Numerical bootstrap

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Introduction

What's bootstrap

- A quantum theory = expectations of all Hermitian operators; Hamiltonian/Lagrangian $\Leftrightarrow$ "probability distribution"
- Constraint on the system $\Rightarrow$ relation between different $\langle O \rangle$'s ("**data**"); independent $\langle O \rangle$'s $\Leftrightarrow$ parameters in the model
- Inequality constraint (e.g. positivity of $\left\langle O^\dagger O \right\rangle$) $\Rightarrow$ allowed range of $\langle O \rangle$'s
- Solving a class of problems without mentioning explicitly the wave function/path integral: hence the name *bootstrap*

Example: conformal bootstrap

- The most famous example: **conformal bootstrap**
- Constraints: (spinless) two-point function

$$\langle \mathcal{O}(x)\mathcal{O}(y)\rangle = \frac{1}{|x-y|^{2\Delta_{\mathcal{O}}}}, \tag{1}$$

three-point function

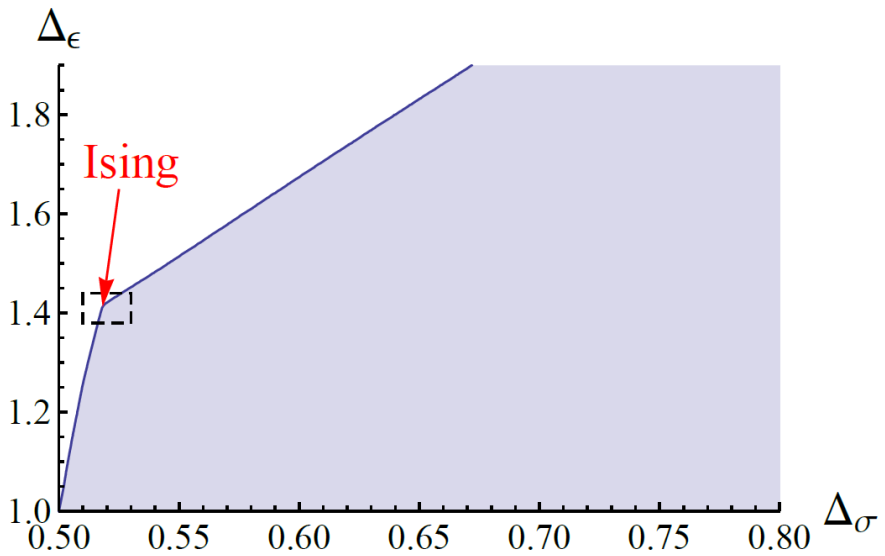
$$\begin{aligned}&\langle \mathcal{A}(x)\mathcal{B}(y)\mathcal{C}(z)\rangle \\ &= \frac{f_{\mathcal{ABC}}}{|x-y|^{\Delta_{\mathcal{A}}+\Delta_{\mathcal{B}}-\Delta_{\mathcal{C}}}|y-z|^{\Delta_{\mathcal{B}}+\Delta_{\mathcal{C}}-\Delta_{\mathcal{A}}}|z-x|^{\Delta_{\mathcal{C}}+\Delta_{\mathcal{A}}-\Delta_{\mathcal{B}}}}\end{aligned} \tag{2}$$

Higher order correlation functions: OPEs.

- Independent parameters: $\{\Delta_{\mathcal{O}}, l_{\mathcal{O}}, f_{\mathcal{ABC}}\}$
- Inequality constraints (self-consistent conditions): determining the range of parameters

Example: conformal bootstrap

- Example of conformal bootstrap: verify whether the critical point of 3D Ising model is a CFT and its position in the allowed region[1]
- Physical picture tells us there are two degrees of freedom: energy density ϵ, spin field σ
- Below is Fig. 3 in the paper: comparing critical exponents of 3D Ising model, and the allowed range from conformal bootstrap



[1] arXiv 1203.6064

Bootstrap for generic systems

How to perform bootstrap for a generic system?

- Correlation functions cannot be determined by countably infinite parameters: no $\{\Delta_{\mathcal{O}}, l_{\mathcal{O}}, f_{\mathcal{ABC}}\}$.
  Solution Store $\langle O_1(x_1)O_2(x_2)\cdots O_n(x_n)\rangle$ separately. Symmetries reduce the size of data: Suppose C is a symmetry,

$$\langle OC\rangle = \langle CO\rangle\,. \tag{3}$$

  Derivation similar to next slide.

Bootstrap for generic systems

How to perform bootstrap for a generic system?

- How to get relations between correlation functions
  Solution Expanding each operator to a linear combination of normal ordered operators. (poor man's OPE)
  Density matrix is determined solely by H, then

$$\langle OH \rangle = \mathrm{tr}(\rho(H)OH) = \mathrm{tr}(H\rho(H)O) = \mathrm{tr}(\rho(H)HO) = \langle HO \rangle \quad (4)$$

  for all operators O. For energy eigenstates (i.e with definite E), we have

$$\langle OH \rangle = E \langle O \rangle , \quad E = \langle H \rangle . \quad (5)$$

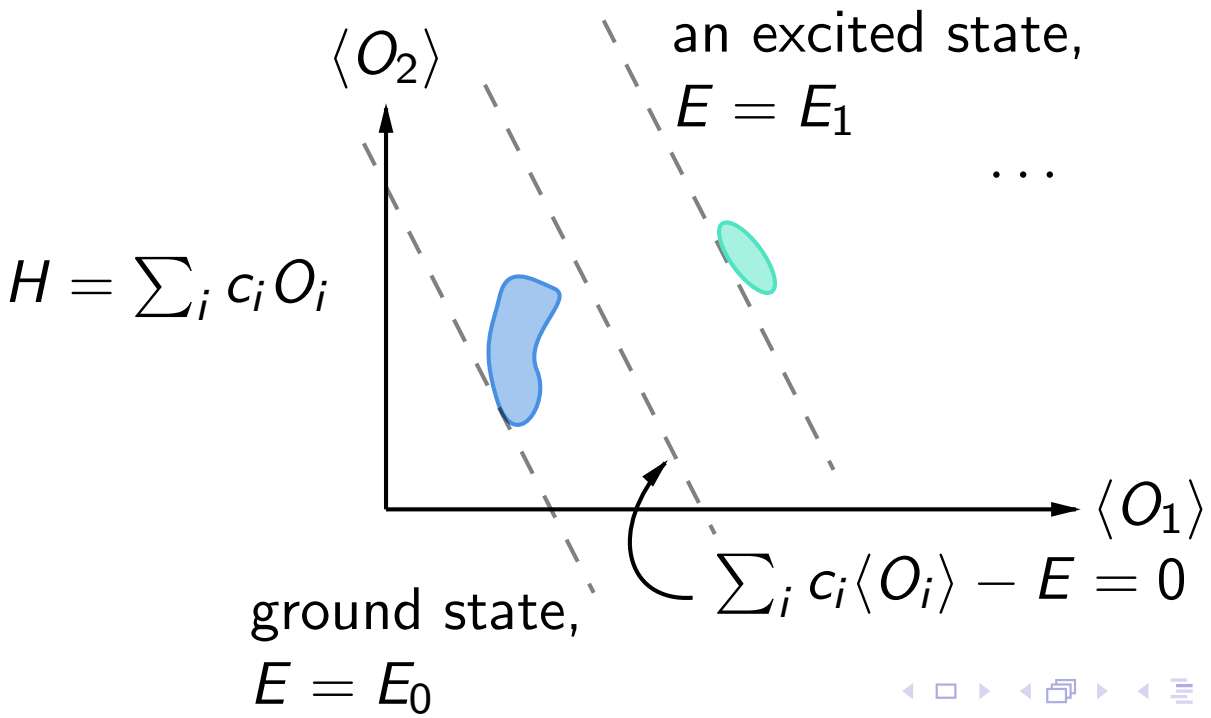
  Thus we break higher order correlation functions into lower order ones.

Bootstrap for generic systems

- The equality constraints used together with the positivity constraint

$$\langle O^\dagger O \rangle \geq 0 \tag{6}$$

  for every O defines an allowed region – the feasible domain for the following optimization.
- To get ground state information, minimize $\langle H \rangle$ globally.
- To get information about excited states, find local minima of $\langle H \rangle$.



Bootstrap for generic systems

The procedure of numerical bootstrap

Input data:

- N basis operators $\{O_i\}$, normal ordered with a length cutoff
- Data of equality constraints: Hamiltonian, symmetry, etc.
- Commutation rules, normal ordering rules, etc. so that $O_i O_j$ can be expanded in terms of $\{O_i\}$
- Hamiltonian $H = \sum_i c_i O_i$

Building the optimization problem:

1. Declare N variables $\{X_i\}$, $X_i = \langle O_i \rangle$ after optimization
2. Impose equality constraints on $\{X_i\}$ according to e.g. $\langle [H, O] \rangle = 0$
3. Imposing semidefinite constraint on $M_{ij} = \langle O_i^\dagger O_j \rangle$ (expanded into linear combination of $\{X_i\}$), so that after optimization $\langle O^\dagger O \rangle \geq 0$ for every O
4. Optimize $\sum_i c_i X_i$

Bootstrap for generic systems

Why we need numerical bootstrap

- Because it doesn't fail with strong non-perturbative effects.[2]
- Because if done correctly, it gives the *lower* bound of ground state energy
  - Density matrix = linear functional $\mathcal{F}$ from operators to numbers
  - Predicted $E_0 = \min_{\mathcal{F}\text{constrained}} \mathcal{F}[H]$
  - Real ground state also constrained $\Rightarrow$ real $E_0 >$ predicted E_0

[2] arXiv 2108.11416

Bootstrap for generic systems

Some technical aspects of the problem

When building the optimization problem:

- A little symbolic calculation required
- Auto normal ordering of $O_i O_j$ given the operator algebra
- Auto commutator: $[A, B]$ = normal ordered AB - normal ordered BA

Bootstrap for generic systems

For optimization itself

- **Linear semidefinite programming (linear SDP)** when using $\langle [H, O] \rangle = 0$ ($\langle HO \rangle$ and $\langle OH \rangle$ being linear combination of $\{O_i\}$)
  - Convex optimization[3]
  - Mature solvers like SCS[4] or CSDP[5]
- **Nonlinear semidefinite programming (nonlinear SDP)** when using $\langle HO \rangle = E \langle O \rangle$ because there are optimization variables in E
  - No solver mature enough[6]

[3] See Wikipedia

[4] https://github.com/cvxgrp/scs

[5] https://github.com/coin-or/Csdp

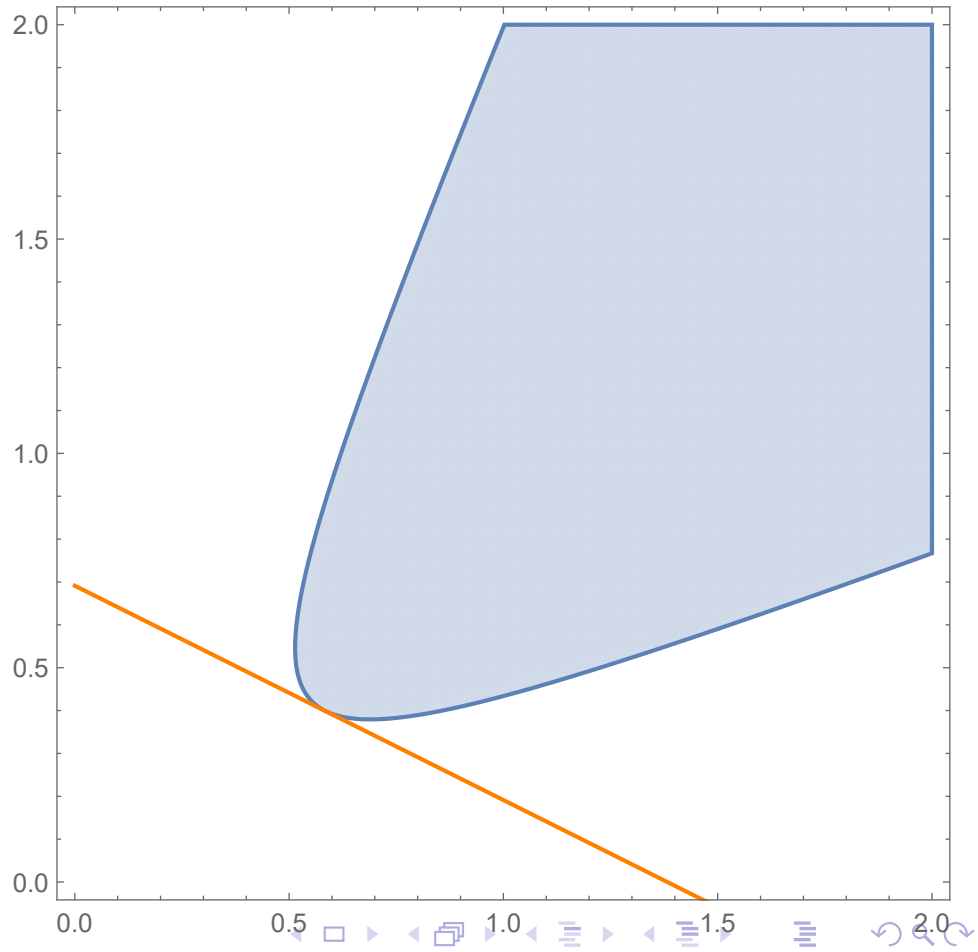
[6] See the discussion before Sec. 1.1 in arXiv 2108.04830. Also, no solver supporting both SDP and nonlinear programming (NLP) is listed in the solver list of JuMP.jl.

Bootstrap for generic systems

- linear SDP (constraints: $\langle [O, H] \rangle = 0$, thermal states allowed) easy
- nonlinear SDP (constraints: $\langle OH \rangle = E \langle O \rangle$, no thermal states) hard

Example of linear SDP (and why it's easy)

$$\begin{aligned} \max\ & M_{11} + 2M_{12}, \text{ s.t.} \\ & M = M^{\top},\ M \geq 0, \\ & M_{11} + M_{12} + M_{13} = -0.5, \\ & M_{22} = 2M_{11} + 3M_{12} + 1, \\ & M_{23} + 4M_{11} = 0, \\ & M_{33} = 4M_{11} + 5M_{12}. \end{aligned}$$



- Convex feasible domain
- Linear objective $\Rightarrow$ minimum at the edge

Example: x^4 anharmonic oscillator

Consider the anharmonic oscillator[7], a famous failure of perturbation theory[8]

$$H = x^2 + p^2 + gx^4. \tag{7}$$

- Symmetry: $x \to -x \Rightarrow \langle x^n \rangle = 0$ with odd n
- Deriving equality constraints:
  - $\mathcal{O} = x^s$ and $\mathcal{O} = x^t p$ in $\langle [H, \mathcal{O}] \rangle = 0$
  - $\mathcal{O} = x^{t-1}$ in $\langle \mathcal{O} H \rangle = E \langle \mathcal{O} \rangle$
- So finally we have

$$\begin{aligned} &E = 2\left\langle x^2 \right\rangle + 3g\left\langle x^4 \right\rangle, \\ &4tE\left\langle x^{t-1} \right\rangle + t(t-1)(t-2)\left\langle x^{t-3} \right\rangle - 4(t+1)\left\langle x^{t+1} \right\rangle \\ &\quad - 4g(t+2)\left\langle x^{t+3} \right\rangle = 0 \end{aligned} \tag{8}$$

- Only independent variables: $\left\langle x^2 \right\rangle$ and E, so nonlinear SDP is possible
- SDP constraint: $M_{ij} = \left\langle x^{i+j} \right\rangle, M \geq 0$

[7] The example is provided in arXiv 2004.10212

[8] Carl M. Bender and Tai Tsun Wu, Anharmonic Oscillator. Phys. Rev. 184, 1231.

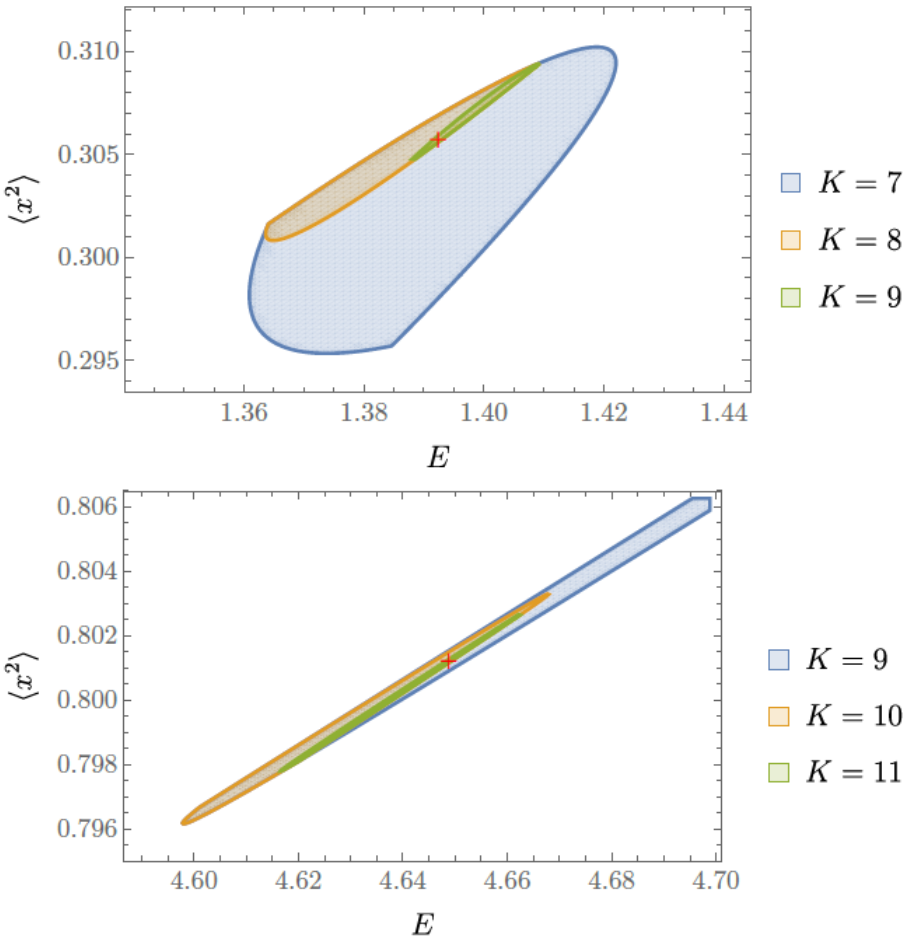
Example: x^4 anharmonic oscillator

- Reproduce Fig. 1 in arXiv 2004.10212 by brutal force searching
- Numerical bootstrap can be quite precise! (high resolution Mathematica plotting required to find the allowed region)

```
expectedX[0] := 1;
expectedX[2] := x2;
expectedX[4] := 1/(3 g) (E0 - 2 x2);
expectedX[u_?EvenQ] :=
1 / (4 g ((-3 + u) + 2)) *
(4 (-3 + u) E0 expectedX[(-3 + u) - 1]
+ (-3 + u) ((-3 + u) - 1) ((-3 + u) - 2)
    expectedX[(-3 + u) - 3]
- 4 ((-3 + u) + 1) expectedX[(-3 + u) + 1]);

matPositive[K_] :=
Table[expectedX[i+j], {i, 0, K}, {j, 0, K}];

RegionPlot[
AllTrue[Eigenvalues[matPositive[9] /. g -> 1]
    # >= 0 &],
{E0, 1.35, 1.44}, {x2, 0.294, 0.311},
PlotPoints -> 100]
```



Example: x^4 anharmonic oscillator

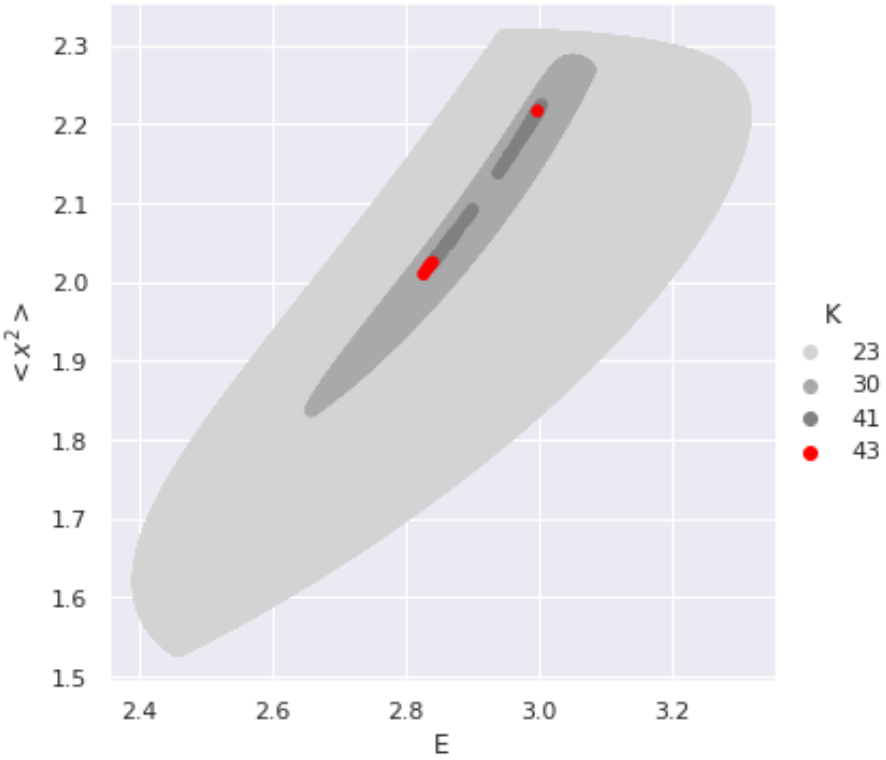
Benchmark

- Solving the Schrödinger equation with finite difference method with $\Delta x = 0.05$: $E_0 = 1.3919$
- Numerical bootstrap with $K = 11$: $E_0 = 1.3922$

More examples

Double-well potential[9]

- Another famous non-perturbative model (instantons between the wells)
- $$H = p^2 - m^2 x^2 + g x^4 + \mathcal{V}_0 \quad (9)$$
- Error between predicted split between the ground state and the first excited state and the dilute instanton approximation goes down as the two wells are separated.



[9] See arXiv 2108.11416

More examples

Matrix model[10]

- Impossible to solve otherwise
- A specific case associated with M-theory[11]
- (Inherent) nonlinear constraints
  - Relaxed bootstrap in Sec. 4 in arXiv 2108.04830
  - trust-region sequential SDP in Xizhi Han's code

[10] See arXiv 2108.04830 and arXiv 2004.10212

[11] arXiv hep-th 9610043

More examples

Hubbard model[12]

Bootstrapping of models in condensed matter physics – No sign problem!

$n = 1$	$U = 2$	$U = 4$	$U = 6$	$U = 8$
$E_{\mathrm{lb}}\|_{K=7}$	-1.221	-0.913	-0.705	-0.565
$E_{\mathrm{lb}}\|_{K=\infty}$	–	–	$-0.66(2)$	$-0.54(2)$
E_{AFQMC}	$-1.1763(2)$	$-0.8603(2)$	$-0.6568(3)$	$-0.5247(2)$
E_{DMET}	$-1.1764(3)$	$-0.8604(3)$	$-0.6562(5)$	$-0.5234(10)$
E_{DMRG}	$-1.176(1)$	$-0.8605(5)$	$-0.6565(1)$	$-0.5241(1)$
$n = 0.875$	$U = 2$	$U = 4$	$U = 6$	$U = 8$
$E_{\mathrm{lb}}\|_{K=7}$	-1.316	-1.103	-0.963	-0.867
$E_{\mathrm{lb}}\|_{K=\infty}$	–	–	$-0.86(5)$	$-0.77(3)$
E_{DMET}	$-1.2721(6)$	$-1.031(3)$	$-0.863(13)$	$-0.749(7)$

- Operator space cutoff: $l(c^{(\dagger)}_{x_1\sigma_1}\cdots c^{(\dagger)}_{x_r\sigma_r}) = r + \sum_{i=1}^{r}\|x_i\|_1 \leq K$
- Ground state energy lower bounded

[12] See 2006.06002.

Discussion

What can be immediately done

- Bootstrapping anharmonic oscillator by linear SDP
- Reproduce the results of Hubbard model

Future perspectives

- Bootstrapping a *class* of models (e.g. "all possible models made by x and p")
  - Extending what is done in conformal bootstrap (e.g. "all possible CFTs made by σ and ϵ") to all kind of models
- Extracting thermal information from $\langle [O, H] \rangle = 0$ bootstraps
- What constraints are effective?
  - Can wave function ansatz (e.g. DMRG) provide some hints?