Inverse Scattering

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Computed tomography solved the problem of determining what's inside an object using energy that traveled in straight lines as was only attenuated by the object. A more difficult but relevant problem is how to determine what's inside an object using energy that scatters as it propagates through an object. The classic problem of this type is called inverse scattering. It is an important problem that has seen only limited practical use due to the complexity of its solution.

1 Scalar field Equation

The starting point of our discussion of inverse scattering is the assumption that the scalar field satisfies the wave equation with propagation speed c, and source term $q(\mathbf{x})$:

$$\nabla^2 \hat{u}(\mathbf{x}, t) = \frac{1}{c^2} \frac{\partial^2 \hat{u}(\mathbf{x}, t)}{\partial t^2} + \hat{q}(\mathbf{x}, t).$$

Further, it is assumed that the time variation is harmonic (sinusoidal) so that

$$\begin{aligned} \hat{u}(\mathbf{x}, t) &= u(\mathbf{x}) e^{-j2\pi vt} \\ \hat{q}(\mathbf{x}, t) &= q(\mathbf{x}) e^{-j2\pi\nu t} \end{aligned}$$

Then,

$$\nabla^2 u(\mathbf{x}) + 4\pi^2 k^2 u(\mathbf{x}) = q(\mathbf{x}),$$

where $k = \frac{\nu}{c} = \frac{1}{\lambda}$ where λ is the wavelength of the radiation. This relation is called the Helmholtz equation.

There are many inverse problems that we can identify form this basic scalar relationship depending on what is viewed as the "input" and what is the "output". If the input is considered the field on some closed surface Σ_1 and the output is the field on another closed surface Σ_2, then we have the inverse diffraction problem. If the input is viewed as the source function $q(\mathbf{x})$ in some finite region D and the output is the field on some surface closed Σ_1 then we have the inverse source problem. Both of these problems are linear. Inverse-scattering is a non-linear problem that also derives from this scalar relationship.

To elucidate the inverse diffraction and inverse source problem we need to find an explicit expression for u. To do this we will be using some mathematics that you already have some familiarity with (but have only seen applied in a limited fashion in 1 dimensional problms). To understand better what we are going to do in 3-dimensional space, we will introduce an analogy with systems that process 1-d signals which you may be more familiar with.

2 1-D analogy

Consider the ordinary differential equation (ODE) with constant coefficients

$$\frac{d^2 y(t)}{dt^2} + a_0 y(t) = x(t)$$

This specifies some relation between y and x, but not uniquely. Suppose z satisfies

$$z''(t) + a_0 z(t) = 0.$$

Then, if $y_p(t)$ satisfies the given relationship then $y(t) = y_p(t) + Cz(t)$ also satisfies the relationship where C is any constant value, so clearly we have not determined a unique result unless we add additional constraints the problem must solve. These additional constraints are auxilliary conditions and are most often discussed in terms of "boundary" or "initial" conditions. You've learned previously that "initial-rest" conditions transformed every linear ODE into a shift-invariant system, but we want to generalize this result. Because impulse responses are so useful for linear systems, we want to define one for this system and see what results. In other words, we define a function to be the output when an impulse at $t'$is placed into the system:

$$\frac{d^2h(t;t')}{dt^2} + a_0 h(t;t') = \delta(t-t').$$

Now, notice that if we assume $t' \in (a,b)$ then,

$$\begin{aligned}
\int_a^b \frac{d}{dt}\left(y\frac{dh}{dt} - h\frac{dy}{dt}\right)dt &= \left. y\frac{dh}{dt} - h\frac{dy}{dt}\right|_a^b \\
\int_a^b \left[y\frac{d^2h(t;t')}{dt} - h(t;t')\frac{d^2y}{dt^2}\right]dt &= \left. y\frac{dh}{dt} - h\frac{dy}{dt}\right|_a^b \\
\int_a^2 \{y(t)[\delta(t-t') - a_0h(t;t')] - h(t;t')[x(t) - a_0y(t)]\}\,dt &= \left. y\frac{dh}{dt} - h\frac{dy}{dt}\right|_a^b \\
\int h(t;t')\,x(t) + \left. y(t)\frac{dh(t;t')}{dt} - h(t;t')\frac{dy(t)}{dt}\right|_{t=a}^b &= y(t').
\end{aligned}$$

So, we see that the relationship between x and y is only linear equation if we can get rid of the second term. Otherwise it is an affine equation. To specify $h(t;t')$ fully we still have to specify auxilliary conditions. It is easiest in this formulation to specify boundary conditions. If we have initial rest so that $y(a) = y'(a) = 0$ then choosing $h(b;t') = \frac{dh}{dt}(b;t') = 0$ will give a linear system.

We will be doing a similar bit of analysis but in multiple dimensions. We will then end-up with an explict formula for u using the impulse response of the system. In multiple dimensions, the impulse response is also called the Green's function because the integral relationship is called Green's identity.

3 Explicit scalar field relationship

Green's identity for any two scalar fields can be extended to higher dimensions. (It is just application of the divergence theorem to $u\nabla G - G\nabla u$). The result is:

$$\int_V \left(u\nabla^2 G - G\nabla^2 u\right)dV = \oint_S \left(u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n}\right)dS.$$

where V is any volume bounded by S and n is the normal direction to the boundary S. Adding and subtracting $4\pi^2k^2Gu$ on the left side produces

$$\int_V \left[u\left(\nabla^2 G + 4\pi^2k^2G\right) - G\left(\nabla^2 u + 4\pi^2k^2u\right)\right]dV = \oint_S \left(u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n}\right)dS.$$

Let u be the scalar field of interest and let G be the scalar field that satisfies

$$\nabla^2 G(\mathbf{x};\mathbf{x}') + 4\pi^2k^2G(\mathbf{x};\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}') \tag{1}$$

which makes G a Green's function of this differential equation.

Notice that we have not specified G completely yet until we fix some boundary conditions. Thus, just as the Helmholtz equation can define several distinct linear operators, the Green's function equation can provide a linear kernel for each of those operators by some choice of the boundary conditions. For each of these Green's functions, interchanging the role of $\mathbf{x}$ and $\mathbf{x}'$ does not change the defining differential equation, thus $G(\mathbf{x};\mathbf{x}') = G(\mathbf{x}';\mathbf{x})$ and we will therefore not be too concerned about specifying whether or not differentiation/integration acts on $\mathbf{x}$ or $\mathbf{x}'$. In general $\mathbf{x}'$ will be the "source" or object coordinates while $\mathbf{x}$ will be the observation, or data coordinates. We will generally integrate over $\mathbf{x}'$.

Using Eq. (1) we can write Green's identity as

$$u(\mathbf{x}) = \int_V GqdV + \oint_S \left(u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n} \right) dS$$

for any arbitrary volume and any scalar function G satisfying Eq. (1).

4 Inverse diffraction

For inverse diffraction, the unknown object $m(\mathbf{x})$ is the field constrained to a closed surface,Σ_1:

$$m(\mathbf{s}) = u(\mathbf{x})|_{\Sigma_1},$$

the data $d(\mathbf{s})$ are the measured values of the field on the closed surface Σ_2. In between Σ_1 and Σ_2 we assume that there are no sources $q(\mathbf{x}) = 0$. Notice that $m(\mathbf{s})$ and $d(\mathbf{s})$ are two-variable functions because they are restricted to a surface in 3-dimensional space. We would like to find a kernel $K(\mathbf{s};\mathbf{s}')$ that makes explicit the abstract linear operation $d = Am$:

$$d(\mathbf{s}) = \int K(\mathbf{s};\mathbf{s}')\, m(\mathbf{s}')\, d\mathbf{s}'.$$

Now, to completely specify this problem within some domain we need to define additional auxiliary conditions on u. One way to do this is to require that u be an outward traveling wave as $r \to \infty$. This is accomplished via the *Sommerfeld radiation* conditions requiring that

$$\lim_{r\to\infty} r\left(\frac{\partial}{\partial r} - j2\pi k\right) u(\mathbf{x}) = 0,$$

where $r = |\mathbf{x}|$. These conditions just mean that as r gets big we can write

$$u(\mathbf{x}) \approx \frac{e^{j2\pi kr}}{r} u_\infty(\theta,\phi)$$

where $u_\infty(\theta,\phi)$ is some arbitrary *far-field radiation pattern.*

With u better specified, we can find the desired kernel through the Green's function formalism previously explained. Define the volume V to be the space bounded by the surfaces Σ_1 and a sphere at $r = \infty$. Then, in V, there are no sources, so $q(\mathbf{x}) = 0$, thus the solution to the Helmholtz equation is

$$u(\mathbf{x}) = \oint_S u\frac{\partial G}{\partial n} dS - \oint G\frac{\partial u}{\partial n} dS.$$

Choose G to be zero on Σ_1 and satisfy Sommerfield radiation conditions at infinity. This specifies G completely. The second integral is zero on Σ_1 (because $G = 0$ by design) and at infinity the integral is

$$\lim_{r\to\infty} \int_0^{2\pi} \int_0^{\pi} \frac{e^{j2\pi kr}}{r} G_\infty(\phi,\theta) \frac{e^{j2\pi kr}}{r} \left[j2\pi k - \frac{1}{r} \right] u_\infty(\phi,\theta)\, r d\theta d\phi \quad = \quad 0.$$

For exactly the same reason, the integral at infinity for the first integral is also zero. Therefore, the value of $u(\mathbf{x})$ can be computed entirely from it's value on the surface Σ_1.

$$u(\mathbf{x}) = \int_{\Sigma_1} \left. \frac{\partial G(\mathbf{x};\mathbf{x}')}{\partial n'} \right|_{\mathbf{x}'=\Sigma_1} m(\mathbf{s}')\, d\mathbf{s}',$$

where it must be remembered that $d\mathbf{s}$ is an area measure. Thus, we see that to relate the field on surface Σ_2 to the field on surface Σ_1 we have the linear system:

$$u(\mathbf{s}) = \int_{\Sigma_1} K(\mathbf{s};\mathbf{s}')\, m(\mathbf{s}')\, d\mathbf{s}'$$

where

$$K(\mathbf{s};\mathbf{s}') = \left.\frac{\partial G(\mathbf{x};\mathbf{x}')}{\partial n'}\right|_{\mathbf{x}'=\Sigma_1,\mathbf{x}=\Sigma_2}.$$

In general, it may be a challenge to find K for arbitrary surfaces, and it may be necessary to compute K numerically. When Σ_1 and Σ_2 are spheres of radius a_1 and a_2 it is possible to find an expression for K. In that case we note that $\mathbf{s} = [\theta, \phi]$ and $d\mathbf{s} = r^2 \sin\theta d\theta d\phi$ where r is the radius of the integration surface. Also, the normal to the integration surface is r $(n = r)$. The derivation for $K(\mathbf{s};\mathbf{s}')$ in that case is given in the Appendix.

4.1 Inverse Source

The inverse source problem is to determine $q(\mathbf{x})$ given measurements of $u(\mathbf{x})$ in some region outside of the source region. Often measurements of $u(\mathbf{x})$ are made only over a surface. Using the Green's function formalism we write

$$u(\mathbf{x}) = \int_V G(\mathbf{x};\mathbf{x}')\, q(\mathbf{x}')\, d\mathbf{x}' + \oint_S \left[u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n}\right] dS.$$

Choose the volume to be all of space, and select out-going waves only for both u and G so that the surface integral is 0. Then it can be shown that

$$G(\mathbf{x};\mathbf{x}') = -\frac{e^{j2\pi k|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}$$

and

$$u(\mathbf{x}) = -\int_D \frac{e^{j2\pi k|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} q(\mathbf{x}')\, d\mathbf{x}'.$$

or in the Fourier-domain:

$$U(\mathbf{f}) = Q(\mathbf{f})\, H(\mathbf{f})$$

where

$$H(\mathbf{f}) = \mathfrak{F}\left\{-\frac{1}{4\pi|\mathbf{x}|} e^{j2\pi k|\mathbf{x}|}\right\}$$

This expression provides the explicit relationship between object and measurements.

In the far-field, the inverse problem is more difficult (because more information is lost), but it can be understood somewhat more easily. It also provides a good characterization of non-radiating sources. In the far-field case we approximate $|\mathbf{x}-\mathbf{x}'| \approx |\mathbf{x}|$ in the denominator and $|\mathbf{x}-\mathbf{x}'| = |\mathbf{x}| - \frac{\mathbf{x}\cdot\mathbf{x}'}{|\mathbf{x}|}$ in the numerator. Thus, if we define $\mathbf{s} = \mathbf{x}/|\mathbf{x}|$, then the far-field observations are

$$u(\mathbf{x}) \approx -\frac{e^{j2\pi k|\mathbf{x}|}}{4\pi|\mathbf{x}|}\int e^{-j2\pi k\mathbf{s}\cdot\mathbf{x}'} q(\mathbf{x}')\, d\mathbf{x}' = -\frac{e^{j2\pi kr}}{4\pi r} u_\infty(\mathbf{s})$$

If the far-field measurements $d(\mathbf{s}) = \int e^{-j2\pi k\mathbf{s}\cdot\mathbf{x}'} q(\mathbf{x}')\, d\mathbf{x}'$ vanish then using the uniqueness of Eq. (5) we can assert that the sources must produce a vanishing field on any sphere of radius a_1 (i.e. the sources don't radiate anywhere).

But, it is also clear that

$$g(\mathbf{s}) = u_\infty(\mathbf{s}) = Q(k\mathbf{s}),$$

which is the Fourier transform of q evaluated on the sphere of radius k centered at the origin). This sphere of radius k is called the *Ewald* sphere. This observation allows us to conclude that *the set of non-radiating sources with support in $\mathcal{D}$ is the set of all functions $q(\mathbf{x})$ whose Fourier transform vanishes on the Ewald sphere.*

Notice that this statement is true in both the near and far field, because not only did we use the far-field observation that the angular measurements (radiation pattern) are the Fourier transform of the source object evaluated on the sphere of radius k, but we also used the uniqueness of the far-field inverse-diffraction problem. The observation that the far-field measurements of the angular dependence of the radiation are just the Fourier-transform of the source evaluated on a sphere is an analog to the projection theorem. The notable difference is that the data themselves are equivalent to the Fourier measurements (without taking Fourier transforms of the data). Notice this also shows the difficulty in identifying the sources from far-field measurements at a single frequency — only one sphere of the 3-D Fourier-transform has been measured. Several spheres would need to be measured (perhaps by using different frequencies) in order to obtain a good estimate of the distribution of the scatterers.

5 Inverse Scattering

The inverse scattering problem attempts to determine something about an object by illuminating it with some form of wave energy and recording the scattered response. It is a difficult, nonlinear problem. We will look at the non-linear problem and then linearize it using a common approximation.

Assume no "real" sources inside of the domain D, but allow the wavenumber, k to vary with position. The scalar Helmholtz equation is

$$\nabla^2 u(\mathbf{x}) + 4\pi^2 k^2(\mathbf{x}) u(\mathbf{x}) = 0$$

is satisfied everywhere in space. Let $k^2(\mathbf{x}) = k^2(1 - m(\mathbf{x}))$ so that $m(\mathbf{x})$ is zero outside of the domain of interest and varies inside. This transforms the inhomogeneous Helmholtz equation into

$$\nabla^2 u(\mathbf{x}) + 4\pi^2 k^2 u(\mathbf{x}) = 4\pi^2 k^2 m(\mathbf{x}) u(\mathbf{x})$$

so that $4\pi^2 k^2 mu$ acts as a "virtual" source.

Typically, the field is broken up into an incident field $u_i(\mathbf{x})$ which satisfies the source-free Helmholtz equation (often it is considered a plane-wave: $u_i(\mathbf{x}) = \exp[i2\pi k \mathbf{s}_0 \cdot \mathbf{x}]$) and the scattered field. Because $\nabla^2 u_i + 4\pi^2 k^2 u_i = 0$, we can write

$$\nabla^2 u_s + 4\pi k^2 u_s = 4\pi^2 k^2 m(u_i + u_s)$$

The Green's function formalism of the inverse source problem allows writing the outgoing scattered wave as

$$u_s(\mathbf{x}) = -\pi k^2 \int_D \frac{e^{j2\pi k|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} u(\mathbf{x}') m(\mathbf{x}') d\mathbf{x}'$$

which is an implicit equation showing the relationship between the total field (*i.e.* incident plus scattered field) and the inhomogeneity. The presence of u inside the integrand makes this a non-linear inverse problem. It can be solved by discretizing the problem to relate discrete u and m and then minimizing some functional (*e.g.* least-squares) between the measured data and the computed data. A nonlinear conjugate gradient method (*e.g.* Polak-Rubiere), which is quite similar in principle to the linear conjugate gradient method, is often used to find m. Regularization is typically done by constraining the estimate of m to be band-limited at each iteration (It can be seen that this overall approach is a generalization of the projected Landweber method to nonlinear problems).

There are two linearizations commonly employed when possible. The first is the Born approximation which is valid when $m(\mathbf{x}')$ is a weak-scatterer (most of the incident energy is unscattered). The second linearization is the Rytov approximation which is valid if the scatterer is slowly varying. As both can be shown to give the same results in the far field, we consider only the Born approximation.

The Born approximation recognizes that when there is weak scattering, the total field is dominated by the incident field which allows writing (*e.g.* for a plane-wave incident field).

$$u_s(\mathbf{x}) = -\pi k^2 \int_D \frac{e^{j2\pi k|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} \exp[i2\pi k \mathbf{s}_0 \cdot \mathbf{x}'] m(\mathbf{x}') d\mathbf{x}'.$$

This is now a linear problem equivalent to the inverse source problem where we identify.

$$q(\mathbf{x}) = 4\pi^2 k^2 \exp[i2\pi k \mathbf{s}_0 \cdot \mathbf{x}'] m(\mathbf{x}').$$

Thus all the analysis of the inverse source problem applies to the case of the linearized inverse scattering problem. The SVD is the same and the same problems of non-uniqueness can occur for "non-radiating" sources. In particular, it was shown that the non-radiating sources have a Fourier transform that vanishes on the Ewald sphere: $Q(k\mathbf{s}) = 0$. But, clearly it can be seen (via the Fourier-shift theorem) that $4\pi^2 k^2 M(\mathbf{f} - k\mathbf{s}_0) = Q(\mathbf{f})$. Therefore the "invisible objects" under illumination by a plane wave are those where $M(k(\mathbf{s} - \mathbf{s}_0)) = 0$ so that the Fourier transform of the inhomogeneity is zero on the "shifted" Ewald sphere.

The fact that the **far-field**, **weakly scattered** measurements are the value of the Fourier-transform of the object on the shifted Ewald sphere has useful implications for reconstruction. More precisely, we know from inverse source theory that

$$u_s(\mathbf{x}) \approx -\frac{e^{i2\pi kr}}{4\pi r} u_{s\infty}(\mathbf{s})$$

and

$$u_{s\infty}(\mathbf{s}) = Q(k\mathbf{s}).$$

Thus,

$$u_{s\infty}(\mathbf{s}) = 4\pi^2 k^2 M(k(\mathbf{s} - \mathbf{s}_0))$$

and measurements of the scattered far-field radiation pattern provide samples of the Fourier transform of the object evaluated on the sphere centered at $k\mathbf{s}_0$ with radius k. This is the analog of the Fourier slice theorem in diffraction tomography. Note the differences. The data are measured directly in Fourier space and the values correspond to the 3-D Fourier transform around a sphere in space. By varying $\mathbf{s}_0$, and measuring the full radiation pattern one can sweep through all of the Fourier domain up to a radius of $2k$. With all of these data an inverse Fourier transform can produce the desired result.

A Inverse diffraction Green's function

To find $G(r, \theta, \phi; r', \theta', \phi')$ for the Helmholtz equation with auxilliary conditions of zero-valued at $r = a_1$ and Sommerfield radiation conditions at $r = \infty$, we solve its defining differential equation by expressing G in component form on an orthonormal basis of the space (θ, ϕ). A particularly useful basis which has nice properties with respect to the Laplacian operator is provided by the spherical harmonics:

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi}$$

where $P_l^m(x)$ is an associated Legendre function, and l ranges from 0 to ∞ while m ranges from $-l$ to l. These functions satisfy

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta Y_{l'm'}^*(\theta, \phi) Y_{l,m}(\theta, \phi) = \delta_{l'l}\delta_{m'm}$$

and

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi) = \delta(\phi - \phi') \delta(\cos\theta - \cos\theta').$$

So, if we define the inner-product over the (θ, ϕ) space as

$$(g, h) = \int_0^{2\pi} \int_0^{\pi} g(\theta, \phi) h^*(\theta, \phi) \sin\theta d\theta d\phi$$

we can see that

$$(Y_{l,m}, Y_{l',m'}) = \delta_{l'l}\delta_{m'm}$$

and the Y_{lm} form an orthonormal basis over that space.

So, we should be able to decompose the angular dependence of G on this basis

$$G(r, \theta, \phi; \mathbf{x}') = \sum_l \sum_m G_{lm}(r; \mathbf{x}') Y_{lm}(\theta, \phi).$$

Also, in spherical coordinates we have

$$\begin{aligned}\delta\left(\mathbf{x}-\mathbf{x}'\right) &= \frac{1}{r^2}\delta\left(r-r'\right)\delta\left(\cos\theta-\cos\theta'\right)\delta\left(\phi-\phi'\right)\\ &= \sum_l\sum_m\frac{1}{r^2}\delta\left(r-r'\right)Y^*_{lm}\left(\theta',\phi'\right)Y_{lm}\left(\theta,\phi\right).\end{aligned}$$

Thus, the differential equation for G is

$$\sum_{l,m}\nabla^2\left[G_{lm}\left(r;\mathbf{x}'\right)Y_{lm}\right]+4\pi^2k^2\sum_{l,m}G_{lm}\left(r;\mathbf{x}'\right)Y_{lm}=\sum_l\sum_m\frac{1}{r^2}\delta\left(r-r'\right)Y^*_{lm}\left(\theta',\phi'\right)Y_{lm}\left(\theta,\phi\right).$$

Note that in spherical coordinates

$$\nabla^2\Phi\leftrightarrow\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r\Phi\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2}.$$

In addition

$$\begin{aligned}\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y_{lm}}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2Y_{lm}}{\partial\phi^2} &= \left[\frac{m^2}{\sin^2\theta}-l\left(l+1\right)\right]\frac{Y_{lm}}{r^2}-\frac{m^2Y_{lm}}{r^2\sin^2\theta}\\ &= -l\left(l+1\right)\frac{Y_{lm}}{r^2}.\end{aligned}$$

Thus,

$$\nabla^2\left(G_{lm}Y_{lm}\right)=\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(rG_{lm}\right)-\frac{l\left(l+1\right)G_{lm}}{r^2}\right]Y_{lm}\left(\theta,\phi\right)$$

and the differential equation is

$$\sum_{m,l}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(rG_{lm}\right)-\frac{l\left(l+1\right)G_{lm}}{r^2}+4\pi^2k^2G_{lm}\right]Y_{lm}\left(\theta,\phi\right)=\sum_{l,m}\frac{1}{r^2}\delta\left(r-r'\right)Y^*_{lm}\left(\theta',\phi'\right)Y_{lm}\left(\theta,\phi\right).$$

Take the inner product of both sides of this equation with $Y_{l'm'}$ and integrate (or identify coefficients in the Y_{lm} expansion) to get

$$r\frac{\partial^2}{\partial r^2}\left[rG_{lm}\left(r;\mathbf{x}'\right)\right]-l\left(l+1\right)G_{lm}\left(r;\mathbf{x}'\right)+4\pi^2k^2r^2G_{lm}\left(r;\mathbf{x}'\right)=\delta\left(r-r'\right)Y^*_{lm}\left(\theta',\phi'\right).$$

It is clear that the θ' and ϕ' dependence of $G_{lm}\left(r;\mathbf{x}'\right)$ is $Y^*_{lm}\left(\theta',\phi'\right)$ so that

$$G_{lm}\left(r;\mathbf{x}'\right)=G_{lm}\left(r;r'\right)Y^*_{lm}\left(\theta',\phi'\right),$$

where $G_{lm}\left(r;r'\right)$ satisfies

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial kr}G_{lm}\right)+\left[4\pi^2k^2r^2-l\left(l+1\right)\right]G_{lm}=\delta\left(r-r'\right).$$

When $r\neq r'$ this is the differential equation for spherical Bessel functions ($j_n\left(2\pi kr\right)$, $y_n\left(2\pi kr\right)$, $h^{(1)}_n\left(2\pi kr\right)$ and $h^{(2)}_n\left(2\pi kr\right)$). Therefore for $r>r'$

$$G^>_{lm}\left(r;r'\right)=A_>\left(r'\right)h^{(1)}_l\left(2\pi kr\right)+B_>\left(r'\right)h^{(2)}_l\left(2\pi kr\right),$$

while for $r<r'$ we may have

$$G^<_{lm}\left(r;r'\right)=A_<\left(r'\right)h^{(1)}_l\left(2\pi kr\right)+B_<\left(r'\right)h^{(2)}_l\left(2\pi kr\right).$$

We require that these two expressions give the same relationship at $r = r'$. To match the boundary condition that G represents an outward going wave at $r = \infty$ (Sommerfield raditiation condition) we require that $B_> = 0$. To match the boundary conditions that $G = 0$ when $r = a_1$ we require that

$$A_< h_l^{(1)}(2\pi k a_1) = -B_< h_l^{(2)}(2\pi k a_1)\,. \tag{2}$$

Matching boundary conditions requires that

$$(A_> - A_<)\, h_l^{(1)}(2\pi k r') = B_< h_l^{(2)}(2\pi k r')\,. \tag{3}$$

Finally, integrate the differential equation around $r = r'$ to get

$$\left[\frac{\partial G_{lm}^{>}}{\partial r} - \frac{\partial G_{lm}^{<}}{\partial r}\right]_{r=r'} = \frac{1}{r'^2}.$$

These four constraints allow us to determine the coefficients. The last constraint is

$$A_> \frac{\partial h_l^{(1)}(2\pi k r')}{\partial r} - A_< \frac{\partial h_l^{(1)}(2\pi k r\prime)}{\partial r} - B_< \frac{\partial h_l^{(2)}(2\pi k r')}{\partial r} = \frac{1}{r'^2}.$$

$$(A_> - A_<)\, h_l^{(1)\prime} - B_< h_l^{(2)\prime} = \frac{1}{2\pi k r'^2}. \tag{4}$$

Because we will be using the Green's function only when $r > r'$, we only need to find $A_>$. This is accomplished by substituting Eq. (3) into Eq. (4) and solving for $B_<$. Then use Eq. (2) for $A_<$. The result is

$$B_< \left[h_l^{(2)}(2\pi k r') \frac{h_l^{(1)\prime}(2\pi k r')}{h_l^{(1)}(2\pi k r')} - h_l^{(2)\prime}(2\pi k r')\right] = \frac{1}{2\pi k r'^2}$$

or using

$$h_l^{(2)} h_l^{(1)\prime} - h_l^{(1)} h_l^{(2)\prime} = \frac{2i}{4\pi^2 k^2 r'^2}$$

we get

$$B_< = \frac{2\pi k}{2i} h_l^{(1)}(2\pi k r')\,.$$

Thus,

$$A_<(r') = -\frac{2\pi k}{2i} h_l^{(1)}(2\pi k r') \frac{h_l^{(2)}(2\pi k a_1)}{h_l^{(1)}(2\pi k a_1)}$$

and

$$\begin{aligned} A_>(r') &= B_< \frac{h_l^{(2)}(2\pi k r')}{h_l^{(1)}(2\pi k r')} + A_< \\ &= \frac{2\pi k}{2i}\left[h_l^{(2)}(2\pi k r') - h_l^{(2)}(2\pi k a_1) \frac{h_l^{(1)}(2\pi k r')}{h_l^{(1)}(2\pi k a_1)}\right] \end{aligned}$$

Therefore, the Green's function is

$$G(\mathbf{x}; \mathbf{x}') = \sum_{m,l} G_{ml}(r; r')\, Y_{lm}(\theta, \phi)\, Y_{lm}^*(\theta', \phi')\,.$$

To get the kernel $K(\mathbf{s}; \mathbf{s}')$ we need to take the derivative of this expression with respect to r' and evaluate at $r' = a_1$ and $r = a_2$ (note $a_2 > a_1$)

$$\frac{\partial G}{\partial r'} = 4\pi^2 \frac{k^2}{2i} \sum_{m,l} \left[h_l^{(2)\prime}(2\pi k r') - h_l^{(2)}(2\pi k a_1) \frac{h_l^{(1)\prime}(2\pi k r')}{h_l^{(1)}(2\pi k a_1)}\right] h_l^{(1)}(2\pi k r)\, Y_{lm}(\theta, \phi)\, Y_{lm}^*(\theta', \phi')\,.$$

$$\left.\frac{\partial G}{\partial r'}\right|_{r'=a_1} = \frac{1}{a_1^2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{h_l^{(1)}(2\pi kr)}{h_l^{(1)}(2\pi ka_1)}Y_{lm}(\theta,\phi)\,Y_{lm}^*(\theta',\phi').$$

Thus the solution for $u(\mathbf{x})$ for $r > a_1$ is

$$\begin{aligned} u(\mathbf{x}) &= \sum_{l=0}^{\infty}\frac{h_l^{(1)}(2\pi kr)}{h_l^{(1)}(2\pi ka_1)}\sum_{m=-l}^{l}Y_{lm}(\theta,\phi)\int_0^{2\pi}\int_0^{\pi}f(\theta',\phi')\,Y_{lm}^*(\theta',\phi')\sin\theta' d\theta' d\phi' \\ &= \sum_{l=0}^{\infty}\frac{h_l^{(1)}(2\pi kr)}{h_l^{(1)}(2\pi ka_1)}\sum_{m=-l}^{l}(f,Y_{lm})\,Y_{lm}(\theta,\phi). \end{aligned}$$

B Inversion using SVD

From the analysis in the preceding section, it can be seen that the relationship between the field on two concentric spheres is

$$d(\mathbf{s}) = \int_0^{2\pi}\int_0^{\pi}K(\mathbf{s};\mathbf{s}')\,m(\theta',\phi')\sin\theta' d\theta d\phi,$$

where

$$K(\mathbf{s};\mathbf{s}') = \sum_{lm}\frac{h_l^{(1)}(2\pi ka_2)}{h_l^{(1)}(2\pi ka_1)}Y_{lm}(\theta,\phi)\,Y_{lm}^*(\theta',\phi').$$

or in other words

$$d = Am = \sum_{l=0}^{\infty}\frac{h_l^{(1)}(2\pi ka_2)}{h_l^{(1)}(2\pi ka_1)}\sum_{m=-l}^{l}(m,Y_{lm})\,Y_{lm}(\theta,\phi).$$

(Remember the $\sin\theta$ weighting in the definition of the inner product). In this formula,

$$h_l^{(1)}(z) = j_l(z) + in_l(z)$$

is a spherical Hankel function (spherical Bessel functions of the third kind). It can be defined as

$$h_l^{(1)}(z) = \sqrt{\frac{\pi}{2z}}\left(J_{l+\frac{1}{2}}(z) + iY_{n+\frac{1}{2}}(z)\right).$$

where $J_\nu(z)$ and $Y_\nu(z)$ are Bessel functions of the first and second kinds. Explicit formulas suitable for small l are

$$\begin{aligned} j_l(z) &= -z^l\left(-\frac{1}{z}\frac{d}{dz}\right)^l\left(\frac{\sin z}{z}\right) \\ n_l(z) &= -z^l\left(-\frac{1}{z}\frac{d}{dz}\right)^l\left(\frac{\cos z}{z}\right) \end{aligned}$$

giving

$$h_l^{(1)}(z) = -i(-z)^l\left(\frac{1}{z}\frac{d}{dz}\right)^l\frac{e^{iz}}{z}.$$

An explicit expression is

$$h_l^{(1)}(z) = i^{-(l+1)}\frac{e^{iz}}{z}\sum_{k=0}^{l}\frac{(l+k)!}{k!\,(l-k)!}(-2iz)^{-k}$$

For large l this function has the expansion ($z > 0$),

$$h_l^{(1)}(z) \approx -\frac{i\sqrt{2}}{z\sqrt{e}}\left(\frac{2l+1}{ez}\right)^l.$$

The first few are

$$
\begin{aligned}
h_0^{(1)}(z) &= \frac{e^{iz}}{iz} \\
h_1^{(1)}(z) &= -\frac{e^{iz}}{z}\left(1+\frac{i}{z}\right) \\
h_2^{(1)}(z) &= \frac{ie^{iz}}{z}\left(1+\frac{3i}{z}-\frac{3}{z^2}\right) \\
h_3^{(1)}(z) &= \frac{e^{iz}}{z}\left(1+\frac{6i}{z}-\frac{15}{z^2}-\frac{15i}{z^3}\right).
\end{aligned}
$$

For large argument ($z \gg 1$), the limit is

$$h_l^{(1)}(z) = (-i)^{l+1}\frac{e^{iz}}{z}.$$

This preceding analysis determines the kernel explicitly in terms of an eigenvalue decomposition (note the eigenvalues are not real therefore it is not the SVD decomposition—but it is closely related). The eigenvalues are $\lambda_l = \frac{h_l^{(1)}(ka_2)}{h_l^{(1)}(ka_1)}$ with multiplicity $2l+1$. To obtain the singular value decomposition we must look at the eigenvector-eigenvalue decomposition of A^*A or A^*A. Equivalently we can use the eigenvalue decomposition and note that

$$\lambda_l = |\lambda_l|\, e^{j\angle\lambda_l}.$$

Thus, if we identify $\sigma_l = |\lambda_l|$ and then choose $v_{lm} = Y_{lm}$ while $u_{lm} = \lambda_l / |\lambda_l|\, Y_{lm}$. We have the singular value decomposition.

The generalized inverse is

$$m^\dagger = A^\dagger d = \sum_{l=0}^{\infty}\frac{1}{\lambda_l}\sum_{m=-l}^{l}(d, Y_{lm})\, Y_{lm}(\theta,\phi).$$

This estimate can behave poorly because $\sigma_l \to 0$ as $l \to \infty$ is not regularized. To regularize we can apply a filter directly in σ_l space and obtain

$$m_\mu = A_\mu d = \sum_{l=0}^{\infty}\frac{W_{l,\mu}}{\lambda_l}\sum_{m=-l}^{l}(g, Y_{lm})\, Y_{lm}(\theta,\phi).$$

A good understanding of the inverse problem can be obtained by observing the spectrum of the eigenvalues. Where these get close to zero information about the corresponding component of f is lost and we must regularize to control $f^\dagger$. Note that as $l \to \infty$ we get

$$\lambda_l \approx \left(\frac{a_1}{a_2}\right)^{l+1} = \exp\left[-(l+1)\log\frac{a_2}{a_1}\right].$$

This exponential decay in the singular values indicates a difficult inverse problem especially as $\frac{a_2}{a_1} \gg 1$. For small values of l you can use

$$\lambda_l = \sqrt{\frac{a_1}{a_2}}\frac{J_{l+0.5}(2\pi k a_2) + jY_{l+0.5}(2\pi k a_2)}{J_{l+0.5}(2\pi k a_1) + jY_{l+0.5}(2\pi k a_1)}.$$

In the far field we use the expansion

$$h_l^{(1)}(z) \approx (-i)^{l+1}\frac{e^{iz}}{z}$$

to note that

$$u(r,\theta,\phi) \approx \frac{e^{i2\pi kr}}{2\pi kr}\sum_{l=0}^{\infty}\frac{(-i)^{l+1}}{h_l^{(1)}(2\pi k a_1)}\sum_{m=-l}^{l}(m, Y_{lm})\, Y_{lm}(\theta,\phi).$$

If we consider

$$d(\theta,\phi) = u_\infty(\theta,\phi) = \sum_{l=0}^{\infty} \frac{(-i)^{l+1}}{h_l^{(1)}(2\pi k a_1)} \sum_{m=-l}^{l} (m, Y_{lm}) Y_{lm}(\theta,\phi) \tag{5}$$

to be the far-field data, then the eigenvalues of the far-field operator are

$$\lambda_l = \frac{(-i)^{l+1}}{h_l^{(1)}(2\pi k a_1)}$$

which for large l becomes

$$|\lambda_l^\infty| \approx \exp\left[-l \log\left(l/\pi k a_1\right)\right],$$

demonstrating a potentially much larger rate of decay than in the near-field case where $a_2/a_1 \approx 1$.

C Inverse source using SVD

Define the measurement surface to be a sphere of radius a_2 with $a_2 > |D|$. We can expand the Green's function in a spherical-harmonic basis as follows

$$\frac{e^{i2\pi k|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} = i2\pi k \sum_{l=0}^{\infty} j_l\left(2\pi k \min\{r,r'\}\right) h_l^{(1)}\left(2\pi k \max\{r,r'\}\right) \sum_{m=-l}^{l} Y_{lm}(\theta,\phi) Y_{lm}^*(\theta',\phi').$$

Therefore, the data $d(\mathbf{s}) = u(a_2,\theta,\phi)$ is

$$d(\mathbf{s}) = Aq = -i2\pi k \sum_{l=0}^{\infty} h_l^{(1)}(2\pi k a_2) \sum_{m=-l}^{l} Y_{lm}(\theta,\phi) \int_D j_l(2\pi k r') Y_{lm}^*(\theta',\phi') q(r,\theta',\phi') r'^2 \sin\theta' dr d\theta' d\phi'.$$

This provides an explicit decomposition of the operator for the inverse source problem. We can use it to find the SVD. Let D be a sphere of radius a. Then, choose $u_{lm} = Y_{lm}(\theta,\phi)$ (as we know this constitutes an orthonormal basis). It is clear that

$$A^* d = i2\pi k \sum_{l=0}^{\infty} h_l^{(1)*}(2\pi k a_2) \sum_{m=-l}^{l} j_l(2\pi k r') Y_{lm}(\theta',\phi') \int Y_{lm}^*(\theta,\phi) g(\theta,\phi) \sin\theta d\theta d\phi$$

Then

$$AA^* d = \sum_{l,m} 4\pi^2 k^2 \left|h_l^{(1)}(2\pi k a_2)\right|^2 \left[\int_0^a r^2 j_l^2(2\pi k r) dr\right] (d, Y_{lm}) Y_{lm}(\theta,\phi).$$

Thus we see that

$$\sigma_l = 2\pi k \left|h_l^{(1)}(2\pi k a_2)\right| \left[\int_0^a r^2 j_l^2(2\pi k r) dr\right]^{1/2}.$$

We can find the orthonormal v_{lm} using

$$v_{lm} = \frac{1}{\sigma_l} A^* u_{lm}$$

giving

$$v_{lm} = i\frac{2\pi k}{\sigma_l} h_l^{(2)}(2\pi k a_2) j_l(2\pi k r) Y_{lm}(\theta,\phi).$$

Thus, we can write

$$d = Aq = \sum_{l=0}^{\infty} \sigma_l \sum_{m=-l}^{l} (q, v_{lm}) u_{lm}.$$

This is not a complete singular value decomposition, because we have not shown that the v_{lm} constitute a complete basis of the source space (it doesn't in fact). What we have is a "partial" SVD of the operator.

There are zero-valued singular values corresponding to the part of $\mathbb{R}^3$ that is not spanned by v_{lm}. This means that the inverse problem is not unique. Notice, that if (q, v_{lm}) is ever zero for all l, m and non-zero q then that value of q could be added to any other source and give the same measurements. These null functions are called non-radiating sources. For example is $q = q_r(r)\, q_{\mathbf{s}}(\theta, \phi)$ and q_r is chosen such that $\int r^2 j_l(2\pi kr)\, q_r(r)\, dr = 0$ for all l, then q is a non-radiating source.

The generalized inverse can be written

$$q^{\dagger} = A^{\dagger} d = \sum_{l=0}^{\infty} \frac{1}{\sigma_l} \sum_{m=-l}^{l} (d, u_{lm})\, v_{lm}$$

or

$$q = i2\pi k \sum_{l=0}^{\infty} \frac{h_l^{(2)}(2\pi k a_2)}{\sigma_l^2} \sum_{m=-l}^{l} \left[\int d(\theta', \phi)\, Y_{lm}^{*}(\theta', \phi') \sin\theta d\theta d\phi \right] j_l(2\pi kr)\, Y_{lm}(\theta, \phi).$$

For large l, the singular values can be understood by approximating

$$j_l(z) \approx \frac{1}{\sqrt{2(2l+1)z}} \left(\frac{ez}{2l+1} \right)^{l+1/2}.$$

Thus,

$$\int_0^a r^2 j_l^2(2\pi kr)\, dr \approx \frac{1}{2\pi k} \int_0^a dr \frac{r}{4l+2} \left(\frac{e2\pi kr}{2l+1} \right)^{2l+1} = \frac{a^{2l+3}(2\pi k)^{2l}}{(4l+2)(2l+3)} \left(\frac{e}{2l+1} \right)^{2l+1}$$

and

$$\begin{aligned} \sigma_l &= \frac{\sqrt{2}}{a_2\sqrt{e}} \left(\frac{2l+1}{e2\pi k a_2} \right)^{l} \sqrt{\frac{a^{2l+3}(2\pi k)^{2l}}{(4l+2)(2l+3)}} \left(\frac{e}{2l+1} \right)^{l+1/2} \\ &= (2\pi k a_2)^{-l} \sqrt{\frac{2a^{2l+3}(2\pi k)^{2l}}{a_2(4l+2)(2l+1)(2l+3)}} \\ &\approx \exp\left[-l \log(a_2/a)\right] \end{aligned}$$

The SVD of the far field operator is a little bit different. We have changed slightly our notion of the measurements from $u(a_2, \theta, \phi)$ to $u_{\infty}(\theta, \phi)$. This does not change u_{lm}, but the singular values become

$$\sigma_l = \sqrt{\int_0^a r^2 j_l^2(2\pi kr)\, dr}$$

while

$$v_{lm}(\mathbf{x}') = \frac{i^l}{\sigma_l} j_l(2\pi kr')\, Y_{lm}(\theta', \phi').$$