The Hadamard glass

A "glass" is broadly defined as a system that, because of slow kinetics, is not in thermal equilibrium. By definition, such systems are beyond the scope of traditional statistical mechanics. Nevertheless, glasses are one of the most intensely studied and vigorously debated subjects in all of statistical mechanics. Most theoretical studies have focussed on systems with "quenched disorder", where the Hamiltonian has many random parameters. "Spin-glasses" — magnetic systems with random interaction parameters — are the best known class of such models. Systems without quenched disorder, where the Hamiltonian has a high degree of symmetry and few parameters, also exhibit glassy behavior. Homogeneous, covalently bonded materials, or "network glasses", are the best known systems in this class.

This project features a new theoretical "toy" model of a glass in the under-represented world of systems without quenched disorder. While displaying glassy behavior, this toy model has the virtue that computational studies can access the equilibrium properties that are out of reach in more realistic systems. For example, there is much speculation on the existence and nature of true thermodynamic transitions in glasses, in a hypothetical world without slow kinetics. Our toy model has such a transition and it is first-order.

The model has $n \times n$ orthogonal matrices U as its variables and Hamiltonian

$$H(U) = -\sqrt{n} \sum_{i=1}^{n} \sum_{j=1}^{n} |U_{ij}|.$$

Note that replacing $|U_{ij}|$ with $|U_{ij}|^2$ would make $H(U)$ a constant, independent of U (and trivialize the model). It's easy to see that H is minimized by a U that has all equal matrix elements in absolute value, that is, $|U_{ij}| = 1/\sqrt{n}$. Such matrices, or rather the ± 1 matrices one gets after multiplying by $\sqrt{n}$, are called *Hadamard matrices*. Hadamard matrices exist for $n = 1, 2$ and, it is believed, all n that are multiples of 4[1]. By limiting ourselves to n that are multiples of 4 we at least know the ground states of our model. On the other hand, there are many Hadamard matrices at the orders where they exist, in fact many more than is accounted for by simply permuting or applying a sign change to rows and columns[2].

Despite the abundance of Hadamard matrices, finding them by minimizing the Hamiltonian $H(U)$ is difficult! This is what makes this model glass-like. The partition function for the model is

$$Z(\beta) = \int dU \; e^{-\beta H(U)},$$

[1] This is the Hadamard matrix conjecture. The smallest open case is $n = 668$.

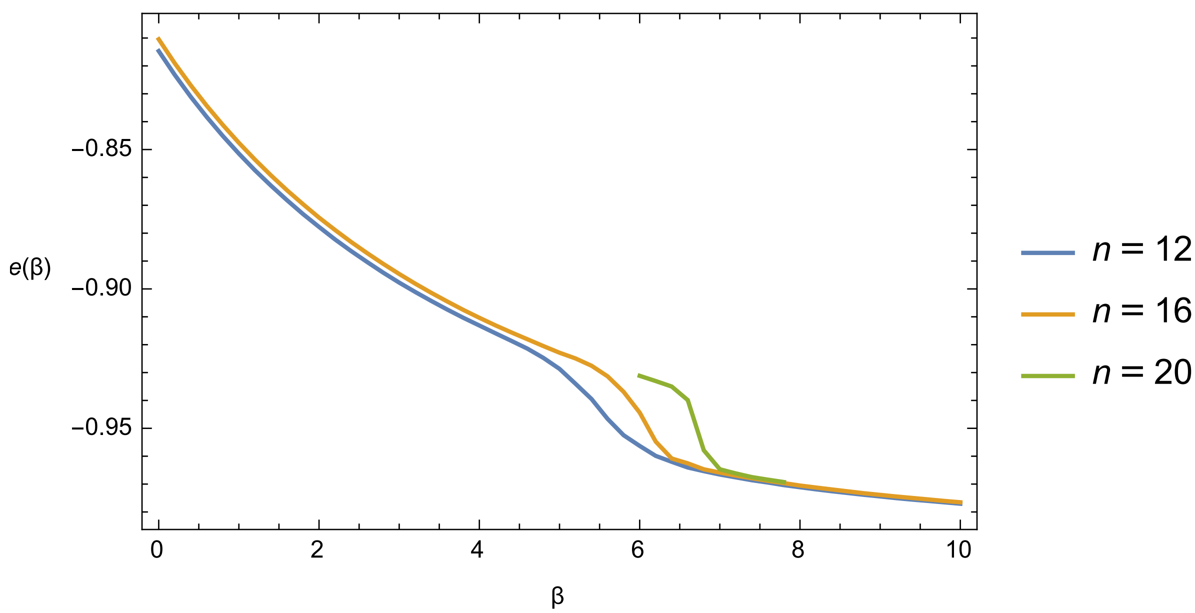
[2] Even declaring matrices related by these symmetries as equivalent, there are 3, 60, 487, and 13,710,027 inequivalent Hadamard matrices of order 20, 24, 28, and 32.

where the integral is with respect to the uniform measure on the space of orthogonal matrices[3]. I simulated this model with the standard Metropolis algorithm and computed the expectation value of the energy density,

$$e(\beta) = \frac{1}{n^2}\langle H \rangle.$$

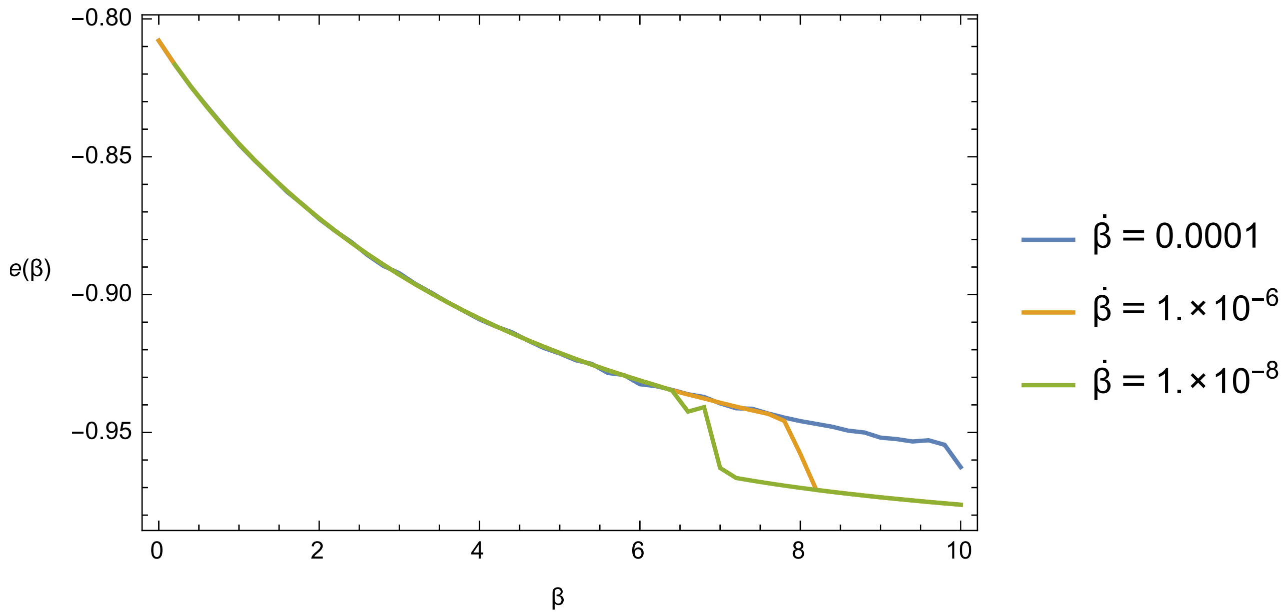
I used Givens rotations for my elementary transitions, where I select a random pair of rows (or columns) and apply a random rotation just to them. The range of the random angle was adjusted to get a 50% Metropolis acceptance rate (as β increased the range of the random angles decreased, as expected).

Below are plots of $e(\beta)$ for three system sizes:



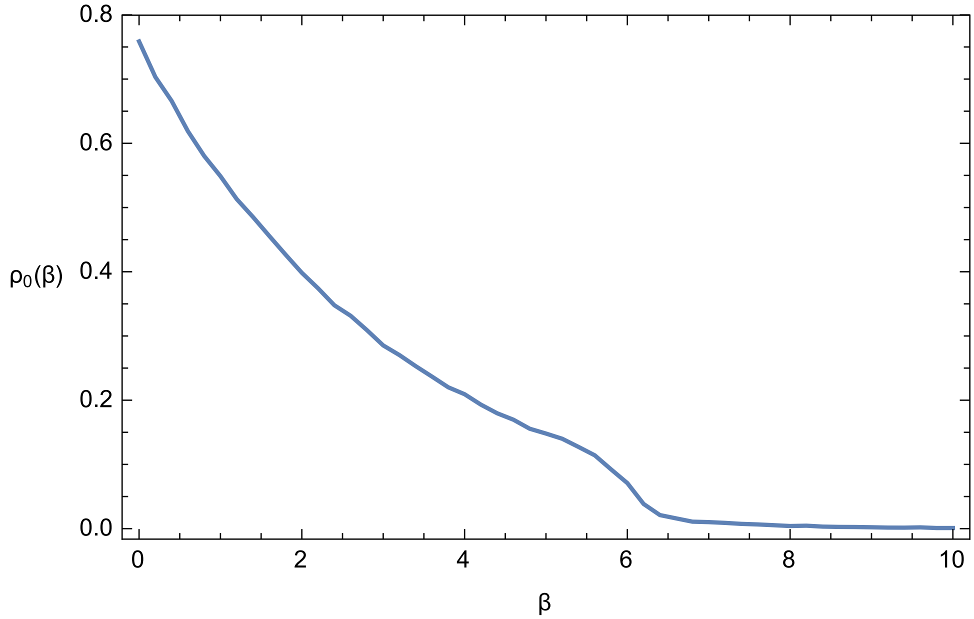
The curves for $n = 12$ and $n = 16$ are well converged when I apply 10^6 Givens rotations before advancing to the next, higher β. However, this number of Metropolis transitions is completely inadequate to equilibrate the $n = 20$ system. The plot on the next page shows the effect, on the $n = 20$ system, of increasing and slowing the cooling rate by a factor of 100. The converged plot above for $n = 20$ used 10^9 Givens rotations per data point. I suspect that the $n = 24$ system may be the largest which can be equilibrated with modest resources.

[3]The unique measure that is invariant under arbitrary rotations, also known as the Haar measure.



As you can see, even modest sized systems when cooled very slowly will not make the transition to the lower energy branch. This is the signature of glassy behavior. In this toy model we have the benefit of knowing a lower energy branch exists, and with great effort can establish the equilibrium transition. The plot comparing the different system sizes shows the transition is first order, because $e(\beta)$ is developing a discontinuity as the system size increases.

What can we say about the two phases of the Hadamard system? At the transition the two phases can be in equilibrium with each other, like water and ice. But is it really just *two* phases? After all, there are many ground states in this system! For the sake of glass phenomenology I find it useful to continue to think in terms of just two phases. In fact, for this system I have been able to define an equilibrium order parameter ρ_0 that is non-zero only in the high temperature phase. Below is a plot of ρ_0 for the $n = 16$ system. When the system fails to make the transition to the low temperature phase, because the cooling rate is not sufficiently slow, ρ_0 remains non-zero. My order parameter therefore serves to identify the "glass phase" even when phase equilibrium is not established. I hesitate to tell you how I define ρ_0 because it will prejudice your thinking about this model and glassiness in general.



If you choose to work on this project, here are the specific tasks.

- Read *Glass Transition Thermodynamics and Kinetics* by F. H. Stillinger and P. G. Debenedetti (Annu. Rev. Condens. Matter Phys. 2013, 4: 263-85).
- Prove that the ground states of the Hamiltonian $H(U)$ are Hadamard matrices (for those n where Hadamard matrices exist).
- Implement a Hadamard model simulator that is fast enough to equilibrate the $n = 20$ system. Compare the transition temperatures for sizes $n = 12, 16, 20$. I was able to account for the systematic decrease in the transition temperature with n by assuming that the entropy and energy change of the ordered phase are both non-extensive, that is, they scale in a way that is subdominant to the n^2 scaling of entropy and energy in the disordered phase. Two examples of subdominant scaling are n^ϕ, $\phi < 2$, and $n \log n$.
- Invent an order parameter that distinguishes the two equilibrium phases.