On the regularization and optimization in quantum detector tomography

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Abstract

Quantum detector tomography (QDT) is a fundamental technique for calibrating quantum devices and performing quantum engineering tasks. In this paper, we utilize regularization to improve the QDT accuracy whenever the probe states are informationally complete or informationally incomplete. In the informationally complete scenario, without regularization, we optimize the resource (probe state) distribution by converting it to a semidefinite programming problem. Then in both the informationally complete and informationally incomplete scenarios, we discuss different regularization forms and prove the mean squared error scales as $O(1/N)$ or tends to a constant with $N$ state copies under the static assumption. We also characterize the ideal best regularization for the identifiable parameters, accounting for both the informationally complete and informationally incomplete scenarios. Numerical examples demonstrate the effectiveness of different regularization forms and a quantum optical experiment test shows that a suitable regularization form can reach a reduced mean squared error.

Key words: Quantum system identification, quantum detector tomography, quantum system, regularization

1 Introduction

In the past decades, significant progress has been achieved in a variety of fields of quantum science and technology, including quantum computation \cite{1}, quantum communication \cite{2} and quantum sensing \cite{3}. In these applications, it is often necessary to develop efficient estimation methods to acquire information about quantum systems and quantum system identification has attracted wide attention \cite{4,5,6}. In quantum estimation and quantum system identification, a common and essential step is to perform measurement on the quantum system of interest. Quantum detector tomography (QDT), as the standard technique to characterize an unknown measurement process, is fundamental for device...
benchmarking and subsequent tasks such as quantum state tomography (QST) [7,8], quantum Hamiltonian identification [10,11,12,13,14,15], quantum process tomography [16,17,18] and quantum control [19].

When the operators describing a detector are diagonal in the Fock state basis, they are called phase-insensitive (otherwise phase-sensitive) detectors and can be straightforwardly identified using function fitting [20] or convex optimization [21,22,23]. For phase-sensitive detectors, generally they can not be simultaneously diagonalized and their reconstruction is thus more complicated. Existing methods include Maximum Likelihood Estimation [24,25], linear regression [26], convex-quadratic optimization [27,28], and analytical two-stage solution [29]. Specially, binary detectors can always be simultaneously diagonalized and thus their estimation has an analytical scheme based on Frobenius-norm projection [30].

For $d$-dimensional QDT, we prepare $M$ different types of quantum states and the total number of copies of these states $N$ is called resource number. Many identification algorithms assume the experimental resource is diverse enough in QDT, i.e., any detector can be uniquely determined by the measurement outcome statistics. This scenario is called informationally complete (I.C.) [31,32] and the opposite scenario is called information incomplete (I.I.). In practice, the I.C. condition may not be satisfied for QDT, which results in an I.I. scenario (e.g. when $M < d^2$ for a $d$-dimensional detector). In the I.I. scenario and in certain I.C. scenarios where the probe states lie close to the I.I. set although they are still in I.C. set, the QDT problem is ill-conditioned. To solve this problem, convex optimization methods with regularization were proposed in [21,22] for phase-insensitive detectors and in [27,28] for phase-sensitive detectors. In experiments, a regularized least-square method was used in [33,34] for phase-insensitive detectors. However, there is still a lack of closed form solutions for QDT with regularization in these existing methods. To solve this problem, we develop QDT with regularization inspired by classical transfer function identification. In the previous literature, a kernel-based regularization was proposed in [35,36,37,38,39], which can cope with bias–variance trade-off. For kernel-based regularization, an important problem is how to design a suitable kernel matrix. Refs. [37,40] proposed different kernels and Refs. [41,42,43,44] discussed how to tune hyper-parameters in the kernel matrix and the asymptotic properties of these parameters. Further work about kernel-based regularization was studied in [45,46,47,48].

In this paper, we develop regularization methods in QDT which are applicable to both phase-insensitive and phase-sensitive detectors. We give a closed form solution, applicable to both the cases of I.C. and I.I. We then discuss different regularization forms and explain the advantages of using regularization in QDT. We consider no regularization as a special case. In the I.C. scenario, a common step (see e.g. [29,30]) is to uniformly distribute the resource for each quantum state as $N/M$, which is often not the optimal distribution. Without regularization, we discuss how to optimize the resource distribution for different types of probe states based on minimizing the mean squared error (MSE) of QDT. We convert this optimization problem into a semidefinite programming (SDP) problem, which can be solved efficiently. In comparison, if the resource distribution is given, the probe state design problem was discussed in [49]. In both the I.C. and I.I. scenarios, we also prove that under the static assumption (specific definitions in Section 4.1), the MSE scales as $O(1/N)$ or tends to a constant, and we characterize when the MSE can reach the optimal scaling $O(1/N)$. We propose an exact characterization of the best regularization for identifiable parameters to achieve the minimum MSE, allowing the probe states to be I.C. or I.I. In the I.C. scenario, we obtain the same best regularization form as proposed in [32]. We also prove the best regularization can reach the optimal scaling $O(1/N)$ even in the I.I. scenario. Numerical examples demonstrate that the optimization of resource distribution and regularization can reduce the MSE. Then we give the reason why adaptive rank-1 regularization motivated from the best regularization fails to show an $O(1/N)$ scaling in QDT, and we find an indication that full-rank regularization might be better. Finally, we apply our algorithm to quantum optical experiments using two-mode coherent states for binary detectors. The experimental results show that the adaptive regularization has a lower MSE compared with the Tikhonov regularization method in [29]. The main contributions of this paper are summarized as follows.

(i) A closed form of regularized QDT solution is established with different regularization forms in the I.C. and I.I. scenarios. The motivations and advantages to apply regularization in QDT are discussed.

(ii) Without regularization, we optimize the resource (probe state) distribution by converting it to a semidefinite programming (SDP) problem in the I.C. scenario.

(iii) Under the static assumption, we prove that the MSE scales as $O(1/N)$ or tends to a constant and we characterize when the MSE can reach the optimal scaling $O(1/N)$. In addition, an exact characterization of the best regularization for identifiable parameters to achieve the minimum MSE is given in the I.C. and I.I. scenarios.

(iv) Simulation results are provided to verify the effectiveness of resource distribution optimization and regularized QDT. Quantum optics experimental results are presented to demonstrate the necessity of choosing a proper regularization form to further reduce the QDT error.

This paper is organized as follows. In Section 2, we introduce the background knowledge and weighted least
squares for QDT. In Section 3 we discuss different regularization forms for QDT. In Section 4 we characterize the scaling of MSE under static assumptions and the best regularization for identifiable parameters. In Section 5 we give numerical examples and in Section 6 we present experimental results. Conclusions are presented in Section 7.

Notation: For a matrix $A$, $A \geq 0$ means $A$ is positive semidefinite. The conjugation and transpose $(T)$ of $A$ is $A^\dagger$. The trace of $A$ is $\text{Tr}(A)$. The rank of $A$ is $\text{Rank}(A)$. The identity matrix is $I$. The real and complex domains are $\mathbb{R}$ and $\mathbb{C}$, respectively. The tensor product is $\otimes$. The set of all $d$-dimensional complex/real vectors is $\mathbb{C}^d/\mathbb{R}^d$. Row and column vectors also denoted as $|\psi\rangle$ and $\langle\psi|$.

The Frobenius norm for a matrix and 2-norm for a vector are $\|\cdot\|$. The Kronecker delta function is $\delta_{ij} = 1$ if $i=j$ and $0$ otherwise. The Pauli matrices are $\sigma_x, \sigma_y, \sigma_z$.

## 2 Preliminaries and identification algorithm

Here we present the background knowledge and briefly introduce the QDT identification algorithm in [29]. Based on this QDT identification algorithm, we introduce weighted least squares (WLS) in QDT and explain its advantages.

### 2.1 Quantum state and measurement

For a $d$-dimensional quantum system, its state can be described by a $d \times d$ Hermitian matrix $\rho$, which satisfies $\rho \geq 0$ and $\text{Tr}(\rho) = 1$. When $\rho = |\psi\rangle \langle \psi|$ for some $|\psi\rangle \in \mathbb{C}^d$, we call $\rho$ a pure state. Otherwise, $\rho$ is called a mixed state, and can be represented using pure states $\{|\psi_i\rangle\}$ as $\rho = \sum_i c_i |\psi_i\rangle \langle \psi_i|$ where $c_i \in \mathbb{R}$ and $\sum_i c_i = 1$ with $c_i \geq 0$.

A set of operators $\{P_{ij}\}_{i=1}^n$ named Positive-operator-valued measure (POVM) characterizes a corresponding detector as a measurement device. Each POVM element $P_i$ is Hermitian and positive semidefinite, and together they satisfy the completeness constraint $\sum_{i=1}^n P_i = I$. When the measurements corresponding to $\{P_i\}$ are performed on $\rho$, the probability of obtaining the $i$-th result is given by the Born’s rule

$$p_i = \text{Tr}(P_i \rho). \quad (1)$$

From the completeness constraint, we have $\sum_i p_i = 1$.

### 2.2 Problem formulation of QDT

Suppose the true values of the POVM elements are $\{P_i\}_{i=1}^n$. We design $M$ different types of quantum states $\rho_j$ (called probe states) and record the measurement results $\hat{p}_{ij}$ as the estimate of $p_{ij} = \text{Tr}(P_i \rho_j)$. Each probe state has resource number $N_j$ (i.e., $N_j$ copies) and the total resource number is $N = \sum_{j=1}^M N_j$. Given experimental data $\{\hat{p}_{ij}\}$, the problem of QDT [29] can be formulated as

$$\min_{\{\hat{p}^*_i\}} \sum_{i=1}^n \sum_{j=1}^M \left[ \hat{p}_{ij} - \text{Tr} \left( \hat{P}_i \rho_j \right) \right]^2 \quad (2)$$

such that $\hat{P}_i = \hat{P}_i^\dagger, \hat{P}_i \geq 0$ for $1 \leq i \leq n$ and $\sum_{i=1}^n \hat{P}_i = I$.

Let $\{\Omega_i\}_{i=1}^d$ be a complete basis set of orthonormal operators with dimension $d$. Informationally let $\text{Tr}(\Omega_i^\dagger \Omega_j) = \delta_{ij}$, $\Omega_i = \Omega_i^\dagger$ and $\text{Tr}(\Omega_i) = 0$ except $\Omega_1 = I/\sqrt{d}$. Then we can parameterize the detector and probe states as

$$P_i = \sum_{a=1}^d \lambda_a^i \Omega_a, \rho_j = \sum_{b=1}^d \phi_b^j \Omega_b. \quad (3)$$

Using Born’s rule, we obtain

$$p_{ij} = \sum_{a=1}^d \phi_a^j \lambda_a^i \triangleq \phi_j^T \lambda_i, \quad (4)$$

where $\phi_j \triangleq \left( \phi_1^j, \ldots, \phi_d^j \right)^T$ and $\lambda_i \triangleq \left( \lambda_1^i, \ldots, \lambda_d^i \right)^T$ are the parameterization vectors of $\rho_j$ and $P_i$, respectively. Suppose the outcome for $P_i$ of $\rho_j$ appears $n_{ij}$ times, and then $\hat{p}_{ij} = n_{ij} / N_j$. Denote the estimation error as $e_{ij} = \hat{p}_{ij} - p_{ij}$. According to the central limit theorem, $e_{ij}$ converges in distribution to a normal distribution with mean zero and variance $(p_{ij} - p_i^2) / N_j$. We thus have the least squares (LS) equation

$$\hat{p}_{ij} = \phi_j^T \lambda_i + e_{ij}. \quad (5)$$

To propose least squares (LS) and weighted least squares (WLS) solutions in QDT, in the following we write down and solve the linear equation for each POVM element individually. This can be achieved by rearranging the data after implementing all the measurements. Collect the parameterization of the probe states as $X = (\phi_1, \phi_2, \ldots, \phi_M)^T$. For the $i$-th POVM element $P_i$, let

$$\hat{y}_i \triangleq (\hat{p}_{i1}, \hat{p}_{i2}, \ldots, \hat{p}_{iM})^T, \quad y_i \triangleq (1, \ldots, 1)_{1 \times M}^T = \sum_i \hat{y}_i,$$

$$d_{d \times 1} \triangleq (\sqrt{d}, 0, \ldots, 0)^T, \quad e_i \triangleq [e_{i1}, \ldots, e_{iM}]^T.$$
Define $\bar{y}_i \triangleq \hat{y}_i - \frac{1}{n} y_0$ and $\theta_i \triangleq \lambda_i - \frac{1}{n} d$. Then we have
\[
\bar{y}_i = X \theta_i + e_i.
\] (6)

Now the QDT problem can be transformed into the following form:

**Problem 1** For $1 \leq i \leq n$, given experimental data $\bar{y}_i$, solve $\min_{\hat{P}_i} \| \bar{y}_i - X \hat{\theta}_i \|^2$ with $\hat{P}_i \geq 0$, where $\lambda_i = \theta_i + \frac{1}{n} d$ is the parametrization of $\hat{P}_i$.

### 2.3 Weighted least squares in QDT

To solve Problem 1, the standard LS solution is
\[
\hat{\theta}_{i,LS} = (X^T X)^{-1} X^T \bar{y}_i,
\] (7)
and then the estimator for each detector is $\hat{\lambda}_{i,LS} = \hat{\theta}_{i,LS} + \frac{1}{n} d$, which is equivalent to equation (9) in [29].

Although all the estimation errors $e_{ij}$ have zero mean, they have different variances, which is called heteroscedasticity in statistics. The constrained least squares as equation (6) in [29] and standard LS (7) do not consider heteroscedasticity. However, WLS considers the heteroscedasticity property and has optimal MSE. We thus consider WLS estimate
\[
\hat{\theta}_{i,WLS} = (X^T W_i X)^{-1} X^T W_i \bar{y}_i,
\] (8)
where
\[
W_i = \text{diag} \left( \frac{N_1}{p_{i1} - p_{i1}^2}, \ldots, \frac{N_M}{p_{iM} - p_{iM}^2} \right)
\] (9)
is the weighting matrix. We assume that $p_{ij}$ is not equal to 0 or 1, which is reasonable because $p_{ij} \in [0, 1]$ and generally the probability for $p_{ij} = 0$ or 1 is 0 in theory. The following are the two main advantages of using WLS:

- We can normalize the estimation errors to normal Gaussian errors and solve the heteroscedasticity problem. With increasing measurements, each $e_{ij}$ will converge asymptotically to a Gaussian random variable with mean zero and variance $\sigma_{ij} = (p_{ij} - p_{ij}^2)/N_j$.

Thus, we have $E(e_i e_j^T) = W_i^{-1}$. Define $Q_i \triangleq \sqrt{W_i}^{-1}/\sigma$, $\bar{y}_i \triangleq \hat{Q}_i^{-1} \bar{y}_i$, $\hat{X}_i \triangleq \hat{Q}_i^{-1} X$, $e_i \triangleq \hat{Q}_i^{-1} e_i$ and the model equivalent to (6) is
\[
\bar{y}_i = \hat{X}_i \theta_i + \bar{e}_i,
\] (10)
where the variance of $\bar{e}_i$ is $\sigma^2 I$ and the practical asymptotic WLS (AWLS) estimate is
\[
\hat{\theta}_{i,AWLS} = (X^T \hat{W}_i X)^{-1} X^T \hat{W}_i \hat{\bar{y}}_i
\] (11)
\[
= (\hat{X}_i^T \hat{X}_i)^{-1} \hat{\bar{X}}_i^T \hat{\bar{y}}_i.
\] (12)
The difference between $\hat{\theta}_{i,AWLS}$ and $\hat{\theta}_{i,WLS}$ is asymptotically small in comparison with $\hat{\theta}_{i,WLS}$ [9]. Thus, the estimate (11) is accurate enough and asymptotically coincides with (8). Using the LS estimate (7) or WLS estimate (10), we can obtain a POVM estimate $\hat{E}_i = \sum_{a=1}^{d^2} \left( \hat{\theta}_{i,LS/WLS} + \frac{1}{n} d \right)_{a\bar{a}}$ and
\[
E(\| \hat{E}_i - P_i \|^2) = \text{Tr} \left( \text{MSEM} \left( \hat{\theta}_i \right) \right).
\] (13)

Thus, all the variances of the estimation errors are normalized to $\sigma^2$.

- For any unbiased linear estimator $\hat{\theta}_i$ for $\theta_i$, we have [9]
\[
\text{MSEM} \left( \hat{\theta}_{i,LS} \right) = \min \left\{ \left( X^T W_i X \right)^{-1} \right\}
\] (14)

\[
= \left( X^T W_i X \right)^{-1} \leq \text{MSEM} \left( \hat{\theta}_i \right),
\] (15)

where MSEM $(\cdot)$ is the MSE matrix. The MSE of all the POVM elements is
\[
E \left( \sum_{i=1}^{n} \| \hat{P}_i - P_i \|^2 \right) = \sum_{i=1}^{n} E \left( \| \hat{E}_i - P_i \|^2 \right)
\] (16)
\[
= \sum_{i=1}^{n} \text{Tr} \left( \text{MSEM} \left( \hat{\theta}_i \right) \right).
\] (17)

We call the error $E(\| \hat{E}_i - P_i \|^2)$ the LS MSE for the $i$-th POVM element. Note that $\{ \hat{E}_i \}_{i=1}^M$ may have negative eigenvalues due to the noise or error in the measurement results. Thus, we need further correction to obtain a positive semidefinite estimate $\{ \hat{P}_i \}_{i=1}^M$ and in this paper,
we utilize the algorithm in [29] to achieve this. We refer to the error $E[||\hat{P}_i - P_i||^2]$ as the final MSE for the $i$-th POVM element.

Remark 1. One may notice that (4) has the same linear regression form $y = X\theta + e$ as transfer function identification in system identification [37]. However, there are some differences between QDT and transfer function identification for classical (non-quantum) systems. First, in QDT, more measurement data will only enhance the data accuracy in $y$ and the dimension of $y$ is fixed with given probe states. In transfer function identification, the dimension of $y$ increases for more data. Second, the parameterization matrix $X$ is determined by the given probe states and $XTX$ can be singular (e.g., $M < d^2$) in QDT. In transfer function identification, $X$ depends on the input data and measurement data. In practice, $XTX$ is therefore always invertible but the condition number may be large. Thus, the standard LS cannot give an accurate estimate. Finally, the variance of the noise $e$ is often assumed to be a constant in transfer function identification. However, in QDT, the variances of noise are usually different and decrease as $O(1/N)$ where $N$ is the resource number.

3 Regularization in QDT

In QDT, when the different types of probe states are similar or I.I., leading to an ill-conditioned problem, convex optimization methods with regularization were proposed in [21,22] for phase-insensitive detectors and in [27,28] for phase-sensitive ones. The motivation of introducing regularization is to mitigate the ill-conditioned property. For phase-insensitive detectors, the regularization form is chosen such that the diagonal elements of the reconstructed detector have smooth variations [28]. However, for phase-sensitive detectors, a suitable regularization form is not easy to find. In addition, convex optimization methods cannot give a closed form solution. Therefore, in this section, we use regularization in the WLS of QDT which can give a closed form solution.

3.1 Regularized weighted least squares

In the ill-conditioned scenario, the condition number of $\tilde{X}_iT\tilde{X}_i$ can be large or even infinite. To solve this problem, we add regularization in the weighted model [15] as

$$\left\|\tilde{y}_i - \tilde{X}_i\theta_i\right\|^2 + \theta_i^T D_i \theta_i,$$

where $D_i$ is positive semi-definite and called a regularization matrix. Denote $R_i \triangleq \tilde{X}_iT\tilde{X}_i$. After we add regularization, the estimate is changed to be

$$\hat{\theta}_{i,\text{RWLS}} = (R_i + D_i)^{-1} \tilde{X}_i^T \tilde{y}_i.$$  

The expectation of $\hat{\theta}_{i,\text{RWLS}}$ is

$$E\left(\hat{\theta}_{i,\text{RWLS}}\right) = (R_i + D_i)^{-1} R_i \theta_i.$$  

The bias is

$$\theta_{i,\text{RWLS}}^{\text{bias}} \triangleq E\left(\hat{\theta}_{i,\text{RWLS}}\right) - \theta_i = -(R_i + D_i)^{-1} D_i \theta_i.$$  

Define

$$\hat{\theta}_i \triangleq \hat{\theta}_{i,\text{RWLS}} - E\left(\hat{\theta}_{i,\text{RWLS}}\right) = (R_i + D_i)^{-1} \tilde{X}_i^T (\tilde{y}_i - \tilde{X}_i\theta_i)$$

and then the MSE matrix of $\hat{\theta}_{i,\text{RWLS}}$ is

$$\text{MSEM}\left(\hat{\theta}_{i,\text{RWLS}}\right) = E\left[\left(\hat{\theta}_{i,\text{RWLS}} - \theta_i\right)\left(\hat{\theta}_{i,\text{RWLS}} - \theta_i\right)^T\right]$$

$$= E\left(\hat{\theta}_i \hat{\theta}_i^T\right) + \theta_{i,\text{RWLS}}^{\text{bias}} \theta_{i,\text{RWLS}}^{\text{bias}}^T$$

$$= (R_i + D_i)^{-1} (\sigma^2 R_i + D_i \theta_i^T D_i^T) (R_i + D_i)^{-1}.$$  

An MSE matrix similar to (23) can be found in [37] for transfer function identification with standard LS estimation. The LS MSE of QDT is $\text{Tr}(\text{MSEM})$ and depends on the true parameter $\theta_i$. When the probe states are I.C., we can obtain an estimate without regularization (i.e., $D_i = 0$) and the MSE matrix becomes

$$\text{MSEM}\left(\hat{\theta}_{i,\text{RWLS}}\right) = \sigma^2 R_i^{-1},$$

which is independent of the true parameter $\theta_i$. Based on the development in classical system identification, several motivations of applying regularization in QDT are as follows:

(i) Regularization is a typical solution to ill-conditioned problems. In the field of classical transfer function identification (see e.g., [41]), the input signal is band-limited, and then the matrix $R_i$ may become ill-conditioned as the amount of data increases. Similarly in QDT, the input probe states can be “band-limited”, in the sense that the types of the probe states are not rich enough (especially when coherent states are employed) which leads to the conversion from I.C. to I.I. This current incapability of realizing perfect number states endows the bias-variance trade-off. The regularization estimation is biased as (21), which can lead to an MSE smaller than that of the standard LS estimation both in the I.C. and I.I. scenarios.

(ii) From an alternative point of view, regularization leverages the bias-variance trade-off. The regularization estimation is biased as (21), which can lead to an MSE smaller than that of the standard LS estimation both in the I.C. and I.I. scenarios.
There are also differences of applying regularization between QDT and classical system identification. All physical POVM elements must be positive semidefinite and sum to identify, which may affect or even guide the design of the specific regularization form in QDT. For example, Ref. [29] noted that POVM elements satisfying these physical constraints always have eigenvalues in [0, 1]. Direct LS estimation for ill-conditioned QDT usually gives a large $||\hat{\theta}_i||$, which may have eigenvalues outside [0, 1] and become nonphysical. Therefore, the regularization $\hat{\theta}_i^T D_i \hat{\theta}_i$ is added to the cost function in [29] as a penalty term, promoting the satisfaction of the physical constraints. Apart from this, other differences will be detailed in Sec. 3.2.3.

Regularized weighted regression is also applied in quantum state tomography. For example, in [9], their motivation is that the quantum state $\rho$ is usually of low rank and thus it is reasonable to add a Tikhonov regularization as Sec. 3.2.2. However, in QDT, the POVM elements are not always of low rank. For example, in the continuous-variable optical experiment in the paper and in [21, 22, 28], the POVM elements are all full-rank. Thus we introduce and discuss more regularization forms in Sec. 3.2.

### 3.2 Different regularization forms in QDT

Here we discuss different regularization forms in QDT. Firstly, we consider no regularization (i.e., $D_i = 0$) as a special regularization form in the I.C. scenario. Since the MSE in (24) does not depend on true parameter $\theta_i$, we propose resource distribution optimization of $N_j$ to minimize the LS MSE with given probe states. Then we present some common regularization forms. With regularization, the LS MSE in (23) depends on true parameter $\theta_i$. Thus we cannot optimize resource distribution as without regularization and we use a uniformly distributed $N_j = N/M$.

#### 3.2.1 Without regularization

Without regularization, Refs. [29, 30] choose $N_j = N/M$ for given probe states, which is often not the optimal distribution. Similar input design problems in classical systems and control have been widely studied and there are many existing results, e.g., D,A,E-optimal input design [51]. Here, we formulate and solve the problem within the framework of A-optimal design problem, where the trace of the covariance matrix (i.e., MSE) is minimized.

Let $\eta_j = \frac{N_j}{N}$, and the optimization of resource distribution problem can be formulated as

$$\min_{\{\eta_j\}} \sum_{j=1}^{N} \text{Tr} \left( \sum_{j=1}^{M} (\eta_j w_{ij} \phi_j \phi_j^T) \right)^{-1}$$

subject to $\eta_j \geq 0$, $\sum_{j=1}^{M} \eta_j = 1$.

where $\phi_j$ is the given parameterization vectors of $\rho_j$ and $w_{ij}$ is the weighted constant which we may obtain from a prior information. If we do not have a prior information, we can set $w_{ij} = 1$. This optimization problem is convex and it can be converted to a semidefinite programming (SDP) problem

$$\min_{\{\eta_j\}_{j=1}^{M}, \{u_k\}_{k=1}^{d^2}} \sum_{k=1}^{d^2} u_k$$

subject to $\sum_{j=1}^{M} \eta_j w_{ij} \phi_j \phi_j^T u_k \geq 0$,

$$1 \leq k \leq d^2, 1 \leq i \leq n,$$

$$\eta_j \geq 0, \sum_{j=1}^{M} \eta_j = 1,$$

where $u_k$ is the $k$-th unit vector. Using CVX [52, 53], we can solve (26) efficiently. Note that $N_j = \eta_j N$ may not be an integer, and we need to round it up or down. In comparison, if the resource distribution is given, the probe state design problem was discussed in [49] based on minimizing an upper bound on the MSE and the condition number.

#### 3.2.2 Tikhonov regularization

A most common regularization form is in a Tikhonov sense [21]. In QDT, a natural method is to choose regularization matrix as

$$D_i^{\text{Tikhonov}} = cI,$$

where $c$ is a positive constant. Ref. [29] did not use WLS and chose $D_i = \frac{c}{N}I$ which is Tikhonov regularization, because

$$\hat{\theta}_{i,\text{RWLS}} = \left( X^T X + \frac{c}{N} I \right)^{-1} X^T \bar{y}_i$$

$$= \left( X^T N I X + cI \right)^{-1} X^T N I \bar{y}_i,$$

where the weighted matrix is $NI$ instead of (14).

#### 3.2.3 Kernel-based regularization

In transfer function identification, Refs. [35, 36, 37, 38] proposed kernel-based regularization and explained reg-
ularization in a Bayesian perspective. We assume the true parameter $\theta_i$ is a random variable and has a Gaussian distribution with zero mean and covariance matrix $S_i$:

$$\theta_i \sim \mathcal{N}(0, S_i).$$

Therefore, the posterior estimate is

$$\hat{\theta}_i^{\text{post}} = (S_i R_i + \sigma^2 I)^{-1} S_i F_i$$

$$= (R_i + \sigma^2 S_i^{-1})^{-1} F_i,$$

where $F_i \triangleq \hat{X}_T^T \hat{y}_i$. If $S_i$ is singular, we can use the first equality of (30) to obtain the estimate. This posterior estimate is the same as the regularized estimate if the regularization matrix $D_i$ is chosen as $37$

$$D_i = \sigma^2 S_i^{-1}.$$

This gives an insight into how to choose the regularization matrix $D_i$ or kernel matrix $S_i$: Let it reflect the correlations of the parameters $37$.

To use the kernel-based regularization in QDT, we need to solve two problems

(i) In the Bayesian perspective for kernel-based regularization, the mean of the unknown parameters is zero. But in QDT, the mean of the unknown parameters $\lambda_i$ is usually not zero.

(ii) Heteroscedasticity: In transfer function identification, it is usually assumed that the noises have the same variances. But the estimation errors $e_2$ usually have different variances in QDT.

The first problem is solved by modeling in $0$ where the unknown parameter $\theta_i$ becomes zero-mean. For the second problem, WLS $14$ solves the heteroscedasticity problem.

There are two advantages of using kernel-based regularization in QDT compared with using kernel-based regularization in transfer function identification:

(i) In transfer function identification, we need to identify the variance of the noise firstly, while we already know the approximate variance of the estimation error in QDT from measurement data.

(ii) In transfer function identification, the problem dimension increases as more data are generated, resulting in increased difficulty. While in QDT, more data will only enhance the data accuracy and the dimension is fixed with given probe states.

One limit using kernel-based regularization in QDT is that without prior knowledge the parameter $\theta_i$ does not have the property of impulse responses of transfer functions which usually decay exponentially $37$. In this paper, we mainly choose DI kernel which only represents the auto-correlation for each coefficient of QDT as

$$S_i^{\text{DI}}(k, j) = \begin{cases} c \mu^k, & \text{if } k = j, \\ 0, & \text{otherwise}, \end{cases}$$

where $c \geq 0$, $0 \leq \mu \leq 1$. If we have more prior knowledge such as the correlation between different coefficients, we can design more suitable kernels as in transfer function identification. For example, when the detector is close to a phase-insensitive detector, i.e., the POVM elements are close to diagonal matrices in the Fock state basis, the true value $\theta_i$ is close to sparse, which is similar to the decay behavior of impulse responses for stable transfer functions in system identification. Therefore, we can apply TC and DC kernels $37$ in transfer function identification

$$S_i^{\text{TC}}(k, j) = c \min (\mu^j, \mu^k),$$

where $c \geq 0$, $0 \leq \mu \leq 1$ and

$$S_i^{\text{DC}}(k, j) = c \mu_1^{j-k} \mu_2^{k+j}/2,$$

where $c \geq 0$, $-1 \leq \mu_1 \leq 1$ and $0 \leq \mu_2 \leq 1$.

3.2.4 Best regularization (in the I.C. scenario)

For true parameter $\theta_i$, two natural questions are whether there exists an optimal regularization matrix and if there exists an optimal regularization matrix, does it depend on $\theta_i$? Ref. $37$ has discussed these problems in transfer function identification and the result also holds for QDT. The MSE matrix in $23$ can be rewritten using $S_i$ as

$$\text{MSEM} \left( \hat{\theta}_{i, \text{RWLS}} \right) = (S_i R_i + \sigma^2 I)^{-1} (\sigma^2 S_i R_i S_i i$$

$$+ \sigma^4 \theta_i \theta_i^T) (R_i S_i + \sigma^2 I)^{-1}.$$

When $R_i$ is invertible, the following inequality $37$

$$\text{MSEM} \left( \hat{\theta}_{i, \text{RWLS}} \right) \big|_{S_i = K} \geq \text{MSEM} \left( \hat{\theta}_{i, \text{RWLS}} \right) \big|_{S_i = \theta_i \theta_i^T}$$

holds for any $K \geq 0$. Later, in Theorem $2$ we will extend this inequality to the case where $R_i$ is singular. Thus, ideally the best choice of regularization always includes

$$S_i^{\text{best}} = \theta_i \theta_i^T,$$

which yields the corresponding optimal regularized estimate

$$\tilde{\theta}_i^{\text{best}} = (\theta_i \theta_i^T R_i + \sigma^2 I)^{-1} \theta_i \theta_i^T F_i,$$

with $R_i = \tilde{X}_i^T \tilde{X}_i$ and $F_i = \tilde{X}_i^T \tilde{y}_i$. The theoretically best regularization depends on the unknown parameter and cannot be used in practice.
A natural question is that, is \( \theta_i\theta_i^T \) the only choice for \( S_i \) to result in the best regularization? Ref. [44] has given a positive answer for the I.C. scenario. For the I.I. scenario we will give a negative answer in Sec. 4.2.

3.2.5 Adaptive regularization

As motivated by the best regularization, we can propose adaptive regularization with rank-1 kernel matrix which is similar to the rank-1 kernel matrix for transfer function identification in [44]. Firstly, we consider a two-step adaptive regularization. In the first step, we use Tikhonov or kernel-based regularization and we can obtain a rough estimate \( \hat{\theta}_i \) with certain kernel matrix \( S_i^{(1)} \). Then in the second step, we repeat using the measurement data in the first step, but now the regularization matrix is adaptively chosen as

\[
S_i^{\text{rank-1}} = \hat{\theta}_i \left( \hat{\theta}_i^T \right)^T.
\] (39)

The following analysis and Theorem 4 in the next section indicate that full-rank kernel matrix may be better than rank-1 kernel matrix, because a full-rank \( S_i \) does not induce a dimension reduction from \( R(B) \) to \( R(S_iB) \). Therefore, we also consider to use full-rank kernel matrix as

\[
S_i^{\text{full-rank}} = S_i^{\text{rank-1}} + S_i^{\text{DI/TC}/DC},
\] (40)

in Sec. 5.

It is an important problem to determine the kernel matrix and some different kernels are proposed in transfer function identification. For a structure-given kernel matrix, optimization of the hyper-parameters (such as \( c, \mu \) in [42]) in the kernel matrix has been discussed in [47,49,41]. However, the question of how to choose the optimal adaptive kernel matrix is still an open problem.

4 Characterizing the MSE of QDT with regularization

4.1 On the MSE scaling

To analyze the performance of different regularization methods, we characterize the asymptotic behavior of the estimation error, e.g., MSE. Without loss of generality, we can always normalize the variances of the estimation errors to 1, i.e., \( \sigma^2 = 1 \) in [11]. We give the following assumptions.

**Assumption 1** The probe state parameterization matrix \( X \) is given. The kernel matrix \( S_i \) is given. For each \( 1 \leq j \leq n \), \( \lim_{N \to \infty} \frac{N}{N} = h(j) \) where \( h(j) \) is a constant in \([0,1]\) depending on \( j \).

We refer to Assumption 1 as the static assumption. With Assumption 1 the probe state parameterization matrix and kernel matrix are given as constant matrices which do not change in our analysis and the resource distribution for each probe state can change as \( N \) increases. But the limit of the ratio is a constant and can be 0 or 1. We say that the random sequence \( \{\xi_N\} \) converges almost surely to a random variable \( \xi \) if \( P (\lim_{N \to \infty} ||\xi_N - \xi||_2 = 1) = 1 \), which can be written as \( \xi_N \xrightarrow{a.s.} \xi \) as \( N \to \infty \). For the weighted matrix \( \hat{W}_i \), its deviation from the true value \( W_i \) has been derived in [9] as

\[
\hat{W}_i = \text{diag} \left( \frac{N_1}{\hat{p}_{i1} - \hat{p}_{i1}}, \ldots, \frac{N_M}{\hat{p}_{iM} - \hat{p}_{iM}} \right)
= \left( 1 + O \left( \frac{1}{\sqrt{N}} \right) \right) W_i.
\] (41)

We define

\[
B \triangleq \lim_{N \to \infty} \frac{X^T W_i X}{N}, \quad \hat{B}_N \triangleq \frac{X^T \hat{W}_i X}{N},
\] (42)

where the normalized weighted parameterization matrix \( \hat{B}_N = \left( 1 + O \left( \frac{1}{\sqrt{N}} \right) \right) B \) for constant matrix \( B \) because \( \lim_{N \to \infty} \frac{N}{N} = \text{constant} \). Therefore, \( \hat{B}_N \xrightarrow{a.s.} B \) as \( N \to \infty \).

We denote \( R(X) \) as the range space of \( X \) and \( N(X) \) as the null space of \( X \). Then we propose the following theorem to characterize the MSE.

**Theorem 1** In the regularization-based QDT, if the \( i \)-th POVM element satisfies the static assumption, then its LS MSE \( \mathbb{E} \left\| \hat{P}_i - P_i \right\|^2 \) and final MSE \( \mathbb{E} \left\| \hat{P}_i - P_i \right\|^2 \) both scale as \( O(1/N) \) if and only if the true values of the unknown parameters satisfy \( \theta_i \in R(S_iB) \). Otherwise, the LS MSE \( \mathbb{E} \left\| \hat{P}_i - P_i \right\|^2 \) converges to a positive value.

**Proof.** For the \( i \)-th POVM element, according to [35] and \( \sigma^2 = 1 \), the MSE is

\[
\text{Tr} \left[ \mathbb{E} \left\| S_iR_i + I \right\|^2 \right]
= \text{Tr} \left[ (S_iR_i + I)^{-1} \left( S_iR_iS_i + \theta_i\theta_i^T \right) (R_iS_i + I)^{-1} \right]
= \text{Tr} \left[ \{ (S_iR_i + I) (R_iS_i + I)^{-1} (S_iR_iS_i + \theta_i\theta_i^T) \} \right],
\] (43)

where \( R_i = X^T W_i X \). We define

\[
A_1 \triangleq (S_iR_i + I) (R_iS_i + I) = \left( N S_i \hat{B}_N + I \right) \left( N \hat{B}_N S_i + I \right),
\] (44)

and

\[
A_2 \triangleq S_i R_i S_i = N S_i \hat{B}_N S_i.
\] (45)
Now the MSE becomes $\text{Tr} \left(A_1^{-1}(A_2 + \theta_i \theta_i^T)\right)$.

We then introduce the following lemma

**Lemma 1** For an $n \times n$ complex matrix $T$, the following statements are equivalent:

1. $T = AB$, where $A, B \succeq 0$;
2. $T = AB$, where $A > 0$ and $B \succeq 0$;
3. $T$ is similar to a nonnegative diagonal matrix.

From Lemma 1, $S_i B$ is similar to a nonnegative diagonal matrix and we assume $S_i B = Q^{-1} \Sigma \Omega Q$ where $\Sigma_1 = \text{diag}(\Sigma_{11}, \Sigma_{12})$ and $\Sigma_{11}$ is a $k \times k$ positive diagonal matrix, $\Sigma_{12}$ is a $(d^2 - k) \times (d^2 - k)$ zero matrix. Therefore, $NS_i B + I$ can also be diagonalized by $Q$ as

$$NS_i B + I = Q^{-1} \text{diag}(\{\tau_1, \ldots, \tau_d^2\}) Q = Q^{-1} \text{diag}(N \Sigma_{11} + I_k, I_{d^2-k}) Q,$$

where $\tau_1 \geq \cdots \geq \tau_d > 0$, $\tau_j = O(N)$ for $1 \leq j \leq k$ and $\tau_j = 1$ for $k + 1 \leq j \leq d^2$ and the corresponding eigenvectors are $\{u_j\}_{j=1}^{d^2}$. As $N \to \infty$, we have

$$\lim_{N \to \infty} (NS_i B + I)^{-1} = \lim_{N \to \infty} Q^{-1} \text{diag}(N \Sigma_{11} + I_k, I_{d^2-k})^{-1} Q = Q^{-1} \text{diag}(0, I_{d^2-k}) Q,$$

and thus $(NS_i B + I)^{-1}$ tends to a constant matrix. Since

$$I - (NS_i B + I)^{-1} = (NS_i B + I)^{-1} NS_i B,$$

it is also a bounded matrix and tends to a constant matrix as $N \to \infty$. Let the spectral decomposition of $B$ be

$$B = V \Sigma_2 V^T = V \text{diag}(\Sigma_{21}, 0) V^T.$$

Thus, the Moore-Penrose inverse of $B$ is

$$\hat{B} = V \text{diag}(\Sigma_{21}^{-1}, 0) V^T,$$

which is a constant matrix and $BBB = B$.

Therefore, the first term of MSE is

$$\text{Tr} \left(A_1^{-1}A_2\right) \overset{a.s.}{\to} \text{Tr} \left((NBS_i + I)^{-1} (NS_i B + I)^{-1} NS_i BS_i\right) = \frac{1}{N} \text{Tr} \left((NS_i B + I)^{-1} NS_i B \cdot \hat{B} \cdot NBS_i (NBS_i + I)^{-1}\right) = O\left(\frac{1}{N}\right),$$

because the term $\text{Tr}(\cdot)$ is bounded and tends to a constant. Therefore, the first term of MSE always scales as $O\left(\frac{1}{N}\right)$. Then we discuss the scaling of the second part of MSE

$$\text{Tr} \left(A_1^{-1}\theta_i \theta_i^T\right) \overset{a.s.}{\to} \text{Tr} \left(NBS_i + I\right)^{-1} (NS_i B + I)^{-1} \theta_i.$$

If $\theta_i$ is a linear combination of $u_j$ for $1 \leq j \leq k$, we have

$$\text{Tr} \left(A_1^{-1}\theta_i \theta_i^T\right) = O(\frac{1}{N^2}).$$

Otherwise, if $\theta_i$ is not a linear combination of $u_j$, $1 \leq j \leq k$, $\text{Tr} \left(A_1^{-1}\theta_i \theta_i^T\right)$ tends to a positive number independent of $N$.

Therefore, for the LS MSE $\mathbb{E}\|\hat{E}_i - P_i\|^2$, it scales as $O(1/N)$ if and only if the true parameter $\theta_i$ is a linear combination of $u_j$ for $1 \leq j \leq k$, i.e., $\theta_i \in R(S_i B)$.

Since $\{\hat{E}_i\}_{i=1}^{n}$ may have negative eigenvalues, we use the algorithm in [29] to further obtain a positive semidefinite estimate $\{\hat{P}_i\}_{i=1}^{n}$. The error analysis in [29] has shown that

$$\sum_{i=1}^{n} \|\hat{P}_i - P_i\|^2 = (dn + 2\sqrt{dn} + 1)O\left(\mathbb{E} \sum_{i=1}^{n} \|\hat{E}_i - P_i\|^2\right).$$

Therefore, if $\mathbb{E} \sum_{i=1}^{n} \|\hat{E}_i - P_i\|^2 = O(1/N)$, we have $\mathbb{E} \sum_{i=1}^{n} \|\hat{P}_i - P_i\|^2 = O(1/N)$ and thus the final MSE $\mathbb{E} \|\hat{P}_i - P_i\|^2$ also scales as $O(1/N)$. Using (46) and (51), if the true parameter $\theta_i$ is not the linear combination of $u_j$ for $1 \leq j \leq k$, i.e., $\theta_i \notin R(S_i B)$, the LS MSE $\mathbb{E} \|\hat{E}_i - P_i\|^2$ tends to a positive value.

**Remark 2** In Theorem 1, when $\theta_i \notin R(S_i B)$, the behavior of the final MSE $\mathbb{E} \|\hat{P}_i - P_i\|^2$ is still difficult to characterize. This problem does not exist for a full-rank detector when the resource number $N$ is large enough, because the LS or WLS estimate already satisfies the positive semidefinite constraint and we do not need to correct $\hat{E}_i$.

Note that when $S_i B$ is full-rank, i.e., $S_i$ and $B$ are both positive definite, the condition $\theta_i \in R(S_i B)$ is always satisfied. Therefore, the MSE always scales as $O(1/N)$. Thus, when the types of different probe states are I.C., for any positive definite kernel matrix $S_i$, the MSE always scales as $O(1/N)$. However, when the probe states are I.I., the condition $\theta_i \in R(S_i B)$ is difficult to be satisfied in practice. Thus, without special prior knowledge, for almost all regularization forms, the LS MSE will tend to a constant when $N$ tends to infinity. In addition, as $M$ decreases, for given $S_i$, this condition may become
more difficult to be satisfied because \( R(S, B) \) may become smaller. Thus, rank-1 adaptive regularization as in (39) is not a good choice and full-rank kernel matrix as in (40) may be better. The above analysis can help understand the boundary of the ability of employing regularization in QDT.

Remark 3 A similar problem was also discussed as Theorem 2.1 in [47] for transfer function identification in the I.C. scenario. There a condition to realize unbiased estimation of the true parameters with regularization was given. Here, by allowing the probe states to be I.C. or I.I., we give a stronger result about the scaling of LS MSE as \( O(1/N) \) or tends to a constant for QDT. Our result can also be applied to the case when the variance of noise scales as \( O(1/N) \), which is typical in the scenario where only statistical noise is considered in quantum measurement.

4.2 On the best regularization allowing I.I.

We now consider the best regularization which has minimum MSE. It is given by (37) in the I.C. scenario. Here we aim to characterize the I.I. case. From (46) we know \( NS_iB + I \) is always invertible. Define

\[
L_i \triangleq (NS_iB + I)^{-1},
\]

and thus

\[
I + L_i = (NS_iB + I)^{-1} NS_iB = -NL_iS_iB.
\]

Therefore, we have

\[
(I + L_i) B = -NL_iS_iB \bar{B}.
\]

Then we propose the following theorem to characterize the best kernel matrix, allowing \( B \) to be singular.

**Theorem 2** For the \( i \)-th POVM element with true parameter \( \theta_i \) and normalized weighted parameterization matrix \( B \) as (48), define \( \Gamma \triangleq \{ M \mid M = \theta_i \theta_i^T + V \text{ diag } (0, Z_3) V^T, Z_3 \geq 0, \dim(Z_3) = d^2 - \text{rank}(B) \} \). If \( \theta_i \in R(B) \), then \( S_i \) achieves the minimum of the LS MSE \( \mathbb{E} \| \hat{E}_i - P_i \|^2 \) (i.e., \( S_i \) is the best regularization) if and only if \( S_i \in \Gamma \).

**Proof.** For the LS MSE \( \| \hat{E}_i - P_i \|^2 \) with kernel matrix \( S_i \), using (44) and (45), it can be rewritten as

\[
\text{Tr} [\text{MSEM} | S_i] = \text{Tr} \left[ (NS_iB + I)^{-1} (NS_iBS_i + \theta_i \theta_i^T) (NBS_i + I)^{-1} \right] = \text{Tr} \left[ \frac{(I + L_i) \hat{B} (I + L_i)^T}{N} + L_i \theta_i \theta_i^T L_i^T \right],
\]

and thus

\[
\text{Tr} \left[ \frac{(I + L_i) \hat{B} (I + L_i)^T}{N} + 2L_i \theta_i \theta_i^T = 0 \right].
\]

If there exists \( S_i \geq 0 \) so that (58) holds for the corresponding \( L_i|S_i \), then such an \( S_i \) is the optimal solution to minimize the MSE (57). We tentatively plug \( S_i \) in (58), which (using (56)) becomes

\[
2L_i \left( -S_iB \bar{B} + \theta_i \theta_i^T \right) = 0,
\]

equivalent to

\[
\bar{B}BS_i = \theta_\beta \theta_\beta^T.
\]

Since \( \theta_i \in R(B) \), we let \( \theta_i = Bb \) and then (59) becomes

\[
V \left[ I_{21} \begin{matrix} 0 \\ 0 \end{matrix} \right] V^T S_i = \left[ \begin{matrix} Z_1 \\ Z_2 \end{matrix} \right].
\]

Then (60) can be simplified as

\[
I_{21} \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} = \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix},
\]

and thus

\[
Z_1 = \Sigma_{21} pp^T \Sigma_{21} 0, Z_2 = 0.
\]

Since

\[
\theta_i \theta_i^T = V \left[ \Sigma_{21} pp^T \Sigma_{21} 0 \right] V^T,
\]
all solutions to (59) can be expressed as

\[ S_i = V \begin{bmatrix} \Sigma_{21} p p^T \Sigma_{21} & 0 \\ 0 & Z_3 \end{bmatrix} V^T = \theta_i \theta_i^T + V \begin{bmatrix} 0 & 0 \\ 0 & Z_3 \end{bmatrix} V^T, \]

where \( Z_3 \) is positive semidefinite. Therefore, the solution set of (59) is exactly characterized by \( \Gamma \) where

\[ \Gamma \triangleq \{ M \mid M = \theta_i \theta_i^T + V \text{ diag} (0, Z_3) V^T, \ Z_3 \geq 0, \dim(Z_3) = d^2 - \text{rank}(B) \}. \]  

(66)

For all the best regularizations \( S_i \) in \( \Gamma \), we have \( S_i B = \theta_i \theta_i^T B \). This gives the minimum value of the MSE, which can be calculated as

\[
\text{Tr} (\text{MSEM} \mid_S, i \in \Gamma) = \text{Tr} \left( \text{MSEM} \mid_{\theta_i \theta_i^T} \right) \\
= \text{Tr} \left[ (N \theta_i \theta_i^T B + I)^{-1} (N \theta_i \theta_i^T B \theta_i \theta_i^T + \theta_i \theta_i^T) (N B \theta_i \theta_i^T + I) \right] \\
= \text{Tr} \left[ \theta_i \theta_i^T (N B \theta_i \theta_i^T + I)^{-1} \right].
\]

(67)

**Remark 4** Note that the best regularization can minimize \( \mathbb{E} \| \hat{E}_i - P_i \|^2 \) instead of \( \mathbb{E} \| \hat{P}_i - P_i \|^2 \). The question to choose the best regularization to minimize the final MSE \( \mathbb{E} \| \hat{P}_i - P_i \|^2 \) where \( \hat{P}_i \geq 0 \) is still an open problem. Moreover, in practice, we do not know the true values of \( B \) and \( \theta_i \). One possible solution is to use a rough estimate \( \hat{\theta}_i \) and \( \hat{B}_N \) to replace \( \theta_i \) and \( B \) in \( \Gamma \). In this case, there may exist an optimal choice of \( Z_3 \) to achieve the minimum MSE and we leave it as an open problem.

Here, we compare Theorem 1 and Theorem 2. If \( \theta_i \in R(B) \), then for any full-rank kernel matrix \( S_i \), \( \theta_i \in R(S_i B) \) and thus the MSE scales as \( O(1/N) \). For any \( S_i \in \Gamma \), we can obtain the minimum MSE. In addition, \( \theta_i \in R(\theta_i \theta_i^T B) = R(S_i B) \), and thus the MSE also scales as \( O(1/N) \). If \( \theta_i \in N(B) \), all the ideal measurement data \( p_{ij} \) are zero, i.e., we cannot obtain any information from the measurement data. Therefore, \( \theta_i \) is not identifiable. If \( \theta_i = \theta_{i,1} + \theta_{i,2} \) where \( \theta_{i,1} \neq 0, \theta_{i,1} \in R(B) \) and \( \theta_{i,2} \neq 0, \theta_{i,2} \in N(B) \), then \( \theta_{i,1} \) is identifiable and \( \theta_{i,2} \) is not identifiable. Therefore, we only aim to identify \( \theta_{i,1} \) and the discussion is the same as \( \theta_i \in R(B) \).

We then consider two special cases. The first one is that \( B \) is full-rank. Therefore, \( \theta_i \in R(B) \) is always satisfied and the unique best kernel matrix is \( S_i = \theta_i \theta_i^T \) which is the same as [37]. The second one is \( S_i = \gamma \theta_i \theta_i^T \) where \( \gamma \) is a positive constant. Even if \( \theta_i \notin R(B) \), we still have \( \theta_i \in R(S_i B) \), otherwise \( R(S_i B) = 0 \), thus the MSE also scales as \( O(1/N) \). Note that all the above discussion is based on the assumption that \( N \) tends to infinity. When \( N \) is small, the performance of the regularization forms will be shown through simulation in Sec. 5.

### 5 Numerical simulation

In this section, the evaluation index is the sum of final MSEs \( \mathbb{E} \sum_{i=1}^{n} \| \hat{P}_i - P_i \|^2 \) and we discuss two commonly used classes of probe states for QDT. The first one involves \( d \) dimensional pure states \( \rho = |\psi\rangle \langle \psi| \) where \( |\psi\rangle \) is the superposition of \( d \) dimensional Fock states as

\[
|\psi\rangle = \sum_{i=1}^{d} c_i |i\rangle.
\]

(68)

In [49], an analysis indicates that pure states may perform better than mixed states for QDT to minimize MSE.

Another class of commonly used probe states for QDT is the coherent states, because they are more straightforward to be prepared. A coherent state is denoted as \( |\alpha\rangle \) where \( \alpha \in \mathbb{C} \) and it can be expanded using Fock states as

\[
|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{i=0}^{\infty} \frac{\alpha^i}{\sqrt{i!}} |i\rangle.
\]

(69)

Coherent states are in essence infinite dimensional. Denote the corresponding \( d \)-dimensional truncation as

\[
|\alpha_d\rangle \triangleq e^{-|\alpha_d|^2/2} \sum_{i=0}^{d-1} \frac{\alpha_d^i}{\sqrt{i!}} |i\rangle.
\]

To estimate a \( d \) dimensional detector, in the simulation we assume that the outcomes generated by the residual signal \( \text{Tr} [[|\alpha\rangle - |\alpha_d\rangle] (|\alpha\rangle - |\alpha_d\rangle)] \) are all included in the outcomes of the last POVM element. Since we truncate the coherent state in \( d \)-dimension, \( \text{Tr} (|\alpha_d\rangle \langle \alpha_d|) < 1 \) but for pure states in [68] \( \text{Tr} (|\rho|) = 1 \). Here we discuss resource distribution optimization without regularization and different regularization forms under the uniformly distributed resources.

When applying kernel-based regularization, an important problem is to determine the hyper-parameters (such as \( c, \mu \) in [32], [33] and [34]) in the kernel matrix \( S_i \). In this paper, we apply the same kernel matrix for all the POVM elements and use cross-validation in [37] to determine these hyper-parameters:
Fig. 1. The error scalings of different regularization forms with WLS using 20 types of 4 dimensional pure states. When the resource number \( N > 10^6 \), all the MSEs scale as \( O(1/N) \) satisfying Theorem 1. The best regularization is \( \theta_i^\text{best} = \theta_i \theta_i^T \) which is the lower bound of MSE and depends on true value of \( \theta_i \). Therefore, it cannot be used in practice and we aim to achieve regularization closest to the best regularization.

(1) Split the probe states randomly into two parts: an estimation data part with probe state parameterization matrix \( X_1 \) and a validation data part with probe state parameterization matrix \( X_2 \).

(2) Collect all the hyper-parameters in a vector \( \omega \). Then estimate the detector as \( \hat{\theta}_i \) using the measurement data from \( X_1 \) for different candidate values of hyper-parameters \( \omega \in \bar{\Omega} \) where \( \bar{\Omega} \) is a finite set in our paper.

(3) Using the validation data from \( X_2 \), we find

\[
\omega_0 = \arg\min_{\omega \in \bar{\Omega}} \sum_{i=1}^n \| \bar{y}_i - X_2 \hat{\theta}_i(\omega) \|^2. \tag{70}
\]

The model can then be re-estimated for this \( \omega_0 \) using all the probe states. Other methods to determine the hyper-parameters can also be found in [37,41].

5.1 Superposed Fock states

We consider a 4 dimensional three-valued phase-sensitive detector as

\[
P^{(4)}_1 = \begin{bmatrix}
0.1 & 0 & 0.002 - 0.005i & 0.003 + 0.007i \\
0 & 0.2 & 0 & 0 \\
0.002 + 0.005i & 0 & 0.3 & 0 \\
0.003 - 0.007i & 0 & 0 & 0.4
\end{bmatrix},
\]

\[
P^{(4)}_2 = \begin{bmatrix}
0.2 & 0.001 + 0.002i & 0 & 0 \\
0.001 - 0.002i & 0.2 & 0 & 0 \\
0 & 0 & 0.3 & 0 \\
0 & 0 & 0 & 0.4
\end{bmatrix},
\]

\[
P^{(4)}_3 = I - P^{(4)}_1 - P^{(4)}_2.
\]

Using the algorithm in [57,58], we generate 20 different types of 4 dimensional pure states. To determine the hyper-parameters in the DI kernel, we use 16 pure states as estimation data and 4 pure states as validation data. We use different regularization forms including no regularization \((27)\) with \( c = 0 \), Tikhonov regularization \((27)\) with \( c = 10 \), kernel-based regularization \((32)\) with \( c = 0.1, \mu = 0.9 \), rank-1 adaptive regularization, full-rank adaptive regularization (see Sec. 4) and the best regularization \((37)\). The best regularization is the lower bound of MSE and depends on true value of \( \theta \). Therefore, it cannot be used in practice and we aim to achieve regularization closest to the best reg-
ularization. For rank-1 adaptive regularization, we use kernel-based regularization (32) with $c = 0.1, \mu = 0.9$ in step 1 and (39) in step 2. For full-rank adaptive regularization, we use kernel-based regularization (32) with $c = 0.1, \mu = 0.9$ in step 1 and (40) in step 2. For each resource number, we run the algorithm 100 times and obtain the average MSE and standard deviation.

The results are shown in Fig. 1. The best regularization scales as $O(1/N)$ satisfying Theorem 1. When the resource number $N < 10^6$, the MSEs of kernel-based regularization and adaptive regularization are a little smaller than Tikhonov regularization and no regularization. In addition, full-rank adaptive regularization has a little smaller MSE than rank-1 adaptive regularization. When the resource number $N > 10^6$, all the MSEs scale as $O(1/N)$ satisfying Theorem 1.

Since these 4 dimensional pure states are I.C., without regularization, we also consider resource distribution optimization. We compare the MSE of the case with averagely distributed resources $N/M$ (“Average” in Fig. 2) and the MSE of the case with optimized resource distribution (“Optimized” in Fig. 2) by solving (26). For each resource number $N$, we run the algorithm 100 times and obtain the average MSE and standard deviation. The results are shown in Fig. 2. We can obtain a lower MSE with resource distribution optimization and both MSEs scale as $O(1/N)$ when $N > 10^5$.

Then we generate only 10 random types of 4 dimensional pure states. To determine the hyper-parameters in the different kernels, we use 8 pure states as the estimation data and 2 pure states as the validation data. Here we assume that we have the prior knowledge that the true detector is close to a phase-insensitive detector. Therefore, we use the Moore-Penrose inverse of $X^T X$ to obtain an estimate instead of (16), which is called “no regularization” in Fig. 3. The best regularization also scales as $O(1/N)$ satisfying Theorem 1. Kernel-based regularization has the minimum MSE compared with other regularization forms because DC kernel utilizes the prior knowledge on the sparsity of coefficients. In addition, the MSEs of adaptive regularizations are always a little smaller than Tikhonov regularization and no regularization when $N < 10^5$.

Hence we change DI kernel to DC kernel (34) with $c = 0.1, \mu_1 = 0.2, \mu_2 = 0.9$ in this case and the results are shown in Fig. 4. In this I.I. scenario, there does not exist a unique solution for WLS (16) without regularization. Therefore, we use the Moore-Penrose inverse of $X_i^T X_i$ to obtain an estimate instead of (16), which is called “no regularization” in Fig. 4. The best regularization also scales as $O(1/N)$ satisfying Theorem 1. Kernel-based regularization has the minimum MSE compared with other regularization forms because DC kernel utilizes the prior knowledge on the sparsity of coefficients. In addition, the MSEs of adaptive regularizations are always a little smaller than Tikhonov regularization and no regularization when $N < 10^5$.
kernel matrix $S_i^{(1)}$, the condition $\theta_i \notin R(S_i^{(1)})B$ is usually not satisfied in the I.I. scenario. Thus, the estimate $\hat{\theta}_i^0$ is biased and MSE tends to a positive constant $c$ as

$$\lim_{N \to \infty} \mathbb{E} \| \theta_i - \hat{\theta}_i^0 \| = c > 0. \quad (73)$$

Then in the second step, if we choose regularization as $(39)$, $\theta_i \notin R(S_i^{\text{rank-1}})B$ because the only one vector in $R(S_i^{\text{rank-1}})B$ is $\hat{\theta}_i^0$ and $\lim_{N \to \infty} \mathbb{E} \| \theta_i - \hat{\theta}_i \| = c > 0$. Moreover, even if we use multi-step regularization with rank-1 kernel matrix as above, the estimation result is still biased and MSE always tends to a constant, because the number of adaptive steps is always finite. As $N$ increases, except the best regularization, all the MSEs tend to constants as predicted by Theorem 1 because $\theta_i \in R(S_iB)$ does not hold.

**5.2 Coherent states**

Since coherent states are truncated, we consider a larger dimensional three-valued phase-sensitive detector as

$$P_1^{(8)} = U_1 \text{diag} \left( P_1^{(4)}, P_1^{(4)} \right) U_1^\dagger,$$
$$P_2^{(8)} = U_2 \text{diag} \left( P_2^{(4)}, P_2^{(4)} \right) U_2^\dagger,$$
$$P_3^{(8)} = I - P_1^{(8)} - P_2^{(8)}, \quad (74)$$

where $d = 8$ and $U_1, U_2$ are random unitary matrices [59, 58]. We also ensure $P_3^{(8)}$ is positive semidefinite.

Since coherent states are more similar to each other, we generate 640 random different types of coherent states using the probe state preparation in [29] where the real part and imaginary part of $\alpha$ are randomly generated in the interval $[-1, 1]$. We use different regularization forms including no regularization $(27)$ with $c = 0$, Tikhonov regularization $(27)$ with $c = 10$, kernel-based regularization $(32)$ with $c = 0.2, \mu = 0.9$, rank-1 adaptive regularization, full-rank adaptive regularization (see Sec. 4) and the best regularization (37). For rank-1 adaptive regularization, we use kernel-based regularization $(32)$ with $c = 0.2, \mu = 0.9$ in step 1 and (39) in step 2. For full-rank adaptive regularization, we use kernel-based regularization $(32)$ with $c = 0.2, \mu = 0.9$ in step 1 and (40) in step 2. For each resource number, we run the algorithm 100 times and obtain the average MSE and standard deviation.

The results are shown in Fig. 5. When $N < 10^8$, the MSEs of kernel-based regularization and adaptive regularization are a little smaller than Tikhonov regularization and no regularization. In addition, full-rank adaptive regularization has a little smaller MSE than rank-1 adaptive regularization. When $N > 10^8$, all the MSEs scale as $O(1/N)$ satisfying Theorem 1. Since these coherent states are I.C., we also consider resource distribution optimization without regularization. The simulation results are shown in Fig. 6. We can also obtain a lower MSE with resource distribution optimization and both MSEs scale as $O(1/N)$ for $N > 10^7$. Then using the same algorithm in [29], we generate only 48 random types of coherent states where real parts and imag-
Fig. 5. The error scalings of different regularization forms with WLS using 640 types of coherent states. When $N > 10^8$, all the MSE scales as $O(1/N)$ satisfying Theorem 1. The best regularization is $S_{best} = \theta_i\theta_i^T$ which is the lower bound of MSE and depends on true value of $\theta_i$. Therefore, it cannot be used in practice and we aim to achieve regularization closest to the best regularization.

6 Experimental examples

We consider the same quantum optical experimental system for QDT in [60] and [29]. Ref. [29] used Tikhonov regularization based on standard LS to complete the QDT. Here, we consider the same experimental data and employ kernel-based regularization based on WLS instead to further improve the QDT accuracy.

6.1 Experimental setup

The entire experimental setup is given in Fig. 8 which determines the structure of the detector to be estimated. More details about this setup can be found in [29,60]. It leads to block-diagonal binary detectors $P_0 + P_1 = I$ as

$$P_i = L_1^{(i)} \oplus L_2^{(i)} \oplus \cdots \oplus L_m^{(i)},$$

(75)

where $m$ is the number of different blocks and $L_j^{(i)} \geq 0$ is $d_j \times d_j$ dimensional, with $\sum_{j=1}^m d_j = d$. Hence, we need to identify each block $L_j^{(i)}$. Two-mode coherent states are prepared for detector tomography by using an adequately attenuated continuous-wave (CW) fiber coupled laser as depicted in the green dashed box in Fig. 8 [29,60].

We express the general two-mode coherent state without global phase as $|\alpha, \beta e^{i\delta}\rangle$ ($\delta \in \mathbb{R}, \alpha, \beta \geq 0$), which
Fig. 7. The error scalings of different regularization forms with WLS using 48 types of coherent states. Except the best regularization, all the MSEs tend to constants as predicted by Theorem 1 and Remark 2 because \( \theta_i \in R(S,B) \) does not hold. Using true parameters \( \theta_i \), the best regularization is \( S_{\text{best}}^i = \theta_i \theta_i^T \) and thus \( \theta_i \in R(S,B) \) always holds. According to Theorem 1, the best regularization scales as \( O \left( \frac{1}{N} \right) \) for arbitrary detectors.

6.2 Result comparison

Ref. [29] considered experiments for two different sets of detectors, denoted as Group I and Group II, respectively, and the basis of the POVM elements is the two-mode Fock state basis as \( \{ |0,0\rangle, |1,0\rangle, |0,1\rangle, |2,0\rangle, |1,1\rangle, |0,2\rangle \} \). For the true value of Group I, \( P_1 = L_1^{(1)} \oplus L_2^{(1)} \oplus L_3^{(1)} \), and we have \( L_1^{(1)} = 2.91 \times 10^{-4} \), \( L_2^{(1)} = \begin{bmatrix} 0.202 & 0.00109i \\ -0.00109i & 0.202 \end{bmatrix} \), and

\[
L_3^{(1)} = \begin{bmatrix} 0.363 & 0.00123i & 1.20 \times 10^{-6} \\ -0.00123i & 0.363 & 0.00123i \\ 1.20 \times 10^{-6} & -0.00123i & 0.363 \end{bmatrix}.
\]
For the true value of Group II, we have $L^{(1)}_{1} = 1.27 \times 10^{-4}$,

$$L^{(1)}_{2} = \begin{bmatrix} 0.0763 & -0.0440 + 0.0879i \\ -0.0440 - 0.0879i & 0.127 \end{bmatrix},$$

and $L^{(1)}_{3} = \begin{bmatrix} 0.147 & -0.0574 + 0.115i 0.00580 + 0.00773i \\ -0.0574 - 0.115i & 0.184 - 0.0543 + 0.109i \\ 0.00580 - 0.00773i -0.0543 - 0.109i & 0.238 \end{bmatrix}$.

Ref. [29] recorded $10^6$ measurement outcomes for each input state, and repeated the process 6 times. We use these measurement data to identify the detectors and also plot the identification results using simulated measurement data as a comparison in Fig. 9 and Fig. 10.

For the QDT problem, Ref. [29] employed Tikhonov regularization with standard LS estimation, where they chose $D_{\text{Tikhonov}} = \frac{10^4}{N} I$ and the estimation is given in [28], while here we use rank-1 adaptive regularization and full-rank adaptive regularization with WLS. Since the result of kernel-based regularization is similar to adaptive regularization, we only show the results of adaptive regularization.

To determine the hyper-parameters in the DI kernel, we use 15 probe states as estimation data and 4 probe states as validation data. In Group I, we choose $c = 0.001$, $\mu = 0.8$ in (32) in step 1 and (39) in step 2 for rank-1 adaptive regularization and for full-rank adaptive regularization, we choose $c = 0.0008$, $\mu = 0.9$ in (32) in step 1 and (40) in step 2. The results are shown in Fig. 9. Adaptive regularization (WLS) performs better than Tikhonov regularization (LS) in [29], especially for large resource number $N$. In addition, the MSE of full-rank adaptive regularization is a little smaller than rank-1 adaptive regularization. In Group II, for rank-1 adaptive regularization, we choose $c = 0.0008$, $\mu = 0.9$ in (32) in step 1 and (39) in step 2 and for full-rank adaptive regularization, we choose $c = 0.0008$, $\mu = 0.9$ in (32) in step 1 and (40) in step 2. The results are shown in Fig. 10. Adaptive regularization (WLS) performs better than Tikhonov regularization (LS) when $N > 10^{2.5}$ and the MSE of full-rank adaptive regularization is always a little smaller than rank-1 adaptive regularization. Moreover, the MSE of Group II is a little larger than that of Group I because the amplitudes of nondiagonal elements in Group II are significantly larger than zero.

7 Conclusion

In this paper, using regularization, we improve QDT accuracy with given probe states. In the I.C. and I.I. scenarios, we have employed WLS estimation, discussed different regularization forms, proved the scaling of MSE under the static assumption and characterized the best regularization. In the I.C. scenario, without regularization, we have studied resource distribution optimization and converted it to an SDP problem. The numerical examples have demonstrated the effectiveness of different regularization forms and resource distribution optimization. In a quantum optical experiment, our adaptive regularization with WLS has achieved lower mean squared errors compared with Tikhonov regularization with LS. It remains an open problem how to choose the kernel optimally in adaptive regularization.
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