

Effect of environmental changes on system periodicity as observed through Markov chains

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When dealing with physical systems in the real world, one might need to determine the causes of statistical complexity due to environmental variables and how complexity evolves over time. In many of these systems, we can only observe and measure certain variables over time, and must determine what causal states exist in the system from this data and how they fluctuate with changes to environmental variables. Once a description of causal states is created, one can calculate the statistical complexity and draw conclusions on the effects of these environmental variables. This paper tests this idea by analyzing behavior of a particle undergoing simple harmonic oscillation under different system conditions and showing how the statistical complexity of the system aligns with this idea.

To create data, simulations were performed with a Langevin dynamics (LD) program. LD is a subset of molecular dynamics that allows for friction and interaction of the object with the environment through random collisions. The ODE system is

$$\begin{aligned}\dot{r} &= v \\ m\dot{v} &= f(r, t) - \alpha v + \beta(t)\end{aligned}$$

with α being the coefficient of friction and $\beta(t)$ a Gaussian random variable such that

$$\begin{aligned}\langle \beta(t) \rangle &= 0 \\ \langle \beta(t)\beta(t') \rangle &= 2\alpha k_B T \delta(t - t')\end{aligned}$$

One can see that this system is dependent on the temperature and coefficient of friction. These two variables are the ones that will be changed in order to observe changes in the system.

The integrator used was a particular Verlet algorithm developed by Grønbech-Jensen and Farago. Both equations are correct to second order.

$$\begin{aligned}r^{n+1} &= r^n + bdtv^n + \frac{bdt^2}{2m}f^n + \frac{bdt}{2m}\beta^{n+1} \\ v^{n+1} &= av^n + \frac{dt}{2m}(af^n + f^{n+1}) + \frac{b}{m}\beta^{n+1}\end{aligned}$$

where

$$b \equiv \frac{1}{1 + \frac{\alpha}{2m}}$$

$$a \equiv \frac{1 - \frac{\alpha}{2m}}{1 + \frac{\alpha}{2m}}$$

and where

$$\beta^{n+1} \equiv \int_{t_n}^{t_{n+1}} \beta(t') dt'$$

is a Gaussian random number with $\langle \beta^n \rangle = 0$ and $\langle \beta^n \beta^l \rangle = 2\alpha k_B T dt \delta_{n,l}$. It has been shown by Grønbech-Jensen and Farago that for a simple, undamped continuous time harmonic oscillator, there is a formal stability limit of $\Omega_0 dt < 2$ for this integrator, where $\Omega_0 = \sqrt{\kappa/m}$ is the resonance frequency oscillator.

Various simulations were run for different temperature and friction scales, from order 0 to 1 with the forcing function for the simple harmonic oscillator. The simulations were run with spring constant $\kappa = 2.0$ for a particle with mass $m = 1.0$. The time step used was $dt = 1.3$, just under the maximum time step allowed ($dt = \sqrt{2}$) for the Verlet integrator with the given κ and m . The location of the particle was recorded at every time step as being to the left (equivalent to a zero) or the right (equivalent to a 1) of equilibrium. The initial velocity and position for each simulation were chosen from a uniform random distribution on $[-1, 1]$. Since this is a simple harmonic oscillator, the period of the particle's oscillation does not change with the initial energy in the system, so no special considerations were necessary for ensuring that each simulation would have equivalent behavior. Each simulation was run for over a 100 time steps, but only 35 were used at most for each parameter set due to time constraints on running analyzing code. Each parameter set had 100,000 iterations each to calculate the probabilities given.

For each set, the transition probabilities were calculated. For example, if the word '0100' has already been observed, we want to know the probability of next observing a '0' (hence now having the word '01000') and the probability of next observing a '1' (and now having '01001'). This is calculated by calculating the conditional probability of seeing the current word of length n given we have seen the same word truncated to length $n - 1$. The probabilities that I have given are these transition probabilities.

Detail the results for each scenario. Give tables of transition probabilities, or at least transitions for a hand full of words for each one.

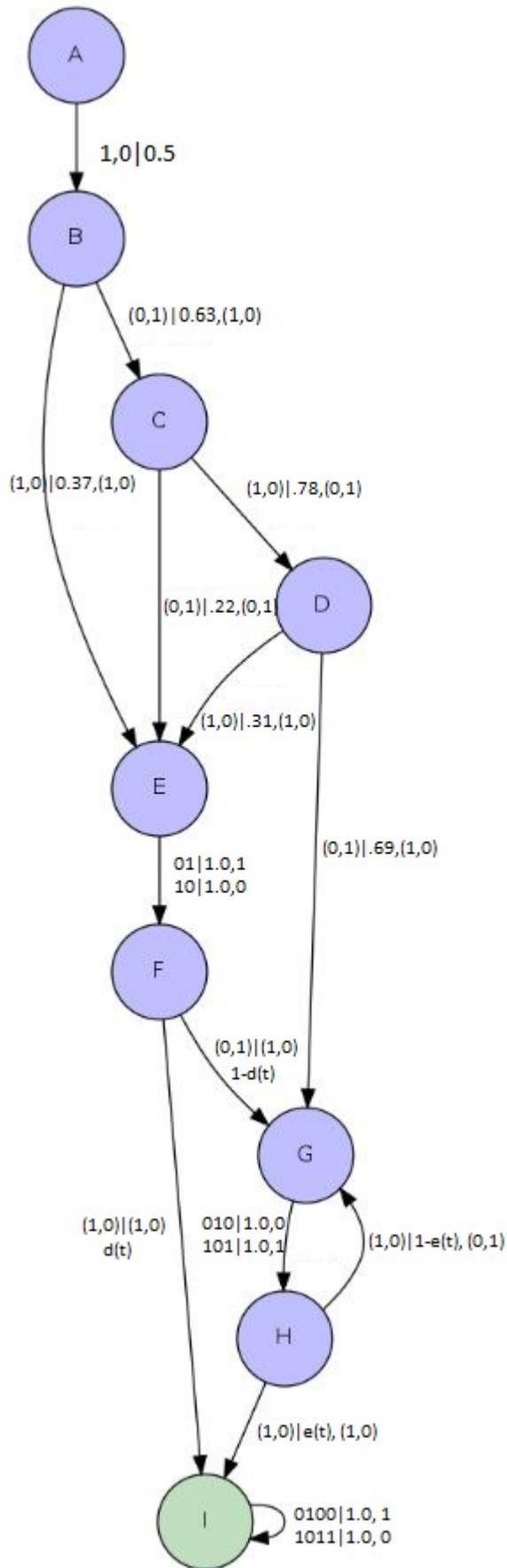
All were highly symmetric. If it occurred on one side of the tree, it also occurred with the same probabilities on the other side with differences in the thousandths place. (This is the source of discrepancies that you may see in these tables when probabilities don't add up quite to 1.)

$$\alpha = 0.0$$

In the table below are a sample of the allowed words and their transition probabilities as would appear in the parse tree.

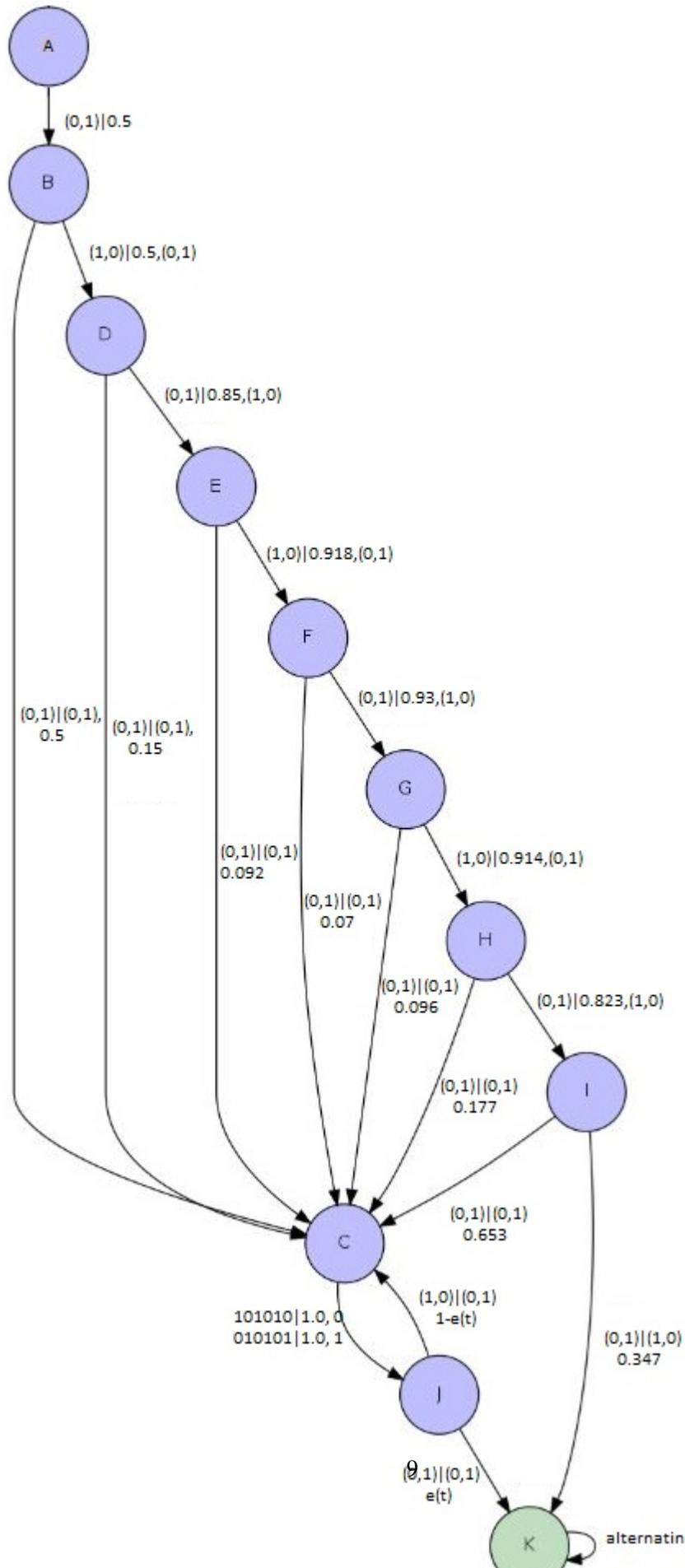
| | | | | | | | | | | | | | | |
|------------------------|--------|--------|--------|--------|---|--------|--------|--------|---|--------|--------|---|---|--------|
| 1001011010010110100100 | 0.4996 | 0.6334 | 0.2201 | 1 | 1 | 0.8333 | 1 | 1 | 1 | 0.8145 | 1 | 1 | 1 | 0.7970 |
| 1001011010010010110100 | 0.4996 | 0.6334 | 0.2201 | 1 | 1 | 0.8333 | 1 | 1 | 1 | 0.1855 | 1 | 1 | 1 | 1 |
| 0100101101001011010010 | 0.5004 | 0.6334 | 0.7784 | 0.3122 | 1 | 1 | 0.9143 | 1 | 1 | 1 | 0.8854 | 1 | 1 | 1 |
| 0101101101001011010010 | 0.5004 | 0.6334 | 0.7784 | 0.6878 | 1 | 1 | 1 | 0.1020 | 1 | 1 | 1 | 1 | 1 | 1 |

The first letter is about 50/50, which makes sense as the initial position is determined with a uniform distribution of $[-1, 1]$, so there should be equal probability of starting on either side. From there, there is an initial "parsing" section for the letters at positions 2,3, and 4. Going down the path that has higher probability will keep you in the initial parse section, while all of the lower probability paths then go into a deterministic stretch. In this case, our first initial stretch is length 2, and happens after the parsing gets the same letter twice (ie sees a 00 or a 11), and the deterministic portion is 10 if 00 or 01 if 11. The last branching point is about 31/69 (a ratio that is repeated in almost all of the different scenarios). The 30 path goes to the deterministic length-2 path, while the 60 skips that and continues onto the main pattern with the length-3 deterministic stretch. The main body of the pattern is that there is a deterministic length-3 segment dependent on what was just seen and which factors in strongly to the next section. If you had 0 previously, you will more likely have the deterministic set 010 than 101, and vice versa for having a 1 previously due to the symmetry. Once you go into the lower probability transition, it appears it's completely deterministic from there, with 1010,0101 alternating after that. At the end of the length, you either return back to the beginning of the same deterministic length or continue onto a longer one. (This pattern is also repeated in most systems, until washed out by white noise.) In this scenario, it seems that the set up is completely deterministic at the end. The final deterministic pattern becomes "00101101" in this case. We will need to analyze longer word lengths here, but that will take time, and I ran out of that here. The probabilities at splittings seem to be oscillating around 33/66 as time goes on. This structure remained the same for all temperatures as $\alpha = 0$ removes both the friction and stochastic properties of the system. In the machine below, we have $0 < d(t), e(t) < 0.5$, as these depended solely upon the word length and not on the actual previous history.



$$T = 0.0, \alpha = 1.0$$

On the next page are some select words from the allowed words for this scenario. The structure here is similar to that from before. The first letter is also 50/50, and there is an initial parsing section at the beginning that last for 6 additional letters. After, there is a deterministic length-6 section, and you repeat the deterministic length-6 section as long as you continue on the high probability pathway. If you hit the low-probability pathway, you then go into a length-22 deterministic segment. The letter structure of the deterministic portions is the same as before, as an alternating sequence. The deterministic lengths appear to get longer and longer as time goes on. This is equivalent to the particle slowing down from friction but not gaining more chaos from the temperature. One could rationalize that in the limit the set is completely deterministic alternating loop, but we never actually will achieve that.



$$T = 1 \times 10^{-5}, \alpha = 1.0$$

The system is non-Markovian and cannot be represented in terms of transitions any more. A different style will be required in order to describe this system with this algorithm.

| | | | | | | | | | | |
|------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 1010000000 | 0.4995 | 0.5081 | 0.8416 | 0.9173 | 0.0698 | 0.0216 | 0.6475 | 0.1990 | 0.4474 | 0.3529 |
| 1010100000 | 0.4995 | 0.5081 | 0.8416 | 0.9173 | 0.9302 | 0.9105 | 0.1961 | 0.1630 | 0.6595 | 0.3027 |
| 1010001000 | 0.4995 | 0.5081 | 0.8416 | 0.9173 | 0.0693 | 0.0216 | 0.3525 | 0.5385 | 0.6607 | 0.3514 |

$$T = 1 \times 10^{-12}, \alpha = 1.0$$

The patterns and the probabilities remain exactly the same as for $T = 0$ until around letter 9, whereas it switches to the same pattern as appear for $T = 1 \times 10^{-5}$. It is reasonable to assume that change occurs in the system due to the velocity and spring force becoming too small compared to the temperature effect as time goes on.

Conclusions

These appear to match our expectations and tell us more about the internal structure. LD method predicts that the stochasticity of the simulation is dependent upon having both α and T greater than 0, as we saw when the system could no longer be represented as Markovian. LD also predicts that relaxation to equilibrium is dependent upon having no stochasticity but with some dampening, as we saw when the periodicity was increased in the deterministic lengths of the system. With this partitioning of physical space, we were able to reasonably observe changes to the periodicity, and should therefore be able to reliably draw conclusions with this method for other potentially periodic systems from experimental data.