An inverse problem for data-driven prediction in quantum mechanics

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Outline

Forgetting the physics and predicting only with data

Data determine the evolution

The initial-to-final-state inverse problem

A scheme to solve this inverse problem

How much further can we go?

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The initial-value problem

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- If the motion takes place under the influence of an electric potential either $V(\mathrm{x})$ or $V(\mathrm{t},\mathrm{x})$
$$\begin{cases} i\partial_{\mathrm{t}} u = -\Delta u + Vu & \text{in } (0,T)\times\mathbb{R}^n, \\ u(0,.) = f & \text{in } \mathbb{R}^n. \end{cases}$$

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- **Phenomenology-driven prediction**: it requires the knowledge of
$$-\Delta + V.$$

The data-driven approximate prediction problem

- For $N \in \mathbb{N}$, we define the **initial-to-final-state set with N elements**

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- This means to me: "*Let's forget physics and predict only with data.*"

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For $V \in L^1((0,T);L^\infty(\mathbb{R}^n))$:

- **The evolution map**

$$\mathcal{U} : f \in L^2(\mathbb{R}^n) \mapsto u \in C([0,T];L^2(\mathbb{R}^n))$$

is linear and bounded.

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- $\mathcal{D}_N$ consists of N points in the graph of $\mathcal{U}_T$.

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Theorem (C & Ruiz)

Assume $V_1(t,x)$ and $V_2(t,x)$ to have super-exponential decay with $n \geq 2$. Then,

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$$\mathcal{U}^1_T = \mathcal{U}^2_T \Rightarrow \mathcal{U}^1 = \mathcal{U}^2.$$

- Non-trivial: if $\mathcal{U}_t : f \longmapsto u(t,\cdot)$

$$\left.\begin{array}{l} i\dfrac{d}{dt}\mathcal{U}^j_t = H^j_t\mathcal{U}^j_t \quad \text{in } (0,T),\ j\in\{1,2\} \\ \mathcal{U}^1_T = \mathcal{U}^2_T. \end{array}\right\} \Rightarrow \mathcal{U}^1_t = \mathcal{U}^2_t \ \ \forall t(0,T).$$

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3. Reconstruction:
$$\mathcal{U}_T \longmapsto V?$$

Uniqueness: the case $V_1(\mathrm{t},\mathrm{x})$ and $V_2(\mathrm{t},\mathrm{x})$

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$$\mathcal{U}_T^1 = \mathcal{U}_T^2 \Rightarrow V_1 = V_2.$$

Uniqueness: the case $V_1(x)$ and $V_2(x)$

- We need $V \in L^1(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$ and **super-linear decay**

$$\sum_{j \in \mathbb{N}_0} 2^j \|V\|_{L^\infty(D_j)} < \infty,$$

where

$$D_0 = \{x \in \mathbb{R}^n : |x| \leq 1\}, \quad D_j = \{x \in \mathbb{R}^n : 2^{j-1} < |x| \leq 2^j\}, \forall j \in \mathbb{N}.$$

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Theorem (Cañizares, C, Parissis & Zacharopoulos)

Assume $V_1(\mathrm{x})$ and $V_2(\mathrm{x})$ to have super-linear decay with $n \geq 2$. Then,

$$\mathcal{U}_T^1 = \mathcal{U}_T^2 \Rightarrow V_1 = V_2.$$

Related results

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- Time-dependent Hamiltonian by Aïcha, Choulli, Eskin, Kian, Soccorsi, Tetlow...

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The orthogonality relation

Proposition

Given $V_1, V_2 \in L^1((0,T); L^\infty(\mathbb{R}^n))$. *We have*

$$\mathcal{U}_T^1 = \mathcal{U}_T^2 \quad \Longrightarrow \quad \int_\Sigma (V_1 - V_2) u_1 \overline{v_2} = 0,$$

for all u_1 *and* v_2 *in* $C([0,T]; L^2(\mathbb{R}^n))$ **physical solutions** *of*

$$(i\partial_t + \Delta - V_1)u_1 = (i\partial_t + \Delta - \overline{V_2})v_2 = 0 \text{ in } \Sigma = (0,T) \times \mathbb{R}^n.$$

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- Density of the product $u_1 \overline{v_2}$ would allow to conclude

$$V_1 = V_2.$$

Simplification of the problem

Assume to $F \in L^1(\mathbb{R} \times \mathbb{R}^n)$ satisfy that

$$\int_{\mathbb{R}\times\mathbb{R}^n} Fu\overline{v} = 0$$

for all physical solutions $(i\partial_t + \Delta)u = 0$ and $(i\partial_t + \Delta)v = 0$.

- Can we ensure that $F = 0$?

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$$\int_{\mathbb{R}\times\mathbb{R}^n} F(t,x)\, e^{-i(|\kappa|^2 t - \kappa\cdot x)}\, \overline{e^{-i(|\eta|^2 t - \eta\cdot x)}}\, \mathrm{d}(t,x) = 0 \qquad \forall \kappa, \eta \in \mathbb{R}^n.$$

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- Hence $\widehat{F}(|\kappa|^2 - |\eta|^2, \eta - \kappa) = 0$ for all $\kappa, \eta \in \mathbb{R}^n$.

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$$\kappa = -\frac{1}{2}\Big(1 + \frac{\tau}{|\xi|^2}\Big)\xi, \qquad \eta = \frac{1}{2}\Big(1 - \frac{\tau}{|\xi|^2}\Big)\xi;$$

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- By the injectivity of the Fourier transform, we have that $F(t, x) = 0$ for a.e. $(t, x) \in \mathbb{R} \times \mathbb{R}^n$.

Back to the full problem

- Recall that
$$\int_\Sigma (V_1 - V_2) u_1 \overline{v_2} = 0,$$
for all u_1 and v_2 physical solutions of $(i\partial_t + \Delta - V_1)u_1 = 0$ and $(i\partial_t + \Delta - \overline{V_2})v_2 = 0$.

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- The correction $u_1^\flat$ and $v_2^\flat$ should be negligible with respect to the free space solutions.
- How can we do that?

Complex geometrical optics

- Solutions with exponential growth

$$(t, x) \in \mathbb{R} \times \mathbb{R}^n \mapsto e^{i|\nu|^2 t + \nu \cdot x}$$

with $\nu \in \mathbb{R}^n \setminus \{0\}$.

Complex geometrical optics

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- For $(\tau, \xi) \in \mathbb{R} \times \mathbb{R}^n$ so that $\xi \neq 0$, we choose

$$\kappa = -\frac{1}{2}\Big(1 + \frac{\tau}{|\xi|^2}\Big)\xi, \qquad \eta = \frac{1}{2}\Big(1 - \frac{\tau}{|\xi|^2}\Big)\xi, \qquad \nu \cdot \xi = 0, \ \ \nu \neq 0;$$

and

$$u_1(t,x) = e^{i|\nu|^2 t + \nu \cdot x}\big(e^{-i(|\kappa|^2 t - \kappa \cdot x)} + u_1^\flat(t,x)\big),$$
$$v_2(t,x) = e^{i|\nu|^2 t - \nu \cdot x}\big(e^{-i(|\eta|^2 t - \eta \cdot x)} + v_2^\flat(t,x)\big).$$

These solutions are called **complex geometrical optics** (CGO).

Challenges of the proof

- Construction of the correction terms: $u_1^\flat$ and $v_2^\flat$. New inequalities for the Fourier multiplier yielding the correction terms, and making them negligible. More about it in a few slides.

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- Construction of the correction terms: $u_1^\flat$ and $v_2^\flat$. New inequalities for the Fourier multiplier yielding the correction terms, and making them negligible. More about it in a few slides.
- CGO solutions are not physical. Hence, the orthogonality relation has to be extended. This is why we need the potentials to decay super-exponentially. This has been previously addressed in the literature Novikov, Khenkin, Uhlmann, Vasy... However, some difficulties have arisen in our situation.

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Unbounded potentials

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- it has **local critical singularities**: $(a, b) \in [1, \infty] \times [1, \infty]$

$$\mathbf{1}_K(\mathrm{x}) V \in L^a((0, T); L^b(\mathbb{R}^n)); \;\; 2 - \frac{2}{a} = \frac{n}{b} \text{ with } (a, b) \neq \left(\infty, n/2\right)$$

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Theorem (C, Ruiz)

Assume $V_1(\mathrm{t}, \mathrm{x})$ and $V_2(\mathrm{t}, \mathrm{x})$ to have local critical singularities and super-exponential decay with $n \geq 2$. Then,

$$\mathcal{U}_T^1 = \mathcal{U}_T^2 \Rightarrow V_1 = V_2.$$

Challenges addressed

- Construction of the correction terms of the CGO:

$$u_1 = e^{i|\nu|^2 t + \nu \cdot x}\left(u_1^\sharp + u_1^\flat\right),$$
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- We have proved appropriate estimates to construct the correction terms for potentials that present local critical singularities and super-exponential decay. For the construction, we use a trick[1] inspired in the Birman–Schwinger principle.

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- We have proved appropriate estimates to construct the correction terms for potentials that present local critical singularities and super-exponential decay. For the construction, we use a trick[1] inspired in the Birman–Schwinger principle.
- CGO solutions are not physical. Hence, the orthogonality relation has to be extended. This is why we need the potentials to decay super-exponentially.

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Correction term of the CGO solution

Recall that CGO is a solution of

$$(i\partial_t + \Delta - V)u = 0 \text{ in } \mathbb{R} \times \mathbb{R}^n,$$

in the form

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Since $(i\partial_t + \Delta)(e^{i|\nu|^2 t + \nu \cdot x} u^\sharp) = 0$ in $\mathbb{R} \times \mathbb{R}^n$ we have that

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- Using Fourier transform we can find an inverse S_ν for $i\partial_t + \Delta + 2\nu \cdot \nabla$. In the next slide.
- Multiplication by V can be thought of as a perturbation.
- Is the operator $S_\nu \circ V$ quantitatively or qualitatively smaller than Id?

$$(\mathrm{Id} - S_\nu \circ V)u^\flat = S_\nu(Vu^\sharp).$$

How to capture this smallness

- To capture the smallness of $S_\nu \circ V$ one has to understand the interactions between S_ν and V.
- Since we want $\mathbf{1}_K(\mathrm{x})V \in L^a((0,T);L^b(\mathbb{R}^n))$, we need to study the boundedness of S_ν in mixed-norm Lebesgue spaces.

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The operator S_ν is the Fourier multiplier

$$S_\nu f(t,x) = \frac{1}{(2\pi)^{\frac{n+1}{2}}} \int_{\mathbb{R}\times\mathbb{R}^n} e^{i(t\tau + x\cdot\xi)} \frac{1}{-\tau - |\xi|^2 + i2\nu\cdot\xi} \widehat{f}(\tau,\xi)\,\mathrm{d}(\tau,\xi),$$

which solves $(i\partial_{\mathrm{t}} + \Delta + 2\nu\cdot\nabla)u = f$ in $\mathbb{R}\times\mathbb{R}^n$.

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which solves $(i\partial_\mathrm{t} + \Delta + 2\nu\cdot\nabla)u = f$ in $\mathbb{R}\times\mathbb{R}^n$. The set

$$\Gamma_\nu = \{(\tau,\xi) \in \mathbb{R}\times\mathbb{R}^n : -\tau - |\xi|^2 + i2\nu\cdot\xi = 0\}$$

is a paraboloid of codimension 2.

How to bound S_ν

There are two types of situations: near and far from Γ_ν.

- Far from Γ_ν the symbol

$$\frac{\mathbf{1}_{\mathrm{far}(\Gamma_\nu)}}{-\tau - |\xi|^2 + i2\nu \cdot \xi}$$

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- When the symbol is supported near Γ_ν, the multiplier can be understood as a restriction-and-then-extension set-up in two different sense:

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- Restriction-and-then-extension either in the paraboloid

$$\{(\tau,\xi)\in\mathbb{R}\times\mathbb{R}^n : \tau = -|\xi|^2\},$$

  or the hyperplane

$$\{(\tau,\xi)\in\mathbb{R}\times\mathbb{R}^n : \nu\cdot\xi = 0\}.$$

Estimates with gain in $|\nu|$

Theorem (C, Ruiz)

Consider $n \in \mathbb{N}$. There exists an absolute constant $C > 0$ such that

$$\sup_{j \in \mathbb{N}_0} \left(2^{-j/2} \|S_\nu f\|_{L^2(\Omega_j^{\hat{\nu}})} \right) \leq \frac{C}{|\nu|} \sum_{k \in \mathbb{N}_0} 2^{k/2} \|f\|_{L^2(\Omega_k^{\hat{\nu}})}$$

for all $f \in \mathcal{S}(\mathbb{R} \times \mathbb{R}^n)$.

Here $\hat{\nu} = \nu/|\nu|$ and

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- The decay in $|\nu|$ makes the correction terms negligible.

Estimates with no gain in $|\nu|$

Theorem (C, Ruiz)

Consider $n \in \mathbb{N}$ and $(q, r) \in [1, 2] \times [1, 2]$ such that

$$2 - \frac{2}{q} = \frac{n}{r} - \frac{n}{2},$$

with $(q, r) \neq \big(2, 2n/(n+2)\big)$. There exists a constant $C > 0$ that only depends on n, q and r such that

$$\|S_\nu f\|_{L^{q'}(\mathbb{R};L^{r'}(\mathbb{R}^n))} \leq C\|f\|_{L^q(\mathbb{R};L^r(\mathbb{R}^n))}$$

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Remark

We hope this estimate to be extended to $(q, r) = \big(2, 2n/(n+2)\big)$ for $n \geq 3$ —the Keel–Tao end-point. Then, $\mathbf{1}_K V \in C([0, T]; L^{n/2}(\mathbb{R}^n))$ with $n \geq 3$ would be an admissible local singularity.

Uniqueness should hold for Yukawa-type potentials

We want to consider $V = V(\mathrm{t}, \mathrm{x})$ so that for some compact $K \subset \mathbb{R}^n$:

- it has **local critical singularities**: $(a, b) \in [1, \infty] \times [1, \infty]$

$$\mathbf{1}_K(\mathrm{x}) V \in L^a((0, T); L^b(\mathbb{R}^n)), \quad 2 - \frac{2}{a} = \frac{n}{b} \text{ with } (a, b) \neq \left(\infty, n/2\right);$$

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Conjecture (C)

Assume $V_1(\mathrm{t}, \mathrm{x})$ and $V_2(\mathrm{t}, \mathrm{x})$ to have local critical singularities and a small-exponential decay with $n \geq 2$. Then,

$$\mathcal{U}_T^1 = \mathcal{U}_T^2 \Rightarrow V_1 = V_2.$$

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- There is a way of understanding what computational or data scientists mean when they say that in prediction the physics can be forgotten if you have enough data.

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- For $V(\mathrm{t}, \mathrm{x})$, we need to use CGO solutions to make the correction terms negligible, the orthogonality relation has to be extended for exponential solutions. This requires the potentials to have a super-exponentially decay.
- To ensure that the correction term become negligible we exploit the trace properties of the Fourier transform on hyperplanes.
- In order for the potentials to present local critical singularities, we need to prove suitable estimates for the correction terms in mixed-norm Lebesgue spaces—in the spirit of Strichartz inequalities.