Volume of classical and quantum ensembles: geometric approach to entropy and information

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Abstract

It is shown for classical and quantum ensembles that there is a unique quantity which has the properties of a “volume”. This quantity is a function of the ensemble entropy, and hence provides a geometric interpretation for the latter. It further provides a simple geometric picture for deriving and unifying a number of results in classical and quantum information theory, and for discussing entropic uncertainty relations.

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Classical and quantum ensembles make natural appearances in many different contexts. These include, for example, equilibrium ensembles in statistical mechanics; signal-state ensembles in communication theory; dynamical ensembles corresponding to Brownian or chaotic diffusion; and ensembles corresponding to the classical limits of various quantum states.

In each of the above contexts it is often fruitful to employ the notion of a “volume” associated with the ensemble. For example, derivations in statistical mechanics often involve counting “microstates” in a volume of small thickness containing a constant-energy surface \[1\]. Shannon’s theorem for information transfer, in the case of signals subject to quadratic energy and noise constraints, can be proved by considering the ratios of spherical volumes in high-dimensional spaces \[2\]. In Ornstein-Uhlenbeck diffusion the evolution of a Gaussian ensemble is usefully depicted by a “distribution ellipsoid” (with principal axis lengths corresponding to root-mean-square variances) \[3\], where the ellipsoid volume is a clear measure of the “spread” of the ensemble. Finally, minimum phase-space volumes on the order of \(\hbar^n\) play a fundamental role in the classical limit of quantum mechanics \[4\].

The above examples raise the question of whether there is in fact some general measure of “volume” for classical and quantum ensembles, which may be usefully employed in all of the above contexts but which is not restricted in application or interpretation to various special cases. Thus, for example, the measure \(\Delta x \Delta p\) for an ensemble of systems with a 2-dimensional phase space is not suitable, because (i) it is not invariant under canonical/unitary transformations; (ii) it has no natural generalisation to finite-dimensional quantum systems; and (iii) while it leads to useful geometric information bounds \[5\], these are only exact in particular cases.

It will be seen here that there is indeed a natural measure of “ensemble volume”. This measure is a function of the Gibb’s entropy for classical ensembles and of the von Neumann entropy for quantum ensembles, and hence provides a unified geometric interpretation for these quantities.

Before writing down this volume measure, it is useful to consider four simple properties which uniquely define it (up to a normalisation constant). The first is an invariance property, while the remaining three are geometric in nature. It is convenient to state these properties in a form independent of whether the ensemble is classical or quantum, as a common geometric viewpoint is desirable. Thus, \(\Gamma\) will be allowed to denote either a classical phase space or a quantum Hilbert space; \(\rho\) either a probability distribution on phase space or a density operator on Hilbert space; and \(\text{Tr}_\Gamma[\cdot]\) either integration over a classical phase space or the trace over a quantum Hilbert space.
space. Moreover, \( \Gamma_{12} \) will denote the phase space or Hilbert space corresponding to an ensemble of composite systems with subsystem spaces \( \Gamma_1 \) and \( \Gamma_2 \), i.e., \( \Gamma_{12} \) denotes \( \Gamma_1 \times \Gamma_2 \) for classical ensembles and \( \Gamma_1 \otimes \Gamma_2 \) for quantum ensembles.

Consider now a volume measure \( V(\rho) \) which satisfies the following properties:

(i) **Invariance Property:** \( V(\rho) \) is invariant under all canonical transformations (these are represented by unitary transformations for quantum ensembles). Note that this property ensures that the volume is a function of the ensemble alone, independently of a particular co-ordinatisation or measurement basis.

(ii) **Cartesian Property:** If \( \rho \) describes two uncorrelated ensembles \( \rho_1 \) and \( \rho_2 \) on \( \Gamma_1 \) and \( \Gamma_2 \) respectively, then

\[
V(\rho) = V(\rho_1)V(\rho_2). \tag{1}
\]

This property is exactly analogous to the geometric property that area equals length times breadth, and is illustrated in Fig. 1. Note that \( \rho \) is the product \( \rho_1 \rho_2 \) for classical ensembles, and the tensor product \( \rho_1 \otimes \rho_2 \) for quantum ensembles.

(iii) **Projection Property:** If \( \rho \) describes an ensemble of composite systems on \( \Gamma_{12} \) then

\[
V(\rho) \leq V(\rho_1)V(\rho_2), \tag{2}
\]

where \( \rho_1, \rho_2 \) denote the “projections” of \( \rho \) onto \( \Gamma_1, \Gamma_2 \) respectively (i.e., \( \rho_1 = \text{Tr}_{\Gamma_2}[\rho], \rho_2 = \text{Tr}_{\Gamma_1}[\rho] \)). This property is exactly analogous to the geometric property that a volume is less than or equal to the product of the lengths obtained by its projection onto orthogonal axes, and is illustrated in Fig. 2. Note that \( \rho_1, \rho_2 \) denote the marginal distributions corresponding to \( \Gamma_1, \Gamma_2 \) for classical ensembles, and the reduced density operators corresponding to \( \Gamma_1, \Gamma_2 \) for quantum ensembles.

(iv) **Uniformity Property:** If \( \rho' \) and \( \rho'' \) denote two non-overlapping ensembles (i.e., \( \text{Tr}[\rho' \rho''] = 0 \)), with equal volumes \( V(\rho') = V(\rho'') = V \), then an arbitrary mixture \( \rho \) of \( \rho' \) and \( \rho'' \) has volume no greater than \( 2V \), where the latter corresponds to the volume of an equally-weighted mixture, i.e.,

\[
V(\rho) \leq V(\rho'/2 + \rho''/2) = 2V. \tag{3}
\]

Thus uniform mixtures maximise ensemble volume.

One has the following result:
Theorem: Any (continuous) measure of volume satisfying properties (i)-(iv) above has the form

\[ V(\rho) = K(\Gamma)e^{S(\rho)}, \]  

where \( S(\rho) \) denotes the ensemble entropy

\[ S(\rho) = -\text{Tr}[\rho \ln \rho], \]  

and \( K(\Gamma) \) is a constant which may depend on \( \Gamma \), and satisfies

\[ K(\Gamma_{12}) = K(\Gamma_1)K(\Gamma_2). \]  

The proof will be given elsewhere for reasons of space, and primarily relies on applying properties (i)-(iv) to an arbitrarily large number of independent copies of a given ensemble \( \rho \). To indicate its plausibility here, consider a quantum ensemble with eigenvalue distribution \( \{\lambda_j\} \). Properties (i), (ii) and (iv) are certainly satisfied by the “Renyi” volumes \((\sum_j (\lambda_j^{\alpha})^\beta)\) with \((1 - \alpha)\beta = 1\), together with a term \( K(\Gamma) \) satisfying Eq. (6). A result of Renyi implies then that the projection property (iii) is satisfied only in the limit \( \alpha \to 1 \), yielding Eqs. (4) and (5).

The universal geometric interpretation of the volume measure in Eq. (4) contrasts with ensemble entropy, for which the only context-independent interpretation to date appears to be as a somewhat vague measure of “uncertainty” or “randomness”, which has a limited and purely heuristic usefulness. Indeed, it is perhaps conceptually more useful to define ensemble entropy as the logarithm of the ensemble volume \( V(\rho) \), thus providing a geometric picture for many of its properties. Applications of the volume measure in Eq. (4) to various contexts will now be discussed.

First, in the statistical mechanics context, the Gibbs relation \( S_{th} = kS(\rho) \) between thermodynamic entropy and ensemble entropy for equilibrium ensembles can be rewritten via Eqs. (4) and (5) as

\[ S_{th} = k \ln[V(\rho)/K(\Gamma)]. \]  

Thus, the thermodynamic entropy is (up to an additive constant) proportional to the logarithm of the ensemble volume. Note further from Eq. (7) and the third law of thermodynamics (that thermodynamic entropy vanishes at absolute zero), that \( K(\Gamma) \) should correspond to a minimum “zero-temperature” ensemble volume. For quantum ensembles one has from Eqs. (4) and (5) that \( V(\rho) = K(\Gamma) \) for pure states, i.e., the quantum zero-temperature volume is just that of a pure state on \( \Gamma \). However, classical ensembles violate
the third law [1] and \( K(\Gamma) \) remains arbitrary in this case (but see Eq. (18) below).

The geometric expression (7) is very similar to the original Boltzmann relation \( S_{th} = k \ln W \), where \( W \) is the number of distinct microstates or “elementary complexions” consistent with the thermodynamic description. Indeed, from the above discussion it follows that Eq. (7) provides a precise geometric interpretation of the Boltzmann relation for equilibrium ensembles: thermodynamic entropy is proportional to the logarithm of the number of non-overlapping zero-temperature (or “microstate”) volumes contained within the total volume of the ensemble.

Second, in the communication context, consider a communication channel where signal states \( \rho_1, \rho_2, \ldots \) are transmitted with prior probabilities \( p_1, p_2, \ldots \) respectively [10]. The ensemble of signal states itself corresponds to the mixture

\[
\rho = \sum_i p_i \rho_i. \tag{8}
\]

As a warm-up exercise, suppose that the signal states all have volumes greater than some minimum volume \( V_0 \) (e.g., due to noise in the channel). From the uniformity property (iv) it follows that the maximum possible number of non-overlapping signal volumes available for a given signal ensemble \( \rho \) is bounded by \( V(\rho)/V_0 \). Hence the maximum amount of error-free data, \( I_1 \), which can be gained by a single measurement at the receiver (measured in terms of the number of binary digits required to represent the data), is bounded by

\[
I_1 \leq \log_2(V(\rho)/V_0). \tag{9}
\]

For example, if the channel is quantum one may always take \( V_0 = K(\Gamma) \) (i.e., the volume of a pure state). Eqs. (4) and (9) then immediately yield the single-measurement quantum information bound

\[
I^Q_1 \leq S(\rho) \log_2 e, \tag{10}
\]

which may be recognised as a special case of Holevo’s bound in quantum communication theory [11] (see also below).

More generally, one may seek to improve information transfer by coding data into blocks of signal states, of some length \( L \), and restricting transmission to particular blocks of signals [8]. These may be referred to as “block-signals”, to distinguish them from the individual signals \( \{\rho_i\} \). The ensemble of block signals will be denoted by \( \rho^{(L)} \). Under the constraint
that state \( \rho_i \) still appears with relative frequency \( p_i \) per individual signal transmission, one has

\[
V(\rho^{(L)}) \leq V(\bar{\rho}_1) \ldots V(\bar{\rho}_L) \leq [V(\rho)]^L,
\]

where \( \bar{\rho}_l \) is the average \( l \)-th component of the transmitted block-signals; the first inequality follows from the projection property (iii); and the second inequality from the concavity property

\[
\sum_l L^{-1} S(\bar{\rho}_l) \leq S(\sum_l L^{-1} \bar{\rho}_l) = S(\rho)
\]

of entropy and Eqs. (4), (6) and (8).

Further, for \( L \) sufficiently large, the strong law of large numbers guarantees that most block-signals are “typical” in the sense of Shannon [8], i.e., the number of times that a signal state \( \rho_i \) appears in a given block-signal is approximately \( p_i L \), except for a set of block-signals with a total probability of occurrence approaching zero as \( L \) is increased (and hence which may be ignored). It then follows immediately from the Cartesian property (1) that the volume of a typical block signal \( \alpha \) is approximately

\[
V_\alpha = \prod_i [V(\rho_i)]^{p_i L}
\]

(and approaches it arbitrarily closely in the limit of large \( L \)).

Exactly as per the derivation of Eq. (9), the amount of error-free data \( I \) which can be gained per individual transmitted signal, by measurements on block-signals, is geometrically bounded in the limit of arbitrarily large block size by

\[
I \leq L^{-1} \log_2 [V(\rho^{(L)})/V_\alpha].
\]

From Eqs. (4), (11) and (13) this yields the general upper bound

\[
I \leq [S(\rho) - \sum_i p_i S(\rho_i)] \log_2 e.
\]

For classical ensembles, Eq. (15) may be recognised as the Shannon bound for discrete memoryless channels [8], while for quantum ensembles it may be recognised as the Holevo bound for such channels [11, 12, 13]. The unified derivation of these bounds from simple volume considerations is a central result of this paper. It is particularly valuable in the quantum case, as existing derivations of the Holevo bound are mathematically rather technical [11, 13, 14].
It has recently been shown \[15\] that the Holevo bound \[15\] is in fact tight, in the sense of being achievable arbitrarily closely for sufficiently large block sizes by choosing a suitable set of typical block-signals for transmission and making appropriate measurements on these block-signals at the receiver. Geometrically, this result corresponds to being able to choose up to \[V(\rho)]L/V\alpha\) non-overlapping block-signal volumes, in the limit of arbitrarily large \(L\), and it would be valuable if a geometrically-based proof of this could be given. Since the total number of typical signal-blocks may be estimated as \(\exp(-L \sum_i p_i \ln p_i)\) \[8\], tightness of bound Eq. (15) immediately implies the Lanford-Robinson inequality \[16\]

\[
S(\rho) - \sum_i p_i S(\rho_i) \leq -\sum_i p_i \ln p_i.
\]  

Next, in the diffusion context, consider a Gaussian classical ensemble with root-mean-square variances \(\Delta x_1, \ldots, \Delta x_n, \Delta p_1, \ldots, \Delta p_n\) relative to the principal axes (these variances and axes will in general vary in time for Ornstein-Uhlenbeck diffusion processes \[3\]). The ensemble volume may then be calculated from Eq. (4) as

\[
V(\rho) = K(\Gamma) \prod_{j=1}^{n} 2\pi e \Delta x_j \Delta p_j,
\]  

which is directly proportional to the volume of the corresponding “distribution ellipsoid” (with equality for the choice \(K(\Gamma) = n!(2e)^{-n}\)). This volume is moreover invariant under all canonical transformations. Note that trivially from Eq. (4) irreversible dynamical processes are characterised by a strictly increasing ensemble volume.

Consider finally a classical ensemble \(\rho_C\) which is the “classical limit” of some quantum ensemble \(\rho_Q\), i.e., the physical properties of \(\rho_C\) approximate those of \(\rho_Q\). For the case of a spinless particle on a 2n-dimensional phase space one can obtain a relationship between the constants \(K(\Gamma_C)\) and \(K(\Gamma_Q)\) in Eq. (4) by requiring that the ensemble volumes \(V(\rho_C)\) and \(V(\rho_Q)\) are approximately equal for such ensembles. Since these constants are independent of the dynamics of the ensemble it suffices to choose an equilibrium ensemble of isotropic oscillators. Equating \(V(\rho_C)\) and \(V(\rho_Q)\) in the high-temperature limit then yields

\[
K(\Gamma_Q) = h^n K(\Gamma_C),
\]  

for the volume of a pure state, where \(h\) is Planck’s constant.
Eq. (18) can be used to derive semi-classical uncertainty relations from geometric considerations. For two corresponding ensembles $\rho_Q$ and $\rho_C$ as above the position and momentum entropies $S(\rho_X)$ and $S(\rho_P)$ will be approximately equivalent for either ensemble, and further

$$\exp(S(\rho_X)) \exp(S(\rho_P)) \geq \exp(S(\rho_C))$$  \hspace{1cm} (19)

holds for the classical ensemble from the projection property (ii) applied to projections onto the position and momentum axes rather than spaces $\Gamma_1$ and $\Gamma_2$ \cite{17}. Eqs. (4), (18) and (19) yield

$$S(\rho_X) + S(\rho_P) \approx n \ln h. $$  \hspace{1cm} (20)

This semi-classical entropic uncertainty relation, holding for quantum ensembles which have classical limits, arises directly from the existence of a minimum volume for quantum ensembles. Following the method of \cite{18}, the corresponding semi-classical Heisenberg uncertainty relation

$$\Delta x \Delta p \approx \hbar/e$$  \hspace{1cm} (21)

follows for the $n = 1$ case. Eqs. (20) and (21) are close to the exact results for general quantum ensembles \cite{18} (where, e.g., $e$ is replaced by 2 in Eq. (21)).

In conclusion, an essentially unique measure of volume for classical and quantum ensembles has been found, related to ensemble entropy, which provides a geometric tool for any context in which ensembles appear. This measure is universal in the sense that it may be defined by theory-independent concepts of invariance, uncorrelated ensembles, projection, and non-overlapping ensembles (properties (i)-(iv)). Applications include a precise geometric interpretation of the Boltzmann relation; a unified derivation of results in classical and quantum information theory based on simple geometric properties; an invariant generalisation of "ellipsoid volume" for diffusion problems; and a geometric derivation of semi-classical uncertainty relations.

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FIGURE CAPTIONS

FIG. 1. Two uncorrelated ensembles $\rho_1$ and $\rho_2$ on spaces $\Gamma_1$ and $\Gamma_2$ respectively (shown here compressed to 1-dimensional axes), have respective volumes $V(\rho_1)$ and $V(\rho_2)$ as indicated by the darkened axis regions. The Cartesian property Eq. (1) states that the corresponding joint ensemble $\rho$ has a “rectangular” volume $V(\rho) = V(\rho_1)V(\rho_2)$, i.e., $V(\rho)$ corresponds to the Cartesian product of volumes $V(\rho_1)$ and $V(\rho_2)$.

FIG. 2. An ensemble $\rho$ on the product space of $\Gamma_1$ and $\Gamma_2$ has a volume $V(\rho)$ indicated by the solid closed curve. The corresponding projected (or “reduced”) ensembles $\rho_1$ and $\rho_2$ on $\Gamma_1$ and $\Gamma_2$ respectively have projected volumes $V(\rho_1)$ and $V(\rho_2)$, indicated by the darkened axis regions. The projection property Eq. (2) states that $V(\rho)$ can be no greater than the volume of the rectangular region formed by the dashed lines, i.e., than the product of the projected volumes.
\[ V(\rho_1) \]
