Ergodicity in theory and in practice

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The term ergodicity did not originally refer to the equality of time and ensemble averages. Rather, by 'ergodic' Boltzmann referred to a dynamical property of a system that would bring about this equality. In this talk we will take a tour of the various classical attempts to pin down Boltzmann's notion from a mathematical standpoint, and why these often have limited usage in practice. Two fundamental difficulties are that a) real systems are never observed for an infinitely long time and b) real data sets are therefore limited to contain finitely many points to perform statistical analyses on them. Our work proposes a new characterisation of ergodicity intended to overcome these difficulties. This new definition, inspired in part by Khinchin, relies on the idea that, to be ergodic, any single trajectory of an observable should sample the same underlying distribution as the thermodynamic equilibrium ensemble's distribution. To implement this definition, we introduce a 2-sample metric between empirical probability distributions to assess how similar 2 finite realisations of sampled time and ensemble trajectories for a specified observable may be. Even if the underlying distributions are identical, the finiteness of the sampling implies that the measured distance between these empirical distributions will never be exactly zero. In this work, we take seriously the fact that, once a specific distance value is obtained for one trajectory, how small it is may allow one to indicate a "degree of ergodicity" rather than adopting a full binary conception of the term for an observable or even an entire dynamical system. Some degree of ergodicity may indeed be sufficient for some purposes while other situations may require a higher degree of ergodicity. We benchmark our analysis on the Kob-Andersen model, a lattice glass former, which was shown to be non-ergodic (in the sense of metric transitivity) for all system sizes for certain parameter values of the model, but to display a non-ergodic -> "quasi-ergodic" crossover as the system size is increased at fixed particle density [2]. We find that there is a substantial dependence in the initial conditions allowing us to provide a statistical description of the ergodic character of the system.

References

[1] F. Paillusson, D. Frenkel, Probing Ergodicity in Granular Matter, Phys. Rev. Lett., 109, 208001 (2012).
[2] Toninelli et al., Cooperative Behavior of Kinetically Constrained Lattice Gas Models of Glassy Dynamics, J. Stat. Phys., 120, 167 (2005).