LA-UR-24-32118

Convex methods in quantum field theory

Scott Lawrence

Based in part on `arXiv:2408.11766`

and on `arXiv:2411.xxxxx` (with Brian McPeak and Duff Neill)

14 November 2024

Los Alamos NATIONAL LABORATORY

NNSA National Nuclear Security Administration

Outline

$$\langle \Psi | \Psi \rangle \geq 0$$

Part I

An overview of convex ("bootstrap") methods

Part II

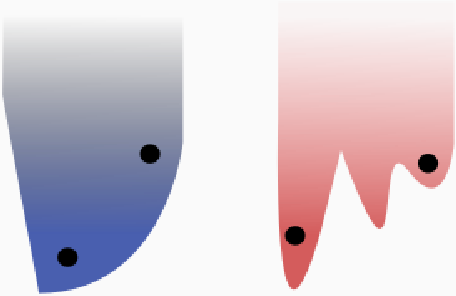
Spectral inversion via Lagrange duality

$$\langle\Psi|\Psi\rangle \geq 0$$

We'll work with operators (and expectations) instead of states:

$$\langle\mathcal{O}^\dagger\mathcal{O}\rangle \geq 0$$

This is a *convex constraint*.



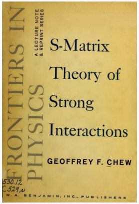
A historical note

A physics schoolbook circa 1880 supposedly contained a problem:

"Why can not a man lift himself by pulling up on his bootstraps?"

Prior to QCD: constrain strong interactions by **unitarity** and various symmetries.

No Lagrangian needed!



The numerical "conformal bootstrap" finally succeeeded at this (general) program last decade, via convex optimization.

Since then, we've started calling all convex optimization-based numerical methods in physics "bootstrap".

(See also: "booting" a computer, and the statistical bootstrap.)

Part I

Bootstrap methods in quantum mechanics

The space of density matrices

For some set of N operators $\{\mathcal{O}_i\}$...

$$\langle \mathcal{O}_i \rangle \equiv \mathrm{Tr}\, \rho \mathcal{O}_i$$

Now consider $\mathbb{R}^N$, the set of possible expectations of $\mathcal{O}_\bullet$. Think of this as a projection of the space of density matrices ρ.

- $\langle \mathcal{O}^\dagger \mathcal{O} \rangle \geq 0$ for all $\mathcal{O}$
- $\langle I \rangle = 1$ (the trace of ρ)

The constrained space is convex!

Any projected density matrix obeys these constraints, and any point in this set is the projection of some density matrix.

Finally, for computational convenience we re-write:

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle \geq 0 \Longrightarrow \langle \mathcal{O}_i^\dagger \mathcal{O}_j \rangle \succeq 0$$

Convex optimization: interior-point methods

Intuitively, convex functions (over convex spaces) are easy to minimize. **How do we actually do this?**

$$\text{minimize } f(x) \text{ subject to } g(x) \geq 0$$

1. Find any strictly feasible point ($g(x) > 0$)
2. Write down a barrier function :

$$\phi(x) = -\log g(x)$$

3. Set $t = 1$ and minimize

$$f_t(x) = f(x) + t^{-1} g(x)$$

4. Assign $t \to 2t$ and repeat until convergence

First (as far as I know) method like this described in [Dikin 1967].

Good introductory text is [Boyd-Vandenberghe 2004].

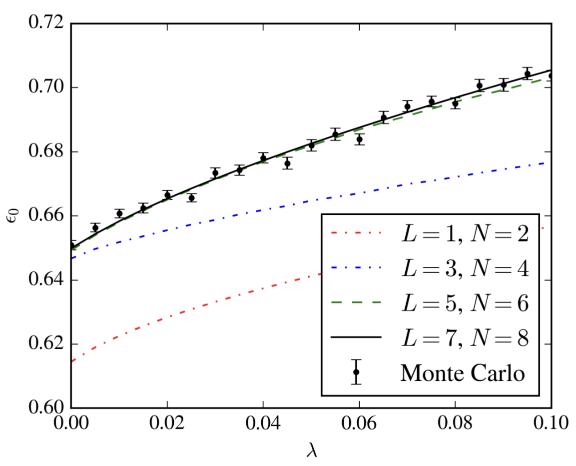
"Bootstrapping" quantum mechanics

We can efficiently compute (quite tight, in practice) **lower bounds** on ground state energies. Impose the usual constraints on $\langle \mathcal{O}^\dagger O \rangle$, and then minimize $\langle H \rangle$.

- The space to optimize over is convex (as discussed).
- The function being minimized is linear, and therefore convex.
- Why are these lower bounds? Any density matrix (including the true ground state) has some projection consistent with these bounds.

Dual to the variational method.

Demonstration: ϕ^4 on the lattice



For ϕ^4 field theory in one spatial dimension, with $m = 0.2$, at infinite volume. From [**SL** `2111.13007`].

Other (quantum mechanical) successes

Eigenstates: [Berenstein-Hulsey 2108.08757] [Berenstein-Hulsey 2109.06251]

Matrix quantum mechanics: [Han-Hartnoll-Kruthoff 2004.10212]

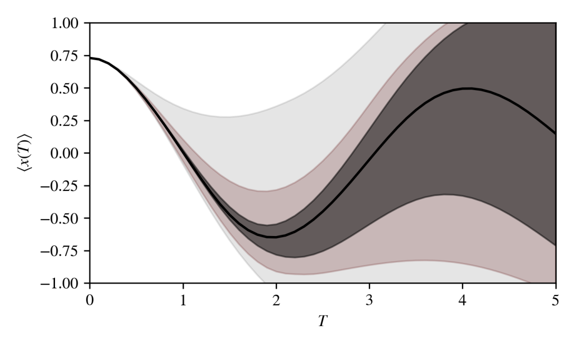
PT-symmetric or non-Hermitian systems: [Li 2202.04334] [Khan+ 2202.05351] [Khan-Rathod 2409.06784]

Finite fermion density: [Barthel-Hübener 2012] [**SL** 2211.08874]

See also related ideas in [Heller+ 2305.07703] regarding relativistic hydrodynamics, and the modern numerical S-matrix bootstrap.

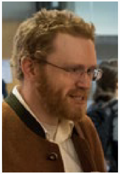
Real-time dynamics

Instead of tracking only a density matrix, we can track *time-dependent* expectations $\langle \mathcal{O} \rangle$. There is an additional linear constraint: $\frac{d}{dt}\langle \mathcal{O} \rangle = i\langle [H, \mathcal{O}] \rangle$.



$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{1}{2}\hat{x}^2 + \frac{1}{4}\hat{x}^4$$

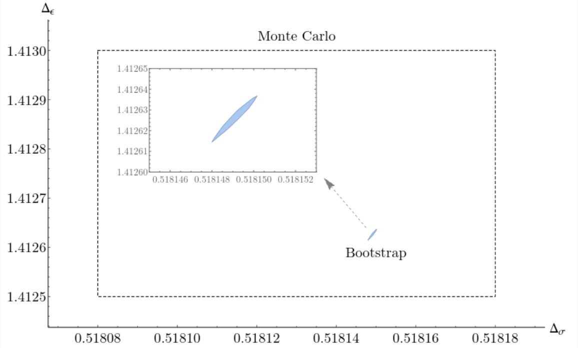
Brian McPeak



Duff Neill

The conformal bootstrap (briefly and crudely)

Positivity *in radial quantization* (inequalities), combined with crossing symmetry, defines the convex space.



See [Kos+ 1603.04436], or [Poland-Rychkov-Vichi 1805.04405] for a review.

Part II

Spectral inversion from Lagrange duality

Spectral reconstruction problems

$$C^{(E)}(\tau) = \int_0^\infty d\omega\, \rho(\omega) \frac{\cosh \omega \left(\frac{\beta}{2} - \tau\right)}{\sinh \frac{\beta\omega}{2}}$$

Given a finite set of measurements of the Euclidean correlator $C_i = C^{(E)}(\tau_i)$, with (correlated) Gaussian errors Σ_{ij}, estimate the smeared spectral density:

$$\tilde{\rho}_\sigma(\omega_0) \equiv \int_0^\infty d\omega\, \rho(\omega) e^{-\frac{(\omega-\omega_0)^2}{\sigma^2}}$$

Or, the (smeared) real-time correlator:

$$\tilde{C}_\sigma(t) \equiv \int dt' e^{-\frac{(t-t')^2}{\sigma^2}} \int d\omega\, \rho(\omega) \sin \omega t'$$

There are some questions we do not ask. Neither $\rho(\omega)$ nor $C(t)$ can be meaningfully constrained.

Spectral reconstruction as convex optimization

The spectral density functions $\rho(\omega)$ are constrained by $\rho(\omega \geq 0)$.

The lattice data provides further constraints. If there are no errors, these are linear constraints (certain integrals of $\rho(\omega)$ are known). With errors, these are convex inequalities:

$$v[\rho]^T \Sigma v[\rho] \leq F_{\max} \text{ where } v[\rho] \equiv C_i - \int \rho(\omega) K_i(\omega)$$

($F_{\max}$ must be chosen to define some confidence interval.)

The space $\{\rho(\omega)\}$, consistent with positivity and the lattice data, is convex.

Now consider some integral:

$$\mathcal{C}[\rho] = \int \mathcal{K}(\omega)\rho(\omega)$$

It's a linear function of a convex (infinite-dimensional) space.

Lagrangians

$$\text{minimize } f(x) \text{ subject to } g(x) \geq 0$$

We define a Lagrange function (or "Lagrangian")

$$L(x, \lambda) = f(x) - \lambda g(x)$$

Now notice that the optimal value p^* is given by

$$p^* = \min_x \max_{\lambda \geq 0} L(x, \lambda)$$

In general, we introduce one Lagrange multiplier (like λ) for every inequality.

$$L[\rho(\omega), \lambda(\omega), \mu] = \int \rho(\omega)\left(\mathcal{K}(\omega) - \lambda(\omega)\right) - \mu\left(F_{\max} - v^T[\rho]\Sigma v[\rho]\right)$$

The dual problem

$$p^* = \min_x \max_{\lambda \geq 0} L(x, \lambda)$$

We can define a dual problem by swapping the order of optimizations

$$d^* = \max_{\lambda \geq 0} \min_x L(x, \lambda)$$

Under "reasonable" conditions, we have $p^* = d^*$; and we always have $d^* \leq p^*$.

The dual is generally more "pleasant" to work with.

Roughly speaking, dual degrees of freedom "come from" primal constraints. In the spectral case, we get one Lagrange multiplier for each Euclidean data point.

Computing the Lagrange dual

For simplicity, restrict to the case with no statistical errors.

$$L[\rho(\omega), \lambda(\omega)] = \int \rho(\omega)\left(\mathcal{K}(\omega) - \lambda(\omega)\right)$$

The primal optimum: $p^* = \min_\rho \max_{\lambda \geq 0} L[\rho, \lambda]$.
Here the minimization over ρ is subject to $\int \rho K_i = C_i$.

Swapping the min/max order, the Lagrange dual function is defined:

$$g(\lambda) = \min_\rho \int \rho(\omega)\left(\mathcal{K}(\omega) - \lambda(\omega)\right)$$

The minimization is unbounded below *unless* the linear constraint tells us the value. In other words, the only permitted λ are of the form

$$\lambda(\omega) = \mathcal{K}(\omega) + \ell_i K_i(\omega).$$

We can now evaluate $g(\ell) = \ell_i C_i$, defining the dual optimization problem

$$\text{maximize } \ell_i C_i \text{ subject to } \mathcal{K}(\omega) - \ell_i K_i(\omega) \geq 0 \text{ (for all } \omega)$$

Enforcing an infinite number of constraints

With statistical errors, the dual problem reads:

$$\text{maximize } \ell^T C - \frac{F_{\max}}{4\mu}\ell^T M^{-1}\ell - \mu$$
$$\text{subject to } \mathcal{K}(\omega) - \sum_i \ell_i K_i(\omega) \geq 0$$
$$\text{and } \mu \geq 0$$

Recall the interior-point method at the beginning of this talk:

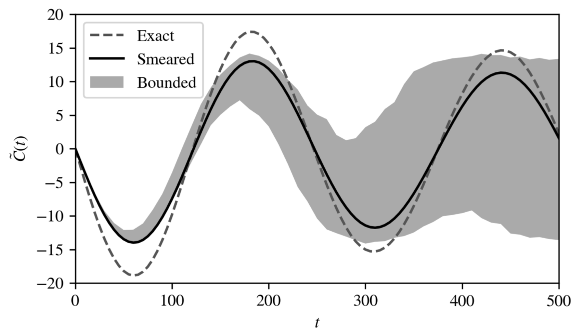
We need only write a barrier function!

$$b[\lambda, \mu] = -\int_0^\infty d\omega \, \log \lambda - \log \mu$$

Done.

Check: Anharmonic oscillator

Computing $\mathrm{Im}\langle x(t)x(0)\rangle$ with $L = \frac{1}{2}(\partial x)^2 + \frac{\omega^2}{2}x^2 + \frac{\lambda}{4}x^4$

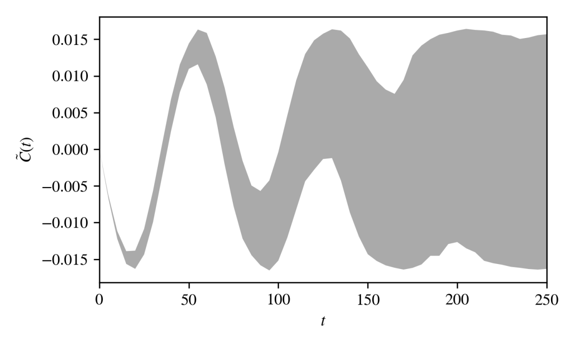


Calculation done on a 100-site lattice, with $\omega^2 = 10^{-4}$ and $\lambda = 10^{-5}$. A total of 3×10^{-4} samples used.

[**SL** `2408.11766`]

Linear response in ϕ^4 theory (2+1 dimensions)

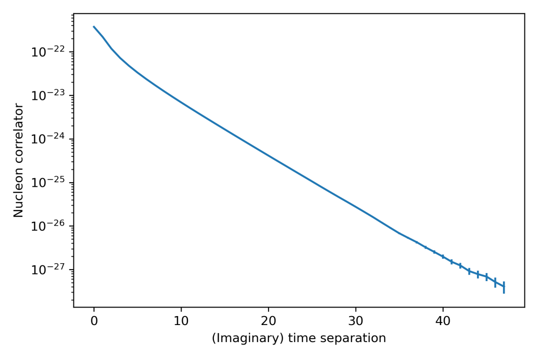
Computing $\mathrm{Im}\,\langle\phi(t)\phi(0)\rangle$ with $L = \frac{1}{2}(\partial\phi)^2 + \frac{m^2}{2}\phi^2 + \frac{\lambda}{4}\phi^4$



Calculation done on a $16^2 \times 80$ lattice, with $m^2 = 0$ and $\lambda = 10^{-2}$.
A total of $\sim 2 \times 10^5$ (imperfectly decorrelated) samples used.
[**SL** `2408.11766`]

Moving to lattice QCD

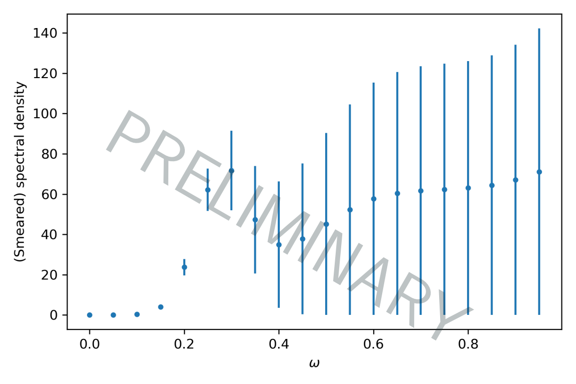
Not all calculations respect reflection positivity!



Easy: ignore the first few data points. Correct: drop (in a controlled way) positivity assumption on $\rho(\omega > \omega_0)$.

(MILC data, courtesy of Rajan Gupta and Jun-Sik Yoo)

Lattice data: nucleon



From a $96^3 \times 192$ lattice with $a = 0.057$ fm; physical pion mass.

Spectral density smeared with $\sigma = 0.05$.

Some open problems

Quantum-mechanical bootstrap:

- How to bootstrap "non-analytic" interactions? Concrete example: I give you a *tabulation* of $V(x)$, and ask for the ground state of $\hat{H} = \hat{p}^2 + V(\hat{x})$. *Nota bene:* Switching to second quantization is cheating.

Spectral inversion:

- Demonstrate bounds on the off-diagonal spectral function (from correlators $\langle \mathcal{O}_1(t)\mathcal{O}_2(0)\rangle$).
- How much does incorporating Schwinger-Dyson relations tighten this bound?