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FAST ALGORITHMS FOR THE INTEGRAL EQUATIONS OF THE INVERSE SCATTERING PROBLEM†

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The Gelfand-Levitan and Marchenko equations of inverse scattering theory are integral equations with Toeplitz and Hankel kernels respectively. It is shown that these facts can be used to reduce the integral equations to differential equations which can be solved with an order of magnitude less computation than generally envisaged.

1. In solving the inverse scattering problem it is conventional to use one of two approaches, that due to Gelfand-Levitan (perhaps as modified by Krein), or that due to Marchenko (cf. the surveys [1], [2]). Both lead to integral equations. In this note, we indicate how the special structure of the kernels in these equations can be exploited to develop fast algorithms solving them--fast in the sense that if a discretization into N small time intervals is made, the number of calculations grows as $0(N^2)$ rather than, as normal, $0(N^3)$. These reductions are based on special algorithms developed in [4], [5] for integral equations with Toeplitz and Hankels kernels.

2. We shall consider the S-wave case, and for convenience we shall assume there are no bound states. Assuming that a phase shift $\delta(\cdot)$ is given satisfying the standard conditions, the Gelfand-Levitan-Krein procedure is as follows. Define

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$$F(k) = \exp\left[-\frac{2}{\pi}\int_0^\infty \frac{\delta(k')}{k'^2-k^2}\,k'\,dk'\right] \qquad (2.1)$$

and

$$H(r) = \frac{1}{\pi}\int_0^\infty \cos kr\left[\frac{1}{|F(k)|^2} - 1\right]dk \qquad (2.2)$$

Let $\Gamma_{2r}(\cdot)$ be the solution of the integral equation

$$\Gamma_{2r}(u) + H(u) + \int_0^{2r} \Gamma_{2r}(s)H(s-u)\,ds = 0,\ 0 \leq u \leq 2r \qquad (2.3)$$

Then the potential is [1], [2]

$$V(r) = -2\frac{d}{dr}[\Gamma_{2r}(2r)] + 4\,\Gamma_{2r}^2(2r) \qquad (2.4)$$

Defining $a(2r;2r-u) = -\Gamma_{2r}(u)$, one can rewrite (2.3) as

$$\underset{T}{a(T;s)} + \int_0^{} a(T;u)H(u-t)\,du = H(T-s),\ 0 \leq s \leq T \qquad (2.5)$$

The Toeplitz nature of the kernel $H(u-t)$ can then be exploited to show that the integral equation can be reduced to a differential equation form which is easier to solve [4]. The relevant differential equation turns out to be [3], [4]

$$\left[\frac{\partial}{\partial t} + \frac{\partial}{\partial s}\right] a(t;s) = -a(t;t-s)a(t;0) \qquad (2.6)$$

To see the potential advantages of this reduction, we examine a (naive) way of solving it numerically. Consider a discretized version of (2.6) with $\alpha(j;\ell) = a(j\Delta;\ell\Delta)$. Suppose that $\alpha(k,\ell)$ is known for $0 \leq \ell \leq k \leq j$. Then (2.5) yields

$$\alpha(j+1,\ell+1) = \alpha(j,\ell) - \alpha(;j-\ell)\alpha(\ell;0)\Delta \qquad (2.7)$$

while $\alpha(j+1,0)$ comes from (2.5) as

$$\alpha(j+1;0) = H((j+1)\Delta,0) - \sum_{\ell=1}^{j+1} \alpha(j+1;\ell)H(\ell\Delta;0)\Delta \qquad (2.8)$$

Moreover, to get $\alpha(j;\ell)$ for any $\ell \leq j$ takes proportional to j^2 operations; this compares with the order of j^3 op-

erations needed to find $a(\cdot)$ via a direct discretization of Eq. (2.5). Note that this recursive solution method allows us to easily accommodate increased values of the upper limit T in (2.5).

3. The Marchenko calculations of $V(r)$ [1], [2] start with the definitions

$$S(k) = \exp[2i\delta(k)], \quad A_0(t) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} [S(k)-1]e^{ikt}\,dk \qquad (3.1)$$

Next one defines $A(r,t)$ for $0 \leq r \leq t$ as the solution of

$$A(r,t) = A_0(r+t) + \int_r^{\infty} A(r,s)A_0(s+t)\,ds \qquad (3.2)$$

with the result that

$$V(r) = -2\,\frac{dA(r,r)}{dr} \qquad (3.3)$$

The integral equation (3.2) has a Hankel kernel, which fact can be exploited by a method patterned after that in [5]. The first step is to introduce a second integral equation for a "dual" quantity

$$\tilde{A}(r,t) = A_0(r+t) - \int_r^{\infty} \tilde{A}(r,s)A_0(s+t)\,ds \qquad (3.4)$$

(This equation is discussed further below.) From (3.2) and (3.4), using the Hankel structure of the kernel A_0 one can derive the following coupled equations:

$$\frac{\partial}{\partial r}\tilde{A}(r,t) - \frac{\partial}{\partial t}A(r,t) = [A(r,r) - \tilde{A}(r,r)]\tilde{A}(r,t) \qquad (3.5)$$

$$\frac{\partial}{\partial t}\tilde{A}(r,t) - \frac{\partial}{\partial r}A(r,t) = [A(r,r) + \tilde{A}(r,r)]A(r,t) \qquad (3.6)$$

To see the potentialities of these equations, we consider a simple discretization as

$$-\tilde{\alpha}(j-1,i) =$$

$$-\tilde{\alpha}(j,i) - \alpha(j,i) + \alpha(j,i+1) + \Delta[\alpha(j,j) - \tilde{\alpha}(j,j)]\tilde{\alpha}(j,i) \qquad (3.7)$$

$$-\alpha(j-1,i) =$$

$$\tilde{\alpha}(j,i) - \tilde{\alpha}(j,i+1) + \alpha(j,i) + \Delta[\alpha(j,j) + \tilde{\alpha}(j,j)]\alpha(j,i) \qquad (3.8)$$

If $\tilde{\alpha}(k,i)$ and $\alpha(k,i)$ are known for all $j \leq k \leq i$, (3.7) supplies $\tilde{\alpha}(j-1,i)$ and (3.8) supplies $\alpha(j-1,i)$ for all $i \geq j$. The quantities $\tilde{\alpha}(j-1,j-1)$ and $\alpha(j-1,j-1)$ are obtained by discretizing (3.4) on the diagonal $t = r$. The scheme needs to be initialized by solving (3.2) and (3.4) for some large fixed r'. Then the scheme recursively obtains values at discrete points of $A(r,s)$ for $r < r'$. With $[r,r']$ discretized into N subintervals, the calculations grow at a rate $0(N^2)$.

4. We describe why the added equation (3.4) has a solution. Let a superscript hat denote an operator associated with an integral kernel. Define $\Delta(t,s) = \delta(t+s)$, then $\hat{\Omega} = \hat{H} - \hat{H}\hat{\Delta}$ has

$$\Omega(t,s) = \frac{2}{\pi}\int_0^\infty \sin kt \left[\frac{1}{|F(k)|^2} - 1\right] \sin ks \, dk$$

and $\hat{\Theta} = \hat{H} + \hat{H}\hat{\Delta}$ has

$$\Theta(t,s) = \frac{2}{\pi}\int_0^\infty \cos kt \left[\frac{1}{|F(k)|^2} - 1\right] \cos ks \, dk$$

Evidently, $I + \hat{\Omega} > 0$, $I + \hat{\Theta} > 0$. Now it is shown in [2] that there exists a Volterra operator $\hat{\Pi}$ for which $(I+\hat{\Pi})(I+\hat{H})(I+\hat{\Pi}^a) = I$ and

$$(I-\hat{A}_0) = (I+\hat{\Pi})(I+\hat{\Omega})(I+\hat{\Pi}^a) = I + (I+\hat{\Pi})\hat{H}\hat{\Delta}(I+\hat{\Pi}^a) \quad (4.1)$$

Here $A_0 = A_0(t+s)$ is restricted to $0 \leq t,s < \infty$. It follows that

$$I+\hat{A}_0 = (1+\hat{\Pi})(I+\hat{\Theta})(I+\hat{\Pi}^a) > 0$$

and therefore that (3.4) is solvable.

5. The numerical schemes used above were meant only to illustrate the order-of-magnitude reductions possible by exploiting the special Toeplitz or Hankel structure of the kernels. More work needs to be done on the numerical analysis aspects of these schemes and equations.

6. The above ideas suggest that extension to matrix problems could well be profitable. (Such extensions are known to be possible for solving integral equations with Toeplitz and

Hankel kernels.) Also, the role of the dual integral equation (3.4) needs to be further investigated. What about equations with non-Toeplitz or non-Hankel kernels? It has been shown that the above algorithms can be extended to arbitrary kernels, but the amount of computation goes up by a factor related to a suitably defined "index" of non-Toeplitzness or non-Hankelness of the kernel--see [3], [4]. The role of such possibilities in more general versions of the inverse scattering problem remains to be investigated.

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