

Quantum tomography based on quantum trajectories

> Quantum Control Theory:
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Quantum tomography versus quantum filtering
Likelihood function calculations via adjoint states
Discrete time case
Continuous time case

MaxLike estimations with experimental data
Process tomography for QND measurement of photons State tomography of a quantum Maxwell demon

Fisher information and low-rank MaxLike estimates
Appendix: asymptotics for multi-dimension Laplace integrals and boundary corrections

## Quantum state tomography based on POVM, $\quad \sum_{j} \pi_{j}=\boldsymbol{I}$

- Tomography of $\rho$ via $N$ independent measurements $\boldsymbol{Y}$ associated to POVM: probability $\operatorname{Tr}\left(\rho \pi_{j}\right)$ of each measurement outcome $j$ given by $\pi_{j}$; for $\boldsymbol{N}_{j}$ the number of $j$ outcomes, $\boldsymbol{Y} \equiv\left(\boldsymbol{N}_{j}\right)$ with $\sum_{j} \boldsymbol{N}_{j}=\boldsymbol{N}$, the number of measurements.
- Several estimation methods:

MaxEnt: $\rho_{\text {ME }}$ maximizes $-\operatorname{Tr}(\rho \log (\rho))$ under the constraints $\left|\operatorname{Tr}\left(\rho \pi_{j}\right)-\boldsymbol{N}_{j} / N\right| \leq \epsilon$ (Bužek et al, Ann. Phys. 1996).
Compress Sensing: $\rho_{C S}$ minimizes $\operatorname{Tr}(\rho)$ under the constraints
$\left|\operatorname{Tr}\left(\rho \pi_{j}\right)-\boldsymbol{N}_{\boldsymbol{j}} / N\right| \leq \epsilon($ Gross et al PRL2010)
MaxLike: $\rho_{M L}$ maximizes the likelihood function,
$\rho \mapsto \mathbb{P}(\boldsymbol{Y} \mid \rho)=\prod_{j}\left(\operatorname{Tr}\left(\rho \pi_{j}\right)\right)^{N_{j}}$ (see, e.g.,
Lvovsky/Raymer RMP 2009)
Bayesian Mean: $\rho_{\text {BM }} \propto \int \rho \mathbb{P}(\boldsymbol{Y} \mid \rho) \mathbb{P}_{0}(\rho) d \rho$ where $\mathbb{P}_{0}$ is some prior distribution $\mathbb{P}_{0}(\rho) d \rho$ (see, e.g., Blume-Kohout NJP2010).
Low rank, high dimensional systems: see, e.g, PhD thesis "Efficient and Robust Methods for Quantum Tomography" of Charles Heber Baldwin, University of New Mexico, December 2016.

## Quantum filtering / tomography with quantum trajectories $\boldsymbol{Y}=\left(\boldsymbol{y}_{t}^{(n)}\right)$

Filtering: estimation of the quantum state $\rho_{t}$ at time $t>0$ from the measurement trajectory $\left[0, t\left[\ni \tau \mapsto \boldsymbol{y}_{\tau}\right.\right.$ and the initial state $\rho_{0}$; see Belavkin semilar contributions (links with Monte-Carlo quantum-trajectories).
State tomography: estimation of the initial state $\rho_{0}=\rho$ from a collection of $N$ measurement trajectories: $\boldsymbol{Y}=\left(\boldsymbol{y}_{t}^{(n)}\right)$ with $n \in\{1, \ldots, N\}$ and $t \in[0, T]$.
Process tomography: estimation of a parameter p from a known initial state $\rho$ and a collection of $N$ measurement trajectories $\boldsymbol{Y}$.
This talk: MaxLike estimation with decoherence and measurement imperfections (PhD thesis of Pierre Six, November 2016):

1. How to compute the likelihood function $\mathbb{P}(\boldsymbol{Y} / \rho, \mathbf{p})$ and its gradient from the stochastic master equation governing filtering (P. Six et al. PRA 2016).
2. For state estimation: variance computation based on asymptotic expansions of Laplace integrals for low rank MaxLike estimates (P. Six /PR, chapter in Lecture Notes in Control and Information Sciences no 473, April 2017).

## Regular MaxLike estimation of a parameter $p$

Log-likelihood function $f(p)=\log (\mathbb{P}(\boldsymbol{Y} \mid p))$ admits a unique maximum at $p_{M L}\left(\nabla f\left(p_{M L}\right)=0\right)$ with a negative definite Hessian $\left(\nabla^{2} f\left(p_{M L}\right)<0\right)$.
$f$ coming from $N$ independent realisations: $f(p) \equiv N \bar{f}(p)$ with asymptotics for $N \mapsto+\infty$ of the Laplace integrals connecting

- Bayesian Mean $p_{B M}$ and MaxLike estimation $p_{M L}$ :

$$
p_{B M}=\frac{\int p e^{N \bar{f}(p)} \mathbb{P}_{0}(p) d p}{\int e^{N \bar{f}(p)} \mathbb{P}_{0}(p) d p}=p_{M L}+O(1 / N) .
$$

with any smooth prior distribution $\mathbb{P}_{0}(p) d p$

- Bayesian variance and Fisher information $\bar{F}_{M L}=-\nabla^{2} \bar{f}\left(p_{M L}\right)$ :

$$
\frac{\int\left\|p-p_{M L}\right\|^{2} e^{N \bar{f}(p)} \mathbb{P}_{0}(p) d p}{\int e^{N \bar{f}(p)} \mathbb{P}_{0}(p) d p}=\operatorname{Tr}\left(\left(\bar{F}_{M L}\right)^{-1}\right) /(2 N)+O\left(1 / N^{2}\right)
$$

Confidence intervals based on $-\nabla^{2} f\left(p_{M L}\right)$.

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## Discrete-time models of open quantum systems

Four features ${ }^{1}$ :

1. Bayes law: $\mathbb{P}\left(\mu^{\prime} / \mu\right)=\mathbb{P}\left(\mu / \mu^{\prime}\right) \mathbb{P}\left(\mu^{\prime}\right) /\left(\sum_{\nu^{\prime}} \mathbb{P}\left(\mu / \nu^{\prime}\right) \mathbb{P}\left(\nu^{\prime}\right)\right)$,
2. Schrödinger equations defining unitary transformations.
3. Randomness, irreversibility and dissipation induced by the measurement of observables with degenerate spectra.
4. Entanglement and tensor product for composite systems.

## $\Rightarrow$ Discrete-time models

Take a set of operators $\boldsymbol{M}_{\mu}$ satisfying $\sum_{\mu} \boldsymbol{M}_{\mu}^{\dagger} \boldsymbol{M}_{\mu}=\boldsymbol{I}$ and a left stochastic matrices $\left(\eta_{\boldsymbol{y}_{t}, \mu}\right)$. Consider the following Markov process of state $\rho$ (density op.) and measured output $\boldsymbol{y}$ :

$$
\rho_{t+1}=\frac{\boldsymbol{K}_{y_{t}}\left(\rho_{t}\right)}{\operatorname{Tr}\left(K_{y_{t}}\left(\rho_{t}\right)\right)}, \text { with proba. } \mathbb{P}_{\boldsymbol{y}_{t}}\left(\rho_{t}\right)=\operatorname{Tr}\left(\boldsymbol{K}_{\boldsymbol{y}_{t}}\left(\rho_{t}\right)\right)
$$

with $\boldsymbol{K}_{\boldsymbol{y}}(\rho)=\sum_{\mu=1}^{m} \eta_{\boldsymbol{y}, \mu} \boldsymbol{M}_{\mu} \rho \boldsymbol{M}_{\mu}^{\dagger}$. It is associated to the Kraus map (ensemble average, quantum channel)

$$
\mathbb{E}\left(\rho_{t+1} \mid \rho_{t}\right)=\boldsymbol{K}\left(\rho_{t}\right)=\sum_{\boldsymbol{y}} \boldsymbol{K}_{\boldsymbol{y}}\left(\rho_{t}\right)=\sum_{\mu} \boldsymbol{M}_{\mu} \rho_{t} \boldsymbol{M}_{\mu}^{\dagger}
$$

${ }^{1}$ See the book of S. Haroche and J.M. Raimond.

## Computation of the likelihood function via the adjoint state (1)

- Denote by $\mathbb{P}_{n}(\rho, \mathrm{p})$ the probability of getting measurement trajectory $n,\left(\boldsymbol{y}_{t}^{(n)}\right)_{t=0, \ldots, T}$, knowing the initial state $\rho_{0}^{(n)}=\rho$ and parameter p .
- Since $\rho_{t+1}^{(n)}=\frac{\boldsymbol{K}_{y_{t}^{(n)}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right)}{\operatorname{Tr}\left(\boldsymbol{K}_{y_{t}^{(n)}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right)\right)}$ with $\operatorname{Tr}\left(\boldsymbol{K}_{\boldsymbol{y}_{t}^{(n)}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right)\right)$ the probability of having detected $\boldsymbol{y}_{t}^{(n)}$ knowing $\rho_{t}^{(n)}$ and $\mathbf{p}$, a direct use of Bayes law yields

$$
\mathbb{P}_{n}(\rho, \mathbf{p})=\prod_{t=0}^{T} \operatorname{Tr}\left(\boldsymbol{K}_{\boldsymbol{y}_{t}^{(n)}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right)\right)=\operatorname{Tr}\left(\boldsymbol{K}_{y_{T}^{(n)}}^{\mathrm{p}} \circ \ldots \circ \boldsymbol{K}_{y_{0}^{(n)}}^{\mathrm{p}}(\rho)\right) .
$$

## Computation of the likelihood function via the adjoint state (2)

- With adjoint map $\boldsymbol{K}_{y}^{\mathrm{p} *}\left(\forall A, B, \operatorname{Tr}\left(\boldsymbol{K}_{y}^{\mathrm{p}}(A) B\right) \equiv \operatorname{Tr}\left(A \boldsymbol{K}_{y}^{\mathrm{p} *}(B)\right)\right)$ : $\mathbb{P}_{n}(\rho, \mathrm{p})=\operatorname{Tr}\left(\boldsymbol{K}_{\boldsymbol{y}_{T}^{(n)}}^{\mathrm{p}} \circ \ldots \circ \boldsymbol{K}_{\boldsymbol{y}_{0}^{(n)}}^{\mathrm{p}}(\rho) \quad \boldsymbol{I}\right)=\operatorname{Tr}\left(\begin{array}{ll}\rho & \boldsymbol{K}_{\boldsymbol{y}_{0}^{(n)}}^{\mathrm{p} *} \circ \ldots \circ \boldsymbol{K}_{\boldsymbol{y}_{T}^{(n)}}^{\mathrm{p} *}(\boldsymbol{I})\end{array}\right)$.
- Normalized adjoint quantum filter ${ }^{2} E_{t}^{(n)}=\frac{\boldsymbol{K}_{y_{t}^{(n)}}^{p}\left(E_{t+1}^{(n)}\right)}{\operatorname{Tr}\left(\boldsymbol{K}_{y_{t}{ }^{(n)}}^{\left(n_{t+1}\right)}\left(E_{t+1)}^{(n)}\right)\right.}$ with

$$
\begin{aligned}
& E_{T+1}^{(n)}=\boldsymbol{I} / \operatorname{Tr}(\boldsymbol{I}) \text {, we get } \\
& \mathbb{P}_{n}(\rho, \mathbf{p})=\prod_{t=T}^{0} \operatorname{Tr}\left(\boldsymbol{K}_{\boldsymbol{y}_{t}^{(n)}}^{\mathbf{p} *}\left(E_{t+1}^{(n)}\right)\right) \operatorname{Tr}\left(\rho E_{0}^{(n)}\right) \triangleq g_{n}(\boldsymbol{Y}, \mathbf{p}) \operatorname{Tr}\left(\rho E_{0}^{(n)}\right) .
\end{aligned}
$$

- A simple expression of the gradients:

$$
\nabla \rho \log \mathbb{P}_{n}=\frac{E_{0}^{(n)}}{\operatorname{Tr}\left(\rho E_{0}^{(n)}\right)}, \quad \nabla_{\mathfrak{p}} \log \mathbb{P}_{n} \cdot \delta \mathbf{p}=\sum_{t=0}^{T} \frac{\operatorname{Tr}\left(E_{t+1}^{(n)} \nabla_{\mathrm{p}} \boldsymbol{K}_{\boldsymbol{y}_{t}^{(n)}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right) \cdot \delta \mathbf{p}\right)}{\operatorname{Tr}\left(E_{t+1}^{(n)} \boldsymbol{K}_{\mathbf{y}_{t}^{(n)}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right)\right)},
$$

MaxLike tomography based on $N$ trajectories data $\boldsymbol{Y}=\left(\boldsymbol{y}_{t}^{(n)}\right)$
From $\mathbb{P}_{n}(\rho, \mathfrak{p})=g_{n}(\boldsymbol{Y}, \mathfrak{p}) \operatorname{Tr}\left(\rho E_{0}^{(n)}\right)$ we have

$$
\mathbb{P}(\rho, \mathfrak{p}) \triangleq \prod_{n=1}^{N} \mathbb{P}_{n}(\rho, \mathfrak{p})=\left(\prod_{n=1}^{N} g_{n}(\boldsymbol{Y}, \mathfrak{p})\right)\left(\prod_{n=1}^{N} \operatorname{Tr}\left(\rho E_{0}^{(n)}\right)\right) .
$$

- MaxLike state tomography: p is known and $\rho_{M L}$ maximizes

$$
\rho \mapsto \sum_{n=1}^{N} \log \left(\operatorname{Tr}\left(\rho E_{0}^{(n)}\right)\right)
$$

a concave function on the convex set of density operators $\rho$ : a well structured convex optimization problem.

- MaxLike process tomography: $\rho$ is known and $p_{M L}$ maximizes $p \mapsto f(p)=\log \mathbb{P}(\rho, p)$ those gradient is given by

$$
\nabla_{\mathfrak{p}} f(\mathbf{p}) \cdot \delta \mathbf{p}=\sum_{n=1}^{N} \sum_{t=0}^{T} \frac{\operatorname{Tr}\left(E_{t+1}^{(n)} \nabla_{\mathrm{p}} \boldsymbol{K}_{y_{t}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right) \cdot \delta \mathbf{p}\right)}{\operatorname{Tr}\left(E_{t+1}^{(n)} \boldsymbol{K}_{y_{t}^{\mathrm{p}}}^{\mathrm{p}}\left(\rho_{t}^{(n)}\right)\right)}
$$

The Hessian $\nabla_{\mathrm{p}}^{2} f$ can be computed similarly (Fisher information).

## Continuous/discrete-time Stochastic Master Equation (SME)

Discrete-time models: Markov chains $\rho_{t+1}=\frac{K_{y_{t}}\left(\rho_{t}\right)}{\operatorname{Tr}\left(K_{y_{t}}\left(\rho_{t}\right)\right)}$, with
$\boldsymbol{K}_{\boldsymbol{y}_{\boldsymbol{t}}}\left(\rho_{t}\right)=\sum_{\mu=1}^{m} \eta_{\boldsymbol{y}_{\boldsymbol{t}}, \mu} \boldsymbol{M}_{\mu} \rho_{t} \boldsymbol{M}_{\mu}^{\dagger}$, and proba. $\mathbb{P}_{\boldsymbol{y}_{\boldsymbol{t}}}\left(\rho_{t}\right)=\operatorname{Tr}\left(\boldsymbol{K}_{\boldsymbol{y}_{\boldsymbol{t}}}\left(\rho_{t}\right)\right)$.
Ensemble averages correspond to Kraus linear maps
$\mathbb{E}\left(\rho_{t+1} \mid \rho_{t}\right)=\boldsymbol{K}\left(\rho_{t}\right)=\sum_{\boldsymbol{y}} \boldsymbol{K}_{\boldsymbol{y}}\left(\rho_{t}\right)=\sum_{\mu} \boldsymbol{M}_{\mu} \rho_{t} \boldsymbol{M}_{\mu}^{\dagger} \quad$ with $\quad \sum_{\mu} \boldsymbol{M}_{\mu}^{\dagger} \boldsymbol{M}_{\mu}=\boldsymbol{I}$
Continuous-time models: stochastic differential systems (see, e.g., Barchielli/Gregoratti, 2009)

$$
\begin{aligned}
d \rho_{t}=\left(-\frac{i}{\hbar}\right. & {\left.\left[\boldsymbol{H}, \rho_{t}\right]+\sum_{\nu} \boldsymbol{L}_{\nu} \rho_{t} \boldsymbol{L}_{\nu}^{\dagger}-\frac{1}{2}\left(\boldsymbol{L}_{\nu}^{\dagger} \boldsymbol{L}_{\nu} \rho_{t}+\rho_{t} \boldsymbol{L}_{\nu}^{\dagger} \boldsymbol{L}_{\nu}\right)\right) d t } \\
& +\sum_{\nu} \sqrt{\eta_{\nu}}\left(\boldsymbol{L}_{\nu} \rho_{t}+\rho_{t} \boldsymbol{L}_{\nu}^{\dagger}-\operatorname{Tr}\left(\left(\boldsymbol{L}_{\nu}+\boldsymbol{L}_{\nu}^{\dagger}\right) \rho_{t}\right) \rho_{t}\right) d W_{\nu, t}
\end{aligned}
$$

driven by Wiener processes $d W_{\nu, t}$, with measurements $d y_{\nu, t}$, $\boldsymbol{d} \boldsymbol{y}_{\nu, \boldsymbol{t}}=\sqrt{\eta_{\nu}} \operatorname{Tr}\left(\left(\boldsymbol{L}_{\nu}+\boldsymbol{L}_{\nu}^{\dagger}\right) \rho_{t}\right) d t+d W_{\nu, t}$, detection efficiencies $\eta_{\nu} \in[0,1]$ and Lindblad-Kossakowski master equations ( $\eta_{\nu} \equiv 0$ ):

$$
\frac{d}{d t} \rho=-\frac{i}{\hbar}[\boldsymbol{H}, \rho]+\sum_{\nu} \boldsymbol{L}_{\nu} \rho \boldsymbol{L}_{\nu}^{\dagger}-\frac{1}{2}\left(\boldsymbol{L}_{\nu}^{\dagger} \boldsymbol{L}_{\nu} \rho+\rho \boldsymbol{L}_{\nu}^{\dagger} \boldsymbol{L}_{\nu}\right)
$$

## Continuous/discrete-time diffusive SME

The Belavkin quantum filter

$$
\begin{aligned}
d \rho_{t}=\left(-\frac{i}{\hbar}\right. & {\left.\left[\boldsymbol{H}, \rho_{t}\right]+\sum_{\nu} \boldsymbol{L}_{\nu} \rho_{t} \boldsymbol{L}_{\nu}^{\dagger}-\frac{1}{2}\left(\boldsymbol{L}_{\nu}^{\dagger} \boldsymbol{L}_{\nu} \rho_{t}+\rho_{t} \boldsymbol{L}_{\nu}^{\dagger} \boldsymbol{L}_{\nu}\right)\right) d t } \\
& +\sum_{\nu} \sqrt{\eta_{\nu}}\left(\boldsymbol{L}_{\nu} \rho_{t}+\rho_{t} \boldsymbol{L}_{\nu}^{\dagger}-\operatorname{Tr}\left(\left(\boldsymbol{L}_{\nu}+\boldsymbol{L}_{\nu}^{\dagger}\right) \rho_{t}\right) \rho_{t}\right) d W_{\nu, t}
\end{aligned}
$$

with $d W_{\nu, t}=\boldsymbol{d} \boldsymbol{y}_{\nu, \boldsymbol{t}}-\sqrt{\eta_{\nu}} \operatorname{Tr}\left(\left(\boldsymbol{L}_{\nu}+\boldsymbol{L}_{\nu}^{\dagger}\right) \rho_{t}\right) d t$ given by the measurement signal $d y_{\nu, t}$, is always a stable filtering process. ${ }^{3}$ Using Itō rules, it can be written as a "discrete-time" Markov model ${ }^{4}$

$$
\rho_{t+d t}=\boldsymbol{K}_{d \boldsymbol{y}_{t}}\left(\rho_{t}\right) / \operatorname{Tr}\left(\boldsymbol{K}_{d y_{t}}\left(\rho_{t}\right)\right)
$$

with partial Kraus maps $\boldsymbol{K}_{\boldsymbol{d} \boldsymbol{y}_{t}}\left(\rho_{t}\right)=\boldsymbol{M}_{\boldsymbol{d} \boldsymbol{y}_{t}} \rho_{t} \boldsymbol{M}_{\boldsymbol{d} \boldsymbol{y}_{t}}^{\dagger}+\sum_{\nu}\left(1-\eta_{\nu}\right) \boldsymbol{L}_{\nu} \rho_{t} \boldsymbol{L}_{\nu}^{\dagger} d t$

$$
\boldsymbol{M}_{d \boldsymbol{y}_{t}}=\boldsymbol{I}+\left(-\frac{i}{\hbar} \boldsymbol{H}-\frac{1}{2}\left(\sum_{\nu} \boldsymbol{L}_{\nu}^{\dagger} \boldsymbol{L}_{\nu}\right)\right) d t+\sum_{\nu} \sqrt{\eta_{\nu}} \boldsymbol{d} \boldsymbol{y}_{\nu, \boldsymbol{t}} \boldsymbol{L}
$$

where the probability of outcome $\boldsymbol{d} \boldsymbol{y}_{\boldsymbol{t}}=\left(d y_{\nu, t}\right)$ reads:
$\mathbb{P}\left(\boldsymbol{d} \boldsymbol{y}_{\boldsymbol{t}} \in \prod_{\nu}\left[\xi_{\nu}, \xi_{\nu}+\boldsymbol{d} \xi_{\nu}\right] / \rho_{t}\right)=\operatorname{Tr}\left(\boldsymbol{K}_{\boldsymbol{\xi}}\left(\rho_{t}\right)\right) \prod_{\nu} e^{-\xi_{\nu}^{2} / 2 d t} \frac{d \xi_{\nu}}{\sqrt{2 \pi d t}}$
${ }^{3}$ H. Amini et al., Russian J. of Math. Physics, 2014, 21, 297-315.
${ }^{4}$ PR, J. Ralph PRA2015; see also PhD thesis of Ph. Campagne-Ibracq (2015) and of P. Six (2016).

## Quantum tomography versus quantum filtering

## Likelihood function calculations via adjoint states Discrete time case Continuous time case

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corrections


- The probability $\mathbb{P}\left(y \mid \phi_{R}, n\right)$ to get $y \in\{g, e\}$ knowing the Ramsey angle $\phi_{R}$ and the number of photon(s) $n \in\{0,1,2, \ldots\}$ :
$\mathbb{P}\left(y \mid \phi_{R}, n\right)=1+\epsilon_{y}\left(A+B_{c}(n) \cos \phi_{R}+B_{s}(n) \sin \phi_{R}\right)$ with $\epsilon_{e / g}= \pm 1$. depends on the parameters $\mathbf{p}=\left(B_{c}(n), B_{s}(n)\right)_{n \in\{0,1, \ldots,\}}$.
- The Kraus maps $\boldsymbol{K}_{y}^{\mathrm{p}}$ based on known cavity decay and thermal photons.


## A priori calibration ${ }^{5}$ (black dots) versus MaxLike (blue dots)



MaxLike estimation of 32 parameters p based on $N=8000$ trajectories of $T=6000$ outcome measurements.
${ }^{5}$ T. Rybarczyk, B. Peaudecerf, M. Penasa, S. Gerlich, B. Julsgaard, K. MøImer, S. Gleyzes, M. Brune, J. M. Raimond, S. Haroche, and I. Dotsenko. Forward-backward analysis of the photon-number evolution in a cavity. PRA 2015.

## A quantum Maxwell demon experiment arXiv:1702.01917v1


(a) After preparation in a thermal or quantum state the system S (superconducting qubit) state is recorded into the demon's quantum memory $D$ (microwave cavity) via a pulse that populates the cavity mode only if the qubit is in the ground state. This information is used to extract work which charges a battery with one extra photon: system S emits this photon only when the demon's cavity is empty. The memory reset is performed by cavity relaxation.
(b) When the system starts in a quantum superposition of the demon and system are entangled after the record step.

## Tomography of the demon after the work extraction step



Computations are based on a truncation to 20 photons How to define the confidence intervals for low rank $\rho_{M L}$ ?

## Outline

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## Asymptotic when $\rho_{M L}$ is on the boundary

- To bypass boundary problem, consider Bayesian estimate instead of MaxLike ones

$$
\rho_{B M}=\frac{\int \rho \mathbb{P}(\boldsymbol{Y} \mid \rho) \mathbb{P}_{0}(\rho) d \rho}{\int \mathbb{P}(\boldsymbol{Y} \mid \rho) \mathbb{P}_{0}(\rho) d \rho}
$$

with some prior distribution $\mathbb{P}_{0}(\rho) d \rho$.

- When the likelihood $\exp (f(\rho)) \equiv \mathbb{P}(\boldsymbol{Y} \mid \rho)$ is concentrated ( $f=\boldsymbol{N} \bar{f}$ with $N \gg 1$ ) around its maximum $\rho_{M L}$ that lies on the boundary ( $\rho_{M L}$ not full rank), how to compute the first terms of an asymptotic expansion versus $N$ of

$$
\int \operatorname{Tr}(\rho A)^{r} \exp (N \bar{f}(\rho)) \mathbb{P}_{0}(\rho) d \rho
$$

for any operator $A$ and exponent $r$ and for some prior distribution $\mathbb{P}_{0}(\rho)$ d $\rho$ (e.g., Gausssian unitary ensemble).

- Since all functions are analytic such an asymptotic expansion versus $N$ always exists: Integration by parts, Watson's lemma, Laplace's method, stationary phase, steepest descents, Hironaka's resolution of singularities ${ }^{6}$, "singular learning" ${ }^{7}$

[^0]
## Geometric optimality condition for the log-likelihood function

Assume that $\rho_{M L}$ is an argument of the maximum of

$$
f: \mathcal{D} \ni \rho \mapsto \sum_{\mu \in \mathcal{M}} \log \left(\operatorname{Tr}\left(\rho E^{(\mu)}\right)\right) \in[-\infty, 0]
$$

over $\mathcal{D}$ (the set of density operators, $E^{(\mu)} \in \mathcal{D}$.). Then necessarily, $\rho_{M L}$ satisfies the following conditions:

- $\operatorname{Tr}\left(\rho_{M L} E^{(\mu)}\right)>0$ for each $\mu \in \mathcal{M}$;
$-\left[\rho_{M L},\left.\nabla f\right|_{\rho_{M L}}\right]=0$, where $\left.\nabla f\right|_{\rho_{M L}}=\sum_{\mu \in \mathcal{M}} \frac{E^{(\mu)}}{\operatorname{Tr}\left(\rho_{M L} E^{(\mu)}\right)}$ is the gradient of $f$ at $\rho_{M L}$ for the Frobenius scalar product;
- there exists $\lambda_{M L}>0$ such that $\lambda_{M L} P_{M L}=\left.P_{M L} \nabla f\right|_{\rho_{M L}}$ and $\left.\nabla f\right|_{\rho_{M L}} \leq \lambda_{M L} I$, where $P_{M L}$ is the orthogonal projector on the range of $\rho_{M L}$ and $l$ is the identity operator.

These conditions are also sufficient and characterize the unique maximum when, additionally, the vector space spanned by the $E^{(\mu)}$ 's coincides with the set of Hermitian matrices.

## Geometric asymptotic expansions of Bayesian mean and variance

For any Hermitian operator $A$, its Bayesian mean and variance read:

$$
I_{A}(N)=\frac{\int_{\mathcal{D}} \operatorname{Tr}(\rho A) e^{N t(\rho)} \mathbb{P}_{0}(\rho) \mathrm{d} \rho}{\int_{\mathcal{D}} e^{N t(\rho)} \mathbb{P}_{0}(\rho) \mathrm{d} \rho}, \quad V_{A}(N)=\frac{\int_{\mathcal{D}}\left(\operatorname{Tr}(\rho A)-I_{A}(N)\right)^{2} e^{N t(\rho)} \mathbb{P}_{0}(\rho) \mathrm{d} \rho}{\int_{\mathcal{D}} e^{N t(\rho)} \mathbb{P}_{0}(\rho) \mathrm{d} \rho} .
$$

Denote by $\rho_{M L}$ the unique maximum of $f$ on $\mathcal{D}$ and by $P_{M L}$ the orthogonal projector on its range. In addition to the necessary and sufficient geometric conditions above, assume that $\operatorname{ker}\left(\lambda_{M L} I-\left.\nabla f\right|_{\rho_{M L}}\right)=\operatorname{ker}\left(I-P_{M L}\right)$.
$I_{A}(N)=\operatorname{Tr}\left(A \rho_{M L}\right)+O(1 / N), \quad V_{A}(N)=\operatorname{Tr}\left(A_{\|}\left(F_{M L}\right)^{-1}\left(A_{\|}\right)\right) / N+O\left(1 / N^{2}\right)$
where $B_{\|}$is an orthogonal projection

$$
B_{\|}=B-\frac{\operatorname{Tr}\left(B P_{M L}\right)}{\operatorname{Tr}\left(P_{M L}\right)} P_{M L}-\left(I-P_{M L}\right) B\left(I-P_{M L}\right) ;
$$

and where $\boldsymbol{F}_{M L}$ is a linear super-operator, corresponds to the Hessian at $\rho_{M L}$ of some restriction of $f$ and generalizes the Fisher information matrix:

$$
F_{M L}(X)=\sum_{\mu} \frac{\operatorname{Tr}\left(X E_{\|}^{(\mu)}\right)}{\operatorname{Tr}^{2}\left(\rho_{M L} E^{(\mu)}\right)} E_{\|}^{(\mu)}+\left(\lambda_{M L} I-\left.\nabla f\right|_{\rho_{M L}}\right) x \rho_{M L}^{+}+\rho_{M L}^{+} X\left(\lambda_{M L} I-\left.\nabla f\right|_{\rho_{M L}}\right)
$$

with $\rho_{M L}^{+}$the Moore-Penrose pseudo-inverse of $\rho_{M L}$.

## Concluding remarks

- Low-rank approximations and efficient numerical schemes for computations of $\rho_{M L}$, the adjoint states $E^{(n)}, \ldots$
- Asymptotics when the log-likelihood function is not strongly concave, when $\operatorname{ker}\left(\lambda_{M L} I-\left.\nabla f\right|_{\rho M L}\right) \neq \operatorname{ker}\left(I-P_{M L}\right) \ldots$
- Process tomography: log-likelihood function not concave ...
- Parameter estimation along quantum trajectories (in real-time)
- Thematic quarter at Institut Henri Poincaré in Paris next Spring 2018 gathering experimental physicists and theoreticians.


## April $16^{\text {th }}$ to July $13^{\text {th }}, 2018$

Organized by:
Etienne Brion, Université Paris-Sud, ENS Paris-Saclay, CNRS Eleni Diamanti, Université Pierre et Marie Curie \& CNRS
Alexei Ourjoumtsev, Collège de France \& CNRS
Pierre Rouchon, Mines ParisTech \& Inria

## Measuremenir zand conitiol of quaintum sustemls: theori and experiments

CIRM Pre-school at Marseille
Modeling and control
of open quantum systems
April $16^{\text {th }}-20^{\text {th }} \cdot 2018$

Observability and estimation
in quantum dynamics
May $15^{\text {th }}$ to $17^{\text {th }}, 2018$
Quantum control and feedback: foundations and applications June $5^{\text {th }}$ to $7^{\text {th }}, 2018$

## PRACQSYS 2018:

Principles and Applications of Control in Quantum Systems
July $2^{\text {nd }}$ to $6^{\text {th }}, 2018$

## Program coordinated by the Centre Emile Borel at IHP

Participation of Postdocs and PhD Students is strongly encouraged Scientific program at: https://sites.google.com/view/mcqs2018/home

Registration is free however mandatory at: www.ihp.fr Deadline for financial support:September 15 ${ }^{\text {h }}, 2017$ Contact:meqs2018@ihp.fr

Sylvie Lhermitte: CEB Manager


## Asymptotics for multi-dimension Laplace integrals (1)

Theorem (interior max) $\mathcal{I}_{g}(N)=\int_{z \in(-1,1)^{n}} g(z) \exp (N f(z)) \mathrm{d} z$ with $f$ and $g$ analytic functions of $z$ on a compact neighbourhood of $\overline{\mathcal{D}}$, the closure of $\mathcal{D}$. Assume that $f$ admits a unique maximum on $\overline{\mathcal{D}}$ at $z=0$ with $\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{0}$ negative definite.
If $g(0) \neq 0$, we have the following dominant term in the asymptotic expansion of $\mathcal{I}_{g}(N)$ for large $N$ :

$$
\mathcal{I}_{g}(N)=\left(\frac{g(0)(2 \pi)^{n / 2} e^{N f(0)} N^{-n / 2}}{\sqrt{\left|\operatorname{det}\left(\left.\frac{\partial{ }^{2 f}}{\partial z^{2}}\right|_{0}\right)\right|}}\right)+O\left(e^{N t(0)} N^{-n / 2-1}\right) .
$$

If $g(0)=0$, with $\left.\frac{\partial g}{\partial z}\right|_{0}=0$, then we have:

$$
\begin{aligned}
\mathcal{I}_{g}(N)=\left(\frac{\operatorname{Tr}\left(-\left.\frac{\partial^{2} g}{\partial z^{2}}\right|_{0}\left(\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{0}\right)^{-1}\right)(2 \pi)^{n / 2}}{2 \sqrt{\left|\operatorname{det}\left(\left.\frac{\partial^{f} f}{\partial z^{2}}\right|_{0}\right)\right|}}\right) & e^{N f(0)} N^{-n / 2-1} \\
& +O\left(e^{N f(0)} N^{-n / 2-2}\right) .
\end{aligned}
$$

## Asymptotics for Bayesian integrals (1')

Corollary (interior max): Assume that $f$ admits a unique maximum on $\overline{\mathcal{D}}$ at $z=0$ with $\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{0}$ negative definite. Then we have the following asymptotic for any analytic function $g(z)$ :

$$
\mathcal{M}_{g}(N) \triangleq \frac{\int_{z \in(-1,1)^{n}} g(z) \exp (N f(z)) \mathrm{d} z}{\int_{z \in(-1,1)^{n}} \exp (N f(z)) \mathrm{d} z}=g(0)+O\left(N^{-1}\right)
$$

We have also:

$$
\begin{array}{r}
\mathcal{V}_{g}(N) \triangleq \frac{\int_{z \in(-1,1)^{n}}\left(g(z)-\mathcal{M}_{g}(N)\right)^{2} \exp (N f(z)) \mathrm{d} z}{\int_{z \in(-1,1)^{n}} \exp (N f(z)) \mathrm{d} z} \\
=\frac{\operatorname{Tr}\left(-\left.\frac{\partial^{2} g}{\partial z^{2}}\right|_{0}\left(\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{0}\right)^{-1}\right)}{2 N}+O\left(N^{-2}\right)
\end{array}
$$

## Asymptotics for multi-dimension Laplace integrals (2)

Theorem (boundary max):
$\mathcal{I}_{g}(N)=\int_{\boldsymbol{x} \in(0,1)} \int_{\boldsymbol{z} \in(-1,1)^{n}} \boldsymbol{x}^{m} \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{z}) \exp (\boldsymbol{N f}(\boldsymbol{x}, \boldsymbol{z})) \mathrm{d} \boldsymbol{x} \mathrm{d} \boldsymbol{z}$ with $f$ and $g$ analytic functions of $(x, z)$ on a compact neighbourhood of $\overline{\mathcal{D}}$, the closure of $\mathcal{D}$. Assume that $f$ admits a unique maximum on $\overline{\mathcal{D}}$ at $(x, z)=(0,0)$, with $\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{(0,0)}$ negative definite and $\left.\frac{\partial f}{\partial x}\right|_{(0,0)}<0$. If $g(0,0) \neq 0$, we have the following dominant term in the asymptotic expansion of $\mathcal{I}_{g}(N)$ for large $N$ :

$$
\mathcal{I}_{g}(N)=\left(\frac{g(0,0) m!(2 \pi)^{n / 2} e^{N f(0,0)} N^{-m-n / 2-1}}{\sqrt{\left|\operatorname{det}\left(\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{(0,0)}\right)\right|}\left(-\left.\frac{\partial f}{\partial x}\right|_{(0,0)}\right)^{m+1}}\right)+O\left(e^{N f(0,0)} N^{-m-n / 2-2}\right)
$$

If $g(0,0)=0$, with $\left.\frac{\partial g}{\partial x}\right|_{(0,0)}=0$ and $\left.\frac{\partial g}{\partial z}\right|_{(0,0)}=0$, then we have:

$$
\begin{gathered}
\mathcal{I}_{g}(N)=\left(\frac{\operatorname{Tr}\left(-\left.\frac{\partial^{2} g}{\partial z^{2}}\right|_{(0,0)}\left(\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{(0,0)}\right)^{-1}\right) m!(2 \pi)^{n / 2}}{2 \sqrt{\left|\operatorname{det}\left(\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{(0,0)}\right)\right|}\left(-\left.\frac{\partial f}{\partial x}\right|_{(0,0)}\right)^{m+1}}\right) e^{N f(0,0))} N^{-m-n / 2-2} \\
+O\left(e^{N f(0,0))} N^{-m-n / 2-3}\right) .
\end{gathered}
$$

## Asymptotics for Bayesian integrals (2')

Corollary (boundary max): Assume that $f$ admits a unique maximum on $\overline{\mathcal{D}}$ at $(x, z)=(0,0)$, with $\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{(0,0)}$ negative definite and $\left.\frac{\partial f}{\partial x}\right|_{(0,0)}<0$. Then, we have the following asymptotic for any analytic function $g(x, z)$ :

$$
\mathcal{M}_{g}(N) \triangleq \frac{\int_{x \in(0,1)} \int_{z \in(-1,1)^{n}} x^{m} g(x, z) \exp (N f(x, z)) \mathrm{d} x \mathrm{~d} z}{\int_{x \in(0,1)} \int_{z \in(-1,1)^{n}} x^{m} \exp (N f(x, z)) \mathrm{d} x \mathrm{~d} z}=g(0,0)+O\left(N^{-1}\right)
$$

We have also:

$$
\begin{array}{r}
\mathcal{V}_{g}(N) \triangleq \frac{\int_{x \in(0,1)} \int_{z \in(-1,1)^{n}} x^{m}\left(g(x, z)-\mathcal{M}_{g}(N)\right)^{2} \exp (N f(x, z)) \mathrm{d} x \mathrm{~d} z}{\int_{x \in(0,1)} \int_{z \in(-1,1)^{n}} x^{m} \exp (N f(x, z)) \mathrm{d} x \mathrm{~d} z} \\
=\frac{\operatorname{Tr}\left(-\left.\frac{\partial^{2} g}{\partial z^{2}}\right|_{(0,0)}\left(\left.\frac{\partial^{2} f}{\partial z^{2}}\right|_{(0,0)}\right)^{-1}\right)}{2 N}+O\left(N^{-2}\right)
\end{array}
$$


[^0]:    ${ }^{6}$ An important reference: V.I. Arnold, S.M. Gusein-Zade, and A.N. Varchenko. Singularities of Differentiable Maps, Vol. II. Birkhäuser, Boston, 1985
    ${ }^{7}$ S. Watanabe: Algebraic Geometry and Statistical Learning Theory, Cambridge University Press, 2009.

