Conditional expectations in quantum mechanics and Kirkwood-Dirac quasiprobability distributions

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Executive summary

- There is a (there are) natural notion(s) of conditional expectation $\mathbb{E}_{\hat{\rho}}(\hat{X}|\hat{Y})$ of not necessarily commuting observables in QM, with similar properties as classically probabilistic cond. expectations
- Unlike joint probability distributions of $\hat{X}$, $\hat{Y}$ which in general does not exist
- Quasiprobability distributions do (in great abundance)
- To any quasidistribution with Born marginals we can also associate an alternative conditional expectation
- Coincides with the quantum mechanical one iff the quasiproba. is the Kirkwood-Dirac one.

References

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Conditional expectation, classically

X, Y random variables taking values in finite sets $\mathrm{Ran}(X)$, $\mathrm{Ran}(Y) \subset \mathbb{C}$

Definition of $\mathbb{E}_{\mathbb{P}}(X|Y)$ from joint probability:

- Conditional probabilities $(x \in \mathrm{Ran}(X), y \in \mathrm{Ran}(Y))$

$$\mathbb{P}(X = x | Y = y) = \frac{\mathbb{P}(X = x, Y = y)}{\mathbb{P}(Y = y)}$$

- Conditional expectation of X given that $Y = y$:

$$e_{X|Y}(y) := \sum_{x \in \mathrm{Ran(X)}} x \, \mathbb{P}(X = x | Y = y)$$

- $\mathbb{E}_{\mathbb{P}}(X|Y) := e_{X|Y}(Y)$: random variable

Conditional expectation, classically

Two characterizations:

1. $X \to \mathbb{E}_{\mathbb{P}}(X|Y)$ unique map of rvs X to rvs that are functions of Y such that for all X,

$$\mathbb{E}_{\mathbb{P}}(g(Y)X|Y) = g(Y)\mathbb{E}_{\mathbb{P}}(X|Y)$$
$$\mathbb{E}_{\mathbb{P}}(\mathbb{E}_{\mathbb{P}}(X|Y)) = \mathbb{E}_{\mathbb{P}}(X)$$

2. $\mathbb{E}_{\mathbb{P}}(X|Y)$ is the function $f(Y)$ of Y which minimizes $\mathbb{E}_{\mathbb{P}}(|X - f(Y)|^2)$

Conditional expectation = best predictor of X by a function $f(Y)$ of Y (nonlinear least squares)

Quantum conditional expectation

$\hat{X}$, $\hat{Y}$ observables (self-adjoint operators) on a Hilbert space H with given state $\hat{\rho}$ (mixed or pure)
Define the cond. expectation of $\hat{X}$ given $\hat{Y}$ as either

- *real* function $f(\hat{Y})$ of $\hat{Y}$ which minimizes

$$\mathrm{Tr}((\hat{X} - f(\hat{Y}))^2 \hat{\rho})$$

  (if you want the cond. expect. of an observable to be an observable, i.e. self-adjoint) or

- *complex* function which minimizes

$$\mathrm{Tr}((\hat{X} - f(\hat{Y}))^\dagger (\hat{X} - f(\hat{Y}))\hat{\rho})$$

  (or perhaps $\mathrm{Tr}((\hat{X} - f(\hat{Y}))(\hat{X} - f(\hat{Y}))^\dagger \hat{\rho})$, or some convex combination: choices to be made ...)

Examples

Real (self-adjoint) conditional expectation of momentum operator $\hat{P} = i^{-1}\nabla$ given position operator $\hat{X}$ for pure state $\psi \in L^2(\mathbb{R}^n)$:

$$\mathrm{Im}\frac{\nabla\psi(x)}{\psi(x)} = \nabla S(x), \ \ \psi = Re^{iS} : \ \text{Bohm momentum}$$

Complex version

$$\frac{\nabla\psi(x)}{\psi(x)} = \frac{\langle x|P|\psi\rangle}{\langle x|\psi\rangle} : \text{weak value}$$

Left quantum conditional expectation

Definition
$\mathbb{E}_{\hat\rho}(\hat X|\hat Y) = f(\hat Y)$ where f complex function which minimizes

$$\mathrm{Tr}\left((\hat X - f(\hat Y))^\dagger(\hat X - f(\hat Y))\hat\rho\right);$$

also defined for non-self adjoint $\hat X$, unique a.e. with respect to $d\mathrm{Tr}(\Pi(\lambda)\rho)$, $\Pi(\lambda)$ spectral resolution of $\hat Y$

To simplify: finite dimensional Hilbert space, Π_y spectral projections of $\hat Y$, $y \in \sigma(\hat Y) =$ spectrum of $\hat Y$

$$\mathbb{E}_{\hat\rho}(\hat X|\hat Y) = \sum_{y\in\sigma(\hat Y)} \frac{\mathrm{Tr}(\Pi_y \hat X \hat\rho)}{\mathrm{Tr}(\Pi_y\hat\rho)}\,\Pi_y$$

for states $\hat\rho$ for which the denominator $\neq 0$ for all $y \in \sigma(\hat Y)$

Characterization by *left $\hat{Y}$-equivariance* plus iterated expectations

Theorem $\mathbb{E}_{\hat{\rho}}(\hat{X}|\hat{Y})$ unique function of $\hat{Y}$ such that

1. $\mathbb{E}_{\hat{\rho}}(g(\hat{Y})\hat{X}|\hat{Y}) = g(\hat{Y})\mathbb{E}_{\hat{\rho}}(\hat{X}|\hat{Y})$, $\forall$ functions g
2. $\mathrm{Tr}(\mathbb{E}_{\hat{\rho}}(\hat{X}|\hat{Y})\hat{\rho}) = \mathrm{Tr}(\hat{X}\hat{\rho})$

Equivalent way of writing 2:

$$\mathbb{E}_{\hat{\rho}}(\mathbb{E}_{\hat{\rho}}(\hat{X}|\hat{Y})) = \mathbb{E}_{\hat{\rho}}(\hat{X})$$

where $\mathbb{E}_{\hat{\rho}}(\hat{X}) := \mathrm{Tr}(\hat{X}\hat{\rho})$: *iterated expectations property*

Property 1: *left-$\hat{Y}$ equivariance*

Operational meaning: weak values, conditioned von Neumann measurements

Change notation: $\hat{X}, \hat{Y} \to \hat{A}, \hat{B}$
$\hat{X}$: meter reading, conjugate momentum $\hat{P}$
Meter-system interaction $U(\gamma) = e^{-i\gamma \hat{A}\hat{P}}$ on (tensor-) product Hilbert space
φ: initial meter state (e.g. narrow Gaussian), projection $|\varphi\rangle\langle\varphi|$

Conditioned von Neumann mesurement of meter reading given that $\hat{B} = b$ (post-selection)

$$\mathbb{E}_\gamma(\hat{X}|B = b) = \frac{\mathrm{Tr}(\hat{X}\Pi_b U_\gamma(\hat{\rho} \otimes |\varphi\rangle\langle\varphi|)U_\gamma^*)}{\mathrm{Tr}(\Pi_b U_\gamma(\hat{\rho} \otimes |\varphi\rangle\langle\varphi|)U_\gamma^*)}$$

classical conditional expectation: $\hat{X}$ and $\hat{B}$ commute!

Weak limit

First-order variation in γ:

$$\begin{aligned}\frac{d}{d\gamma}\mathbb{E}^{cl}_{\gamma}(\hat{X}|\hat{B}=b)|_{\gamma=0} &= \mathrm{Re}\,\mathbb{E}_{\hat{\rho}}(\hat{A}|\hat{B}=b)+ \\ &\quad 2\mathrm{Im}\mathbb{E}_{\hat{\rho}}(\hat{A}|\hat{B}=b)\cdot\mathrm{cov}_{\varphi}(\hat{X},\hat{P})\end{aligned}$$

$$\mathrm{cov}_{\varphi}(\hat{X},\hat{P})=\left\langle\frac{1}{2}(\hat{X}\hat{P}+\hat{P}\hat{X})\right\rangle_{\varphi}-\langle\hat{P}\rangle_{\varphi}\langle\hat{X}\rangle_{\varphi}$$

cf. J. Dressel, A. N. Jordan, Significance of the imaginary part of the real value, Phys. Rev. A **85**, 012107 (2012)

Conditional expectation of meter momentum (post interaction)

$$\frac{d}{d\gamma}\mathbb{E}_{\gamma}(\hat{P}|\hat{B}=b)|_{\gamma=0} = 2\mathrm{Im}\,\mathbb{E}_{\hat{\rho}}(\hat{A}|\hat{B}=b)\cdot \mathrm{var}_{\varphi}(\hat{P})$$

where

$$\begin{aligned} \mathrm{var}_{\varphi}(\hat{P}) &= \langle \hat{P}^2\rangle_{\varphi} - \langle \hat{P}\rangle_{\varphi}^2 \\ &= ||\hat{P}\varphi||^2 - \langle\varphi|\hat{P}|\varphi\rangle^2 \end{aligned}$$

(Dressel & Jordan, loc. cit.)

Conditional expectations from quasi-probabilities

$\hat{A}$, $\hat{B}$: simple spectra: $\#\sigma(\hat{A}) = \#\sigma(\hat{B}) = \dim(H)$

$(S_{a,b})_{(a,b)\in\sigma(\hat{A})\times\sigma(\hat{B})}$ basis of $L(H) = \{$ linear operators on $H\}$

Definition *Born-compatible* if (with $\Pi_a^{\hat{A}}, \Pi_b^{\hat{B}}$ spectral projections of $\hat{A}$, $\hat{B}$)

$$\sum_a S_{a,b} = \Pi_b^{\hat{B}}, \ \sum_b S_{a,b} = \Pi_a^{\hat{A}}$$

Then

$$Q_{a,b}(\hat{\rho}) := \mathrm{Tr}(S_{a,b}^{\dagger}\hat{\rho})$$

is a quasi-probability (complex measure of mass 1) on $\sigma(\hat{A}) \times \sigma(\hat{B})$ with Born probabilities of $\hat{A}$ and $\hat{B}$ as marginals:

$$\sum_b Q_{a,b}(\rho) = \mathrm{Tr}(\Pi_a^{\hat{A}}\hat{\rho}), \ \sum_a Q_{a,b}(\rho) = \mathrm{Tr}(\Pi_b^{\hat{B}}\hat{\rho})$$

$T_{a,b}$ dual basis: $\mathrm{Tr}(S^{\dagger}_{a,b} T_{a'b'}) = \delta_{aa'}\delta_{bb'}$

$$\widetilde{Q}_{a,b}(\hat{X}) =_{\mathrm{def.}} \mathrm{Tr}(T^{\dagger}_{a,b}\hat{X}), \quad \hat{X} \in L(H)$$

"Overlap formula"

$$\mathrm{Tr}(\hat{\rho}\hat{X}^{\dagger}) = \sum_{(a,b)\in\sigma(\hat{A})\times\sigma(\hat{B})} \overline{\tilde{Q}_{a,b}(\hat{X})} Q_{a,b}(\hat{\rho})$$

$\hat{X} \Leftrightarrow$ random variable $(a,b) \to \overline{\widetilde{Q}_{a,b}(\hat{X}^{\dagger})}$ on $\sigma(\hat{A}) \times \sigma(\hat{B})$

Born-compatible quasi-probabilistic representation of quantum mechanics on H

Examples

1. Kirkwood-Dirac: $S_{a,b} = \Pi_a^{\hat{A}} \Pi_b^{\hat{B}}$, assuming none of these are 0 (eigenvectors of $\hat{A}$ not perpendicular to any of those of $\hat{B}$)
2. Gross-Wigner on $\mathbb{Z}/n\mathbb{Z} \times \mathbb{Z}/n\mathbb{Z}$
3. Many others (many ways of choosing n^2 independent vectors in $L(H)$ subject to $2n$ conditions where $n = \mathrm{dim}(H)$)

   (Which ones are physically relevant?)

Q-conditional expectation

Definition

1. Quasi-proba that $\hat{A} = a$ given that $\hat{B} = b$:

$$Q_{a|b}(\hat{\rho}) := \frac{Q_{a,b}(\hat{\rho})}{\sum_a Q_{a,b}(\hat{\rho})} = \frac{Q_{a,b}(\hat{\rho})}{\mathrm{Tr}(\Pi_b^{\hat{B}}\hat{\rho})}$$

2. Q-cond. expectation of $\widehat{X}$ given $\widehat{B}$: *operator* defined by

$$\mathbb{E}_{\hat{\rho}}^{Q}(\hat{X}|\hat{B}) = \sum_{b\in\sigma(\hat{B})}\left(\sum_{a\in\sigma(\hat{A})}\overline{\tilde{Q}_{a,b}(\hat{X}^{\dagger})}Q_{a|b}(\hat{\rho})\right)\Pi_b^{\hat{B}}$$

Satisfies the iterated expectation property but is in general not left $\hat{B}$-equivariant, except for KD

Characterization of KD

Theorem We have that for all $\hat{X}$ and all functions f

$$\mathbb{E}^{Q}_{\hat{\rho}}(f(\hat{B})\hat{X}|\hat{B}) = f(\hat{B})\mathbb{E}_{\hat{\rho}}(\hat{X}|\hat{B})$$

iff $(Q, \widetilde{Q})$ is the Kirkwood-Dirac quasiprobability representation; in particular $Q_{ab}(\hat{\rho}) = Q^{KD}_{a,b}(\hat{\rho}) := \mathrm{Tr}(\Pi^{\hat{B}}_{b}\Pi^{\hat{A}}_{a}\hat{\rho})$ and the Q^{KD}-conditional expectation is the quantum conditional expectation (defined by minimisation)

Proof. Characterization of QM cond. expectation implies

$$\sum_{a\in\sigma(\hat{A})} \overline{\tilde{Q}_{a,b}(\hat{X}^{\dagger})}Q_{a,b}(\hat{\rho}) = \mathrm{Tr}(\Pi^{\hat{B}}_{b}\hat{X});$$

$+$ special choice $X = S_{a,b}$

Variational formula for $Q^{KD}_{a,b}$

Variational characterisation of $\mathbb{E}^{Q^{KD}}_{\hat{\rho}}(\hat{X}|\hat{B}) = \mathbb{E}_{\hat{\rho}}(\hat{X}|\hat{B})$ implies that

$$Q^{KD}_{a,b}(\hat{\rho}) = \mathrm{argmin}_{\lambda\in\mathbb{C}}\, \mathbb{E}_{\hat{\rho}}\left(\left|\langle b\rangle_\rho \Pi^{\hat{A}}_a - \lambda \Pi^{\hat{B}}_b\right|^2\right)$$

where $\langle b\rangle_\rho = \mathrm{Tr}(\Pi^{\hat{B}}_b \hat{\rho})$ and $|X|^2 := X^\dagger X$