Shadowing high-dimensional Hamiltonian systems: the gravitational $n$-body problem

Wayne B. Hayes

Department of Computer Science, University of Toronto, Toronto, Ontario, M5S 3G4 Canada

(Dated: March 19, 2022)

A shadow is an exact solution to a chaotic system of equations that remains close to a numerically computed solution for a long time, ending in a glitch. We study the distribution of shadow durations at low dimension and how shadow durations scale as dimension increases up to 300 in a slightly simplified gravitational $n$-body system. We find that “softened” systems are shadowable for many tens of crossing times even for large $n$, while in an “unsoftened” system each particle encounters glitches independently as a Poisson process, giving shadow durations that scale as $1/n$.

PACS numbers: 02.60.-x, 02.70.-c, 05.45.-a, 05.45.Jn, 95.75.P, 05.40.-a, 98.10.+z

The behaviour of dynamical systems is often studied using numerical techniques. A source of error in such studies arises because dynamical systems often display sensitive dependence on initial conditions: two solutions whose initial conditions differ by an arbitrarily small amount generally diverge exponentially away from each other. Since numerical methods introduce errors, it is virtually guaranteed that a numerically computed solution diverges exponentially away from the exact solution with the same initial conditions. This remains true even if integrals of motion such as energy and momentum are conserved to arbitrary precision. Although this fact is widely known, its impact is not well understood.

Fortunately, most studies of dynamical systems do not aim to predict the precise evolution of a particular choice of initial conditions. Instead, the dynamics of the system is sampled in order to study its general behaviour. In such cases, we typically choose initial conditions from a random distribution and would be happy if our numerical solution exhibited behaviour typical of any valid choice of initial conditions from our distribution. In particular, we may be satisfied if our numerical solution closely follows some exact solution whose initial conditions are close to those that we chose.

The study of shadowing provides just such a property: a shadow is an exact solution to a given set of equations that remains close to a numerically computed solution of the same set of equations for a nontrivial duration of time. Although not all numerical simulations are likely to be shadowable, the existence of a shadow is a strong property: it asserts that a numerical solution can be viewed as an experimental observation of an exact solution. As such, within the “observational” error, the dynamics observed in a numerical solution that has a shadow represent the dynamics of an exact solution. There are only two remaining questions (both beyond the scope of this paper): (1) Whether the mathematical model being simulated accurately reflects the system being studied. This is certainly not the case for systems such as the weather (and thus shadowing is probably an inappropriate measure of error), but can be assumed to be the case for others, such as the unsoftened gravitational $n$-body problem. (2) Whether shadows are typical of exact solutions chosen at random. Simple examples exist of shadows that are atypical, although it seems unlikely that atypical shadows are common — lest the numerical solutions we compute would be commonly atypical as well.

Shadows of “noisy” trajectories were first proved to exist in hyperbolic systems. Such systems possess a phase space which is spanned locally by an independent set of stable and unstable directions that remain consistent under the evolution of the system. Few chaotic dynamical systems are globally hyperbolic, but for those that are nearly hyperbolic over finite time intervals, the existence of finite-duration shadows can often be inferred or rigorously proved. If a shadow is viewed as a measure of error of a numerical solution, then the relevant measures are the phase-space distance between corresponding points on the “noisy” and exact trajectories (smaller is better), and the duration over which they remain close together (longer is better). Generally, the smaller the local error in the trajectory, and the more hyperbolic the trajectory, the closer and longer the shadow. In scaling laws were developed for the expected duration of shadows, based upon the distance from zero of finite-time Lyapunov exponents of the system. If an exponent fluctuates about zero over a trajectory, it represents a tangential direction that is uncertain between stable and unstable. This effect, also called unstable dimension variability, is the cause of unshadowability in chaotic systems. If a numerical trajectory is unshadowable, then it is possible (though far from certain) that statistical quantities associated with the numerical trajectory can have significant bias.

To date, most studies of shadowability of chaotic systems have focussed on maps or ODEs with only a few dimensions, and concern has been expressed that fluctuating Lyapunov exponents may be common in high-dimensional systems. Furthermore, since Hamiltonian systems are not globally hyperbolic, there is no reason to expect them to be easily shadowable. In this paper, we demonstrate that trajectories of at least one commonly integrated continuous Hamiltonian system...
(the softened gravitational $n$-body problem) are shadowable for long times with as many as 150 phase-space dimensions (25 particles). We also demonstrate that, for the purpose of shadowing, a large $n$-body system can be viewed as a superposition of many small systems, so that the distribution of shadow durations for a high-dimensional $n$-body system can be approximated using the distribution of shadow durations of many low-dimensional systems.

The trajectories that we will attempt to shadow belong to a slightly simplified gravitational $n$-body problem in which there are $N$ total particles, only $M$ of which move. We do this because the shadowing algorithm we use takes time $O(M^3)$ and we want to simulate a large system with a complex potential while keeping the time to compute a shadow tractable. Each moving particle interacts both with fixed particles and with other moving particles via Newton’s gravitational force law,$\quad F_{ij} = -\frac{Gm_i m_j}{r_{ij}^2 + \varepsilon^2},$

where $F_{ij}$ is the force on particle $i$ from particle $j$, $m_i$ and $m_j$ are their masses, $r_{ij}$ is the distance between them, and $\varepsilon$ is the gravitational softening parameter which, if non-zero, artificially smoothens the gravitational potential in order to approximately emulate a system with more particles than are actually present and to avoid the singularity at $r_{ij} = 0$. We use normalized units in which each particle has mass $1/N$, the system has diameter of order unity, and the crossing time (the average time for a particle to cross the system from one side to the other) is of order unity. We use a variable-order, variable timestep integrator for all integrations. We generate noisy trajectories with local errors of about $10^{-5}$ per crossing time. To find shadows, we use an algorithm described in, optimized to run between two and three orders of magnitude faster. Called iterative refinement, we use the same integrator as the noisy trajectory with tighter tolerance to estimate the full phase-space vector of local errors of the noisy trajectory, and then use a Newton-like correction to refine the trajectory until it has local errors as small as possible. For simple systems, the errors of the refined trajectory can be as small as the machine precision ($10^{-16}$), but the minimum local error achievable with refinement increases as the number of dimensions increases, due to numerical errors in computing the Newton corrections. A trajectory produced by refinement is called a numerical shadow. The existence of a numerical shadow is expected to indicate the existence of an exact shadow of comparable duration.

A system with parameters $N = 100$, $M = 1$, $\varepsilon = 0$ was first shadowed by, who found that the single particle can be shadowed for a few tens of crossing times, and that glitches (the point beyond which a shadow cannot be found) tend to occur more frequently during close approaches with other particles. Combined with the fact that close approaches occur as a stochastic process, we hypothesized that glitches also occur as a stochastic process. Fig. 1 shows a histogram of shadow durations for 1000 $M = 1$ systems. The distribution is well-fit by an exponential curve, suggesting that glitches are encountered as a Poisson process in an unsoftened system.

![FIG. 1: Histogram of shadow durations of 1000 unsoftened gravitational $n$-body systems. Each system has 99 fixed particles and one moving particle. Noisy orbits have local error of about $10^{-5}$ per crossing time; numerical shadows were required to have a maximum local error no bigger than $10^{-14}$. The horizontal axis is in crossing times; the vertical axis is the measured probability density. The distribution fits an exponential curve with a mean glitch rate of about 0.07 per crossing time, indicating that the moving particle encounters glitches as a Poisson process in an unsoftened system.](image)

The robustness of our shadowing algorithm with increasing problem dimension was tested in two ways. First, we contrived a slightly nonlinear Hamiltonian system designed to be easily shadowable (i.e., almost hyperbolic), and successfully shadowed it for 20–50 Lyapunov times on average while the dimension was increased from 2 to 180. Second, we searched for shadows of gravitational systems similar to the above consisting of $99 + M$ particles in which the $M$ moving particles interact only with the 99 fixed particles. Such a system is equivalent to superimposing $M$ uncoupled single-particle systems, and it will encounter glitches as a Poisson process with an aggregate rate $M$ times that of a single-particle system. This results in average shadow durations that scale as $1/M$. This was in fact observed in our simulations, giving us confidence that our shadowing algorithm works as well for large $M$ as it does for small $M$.

Fig. 2 demonstrates that the scaling is still $1/M$ even if the $M$ moving particles interact. This is moderately surprising because it suggests that although particles interact in motion, they do not interact in glitching. A possible explanation is that if $1 < M \ll N$, then the coupling between the $M$ moving particles is weak on average and we can still view the system as the superposition of $M$ single-particle systems. Furthermore, we note...
numerical shadow was required to have a maximum error of $10^{-5}$ per crossing time; each numerical shadow was required to have a maximum error of $10^{-12}$. The points represent sample shadow durations, 30 samples each for $M = 1, 2, \ldots, 19, 20, 25$ and 10 samples each for $M = 30, 35, \ldots, 50$. The “coupled average” line joins their averages, while $55/M^{0.9}$ and $55/M^{1.1}$ are plotted for comparison. The “coupled average” line is statistically indistinguishable from the “uncoupled average” one in which the gravitational interaction between moving particles is deleted, which both validates the robustness of our shadowing algorithm for large $M$, and suggests that even coupled particles encounter glitches independently of one another.

systems in which softening has been set to $\varepsilon = 0.1$, which is approximately half the average inter-particle separation. The differences from Fig. 2 are quite marked. First, the distribution is peaked near 100 crossing times and has a long tail going out to hundreds of crossing times. Second, even though the local errors of the noisy and shadow orbits are identical to those from Fig. 2, the average shadow length has increased by more than an order of magnitude from 14 to 218. Although this is roughly equivalent to the increase in the Lyapunov timescale \cite{10}, the distribution is far from exponential. In fact, the most striking difference from Fig. 2 is that the distribution has a vanishingly small density near zero shadow duration, in striking contrast to a Poisson process. In other words, virtually no particles undergo glitches until several tens of crossing times have occurred. If this remains true even for $M > 1$, then shadowing of softened gravitational systems would be feasible even for large $M$, because the trajectories of all particles in the simulation would remain valid for many crossing times. This question is addressed in Fig. 4, where we plot the average shadow duration for softened systems as a function of $M$, along with the shadow duration predicted by superimposing $M$ single-particle systems. We see that although the duration of shadows for coupled systems decreases as $M$ increases, they decrease much more slowly than $1/M$, and appear to be levelling off at about 50 crossing times. This is consistent with superimposing single-particle trajectories all of which have shadows that last several tens of crossing times, although it is surprising that the shadow durations are slightly longer than that predicted by superimposing single-particle trajectories. Now, if particles

that the cross-section for close approaches is not altered as $M$ increases (which simply changes fixed particles into moving ones), so the argument still holds independent of whether $M \ll N$.

With non-zero softening, \cite{10} found that shadow durations increased significantly, while the correlation between glitches and close approaches decreased. Fig. 3 shows the distribution of shadow durations for 250 $M = 1$
encounter glitches largely independently of one another, and shadow durations for softened systems are long for most particles, then we can hypothesize that reasonable statistical results may be acquired from long simulations of large softened systems as long as only a small number of particles have undergone glitches, and the statistics taken depend on large numbers of particles. Thus, for example, the global spatial distribution of matter in a simulated galaxy may be correct, but the number of escapers from a simulated globular cluster may be incorrect if the stars that escape happen also to be the stars that underwent glitches before escaping.

The difference between the shadow durations for softened vs. unsoftened systems undoubtedly is related to fluctuating Lyapunov exponents as discussed in [1, 2, 3]. Although we have not measured Lyapunov exponents explicitly, we measured a related quantity, namely the expansion and contraction factors across a timestep of the vectors that span the locally expanding and contracting spaces. In a uniformly hyperbolic system, these factors will always be greater and less than 1, respectively. An event of “non-hyperbolicity” can be observed by looking for areas along the trajectory where directions which were previously expanding over long periods instead start to contract, or vice versa. If we plot the expansion and contraction amounts along a trajectory, we find that “non-hyperbolic” events correlate well with the occurrence glitches [2]. If we plot an $M = 1$ particle orbit in three dimensions, we also observe that these events loosely correlate with times when the particle’s orbital geometry changes in an obvious way. We postulate that the locally expanding and contracting directions of a particle in the system are closely related to the geometry of the particle’s orbit, so that changing the geometry of the orbit can cause these local vectors to become inconsistent as time progresses. In an unsoftened system, the geometry of a particle’s orbit can be suddenly and violently changed by a close encounter. In softened systems, however, there is no precise, short-duration “event” which triggers non-hyperbolicity; instead, the geometry of the orbit of a particle changes slowly, so that many crossing times occur before a glitch is likely. This helps to explain Figs. 1 and 2.

In conclusion, we postulate that there is no feasible integration accuracy which will produce long shadows in unsoftened gravitational $n$-body simulations. This does not necessarily mean that such simulations should not be trusted, only that shadowing may be too stringent a measure of error. In contrast, we believe that there does exist a feasible integration accuracy for which softened systems are shadowable for many crossing times even for large $n$. Given the stark dependence of shadow duration on the softening parameter, however, we suspect that until a better understanding is acquired, the shadowability of physical simulations in general will need to be decided on a case-by-case basis.

The author’s software [7] is available on request.

Acknowledgments: We thank Scott Tremaine, Ken Jackson, and James Yorke for thoughtful discussions on this work, and the University of Toronto’s Computing Disciplines Facility for cluster computer time. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada, and the Information Technology Research Centre of Ontario.

[1] S. Dawson, C. Grebogi, T. Sauer, and J. A. Yorke, Physical Review Letters 73, 1927 (3 Oct 1994).
[2] T. Sauer, C. Grebogi, and J. A. Yorke, Physical Review Letters 79, 59 (7 July 1997).
[3] T. D. Sauer, Physical Review E 65, 036220 (2002).
[4] J. D. Farmer and J. J. Sidorowich, Physica D 47, 373 (1991).
[5] S. T. Fryska and M. A. Zohdy, Physics Letters A 166, 340 (1992).
[6] R. M. Corless, Computers Math. Appl. 28, 107 (1994).
[7] D. V. Anosov, Proc. Steklov Inst. Math 90, 1 (1967).
[8] R. Bowen, Journal of Differential Equations 18, 333 (1975).
[9] C. Grebogi, S. M. Hammel, J. A. Yorke, and T. Sauer, Physical Review Letters 65, 1527 (1990).
[10] G. D. Quinlan and S. Tremaine, Monthly Notices of the Royal Astronomical Society 259, 505 (1992).
[11] B. A. Coomes, H. Koçak, and K. J. Palmer, Numerische Mathematik 69, 401 (1995).
[12] W. B. Hayes, Ph.D. thesis, Department of Computer Science, University of Toronto (2001).
[13] Y.-C. Lai, D. Lerner, K. Williams, and C. Grebogi, Physical Review E 60, 5445 (1999).
[14] D. C. Heggie and R. D. Mathieu, in The Use of Supercomputers in Stellar Dynamics, edited by P. Hut and S. L. W. McMillan (Springer-Verlag, 1986), pp. 233–235.
[15] A. C. Hindmarsh, ACM-SIGNUM Newsletter 15, 10 (1980).
[16] L. Spitzer Jr., Dynamical Evolution of Globular Clusters, Princeton series in astrophysics (Princeton University Press, 1987).
[17] W. Hayes, Master’s thesis, Dept. of Computer Science, University of Toronto (1995).
[18] J. Wisdom and M. Holman, The Astronomical Journal 104, 2022 (1992).
[19] This question is not unique to shadowing. For example, even though a symplectic integrator applied to a Hamiltonian problem exactly solves a nearby Hamiltonian problem [12], we could ask if the exactly solved problem is typical of nearby Hamiltonian problems of interest.
[20] The weak coupling assumption is broken when a close approach between two moving particles occurs, but since it is likely to cause a glitch anyway, and our argument need only apply until a glitch occurs, the assumption holds during the time interval we need it to hold.
[21] Note that we did not observe any obvious neutral directions, which is moderately surprising given that Hamiltonian systems are not hyperbolic.
shadow duration

uncoupled average

coupled average

indiv. samples

\( 55/\times 0.9 \)

\( 55/\times 1.1 \)
probability density

shadow duration of 1 particle, softened potential

binsize 5
shadow duration

number of moving particles M, softened potential

coupled average
indiv. samples
450/M^{0.7}
probability density

shadow duration of 1 particle, softened potential

binsize 12.5
shadow duration

number of moving particles $M$, softened potential

- indiv. samples
- coupled average
- overlay average
shadow duration

number of moving particles M, unsoftened potential

coupled average

indiv. samples

55/M^0.9

55/M

55/M^1.1
probability density

shadow duration of 1 particle, local error 1e-12

binsize 5
Probability density of shadow duration of 1 particle, unsoftened potential.

- Binsize 2.5
- Binsize 1.25
- $0.07 \exp(-0.07 \cdot M)$