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Iterative maximum-likelihood reconstruction in quantum homodyne tomography

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Abstract
I propose an iterative expectation maximization algorithm for reconstructing
the density matrix of an optical ensemble from a set of balanced homodyne
measurements. The algorithm applies directly to the acquired data,
bypassing the intermediate step of calculating marginal distributions. The
advantages of the new method are made manifest by comparing it with the
traditional inverse Radon transformation technique.

Keywords: quantum state reconstruction, quantum homodyne tomography,
maximum likelihood

Quantum tomography is a technique of characterizing a state
of a quantum system by subjecting it to a large number of
quantum measurements, each time preparing the system anew.
By varying the configuration of the measurement apparatus,
one acquires the quantum statistics associated with different
bases from which complete information about the state of the
system can be extracted.

The ensemble's density matrix can be evaluated from the
experimental statistical data by a number of techniques. In this
paper we are dealing with one such technique, the *maximum
likelihood* (MaxLik) estimation. Assuming a particular density
matrix $\hat{\rho}$, one can evaluate the likelihood (probability) of
acquiring a particular set of measurement results. The ansatz of
the MaxLik method is to find, among the variety of all possible
density matrices, the one which maximizes the probability
of obtaining the given experimental data set. To date, this
method has been applied to various quantum and classical
problems from quantum phase estimation [1] to reconstruction
of entangled optical states [2, 3].

In the present work we discuss applications of likelihood
maximization to *quantum homodyne tomography*—a method
of characterizing a quantum state of an optical mode by
means of multiple phase-sensitive measurements of its electric
field's quantum noise. Since its proposal [4] and first
experimental implementation [5] in the early 1990s, quantum
homodyne tomography has become a robust and versatile

tool of quantum optics and has been applied in many
different experimental settings. As any statistical method,
it is compatible with the likelihood maximization approach.
Yet so far experimentalists have used a clumsier and less
accurate reconstruction algorithms based on the inverse Radon
transformation. The goal of this paper is to provide an explicit
numerical recipe for the MaxLik reconstruction of a quantum
state from homodyne data and to demonstrate its advantages
by applying it to *bona fide* experimental results.

The applications of the MaxLik estimation to homodyne
tomography have been investigated by Banaszek, who has
reconstructed the photon-number distribution (the diagonal
density matrix elements which correspond to a phase-
randomized optical ensemble) from a Monte Carlo simulated
data set [6, 7]. In a subsequent publication [8], Banaszek
et al discussed the MaxLik estimation of the complete density
matrix, but no explicit reconstruction algorithm has been
presented.

The iterative scheme outlined here is based on that
elaborated by Hradil *et al* for discrete-variable states [2, 9–
11]. Here we give its brief overview. Consider a large set
of von Neumann measurements, each one projecting the state
of the system onto an eigenstate of a measurement apparatus
$|y_j\rangle$. The set of all possible outcomes $\{|y_j\rangle\}$ can be associated
with either one or several measurement bases. Let f_j be
the frequency of occurrences for each outcome. Then, with
the system being in the quantum state $\hat{\rho}$, the likelihood of a

particular data set $\{f_j\}$ is

$$\mathcal{L}(\hat{\rho}) = \prod_j \mathrm{pr}_j^{f_j}, \qquad (1)$$

where $\mathrm{pr}_j = \langle y_j | \hat{\rho} | y_j \rangle = \mathrm{Tr}[\hat{\Pi}_j \hat{\rho}]$ is the probability of the outcome $|y_j\rangle$ and $\hat{\Pi}_j = |y_j\rangle\langle y_j|$ denotes the projection operator.

To find the ensemble $\hat{\rho}$ which maximizes the likelihood (1), one introduces the operator

$$\hat{R}(\hat{\rho}) = \sum_j \frac{f_j}{\mathrm{pr}_j} \hat{\Pi}_j \qquad (2)$$

and notices that for the ensemble ρ_0 that is most likely to produce the observed data set, $f_j \propto \mathrm{pr}_j$. Furthermore, since the $\sum_j \hat{\Pi}_j \propto \hat{1}$, we find $\hat{R}(\hat{\rho}_0) \propto \hat{1}$ and thus

$$\hat{R}(\hat{\rho}_0)\hat{\rho}_0 = \hat{\rho}_0 \hat{R}(\hat{\rho}_0) \propto \rho_0 \qquad (3)$$

as well as

$$\hat{R}(\hat{\rho}_0)\hat{\rho}_0 \hat{R}(\hat{\rho}_0) \propto \rho_0. \qquad (4)$$

The last relation forms the basis for the iterative algorithm. We choose some initial density matrix as, e.g., $\hat{\rho}^{(0)} = \mathcal{N}[\hat{1}]$, and apply repetitive iterations

$$\hat{\rho}^{(k+1)} = \mathcal{N}[\hat{R}(\hat{\rho}^{(k)})\hat{\rho}^{(k)}\hat{R}(\hat{\rho}^{(k)})], \qquad (5)$$

where $\mathcal{N}$ denotes normalization to a unitary trace. Each step will monotonically increase the likelihood associated with the current density matrix estimate, while the latter will asymptotically approach the maximum-likelihood ensemble $\hat{\rho}_0$.[2] This iterative scheme can be viewed as a special case of the classical expectation-maximization algorithm [12].

Now we turn to the main subject of the paper and consider a homodyne tomography experiment performed on an optical mode prepared in some quantum state $\hat{\rho}$. In an experimental run one measures the field quadrature at various phases of the local oscillator. Each measurement is associated with the observable $\hat{X}_\theta = \hat{X}\cos\theta + \hat{P}\sin\theta$, where $\hat{X}$ and $\hat{P}$ are the canonical position and momentum operators and θ is the local oscillator phase.

For a given phase θ, the probability of detecting a particular quadrature value x is proportional to

$$\mathrm{pr}_\theta(x) = \mathrm{Tr}[\hat{\Pi}(\theta, x)\hat{\rho}], \qquad (6)$$

where $\hat{\Pi}(\theta, x) = |\theta, x\rangle\langle\theta, x|$ is the projector onto this quadrature eigenstate. In the Fock (photon number state) basis, the projection operator is expressed as

$$\Pi_{mn}(\theta, x) = \langle m|\hat{\Pi}(\theta, x)|n\rangle = \langle m|\theta, x\rangle\langle\theta, x|n\rangle, \qquad (7)$$

where the overlap between the number and quadrature eigenstates is given by the well known stationary solution of the Schrödinger equation for a particle in a harmonic potential:

$$\langle n|\theta, x\rangle = \mathrm{e}^{in\theta}\left(\frac{2}{\pi}\right)^{1/4}\frac{H_n(\sqrt{2}x)}{\sqrt{2^n n!}}\exp(-x^2), \qquad (8)$$

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[2] We base our iteration scheme on equation (4) rather than (3) in order to ensure the positivity of the density matrix at each step.

with H_n denoting the Hermite polynomials[3].

Because a homodyne measurement generates a continuous value, one cannot apply the iterative scheme (5) directly to the experimental data. One way of dealing with this difficulty is to discretize the data by binning it up according to θ and x and counting the number of events $f_{\theta,x}$ belonging to each bin. In this way, a number of histograms, which represent the marginal distributions of the desired ensemble's Wigner function, can be constructed. They can then be used to implement the above reconstruction procedure.

However, discretization of continuous experimental data will inevitably lead to a loss of precision. To lower this loss, one needs to reduce the size of a single bin and increase the number of bins. In the limiting case of infinitely small bins, $f_{\theta,x}$ takes on the values of either 0 or 1, so the likelihood of a data set $\{(\theta_i, x_i)\}$ is given by

$$\ln\mathcal{L} = \sum_i \ln\mathrm{pr}_{\theta_i}(x_i), \qquad (9)$$

and the iteration operator (2) becomes

$$\hat{R}(\hat{\rho}) = \sum_i \frac{\hat{\Pi}(\theta_i, x_i)}{\mathrm{pr}_{\theta_i}(x_i)}, \qquad (10)$$

where $i = 1 \ldots N$ enumerates individual measurements. The iterative scheme (5) can now be applied to find the ensemble which maximizes the likelihood (9).

In practice, the iteration algorithm is executed with the density matrix in the photon number (Fock) representation. Since the Hilbert space of optical states is of infinite dimension, the implementation of the algorithm requires its truncation so the Fock terms above a certain threshold are excluded from the analysis. This assumption conforms to many practical experimental situations in which the intensities of fields involved are *a priori* limited.

It is instructive to compare the maximum likelihood quantum state estimation with the traditional methods employed in homodyne tomography: reconstruction of the Wigner function by means of the inverse Radon transformation [13] and evaluation of the density matrix using quantum state sampling [14, 15]. Figure 1 shows application of these two techniques to the experimental data from [16]. The data set consists of 14 152 quadrature samples of an ensemble approximating a coherent superposition of the single-photon and vacuum states.

The reconstruction shown in the figure reveals the advantages of the MaxLik technique in comparison with the standard algorithm. First, the finite amount and a discrete character of the data available leads necessarily to statistical noise which prevents one from extracting complete information about a quantum state of infinite dimensions. To deal with this issue, both techniques apply certain assumptions to the ensemble to be reconstructed. While the MaxLik algorithm truncates the Fock space, the filtered back-projection

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[3] Normalization $[\hat{x}, \hat{p}] = \mathrm{i}/2$ is used. The additional phase factor $\mathrm{e}^{in\theta}$ originates from the properties of the phase-space rotation operator [13] $\hat{U}(\theta) = \mathrm{e}^{-i\theta\hat{n}}$. From $\hat{U}^\dagger(\theta)\hat{a}\hat{U}(\theta) = \hat{a}\mathrm{e}^{-i\theta}$ we find for the quadrature operator $\hat{U}^\dagger(\theta)\hat{X}\hat{U}(\theta) = \hat{X}_\theta$ and for its eigenstate $|\theta, x\rangle = \hat{U}^\dagger|0, x\rangle$. From the first and last relations above, we obtain $\langle m|\theta, x\rangle = \mathrm{e}^{i\theta m}\langle m|0, x\rangle$. The quantity $\langle m|0, x\rangle$ is the energy eigenwavefunction of a harmonic oscillator.
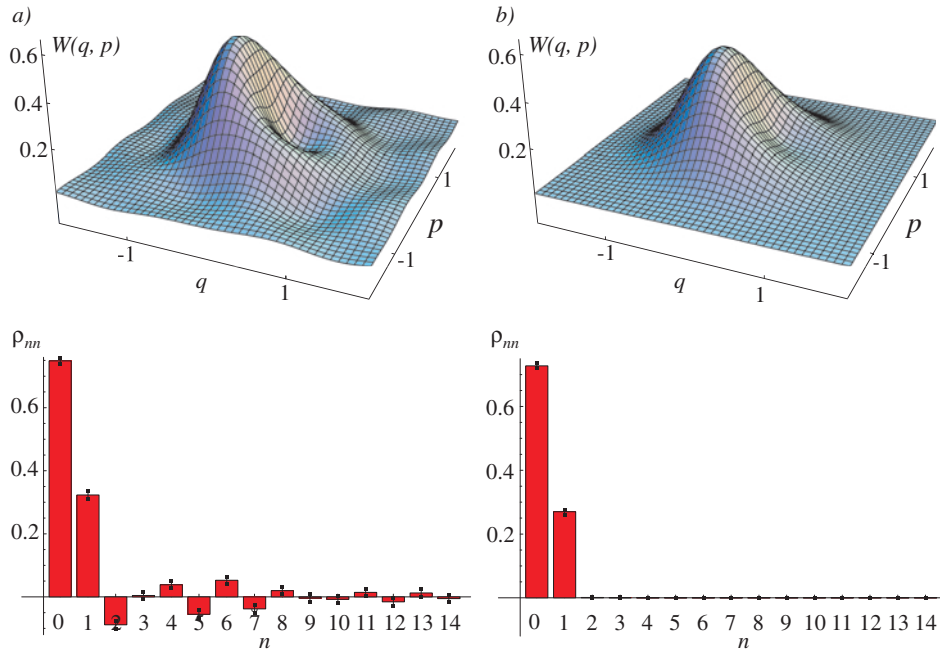
Figure 1. Estimation of an optical ensemble from a set of 14 152 experimental homodyne measurements [16] by means of the inverse Radon transformation (a) and the likelihood maximization algorithm (b). The Wigner function and the diagonal elements of the reconstructed density matrix are shown. The inverse Radon transformation in (a) was performed by means of the filtered back-projection algorithm with the cutoff frequency of 6.3. The statistical uncertainties in (b) were determined by means of a Monte Carlo simulation (see text).

(This figure is in colour only in the electronic version)

imposes low pass filtering onto the Fourier image of the Wigner function[4], i.e. assumes the ensemble to possess a certain amount of 'classicality' [17]. The latter assumption is dictated by mathematical convenience and is much less physically founded than the former. The ripples visible in the Wigner function reconstruction in figure 1(a) are a direct consequence of statistical noise and are associated with unphysical high number terms in the density matrix. Such ripples are typical of the inverse Radon transformation [18, 19].

Second, the back-projection algorithm does not impose any *a priori* restrictions on the reconstructed ensemble. This may lead to unphysical features in the latter, such as negative diagonal elements of the density matrix in figure 1(a). The MaxLik technique, on the other hand, allows us to incorporate the positivity and unity-trace constraints into the reconstruction procedure, thus always yielding a physically plausible ensemble [6, 7].

A third important advantage of the MaxLik technique is the possibility of incorporating the detector inefficiencies. In a practical experiment, the photodiodes in the homodyne detector are not 100% efficient, i.e. they do not transform every incident photon into a photoelectron. This leads to a distortion of the quadrature noise behaviour which needs to be corrected for in the reconstructed ensemble.

A common model for a homodyne detector of non-unitary efficiency η is a perfect detector preceded by a fictitious beam splitter of transmission η. The reflected mode is lost so the incident density matrix undergoes, in transmission through

the imaginary beam splitter, a so-called generalized Bernoulli transformation [13]:

$$\langle m|\hat{\rho}_\eta|n\rangle = \sum_{k=0}^{\infty} B_{m+k,m}(\eta) B_{n+k,n}(\eta) \langle m+k|\hat{\rho}_0|n+k\rangle, \quad (11)$$

where $\hat{\rho}_0$ and $\hat{\rho}_\eta$ are the density matrices of the original and transmitted ensembles, respectively, and $B_{n+k,n} = \sqrt{\binom{n+k}{n}\eta^n(1-\eta)^k}$. Under these circumstances the probability (6) of detecting a quadrature value x becomes

$$\mathrm{pr}_\theta^\eta(x) = \langle \theta, x|\hat{\rho}_\eta|\theta, x\rangle$$

$$= \sum_{m,n=0}^{\infty} \sum_{k=0}^{\infty} B_{m+k,m}(\eta) B_{n+k,n}(\eta) \langle n|\theta, x\rangle\langle \theta, x|m\rangle$$

$$\times \langle m+k|\hat{\rho}_0|n+k\rangle, \quad (12)$$

so the projection operator $\hat{\Pi}(\theta, x)$ becomes replaced by a POVM element given by

$$\hat{E}_\eta(\theta, x) = \sum_{m,n,k} B_{m+k,m}(\eta) B_{n+k,n}(\eta) \langle n|\theta, x\rangle\langle \theta, x|m\rangle$$

$$\times |n+k\rangle\langle m+k|. \quad (13)$$

Aware of the homodyne detector efficiency η, one runs the iterative algorithm (5) and reconstructs the original density matrix $\hat{\rho}_0$ [8].

Theoretically, it is also possible to correct for the detector inefficiencies by applying the inverted Bernoulli transformation *after* an efficiency-uncorrected density matrix has been reconstructed [20]. However, this may give rise to unphysically large density matrix elements associated with high photon numbers. With the inefficiency correction incorporated, as described above, into the reconstruction procedure, such terms do not arise [7].

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[4] The pattern function reconstruction of the density matrix is free from this drawback as it does not involve spectral filtering and relies on truncating the Fock space instead.

It is interesting to discuss the MaxLik reconstruction of the density matrix in comparison with the point-by-point reconstruction of the Wigner function as proposed in [21]. To determine the value of the Wigner function at a specific point (p, q) in the phase space, [21] proposes to apply a phase-dependent shift to the experimental data which corresponds to a displacement of the point (p, q) to the phase space origin. Then one reconstructs a phase-averaged ensemble according to [6, 7], and calculates the value of the Wigner function at the origin of the displaced phase space, which is equal to that at the desired location in the undisplaced phase space.

This scheme may appear more involved than the one proposed here, as one needs to run a separate iteration series for every point in which the Wigner function is to be calculated. However, due to a smaller number of parameters and a simplified iteration step, each iteration takes less time and the series converges faster. The choice of a particular scheme depends on a specific task and on the chosen truncation threshold in the Fock space. It is important to note that the scheme [21] does not impose any *a priori* restrictions on the ensemble being reconstructed, and therefore the latter is not guaranteed to be physically meaningful.

Finally, we discuss statistical uncertainties of the reconstructed density matrix. In generic MaxLik algorithms, they are typically estimated as an inverse of the Fisher information matrix [22, 23] $G = \partial^2 \mathcal{L}(\vec{t})/\partial \vec{t}\, \partial \vec{t}'$, where $\vec{t}$ denotes a set of independent parameters with respect to which the likelihood is evaluated. Because the density matrix elements are not fully independent but bound by the positivity and unity trace constraints, one expresses the density matrix as a product $\hat{\rho} = \hat{T}^\dagger \hat{T}/\mathrm{Tr}[\hat{T}^\dagger \hat{T}]$. Now the constraints for $\hat{\rho}$ are satisfied for any random $\hat{T}$ and one can regard the elements of the latter as free parameters in evaluating the Fisher information [8, 24].

A sensible alternative is offered by a clumsy, yet simple and robust technique of *simulating* the quadrature data that would be associated with the estimated ensemble $\hat{\rho}_{\mathrm{ML}}$ if it were the true state. One generates a large number of random sets of homodyne data according to equation (6), then applies the MaxLik reconstruction scheme to each set and obtains a series of density matrices $\hat{\rho}'_k$, each of which approximates the original matrix $\hat{\rho}_{\mathrm{ML}}$. The average difference $\langle |\hat{\rho}_{\mathrm{ML}} - \hat{\rho}'_k| \rangle_k$ evaluates the statistical uncertainty associated with the reconstructed density matrix.

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