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Convex methods for sign problems

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Based in part on arXiv:2408.11766

and on arXiv:2412.08721 (with Brian McPeak and Duff Neill)

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Outline

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

Part I

Convex methods for real-time dynamics

Part II

Overview and philosophy

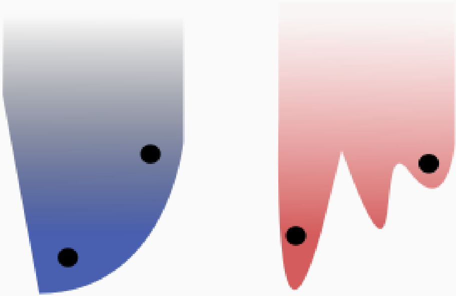
Convex geometry in quantum physics

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

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

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

This is a *convex constraint*.



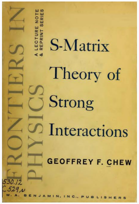
A historical note

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

Convex methods for real-time dynamics

The space of density matrices

$$\mathrm{Tr}\,\rho = 1 \quad \text{and} \quad \rho \succeq 0$$

The density matrix is **positive semi-definite**: $v^\dagger \rho v \geq 0$ for all v.

Expectation values are *projections*.

$$M_{ij} = \langle \mathcal{O}_i^\dagger \mathcal{O}_j \rangle \succeq 0$$

The space of ρ is **convex**. The space of M is a projection of a convex space (also **convex**).

What is the minimum value of $\langle \mathcal{O} \rangle$ consistent with $\rho \succeq 0$?

What is the minimum value of $\langle \mathcal{O} \rangle$ consistent with $M \succeq 0$?

Projections of density matrices

$$\{\hat{x}, \hat{p}\} \qquad M = \begin{pmatrix} \langle \hat{x}^2 \rangle & \langle \hat{x}\hat{p} \rangle \\ \langle \hat{x}\hat{p} \rangle - i & \langle \hat{p}^2 \rangle \end{pmatrix} \succeq 0$$

$$\{\hat{x}, \hat{p}, \hat{x}^2\} \qquad M = \begin{pmatrix} \langle \hat{x}^2 \rangle & \langle \hat{x}\hat{p} \rangle & \langle \hat{x}^2 \rangle \\ \langle \hat{x}\hat{p} \rangle - i & \langle \hat{p}^2 \rangle & \langle \hat{p}\hat{x}^2 \rangle \\ \langle \hat{x}^3 \rangle & \langle \hat{x}^2\hat{p} \rangle & \langle \hat{x}^4 \rangle \end{pmatrix} \succeq 0$$

"So what?" This implies the uncertainty principle:

$$\langle \hat{x}^2 \rangle \langle \hat{p}^2 \rangle \geq \frac{1}{4}$$

and therefore a lower bound on $\langle H \rangle$ of the harmonic oscillator.

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].

The primal approach

Describe a **convex** space:

- One point in this space is the “physical” point.
- The observable of interest is a convex (linear counts) function of this space.
- (Ideally) as more constraints are included, the space shrinks to the physical point.

Use IPM or similar to **bound** the observable.

The space of time-dependent density matrices

$$\rho(t) \succeq 0 \quad (\forall t)$$

As ever, we project to a finite set of operators:

$$M(t) \succeq 0 \quad (\forall t)$$

Heisenberg equations of motion:

$$\frac{d}{dt}\langle \mathcal{O} \rangle = i\langle [H, \mathcal{O}] \rangle$$

provide linear constraints on M:

$$\frac{d}{dt} \operatorname{Tr} CM(t) = \operatorname{Tr} DM(t)$$

This is an **infinite-dimensional** space.

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.

The space of spectral density functions

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:

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

(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:

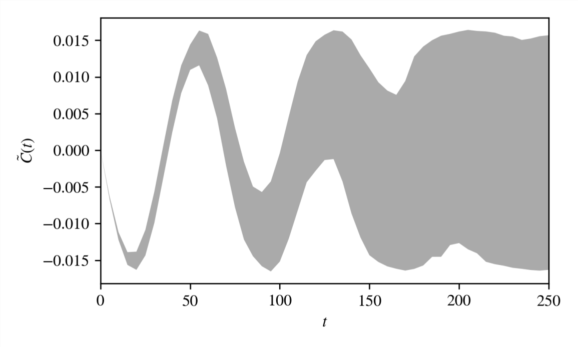
We need only write a barrier function!

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

Done.

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`]

Nonequilibrium dynamics: the dual problem

Primal:
$$\begin{cases} \textbf{minimize} & \operatorname{Tr} OM(T) \\ \textbf{subject to} & M(t) \succeq 0 \\ & \operatorname{Tr} A^{(i)} M(t) = 0 \\ & \operatorname{Tr} B^{(j)} M(0) = b_j \\ & \operatorname{Tr} \left(D^{(k)} - C^{(k)} \frac{d}{dt} \right) M(t) = 0. \end{cases}$$

Lagrangian: $L[M, \Lambda] = \operatorname{Tr} OM(T) - \int_0^T \Lambda(t) M(t)\, dt.$

Dual:
$$\begin{cases} \textbf{maximize} & \lambda_d^{(k)}(0) \operatorname{Tr} C^{(k)} M_0 \\ \textbf{subject to} & \lambda_d^{(k)}(T) C^{(k)} = O \\ & \lambda_a^{(i)}(t) A^{(i)} + \left(D^{(k)} + C^{(k)} \frac{d}{dt} \right) \lambda_d^{(k)} \succeq 0. \end{cases}$$

Discretizing the dual problem

$$\textbf{Dual:}\quad \begin{cases} \textbf{maximize } \lambda_d^{(k)}(0)\operatorname{Tr} C^{(k)} M_0 \\ \textbf{subject to } \lambda_d^{(k)}(T) C^{(k)} = O \\ \qquad \lambda_a^{(i)}(t) A^{(i)} + \left(D^{(k)} + C^{(k)} \frac{d}{dt}\right) \lambda_d^{(k)} \succeq 0. \end{cases}$$

Optimization over $\lambda_\bullet(t)$ is still infinite-dimensional. But we can restrict the search to a finite-dimensional subspace.

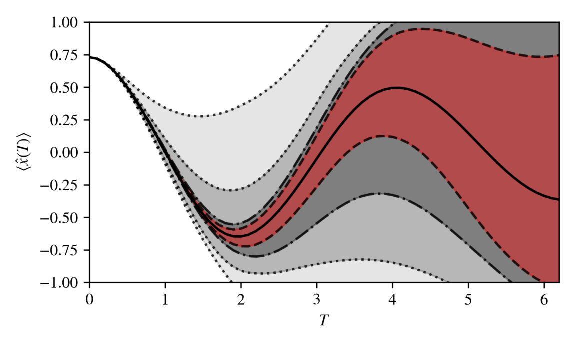
Let $\lambda_\bullet(t)$ be a quadratic spline with K knots.

$$\textbf{maximize } \lambda_d^{(k)}(0)\operatorname{Tr} C^{(k)} M_0$$

$$\textbf{subject to } \Lambda(t, y) \succeq 0 \text{ (for all } t\text{)}.$$

Nonequilibrium dynamics: one anharmonic oscillator

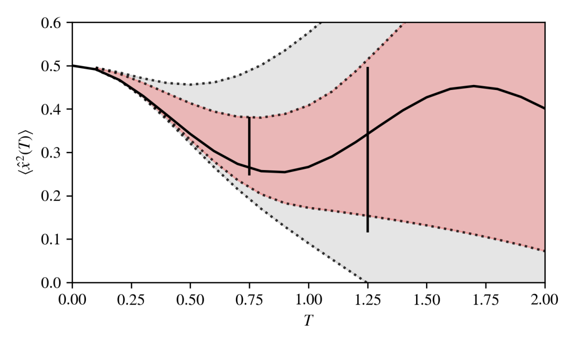
$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2} + \frac{\hat{x}^4}{4} \qquad |\psi(0)\rangle \propto |0\rangle + \frac{1}{2}|1\rangle + \frac{1}{4}|2\rangle$$



N	K	Algebraic	Derivatives	Parameters
4	0	7	7	35
4	3	7	7	77
9	3	56	21	441
9	6	56	21	672

Nonequilibrium dynamics: coupled anharmonic oscillators

$$\hat{H}_0 = \frac{\hat{p}^2 + \hat{q}^2}{2} + \frac{\hat{x}^2 + \hat{y}^2}{2} + \frac{(\hat{x} - \hat{y})^2}{2} \qquad \hat{H} = \hat{H}_0 + \frac{1}{8}(\hat{x}^4 + \hat{y}^4)$$



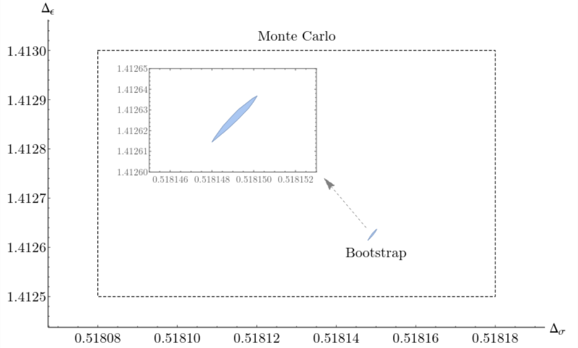
N	K	Algebraic	Derivatives	Parameters
8	0	34	18	138
8	3	34	18	294
26	0	521	103	1769

Part II

Overview and philosophy

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.

Finite fermion density

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

This can be used to obtain lower bounds on $\langle H \rangle$. The dual problem is termed "noncommutative sum-of-squares":

$$H = \sum_i \lambda_i A_i^\dagger A_i + C \Longrightarrow \langle H \rangle \geq C$$

The first numerical QM bootstrap that I know of is [Barthel-Hübener 2012], targeting the Hubbard model. See also [**SL** `2211.08874`].

Constraining the ground state

$$\langle \mathcal{O}^\dagger [H, \mathcal{O}] \rangle \geq 0$$

This statement uniquely fixes the ground state.

I can't find numerical works applying this sort of bound. (Most existing ground-state bounds are lower bounds only, using $\langle \mathcal{O}^\dagger \mathcal{O} \rangle \geq 0$.)

Stay tuned!

There is also a thermal generalization: "energy-entropy balance inequalities".

Bootstrapping the path integral

Without a sign problem, we have statements of the form

$$\int \mathcal{D}\phi \, e^{-S} |f(\phi)|^2 \geq 0$$

With a sign problem, we still have reflection-positivity.[1]

Implemented in the context of Yang-Mills [Kazakov-Zheng 2203.11360] and the Ising model [Cho+ 2206.12538].

[1] Terms and conditions apply! Enquire within.

Philosophy: Maintaining convexity

Here's a constraint true only for eigenstates [Berenstein-Hulsey 2209.14332]:

$$\langle H\mathcal{O}\rangle = E\langle\mathcal{O}\rangle$$

This constraint is not convex when E is unknown!

This is a *minor* problem with only one unknown (you can scan over all possible values of E). Adding unknowns to the Hamiltonian causes *major* problems.

Maintaining convexity of constraints is what lets these methods scale.

Philosophy: The space of proofs

$A = B$ is *two* statements: $A \leq B \wedge A \geq B$.

It should be easier to find pairs of statements if we separate $B_{\pm}$:

$$A \leq B_{+} \wedge A \geq B_{-}$$

A dual-feasible point is **a proof of a bound**.

There is therefore a particular space of proofs which is convex.
The 'strength' of the proof is a convex function on this space.

What types of proofs are missing from this space?

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?