A Combinatorial Dynamics Simulation in Python

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1 Introduction

Recursion relations arise naturally in many contexts. One such can be called combinatorial, since the recursion relation is for a sequence of generating functions which enumerate a collection of objects. We study here a combinatorial recurrence relation arising from enumeration problems for four-valent maps, see for example [BDFG03]. This same recurrence relation also arises naturally in the setting of recurrence coefficients for orthogonal polynomials, see [Dei99] for a general reference, and [Erc11] for results on the asymptotics for these coefficients. We will here ignore the map setting, and will very briefly give the orthogonal polynomial setting as we will use it to derive several important elements for the dynamics. In these notes we reproduce and extend a setting described by Van Assche [VA07].

The recursion relation which we will study for the sequence $\{x_n\}$ is nonlinear, three-term, and time-dependent:

$$4tx_n\left(x_{n+1}+x_n+x_{n-1}\right)+\zeta x_n=\frac{n}{N}.$$

Thinking of x_n as the state of a system at time n, we see that the state at the future time $n+1$ depends upon the current (time n) state of the system as well as the immediate past (time $n-1$) state. A differential equation with time delay is often cast as a higher-order equation without the time delay, and we employ a similar trick here to transform the 1-D system with time delay into a 2-D system in which the state at the next time depends only upon the state at the current time.

Thus the recursion relation, re-cast as a two-dimensional system of nonlinear, time-dependent equations in which each step depends only on the single previous step, can be studied as a discrete dynamical system. The problem then begs to be put on a computer and investigated.

We created a simulation in Python 2 which will calculate and plot the orbit of the system, given any initial conditions. Due to the nature of the system, which has a hyperbolic fixed point and therefore exponential growth of error near this fixed point, the system is actually rather bad to calculate numerically, so verification of the results is especially important for this problem. The integrability of the system and known asymptotic results are essential here.

Section 2 of these notes contains the mathematics of interest, while section 3 describes the numerical simulation and gives a few results, as well as a discussion of the numerical instability of the problem.

2 Mathematical Background

2.1 Orthogonal polynomial setting

Consider the family of orthonormal polynomials $p_n(x) = \gamma_n x^n + \dots$ for positive γ_n with respect to the weight

$$w_\zeta(x) = \exp\left(-N\left(\frac{\zeta}{2}x^2 + tx^4\right)\right), \tag{1}$$

so that

$$\int p_n(x)p_m(x)w_\zeta(x)dx = \delta_{nm}$$

for $n, m \geq 0$. These polynomials satisfy the recurrence relation

$$xp_{n,N}(x) = b_{n+1,N}p_{n+1}(x) + a_{n,N}p_n(x) + b_{n,N}p_{n-1}(x)$$

for $n \geq 0$ and $p_{-1} = 0$. Since the weight is even, the recurrence coefficients $a_{n,N}$ are all zero, and so the family of orthogonal polynomials is entirely defined by the recurrence coefficients $b_{n,N}$. It turns out that these coefficients satisfy a recurrence of their own:

$$4tb_{n,N}^2\left(b_{n+1,N}^2 + b_{n,N}^2 + b_{n-1,N}^2\right) + \zeta b_{n,N}^2 = \frac{n}{N}.$$

2.2 The generalized recursion

Letting $x_n := b_n^2$ (suppressing for now that x_n depends upon N, though it clearly does), we will study the recursion

$$4tx_n\left(x_{n+1} + x_n + x_{n-1}\right) + \zeta x_n = \frac{n}{N}, \tag{2}$$

where t and ζ are parameters (and we will think for now of N as another parameter). The parameter ζ mediates between a purely quartic potential ($\zeta = 0$) and a mixed potential ($\zeta \neq 0$). In particular, the mixed potential case $\zeta = 1$ is a perturbation (for small positive t) of a Gaussian potential and of interest in relation to the map enumeration problems mentioned earlier.

2.3 Comparison to Van Assche

The recursion (2) is studied in [VA07] under slightly different setting and scaling. Van Assche's work stems from a measure

$$w_\rho(x) = |x|^\rho \exp\left(-|x|^m\right)$$

for $\rho > -1$ and $m > 0$. In the case $\rho = 0$ he studies the purely quadratic and the purely quartic cases, and comments that the potential could quite easily be extended to mix these cases. However, for Van Assche's work it is convenient to absorb the 4 in the recursion (2) into the definition of the x_n by defining $x_n = 2b_n^2$. We prefer to leave this constant factor as is, and therefore any of our comparisons to his work differ by a constant.

2.4 The dynamical system formulation

The trick to eliminate time delay by adding a dimension is to define $y_n = x_{n-1}$. Then (2) can be rewritten as the 2-D discrete dynamical system

$$x_n = \frac{n-1}{4tNx_{n-1}} - \frac{\zeta}{4t} - x_{n-1} - y_{n-1} \tag{3a}$$

$$y_n = x_{n-1}. \tag{3b}$$

Notice that the system is time (n) dependent, so one can also view it as three-dimensional.

The initial condition for the system is given as $(x_1, y_1) = (x_1, x_0)$. The system can, of course, be studied for any given initial condition, but the orthogonal polynomial setting gives a specific initial condition to study.

2.5 Initial conditions

The appropriate initial conditions for the orthogonal polynomial recurrence coefficients are $x_0 = 0$ and $x_1 = \dfrac{c_2}{c_0}$ where $c_j = \displaystyle\int x^j w_\zeta(x)dx$ is the j^{th} moment of the measure. The latter is derived from the first equation for the orthogonal polynomials

$$xp_0(x) = b_1 p_1(x) + 0 + b_0 p_{-1}(x)$$

$$x\gamma_0 = b_1 p_1(x)$$

by requiring that $p_1(x) = \dfrac{x\gamma_0}{b_1}$ has norm 1. We then have

$$\begin{aligned}\int p_1(x)p_1(x)w_\zeta(x)dx &= \int \left(\frac{x\gamma_0}{b_1}\right)^2 w_\zeta(x)dx \\ &= \frac{\gamma_0^2}{b_1^2}\int x^2 w_\zeta(x)dx \\ &= 1\end{aligned}$$

so that

$$x_1 = b_1^2 = \gamma_0^2 \int x^2 w_\zeta(x)dx.$$

To discover γ_0 we similarly require that $p_0(x) = \gamma_0$ has norm 1:

$$\begin{aligned}\int p_0(x)p_0(x)w_\zeta(x)dx &= \int \gamma_0^2 w_\zeta(x)dx \\ &= \gamma_0^2 \int w_\zeta(x)dx \\ &= 1\end{aligned}$$

so $\gamma_0^2 = \dfrac{1}{\int w_\zeta(x)dx}$ and thus

$$x_1 = \frac{\displaystyle\int x^2 w_\zeta(x)dx}{\displaystyle\int w_\zeta(x)dx}.$$

2.6 Long-time asymptotics

The leading order behavior of this recursion for large n is

$$x(n) = \frac{-\zeta + \sqrt{\zeta^2 + 48tn/N}}{24t}, \tag{4}$$

so for large n we expect to see $x_n \sim x(n)$.

2.7 Integrability

The recursion (2) satisfies the *discrete Painlevé property*, also known as *singularity confinement*: if x_n is such that it results in a singularity for x_{n+1}, then there exists a $p \in \mathbb{N}$ such that this singularity is confined to $x_{n+1}, \ldots, x_{n+p}$. Furthermore, x_{n+p+1} depends only on x_{n-1}, x_{n-2}, ... (definition from [VA07]).

To verify this property, we let $x_n = \epsilon$ and expand successive terms in a Laurent series in ϵ. Working from

$$x_{n+1} = \frac{n}{4tNx_n} - \frac{\zeta}{4t} - x_n - x_{n-1},$$

we have:

$$\begin{aligned}
x_n &= \epsilon \\
x_{n+1} &= \frac{n}{4tN\epsilon} - x_{n-1} - \frac{\zeta}{4t} - \epsilon \\
x_{n+2} &= -\frac{n}{4tN\epsilon} + x_{n-1} + \frac{n+1}{n}\epsilon + \mathcal{O}(\epsilon^2) \\
x_{n+3} &= -\frac{n+3}{n}\epsilon + \mathcal{O}(\epsilon^2) \\
x_{n+4} &= \frac{n}{n+3}x_{n-1} - \frac{\zeta}{2t(n+3)} + \mathcal{O}(\epsilon).
\end{aligned}$$

Looking at the Laurent expansion, one can see that if x_n is 0 then x_{n+1} and x_{n+2} are singularities with opposite signs, x_{n+3} vanishes again, and x_{n+4} has so fully recovered from the blow-up that it depends only on x_{n-1} (and, of course, n and the parameters in the system). This property is an indicator of integrability.

We define the time-dependent Hamiltonian (is this truly a Hamiltonian??)

$$f_n(x, y) = xy(\zeta + 4tx + 4ty) - \frac{n}{N}x - \frac{n}{N}y. \tag{5}$$

Then the difference of this function evaluated at two successive points in the orbit $(x_{n+1}, y_{n+1}) = (x_{n+1}, x_n)$ and $(x_n, y_n) = (x_n, x_{n-1})$, both at the "same time" n, is

$$f_n(x_{n+1}, x_n) - f_n(x_n, x_{n-1}) = 0$$

and by evaulating the function on the same two points but at the "right" times n and $n-1$, we see

$$f_n(x_{n+1}, x_n) - f_{n-1}(x_n, x_{n-1}) = -\frac{1}{N}\left(x_n + x_{n-1}\right).$$

The calculations of these facts follow:

$$\begin{aligned}
f_n(x_{n+1}, x_n) - f_n(x_n, x_{n-1}) &= x_{n+1}x_n(\zeta + 4tx_{n+1} + 4tx_n) - \frac{n}{N}x_{n+1} - \frac{n}{N}x_n \\
&\quad - x_nx_{n-1}(\zeta + 4tx_n + 4tx_{n-1}) + \frac{n}{N}x_n + \frac{n}{N}x_{n-1} \\
&\quad + 4tx_{n+1}x_nx_{n-1} - 4tx_{n+1}x_nx_{n-1} \\
&= (x_{n+1} - x_{n+1})\left(\zeta x_n - \frac{n}{N} + 4tx_n(x_{n+1} + x_n + x_{n-1})\right) \\
&= 0
\end{aligned}$$

and

$$\begin{aligned}
f_n(x_{n+1}, x_n) - f_{n-1}(x_n, x_{n-1}) &= x_{n+1}x_n(\zeta + 4tx_{n+1} + 4tx_n) - \frac{n}{N}x_{n+1} - \frac{n}{N}x_n \\
&\quad - x_nx_{n-1}(\zeta + 4tx_n + 4tx_{n-1}) + \frac{n-1}{N}x_n + \frac{n-1}{N}x_{n-1} \\
&= \zeta x_{n+1}x_n + 4tx_{n+1}x_{n+1}x_n + 4tx_{n+1}x_nx_n + 4tx_{n+1}x_nx_{n-1} \\
&\quad - \zeta x_nx_{n-1} - 4tx_nx_nx_{n-1} - 4tx_nx_{n-1}x_{n-1} - 4tx_{n+1}x_nx_{n-1} \\
&\quad - \frac{n}{N}x_{n+1} - \frac{1}{N}x_n + \frac{n-1}{N}x_{n-1} \\
&= x_{n+1}(\zeta x_n + 4tx_{n+1}x_n + 4tx_nx_n + 4tx_nx_{n-1}) - \frac{n}{N}x_{n+1} \\
&\quad - x_{n-1}(\zeta x_n + 4tx_nx_n + 4tx_nx_{n-1} + 4tx_nx_{n+1}) + \frac{n}{N}x_{n-1} \\
&\quad - \frac{1}{N}\left(nx_{n+1} + x_n + (n-1)x_{n-1}\right) + \frac{n}{N}x_{n+1} - \frac{n}{N}x_{n-1} \\
&= (x_{n+1} - x_{n-1})\left(\zeta x_n - \frac{n}{N} + 4tx_n(x_{n+1} + x_n + x_{n-1})\right) \\
&\quad - \frac{1}{N}\left(x_n + x_{n-1}\right) \\
&= -\frac{1}{N}\left(x_n + x_{n-1}\right).
\end{aligned}$$

3 The Python simulation

3.1 Input

The input to a simulation comes in three categories: system constraints that have to do with the numerical precision, parameters occurring in the mathematical problem, and initial conditions for the dynamical system.

- *dps* is a system constraint: the Python package mpmath [J+13] allows floating point arithmetic to be made arbitrarily precise. The *dps* is number of decimal places to which each arithmetic calculation will be rounded.
- n_{max} is a system constraint: it is the largest value of n for which x_n will be calculated. To ensure numerical accuracy of the simulation, n_{max} and the *dps* must be balanced, with the decimal precision high enough to allow the simulation to survive the desired length of time.

- ζ is a mathematical parameter: its main function is to mediate between the purely quartic and mixed potential cases.
- t is a mathematical parameter: for the mixed potential case it should be small so that the potential is a perturbation of a Gaussian.
- N is a mathematical parameter: it appears in the potential and is to be generally considered a large parameter. In the literature (e.g. [Erc11]) generally N is taken to be on the same order as n so that in the limit $n, N \to \infty$ their ratio is fixed and nonzero. However, N can also be ignored by fixing it (e.g. [VA07]). In the interplay between *dps* and n_{max}, the larger N is taken for a fixed n_{max}, the greater the decimal precision must be for the simulation to survive.
- x_1 and $y_1 = x_0$ are the initial conditions for the dynamical system: the pair (x_1, y_1) can be specified anywhere in the plane. Alternatively, the initial condition can be taken to be the one appropriate for the orthogonal polynomial setting.

3.2 The recursion and diagnostic calculations

The recursion itself runs: for $2 \leq n \leq n_{max}$, the previously-calculated values

$$x_{n-1}$$
$$x_{n-2}$$

are recalled and then used to compute

$$x_n = \frac{n-1}{4tx_{n-1}} - \frac{\zeta}{4t} - x_{n-1} - x_{n-2}.$$

Next, several diagnostic calculations are performed. To use our knowledge of the asymptotic behavior of the system, we calculate the values

$$x(n) = \frac{-\zeta + \sqrt{\zeta^2 + 48tn}}{24t}$$

for $0 \leq n \leq n_{max}$. Using our knowledge of integrability, the values

$$f_n(x_{n+1}, x_n) - f_n(x_n, x_{n-1})$$

and

$$f_n(x_{n+1}, x_n) - f_{n-1}(x_n, x_{n-1})$$

are calculated for $0 \leq n \leq n_{max}$.

3.3 Output

The simulation results are given as five figures, the first two images of the orbit and the last three to be used as diagnostics to determine whether or not the simulation is accurate over the whole run.

- 3D orbit plot: the 2D time-dependent system (3) is plotted on three axes, (n, x_n, y_n), with time n on one axis.
- 2D projection of orbit plot: the orbit plot is projected onto the (x_n, y_n) plane.
- Diagnostic plot of asymptotic behavior: x_n and $x(n)$ are plotted against n, the first as a set of discrete data points and the latter as a continuous function of n. For large enough values of n, the data points x_n should lie on the curve since $x_n \sim x(n)$.
- Diagnostic plot #1 from integrability: $|f_n(x_{n+1}, x_n) - f_{n-1}(x_n, x_{n-1})|$ and $\left|\frac{x_n + x_{n-1}}{N}\right|$ are plotted against n in a log-lin plot, where the values x_n are all recursively-generated. Up to plotting precision, these two curves are the same. Furthermore, as long as the simulation is still valid, the resulting curve is smooth with the basic shape $\sqrt{n}$.
- Diagnostic plot #2 from integrability: $|f_n(x_{n+1}, x_n) - f_n(x_n, x_{n-1})|$ is plotted against n. As this difference is known to be 0, the plot should show all function values to be a figment only of the numerical precision. Thus, all function values should be smaller than 10^{-dps}, due only to rounding error in the final decimal place.

3.4 Some results

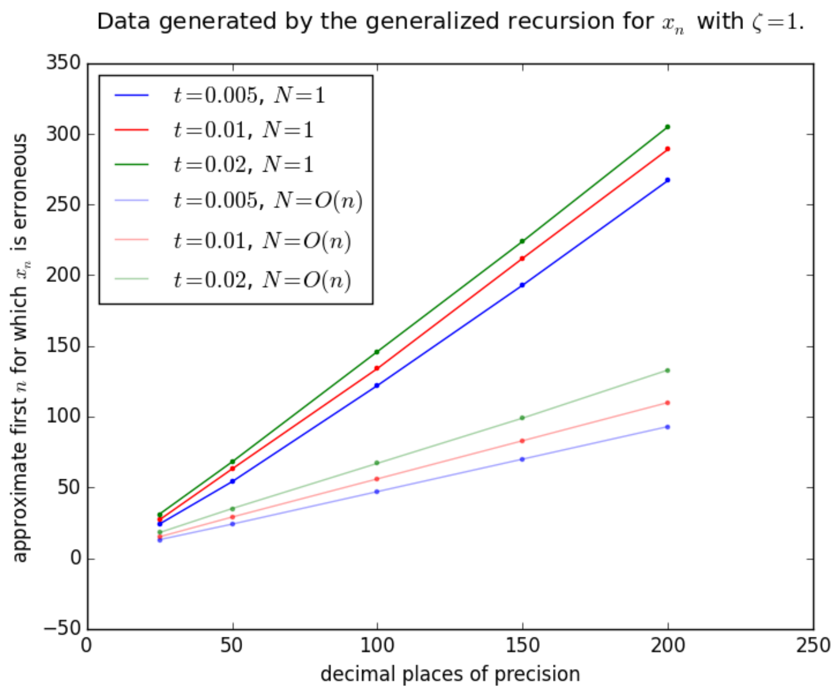
Figure 1 is a simulation of the purely quartic potential, as studied in [VA07]. In particular, Figure 1c is a plot given in that paper. In this case, $x(n) = \sqrt{n/12}$, so for large n we see x_n approaching $\sqrt{12} \approx 3.46$. This is verified in Figure 1b where the orbit (x_n, x_{n-1}) is approaching a point somewhere around $(3.5, 3.5)$.

Figure 2 shows the "typical" picture of a successful simulation in the mixed potential case, including the diagnostic plots which prove that the system was successfully investigated.

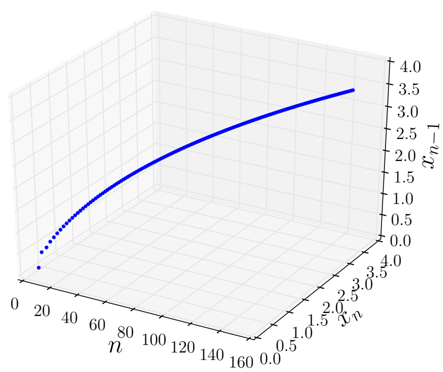
Figure 3 shows a simulation for which n_{max} was set too high. After a certain value of n, the behavior of the x_n's deviates from its asymptotic behavior.

3.5 Effect of decimal precision on survival of simulation

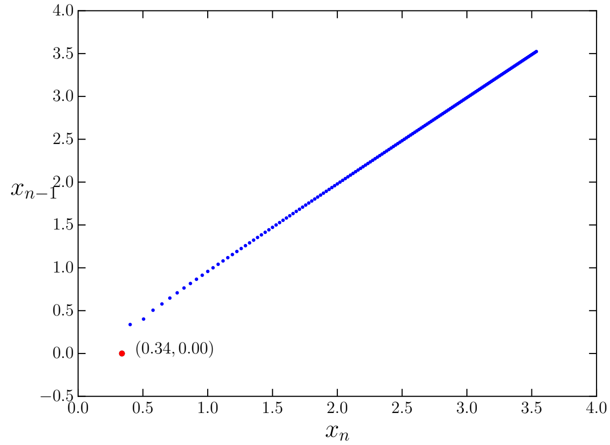
Finally, we include data gathered from many simulations regarding the numerical difficulty of this recursion. The three dark lines are for $N = 1$. We want to be able to look at the asymptotics for n and N of the same order, so the three lighter lines are for N on the same order as n. For these particular simulations, N was taken to be $12.5, 25, 50, 75$, and 100. These numbers were chosen to scale with the decimal precision, and in all cases the simulation barely survives to the order of N, or falls just short.


Data generated by the generalized recursion for x_n with $\zeta=1$.
$t=0.005,\ N=1$
$t=0.01,\ N=1$
$t=0.02,\ N=1$
$t=0.005,\ N=O(n)$
$t=0.01,\ N=O(n)$
$t=0.02,\ N=O(n)$
approximate first n for which x_n is erroneous
decimal places of precision
350
300
250
200
150
100
50
0
−50
0
50
100
150
200
250

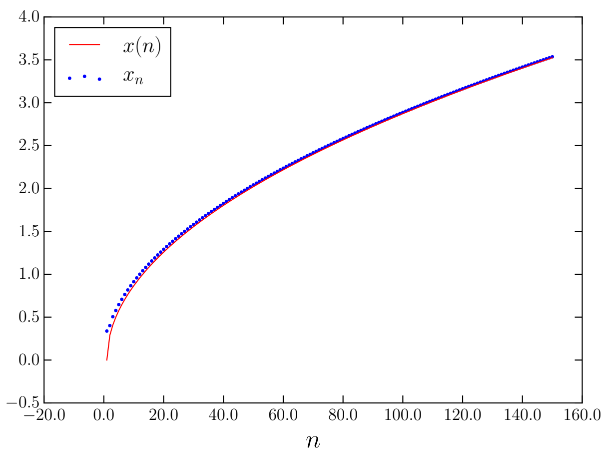
4 Appendix: Large figures



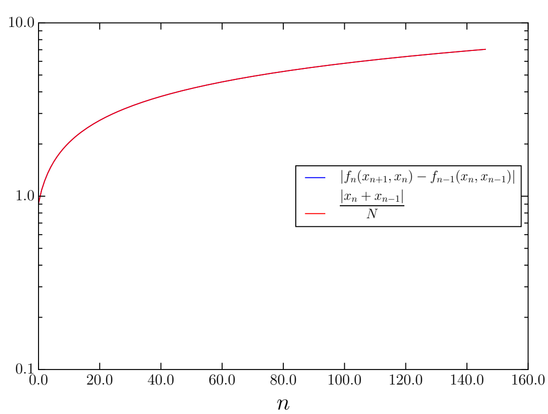
(a) 3D orbit



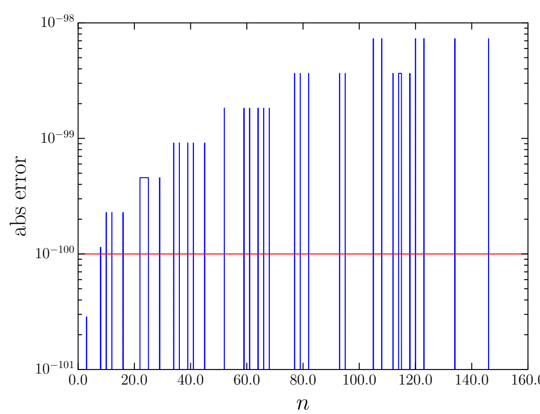
(b) 2D projection of orbit



(c) Diagnostic: asymptotics

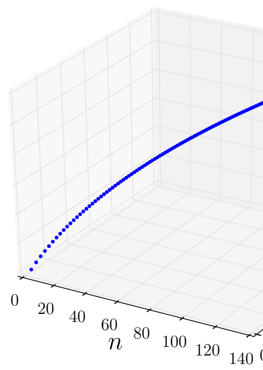


(d) Diagnostic: integrability #1

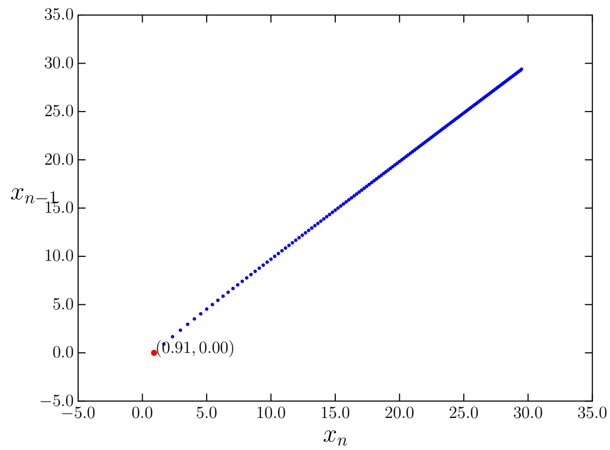


(e) Diagnostic: integrability #2

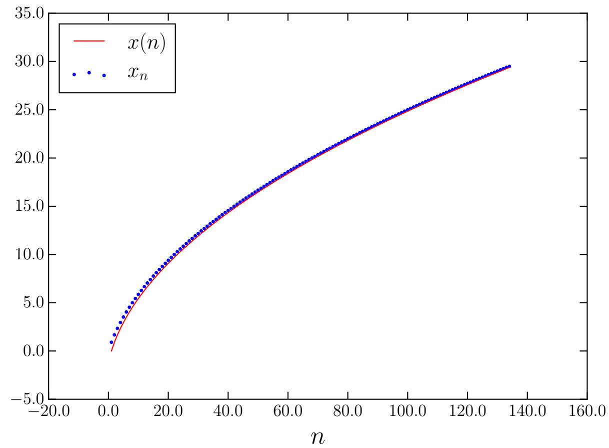
Figure 1: $dps = 100$, $\zeta = 0$, $t = 1$, $N = 1$, $n_{max} = 150$.



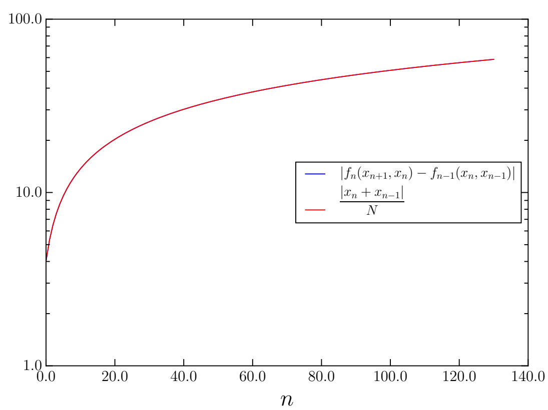
(a) 3D orbit



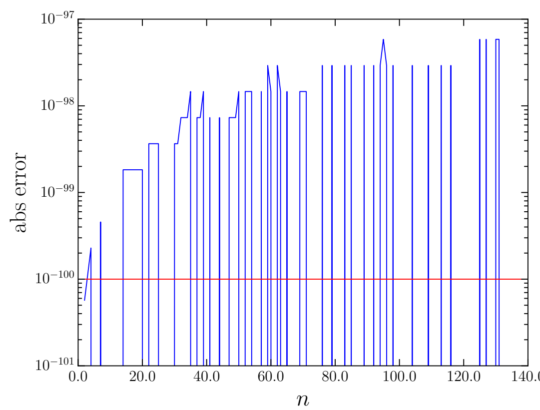
(b) 2D projection of orbit



(c) Diagnostic: asymptotics

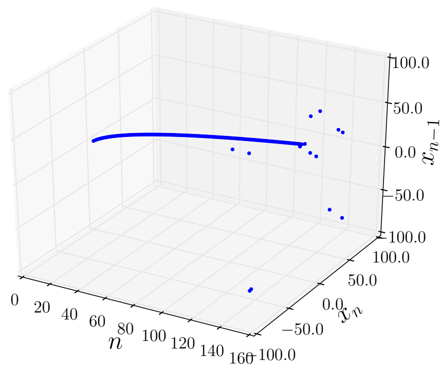


(d) Diagnostic: integrability #1

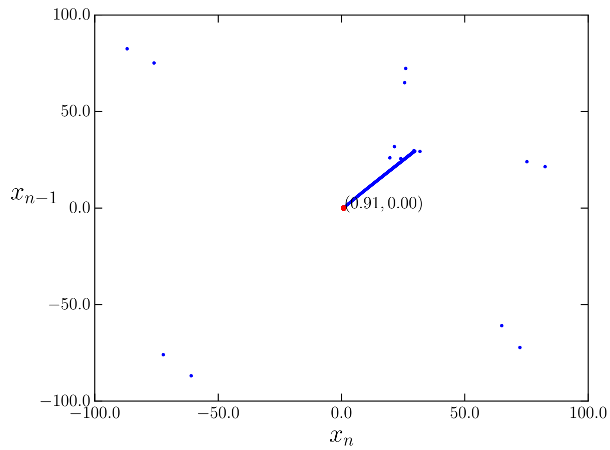


(e) Diagnostic: integrability #2

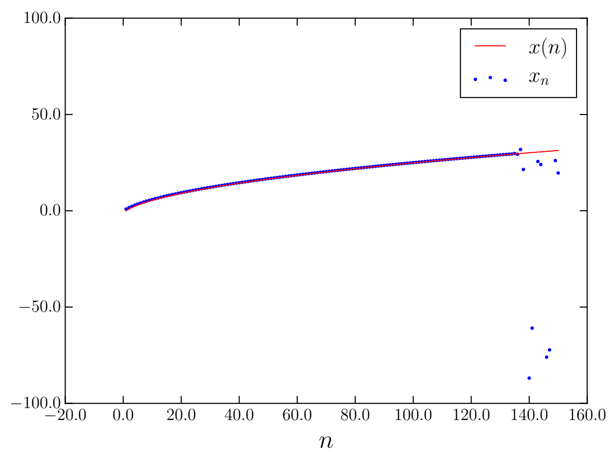
Figure 2: $dps = 100$, $\zeta = 1$, $t = 0.01$, $N = 1$, $n_{max} = 134$.



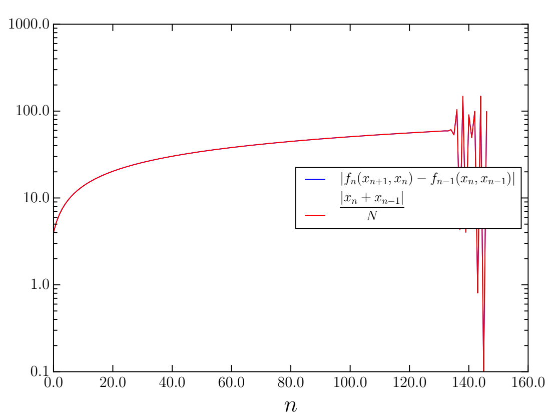
(a) 3D orbit



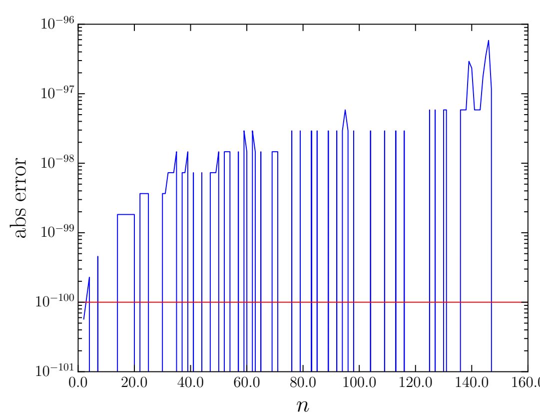
(b) 2D projection of orbit



(c) Diagnostic: asymptotics



(d) Diagnostic: integrability #1



(e) Diagnostic: integrability #2

Figure 3: Simulation: $dps = 100$, $\zeta = 1$, $t = 0.01$, $N = 1$, $n_{max} = 150$.

References

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