Deterministic Systems that Approximate Stochastic Processes: Analysis and Computation

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Outline

1. Motivation
2. Overview
3. White Noise from a System of Oscillators
4. Two Billiards in a Box
5. Conclusion

Motivation

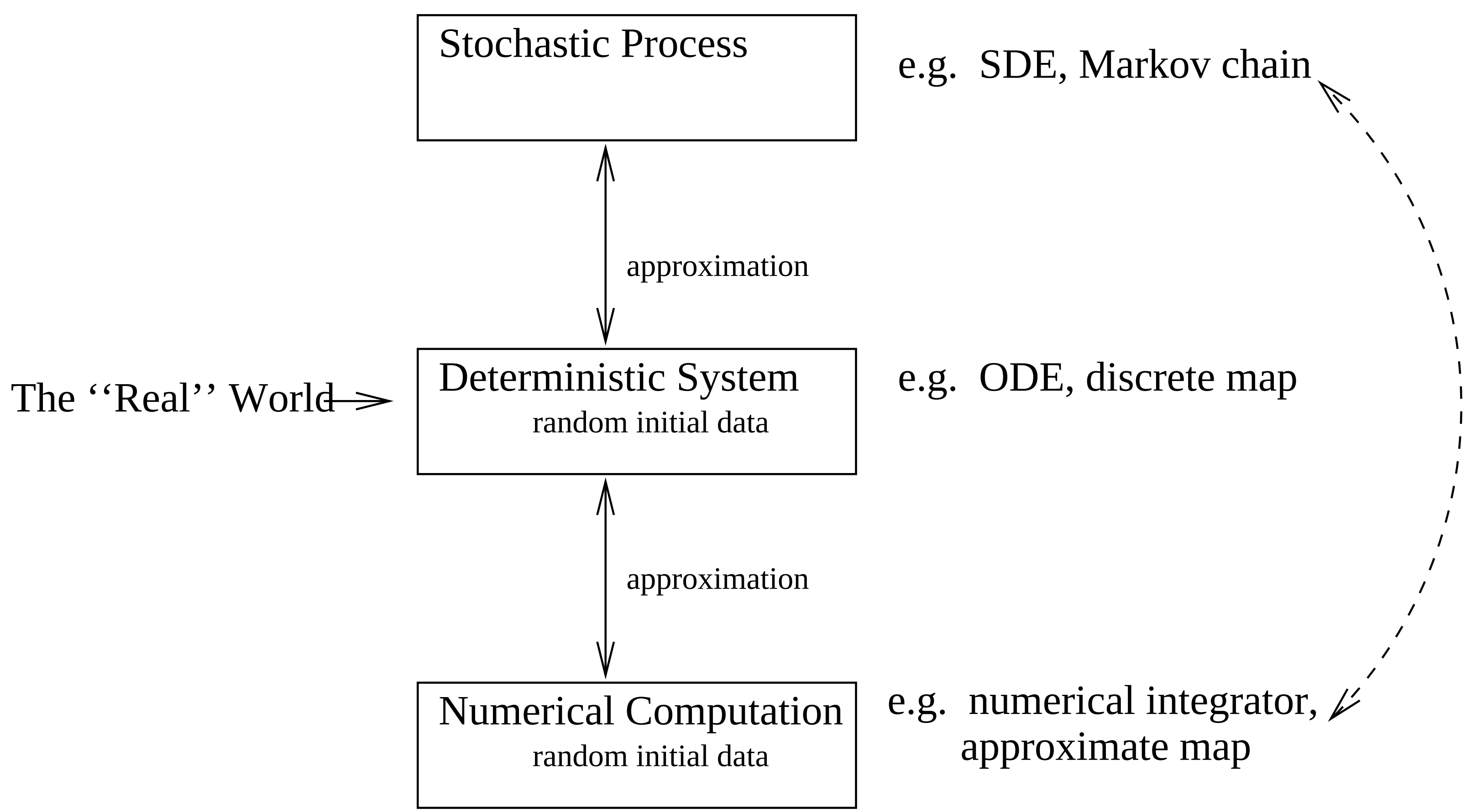
In Molecular Dynamics, physical systems are modelled by

- Deterministic ODEs
- Random Initial Conditions

Certain time-series are believed to be well approximated by stochastic processes

For Numerical Simulations of such systems

- No hope of approximating trajectories well
- Want to show that statistical properties are reproduced accurately


Stochastic Process
e.g. SDE, Markov chain
approximation
The ''Real'' World
Deterministic System
random initial data
e.g. ODE, discrete map
approximation
Numerical Computation
random initial data
e.g. numerical integrator,
approximate map

White Noise from a system of Linear Oscillators

Ref: Cano, Stuart, Suli, Warren (1999)

Suppose we take

$$\ddot{u}_j + j^2 u_j = 0$$

$$u_j(0) = a_j, \quad \dot{u}_j(0) = 0, \quad j = 0, \ldots, N.$$

Let

$$a_0 = \frac{1}{\sqrt{\pi}}\eta_0, \quad a_j = \sqrt{\frac{2}{\pi}}\eta_j, \quad j \geq 1,$$

where $\eta_j, j = 0, \ldots, N$, are independent $\mathcal{N}(0,1)$ r.v.'s.

We get that

$$H_N(t) := \sum_{j=0}^{N} u_j(t) = \sum_{j=0}^{N} a_j \cos(jt).$$

If we integrate $H_N(t)$ we get:

$$\int_0^t H_N(s)dt = \frac{1}{\sqrt{\pi}}\eta_0 t + \sum_{j=1}^{N} \sqrt{\frac{2}{\pi}}\eta_j \frac{1}{j}\sin(jt)$$

As $N \to \infty$ this converges to Brownian Motion uniformly on $[0, \pi]$ (Krylov 1995).

So we can imagine

$$H_N(t) \approx \dot{W}(t), \qquad \text{(white noise)}$$

Particle Driven by White Noise

Consider

$$\dot{z}_N = f(z_N) + H_N(t),$$

$$z_N(0) = z_0.$$

We expect solution of this to approximate solutions to SDE

$$dz = f(z)dt + dW,$$

$$z(0) = z_0,$$

on $[0, \pi]$.

Strong Results Cano, Stuart et al. proved for globally Lipschitz f

$$\|z(\cdot) - z_N(\cdot)\|^2_{L^2(0,T)} \leq \frac{C(T)}{N},$$

and

$$\sup_{t \in (0,T)} \mathbb{E}|z(t) - z_N(t)|^2 \leq \frac{C(T)}{N},$$

for $T \in [0, \pi]$.

Weak Result For sufficiently smooth g and $f \equiv 0$

$$\sup_{z_0 \in \mathbb{R}} |\mathbb{E}g(z(T)) - \mathbb{E}g(z_N(T))| \leq \frac{C}{N}$$

Numerical Analysis

Classical ODE Numerical Analysis: Integrate system of ODEs with time step Δt to get

$$Z_N^n \approx z_N(n\Delta t).$$

For fixed N, as $\Delta t \to 0$,

$$Z_N^n \to z_N(n\Delta t).$$

As Δt gets small enough, it is able to resolve the highest frequencies of the system.

However, we wish to integrate without resolving higher freqencies.

Consider limit

$$N \to \infty, \quad \Delta t \to 0, \quad N\Delta t = \zeta.$$

Prove that

$$Z_N^n \approx z(n\Delta t).$$

Numerical Integration

We solve for $u_j(t), j = 0, \ldots, N$ with the Verlet method:

$$U_j^{n+1} - 2U_j^n + U_j^{n-1} = 0,$$

$$U_j^0 = a_j, , \quad U_j^1 = a_j[1 - \alpha j^2 \Delta t^2],$$

for $\alpha \in [0, 1]$. This is a *symplectic method*: For each oscillator

- conserves phase space volume
- conserves quantity close to energy
- solution bounded for all n if $\zeta = N\Delta t \leq 2$.

We solve for $z_N(t), t \in [0, T]$ with

$$\begin{aligned} Z^{n+1} - Z^n &= \Delta t[\theta f(Z^{n+1}) + (1-\theta) f(Z^n)] \\ &+ \Delta t[\theta H_N^{\Delta t}(t^{n+1}) + (1-\theta) H_N^{\Delta t}(t^n)], \end{aligned}$$

the θ-method.

$\theta = 0$ — forward Euler

$\theta = 1$ — backward Euler

Let z^n denote solution of SDE at $n\Delta t$.

Cano, Stuart et al. show for $n\Delta t \in [0, T]$

$$\mathbb{E}\|z^n - Z^n\|^2 \leq C(T)\Delta t^{2/3}$$

and

$$|\mathbb{E}g(z^n) - \mathbb{E}g(Z^n)| \leq C(n\Delta t)\Delta t^{2/3}$$

for sufficiently smooth g and for linear f.

Advantages

- Can construct on same space as Brownian motion so strong convergence possible.
- Linear and explicitly solvable, can prove lots of things easily.

Shortcomings

- Integer freqencies unrealistic.
- Only valid on $[0, \pi]$.
- Relationship between particle and oscillators unrealistic.

More Realistic System: Heat Bath

Model due to Ford and Kac (1987). A linear Hamiltonian system:

$$\ddot{u}_j + j^2(u_j - q) = 0,$$

$$\ddot{q} + V'(q) = \sum_{j=1}^{N} \gamma^2 (u_j - q)$$

$$u_j(0) = \sqrt{\frac{2}{\pi}}\eta_j, \quad \dot{u}_j(0) = 0, \quad q(0) = q_0, \quad \dot{q}(0) = p_0,$$

where η_j are distributed as $\mathcal{N}(0,1)$.

When N large formally similar to

$$\ddot{Q} + \frac{\gamma^2 \pi}{2} \dot{Q} + V'(Q) - \frac{\gamma^2}{\pi} Q = \dot{W}$$

where

$$Q(0) = q_0, \qquad \dot{Q}(0) = p_0 - \frac{\gamma^2 \pi}{2} q_0,$$

and $W(t)$ is Brownian motion.

In fact, Stuart and Warren (1998) show that for any $T \in [0, \pi]$,

$$\mathbb{E}\{\|q - Q\|^2_{L_\infty(0,T)} + \|\dot{q} - \dot{Q}\|^2_{L_\infty(0,T)}\} \leq C(T) \frac{\ln N^2}{N}.$$

Computation

Solve for u_j as before, with $\alpha \in [0,1]$.

Solve for distinguished particle with parametrized method

$$q^{n+1} = q^n + \Delta t p^{n+\sigma_1},$$

$$p^{n+1} = p^n - \Delta t V'(q^{n+\sigma_2}) + \Delta t \gamma^2 \sum_{j=1}^{n} (U_j^{n+\theta} - q^{n+\phi})$$

where $\sigma_i, \theta, \phi \in [0,1]$.

Convergent method for all choices of parameters. However, only has the correct limiting SDE behaviour with $N\Delta t = \zeta$ if

$$\phi = \theta, \alpha = 1 - \theta.$$

Formally and experimentally verified, not proved rigourously.

Another Direction

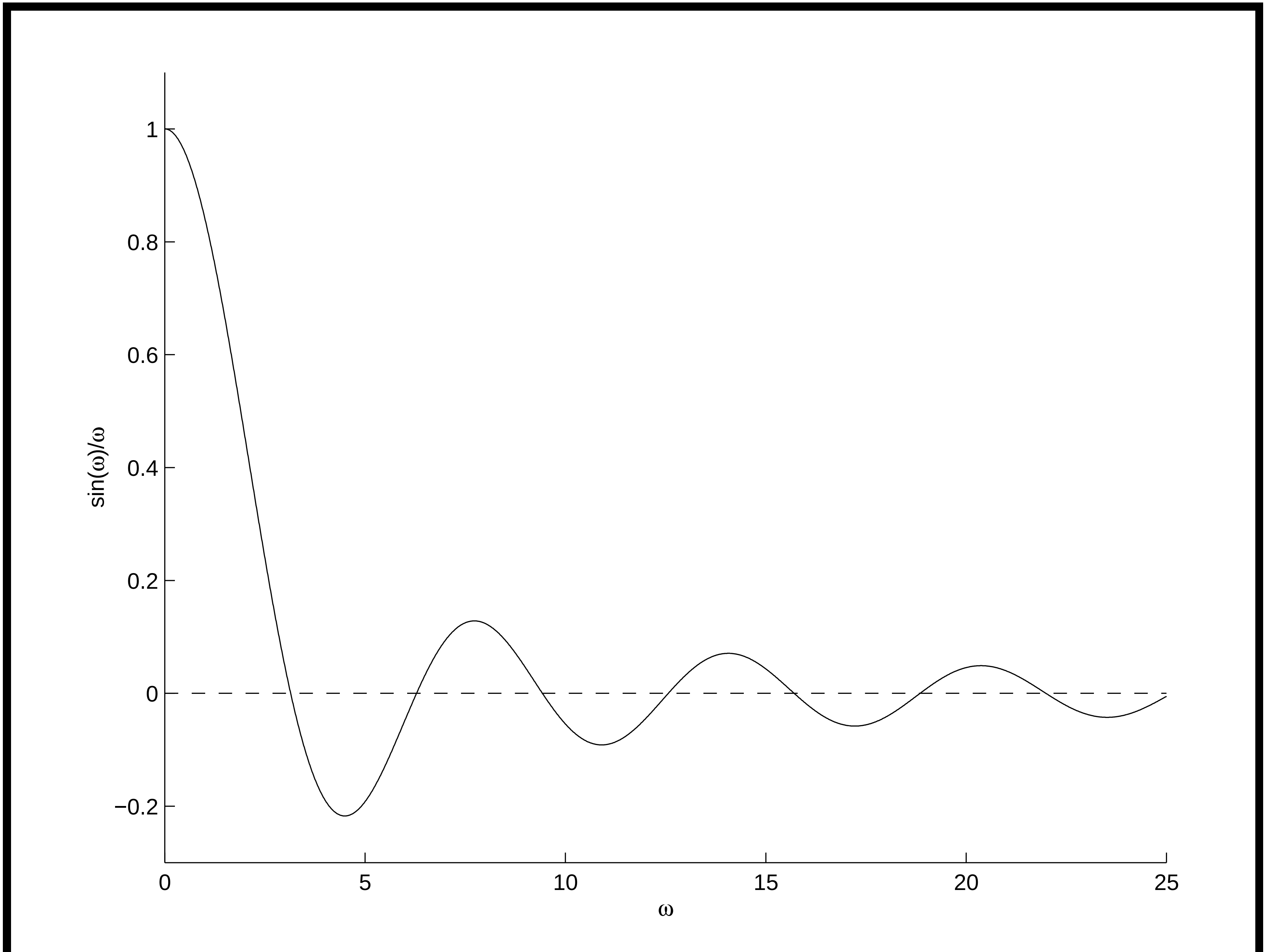
Previous examples depended on Fourier series representation of Brownian motion:

$$W(t) = \frac{1}{\sqrt{\pi}}\eta_0 t + \sum_{j=1}^{\infty} \sqrt{\frac{2}{\pi}}\eta_j \frac{\sin(jt)}{j}, \quad \text{on } [0, \pi].$$

However, we also have Fourier integral represention:

$$W(t) = \int_0^{\infty} \sqrt{\frac{2}{\pi}} \frac{\sin(\omega t)}{\omega} dW(\omega), \quad \text{on } [0, \infty).$$

We want to approximate this integral by system with a finite number of frequencies.


sin(ω)/ω
1
0.8
0.6
0.4
0.2
0
−0.2
0
5
10
15
20
25
ω

Sample at randomly selected frequencies with a random weight.

Approximate

$$W(t) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\sin(\omega t)}{\omega} dW(\omega)$$

with

$$W_n(t) = \sqrt{\frac{2}{\pi}} \sum_{m=1}^{n} \eta_m n^{-1/4} \frac{\sin(\omega_m t)}{\omega_m}$$

where $\eta_m \sim \mathcal{N}(0,1)$ and $\omega_m \sim \mathcal{U}[0, n^{1/2}]$.

Can show

$$W_n(t) \Rightarrow W(t) \quad \text{on } [0,T]$$

for any $T > 0$.

This means, for any bounded continuous $g : C[0,T] \to \mathbb{R}$:

$$\mathbb{E}g(W_n) \to \mathbb{E}g(W).$$

More general case

Let f satisfy some technical conditions.

If

$$I(t) = \int_0^\infty \sin(\omega t) f(\omega) dW(\omega)$$

and

$$I_n(t) = \sum_{m=1}^{n} \eta_m n^{-a/2} sin(\omega_m t) f(\omega_m)$$

where $\eta_m \sim \mathcal{N}(0,1)$, $\omega_m \sim \mathcal{U}[0, n^a]$ and $a \in (0,1)$ then

$$I_n \Rightarrow I \quad \text{ in } [0,T],$$

for all $T > 0$.

Note that as before, we can generate as solution to differential equations:

$$\ddot{u}_m + \omega_m u_m = 0,$$

$$u_m(0) = 0, \quad \dot{u}_m(0) = n^{-1/4}\eta_m \omega_m f(\omega_m), \quad m = 1, \dots, n,$$

setting

$$U_n(t) = \sum_{m=1}^{n} u_m(t).$$

Long Time Averages

We can now ask questions of series on $[0, \infty)$.

Consider approximation to Ornstein-Uhlenbeck Process:

$$U(t) = \int_0^\infty \frac{2}{\pi} \frac{\sin(\omega t)}{\sqrt{1+\omega^2}} dW(\omega)$$

with

$$U_n(t) = \sum_{m=0}^{n} \frac{2}{\pi} n^{-1/4} \eta_m \frac{\sin(\omega_m t)}{\sqrt{1+\omega_m^2}}.$$

Since U is ergodic and has normal invariant measure,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T g(U(t))dt = \mathbb{E} g(N)$$

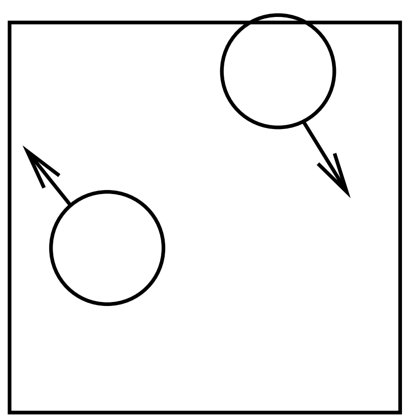
where N is normally distributed.

Question: Does $U_n(t)$ have same limiting property?

A Different System: Two Billiard in a Box

Consider a system of two discs moving in a two-dimensional box.

- No interaction when discs not touching
- Linear spring force if overlapping with each other or walls
- Hamiltonian system
- Conjectured to be ergodic



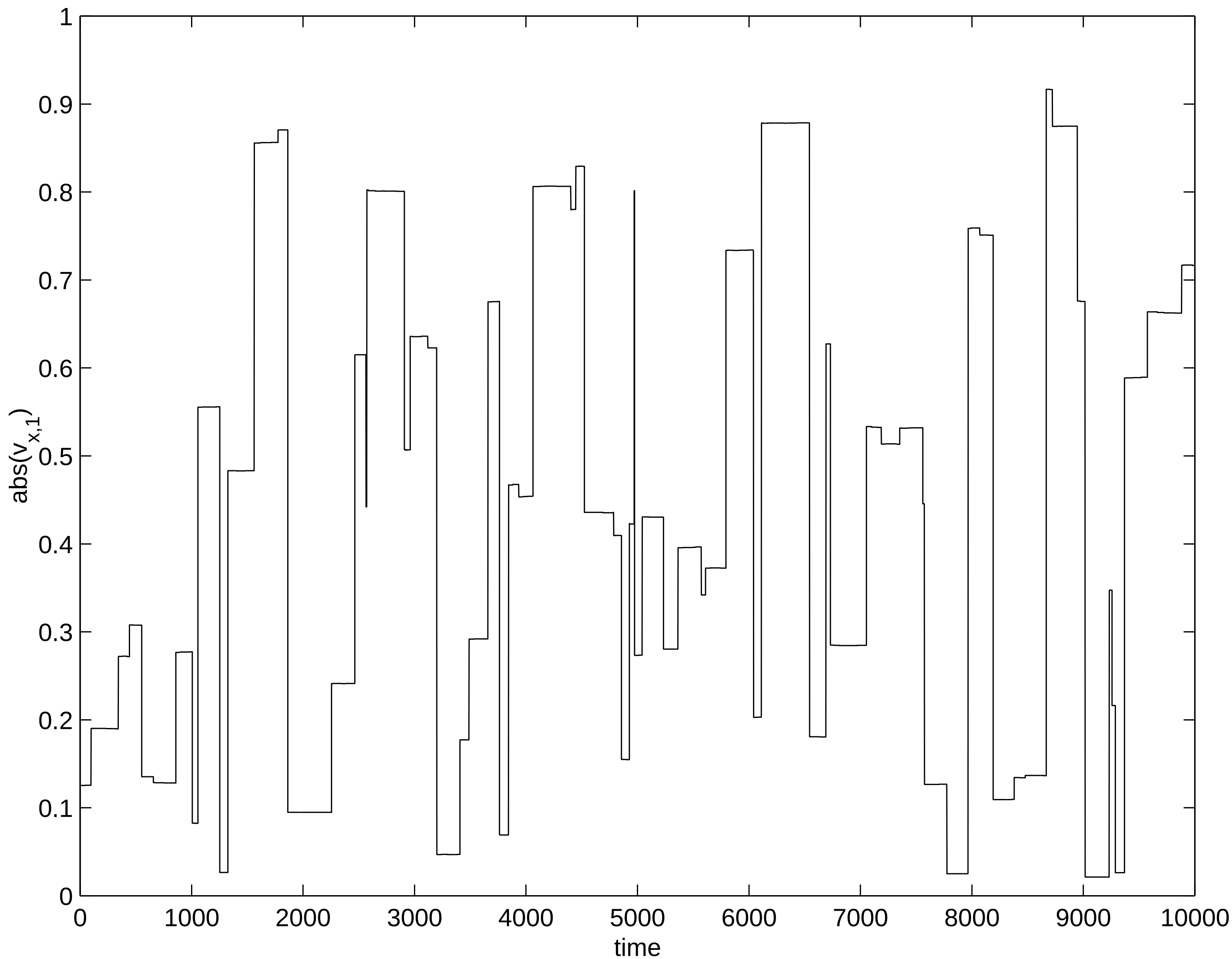
Time Series

Select one velocity coordinate of one particle, $v = v_{x,1}$.

Measure it only at times when discs are not touching.

The statistic $|v|$ is unchanged by collisions with walls.

Series for $|v|$ resembles that of a Continuous Time Markov Chain.



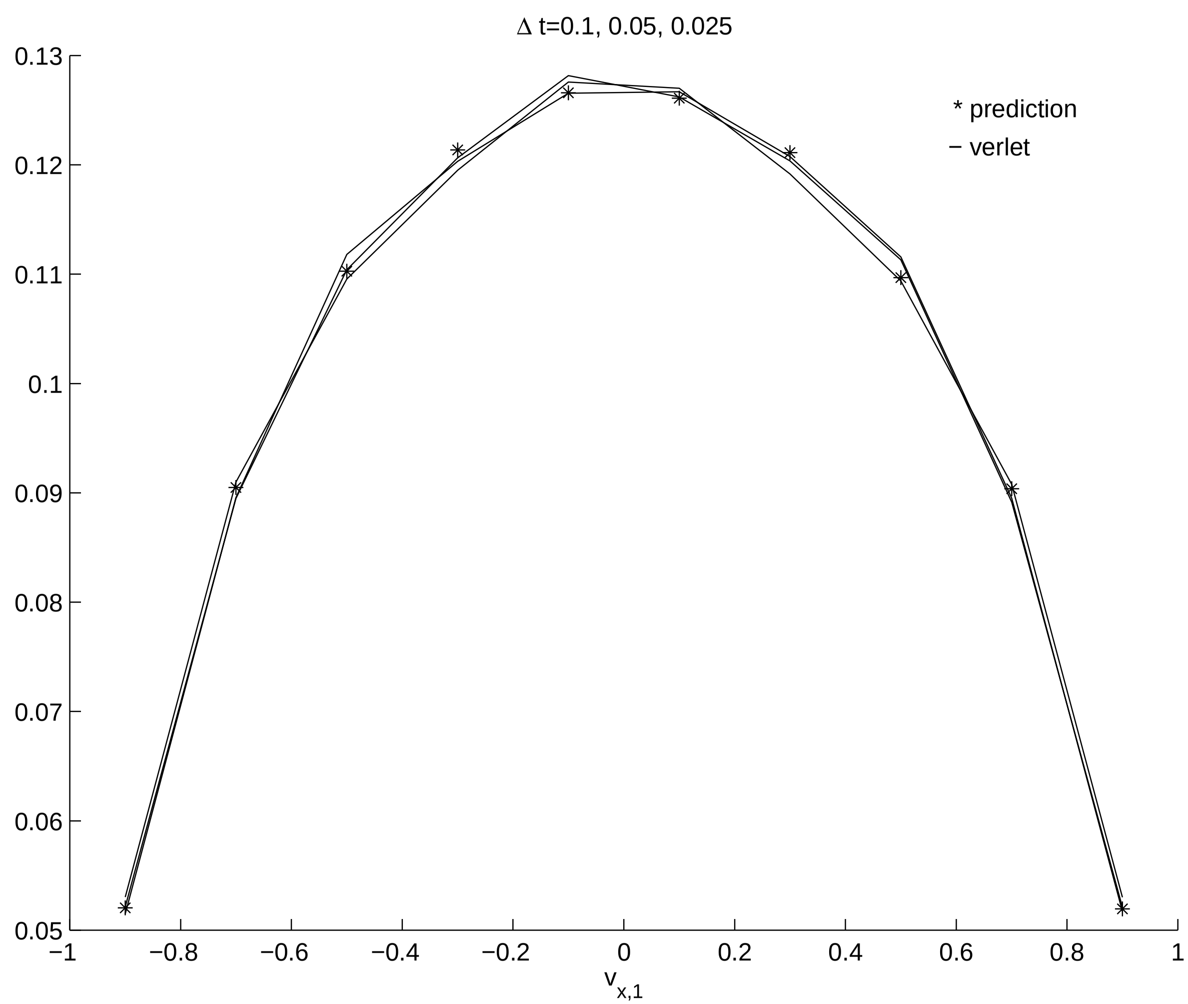
abs(v_{x,1})
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
time

What is invariant distribution of this process?

Compare four different answers.

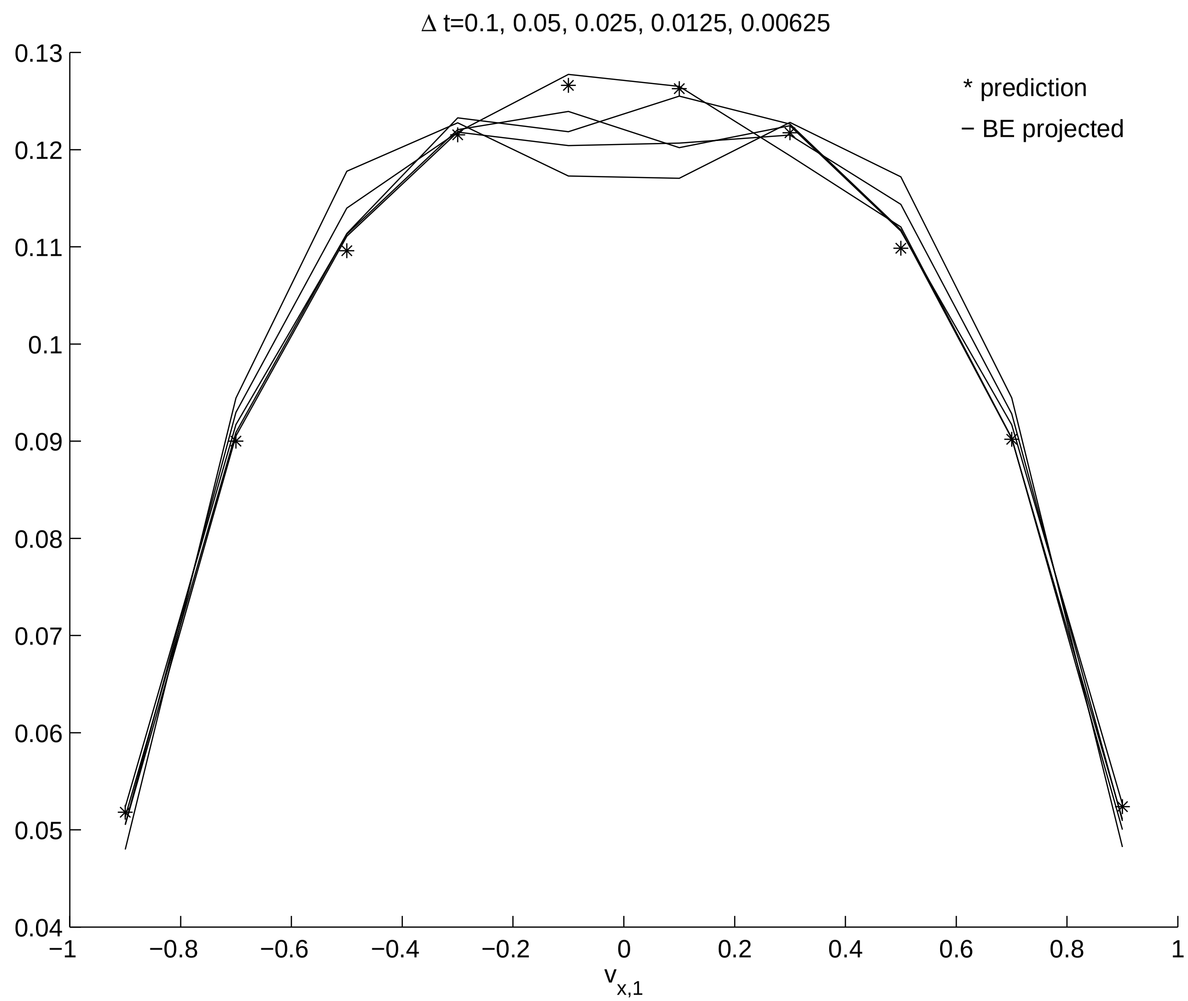
1. **Statistical Mechanics:** Liouville Measure says all energetically accessible states equally likely. (Correct if system is ergodic.)
2. **Verlet Method:** Symplectic integrator as above.
3. **Forward Euler with Projection:** Unstable method made stable by projecting to conserve energy.
4. **Backward Euler with Projection:** Energy-draining method made reasonable by projecting to conserve energy.

Verlet

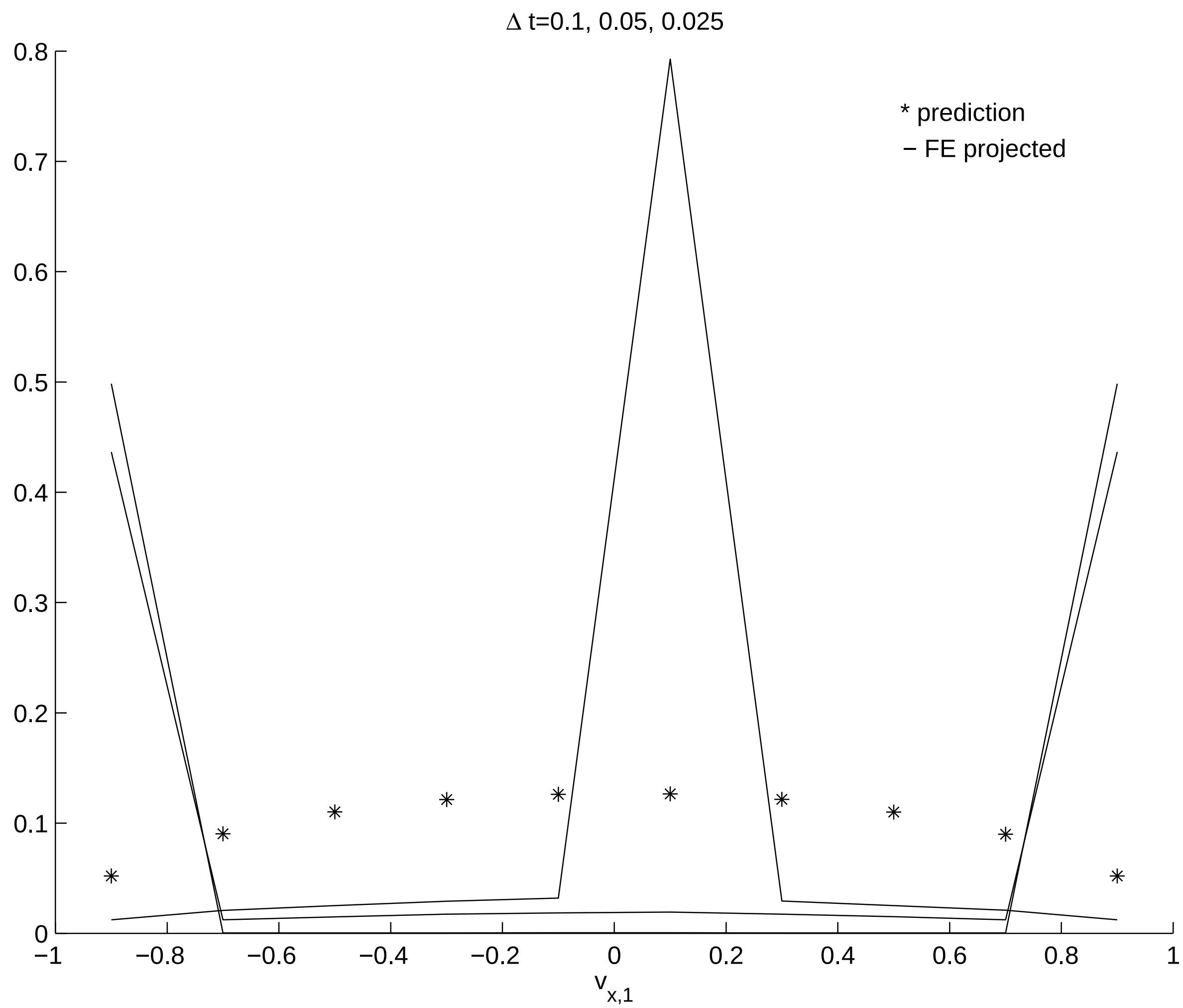


Δ t=0.1, 0.05, 0.025
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
v x,1
* prediction
− verlet

Backward Euler with projection



Forward Euler with projection



Discussion

Verlet Method Symplectic method may have something like Liouville measure.

Backward Euler When particle collides with wall energy is lost. Projection adds energy to both particles. Favours more balanced distribution of energy.

Forward Euler When particle collides with wall energy is gained. Projection removes energy from both particles. Favours unequal distribution of energy. Stable state with one particle having all the energy.

Possible Direction for Analysis

Conjecture: As disc radius goes to 0, time series for $|v_{x,1}|$ for exact system and each numerical approximation is approximately generated by a Continuous Time Markov Chain.

Strategy:

- Determine generator for Markov chain for exact system and each method of approximation.
- Determine invariant measure for these Markov chains.
- Examine which methods approximate invariant measure well.

Conclusion

Numerical methods of similar accuracy from the classical point of view, can have very different properties for approximating statistics.