Alternate Forms of the T-Matrix in Quantum State Tomography

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Abstract

In this paper, we focus on alternate forms of the T-matrix used in the Maximum Likelihood Estimate (MLE) procedure for fitting the experimental data collected in quantum state tomography experiments. In particular, we analyze the single quantum state tomography case, deriving in the process three new valid alternate forms for achieving optimality. These alternative forms then serve as a consistency check, thus enhancing the robustness of the MLE fitting process. One form, in particular, serves as a useful complement to the standard form normally employed. We subsequently provide a generalization of these forms to the case of multiqubit state tomography.

1 Introduction

A T-matrix is a theoretical construct in quantum state tomography to decipher the quantum state from collected experimental data. The data comprise measurements of the Stokes parameters. The quantum state is expressed via a density matrix, which is expressed in terms of the T-matrix and then fitted to the experimental data in an optimization process called the Maximum Likelihood Estimate (MLE) [1]. The aim in the MLE process is to assign appropriate starting values for the T-matrix parameters so that a global (and not a local) minimum is achieved. In an earlier paper [2], we analyzed the T-matrix traditionally used in literature for single qubit state tomography and succeeded in providing novel expressions for the starting values of the T-matrix parameters based on the measured experimental data.

In this note, we provide three alternate forms of the T-matrix and report the results of our analysis, including the corresponding sets of starting values for the different T-matrices that can be used in the MLE optimization technique. These forms then serve as a consistency check on the fits to the density matrix. In particular, one of these alternate forms (called Form B below) compliments the standard form [1-3] (which we call Form A, henceforth) in that where Form A fails, Form B works, and vice versa. The other forms (called Forms C and D below), while still being equally valid forms, are not as easy to implement because the expressions for the starting values allow for a larger region of the Stokes parameter space, where they may become unstable.

While we focus on the T-matrix for single qubit tomography, we provide in Appendix A a generalization for multiqubit tomography. Two-photon quantum tomography has been employed in the past [1].

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2 Alternate Forms of the T-Matrix

For the single qubit tomography, the T-matrix used in literature [1-3] is

\[
T = \begin{bmatrix}
t_1 & 0 \\
t_3 + it_4 & t_2
\end{bmatrix},
\]

and the density matrix \( \rho \) is given by

\[
\rho = \frac{T^\dagger T}{Tr(T^\dagger T)}.
\]

In order to derive alternate forms of the T-matrix, we start with the most general representation of a 2x2 matrix. Consider

\[
T = \begin{bmatrix}
a & c \\
d & b
\end{bmatrix},
\]

where parameters \( a, b, c, \) and \( d \) are complex in general; we also assume in what follows that these complex parameters are completely independent of each other. This definition leads to

\[
\frac{T^\dagger T}{Tr(T^\dagger T)} = \begin{bmatrix}
|a|^2 + |d|^2 & a^*c + bd^* \\
ac^* + bd^* & |c|^2 + |b|^2
\end{bmatrix},
\]

which is Hermitian and has trace equal to 1, by construction. Now any T-matrix representation of a physical density matrix should contain 4 real independent parameters. This is due to the fact that there are two angles \( \theta, \phi \) of the Bloch sphere and a positive “mixed” state parameter less than or equal to 1, to provide a complete description of the quantum state under consideration; a fourth parameter, which we call the “scaling” parameter, is added to the T-matrix to facilitate numerical computation. In order to generate such a form of \( \rho \), which is Hermitian and complex in general, two of the 4 real parameters must combine to form the complex off-diagonal elements of the 2 x 2 density matrix, i.e., one of the two terms in the expression, \( a^*c + bd^* \), of the off-diagonal element of the matrix in Eq. 4 must be zero in order to accommodate the (at most) 4 real parameters that a physical density matrix is constructed from. With these restrictions, four structurally different forms arise:

A) \( c=0 \), with \( a \) and \( b \) real, and \( d \) being complex

Set \( a = t_1, b = t_2, d = t_3 + it_4 \), which leads to

\[
T = \begin{bmatrix}
t_1 & 0 \\
t_3 + it_4 & t_2
\end{bmatrix},
\]

and

\[
\rho = \frac{T^\dagger T}{Tr(T^\dagger T)} = \begin{bmatrix}
t_1^2 + t_2^2 + t_4^2 & t_2(t_3 - it_4) \\
t_2(t_3 + it_4) & t_2^2
\end{bmatrix},
\]

\[
= \begin{bmatrix}
t_1^2 + t_2^2 + t_3^2 + t_4^2 \\
t_1^2 + t_2^2 + t_3^2 + t_4^2
\end{bmatrix},
\]

2
which is the standard from that has been employed in the past [1-3].

B) $d=0$, with $a$ and $b$ real, and $c$ being complex

Set $a = t_2, b = t_1, c = t_3 + it_4$, which leads to

$$T = \begin{bmatrix} t_2 & t_3 + it_4 \\ 0 & t_1 \end{bmatrix},$$

(7)

and

$$\rho = \frac{T^\dagger T}{Tr(T^\dagger T)} = \frac{\begin{bmatrix} t_2^2 & t_2(t_3 + it_4) \\ t_2(t_3 - it_4) & t_1^2 + t_3^2 + t_4^2 \end{bmatrix}}{t_1^2 + t_2^2 + t_3^2 + t_4^2},$$

(8)

which is different from Form A (the standard form) that has been employed in the past [1-3].

C) $a=0$, with $b$ and $c$ real, and $d$ being complex

Set $b = t_2, c = t_1, d = t_3 + it_4$, which leads to

$$T = \begin{bmatrix} 0 & t_2 \\ t_3 + it_4 & t_1 \end{bmatrix},$$

(9)

and

$$\rho = \frac{T^\dagger T}{Tr(T^\dagger T)} = \frac{\begin{bmatrix} t_2^2 + t_4^2 & t_2(t_3 - it_4) \\ t_2(t_3+it_4) & t_1^2 + t_2^2 \end{bmatrix}}{t_1^2 + t_2^2 + t_3^2 + t_4^2},$$

(10)

which is different from Forms A and B.

D) $b=0$, with $a$ and $d$ real, and $c$ being complex

Set $a = t_2, d = t_1, c = t_3 + it_4$, which leads to

$$T = \begin{bmatrix} t_1 & t_3 + it_4 \\ t_2 & 0 \end{bmatrix},$$

(11)

and

$$\rho = \frac{T^\dagger T}{Tr(T^\dagger T)} = \frac{\begin{bmatrix} t_1^2 + t_2^2 & t_2(t_3 + it_4) \\ t_2(t_3 - it_4) & t_1^2 + t_3^2 \end{bmatrix}}{t_1^2 + t_2^2 + t_3^2 + t_4^2},$$

(12)
which is different from Forms A, B, and C. More forms can be derived by interchanging the parameters $t_1$ and $t_2$, interchanging $t_3$ and $t_4$, replacing $t_1$ by $-t_1$, and so forth, but these are not fundamentally different. Do the three additional forms provide any advantage in the MLE process? We have analyzed the above three additional forms. Recalling that the experimental density matrix is expressed in terms of the normalized Stokes parameters:

\[
\rho = \frac{1}{2} \begin{bmatrix}
1 + s_3 & s_1 - is_2 \\
1 + is_2 & 1 - s_3 \\
\end{bmatrix},
\]

with the requirement

\[
s_1^2 + s_2^2 + s_3^2 \leq 1,
\]

where the equality sign holds when the density matrix $\rho$ describes a completely pure state, we give the major results, including the critical starting values for the T-matrix parameters in the MLE optimization process; these are expressed in terms of the experimentally determined Stokes parameters.

3 Analysis of the Alternate Forms

We now report the results of our analysis of these various alternate forms, providing the sets of starting values for each form in the MLE search.

3.1 Form B

1) $\det(\rho)=0$ leads to $t_2^2t_1^2 \geq 0$, which implies

\[
\rho = \begin{bmatrix}
0 & 0 \\
0 & 1 \\
\end{bmatrix}
\]

(15)

when $t_2 = 0$. $t_1 = 0$ leads to a general pure state, as in Form A [2].

2) Comparing Eq. 13 with Eq. 8 then leads to

\[
t_1^2 = \frac{(1 - s_3^2 - s_1^2 - s_2^2)}{(1 + s_3)^2}t_2^2,
\]

(16)

\[
t_3 = \frac{s_1}{1 + s_3}t_2,
\]

(17)

\[
t_4 = -\frac{s_2}{1 + s_3}t_2.
\]

(18)

Eqs. 16, 17, and 18 give expressions for $t_1$, $t_3$, and $t_4$ in terms of the Stokes parameters, $s_1$, $s_2$, and $s_3$, and the parameter $t_2$. With $t_2$, say, fixed at 1, they serve as the starting values in the search for the minimum in the MLE process. When $s_3$ is observed to be close to -1, one may then set $t_2 = 0$ (see Eq. 15), with the remaining parameters $t_1$, $t_3$, and $t_4$ initialized at some arbitrary values chosen to be 1 each, for example.

Further Remarks
Form B is complimentary to Form A in the sense that if one fits the data initially with Form A, then Form B serves as a back-up when the observed value of $s_3$ is close to 1; in this situation, the expressions for the starting values based on Form A (as we saw in [2]) become unstable near $s_3 = 1$, so it is prudent to apply Form B whose starting values are stable near $s_3 = 1$. Similarly, if one chooses to employ Form B in the MLE process, then Form A serves as a backup in the vicinity of $s_3 = 1$.

For completeness, we analyze Forms C and D, and provide expressions of the starting values based on these forms.

### 3.2 Form C

1) $\det(\rho)=0$ leads to $(t_3^2 + t_4^2)t_1^2 \geq 0$, which implies

$$\rho = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

when $t_3 = t_4 = 0$. $t_1 = 0$ leads to a general pure state.

2) Comparing Eq. 13 with Eq. 10 then leads to

$$t_1^2 = \frac{(1 - s_3^2 - s_1^2 - s_2^2)}{s_1^2 + s_2^2} t_2^2,$$

$$t_3 = \frac{(1 + s_3)s_1}{s_1^2 + s_2^2} t_2,$$

$$t_4 = \frac{(1 + s_3)s_2}{s_1^2 + s_2^2} t_2.$$  

Eqs. 20, 21, and 22 give expressions for $t_1$, $t_3$, and $t_4$ in terms of the Stokes parameters, $s_1$, $s_2$, and $s_3$, and the parameter $t_2$. With $t_2$, say, fixed at 1, they serve as the starting values in the search for the minimum in the MLE process. Clearly, when $s_1 \approx s_2 \approx 0$, the above expressions become unstable. Alternate expressions for the starting values of the $t$ parameters must be obtained for such situations; these are likely to be more involved than in the case of Forms B and C.

### 3.3 Form D

1) $\det(\rho)=0$ leads to $(t_3^2 + t_4^2)t_1^2 \geq 0$, which implies

$$\rho = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

when $t_3 = t_4 = 0$. $t_1 = 0$ leads to a general pure state.

2) Comparing Eq. 13 with Eq. 12 then leads to

$$t_1^2 = \frac{(1 - s_3^2 - s_1^2 - s_2^2)}{s_1^2 + s_2^2} t_2^2,$$
t_3 = \frac{(1 - s_3)s_1}{s_1^2 + s_2^2} t_2, \quad (25)

\begin{align*}
t_4 &= \frac{(1 - s_3)s_2}{s_1^2 + s_2^2} t_2. \quad (26)
\end{align*}

Eqs. 24, 25, and 26 give expressions for \( t_1, t_3, \) and \( t_4 \) in terms of the Stokes parameters, \( s_1, s_2, \) and \( s_3, \) and the parameter \( t_2. \) The instability case nears \( s_1 \approx s_2 \approx 0 \) is similar to Form C above.

4 Summary

We have derived four forms of the T-matrix, including the standard form used currently in literature, in the construction of a physical density matrix for the purposes of fitting the experimental data in the MLE optimization procedure. This MLE procedure is often used in quantum state tomography. The three new alternate forms, Forms B, C, and D, can be used for consistency checks. For all the four forms of the T-matrix, the starting values derived from knowledge of experimental data become unstable in some region of the space spanned by the Stokes parameters. In particular, we show that Form B acts as a robust backup to Form A, the standard form, when the latter becomes unstable. While Forms C and D are equally valid forms to choose from, their implementation is relatively more involved due to a larger region of instability, compared to Forms A and B. Our recommendation therefore is to use Form A or Form B in the analysis of single qubit state tomography, with the other acting as a backup. In Appendix A, we give the generalization of Form B to multiple qubit states. The generalization to Form A was given in Ref. [1].

References

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[2] Bhandari, R On Single Qubit Quantum State Tomography. [arXiv:1407.6668 [quant-ph]].

[3] Peters, N., Altepeter, J., Jeffrey, E., Branning, D., and Kwiat, P. Precise Creation, Characterization, and Manipulation of Single Qubits. [http://research.physics.illinois.edu/QI/Photonics/.../QIC-3-503-2003.pdf], September 16, 2003.

A Generalization of T-Matrix to a Multiqubit Case

A T matrix for \( n \) qubits requires \( 2^{2n} \) independent parameters [1]. A general form for Form A, the standard form, was provided in Ref.[1]. Here we provide a generalization of the new Form B given in Eq. 7:

\[
T = \begin{bmatrix} t_{2^n} & t_{2^n+1} + it_{2^n+2} & \ldots & t_{4^n-1} + it_{4^n} \\ 0 & t_{2^n-1} & \ldots & t_{4^n-3} + it_{4^n-2} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & t_1 \end{bmatrix} \quad (A.1)
\]
While the density matrix $\rho$ constructed via Eq. 2 is Hermitian with trace equal to 1, by construction, the requirement, $\det(\rho) \geq 0$, applied to the above form implies

$$t_1 t_2 \ldots t_2^n \geq 0. \tag{A.2}$$

### A.1 $n=1$; the single qubit case

$$T = \begin{bmatrix} t_2 & t_3 + it_4 \\ 0 & t_1 \end{bmatrix}, \tag{A.3}$$

with

$$t_1 t_2 \geq 0. \tag{A.4}$$

### A.2 $n=2$; the two qubit case

$$T = \begin{bmatrix} t_4 & t_5 + it_6 & t_{11} + it_{12} & t_{15} + it_{16} \\ 0 & t_3 & t_7 + it_8 & t_{13} + it_{14} \\ 0 & 0 & t_2 & t_9 + it_{10} \\ 0 & 0 & 0 & t_1 \end{bmatrix}, \tag{A.5}$$

with

$$t_1 t_2 t_3 t_4 \geq 0. \tag{A.6}$$

Similarly, Form C (Eq. 10) and Form D (Eq. 12) can be generalized.