

Microscopic ensemble bootstrap in phase space

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Abstract

The bootstrap method which has been studied under many quantum mechanical models turns out feasible in microcanonical ensemble as well. While the approach in [Y. Nakayama, Modern Physics Letters A **37**, 10.1142/s0217732322500547 (2022)] produces a sector when Energy is negative, in this paper we report a method that has stronger constraints thus resulting in a smaller region. We also study other models to demonstrate the effectiveness of our method.

INTRODUCTION

Bootstrap, a novel yet promising method has been studied in quantum mechanics recently, is a way to utilize the very general self-consistency condition and solve the system numerically [1][2][3], many have reported the accuracy and high precision of the method. And in some case the bootstrap evolves into Dirac's ladder operator approach and can be solved analytically, suggesting some underlying mechanism of this method [4].

Although widely studied in quantum mechanics, one can also apply the method into microcanonical ensembles as the fundamental relations of bootstrap are still applicable and have their classical correspondence (3)(4)(5) as $\hbar \rightarrow 0$.

Nakayama [5] first introduced this method into the classical scenario, despite reporting the feasibility of the approach, when bootstrapping the double well potential he mentioned a peninsula in $E < 0$ which doesn't converge even for larger bootstrap matrices. In this paper, we use a different approach that incorporates more information in phase space and thus exhibiting a much stronger constraint, we will see that the result of double well bootstrap in phase space cancels the sector region in $E < 0$ compared to the x only bootstrap.

We also investigate coulomb potential, a harmonic oscillator and a non relativistic toda model, the first two can be solved analytically via the bootstrap approach which, however, are trivial cases. As for the non relativistic toda model, our approach in phase space once again demonstrates more powerful restriction, maybe over powerful that we can merely see few points in the result if the sample isn't big enough.

Yet a stronger constraint our approach may have, it still cannot converge to the exact solution in some places, like the non relativistic toda model. Not to mention that our approach consumes much more computing power, the size of our bootstrap matrix is $O(n^4)$. But the benefit is that we can easily achieve high precision when the result converges.

MICROCANONICAL ENSEMBLE BOOTSTRAP

Bootstrap Equations and Matrices

Starting with the Hamiltonian we have

$$H = \frac{p^2}{2M} + V(x) \quad (1)$$

for microcanonical ensemble the average of an observable $\mathcal{O}(x, p)$ is

$$\langle \mathcal{O}(x, p) \rangle = \frac{\int dx dp \mathcal{O}(x, p) \delta(E - H)}{\int dx dp \delta(E - H)} \quad (2)$$

and we can easily find that

$$\langle \{H, \mathcal{O}\} \rangle = 0 \quad (3)$$

$$\langle H\mathcal{O} \rangle = E \langle \mathcal{O} \rangle \quad (4)$$

here $\{H, \mathcal{O}\}$ is the poisson bracket. As for the positivity constraints, obviously that for any observable \mathcal{O} we would have

$$\langle \mathcal{O}^* \mathcal{O} \rangle \geq 0 \quad (5)$$

and by writing the observable as a polynomial of certain observable o , $\mathcal{O} = \sum_{i=0}^k a_i o^i$, one can construct a bootstrap matrix which can be defined as

$$\mathcal{M}_{ij} = \langle (o^*)^i o^j \rangle, \quad i, j = 0, 1, \dots, k \quad (6)$$

we can then rewrite the constraints (5) with matrix and vectors

$$\alpha^\dagger \mathcal{M} \alpha \geq 0 \quad (7)$$

as (7) should hold true for any vector α , the bootstrap matrix \mathcal{M} must embody the positive semi definiteness i.e. $\mathcal{M} \succeq 0$, which is essentially an eigenvalue problem

$$\forall (\mathcal{M})_{\text{eigenvalue}} \geq 0 \quad (8)$$

When the observable \mathcal{O} is a coupling of two observables, say, A and B

$$\mathcal{O} = \sum_{i,j=0}^{k-1} a_i b_j A^i B^j \quad (9)$$

$$\mathcal{O}^* \mathcal{O} = \sum_{i_1, j_1, i_2, j_2=0}^{k-1} a_{i_1}^* b_{j_1}^* (B^*)^{j_1} (A^*)^{i_1} A^{i_2} B^{j_2} a_{i_2} b_{j_2} \quad (10)$$

here we define two auxiliary matrices $\mathcal{M}_{ij}^0 = (B^*)^j (A^*)^i$ and $\mathcal{M}_{ij}^1 = A^i B^j$, the constraints may be written as

$$\mathcal{M}_{ij} = \langle (\mathcal{M}^0 \otimes \mathcal{M}^1)_{ij} \rangle, \quad i, j = 0, 1, 2, \dots, k^2 - 1 \quad (11)$$

$$\mathcal{M} \succeq 0 \quad (12)$$

Double Well Potential

The Hamiltonian of a double well potential can be written as

$$H = p^2 - x^2 + x^4 \quad (13)$$

here we consider the observable $\mathcal{O} = x^m p^n$, substitute it as well as the Hamiltonian into (3) and (4), we can obtain two recursion formulas

$$2(2n + m) \langle x^{m+3} p^{n-1} \rangle = 2(m + n) \langle x^{m+1} p^{n-1} \rangle + 2mE \langle x^{m-1} p^{n-1} \rangle \quad (14)$$

$$\langle H x^m p^n \rangle = E \langle x^m p^n \rangle = \langle x^m p^{n+2} \rangle - \langle x^{m+2} p^n \rangle + \langle x^{m+4} p^n \rangle$$

plus $\langle \{H, x^m\} \rangle = 0$, we get

$$\langle x^{m-1} p \rangle = 0 \quad (15)$$

and for simplicity, we here assume that the average of x to the odd powers is 0

$$\langle x^m \rangle = 0, \quad \text{for all odd } m \quad (16)$$

with (14) (15) (15) (16) plus the initial paratemers E and $\langle x^2 \rangle$ we can construct the bootstrap matrix \mathcal{M} . The result when $k = 5$ is shown in Fig. 1. We also reproduced the result in [5] to make a comparison.

In constrast with [5], our result shows no peninsula in where $E < 0$, as we include the information of the momentum. When E turns negative, the curve menifests a similar behavior as the positive part. In our program the scale of the bootstrap matrix is k^4 , which is much larger compared to the single observable bootstrap program with the scale of k^2 . So here the size of our bootstrap matrix is 625, about seven times to the x bootstrap. But

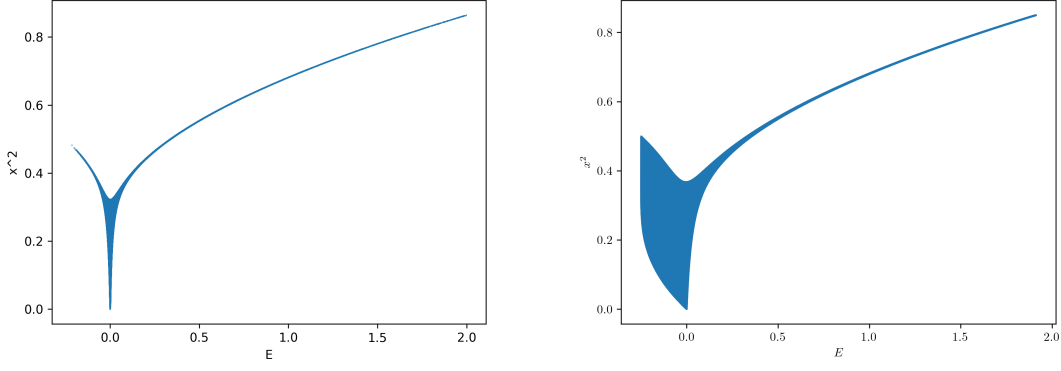


FIG. 1. xp bootstrap with $k = 5$ (left), x only bootstrap with $k = 9$ (right)

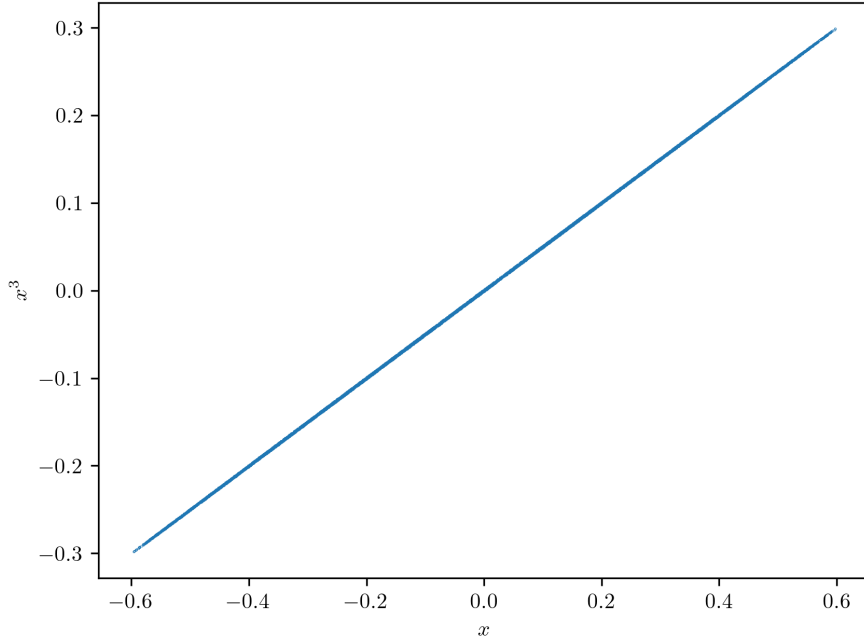


FIG. 2. $\langle x^m p^n \rangle$ bootstrap ($k = 5$) with fixed $E = -0.1$ and $\langle x \rangle = 0.4052$

the region still doesn't shrink even when we set $k = 25$ for the x only bootstrap program, so we conclude that this bootstrap in phase space does have a much stronger constraints than the single observable one.

Like Nakayama has mentioned, $\langle x \rangle$ doesn't have to be zero in classical mechanics, but this method does produce a narrow region upon the assumption (16). So we then study the $\langle x \rangle$ and $\langle x^3 \rangle$ with fixed E and $\langle x^2 \rangle$ using the $\langle x^m p^n \rangle$ bootstrap program, which, still turns

out to be a line in Fig. 2.

NUMERICAL EXAMPLES

CONCLUSIONS

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