

Maximum Likelihood, Minimum Effort

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We provide an efficient method for computing the maximum likelihood mixed quantum state (with density matrix ρ) given a set of measurement outcome in a complete orthonormal operator basis subject to Gaussian noise. Our method works by first changing basis yielding a candidate density matrix μ which may have nonphysical (negative) eigenvalues, and then finding the nearest physical state under the 2-norm. Our algorithm takes at worst $O(d^4)$ for the basis change plus $O(d^3)$ for finding ρ where d is the dimension of the quantum state. In the special case where the measurement basis is strings of Pauli operators, the basis change takes only $O(d^3)$ as well. The workhorse of the algorithm is a new linear-time method for finding the closest probability distribution (in Euclidean distance) to a set of real numbers summing to one.

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The race is not always to the swift nor the battle to the strong, but that's the way to bet—Damon Runyon

As scientists, we are faced again and again with the problem of determining from imperfect data what “really happened” in an experiment. Generally, the more data one has the better the reconstruction of the true events. Even so, the view remains imperfect, so one typically tries only to determine what was the event most likely to have led to the observed data. When quantum mechanics is considered, the situation is harder on the experimentalist, since even the results of perfectly performed measurements may have probabilistic results.

Nevertheless, one can still determine the quantum state of a system by performing many experiments on identically prepared systems and building up good statistics on the outcomes. If the set of experiments is *informationally complete* then the mixed state density matrix describing the system can be determined. This is called quantum state tomography [1–3]. A completely determination of the state would require an infinite number of perfect measurements, which are unobtainable, so instead we concentrate on finding the maximum likelihood state (*cf.* [4]).

We consider an informationally complete set of measurements, each performed many times on identically prepared quantum systems. From the experimental outcomes, we would like to determine the quantum state that gives the observed results with highest probability. This can be a computationally intensive task. For the two qubit experiments of [5], conventional ML solving took more time than the experiments themselves. And it has been reported in [6] that the ML reconstruction for 8 qubits in [7] took *weeks* of computation. Our main result is a fast algorithm for reconstructing this state when the noise is Gaussian. For 8 qubits our algorithm runs in *seconds*.

The rest of the paper is organized as follows: First, we show that the ML state reconstruction problem with

Gaussian noise is equivalent to a least-squares minimization problem on quantum states. Next, we prove that the minimum takes a particularly simple form. Finally, we give a fast algorithm that finds this minimum explicitly and benchmark it against direct minimization.

Reduction to density matrix minimization—Observables in quantum mechanics are Hermitian operators with the expectation value of a Hermitian operator σ applied to a mixed state ρ given by $\text{Tr}(\sigma\rho)$. We can represent the result of an imperfect measurement of such an expectation subject to additive Gaussian noise with variance v as a probability density function $p(m|\rho) = \frac{1}{\sqrt{2\pi v}} e^{-[m - \text{Tr}(\sigma\rho)]^2/(2v)}$.

Given an orthonormal Hermitian operator basis $\{\sigma_i\}_{i=1}^{d^2}$ on $d \times d$ matrices (with $\text{Tr}[\sigma_i \sigma_j] = d\delta_{ij}$), and a particular set of measured values m_{ij} corresponding to j th measurement result of expectation value σ_i applied to the “true state” ρ_0 , we want to find the mixed state ρ , a trace 1 Hermitian matrix with only nonnegative eigenvalues, maximizing the likelihood function

$$\mathcal{L} = \prod_{ij} p^{(i)}(m_{ij}|\rho) = \prod_{ij} \frac{1}{\sqrt{2\pi v}} e^{-[m_{ij} - \text{Tr}(\sigma_i \rho)]^2/(2v)} \quad (1)$$

or

$$\mathcal{L} = \prod_i \left(\frac{1}{\sqrt{2\pi v}} \right)^n e^{-n[m_i - \text{Tr}(\sigma_i \rho)]^2/(2v)}. \quad (2)$$

Here n is the number of measurement results for the expectation of σ_i and $m_i = \sum_{j=1}^n m_{ij}/n$ is the average value of those results. The same ρ that maximizes \mathcal{L} will minimize the log likelihood function

$$\mathcal{L}_{\log} = \sum_i [m_i - \text{Tr}(\sigma_i \rho)]^2. \quad (3)$$

Working in the operator basis of the $\{\sigma_i\}$ s is not convenient, but fortunately the distance is just the Hilbert-Schmidt, or 2-norm, which is basis independent. We show this here for completeness:

Lemma: $\sum_i (m_i - r_i)^2 = \|\mu - \rho\|_2^2 / d$ where $m_i = \text{Tr}[\sigma_i \mu]$ and $r_i = \text{Tr}[\sigma_i \rho]$.

Proof:

$$\begin{aligned} \|\mu - \rho\|_2^2 &= \text{Tr}(\mu - \rho)^2 \\ &= \text{Tr}\left[\left(\sum_i (m_i - \text{Tr} \rho \sigma_i) \sigma_i\right)^2\right] \\ &= \sum_{ij} \text{Tr}[(m_i - \text{Tr} \rho \sigma_i) \sigma_i (m_j - \text{Tr} \rho \sigma_j) \sigma_j] \\ &= \sum_{ij} (m_i - \text{Tr} \rho \sigma_i) (m_j - \text{Tr} \rho \sigma_j) \text{Tr}[\sigma_i \sigma_j] \\ &= d \sum_i (m_i - \text{Tr} \rho \sigma_i)^2 \end{aligned} \quad (4)$$

□

The matrix $\mu = (1/d) \sum_i m_i \sigma_i$ can be thought of as the experimentally noisy view of the density matrix ρ_0 . Note that it is trace one by construction, but may have negative eigenvalues. Calculation of μ from the m_i s is a change of operator basis, and in general requires time $O(d^4)$ (there are d^2 values of i and each σ_i is a $d \times d$ matrix). This will actually be the limiting step in our overall algorithm, as all other steps will be $O(d^3)$ or better. In many cases of interest, however, the operator basis change can be done more quickly. This will be true whenever the matrices representing the σ_i s in the canonical basis are sparse. In particular, if the σ_i s are tensor products of the Pauli matrices

$$\{\sigma_0, \sigma_1, \sigma_2, \sigma_3\} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

on n qubits, so that $d = 2^n$, each σ_i has only d nonzero elements and the change of basis can be carried out in $O(d^3)$ steps.

Now, after the change of basis from the m_i s to μ , our original maximum-likelihood problem has been transformed into the following:

Subproblem 1: Given a trace-one Hermitian matrix μ , find the closest density matrix ρ (a trace-one Hermitian matrix with only nonnegative eigenvalues) under the 2-norm:

$$\|\mu - \rho\|_2^2 = \text{Tr}[(\mu - \rho)^2] = \sum_{ij} |\mu_{ij} - \rho_{ij}|^2 \quad (5)$$

This is immediately familiar as a least squares minimization problem, for which standard minimizer packages are well suited. Indeed, this is how the problem is often solved in practice. Unfortunately, finding the solution can be computationally intensive. In standard state reconstruction algorithms, this is the most expensive step by far (see Fig. 2).

Simple form for the minimum— To improve matters, since the 2-norm is basis independent, we can work in the eigenbasis of μ . Then we observe that the optimum

ρ is diagonal in this basis as well. This is immediate from the form of (5), where any off diagonal terms could only contribute positive amounts to the sum. Thus, the problem reduces to finding the eigenvectors and eigenvalues of μ and picking the d non-negative eigenvalues for ρ that minimize (5). Eigensystem solutions are $O(d^3)$ and good packages exist [8].

We are left with a minimization over d variables, effectively the square root of the difficulty of the original problem. Call the eigenvalues of μ, ρ μ_i, λ_i and arrange them such that $\mu_i \geq \mu_{i+1}$. We now want to minimize $\sum_i (\lambda_i - \mu_i)^2$ such that $\sum_i \mu_i = \sum_i \lambda_i = 1$ and $\lambda_i \geq 0$. Using the method of Lagrange multipliers to impose this constraint, and writing $\lambda_i = x_i^2$ to enforce non-negativity of λ_i we write the objective function

$$\Lambda = \sum_i (x_i^2 - \mu_i)^2 - L \left(\sum_i x_i^2 - 1 \right). \quad (6)$$

Differentiating with respect to x_i we have

$$\frac{\partial \Lambda}{\partial x_i} = 4(x_i^2 - \mu_i)x_i - 2Lx_i = 0. \quad (7)$$

This equation has two solutions, either $x_i = 0$ or

$$x_i^2 = L/2 + \mu_i. \quad (8)$$

Note that L doesn't depend on i so each $\lambda_i = x_i^2$ is either set to zero or given by μ_i plus the very same number. To evaluate L we must pick a set $\mathbf{s} = \{i \text{ such that } x_i \neq 0\}$. Then, summing (8) over i we have $1 = \sum_i x_i^2 = |\mathbf{s}|L/2 + \sum_{i \in \mathbf{s}} \mu_i$ or

$$L/2 = \frac{1}{|\mathbf{s}|} \sum_{i \notin \mathbf{s}} \mu_i \quad (9)$$

and

$$\Lambda = \frac{1}{|\mathbf{s}|} \left(\sum_{i \notin \mathbf{s}} \mu_i \right)^2 + \sum_{i \notin \mathbf{s}} \mu_i^2. \quad (10)$$

Lemma: Consider an i and j with $\mu_i > \mu_j$ with $i \in \mathbf{s}$ and $j \notin \mathbf{s}$. Then Λ_i , the distance function for this case, is always less than or equal to Λ_j , the distance function for a new set $\mathbf{s}' = \mathbf{s} + \{j\} - \{i\}$.

Proof: We can write

$$\Lambda_i = |\mathbf{s}| \left(\frac{L}{2} \right)^2 + \sum_{k \notin \mathbf{s}} \mu_k^2 \quad (11)$$

and for the case with $j \in \mathbf{s}$ and $i \notin \mathbf{s}$

$$\Lambda_j = |\mathbf{s}| \left(\frac{L}{2} + \frac{\mu_i - \mu_j}{|\mathbf{s}|} \right)^2 - \mu_j^2 + \mu_i^2 + \sum_{k \notin \mathbf{s}} \mu_k^2. \quad (12)$$

If we had $\Lambda_j < \Lambda_i$ this would imply

$$L < \frac{\mu_j - \mu_i - |\mathbf{s}|(\mu_i + \mu_j)}{|\mathbf{s}|}. \quad (13)$$

Then we would have

$$\lambda_j = \mu_j + \frac{L}{2} + \frac{\mu_i - \mu_j}{|\mathbf{s}|} < \frac{(|\mathbf{s}| - 1)(\mu_j - \mu_i)}{2|\mathbf{s}|} \leq 0 \quad (14)$$

because $\mu_i \geq \mu_j$. But λ_j must be nonnegative, therefore Λ is never decreased by moving i into and j out of \mathbf{s} .

□

The lemma tells us that all the λ_i s that are zero are together at the end, matching up with the smallest μ_i ’s. Thus, rather than the 2^d possible choices for \mathbf{s} we need only decide where to put the break between zero and nonzero λ_i ’s, for which there are only d choices.

Next, we show that the choice of \mathbf{s} should be the largest set satisfying the constraint that all the λ_i ’s are nonnegative. Starting from Eq. (11), we imagine removing some element j from from \mathbf{s} . Then

$$\Lambda' = \frac{1}{|\mathbf{s}| - 1} \left(|\mathbf{s}| \frac{L}{2} + \mu_j \right)^2 + \mu_j^2 + \sum_{k \notin \mathbf{s}} \mu_k^2 \quad (15)$$

and

$$\begin{aligned} \Lambda' - \Lambda_i &= \frac{1}{|\mathbf{s}| - 1} \left(|\mathbf{s}| \frac{L}{2} + \mu_j \right)^2 + \mu_j^2 - |\mathbf{s}| \left(\frac{L}{2} \right)^2 \\ &= \frac{|\mathbf{s}|}{|\mathbf{s}| - 1} \left(\left(\frac{L}{2} \right)^2 + 2\mu_j \frac{L}{2} + \mu_j^2 \right) \\ &= \frac{|\mathbf{s}|}{|\mathbf{s}| - 1} \left(\frac{L}{2} + \mu_j \right)^2 \geq 0. \end{aligned} \quad (16)$$

In other words, setting any more of the λ_i ’s to zero than necessary increases the distance function. We are now ready to give an algorithm for Subproblem 1.

Fast algorithm for Subproblem 1—

1. Calculate the eigenvalues and eigenvectors of μ . Arrange the eigenvalues in order from largest to smallest. Call these $\mu_i, |\mu_i\rangle$, $1 \leq i \leq d$.
2. Let $i = d$ and set an accumulator $a = 0$.
3. If $\mu_i + a/i$ is non-negative, go on to step 4. Otherwise, set $\lambda_i = 0$ and add μ_i to a . Reduce i by 1 and repeat step 3.
4. Set $\lambda_j = \mu_j + a/j$ for all $j \leq i$.
5. Construct $\rho = \sum_i \lambda_i |\lambda_i\rangle \langle \lambda_i|$.

Fig. 1 works through an example of this algorithm.

Efficiency of the algorithm— The slowest step is step 1, solving the eigensystem, which is $O(d^3)$ (the standard libraries such as LAPACK start and are limited by reducing a Hermitian matrix to tridiagonal form using the Householder method which is $O(d^3)$ [9]). Step 2 is obviously constant time, and step 3 and 4 together are easily seen to be $O(d)$. Step 5 involves a choice of whether one wants the answer in the eigenbasis of μ , in which

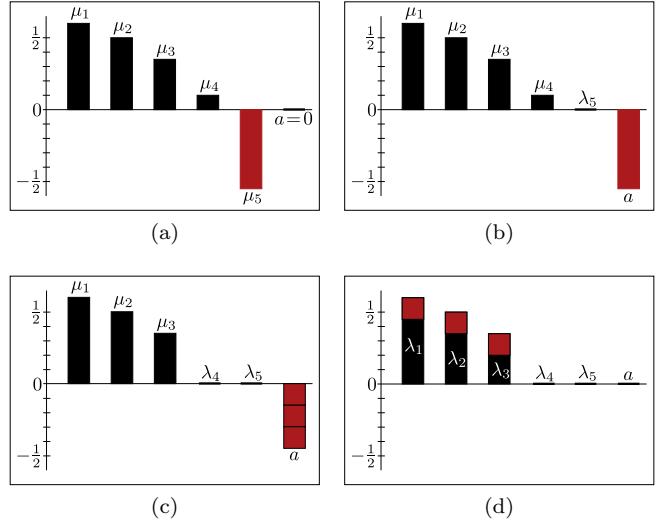


FIG. 1: Example of our algorithm for subproblem 1: (a) We start with $\mu_1 = 3/5$, $\mu_2 = 1/2$, $\mu_3 = 7/20$, $\mu_4 = 1/10$, $\mu_5 = -11/20$, and accumulator $a = 0$. (b) Since $\mu_5 + a/5$ is negative, λ_5 is set to 0 and a to $-11/20$. (c) Since $\mu_4 + a/4$ is negative, λ_4 is set to 0 and $a = -9/20$. (d) Finally, λ_1 , λ_2 , and λ_3 each have $a/3 = -3/20$ added to the corresponding μ . The final result is $\lambda_1 = 9/20$, $\lambda_2 = 7/20$, $\lambda_3 = 1/5$, and $\lambda_4 = \lambda_5 = 0$.

case it has already been computed, or in some other basis, in which case it is $O(d^3)$ or better [10]. Thus, the overall complexity is $O(d^3)$. The actual run-time of an implementation will depend primarily on the eigensystem solver used. Fig. 2 compares the run time of our algorithm with that of a traditional ML optimization.

Discussion— Our argument that the problem of ML state reconstruction reduces to finding the closest density matrix under the 2-norm to a nonphysical candidate matrix μ depended on the measurements of the expectation values of $\text{Tr}(\sigma_i \rho)$ in Eq. (1) having the same Gaussian variance for all i . In practice, this may not be the case. One solution to this is to equalize the variances by simply performing more of the noisier measurements. For example, in circuit quantum electrodynamics (superconducting qubits) quantum non-demolition measurement of a Pauli is performed with $v = 1/(\Gamma\tau)$ where Γ is the measurement rate and τ is the measurement time.

We have focused only on state reconstruction, but it is often desired to perform *process tomography* [11], that is, to determine the quantum input/output relation (a trace-preserving completely-positive map) implemented by an apparatus. Due to the Choi-Jamiolkowski isomorphism [12, 13] such a map can be represented by a density matrix. Thus, the generalization of our result to process tomography should be straightforward.

Finally, we note a connection to classical probability theory. If one considers the eigenvalues μ_i (some of which may be negative) as a noisy view of a *probability distri-*

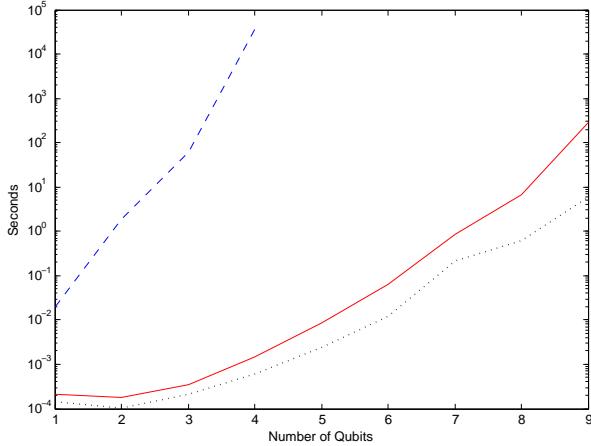


FIG. 2: Run time for reconstruction of random n -qubit pure states mixed with the identity and subjected to Gaussian noise on Pauli measurements. Given a set of measurement outcomes, we generate a candidate matrix μ consistent with the data but with potentially negative eigenvalues. We use two techniques to generate the maximum likelihood density matrix ρ . The top, dashed line, is Matlab’s `fminsearch` used to minimize $\text{Tr}[(\mu - \rho)^2]$ directly. The lowest, dotted line, is our algorithm for Subproblem 1. The middle, solid line, is the Subproblem 1 algorithm together with the basis change from the measurement outcomes to μ . All timings were performed in Matlab on a single core of an Intel E8400 CPU running at 3GHz.

bution, then the algorithm starting from step 2 is an algorithm for finding the nearest proper probability distribution. Furthermore, if the noise is Gaussian, this finds the maximum likelihood probability distribution.

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