}$. Then $N(0, 0)$ should be proportional both to $|e_0\rangle\langle e_0|$ and $|f_0\rangle\langle f_0|$. So that it is null. Same remark for the other $N(i, j)$. Thus $N(\{0, 1\}^{\otimes 2}) = 0 \neq \mathbf{1}$. So that it is null.

The truly quantum feature of quantum statistics lies in that we should decide which measurement is to be carried out. Once we have chosen our measurement, we are left through (A.4) with a classical statistical experiment. This is the case in this article.

As a last remark on the subject, we could have developed a slightly more general formalism, based on C^*-algebras, that would have been parallel to Le Cam formulation of statistics. In practical applications, the formalism above is usually sufficient.

A.2. Quantum homodyne tomography

The system we work with is the harmonic oscillator. Both in classical or quantum mechanics, the harmonic oscillator is a basic and pervading system. It describes, notably, a particle on a line, or a mode of the electromagnetic field (that is monochromatic light), as in our case.

The state of a quantum harmonic oscillator is described by an operator on $L^2(\mathbb{R})$ (this is the Hilbert space **{1}**). There are two important observables corresponding to the canonical coordinates of the particle. If we know the expectation of measuring on a state ρ any operator in the algebra they generate, then we know ρ. Those observables are $\mathbf{P}$, the magnetic field, and $\mathbf{Q}$, the electric field. They satisfy the (canonical) commutation relations:

$$\begin{aligned}[\mathbf{Q}, \mathbf{P}] &= \mathbf{QP} - \mathbf{PQ} \\ &= i\mathbf{1}.\end{aligned}$$

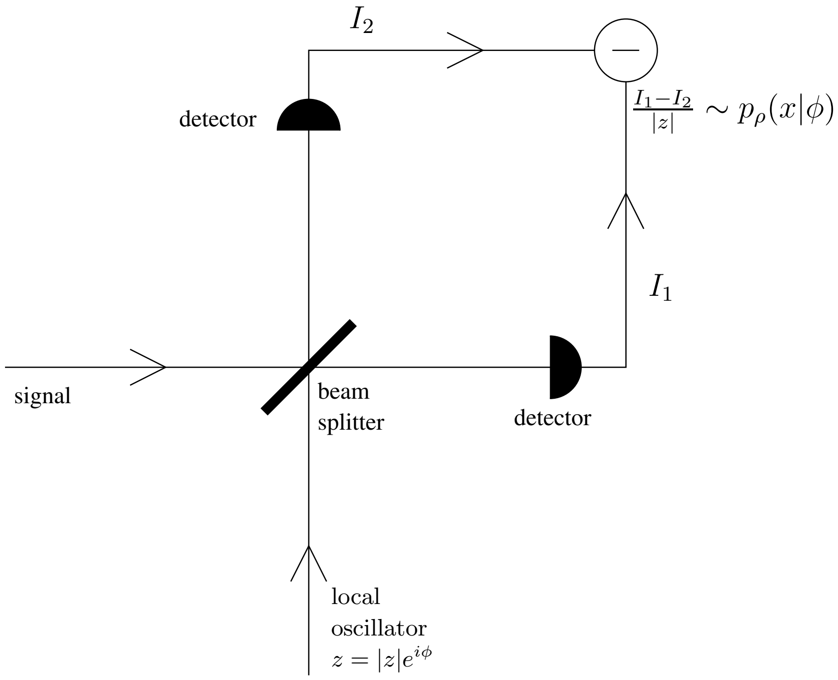

FIGURE 2. Quantum homodyne tomography measurement set-up.

They are realized as:

$$\begin{aligned}(\mathbf{Q}\psi_1)(x) &= x\psi_1(x)\\ (\mathbf{P}\psi_2)(x) &= -i\frac{\mathrm{d}\psi_2(x)}{\mathrm{d}x}\cdot\end{aligned} \tag{A.6}$$

As they do not commute, they cannot be measured simultaneously. However, any linear combination can theoretically be measured. These $\mathbf{X}_\phi = \sin(\phi)\mathbf{Q} + \cos(\phi)\mathbf{P}$ are called *quadratures*.

Using an experimental setup proposed in [21], each of these quadratures could be experimentally measured on a laser beam [20]. The technique is called *quantum homodyne tomography*.

The optical set-up sketched in Figure 2 consists of an additional laser of high intensity $|z| \gg 1$ called the local oscillator, a beam splitter through which the cavity pulse prepared in state ρ is mixed with the laser, and two photodetectors each measuring one of the two beams and producing currents $I_{1,2}$ proportional to the number of photons. An electronic device produces the result of the measurement by taking the difference of the two currents and rescaling it by the intensity $|z|$. A simple quantum optics computation in [17] shows that if the relative phase between the laser and the cavity pulse is chosen to be ϕ then $(I_1 - I_2)/|z|$ has density $p_\rho(x|\phi)$ corresponding to measuring $\mathbf{X}_\phi$.

Knowledge of $P_\rho(x|\phi)$, the law of the result of the measurement $\mathbf{X}_\phi$ on ρ, for all ϕ, is enough to reconstruct the state ρ. As we have seen, the experimentalist may choose ϕ when measuring. We assume that the measurement carried out on each of the n systems in state ρ is the following: first choose ϕ uniformly at random, then measure $\mathbf{X}_\phi$. We get a random variable $\mathbf{Y} = (\mathbf{X}, \Phi)$ with values in $\mathbb{R} \times [0, \pi)$ whose density with respect to the Lebesgue measure is $p_\rho(x, \phi) = \frac{1}{\pi} p_\rho(x|\phi)$.

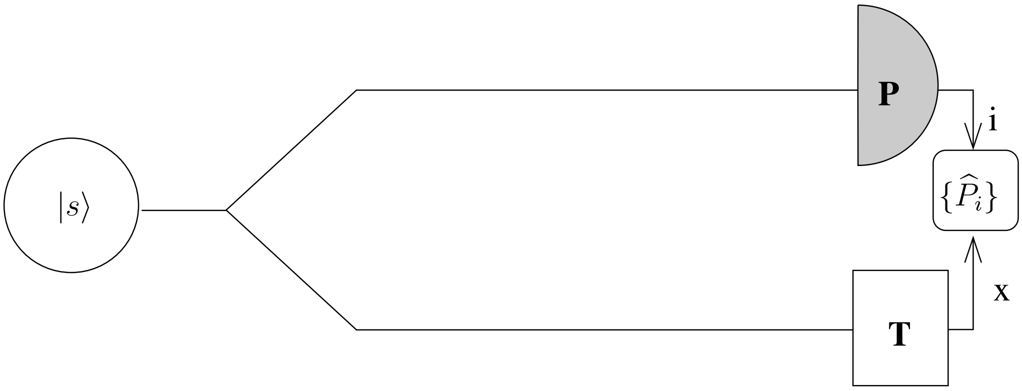

FIGURE 3. Experimental set-up to determine the POVM associated to an unknown photocounter **P**. We use it to measure a known bipartite state $|s\rangle$, jointly with a tomographer **T**. The photocounter gives a result i and the tomographer a result x. From these samples, we construct an estimator $\{\hat{P}_i\}$ of the self-adjoint operators associated to the results $\{i\}$ by the photocounter **P**.

Now we make explicit the links between ρ, $p_\rho(x,\phi)$ and the Wigner function W_ρ. First we write ρ in a particular basis, physically very meaningful, the *Fock basis*, already given in Section 2:

$$\psi_k(x) = H_k(x)\mathrm{e}^{-x^2/2},$$

where H_k is the kth Hermite polynomial, normalized so that the L^2 norm of ψ_k is 1. The projector on ψ_k is the pure state with precisely k photons. We also denote this state by the ket $|k\rangle$.

The matrix entries of p_ρ in this basis are $\rho_{j,k} = \langle \psi_j, \rho\psi_k\rangle$. We can then derive from (A.2) and (A.6) the formula we gave in Section 2:

$$\begin{aligned} \mathbf{T} : \mathcal{S}(L^2(\mathbb{R})) &\longrightarrow L^1(\mathbb{R}\times[0,\pi]) \\ \rho &\mapsto \left(p_\rho : (x,\phi) \mapsto \sum_{j,k=0}^{\infty} \rho_{j,k}\psi_j(x)\psi_k(x)\mathrm{e}^{-i(j-k)\phi}\right). \end{aligned} \tag{A.7}$$

The mapping $\mathbf{T}$ associating P_ρ to ρ is invertible, so we may hope to find ρ from the independent identically distributed results $Y_1, Y_2, \ldots, Y_n$ of the measurements of the n systems in state ρ. This implies notably that p_ρ is another representation of the state.

More explicitly, there are *pattern functions* $f_{j,k}$ [7] against which to integrate p_ρ to find any matrix entry of ρ in the Fock basis, that is:

$$\rho_{j,k} = \int_{-\infty}^{\infty} \mathrm{d}x \int_0^{\pi} \frac{\mathrm{d}\phi}{\pi} p_\rho(x,\phi) f_{j,k}(x)\mathrm{e}^{i(j-k)\phi}.$$

These $f_{j,k}$ are bounded real functions. That inverting the Radon transform is an ill-posed problem can be seen in the behaviour of $f_{j,k}$ when j and k go to infinity. Several formulas were found for these functions [18], among which:

$$f_{j,k}(x) = \frac{\mathrm{d}}{\mathrm{d}x}(\chi_j(x)\phi_k(x)) \tag{A.8}$$

for $k \geq j$, where χ_j and ϕ_k are respectively the square-integrable and the unbounded solutions of the Schrödinger equation:

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{1}{2}x^2\right]\psi=\omega\psi, \quad \omega\in\mathbb{R}.$$

Another one, maybe more practical when it comes to theoretical calculations, or when we add noise (see Sect. 3.6) is:

$$f_{j,k}(x,\phi)=\sqrt{\frac{j!}{k!}}\int_{-\infty}^{\infty}|r|\mathrm{e}^{-\frac{r^2}{2}+2irx}r^{k-j}L_j^{k-j}(r^2)\mathrm{d}r$$

where the L_j^d are the Laguerre polynomials, that is the orthogonal polynomials with respect to the measure $\mathrm{e}^{-x}x^d$ on $\mathbb{R}^+$.

Let's now have a look at the Wigner function. This is a real function of two variables, with integral 1, but that may be negative in places. It can be interpreted as a generalized joint probability density of the electric and magnetic fields q and p. As both cannot be measured simultaneously, the negative patches are not nonsense. On the other hand, any projection on a line of the Wigner function must be a true probability density, as it is the law of $\mathbf{X}_\phi$, which is an observable. In fact, the Wigner function may be seen as the probability density on $\mathbb{R}^2$ resulting from (A.4) when measuring on ρ a "POVM" whose elements are not non-negative, but whose marginals on each line $\mathbb{R}$ are the X_ϕ.

As we have already said in the introduction, p_ρ is the Radon transform of the Wigner function. The Wigner function can be defined by its Fourier transform. This definition tells how to find the Wigner function W of the state from its density matrix ρ:

$$\mathcal{F}_2W(u,v)=\operatorname{tr}\left(\rho\mathrm{e}^{-iu\mathbf{Q}-iv\mathbf{P}}\right). \tag{A.9}$$

On the other hand, the generating function of $p_\rho(\cdot|\phi)$ is

$$\mathbb{E}\left[\mathrm{e}^{itX_\phi}\right] = \operatorname{tr}\left(\rho\mathrm{e}^{it\mathbf{X}_\phi}\right).$$

In other words, $\mathcal{F}_2W(t\cos\phi,t\sin\phi)=\mathcal{F}[p_\rho(\cdot,\phi)](t)$. These relations are known to imply that $p_\rho=\mathbf{R}(W)$ [10] where $\mathbf{R}$ is the Radon transform. Explicitly:

$$p_\rho(x,\phi) = \int_{-\infty}^{\infty}W(x\cos\phi+y\sin\phi,x\sin\phi-y\cos\phi)\mathrm{d}y.$$

The Radon transform is illustrated by Figure 1, given in Section 2.

Finding the Wigner function from the data means then inverting the Radon transform, hence the name of tomography: that is the same mathematical problem as with the brain imagery technique called Positron Emission Tomography.

A.3. Physical origin of the photocounter calibration problem

An experiment usually ends with a measurement. We need, however, an apparatus to measure. And we first have to know what is the meaning of the result the apparatus is giving us: it is not at all obvious *a priori* that if our new thermometer says "31 °C", the temperature cannot be "32 °C". That is why we must *calibrate* our measurement apparatus. In quantum mechanics, this means associating with each result i of our measurement the positive operator $P(i)$, such that P is the POVM (see definition 5.3) corresponding to our measurement.

In [9], a general calibration procedure was introduced. The procedure relies on comparing with an already calibrated apparatus, using entangled states. Let us describe this more precisely in the special case of the photocounter.

A photocounter is an apparatus that aims at counting the photons in a beam. The ideal detector D has therefore POVM elements given by $D(i)=|i\rangle\langle i|$ in the Fock basis. Recall we use the physicists' notation, where $|\cdot\rangle$ is a vector and $\langle\cdot|$ is the associated linear form. Moreover $|i\rangle$ is the vector corresponding to the pure state with i photons, that is the function ψ_i on $L^2(\mathbb{R})$, that we had defined in (2.1).

Models of the noise (non-unit efficiency and dark current) leave the POVM diagonal in this basis. Thus, we are only interested in the diagonal elements of P_i in the Fock basis. To obtain those we send a twin beam state, one of the beams in the photocounter, the other in a homodyne tomographer. We get a result I from the photo-counter, and X from the tomographer (Fig. 3; as we are only interested in the diagonal elements, we shall see that we do not need the phase ϕ, as long as the experimentalist chooses it randomly). We then have to process these outcomes (I, X) to find P.

Mathematically, the twin beam is a system in a state $|s\rangle = \sum_{k=0}^{\infty} b_k |k\rangle \otimes |k\rangle$. This notation (where we may choose the b_k non-negative) means that the underlying Hilbert space is $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$, and that ρ is the pure state that projects on the line spanned by this vector. Here again, $|k\rangle$ is the vector corresponding to the pure state with k photons. Finally $\sum_k b_k^2 = 1$, so that the vector state $|s\rangle$ is normalized and the density operator is $\rho = |s\rangle\langle s|$.

Now, what is the law $p(i, x)$ of the samples we get? By (A.7) we see that the POVM associated to the tomographer is dominated by the Lebesgue measure on $\mathbb{R}\times[0, \pi)$, as in (A.5). That is $\langle j|t_{x,\phi}|k\rangle = \psi_j(x)\psi_k(x)\mathrm{e}^{-i(j-k)\phi}$, where we have denoted $t_{x,\phi}$ the self-adjoint operator associated to the result (x, ϕ) for the POVM of the tomographer. If we forget about ϕ after having chosen it randomly, we then get $\langle j|t_x|k\rangle = \psi_k(x)^2 \mathbf{1}_{j=k}$. We have now all the ingredients for calculating our law, given the notation $\langle k|M_i|k\rangle = M_i^k$.

$$\begin{aligned}
p(i, x) &= \mathrm{tr}\left(\rho(P_i \otimes t_x)\right) \\
&= \langle s|(P_i \otimes t_x)|s\rangle \\
&= \sum_{k_1,k_2} b_{k_1} b_{k_2} (\langle k_1| \otimes \langle k_1|)(P_i \otimes t_x)(|k_2\rangle \otimes |k_2\rangle) \\
&= \sum_{k_1,k_2} b_{k_1} b_{k_2} \langle k_1|P_i|k_2\rangle\langle k_1|t_x|k_2\rangle \\
&= \sum_{k=0}^{\infty} b_k^2 P_i^k \psi_k(x)^2.
\end{aligned}$$

(As a remark, the fourth line shows that the use of the phase would be to retrieve the non-diagonal elements, in which we are not interested.)

We have thus recovered (5.1), and explained how we got the data with which we want to estimate the M_i^m.

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