Assignment 3 Solutions

1. Customize your Hadamard-model simulator — or one of the contributed simulators from the course Github site — to address a number of outstanding features of the model. At a minimum you want to be able to specify, for one run: n, the range and increment for β, and the number of sweeps in the average at each β. The output should list the energy e and heat capacity c at each β, along with estimates of the errors. Here are the simulations for this assignment:

   - For $n = 12$ make plots of $e(\beta)$ and $c(\beta)$ for β between 0 and 10, with sufficiently small increments to resolve the abrupt drop in energy and see the heat capacity peak as a hill rather than a single point. Check that $e(\beta)$ and $c(\beta)$ agree with the high temperature limit from the previous assignment and the equipartition forms $e(\beta) \sim -1 + 1/(4\beta)$, $c(\beta) \sim 1/4$ at large β (where the Hamiltonian can be approximated as a quadratic potential for $n^2/2$ degrees of freedom).
   - Locate the transition β^* for $n =$ 8,12,16, 20 ($n = 24$ is probably out of reach, but you are welcome to try) by the maximum of $c(\beta)$. An outstanding question is whether the apparent increase of $\beta^*(n)$ with n (for those n that have Hadamard ground states) is just a "finite size effect", and $\beta^*(n)$ approaches a finite limit, or whether $\beta^*(n) \propto n^\psi$ for some positive exponent ψ. Which hypothesis is best supported by your four data points?
   - How do the entropy changes $\beta^*\Delta e(\beta^*)$ at the transitions depend on n? For this it will probably be easier to look at plots of $\beta(e(\beta) + 1)$ near the transition, rather than the $c(\beta)$ plots you used to locate β^*.
   - What can you say about the model at the oddly-even sizes $n = 10, 14, 18, 22$, which do not have Hadamard ground states?

   Solution:

   Below are plots/tables of the simulation results.

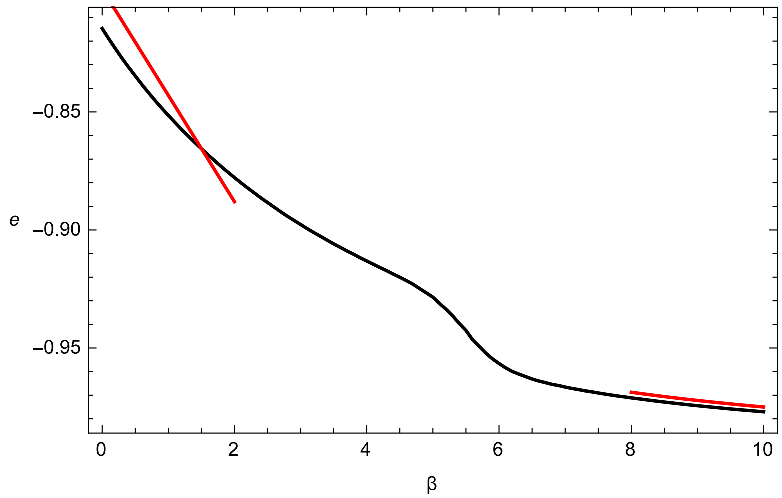

Figure 1: Energy of the $n = 12$ model. Analytical low and high temperature limits (for $n = \infty$) are rendered in red.

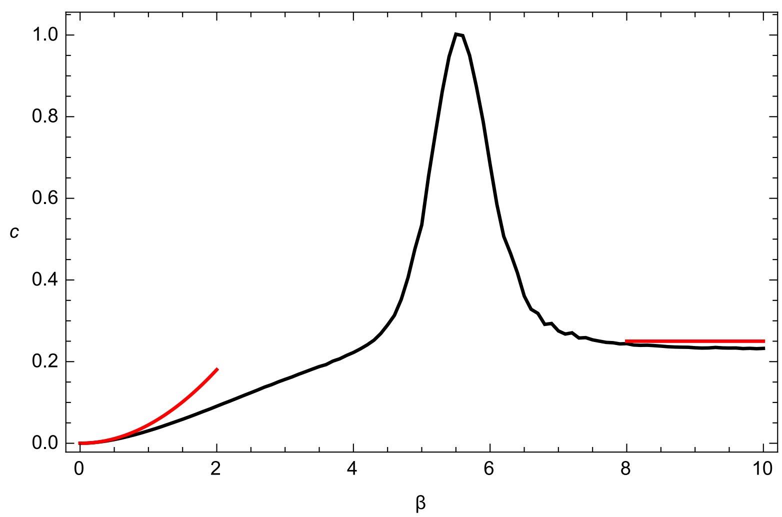

Figure 2: Heat capacity of the $n = 12$ model. Analytical low and high temperature limits (for $n = \infty$) are rendered in red.

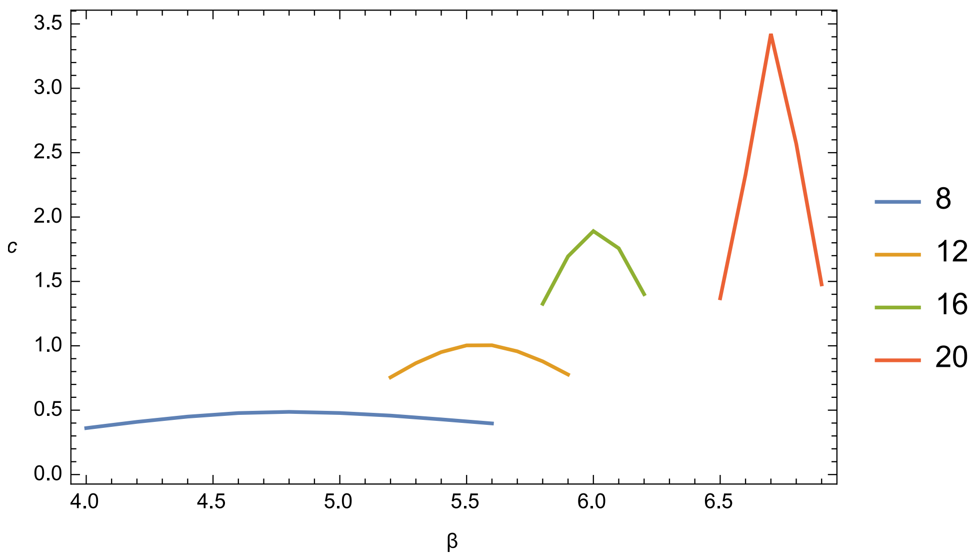

Figure 3: Heat capacity peaks for different system sizes.

Table 1: Estimates of β^* from parabolic fits to the peaks in Figure 3.

n	8	12	16	20
β^*	4.82	5.56	6.01	6.71

Finite size effects are usually much smaller than we are seeing in the behavior of the heat capacity peaks. A power-law growth of the transition temperature with n seems consistent with the data. The slope of the log-log plot of $\beta^*(n)$ vs. n gives exponent $\psi = 0.35$:

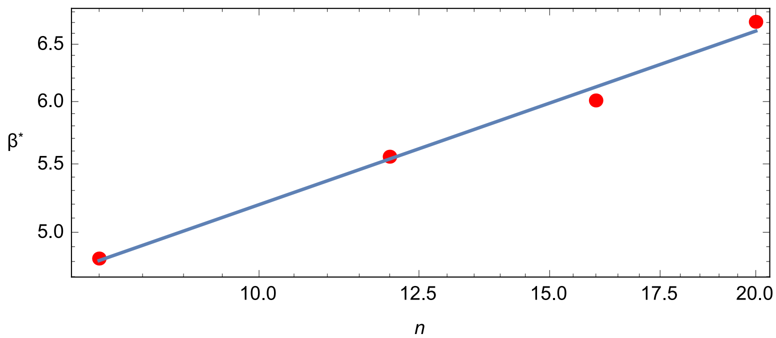

Figure 4: Log-log plot to estimate the exponent ψ.

In Figure 5 we see that the entropy change at the transition appears to stay extensive, consistent with a limiting value at large n.

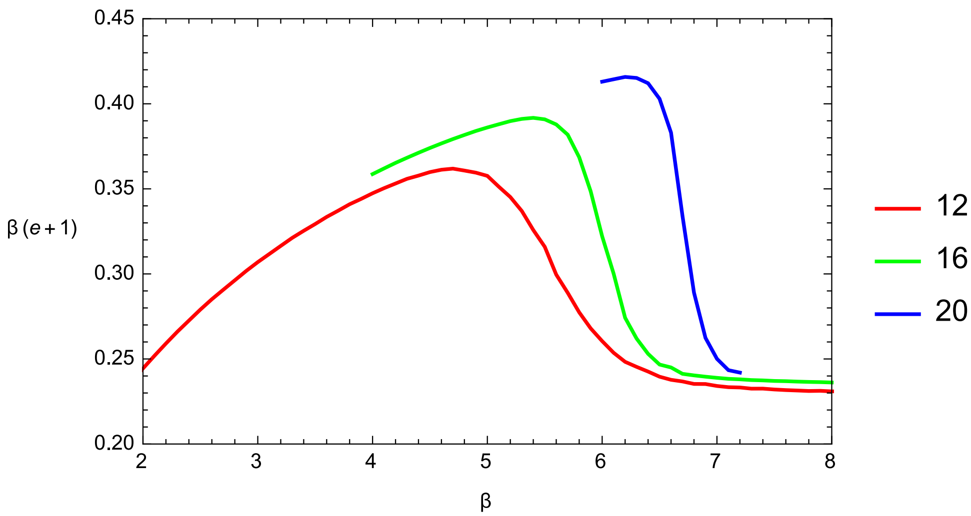

Figure 5: Plots of $\beta(e(\beta)+1)$ for three system sizes.

2. Consider the following very crude model of the low-energy density of states of the $n \times n$ Hadamard model,

$$\rho(E) = \rho_0\, \delta(E - E_0) + \rho_1\, \delta(E - E_1),$$

where the excitation energy $E_1 - E_0 = \Delta = \epsilon\, n^\phi$ is sub-extensive ($\phi < 2$) by the same exponent as the ground state entropy ($\epsilon, \sigma_0, \sigma_1$ are positive constants):

$$\rho_0/\rho_1 = \exp\left(\sigma_0 n^\phi - \sigma_1 n^2\right).$$

Show that this model has a discontinuity in the mean energy in the limit $n \to \infty$, but at a critical value of $\tilde{\beta}$, where $\beta = \tilde{\beta} n^\psi$, for some exponent ψ. Find ψ and also the behavior of the entropy change, $\beta\Delta$, with n.

Solution: After some algebra that makes the exponential part of the n dependence explicit, we obtain the following expression for the average energy:

$$\langle E \rangle = \frac{E_1 + (E_1 - \Delta) e^{(\sigma_0 + \tilde{\beta}\epsilon n^\psi) n^\phi - \sigma_1 n^2}}{1 + e^{(\sigma_0 + \tilde{\beta}\epsilon n^\psi) n^\phi - \sigma_1 n^2}}.$$

From this we see that the exponential n-dependence switches discontinuously for the case

$$\psi + \phi = 2$$

at the rescaled inverse temperature

$$\tilde{\beta}^* = \frac{\sigma_1}{\epsilon}.$$

In the limit $n \to \infty$ we obtain:

$$\langle E \rangle = \begin{cases} E_1, & \tilde{\beta} < \tilde{\beta}^*, \\ E_1 - \Delta, & \tilde{\beta} > \tilde{\beta}^*. \end{cases}$$

Since the simulations (see problem 1) indicate $\psi \approx 0.35$, this simplified model predicts $\phi \approx 2 - 0.35 = 1.65$ for the ground state entropy exponent[1]. The model predicts an extensive entropy change at the transition:

$$\Delta S = \beta^* \Delta = (\tilde{\beta}^* n^\psi)(\epsilon n^\phi) = \sigma_1 n^2.$$

[1] Y. Berra: "It's like déjà vu all over again." (see assignment 1 solutions).

3. On clear nights humans are naturally inclined to define the "constellation graph model", or CGM. The vertices of CGM are stars up to a given magnitude (the threshold of vision) and the rule for edges is that each star/vertex is connected to its nearest neighbor. A fundamental quantity in the CGM is the average number of stars S in a connected cluster — a constellation. The stars in CGM are assumed to be distributed uniformly, and their density is high enough that the sky may be modeled as a flat plane (rather than a sphere).

   In class we showed that every constellation has a unique pair of "core stars", defined by the property that each is the other's nearest neighbor, and

   $$S = \frac{2}{p_{\mathrm{c}}},$$

   where p_{c} is the probability that a randomly selected star is a core star. Calculate p_{c} in the CGM and thereby determine S.

   Solution: Consider a random star c_1 and without generality let its position define the origin in our plane of stars. This star is a core star if and only if the nearest star, c_2, is the other core star of the constellation. Let $\mathbf{r}$ be the position of c_2. The pair c_1 and c_2 are core stars if and only if there are no other stars in a region comprising the union of two disks of radius $r = |\mathbf{r}|$ centered on the two stars. Let $A(r) = ar^2$ be the area of this region. Using high school geometry,

   $$a = \frac{4\pi}{3} + \frac{\sqrt{3}}{2}.$$

   We use the Poisson distribution to determine the probabilities that (i) the region of area d^2r centered on $\mathbf{r}$ contains 1 star (c_2), and (ii) the union-of-disks-minus-centers region, of area $A(r)$, contains 0 stars. In both cases we use for the mean μ of the Poisson distribution,

   $$\mathrm{prob}(k) = \frac{\mu^k}{k!} e^{-\mu},$$

   the product of the area and the density of stars in the plane, ρ. Integrating over the possible positions $\mathbf{r}$ of c_2, weighted by the appropriate probabilities of finding stars, gives us the probability that c_1 is a core star:

$$\begin{aligned} p_{\rm c} &= \int (\rho\, d^2 r)\; e^{-\rho A(r)} \\ &= 2\pi\rho \int_0^\infty r dr\; e^{-\rho a r^2} \\ &= \frac{\pi}{a}. \end{aligned}$$

Using the high school result above we obtain the average number of stars per constellation:

$$S = \frac{2}{p_{\rm c}} = \frac{8}{3} + \frac{\sqrt{3}}{\pi} \approx 3.218.$$

4. In class we calculated two quantities of central importance in the random graph model:

$$\begin{aligned} f &= \sum_{k=1}^{\infty} k \langle n_k \rangle / n \\ s &= \sum_{k=1}^{\infty} k^2 \langle n_k \rangle / n. \end{aligned}$$

We were able to express both of these succinctly in terms of the Lambert w-function defined by

$$w(z) = \sum_{k=1}^{\infty} \frac{k^{k-1}}{k!} z^k,$$

for $|z| < 1/e$ and showed that $w(z)$ satisfies the implicit equation

$$z = w(z) e^{-w(z)}.$$

The quantity s is sometimes referred to as the "size" of finite clusters. An alternative definition of finite cluster size is the following:

$$\tilde{s} = \frac{f}{\sum_{k=1}^{\infty} \langle n_k \rangle / n}.$$

This corresponds to the definition we used in the CGM[2].

[2]Sadly, there are no percolating mega-constellations in the CGM, so always $f = 1$.

(a) Contrast in your own *words* the two definitions of "size".

Solution: The quantity s is a property of the *vertices*: the total number of vertices an average vertex is connected to (including itself), or equivalently, the size of cluster a vertex belongs to, averaged over all vertices in the random graph ensemble. By contrast, $\tilde{s}$ is a property of the *clusters*: the cluster size (number of vertices) averaged over clusters.

(b) Express $\tilde{s}$ explicitly in terms of the w-function. To get started, first show that the function

$$v(z) = \sum_{k=1}^{\infty} \frac{k^{k-2}}{k!} z^k,$$

satisfies the differential equation $v' = (1-w)w'$ (which is easily integrated).

Solution: Working with the Taylor series for $v(z)$ we obtain

$$zv' = w.$$

Next, using the implicit definition of $w(z)$ above to substitute for w/z, we obtain

$$v' = e^w.$$

We can also take the derivative of the implicit definition of $w(z)$; this produces

$$1 = (1-w)e^{-w}w'.$$

Combining the last two equations,

$$v' = (1-w)w',$$

and integrating we obtain

$$v = w - \frac{w^2}{2} + C.$$

Going back to the Taylor series for $v(z)$ and $w(z)$ we see that the constant C is zero.

(c) Using the result of part (b) obtain the explicit formula

$$\tilde{s}(d) = \begin{cases} (1 - d/2)^{-1}, & d < 1 \\ (1 - \tilde{d}(d)/2)^{-1}, & d > 1, \end{cases}$$

where $\tilde{d}(d)$ is the dual-degree function (the non-trivial solution of $\tilde{d}e^{-\tilde{d}} = de^{-d}$). Make a sketch of $\tilde{s}(d)$.

Solution:

$$\begin{aligned} \tilde{s} &= \frac{f}{\sum_{k=1}^{\infty} \langle n_k \rangle / n} \\ &= \frac{w(z)/d}{v(z)/d} \\ &= \frac{1}{1 - w(z)/2}. \end{aligned}$$

This evaluates to two forms, depending on whether the mean degree d is less than or greater than 1 (just as in lecture for the fraction f) . When $d < 1$, $w(de^{-d}) = d$, while for $d > 1$, $w(de^{-d}) = \tilde{d}$ (the dual degree).