Numerical bootstrap

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Numerical methods for strongly correlated systems

Strongly correlated systems

- Fermi liquid: interaction correction of Fermi gas
- Strongly correlated systems: something non-perturbative happens

Numerical approaches

- DQMC: discrete path integral and discrete Hubbard-Stratonovich transformation
- DMRG (MERA, PEPS): tensor network wave function ansatz
- Diagrammatic Monte-Carlo: stochastic summation of Feynman diagrams
- DMFT: self-energy correction + impurity model

What's in common: All with unobservable objects, be it the path integral or wave function or Feynman diagram or ...

Introduction

What's bootstrap

- A model = expectations of all operators
  - Hamiltonian/Lagrangian $\Leftrightarrow$ "probability distribution"
  - independent $\langle O \rangle$'s $\Leftrightarrow$ parameters in the model ("**data**")
- Probability distribution $\Rightarrow$ Equality constraint on $\{\langle O \rangle\}$ without carrying out substantial calculation
  - Trivial example: Wick theorem
  - Conformal symmetry
- Inequality constraint $\Rightarrow$ allowed range of $\langle O \rangle$'s
  - Positivity of $\langle O^\dagger O \rangle$
  - Relaxed equational constraints
- Obtaining estimation of physical quantities without the wave function/path integral ("out of nothing"): 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: $\{\Delta_{\mathcal{O}}, l_{\mathcal{O}}, f_{\mathcal{ABC}}\}$
- Self-consistent conditions: determining the range of parameters

Bootstrap for generic systems

How to perform bootstrap for a generic system?

- The data: Correlation functions cannot be reduced to countably infinite parameters: no $\{\Delta_{\mathcal{O}}, l_{\mathcal{O}}, f_{\mathcal{ABC}}\}$.
  Solution Store the normal-ordered $\{\langle O_i \rangle\}$ set (a basis of the operator space) with a cutoff. This is the data. Using equational constraints to reduce the size of data.
  Example:
  $$\langle px^3 \rangle = \langle x^3 p \rangle - 3\,\mathrm{i}\,\langle x^2 \rangle\,. \tag{3}$$
  Data used: $\{\langle x^3 p \rangle, \langle x^2 \rangle\} \in \{\langle x^m p^n \rangle\}$

Bootstrap for generic systems

How to perform bootstrap for a generic system?

- The equality constraints
  Solution $\rho = \mathrm{e}^{-\beta H}/Z$, $[\rho, H] = 0$, then for all operators O

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

$$\langle [O, H] \rangle = 0 \tag{4}$$

  Similarly, suppose C is a symmetry of the system, we have

$$\langle [O, C] \rangle = 0. \tag{5}$$

  There are linear constraints w.r.t the operator basis $\{O_i\}$.
  For energy eigenstates (i.e with definite but unknown E), we have

$$\langle OH \rangle = E \langle O \rangle , \quad E = \langle H \rangle . \tag{6}$$

  This is a nonlinear constraint.

Bootstrap for generic systems

Example of equality constraint Suppose $H = x^2 + p^2 + x^4$, then

$$\langle [H, xp] \rangle = 0$$

gives linear constraint

$$\langle p^2 \rangle - \langle x^2 \rangle - 2 \langle x^4 \rangle = 0, \tag{7}$$

and

$$\langle xp \cdot H \rangle = E \langle xp \rangle$$

gives nonlinear constraint

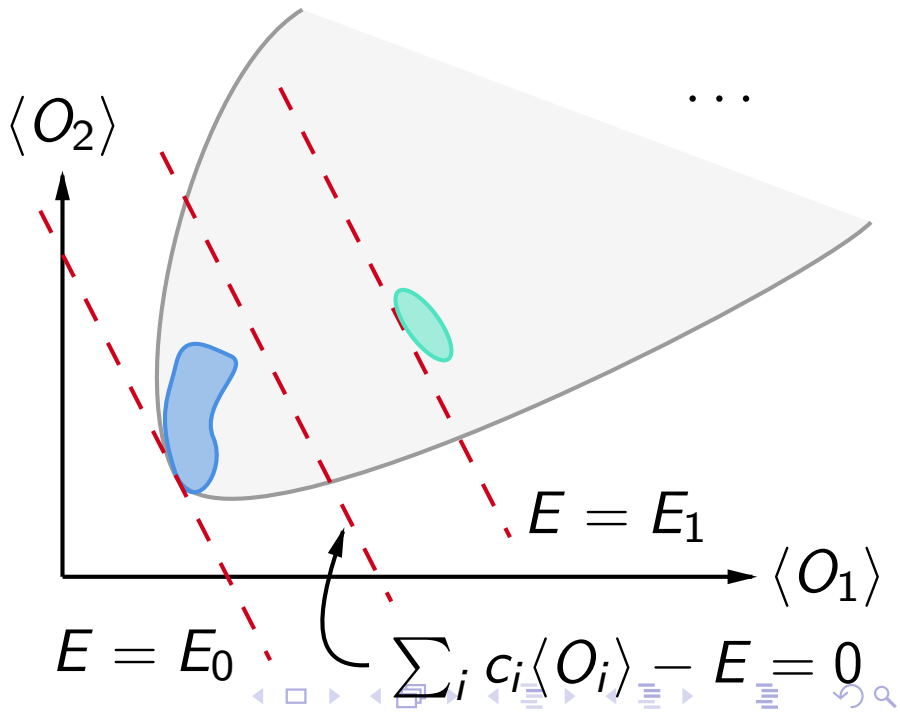
$$\begin{aligned} &\langle xp^3 \rangle + \langle x^3 p \rangle - 2\,\mathrm{i} \langle x^2 \rangle + \langle x^5 p \rangle - 4\,\mathrm{i} \langle x^4 \rangle \\ &- \langle xp \rangle \langle x^2 \rangle - \langle xp \rangle \langle p^2 \rangle - \langle xp \rangle \langle x^4 \rangle = 0. \end{aligned} \tag{8}$$

Bootstrap for generic systems

- The equality constraints together with the positivity constraint $\langle O^\dagger O \rangle \geq 0$ for every O defines a feasible domain.
- This is an **semidefinite programming (SDP)** problem:

$$M_{ij} = \langle O_i^\dagger O_j \rangle = \sum_k c_{ij}^k \langle O_k \rangle , \quad M \geq 0. \tag{9}$$

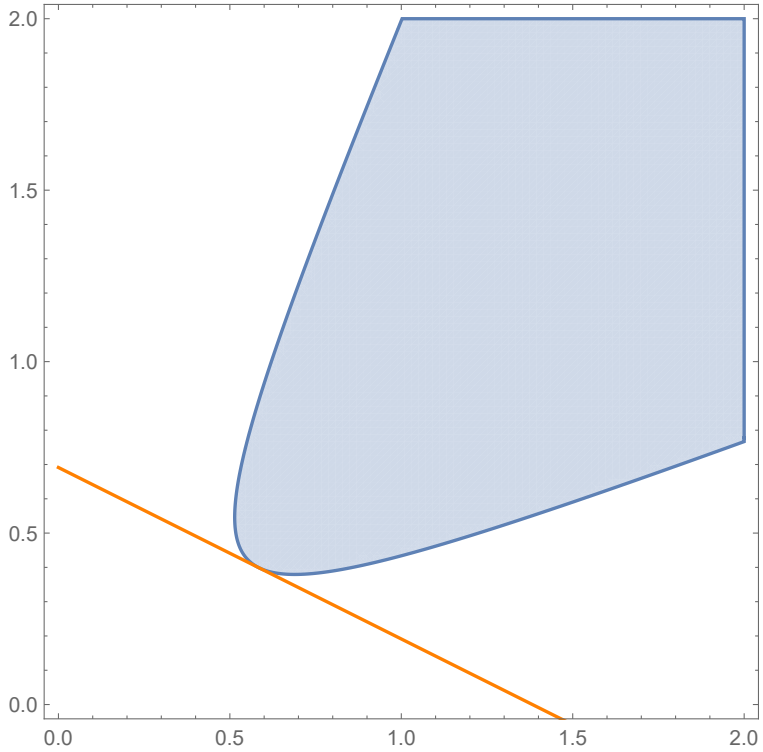
- $\langle [O, C] \rangle = 0$: **linear SDP**, convex feasible domain, min $\langle H \rangle \Leftrightarrow$ ground state information
- $\langle OH \rangle = \langle H \rangle \langle O \rangle$: **nonlinear SDP**, nonconvex feasible domain; a connected component = an eigenstate (or a continuous spectrum)



Bootstrap for generic systems

Some technical aspects of the problem

- **Linear SDP**
  - $\langle [H, O] \rangle = 0$, thermal states allowed
  - Convex optimization[1], Linear objective $\Rightarrow$ minimum at the edge
  - Mature solvers like SCS or CSDP[2]
- **Nonlinear SDP**
  - $\langle HO \rangle = E \langle O \rangle$, there are optimization variables in E, eigenstates only
  - No solver mature enough[3]



[1] See Wikipedia

[2] https://github.com/cvxgrp/scs, https://github.com/coin-or/Csdp

[3] See the discussion before Sec. 1.1 in arXiv 2108.04830. Also, no nonlinear solver supporting SDP is listed in the solver list of JuMP.jl.

Bootstrap for generic systems

The procedure of numerical bootstrap

Input data:

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

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 $\{X_i\}$)

Bootstrap for generic systems

Why we need numerical bootstrap

- Because it doesn't fail with strong non-perturbative effects.[4]
- 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 $E_0 \geq$ predicted E_0
  - Upper and lower bounds for all physical quantities:

$$\min_{E_{\text{lb}} \leq \langle H \rangle_\rho \leq E_{\text{ub}}} \langle O \rangle_\rho \leq \langle O \rangle_{\rho_0} \leq \max_{E_{\text{lb}} \leq \langle H \rangle_\rho \leq E_{\text{ub}}} \langle O \rangle_\rho \tag{10}$$

[4] arXiv 2108.11416

Examples

Anharmonic oscillator and Hubbard model

- Main topics of my thesis

Double-well potential[5]

- Non-perturbative: instanton effect
- Solved in a similar way of the anharmonic oscillator
- Dilute instanton approximation works with two wells well separated

Matrix model[6]

- Hard to solve otherwise
- (Inherent) nonlinear constraints
  - Relaxed bootstrap in Sec. 4 in arXiv 2108.04830
  - trust-region sequential SDP in Xizhi Han's code

[5] See arXiv 2108.11416

[6] See arXiv 2108.04830 and arXiv 2004.10212

Example: x^4 anharmonic oscillator

The anharmonic oscillator[7]: famous failure of perturbation theory[8]

$$H = x^2 + p^2 + gx^4. \tag{11}$$

- Equality constraints from symmetry: $x \to -x \Rightarrow \langle x^n \rangle = 0$ with odd n
- Equality constraints from Hamiltonian:
  - $\mathcal{O} = x^s$ 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

$$\begin{aligned} & E = 2\left\langle x^2 \right\rangle + 3g\left\langle x^4 \right\rangle, \\ & 4tE\left\langle x^{t-1} \right\rangle + t(t-1)(t-2)\left\langle x^{t-3} \right\rangle - 4(t+1)\left\langle x^{t+1} \right\rangle \\ & \quad - 4g(t+2)\left\langle x^{t+3} \right\rangle = 0 \end{aligned} \tag{12}$$

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

[7] The example is provided in arXiv 2004.10212

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

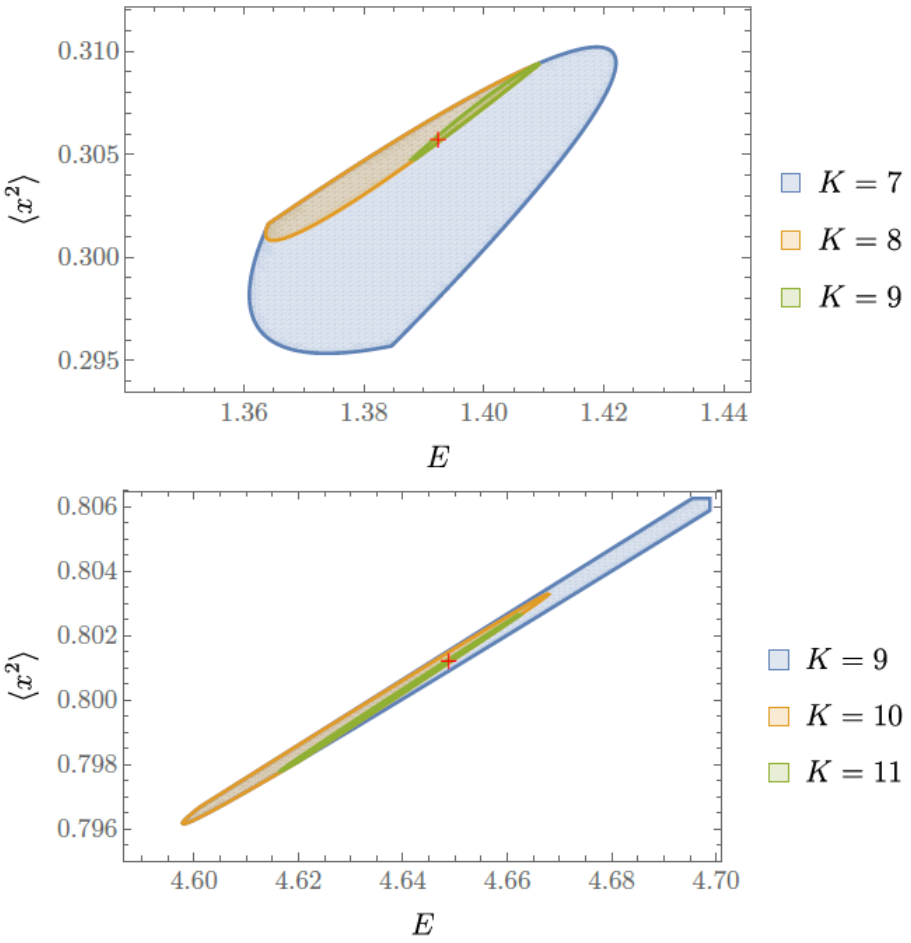
Example: x^4 anharmonic oscillator

- 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 $K = 11$: $E_0 = 1.3922$

Example: x^4 anharmonic oscillator

Linear SDP

- Solver: JuMP and COSMO[9]
- Operator algebra: McCoy formula

$$[x^n, p^m] = \sum_{k=1}^{\min(m,n)} \frac{-(-i\hbar)^k \, n! m!}{k! \, (n-k)! \, (m-k)!} x^{n-k} p^{m-k}. \tag{13}$$

- Operator basis and cutoff: $\{x^m p^n\}$, where $0 \leq m, n \leq 2L$
- Hence for $O_i = x^m p^n$ in $M_{ij} = \langle O_i^\dagger O_j \rangle$, $0 \leq m, n \leq L$
- COSMO only support real variables $\Rightarrow$ Declare two JuMP variables for $\mathrm{Re}\, O$ and $\mathrm{Im}\, O$ (odd $m+n \Rightarrow$ zero expectation, odd $n \Rightarrow$ imaginary, even $n \Rightarrow$ real),

$$M_{ij} \to \mathrm{Re}(M_{ij}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \mathrm{Im}(M_{ij}) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{14}$$

[9] https://jump.dev/JuMP.jl/stable/, https://oxfordcontrol.github.io/COSMO.jl/stable/

Example: x^4 anharmonic oscillator

Result of linear SDP

- Successful when L is small
- But when L is 4. . . Severe convergent problem!
- Both stationary Schrödinger equation and nonlinear SDP estimate $E \approx 1.392$, $\langle x^2 \rangle \approx 0.306$. Not sure whether $L = 4$ converges.
- $L = 5$ takes 80000000 iterations and still doesn't converge.
- Only COSMO works for $L = 4$; SCS and CSDP report infeasibility
- False convergence when `eps_rel` is not small enough (1×10^{-5} not enough; 1×10^{-10} works for $L = 4$)

L	E	$\langle x^2 \rangle$	time consumption
2	1.381	0.313	0.752s, 958 iterations
3	1.387	0.305	2.501s, 1194 iterations
4	1.394	0.306	172375s, 79461867 iterations

Example: x^4 anharmonic oscillator

Possible reasons of the convergence problem

- Too much time is spent on tightening the constraints. Hints:
  - In the solver log of the $L = 4, 5$ cases, first energy goes down and residue goes up, then residue goes down and energy goes up, ...
  - False convergence
  - Solution: eliminate some variables in the optimization problem
- Float precision not enough, introducing fluctuation. Hints:
  - This is the case in conformal bootstrap.
  - Diagnosis: using less precise floats for $L = 2, 3$ and checking if the problem recurs.
  - Solution: same as conformal bootstrap
- The scheme

$$M_{ij} \to \mathrm{Re}(M_{ij}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \mathrm{Im}(M_{ij}) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{15}$$

  is bad. Hints:
  - No convergence problem in Hubbard model. (strange but true ...)
  - Solution: rephrasing the anharmonic oscillator in terms of the creation and annihilation operators

Example: Hubbard model

Hubbard model[10]

$$H = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} c^{\dagger}_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + U \sum_{\boldsymbol{i}} n_{\boldsymbol{i}\uparrow} n_{\boldsymbol{j}\downarrow} \tag{16}$$

is probably the most important strongly correlated electronic model.

- Half filling: small $U \Rightarrow$ Fermi liquid, large $U \Rightarrow$ Heisenberg model (Mott transition, spin-charge separation)
- Doping: t-J model, superconductivity
- Problems of various numerical approaches:
  - DQMC: sign problem when doped away from half-filling, can be tackled in some case[11] but no generic solution[12]
  - DMRG: works well in 1D but slow in 2D

[10] arXiv 2006.06002
[11] arXiv 2204.08777
[12] arXiv cond-mat 0408370

Example: Hubbard model

Linear SDP

- Solver: JuMP and COSMO
- Operator algebra: QuantumAlgebra.jl[13]
- Operator basis and cutoff: normal ordered $\{c^\dagger_{\boldsymbol{i}_1\sigma_1} c^\dagger_{\boldsymbol{i}_2\sigma_2} \cdots c_{\boldsymbol{i}_n\sigma_n}\}$, $n + \sum_{k=1}^{n} \|\boldsymbol{i}_k\|_1 \leq K$
- One JuMP variable for one operator $\Leftarrow$ the whole model is real
- Expectations of operators that do not keep particle number (e.g. $c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} c^\dagger_{3\uparrow} c_{1\uparrow}$) and total spin (e.g. $c^\dagger_{1\uparrow} c_{1\downarrow}$) are zero
- Translational and inversion symmetry: $\langle c^\dagger_{1\uparrow} c_{1\uparrow} \rangle = \langle c^\dagger_{2\uparrow} c_{2\uparrow} \rangle$
- Electron filling: need to be explicitly imposed
  - half filling $\Rightarrow \langle n_1 \rangle = \langle n \rangle_2 = \cdots = 1$
  - doping $\Rightarrow \langle n_1 \rangle = \langle n \rangle_2 = \cdots = 0.75$, etc.
  - *Not* done by chemical potential (which is the case in DQMC but not in DMRG)

[13] https://github.com/jfeist/QuantumAlgebra.jl

Example: Hubbard model

DMRG benchmark

- Using ITensor's fixed quantum number DMRG to find reference values
- The DMRG solution is in the feasible domain (so the implementation is correct)

Example: Hubbard model

1D square lattice

$n_i = 1$		$U = 4$	$U = 6$	$U = 8$	$U = 10$
$K = 10$	E	-0.6202	-0.4580	-0.3574	-0.2913
	$n_{i\uparrow} n_{i\downarrow}$	0.1071	0.0639	0.0406	0.0275
$K = 12$	E	-0.6049	-0.4466	-0.3486	-0.2842
	$n_{i\uparrow} n_{i\downarrow}$	0.1027	0.0618	0.0394	0.0267
Exact	E	-0.5737	-0.4201	-0.3275	-0.2672
	$n_{i\uparrow} n_{i\downarrow}$	0.1002	0.0582	0.0366	0.0248

- Approximately correct, but not as good as Xizhi Han's results
- Converges rather quickly: 20 minutes for $K = 12$, 7×10^5 variables
- Larger $U \Rightarrow$ smaller absolute error, larger relative error

Example: Hubbard model

1D square lattice

- Accuracy with various U
  - Expected: large $U \Rightarrow$ localized electrons, so with our local operators large U means higher accuracy
  - Observed: Larger $U \Rightarrow$ smaller absolute error, larger relative error
  - What's the correct way to evaluate the accuracy of numerical bootstrap?
- Main performance bottleneck: *before* optimization, the step turning QuantumAlgebra.jl operators into JuMP variables

Example: Hubbard model

1D square lattice with doping

$n_i = 0.5$		$U = 4$	$U = 6$	$U = 8$	$U = 10$
$K = 12$	E	-0.7830	-0.7593	-0.7444	-0.7342
	$n_{i\uparrow} n_{i\downarrow}$	0.0168	0.0102	0.0068	0.0048
DMRG	E	-0.7534	-0.7243	-0.7059	-0.6939
	$n_{i\uparrow} n_{i\downarrow}$	0.0189	0.0114	0.0075	0.0052

- Comparison of accuracy between half filling and hole doping
  - Errors larger than half filling
  - Expected: hole doping $\Rightarrow$ iterant electrons, whose behavior can't be captured by local operators $\Rightarrow$ poorer accuracy ✓
- U increase $\Rightarrow$ relative and absolute errors increase??

Example: Hubbard model

2D square lattice

$n_i = 1$		$U = 2$	$U = 4$	$U = 6$	$U = 8$
$K = 8$	E	-1.3164	-1.0491	-0.8626	-0.7276
	$n_{i\uparrow} n_{i\downarrow}$	0.1602	0.1105	0.0784	0.0576
DMRG	E	-1.176(1)	-0.8605(5)	-0.6565(1)	-0.5241(1)
	$n_{i\uparrow} n_{i\downarrow}$	0.188(1)	0.126(1)	0.0809(3)	0.0539(1)

- Time consumption gets larger (no real large-scale results)
- Error analysis
  - The absolute error of E as U shows an increasing tendency (the relative error goes all the way higher)
  - The absolute error of the double occupation decreases, and the relative error shows a decreasing tendency
  - Expected: larger $U \Rightarrow$ smaller error
  - Possible reason: energy bound is not very tight

Conclusion

- Verify the result of nonlinear SDP bootstrap for anharmonic oscillator
- Linear SDP for anharmonic oscillator and convergence problem
- Linear SDP for Hubbard model, 1D, 1D doped and 2D, and error analysis

Future prospects

- Symmetry breaking: so the ground state ρ is not a function of H:

$$\lim_{\beta\to\infty}\frac{1}{Z}\mathrm{e}^{-\beta H}=\frac{1}{2}(|\uparrow\rangle\langle\uparrow|+|\downarrow\rangle\langle\downarrow|)\neq \underbrace{|\uparrow\rangle\langle\uparrow|}_{\text{true ground state}} \tag{17}$$

- Bootstrapping spin models: Heisenberg model, lattice frustration, next neighbor interaction induced frustration, spin liquids, etc.
- Bootstrapping a *class* of models (e.g. "all possible QM models")
  - 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's the entropy?
  - What's the temperature in terms of operator expectations?
- What constraints are effective? (Important for scaling up and interpretation)
  - Can wave function ansatz (e.g. DMRG) provide some hints?
  - Constraints that are "almost" violated are the most important?
  - arXiv 2205.12325: bootstrap and perturbation theory