Rank deficiency and the Euclidean geometry of quantum states

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Rank deficiency

The number of parameters required to characterize an arbitrary state of a d-dimensional quantum system quickly grows to intractable levels:

$$\text{Parameters} = d^2 - 1\,.$$

If there is good reason to believe that the system is well described by a state of bounded rank r, then the number of parameters required to describe the state only scales linearly in the Hilbert-space dimension:

$$\text{Parameters} = r\,(2d - r) - 1\,.$$

The "efficient" parametrization of bounded-rank states causes us to be interested in estimators that tend to return rank-deficient states, such as the maximum-likelihood estimator (MLE).

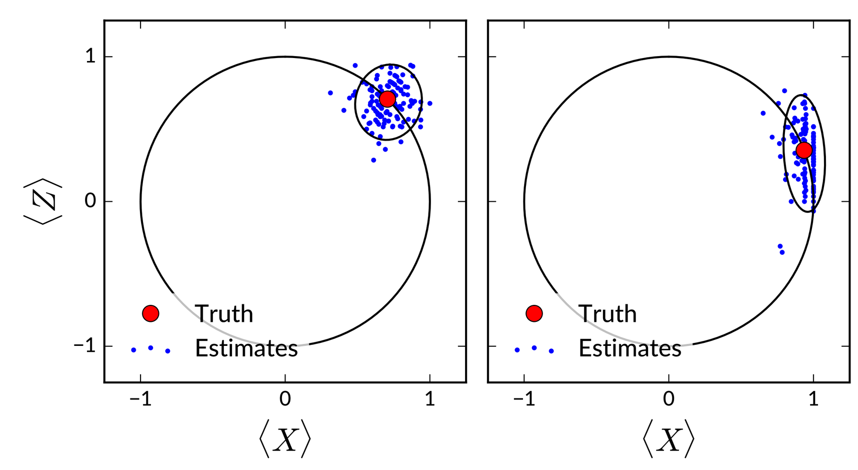
Maximum-likelihood estimation

The maximum-likelihood estimate for the quantum state is the density matrix that assigns the highest probability for obtaining the data:

$$\begin{aligned}\mathcal{L}(\rho \mid \text{data}) &:= \Pr(\text{data} \mid \rho)\\ \widehat{\rho}_{\text{MLE}}(\text{data}) &= \underset{\rho\geq 0,\,\mathrm{tr}[\rho]=1}{\arg\max}\ \mathcal{L}(\rho \mid \text{data})\,.\end{aligned}$$

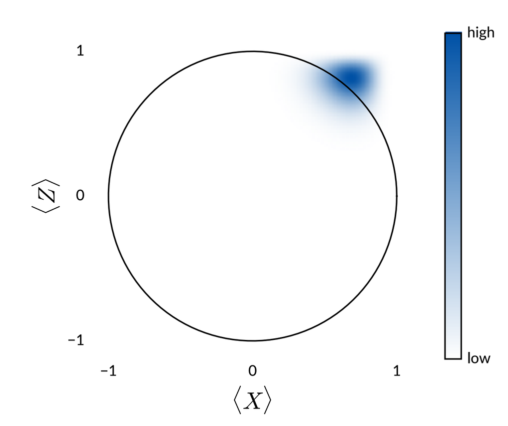
In the absence of boundaries to constrain the estimate, the maximum-likelihood estimator is asymptotically normal. For quantum state estimation, the only boundaries in the problem are those imposed by the positivity constraint, so it is sometimes convenient to perform an unconstrained maximum-likelihood estimate:

$$\widehat{A}_{\text{MLE}}(\text{data}) = \underset{\mathrm{tr}[A]=1}{\arg\max}\ \mathcal{L}(A \mid \text{data})\,.$$



Scatter plots of maximum-likelihood estimates for two different "true" states upon which random Pauli X and Z measurements were performed. Covariance ellipses illustrate the variation of the classical Fisher information within the state space (see bottom panel for more details).

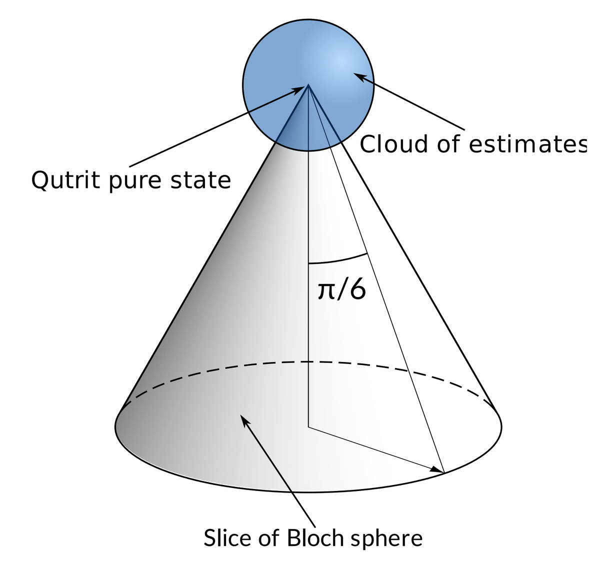
Unconstrained estimate lying outside the set of positive states result in constrained estimates lying on the boundary of the state space due to the convex structure of this problem.



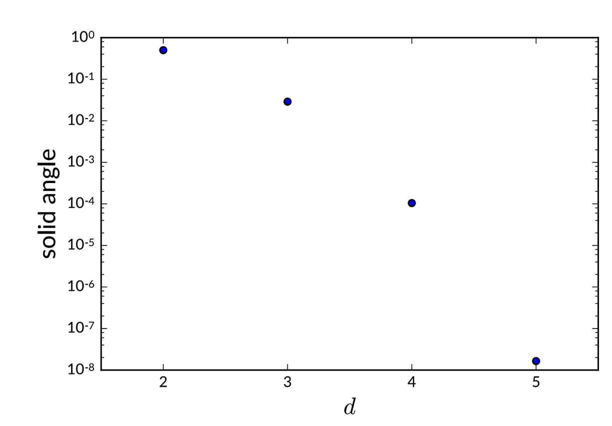
Likelihood functions with the maximum outside the state space reach their maximum value within the state space along the boundary.

State-space geometry

States on the boundary are rank deficient, and therefore offer some amount of parameter reduction. To partially characterize the rank-deficient behavior of maximum-likelihood estimates, we wish to calculate the probability of obtaining a rank-deficient estimate given a pure (rank-1) "true" state. Our initial calculations depend on some naïve assumptions discussed in the panel below.



The probability of obtaining a full-rank estimate has a geometric interpretation as the solid angle of a cone whose base is the state space for a quantum system of one lower Hilbert-space dimension.



The solid angles of the relevant cones fall precipitously as the Hilbert-space dimension grows.

Related Work

For a related geometric approach to model selection, see the poster *An effective state-space dimension for a quantum system* by Travis Scholten.

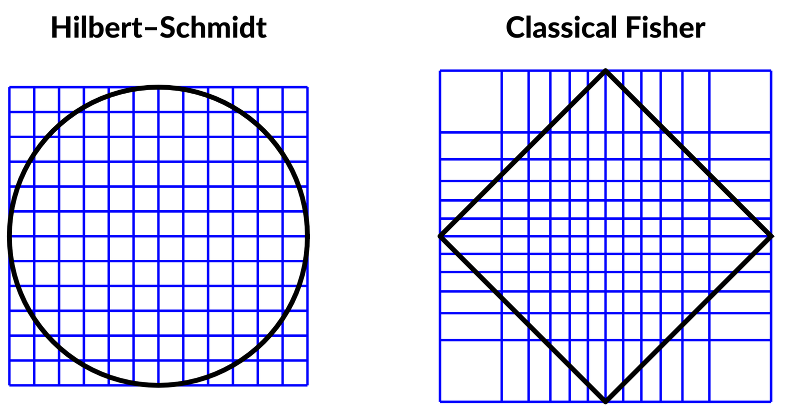
Classical Fisher metric

The solid-angles in the top panel were calculated assuming an isotropic covariance for the maximum-likelihood estimates relative to the Hilbert–Schmidt metric:

$$\left\lVert\rho_1 - \rho_2\right\rVert_{\text{HS}} = \sqrt{\mathrm{tr}\left[(\rho_1 - \rho_2)^2\right]}\,.$$

In general, the covariance of the maximum-likelihood estimates is expressed as the classical Fisher information C for the measurement $\{E^\xi\}_\xi$ being performed, evaluated at the "true" state ρ:

$$\begin{aligned}\rho &= \frac{1}{d}I + x^\alpha X_\alpha\\ C_{\alpha\beta} &= \sum_\xi \frac{\mathrm{tr}[E^\xi X_\alpha]\mathrm{tr}[E^\xi X_\beta]}{\mathrm{tr}[E^\xi\rho]}\\ \mathrm{Cov}\left(\widehat{x}^\alpha, \widehat{x}^\beta\right) &\sim \left[C^{-1}\right]_{\alpha\beta}\,.\end{aligned}$$



Comparison between the Hilbert–Schmidt metric and the classical Fisher metric for Pauli measurements on a rebit. The grid lines on the classical-Fisher diagram form squares where the metric is proportional to the Hilbert–Schmidt metric.

The figure above illustrates just how wildly the classical Fisher information, interpreted as a metric, can deviate from the Hilbert–Schmidt metric. Even for the simple case of a rebit, isotropy is only present along the diagonals.

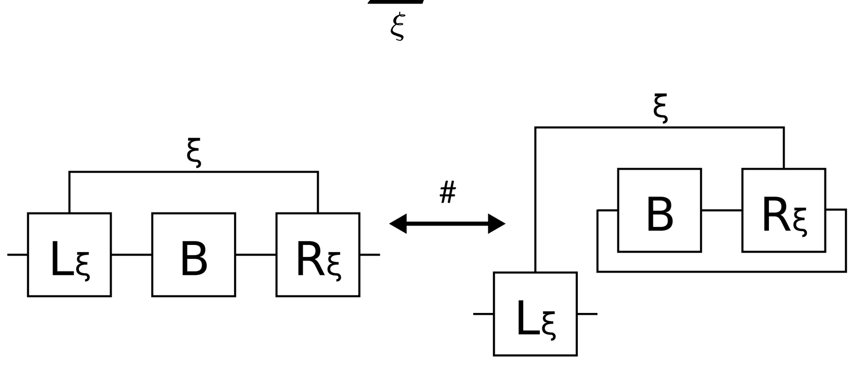
Higher dimensions

The classical Fisher metric has even more interesting behavior in Hilbert spaces of dimension 3 or higher. This behavior is made evident when considering the classical Fisher metric as a superoperator:

$$\mathcal{C}(\odot) = \sum_\xi \frac{E^\xi \odot E^\xi}{\mathrm{tr}[E^\xi\rho]}\,.$$

There is a certain involution on superoperators, denoted here by # (sharp), defined by

$$\begin{aligned}\mathcal{A}: B &\mapsto \sum_\xi L^\xi B R^\xi\\ \mathcal{A}^\sharp: B &\mapsto \sum_\xi \mathrm{tr}[R^\xi B]L^\xi\,.\end{aligned}$$



The # involution represented via a tensor diagram. The exchange of wires corresponds to swapping two indices of a rank-4 tensor.

If $\{E^\xi\}_\xi$ is composed entirely of rank-1 operators (a "lossless" POVM), the superoperator $\mathcal{C}$ is invariant under sharping. This seemingly esoteric observation has interesting consequences, as many widely used metrics (including the Hilbert–Schmidt metric) have associated superoperators that are *not* sharp invariant for Hilbert spaces of dimension 3 or higher. For this reason, the isotropic assumption will *never* be valid for rank-1 measurements.

Further inquiry

Isotropy of the classical Fisher information is a common assumption (see [1], for example). It remains to be seen how misleading this assumption is in practice.

Noisy measurements (for which the POVM contains higher-rank operators) do not generally yield sharp-invariant superoperators. Is it possible for such a measurement to produce an isotropic classical Fisher information, and if so how noisy must it be?

References

[1] *Efficient Method for Computing the Maximum-Likelihood Quantum State from Measurements with Additive Gaussian Noise*, John A. Smolin, Jay M. Gambetta, and Graeme Smith. Phys Rev. Lett. 108, 070502 – Published 17 February 2017

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