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SOME COMMENTS ON QUANTUM PROBABILITY

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This is a short expository lecture* aimed mainly at an audience of classical probability theorists. Strict adherence to rigour is not maintained.

The expectation of a real valued random variable f on a sample space $\Omega = \{1, 2, \ldots, n\}$ with probability distribution $(p_1, p_2, \ldots, p_n)$ can be expressed in two different ways

$$\begin{aligned} \mathbb{E}f = \sum p_j f(j) &= (p_1, p_2, \ldots, p_n) \begin{pmatrix} f(1) \\ f(2) \\ \vdots \\ f(n) \end{pmatrix} \\ &= \mathrm{Tr} \begin{pmatrix} p_1 & 0 & 0 & \ldots & 0 \\ 0 & p_2 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & 0 & \ldots & p_n \end{pmatrix} \begin{pmatrix} f(1) & 0 & \ldots & 0 \\ 0 & f(2) & \ldots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & \ldots & f(n) \end{pmatrix} \end{aligned} \tag{1}$$

If $(\Omega, \mathcal{F}, \mathbb{P})$ is a general probability space and $f : \Omega \to \mathbb{R}$ is a random variable we can write

$$\mathbb{E}f = \int f \, d\mathbb{P} = \mathrm{Tr}(\rho M_f) = \langle 1, M_f 1 \rangle \tag{2}$$

where ρ is the orthogonal projection on the one dimensional subspace $\mathbb{C} \cdot 1$ in the Hilbert space $\mathcal{H} = L^2(\mathbb{P})$, M_f is the selfadjoint operator of multiplication by f and 1 denotes the constant function with value unity.

Thus expectation can be expressed in terms of trace when the probability measure and random variable are interpreted as suitable operators in a Hilbert space. If ρ is a nonnegative selfadjoint operator of unit trace and A is a selfadjoint operator in a Hilbert space $\mathcal{H}$ then we can construct a complete orthonormal basis $\{e_i\}$ such that

$$\rho e_j = p_j e_j \,, \; p_j \geq 0 \,, \quad j = 1, 2, \ldots \,, \; \sum_j p_j = 1$$

and write

$$\begin{aligned} \mathrm{Tr}(\rho A) &= \langle \textstyle\sum_j p_j^{1/2} e_j \otimes e_j \,, \; A \otimes I (\sum_j p_j^{1/2} e_j \otimes e_j) \rangle \\ &= \mathrm{Tr}(\rho' \otimes I) \end{aligned} \tag{3}$$

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where ρ' is the one dimensional orthogonal projection on the subspace $\mathbb{C}\cdot(\sum_j p_j^{1/2} e_j \otimes e_j)$ in $\mathcal{H} \otimes \mathcal{H}$. In other words one can view expectation as a diagonal matrix element of a suitable selfadjoint operator in a suitable Hilbert space. Such an interpretation enables us to widen the scope of classical probability by including in (1) the case of nondiagonal Hermitian matrices or in (2) the case of selfadjoint operators which are not necessarily multiplication by functions. To formalize this procedure we introduce a definition.

DEFINITION. Let $\mathcal{H}$ be a complex separable Hilbert space. Any nonnegative selfadjoint operator of unit trace in $\mathcal{H}$ is called a *state*. Any selfadjoint operator in $\mathcal{H}$ is called an *observable*. If ρ is a state and A is an observable the *expectation* of A in the state ρ is defined to be the (real) scalar $\mathrm{Tr}(\rho A)$ whenever it exists. When A is an orthogonal projection it is called an *event* (or the indicator of an event). The quantity $\mathrm{Tr}(\rho A^n)$ is called the *n-th moment* of A in the state ρ. The function $\varphi(t) = \mathrm{Tr}(\rho e^{itA})$ is called the *characteristic function* of the observable A in the state ρ. If $A = \int_{\mathbb{R}} x\, P^A(dx)$ is the spectral resolution of A then for any Borel set $E \subset \mathbb{R}$, $P^A(E)$ is the *event that the value of A lies in E*. Then the probability measure $E \to \mathrm{Tr}(\rho P^A(E))$ on the Borel σ-algebra of $\mathbb{R}$ is called the *distribution of the observable A in the state* ρ.

If A has countable spectrum $\{x_1, x_2, \ldots\}$ then A is an observable assuming the values x_j with probabilities $\mathrm{Tr}(\rho P^A(\{x_j\}))$ where $P^A(\{x_j\})$ is the projection on the eigensubspace of A for the eigenvalue x_j. When $\dim \mathcal{H} = d \leq \infty$ every observable A assumes at most d values, namely the eigenvalues of A. However, in this case the dimension of the real linear space of all observables is d^2. This is to be compared with the fact that on a sample space of d points every random variable assumes at most d values, but the linear space of all real valued random variables has dimension d.

We denote by $S(\mathcal{H})$ the set of all states in $\mathcal{H}$ and by $Q(\mathcal{H})$ the space of all observables in $\mathcal{H}$. $S(\mathcal{H})$ is a convex set whose extreme points are one dimensional projections, called *pure states*. Such a pure state is determined by a unit vector up to a multiplicative constant of modulus unity called *phase factor*. By abuse of language any unit vector u in $\mathcal{H}$ is called a pure state; truly speaking it stands for the one dimensional projection on the subspace $\mathbb{C}\cdot u \subset \mathcal{H}$.

If $\dim \mathcal{H} = d \leq \infty$ then as we had already remarked $Q(\mathcal{H})$ is a real linear space of dimension d^2. If $\dim \mathcal{H} = \infty$ an observable is said to be *bounded* if the corresponding self-adjoint operator is bounded. The set of all bounded observables is a real linear space. If A, B are any two bounded observables then $AB + BA$ and $i[A, B] = i(AB - BA)$ are also bounded observables.

If u is a pure state, $A \in Q(\mathcal{H})$, $u \in \mathrm{Dom}(A)$ (the domain of A), then the expectation of A in the state u is $m = \langle u, Au \rangle$. If $u \in \mathrm{Dom}(A^2)$ then the variance of A is equal to $\langle u, A^2 u \rangle - \langle u, Au \rangle^2 = \|(A - m)u\|^2$, under the convention that the scalar m and the operator mI are denoted by the same symbol. For any two bounded observables A, B and any pure state u one has the inequality

$$\|(A - m)u\| \, \|(B - m')u\| \geq \tfrac{1}{2} |\langle u, i[A, B] u \rangle| \tag{4}$$

where $m = \langle u, Au \rangle$, $m' = \langle u, Bu \rangle$. If the spectrum of $i[A, B]$ is contained in the

set $\{x : |x| \geq \varepsilon\}$ then the product of the variances of A and B in any pure state is not less than $\varepsilon^2/4$. This is a mathematical description of Heisenberg's uncertainty principle. It must be compared with the fact that the convex set of all probability distributions has extreme points which are degenerate distributions and the variance of every random variable with respect to a degenerate distribution is zero.

For solving problems in quantum probability it is often useful to identify an observable A with the one-parameter group $U_t = \exp itA$, $t \in \mathbb{R}$ of unitary operators. Very often one comes across a strongly continuous unitary representation $g \longmapsto U_g$ of a Lie group G in the Hilbert space $\mathcal{H}$ under consideration, and each one-parameter subgroup (g_t) in G leads to a one-parameter group $V_t = U_{g_t}$ of unitary operators whose Stone generator provides an observable of (physical) significance. If u is a pure state, then the positive definite function $<u, U_g u> = \varphi(g)$ provides all the information about the distributions in the state u of these observables.

We shall now examine how different probability distributions, with support in a subset of cardinality at most n in the real line, can be realized by observables in the n-dimensional Hilbert space $\mathbb{C}^n$ in the pure state

$$u = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{5}$$

where any element of $\mathbb{C}^n$ is expressed as a column vector. To this end consider a probability distribution $p_1, p_2, \ldots, p_n$ over $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}$. Define the complex numbers $\psi_j = p_j^{1/2} \exp i\theta_j$ where $\theta_1, \theta_2, \ldots, \theta_n$ are arbitrary angles. Consider any unitary operator U of the form

$$U = \begin{pmatrix} \psi_1 & * & \ldots & * \\ \psi_2 & * & \ldots & * \\ \vdots & & & \\ \psi_n & * & \ldots & * \end{pmatrix}$$

whose first column in the standard basis of $\mathbb{C}^n$ consists of $\psi_1, \ldots, \psi_n$. Consider the hermitian operator

$$X = U^\dagger \begin{pmatrix} x_1 & & & 0 \\ & x_2 & & \\ & & \ddots & \\ 0 & & & x_n \end{pmatrix} U$$

where $\dagger$ denotes adjoint. If u is defined by (5) then

$$<u, X^r u> = \textstyle\sum_j p_j x_j^r, \quad r = 1, 2, \ldots .$$

In other words the observable X in the state u has the same moments as the random variable assuming values $x_1, \ldots, x_n$ with probabilities $p_1, \ldots, p_n$ respectively. The abundance of choice for the unitary operator U indicates the tremendous flexibility in realising

a concrete statistical model in the context of quantum probability. As U varies over the unitary group of $\mathbb{C}^n$, any probability distribution over $x_1, x_2, \ldots, x_n$ is realised by the observable X in the fixed state u. Let $d = dim\mathcal{H} < \infty$. Consider k linearly independent observables $X_1, X_2, \ldots, X_k$ in $\mathcal{H}$. For any state ρ set

$$\varphi(t_1, t_2, \ldots, t_k) = \mathrm{Tr}\left(\rho e^{i(t_1 X_1 + \ldots + t_k X_k)}\right) \quad ; \qquad t_j \in \mathbb{R} \tag{6}$$

φ is a real analytic function of k variables, $\varphi(0) = 1$ and for fixed $(t_1, t_2, \ldots, t_k)$, $\varphi(tt_1, tt_2, \ldots, tt_k)$ is a positive definite function of t. If the X_j's commute then φ is positive definite in $\mathbb{R}^k$ and hence (by Bochner's theorem) turns out to be the characteristic function of a probability distribution in $\mathbb{R}^k$. Since in this case $X_1, X_2, \ldots, X_k$ can be simultaneously diagonalized by a single orthogonal transformation, the corresponding probability distribution in $\mathbb{R}^k$ has at most d points in its support. In general φ need not be the characteristic function of any distribution in $\mathbb{R}^k$. We do not seem to know which complex valued functions φ of k real variables can be expressed in the form (6).

If A, B are two bounded observables and ρ is a state in $\mathcal{H}$, then the covariance between A and B in the state ρ is the quantity $\mathrm{Cov}(A,B) = \mathrm{Tr}(\rho AB) - \mathrm{Tr}(\rho A)\mathrm{Tr}(\rho B)$. In general $\mathrm{Cov}(A,B)$ is complex. If $A_1, A_2, \ldots, A_k$ are any k observables, then the matrix $(\sigma_{ij}) = (\mathrm{Cov}(A_i, A_j))$ is positive semidefinite, and the observables are said to be ***mutually uncorrelated*** if $\sigma_{ij} = 0$ for $i \neq j$.

An observable A is called a ***spin observable*** if its spectrum is the two point set $\{-1, 1\}$. Suppose $\dim\mathcal{H} = d < \infty$ and ρ is the state $d^{-1}I$ (which is the analogue of uniform distribution in a sample space of d points). In $\mathcal{H}$ one can find $d^2 - 1$ mutually uncorrelated observables of expectation 0 in the state ρ. This is because $\mathrm{Tr}\,AB = \langle A, B\rangle$ is an inner product in the Hilbert space $\Omega(\mathcal{H})$ of dimension d^2. We do not know the maximal number of spin observables of expectation 0 which are mutually uncorrelated in the state ρ. When $d = 2^r$ this maximal number is $d^2 - 1$. This can be seen as follows. Identify $\mathcal{H}$ with the r-fold tensor product $\mathbb{C}^2 \otimes \ldots \otimes \mathbb{C}^2$. Consider the 2×2 matrices σ_0 =identity and

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{7}$$

$\sigma_1, \sigma_2, \sigma_3$ are the well known Pauli matrices whose eigenvalues are ± 1. We have $\rho = d^{-1}\sigma_0 \otimes \ldots \otimes \sigma_0$. First observe that $\sigma_1, \sigma_2, \sigma_3$ are mutually uncorrelated spin observables of expectation 0 in the state σ_0. Let $\mathcal{S}$ denote the set of all observables of the form $A_1 \otimes A_2 \otimes \ldots \otimes A_r$ where each A_i is any one of the operators σ_j, $j = 0, 1, 2, 3$ but not all the A_i's are equal to σ_0. Then $\mathcal{S}$ is a set of $d^2 - 1$ mutually uncorrelated spin observables of expectation 0 in the state ρ.

The problem concerning spin observables mentioned in the preceding paragraph has a classical analogue which is also open *. Suppose Ω is an n point sample space with uniform distribution and n is even. What is the maximal number of mutually uncorrelated random

* Marshall Hall, *Combinatorial Theory*, John Wiley & Sons, New York 1967, Chapter 4, p.206.

variables of expectation 0 on Ω assuming the values ± 1 ? This is related to the problem of Hadamard matrices. If n is divisible by 4 it is a conjecture that the maximal number is $n-1$. If $n = 2^r$ the conjecture is easily shown to be true by considering the matrix $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^{\otimes r}$ of order 2^r whose first row consists of 1's only, remaining rows consist of ± 1 and any two rows are orthogonal.

We now illustrate one of the significant qualitative features of quantum probability by constructing two spin observables A, B such that the spectrum of $A+B$ is the interval $[-2,2]$. Let

$$\mathcal{H} = L_2[0,2\pi] \oplus L_2[0,2\pi] ,$$

so that any element of $\mathcal{H}$ can be expressed as a column vector $\begin{pmatrix} f(\theta) \\ g(\theta) \end{pmatrix}$ of two functions of $\theta \in [0,2\pi]$. Define

$$A\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} f \\ -g \end{pmatrix} \quad ; \quad B\begin{pmatrix} f(\theta) \\ g(\theta) \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ \cos\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} f(\theta) \\ g(\theta) \end{pmatrix} .$$

It is clear that A and B are observables with spectrum equal to the two-point set $\{-1,1\}$. The operator $A+B$ which is matrix multiplication by $\begin{pmatrix} 1+\cos\theta & \sin\theta \\ \sin\theta & -(1+\cos\theta) \end{pmatrix}$ has Lebesgue spectrum of multiplicity 2. In any state A and B have a distribution with support $\{-1,1\}$, but $A+B$ has an absolutely continuous distribution in the interval $[-2,2]$.

There do exist well known examples (from physics) of unbounded observables A, B with absolutely continuous spectra such that for every $\epsilon > 0$ $A+\epsilon B$ is defined as an essentially selfadjoint operator whose closure has discrete spectrum.

The quantum probabilistic analogue of the cartesian product of Borel spaces is the tensor product of Hilbert spaces. If $\mathcal{H}_i$, $i = 1,2,\ldots,n$ are Hilbert spaces and ρ_i is a state in $\mathcal{H}_i$ for each i then $\rho = \rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_n$ is a state in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_n$. If P_i is an event in $\mathcal{H}_i$ for each i and $P = P_1 \otimes P_2 \otimes \ldots \otimes P_n$ then P is an event in $\mathcal{H}$ and $\mathrm{Tr}(\rho P) = \prod_{i=1}^n \mathrm{Tr}(\rho_i P_i)$.

If $\mathcal{B}_i$ denotes the algebra generated by all bounded observables of the form $A_1 \otimes A_2 \otimes \ldots \otimes A_i \otimes I \otimes \ldots \otimes I$, I denoting the identity operator on any Hilbert space, then $\mathcal{B}_1 \subset \mathcal{B}_2 \subset \ldots \mathcal{B}_n$ and the hermitian elements of $\mathcal{B}_i$ describe all the bounded observables concerning the "systems" described by $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_i$. In other words the increasing sequence $\mathcal{B}_i$, $i = 1,2,\ldots,n$ provides the analogue of a filtration in classical probability.

We now make a remark concerning the standard choice of complex Hilbert spaces instead of real ones for doing quantum probability. If $\mathcal{H}_1, \mathcal{H}_2$ are two real spaces of dimension d_1, d_2 respectively then

$$\dim Q(\mathcal{H}_i) = \frac{d_i(d_i+1)}{2}, i = 1,2 \quad ; \quad \dim \mathcal{H}_1 \otimes \mathcal{H}_2 = \frac{d_1 d_2 (d_1 d_2 + 1)}{2}$$

and therefore $\dim(\mathcal{H}_1 \otimes \mathcal{H}_2) > \dim(\mathcal{H}_1) \cdot \dim(\mathcal{H}_2)$ for $d_1, d_2 > 1$. By our method of putting two quantum systems together through tensor products we seem to get more

observables than we should from a purely dimensional point of view. On the other hand if $\mathcal{H}_1, \mathcal{H}_2$ are *complex* Hilbert spaces then $\dim Q(\mathcal{H}_i) = d_i^2$, $\dim Q(\mathcal{H}_1 \otimes \mathcal{H}_2) = (d_1 d_2)^2 = \dim(\mathcal{H}_1) \cdot \dim(\mathcal{H}_2)$ and the anomaly disappears.

The analogue of a Bernoulli trial in quantum probability is the Hilbert space $\mathbb{C}^2$ with the pure state $\binom{1}{0}$. Thus n independent Bernoulli trials are described by the n-fold tensor product $\mathbb{C}^2 \otimes \ldots \otimes \mathbb{C}^2$ and the pure state $\binom{1}{0} \otimes \ldots \otimes \binom{1}{0}$. This Hilbert space is called *baby* or *toy Fock space* in [5]. By letting $n \to \infty$ and making appropriate passage to limits it is possible to construct objects like Fock space, quantum Brownian motion and Poisson process, quantum diffusions, etc. In such a context the Poisson process may be viewed as a "perturbation" of Brownian motion just as the harmonic oscillator in quantum mechanics is viewed as a perturbation of a "free wave". In classical probability one builds the Gaussian model from Bernoulli trials. Quantum probability enables us to construct discrete models like Bernoulli and Poisson distributions from the Gaussian model in a natural way. Unfortunately this cannot be achieved in this short lecture. We have given at the end some of the references where an enthusiast may find more detailed explanations in the light of my comments.

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