Quantum state estimation

Challenges and solutions, methods of statistical inference

—

Arthur Vesperini

Quantum statistics: generalities

Density operators and measurement basis

Quantum statistics: 2-level systems

Classical coin

$$x = 0, 1$$

Quantum coin

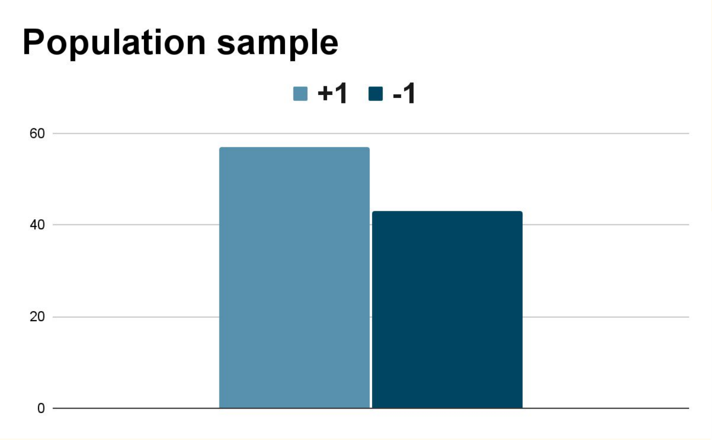
$$|x\rangle = \alpha|0\rangle + \beta|1\rangle$$

Quantum statistics: 2-level systems

Classical coin

$$x = 0, 1$$

$$P(x) = p_0\delta(x) + p_1\delta(x-1)$$



Quantum coin

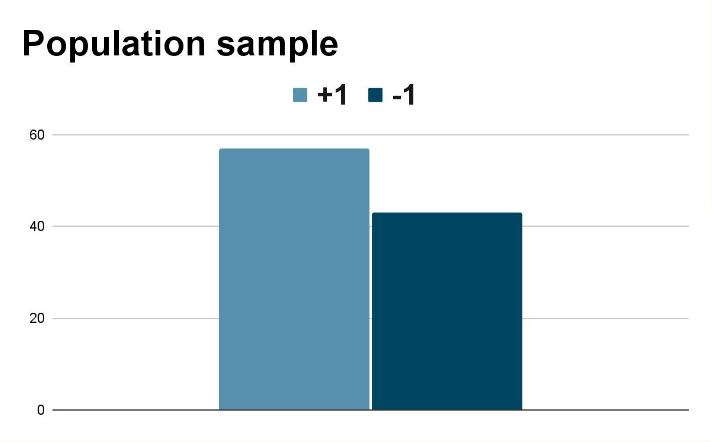
$$|x\rangle = \alpha|0\rangle + \beta|1\rangle$$

Quantum statistics: 2-level systems

Classical coin

$$x = 0, 1$$

$$P(x) = p_0\delta(x) + p_1\delta(x-1)$$



Quantum coin

$$|x\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$P(|x\rangle) = \mathrm{Tr}(\rho|x\rangle\langle x|)$$

$$\rho = \begin{pmatrix} p_0 & p_{01} \\ p_{01}^* & p_1 \end{pmatrix}$$

Quantum statistics: 2-level systems

Qubit / spin-1/2

"Classical" probabilistic mixture (diagonal matrix) of $|0\rangle$ and $|1\rangle$

$$\rho_c = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$$

Pure quantum superposition (off-diagonal "interferences")

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

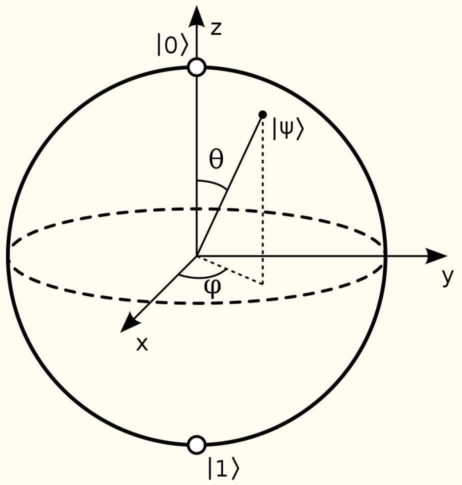
$$\rho_+ = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1| + |0\rangle\langle 1| + |1\rangle\langle 0|)$$

Quantum statistics: 2-level systems

Qubit / spin-1/2

$$\rho = \begin{pmatrix} p_0 & p_{01} \\ p_{01}^* & p_1 \end{pmatrix}$$

$$= \frac{1}{2}(\mathbb{I} + n_x\sigma_x + n_y\sigma_y + n_z\sigma_z)$$



⇒ Tomographic completeness: 3 independent basis of measurement ("*quorum*" of observables).

Quantum statistics: 2-level systems

Classical coin

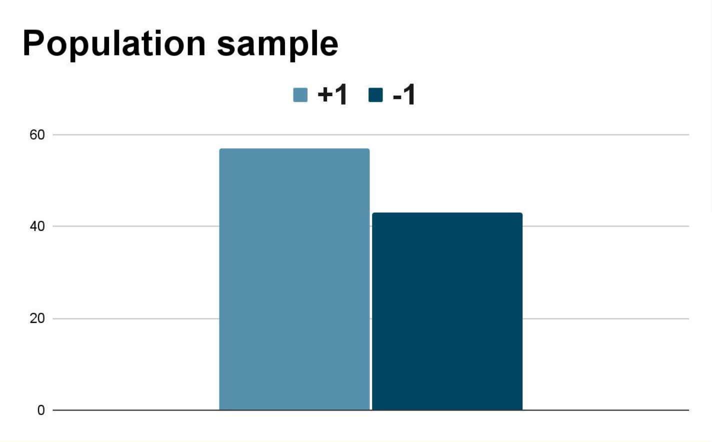
$$x = 0, 1$$

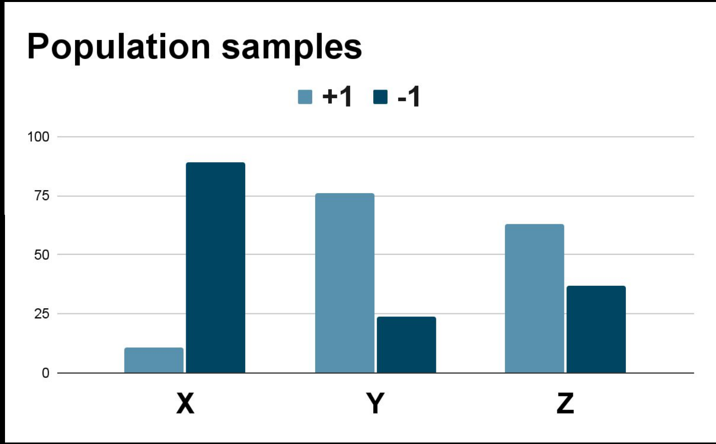
$$P(x) = p_0\delta(x) + p_1\delta(x-1)$$

Quantum coin

$$|x\rangle = \alpha|0\rangle + \beta|1\rangle$$

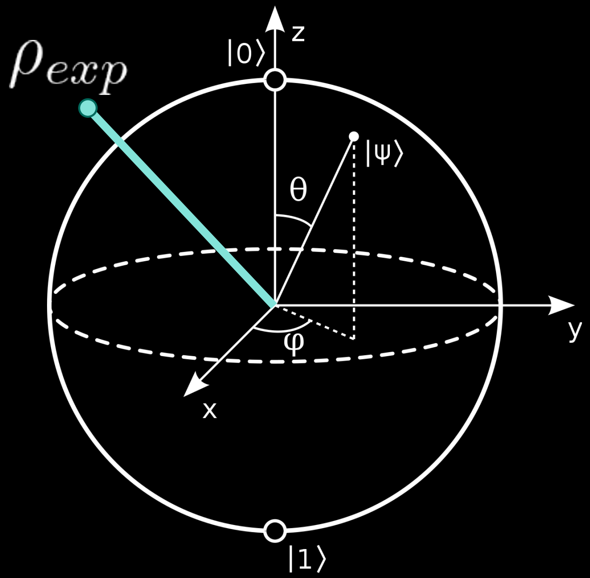
$$P(|x\rangle) = \mathrm{Tr}(\rho|x\rangle\langle x|)$$





Standard scheme: Linear Inversion

The problem of positivity



Main references:
[Řeháček et al., 2001;
Hradil et al., 2004;
Blume-Kohout, 2010]

Linear inversion: principle

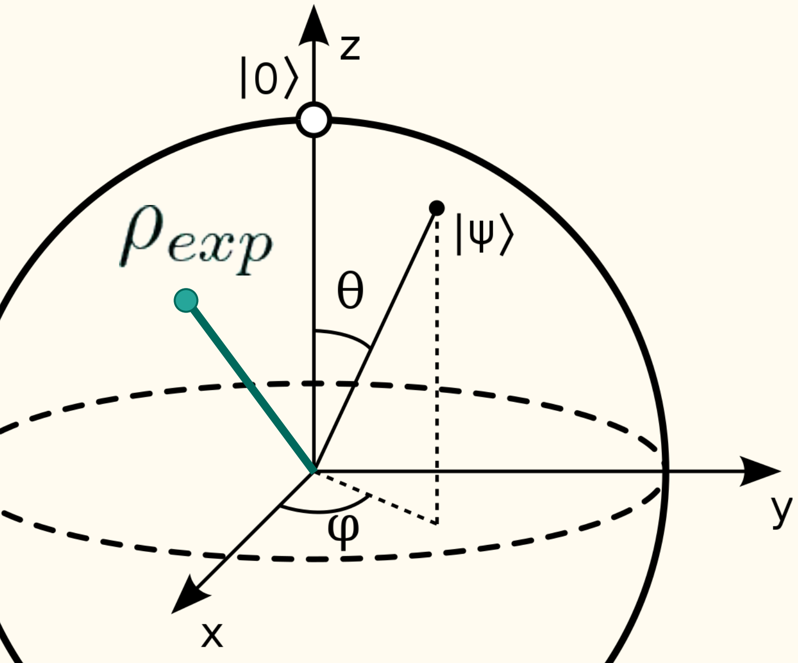
Direct linear inversion

$$f_j = \mathrm{Tr}(\rho_{exp}|x_j\rangle\langle x_j|) = \langle x_j|\rho_{exp}|x_j\rangle$$

$$\Rightarrow \quad \rho_{exp} = \sum_j f_j |x_j\rangle\langle x_j|$$

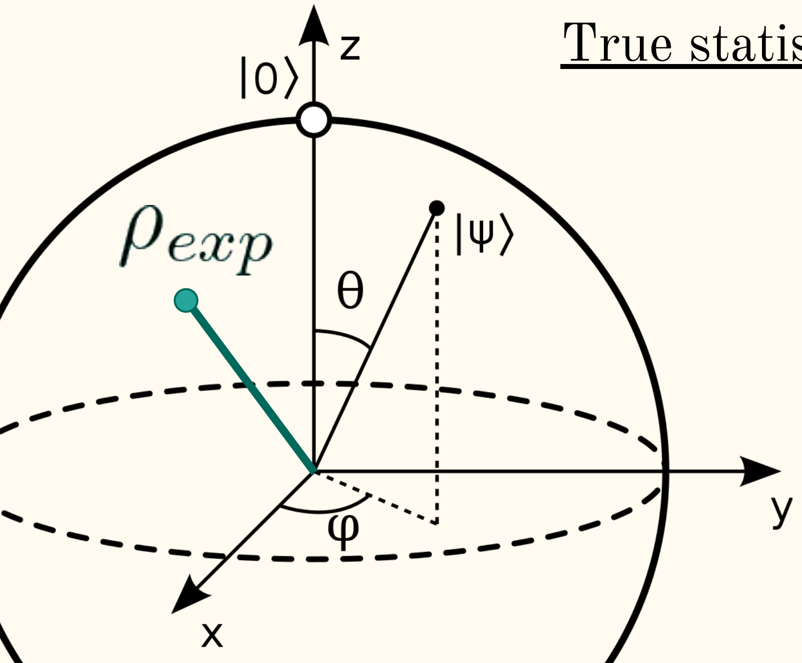
Linear inversion: 2-level systems (qubit/spin-½)

$$\rho_{exp} = \frac{1}{2}(\mathbb{I} + \vec{n}_{exp} \cdot \vec{\sigma})$$



Linear inversion: 2-level systems (qubit/spin-½)

$$\rho_{exp} = \frac{1}{2}(\mathbb{I} + \vec{n}_{exp} \cdot \vec{\sigma})$$

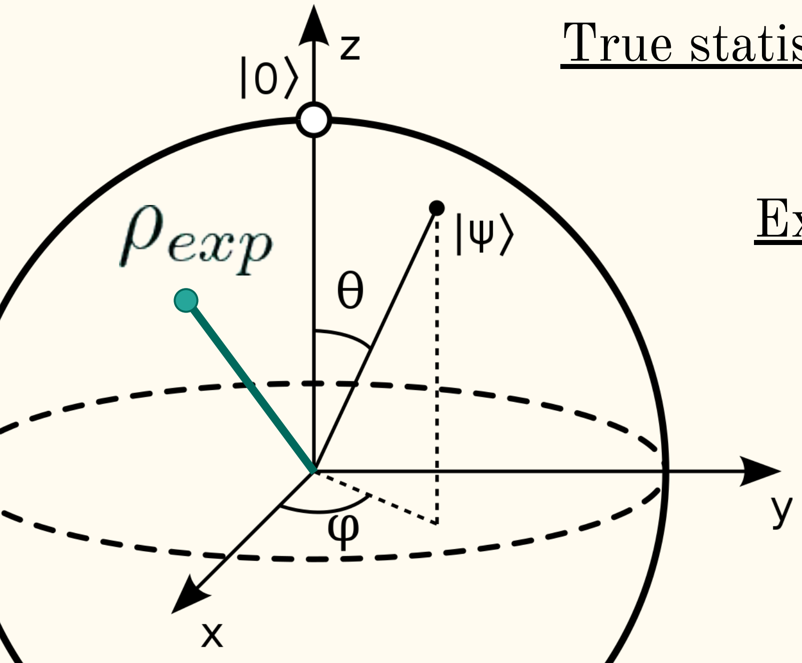


True statistics:

$$\rho = |0\rangle\langle 0| = \frac{1}{2}(\mathbb{I} + \sigma_z)$$

Linear inversion: 2-level systems (qubit/spin-½)

$$\rho_{exp} = \frac{1}{2}(\mathbb{I} + \vec{n}_{exp} \cdot \vec{\sigma})$$



True statistics:

$$\rho = |0\rangle\langle 0| = \frac{1}{2}(\mathbb{I} + \sigma_z)$$

Experimental outcome:

$$\vec{n}_{exp} = \begin{pmatrix} \langle\sigma_x\rangle_{exp} \\ \langle\sigma_y\rangle_{exp} \\ \langle\sigma_z\rangle_{exp} \end{pmatrix} = \begin{pmatrix} f_x - f_{-x} \\ f_y - f_{-y} \\ 1 \end{pmatrix}$$

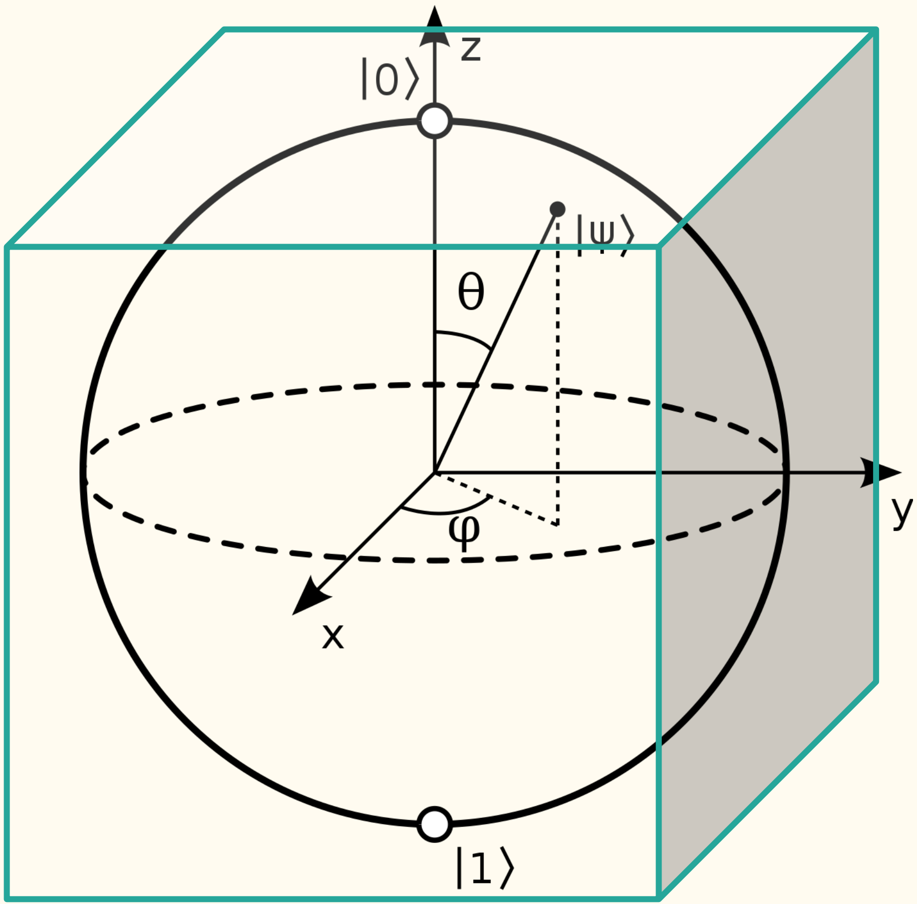
Linear inversion: 2-level systems (qubit/spin-½)

$$|n_i^{exp}| \leq 1$$

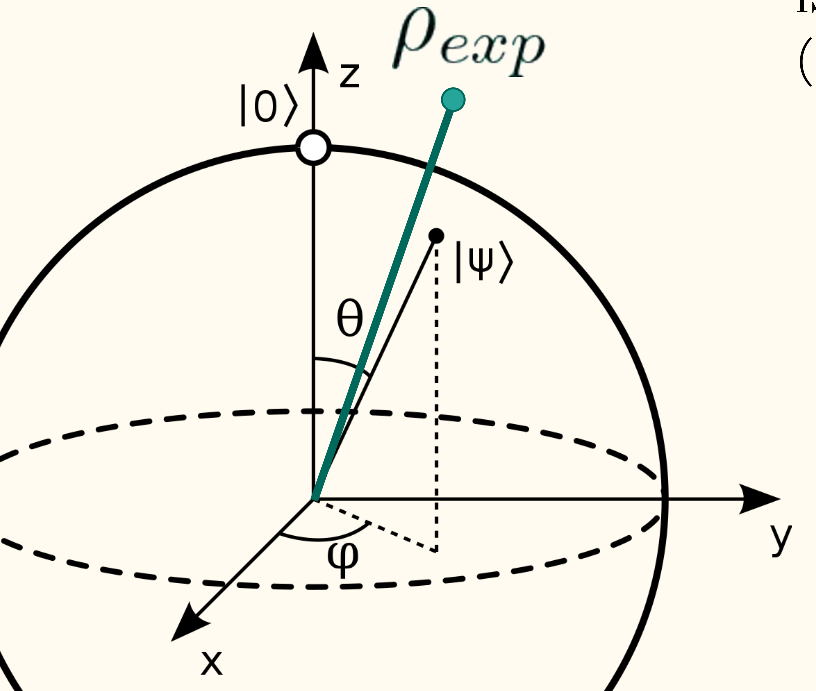
hence $\vec{n}_{exp}$ belongs to a “Bloch cube”.

In particular, we might have:

$$|\vec{n}_{exp}| > 1$$



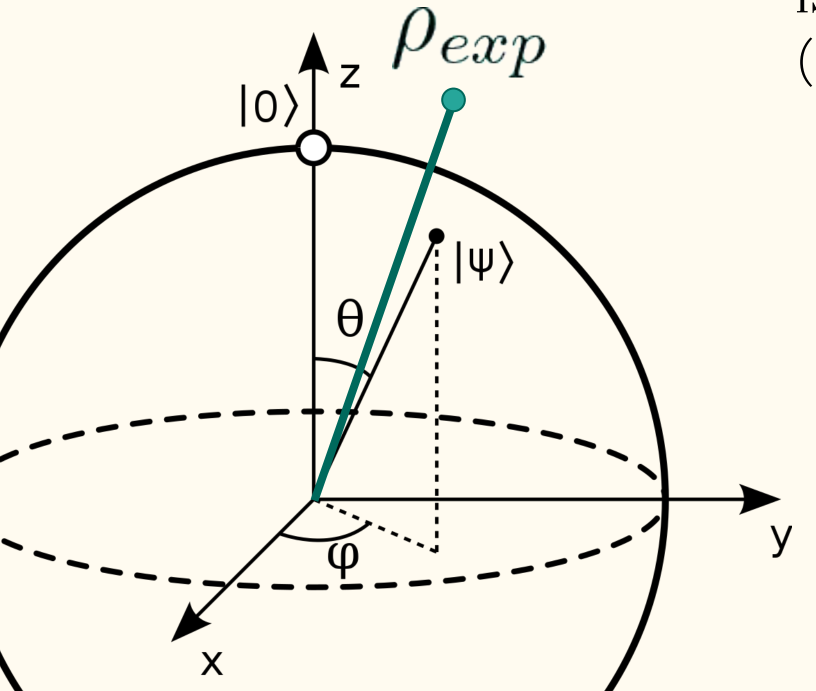
Linear inversion: 2-level systems (qubit/spin-½)



$$p^{exp}_{\pm n} = \lambda_{\pm n} = \frac{1 \pm |\vec{n}|}{2}$$

is negative or greater than one if $|\vec{n}| > 1$ (outside of the Bloch ball).

Linear inversion: 2-level systems (qubit/spin-½)



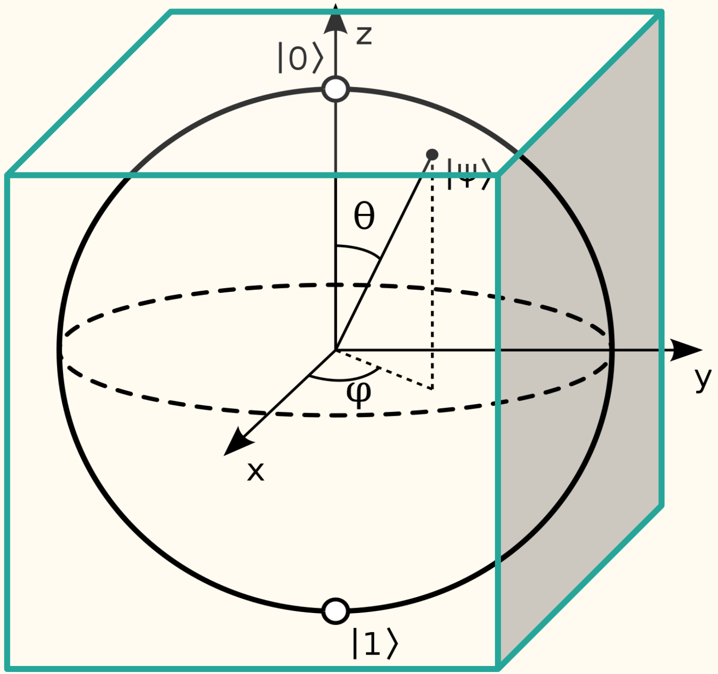
$$p_{\pm n}^{exp} = \lambda_{\pm n} = \frac{1 \pm |\vec{n}|}{2}$$

is negative or greater than one if $|\vec{n}| > 1$ (outside of the Bloch ball).

Generally ill-defined probability weights

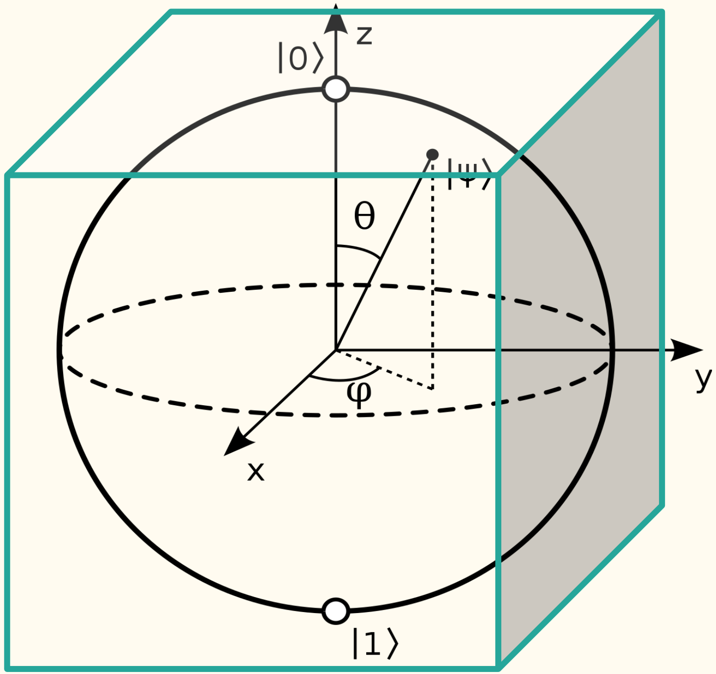
Linear inversion: 2-level systems (qubit/spin-½)

In quantum systems, there always exists an *infinite number of measurement basis*.



Linear inversion: 2-level systems (qubit/spin-½)

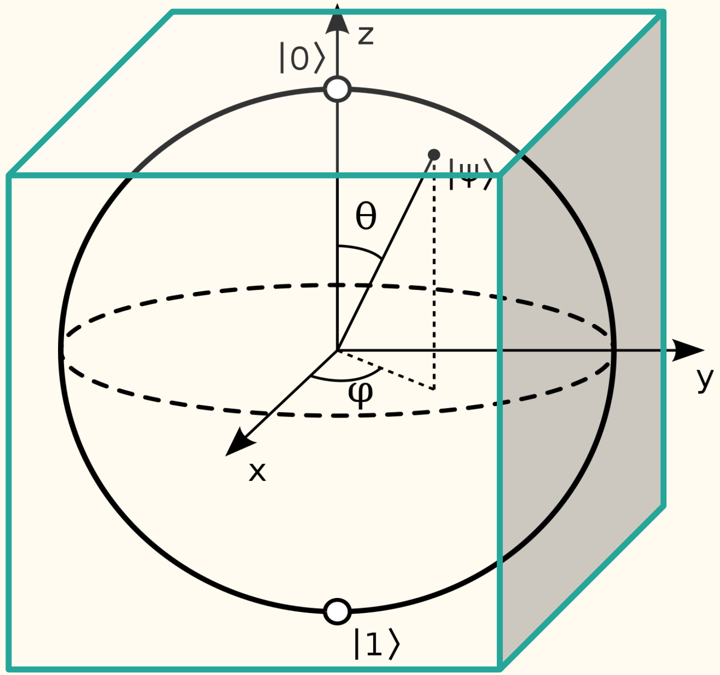
In quantum systems, there always exists an *infinite number of measurement basis*.



Nonnegativity is only guaranteed for the measurement basis of the chosen quorum (axis of the cube).

Linear inversion: 2-level systems (qubit/spin-½)

In quantum systems, there always exists an *infinite number of measurement basis*.

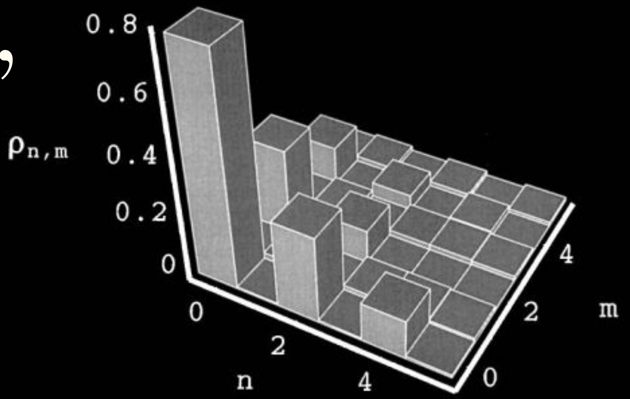


Nonnegativity is only guaranteed for the measurement basis of the chosen quorum (axis of the cube).

One can gets negative probabilities *for observables that have not been measured.*

Maximum Likelihood Estimation

Principle, extremal equation, algorithm and flaws



MLE reconstruction of the density matrix of a single-mode radiation field.
Image from K. Banaszek et al, 1999

Main references:
[Banaszek, 1999;
Řeháček et al., 2001;
Hradil et al., 2004;
Blume-Kohout, 2010]

MLE of quantum states: principle

What state is most likely to have produced a given experimental outcome $\mathcal{M} = \{|x_1\rangle, ..., |x_N\rangle\}$?

Maximizing the likelihood functional:

$$(\mathcal{L}(\rho))^{1/n} = \prod_j^M p(|x_j\rangle|\rho)^{f_j}$$

MLE of quantum states: principle

What state is most likely to have produced a given experimental outcome $\mathcal{M} = \{|x_1\rangle, ..., |x_N\rangle\}$?

Maximizing the likelihood functional:

$$(\mathcal{L}(\rho))^{1/n} = \prod_j^M p(|x_j\rangle|\rho)^{f_j}$$

equivalent to minimizing the statistical distance (Kullback-Leibler divergence):

$$D(\mathbf{f}, \mathbf{p}) = -\sum_j^M f_j \ln(p_j)$$

MLE of quantum states: extremal equation

General solution: extremal equation

$$R\rho_e = \rho_e$$

with $R = \sum_{j}^{M} \frac{f_j}{\langle x_j|\rho_e|x_j\rangle} |x_j\rangle\langle x_j|$

MLE of quantum states: a simple algorithm

If eigenbasis is known, we have $\rho = \sum_k r_k |\psi_k\rangle\langle\psi_k|$,

hence $f_j = \langle x_j|\rho|x_j\rangle = \sum_k r_k |\langle x_j|\psi_k\rangle|^2$

Finding the eigenvalues is a linear positive problem for which converging algorithms are available (e.g. expectation-maximization algorithm).

MLE of quantum states: a simple algorithm

This suggests performing the reconstruction in two steps to be repeated iteratively:

MLE of quantum states: a simple algorithm

This suggests performing the reconstruction in two steps to be repeated iteratively:

- find the most likely eigenvalues in a fixed basis (linear positive problem).

MLE of quantum states: a simple algorithm

This suggests performing the reconstruction in two steps to be repeated iteratively:

- find the most likely eigenvalues in a fixed basis (linear positive problem).

- rotate the eigenbasis in the “good” direction (appropriate rotation found considering the variation of the log-likelihood).

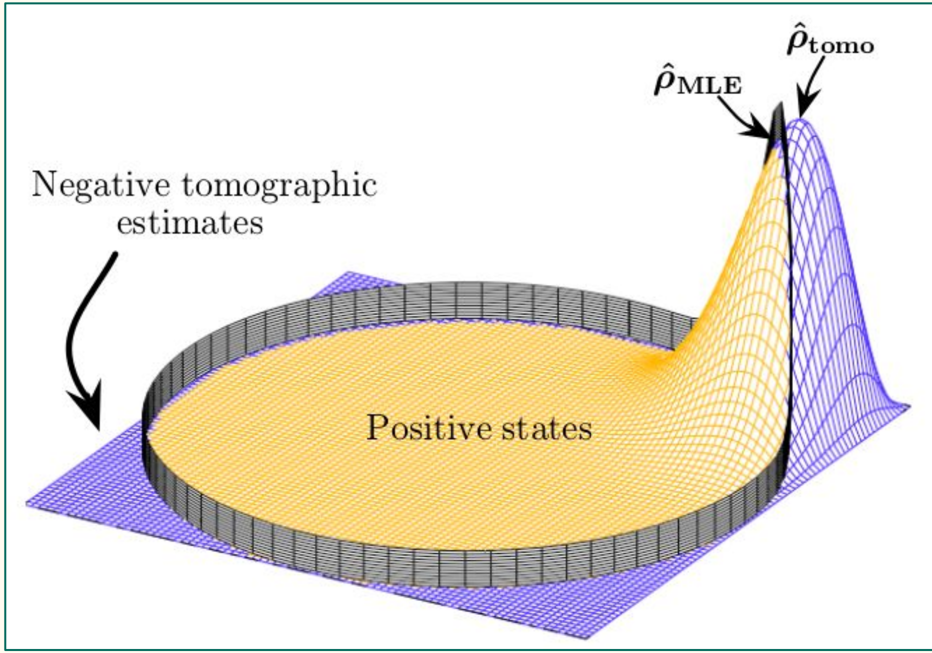
MLE of quantum states: a simple algorithm

This suggests performing the reconstruction in two steps to be repeated iteratively:

- find the most likely eigenvalues in a fixed basis (linear positive problem).
- rotate the eigenbasis in the “good” direction (appropriate rotation found considering the variation of the log-likelihood).

MLE of quantum states: relation to linear inversion

Linear inversion ~ unconstrained MLE

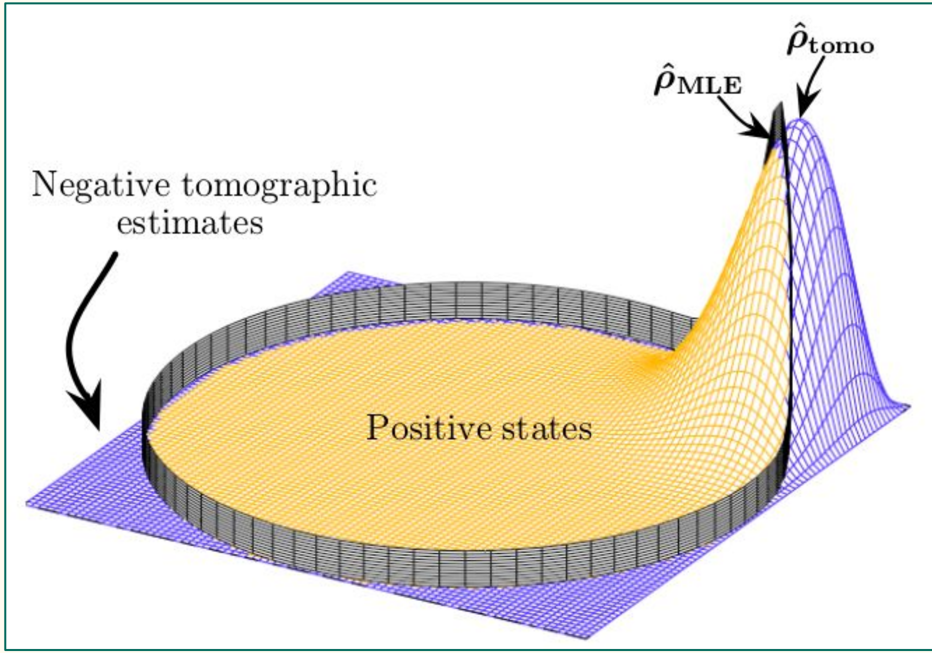


Example of likelihood function, with both constrained and unconstrained maxima shown, in a cross-section of the single-spin Bloch sphere. Figure from [Blume-Kohout, 2010]

MLE of quantum states: relation to linear inversion

Linear inversion ~ unconstrained MLE

- $\rho_{tomo} \geq 0 \implies \max(\mathcal{L}(\rho)) = \mathcal{L}(\rho_{tomo})$

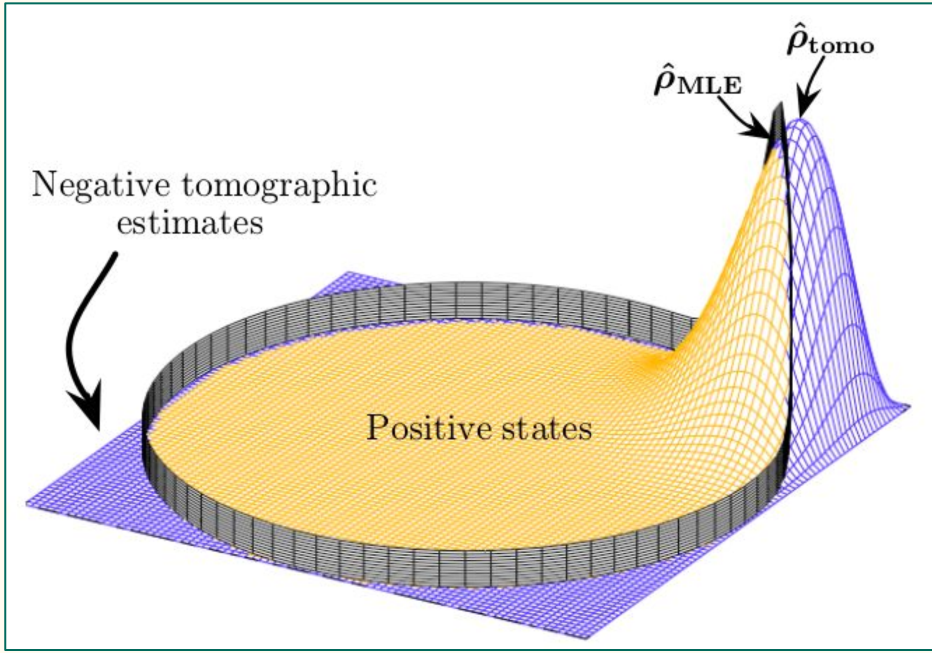


Example of likelihood function, with both constrained and unconstrained maxima shown, in a cross-section of the single-spin Bloch sphere. Figure from [Blume-Kohout, 2010]

MLE of quantum states: relation to linear inversion

Linear inversion ~ unconstrained MLE

- $\rho_{tomo} \geq 0 \implies \max(\mathcal{L}(\rho)) = \mathcal{L}(\rho_{tomo})$
- $\forall \lambda_i^{tomo} < 0 \;,\; \exists \lambda_i^{MLE} = 0$



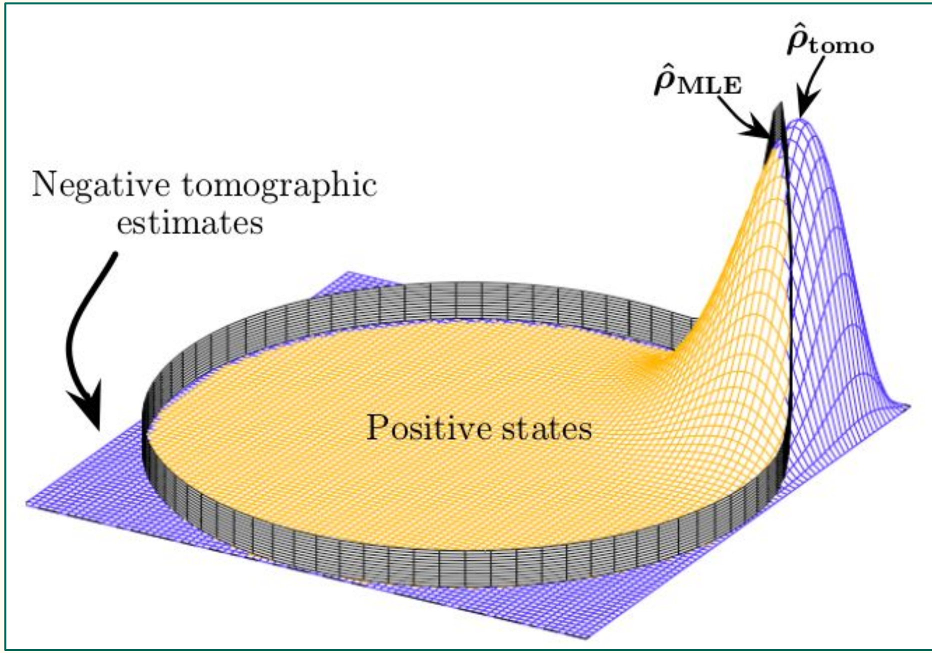
Example of likelihood function, with both constrained and unconstrained maxima shown, in a cross-section of the single-spin Bloch sphere. Figure from [Blume-Kohout, 2010]

MLE of quantum states: relation to linear inversion

Linear inversion ∼ unconstrained MLE

- $\rho_{tomo} \geq 0 \implies \max(\mathcal{L}(\rho)) = \mathcal{L}(\rho_{tomo})$
- $\forall \lambda_i^{tomo} < 0\ ,\ \exists \lambda_i^{MLE} = 0$

A finite number of measurement cannot justify a vanishing probability!



Example of likelihood function, with both constrained and unconstrained maxima shown, in a cross-section of the single-spin Bloch sphere. Figure from [Blume-Kohout, 2010]

MLE and linear inversion of quantum states: flaws

- Generally leads to negative or vanishing probabilities.

MLE and linear inversion of quantum states: flaws

- Generally leads to negative or vanishing probabilities.
- Do not provide well-defined error bars.

MLE and linear inversion of quantum states: flaws

- Generally leads to negative or vanishing probabilities.

- Do not provide well-defined error bars.

Flaws inherent to frequentist approaches to quantum state reconstruction.

Somehow related to the infinite number of observables: the estimation closest from observed frequencies fails to describe unmeasured events.

Bayesian Mean Estimation

Principle, extensivity, pros and cons

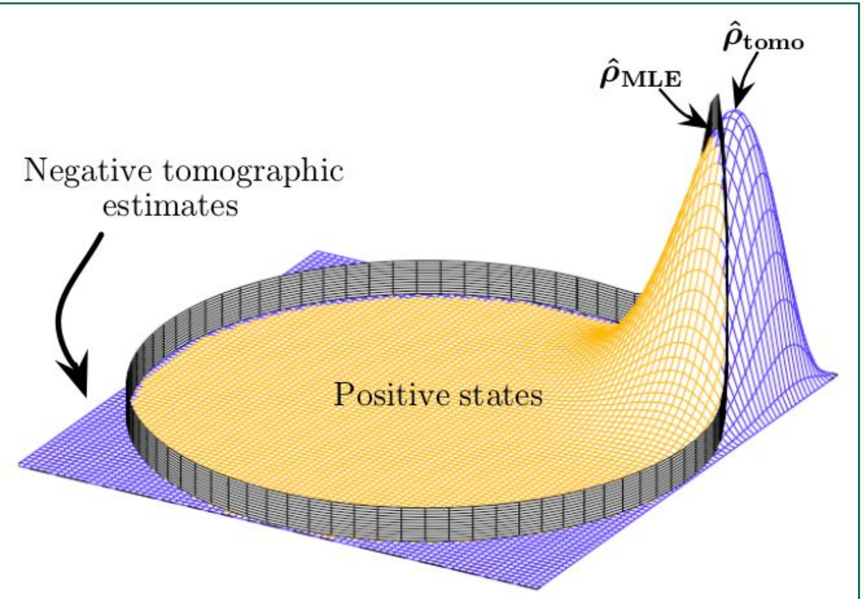
Main reference:
[Blume-Kohout, 2010]

$$p(\rho|\mathcal{M}) = \frac{p(\mathcal{M}|\rho)p(\rho)}{p(\mathcal{M})}$$

Bayes theorem

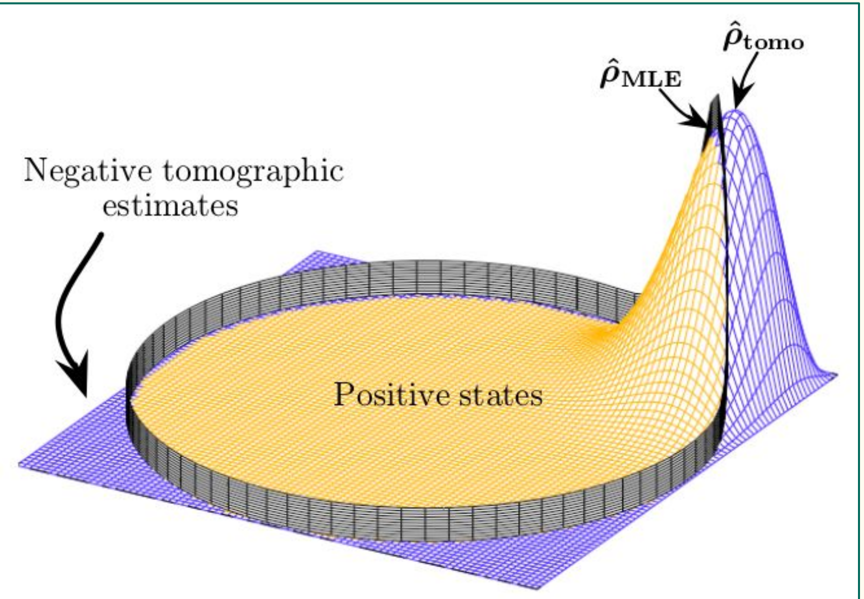
BME of quantum states: principle

$$\rho_B = \int \rho \pi_f(\rho) d\rho = \frac{\int \rho \mathcal{L}(\rho) \pi_0(\rho) d\rho}{\int \mathcal{L}(\rho) \pi_0(\rho) d\rho}$$



BME of quantum states: principle

$$\rho_B = \int \rho \pi_f(\rho) d\rho = \frac{\int \rho \mathcal{L}(\rho) \pi_0(\rho) d\rho}{\int \mathcal{L}(\rho) \pi_0(\rho) d\rho}$$



Provided a reasonable (*robust*) prior was chosen:

- no vanishing probabilities
- extensive with respect to sample size

BME of quantum states is extensive

Extreme example: $\mathcal{M} = \{|0\rangle, ..., |0\rangle\}\,, \quad \pi_0 = c$

$$\rho_B = \int \pi_f(\rho)\rho d\rho$$

$$= \frac{\int (\rho_{00})^N \rho d\rho}{\int (\rho_{00})^N d\rho_{00}} = (N+1)\int (\rho_{00})^N \rho d\rho$$

BME of quantum states is extensive

Extreme example: $\mathcal{M} = \{|0\rangle, ..., |0\rangle\}\,,\quad \pi_0 = c$

$$(\rho_B)_{00} = (N+1)\int (\rho_{00})^{N+1} d\rho_{00} = \frac{N+1}{N+2}$$

$$(\rho_B)_{11} = \frac{1}{N+2}$$

BME of quantum states: pros and cons

- Average over the whole Hilbert space (rather than “one-point estimation”).

BME of quantum states: pros and cons

- Average over the whole Hilbert space (rather than "one-point estimation").

- Plausible reconstructed statistics: extensive in sample size, no vanishing or negative probability.

BME of quantum states: pros and cons

- Average over the whole Hilbert space (rather than "one-point estimation").

- Plausible reconstructed statistics: extensive in sample size, no vanishing or negative probability.

- Provide natural, well-motivated error bars (*honest* estimation).

BME of quantum states: pros and cons

- Average over the whole Hilbert space (rather than “one-point estimation”).

- Plausible reconstructed statistics: extensive in sample size, no vanishing or negative probability.

- Provide natural, well-motivated error bars (*honest* estimation).

- Optimize accuracy (in terms of *operational divergence*).

BME of quantum states: pros and cons

- Average over the whole Hilbert space (rather than "one-point estimation").

- Plausible reconstructed statistics: extensive in sample size, no vanishing or negative probability.

- Provide natural, well-motivated error bars (*honest* estimation).

- Optimize accuracy (in terms of *operational divergence*).

- Sensitive to choice of prior.

BME of quantum states: pros and cons

- Average over the whole Hilbert space (rather than "one-point estimation").
- Plausible reconstructed statistics: extensive in sample size, no vanishing or negative probability.
- Provide natural, well-motivated error bars (*honest* estimation).
- Optimize accuracy (in terms of *operational divergence*).

- Sensitive to choice of prior.
- Relatively low performance (numerical integration, e.g. Metropolis-Hastings algorithm).

Conclusion

Different applications need different methods:

Conclusion

Different applications need different methods:

- Linear inversion: fastest and easiest to implement; still very useful for applications with large number of measurements and low sensitivity to negativity (e.g. X-ray tomography).

Conclusion

Different applications need different methods:

- Linear inversion: fastest and easiest to implement; still very useful for applications with large number of measurements and low sensitivity to negativity (e.g. X-ray tomography).

- MLE: negativity-sensible applications, with few measurements (e.g. entanglement experiments).

Conclusion

Different applications need different methods:

- Linear inversion: fastest and easiest to implement; still very useful for applications with large number of measurements and low sensitivity to negativity (e.g. X-ray tomography).

- MLE: negativity-sensible applications, with few measurements (e.g. entanglement experiments).

- BME: most rigorous and computationally costly, preferred when accurate *prediction* and well-defined error bars are crucial (e.g. quantum computers).

Conclusion

Different applications need different methods:

- Linear inversion: fastest and easiest to implement; still very useful for applications with large number of measurements and low sensitivity to negativity (e.g. X-ray tomography).
- MLE: negativity-sensible applications, with few measurements (e.g. entanglement experiments).

Frequentist approach: **accurate description of the past**

- BME: most rigorous and computationally costly, preferred when accurate *prediction* and well-defined error bars are crucial (e.g. quantum computers).

Bayesian approach: **fitted for predictions of the future**

Bibliography

Banaszek, K., G. M. D'Ariano, M. G. A. Paris, and M. F. Sacchi. 1999. "Maximum-Likelihood Estimation of the Density Matrix." *Physical Review A* 61 (1): 010304. https://doi.org/10.1103/PhysRevA.61.010304.

Blume-Kohout, Robin. 2010. "Optimal, Reliable Estimation of Quantum States." *New Journal of Physics* 12 (4): 043034. https://doi.org/10.1088/1367-2630/12/4/043034.

Hradil, Zdeněk, Jaroslav Řeháček, Jaromír Fiurášek, and Miroslav Ježek. 2004. "3 Maximum-Likelihood Methodsin Quantum Mechanics." In *Quantum State Estimation*, edited by Matteo Paris and Jaroslav Řeháček, 649:59–112. Lecture Notes in Physics. Berlin, Heidelberg: Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-540-44481-7_3.

Řeháček, J., Z. Hradil, and M. Ježek. 2001. "Iterative Algorithm for Reconstruction of Entangled States." *Physical Review A* 63 (4): 040303. https://doi.org/10.1103/PhysRevA.63.040303.

Thanks for your attention.