A computational method in inverse scattering for radial potentials using phase shift data

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Scattering data for a potential in the Schrödinger equation comes in many different forms:

- Phase shift
- S-matrix
- Weyl function
- Spectral density function
- Left and right reflection coefficients
- Jost function
- Scattering amplitude
- ... more exotic choices

Inverse scattering: Given some form of scattering data, find the corresponding potential.

Many analytical and numerical approaches have been developed Most well known ones involve integral equations (Gelfand-Levitan, Marchenko, ...)

But these are not always so well suited to numerical computation due to high operation counts, and certain sources of instability

This presentation: Approach via *overdetermined hyperbolic boundary value problems*, which adapts in a fairly straightforward way to many forms of scattering data (and scattering problems for other differential operators) and has computational advantages

Let $V(x) = V(|x|)$ be a central potential on $\mathbf{R}^3$ which is sufficiently rapidly decaying at ∞.

The Schrödinger equation

$$iu_t = \Delta u + V(x)u$$

has solutions of the form

$$u = e^{-ik^2 t} Y_\ell^m(\theta, \phi) \frac{\psi(|x|)}{|x|}$$

where $\psi = \psi(r)$ satisfies

$$\psi'' + (k^2 - V(r) - \frac{\ell(\ell+1)}{r^2})\psi = 0 \qquad 0 < r < \infty$$

for some $\ell = 0, 1, 2, \ldots$

There exists a physically acceptable solution ψ, unique up to a constant multiple, satisfying

$$\psi(r) = O(r^{\ell+1}) \quad r \to 0$$

The phase shift comes from examining the behavior of this solution as $r \to \infty$:

In the absence of a potential we would have, as $r \to \infty$,

$$\psi(r) = C\sqrt{r}J_{\ell+1/2}(kr) \approx C \sin{(kr - \frac{1}{2}\ell\pi)}$$

With the potential present we get instead

$$\psi(r) \approx C \sin{(kr - \frac{1}{2}\ell\pi + \delta)}$$

for some $\delta = \delta_\ell(k)$. This is the phase shift.

The **inverse problem** is

Determine the potential $V(x)$ given phase shift data $\delta_\ell(k)$.

Two most common special cases:

- Fixed $\ell \in \{0, 1, 2, \dots\}$

- Fixed $k \in \mathbb{R}$

Older history (uniqueness, existence, constructive methods ...)

Levinson 1949, Bargman 1949, Borg 1949, Gelfand-Levitan 1951, Marchenko 1952, Jost-Kohn 1952, Kay 1955, Fadeev 1958, and lots more

Bound state data

For fixed ℓ we may regard

$$\psi = \psi(r,k)$$

defined for $r \geq 0$ and $k \in \mathbb{C}$.

For a finite number of special values of $k = i\kappa_j, \kappa_j > 0$ we may have $\psi \sim e^{-\kappa_j r}$ as $r \to \infty$, in which case $\psi_j \in L^2(0,\infty)$ is a bound state wave function for V.

Denote

$$s_j = \left(\int_0^\infty |\psi_j(r)|^2 \, dr\right)^{-1}$$

The bound state data is

$$\{\kappa_j, s_j\}_{j=1}^n$$

Marchenko's method ($\ell = 0$ case)

- Set

  $$F(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}[1-e^{2i\delta_0(k)}]e^{ikx}\,dk+\sum_{j=1}^{n} s_j e^{-\kappa_j x}$$

- Solve the integral equation

  $$A(x,y)+\int_x^{\infty} A(x,t)F(t+y)\,dt+F(x+y) = 0$$

  for $0 < x < y$

- Obtain the potential as

  $$V(x) = -2\frac{d}{dx}A(x,x)$$

Computational complexity: Assume no bound states for simplicity. Data is $\delta(k)$ sampled at K points.

Fourier transform step is $O(K \log K)$.

Main computational effort is in solving the integral equation, which is a second kind Fredholm equation on a semi-infinite interval for each fixed $x > 0$.

If you want to recover V at N points $x_j = j\Delta x$, discretize everything at these N points to get N $N \times N$ linear systems for total operation count $O(N^4)$.

Below is an $O(N^2)$ alternative (joint work with T. Aktosun)

There is the following sequence of steps:

1. $\delta_0(k) \longmapsto F(x)$ $(O(K \log K))$

2. $F(x) \longmapsto f(k)$ $(O(N^2 + K \log K))$

3. $f(k) \longmapsto g(t)$ $(O(K \log K))$

4. $g(t) \longmapsto V(x)$ $(O(N^2))$

Step 1

Just a Fourier transform but needs to be done the right way due to slow ($O(1/k)$) decay.

Step 2

Solve

$$B(t) + F(t) + \int_0^\infty F(t+s)B(s)\,ds = 0 \qquad t > 0$$

for $B(t)$, $t > 0$.

This can be done in $O(N^2)$ operations, exploiting 'Toeplitz+Hankel' structure.

Then set

$$f(k) = 1 + \int_0^\infty B(t)e^{ikt}\,dt$$

Step 3

Set

$$g(t) = \frac{2}{\pi} \int_0^\infty k \left(\frac{1}{|f(k)|^2} - 1 \right) \sin kt \, dk$$

(Then

$$g(t) = \frac{1}{2\pi} \int_\infty^\infty (M(k) - ik) e^{-ikt} \, dk$$

where $M(k)$ is the Weyl function for V.)

Step 4

The potential

$$V(x), 0 < x < a$$

is related to

$$g(t), 0 < t < 2a$$

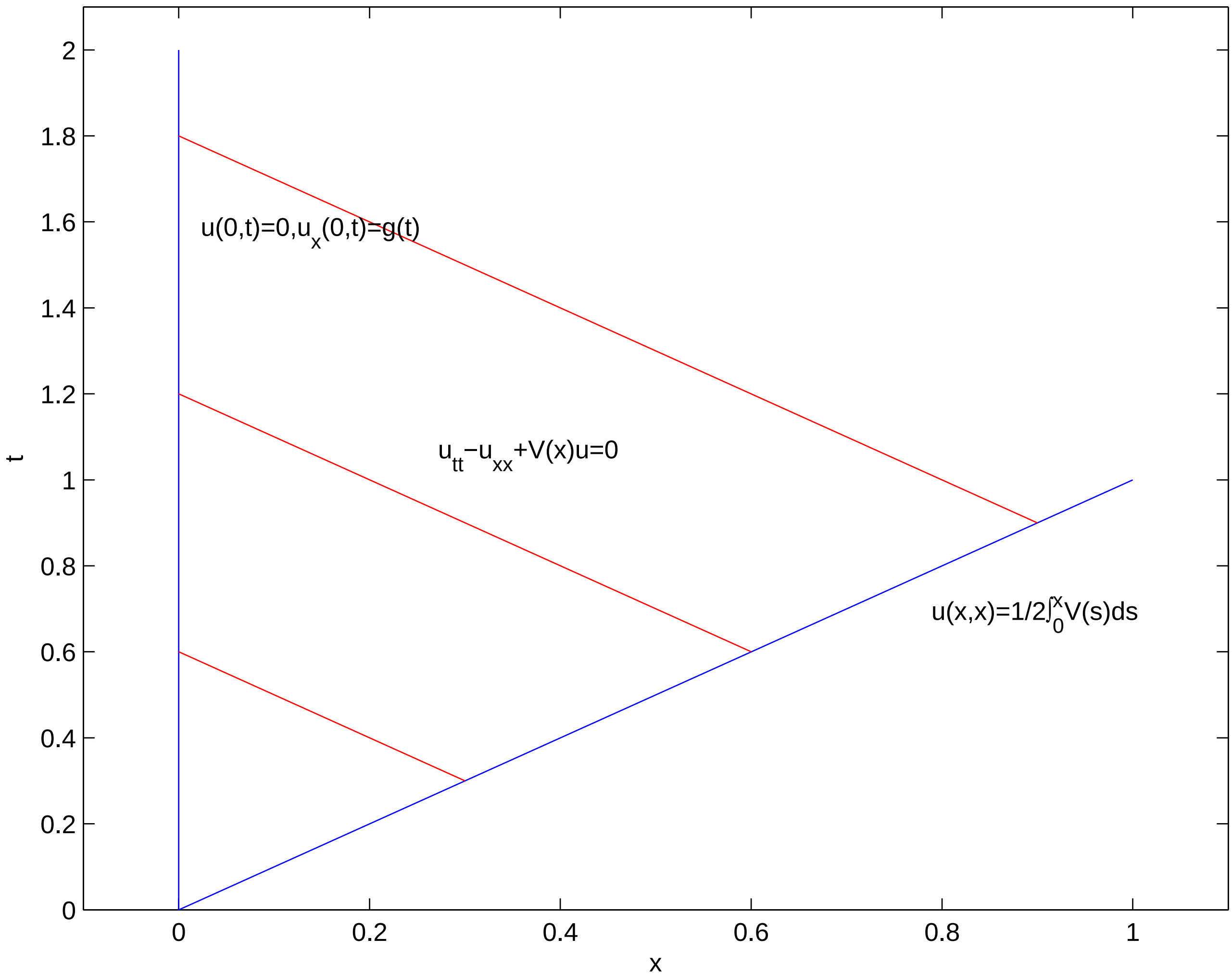
by the following 'overdetermined' hyperbolic boundary value problem.

$$u_{tt} - u_{xx} + V(x)u = 0 \qquad 0 < x < t < 2a - x$$

$$u(0,t) = 0 \qquad 0 < t < 2a$$

$$u_x(0,t) = g(t) \qquad 0 < t < 2a$$

$$u(x,x) = -\frac{1}{2}\int_0^x V(s)\,ds \qquad 0 < x < a$$


u(0,t)=0,u_x(0,t)=g(t)
u_tt−u_xx+V(x)u=0
u(x,x)=1/2∫_0^x V(s)ds
t
x
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

This is one of a collection of problems, in which the Cauchy data on $x = 0$

$$u(0, t) = f(t) \qquad u_x(0, t) = g(t)$$

are prescribed, along with the condition on the characteristic line $t = x$.

It is known that V is uniquely determined by g, there is continuous dependence in appropriate norms, and fast reliable computational methods are available.

The best of these are $O(N^2)$ and rely on a further transformation to an 'impedance form' equation

$$\eta(x)u_{tt} - (\eta(x)u_x)_x = 0$$

(See Bube-Burridge, Santosa-Schwetlick, Corones-Davison-Krueger etc.)

The $\ell \neq 0$ case:

There is a similar integral equation formalism, but there are complications

- The function $F(x)$ is no longer a Fourier transform

- The kernel of the integral equation is no longer a function of the sum of the variables

Computational complexity increases considerably.

Alternative approach ($\ell = 1$ for example):

Theorem of Marchenko states: there exists $V_0(r)$ having phase shift $\delta_1(k)$ for $\ell = 0$.

Furthermore, if

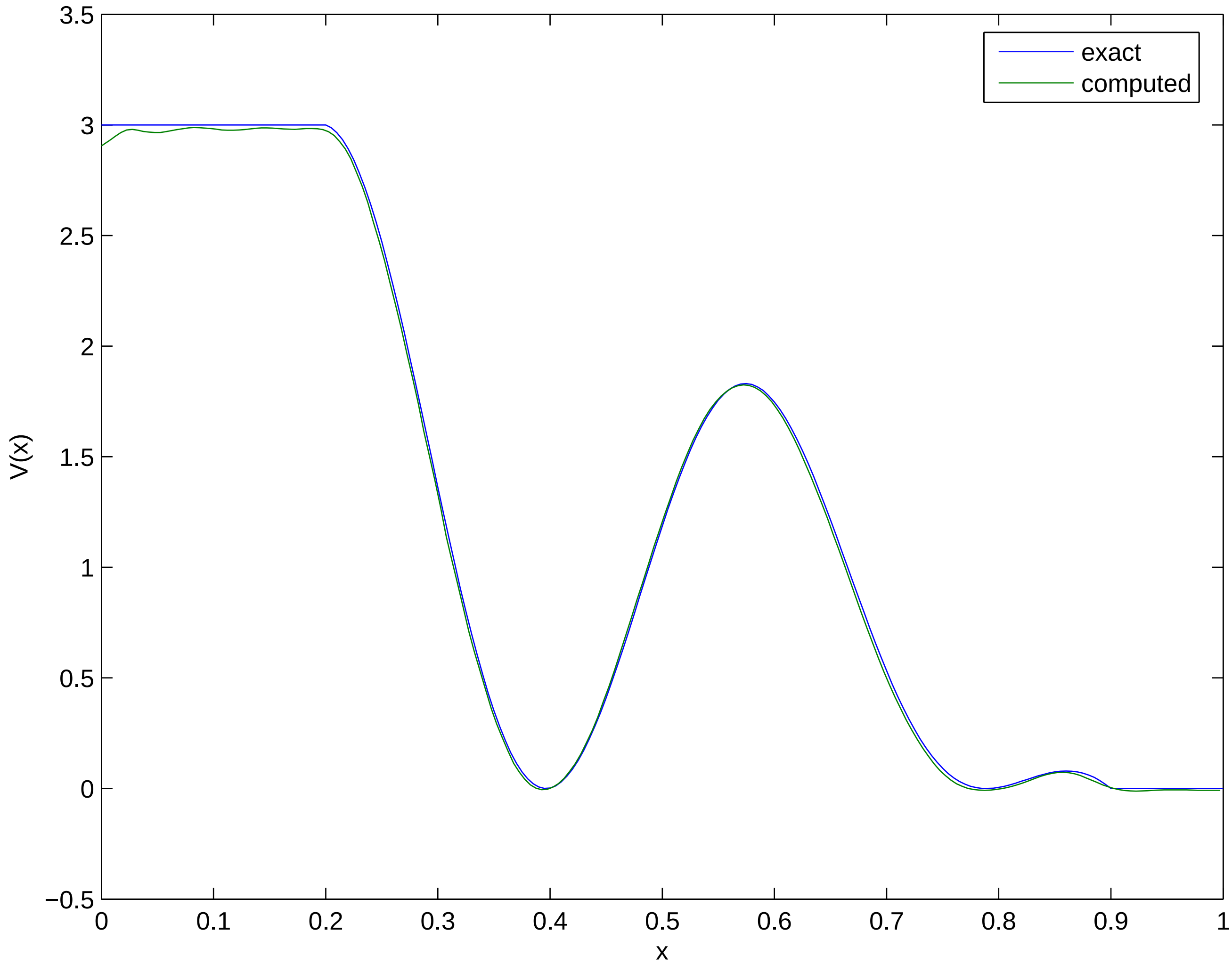
$$\phi'' = V_0 \phi \qquad \phi(0) = 0$$

then

$$V(r) = 2\left(\frac{\phi'(r)}{\phi(r)}\right)^2 - V_0(r) - \frac{2}{r^2}$$

Thus you use the $\ell = 0$ technique with data δ_1 to obtain V_0 and then the above relations to get $V(r)$ (with $O(N)$ work).

Various relations between V_0, V can be proved and exploited


exact
computed
V(x)
x
3.5
3
2.5
2
1.5
1
0.5
0
−0.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1