Notes on Green's functions in inhomogeneous media

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1 Homogeneous media

Suppose we have Poisson's equation with constant coefficients ($= 1$ for simplicity), i.e. in a homogeneous medium, i.e. in "empty space", i.e.

$$-\nabla^2 u = f$$

in some region Ω, with boundary conditions so that this has a unique solution, e.g. Dirichlet boundaries $u|_{d\Omega} = 0$. Then we can write the solution in terms of the Green's function $G_0(\mathbf{x}, \mathbf{x}')$:

$$u(\mathbf{x}) = \int_\Omega G_0(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') d^n \mathbf{x}', \tag{1}$$

in n dimensions, where $-\nabla^2 G_0(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$. For example, if $\Omega = \mathbb{R}^3$, then $G_0(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|}$.

2 Inhomogeneous media

Now, suppose we have non-constant coefficients $c(\mathbf{x}) > 0$, corresponding to an inhomogeneous medium (i.e. different "materials" at different points in space). This could enter Poisson's equation in several ways, for example:

1. $-c\nabla^2 u = f$ — for example, in a stretched string or drum, $1/c$ would be proportional to the density, so $c(\mathbf{x})$ would represent a variable density.

2. $-\nabla \cdot (c\nabla u) = f$ — for example, in electrostatics $\sqrt{c}$ would be proportional to the refractive index; in a stretched string or drum c would be proportional to a tension/elasticity; in a diffusion problem c would be a diffusion coefficient; in a heat-conduction problem c would be proportional to a thermal conductivity.

3. $-\nabla^2 u + cu = f$ — for example, in quantum mechanics this would represent Schrödinger's equation with a variable potential energy c.

4. Various other generalizations and combinations. e.g. a multidimensional Sturm–Liouville equation, $-c_1 \nabla \cdot (c_2 \nabla u) + c_3 u = f$, for different functions $c_{1,2,3}(\mathbf{x})$ (and c_2 could even be a positive-definite matrix).

All of these are of the form $\hat{A}u = f$ where $\hat{A}$ is self-adjoint and positive-definite (assuming zero Dirichlet boundary conditions and an appropriate inner product $\langle u, v \rangle$), as we've seen previously in class, so they should have unique solutions (excluding pathological c functions). However, the solutions may in general be quite different from those of $-\nabla^2 u = f$. **Can we relate them to G_0, the Green's function for empty space?**

2.1 $\quad -c\nabla^2 u = f$

This case is quite trivial to relate to empty space: just rewrite it as $-\nabla^2 u = f/c$ (valid since $c > 0$), in which case we can use eq. (1) to obtain

$$u(\mathbf{x}) = \int_\Omega G_0(\mathbf{x}, \mathbf{x}')\frac{f(\mathbf{x}')}{c(\mathbf{x}')}d^n\mathbf{x}',$$

from which it follows that the Green's function of this problem is $G(\mathbf{x}, \mathbf{x}') = G_0(\mathbf{x}, \mathbf{x}')/c(\mathbf{x}')$.

2.2 $\quad -\nabla \cdot (c\nabla u) = f$

To make it look like empty space, we employ the product rule to write $\nabla(c\nabla u) = (\nabla c) \cdot (\nabla u) + c\nabla^2 u$, obtaining:

$$-\nabla^2 u = \frac{f}{c} + \frac{\nabla c}{c} \cdot \nabla u.$$

If we substitute the right-hand side as if it were "f" in the empty-space problem, from eq. (1), and note that $(\nabla c)/c = \nabla \ln c$, we obtain:

$$u(\mathbf{x}) = \int_\Omega G_0(\mathbf{x}, \mathbf{x}') \left[\frac{f(\mathbf{x}')}{c(\mathbf{x}')} + \nabla'[\ln c(\mathbf{x}')] \cdot \nabla' u(\mathbf{x}') \right] d^n\mathbf{x}'. \tag{2}$$

Notice, however, that the unknown u appears on both the left- and right-hand sides. This is a **volume integral equation**[1] for $u(\mathbf{x})$. There are various numerical methods to solve such "VIE" problems approximately by discretizing space, but we won't cover these in 18.303. However, there are still several lessons to be learned from this equation. First, one can think of the inhomogeneous solution as the sum of "homogeneous" solutions $G_0(\mathbf{x}, \mathbf{x}')$ from the right-hand-sides $f(\mathbf{x}')/c$ at $\mathbf{x}'$ **plus a "scattered" solution** from the solution u creating **new source terms at inhomogeneities** ∇c. Second, there are various general situations where this VIE simplifies considerably. In the following, denote

$$u_0(\mathbf{x}) = \int_\Omega G_0(\mathbf{x}, \mathbf{x}')\frac{f(\mathbf{x}')}{c(\mathbf{x}')}d^n\mathbf{x}',$$

the part of $u(\mathbf{x})$ that *doesn't* come from the inhomogeneity ∇c, the "incident" solution. We then can write $u = u_0 + \hat{B}u$ where $\hat{B}$ is the linear *integral* operator corresponding to $\hat{B}u = \int G_0 \nabla' \ln c \cdot \nabla' u$.

(This terminology of "incident" and "scattered" parts of the solution has its origins in wave-equation problems, where the solution represents a wave propagating outwards from a source f, and is actually bouncing off of objects/inhomogeneities. In the present problem, there is no time dependence so this terminology is only an analogy.)

2.2.1 Piecewise-homogeneous media

The most common and important case of inhomogeneous media is where $c(\mathbf{x})$ is **piecewise-constant**. e.g. in one region you have glass, in another region you have metal, and in another region you have water, each corresponding to a different constant value of c.

For example, suppose we have $\Omega = \mathbb{R}^3$, with $-\nabla \cdot (c\nabla u) = f$ for the situation depicted in figure 1: $c(\mathbf{x}) = c_1$ in some volume V and $= c_2$ outside of V. In this case $\nabla \ln c$ is actually a delta function at the interface, multiplied by the magnitude $\ln c_2 - \ln c_1 = \ln(c_2/c_1)$ of

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[1]More specifically, it is a "second-kind" integral equation, since u appears both inside and outside the integral.
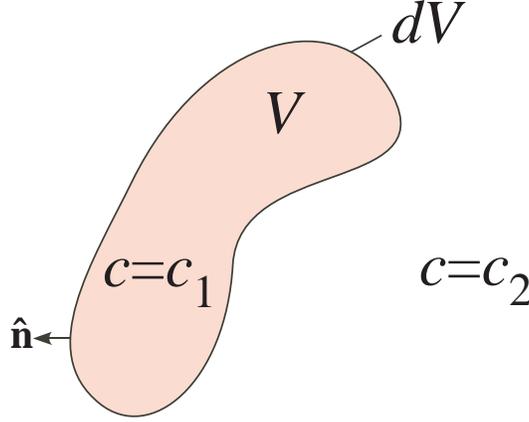
Figure 1: Schematic example of piecewise-constant coefficients $c(\mathbf{x})$: $c(\mathbf{x}) = c_1$ in some region V (with boundary dV, and $\hat{\mathbf{n}}$ denoting the outward unit-normal vector), and $c(\mathbf{x}) = c_2$ otherwise.

the discontinuity, also multiplied by a unit-normal vector $\hat{\mathbf{n}}$ at each point on the interface (giving the direction $\nabla \ln c$). Then the VIE (2) simplifies to u_0 plus a *surface integral*:

$$u(\mathbf{x}) = u_0(\mathbf{x}) + \ln(c_2/c_1) \oiint_{dV} G_0(\mathbf{x}, \mathbf{x}') \nabla' u(\mathbf{x}') \cdot d\mathbf{A}', \tag{3}$$

where $d\mathbf{A}' = \hat{\mathbf{n}} dA'$ is the usual outward-normal differential area in a surface integral. This is now a **surface integral equation** (SIE) for $u(\mathbf{x})$: once we know $\hat{\mathbf{n}} \cdot \nabla u$ on the surface, we can get $\mathbf{u}(\mathbf{x})$ everywhere! Physically, this can be interpreted as "scattering" of the solution off the *interface* between c_1 and c_2, as represented by "source" terms at every $\mathbf{x}' \in dV$.

However, **this isn't quite right**. The problem is that $\nabla u \cdot \hat{\mathbf{n}}$ isn't actually continuous across the interface in general, and so evaluating it on the surface dV is not well-defined. We can see this by looking at the original equation $\nabla \cdot (c \nabla n) = f$: unless f happens to have delta functions right on the dV interface, the quantity $c \nabla u$ must be continuous across the interface in the $\hat{\mathbf{n}}$ direction. That is, $c \nabla u \cdot \hat{\mathbf{n}}$ is continuous, not $\nabla u \cdot \hat{\mathbf{n}}$. So, before we can evaluate a surface integral, we need to rewrite things in terms of $c \nabla u \cdot \hat{\mathbf{n}}$. We can do this, since

$$\nabla[\ln c] \cdot \nabla u = \frac{\nabla c}{c} \cdot \nabla u = \frac{\nabla c}{c^2} \cdot c \nabla u = \nabla \left(-\frac{1}{c} \right) \cdot c \nabla u$$

in eq. (2). And $\nabla(-1/c)$ is also a delta function multiplied by $\hat{\mathbf{n}}$ and the magnitude $\frac{1}{c_1} - \frac{1}{c_2}$ of the discontinuity, and hence we obtain a corrected SIE:

$$u(\mathbf{x}) = u_0(\mathbf{x}) + \left(\frac{1}{c_1} - \frac{1}{c_2} \right) \oiint_{dV} G_0(\mathbf{x}, \mathbf{x}') \left[c(\mathbf{x}') \nabla' u(\mathbf{x}') \right] \cdot d\mathbf{A}', \tag{4}$$

which is well-defined since the integrand is now a continuous quantity across the interface. (And even this is not quite in the form that is used in numerics.)

Like our SIE equations for the case where Ω itself has a boundary, these SIE equations are solved by parameterizing the surface unknowns via some discretization, and then choosing the unknowns so that u satisfies appropriate continuity conditions at the interface dV. The details of this get rather tricky very quickly, but these can yield very efficient computational methods because they only involve unknowns at interfaces and handle homogeneous regions (even infinite homogeneous regions) analytically via G_0.

2.2.2 Born approximation

We have written the solution in the form $u = u_0 + \hat{B}u$, where u_0 is the solution due to f ignoring the inhomogeneity, and $\hat{B}$ is an integral operator giving the "scattered" portion of the solution $\hat{B}u$ due to the inhomogeneity. We can then formally write:

$$
\begin{aligned}
u &= u_0 + \hat{B}u = u_0 + \hat{B}(u_0 + \hat{B}u) = u_0 + \hat{B}u_0 + \hat{B}^2(u_0 + \hat{B}u_0 + \hat{B}^2 u) \\
&= \cdots = \left(\sum_{k=0}^{\infty} \hat{B}^k \right) u_0,
\end{aligned}
$$

which is called a "Born–Dyson" series/expansion (sometimes omitting one name or the other). Equivalently, $(1 - \hat{B})u = u_0$ implies $u = (1 - \hat{B})^{-1}u_0$, and the Taylor series for $(1 - \hat{B})^{-1}$ is $\sum_k \hat{B}^k$.

What does this represent physically? u_0 is the "incident" portion of the solution, before scattering off the inhomogeneity. $\hat{B}u_0$ is the portion of the solution where this "incident" solution has scattered *once* off the inhomogenity, producing a scattered solution

$$
\hat{B}u_0 = \int_{\Omega} G_0(\mathbf{x}, \mathbf{x}')\nabla' \ln c(\mathbf{x}') \cdot \nabla' u_0(\mathbf{x}') d^n\mathbf{x}'.
$$

But of course, *this* portion of the solution *also* scatters off of the inhomogeneity, producing a portion of the solution representing incident solutions that have scattered *twice*:

$$
\hat{B}^2 u_0 = \int_{\Omega} G_0(\mathbf{x}, \mathbf{x}')\nabla' \ln c(\mathbf{x}') \cdot \nabla' \left[\int_{\Omega} G_0(\mathbf{x}', \mathbf{x}'')\nabla'' \ln c(\mathbf{x}'') \cdot \nabla'' u_0(\mathbf{x}'') d^n\mathbf{x}'' \right] d^n\mathbf{x}',
$$

i.e. a u_0 at $\mathbf{x}''$ produces a source term due to $\nabla''c$, which "travels" from $\mathbf{x}''$ to $\mathbf{x}'$ via $G_0(\mathbf{x}', \mathbf{x}'')$, then produces a source at $\mathbf{x}'$ due to $\nabla'c$, then "travels" from $\mathbf{x}'$ to $\mathbf{x}$ via $\mathbf{G}_0(\mathbf{x}, \mathbf{x}')$, and of course this must be integrated over all possible scattering points $\mathbf{x}'$ and $\mathbf{x}''$. Then $\hat{B}^3 u_0$ represents things scattering three times, and so on.[2]

Now, suppose we have a system that is *nearly* homogeneous. e.g. ∇c is small. Then one might expect that the scattered portion $\hat{B}u$ of the solution to be small. In this case, we may be able to approximate this series by keeping only the first two terms—if scattering *once* has small amplitude, then scattering *twice* should have even smaller amplitude. (e.g. if ∇c is small, this could be thought of as expanding as a power series in ∇c, since $\hat{B}^k \sim |\nabla c|^k$.) This is the **Born approximation**:

$$
u(\mathbf{x}) \approx u_0(\mathbf{x}) + \hat{B}u_0,
$$

and is an extremely useful way to think about *nearly homogeneous* problems.

3 Example: Inhomogeneity in a small volume

Suppose we are solving $-\nabla \cdot (c\nabla u) = f$ in $\Omega = \mathbb{R}^3$ with a point source $f(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0)$ at $\mathbf{x}_0$. Furthermore, suppose that $c(\mathbf{x})$ is piecewise-constant as in figure 1, with $c(\mathbf{x}) = c_2$ everywhere except in a volume V, centered at $\mathbf{x}_1$, where $\mathbf{c}(\mathbf{x}) = c_1$. Now, suppose that we want the solution $u(\mathbf{x})$, but are far from V: both the source point $\mathbf{x}_0$ and the desired point $\mathbf{x}$ are far from V, with $|\mathbf{x}_1 - \mathbf{x}_0|$ and $|\mathbf{x}_1 - \mathbf{x}|$ both much bigger than the diameter of V. This is shown schematically in figure 2. In this case, we should expect the effect of the "scattered"

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[2]In quantum mechanics, this kind of series of events is sometimes represented graphically by the notation of "Feynman diagrams," and can be generalized to nonlinear problems and other effectivei inhomogeneities. In that context, this process of summing all possible scattering sequences is sometimes mysteriously described as a "particle exploring all possible paths between two points," but is really just a consequence of particles being described by PDEs (Schrödinger's equation, in single-particle quantum mechanics), rather than ODEs.
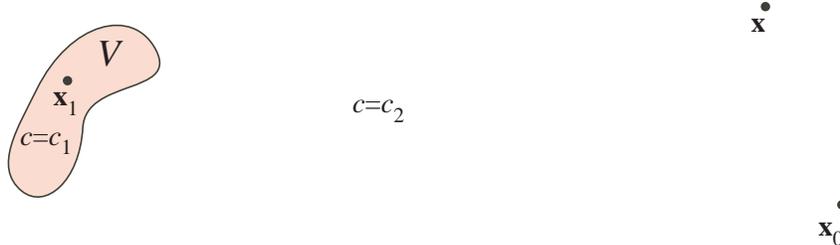
Figure 2: Schematic of problem with an inhomogeneity in a small volume V (centered at $\mathbf{x}_1$): we have a source at $\mathbf{x}_0$ and want the solution at $\mathbf{x}$, with both $\mathbf{x}_0$ and $\mathbf{x}$ much farther from $\mathbf{x}_1$ than the diameter of V.

solution from V to be small at $\mathbf{x}$, and a Born approximation should apply. Furthermore, we will assume $c_1 \approx c_2$ (though not exactly equal!), so that we can neglect the effect of the discontinuity in ∇u mentioned after equation (3) above (which greatly complicates the application of any Born-like approximation in this problem because it would prevent us from using $u \approx u_0$ in V).[3]

In this case,

$$u_0(\mathbf{x}) = G_0(\mathbf{x}, \mathbf{x}_0)/c(\mathbf{x}_0) = \frac{1}{4\pi c_2 |\mathbf{x} - \mathbf{x}_0|},$$

so in the Born approximation we write:

$$u(\mathbf{x}) \approx u_0(\mathbf{x}) + \hat{B} u_0,$$

where the scattered part of the solution, applying the SIE form (4) [valid when $c_1 \approx c_2$], is

$$
\begin{aligned}
\hat{B} u_0 &= \ln(c_2/c_1) \oiint_{dV} G_0(\mathbf{x}, \mathbf{x}') \nabla' u_0(\mathbf{x}') \cdot d\mathbf{A}' \\
&= \ln(c_2/c_1) \iiint_V \nabla' \cdot [G_0(\mathbf{x}, \mathbf{x}') \nabla' u_0(\mathbf{x}')] \, d^3\mathbf{x}' \\
&= \ln(c_2/c_1) \iiint_V \left[\nabla' G_0(\mathbf{x}, \mathbf{x}') \cdot \nabla' u_0(\mathbf{x}') + G_0 \cancel{\nabla'^2 u_0} \right] d^3\mathbf{x}',
\end{aligned}
$$

where in the second line we applied the divergence theorem, and in the third line the product rule led to a $\nabla^2 u_0$ term, where $\nabla^2 u_0 = -\delta(\mathbf{x} - \mathbf{x}_0)$ is zero in V (since $\mathbf{x}_0$ is outside of V).

Now, since V is small compared to the distance from $\mathbf{x}$ and $\mathbf{x}_0$, the distances $|\mathbf{x}' - \mathbf{x}|$ and $|\mathbf{x}' - \mathbf{x}_0|$ hardly change for any $\mathbf{x}' \in V$, and so the $\nabla' G_0$ and $\nabla' u_0$ terms are approximately constant in this integral and we can just pull them out, giving the approximation:

$$\hat{B} u_0 \approx \ln(c_2/c_1) \, \nabla' G_0(\mathbf{x}, \mathbf{x}') \cdot \nabla' u_0(\mathbf{x}')|_{\mathbf{x}'=\mathbf{x}_1} \text{volume}(V).$$

We can compute these gradients explicitly:

$$\nabla' \frac{1}{|\mathbf{x}' - \mathbf{y}|} = -\frac{\mathbf{x}' - \mathbf{y}}{|\mathbf{x}' - \mathbf{y}|^3},$$

and hence:

$$u(\mathbf{x}) \approx \frac{1}{4\pi c_2 |\mathbf{x} - \mathbf{x}_0|} + \ln(c_2/c_1) \frac{(\mathbf{x}_1 - \mathbf{x})}{4\pi |\mathbf{x}_1 - \mathbf{x}|^3} \cdot \frac{(\mathbf{x}_1 - \mathbf{x}_0)}{4\pi c_2 |\mathbf{x}_1 - \mathbf{x}_0|^3} \text{volume}(V). \qquad (5)$$

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[3]It turns out that many people get this wrong in electromagnetism for cases when c_1 and c_2 are very different, as discussed in my paper on a closely related subject, "Roughness losses and volume-current methods in photonic-crystal waveguides," *Appl. Phys. B* **81**, 238–293 (2005): http://math.mit.edu/~stevenj/papers/JohnsonPo05.pdf

Notice that the amplitude of the scattered term vanishes as volume$(V) \to 0$, as expected. Notice that it also depends on the sign of $(\mathbf{x}_1 - \mathbf{x}) \cdot (\mathbf{x}_1 - \mathbf{x}_0)$. Why is that? What does a $\nabla' G_0$ source "mean," physically?

3.1 Dipole sources

Consider the following problem in $\Omega = \mathbb{R}^3$, requiring as usual that solutions vanish at ∞:

$$-\nabla^2 D_{\mathbf{p}}(\mathbf{x}, \mathbf{x}') = -\mathbf{p} \cdot \nabla \delta(\mathbf{x} - \mathbf{x}') = +\mathbf{p} \cdot \nabla' \delta(\mathbf{x} - \mathbf{x}').$$

This is like the Green's function equation, except now we have put the *derivative* of a delta function on the right-hand side, with some constant vector $\mathbf{p}$ (the "dipole moment"). Recall what the derivative of a delta function is:

$$[-\mathbf{p} \cdot \nabla \delta(\mathbf{x} - \mathbf{x}')]\{\phi\} = [\delta(\mathbf{x} - \mathbf{x}')]\{\mathbf{p} \cdot \nabla \phi\} = \mathbf{p} \cdot \nabla \phi|_{\mathbf{x}'} = \lim_{\epsilon \to 0} \frac{\phi(\mathbf{x}' + \epsilon \mathbf{p}) - \phi(\mathbf{x}' - \epsilon \mathbf{p})}{2\epsilon},$$

and hence (similar to pset 5 of 2010 or pset 7 of 2011),

$$-\mathbf{p} \cdot \nabla \delta(\mathbf{x} - \mathbf{x}') = \lim_{\epsilon \to 0} \frac{\delta(\mathbf{x} - \mathbf{x}' - \epsilon \mathbf{p}) - \delta(\mathbf{x} - \mathbf{x}' + \epsilon \mathbf{p})}{2\epsilon}.$$

That is, the derivative of a delta function is a limit of limit of *two* delta functions of *opposite* sign, displaced proportional to $\mathbf{p}$. In 8.02, where delta functions are "point charges," this is what you would have called an "electric dipole."

We can solve for $\mathbf{D_p}$ quite easily, because we know the solution G_0 to $-\nabla^2 G_0(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$, and ∇ and ∇' derivatives can be interchanged in their order:

$$-\mathbf{p} \cdot \nabla \delta(\mathbf{x} - \mathbf{x}') = \mathbf{p} \cdot \nabla' [\delta(\mathbf{x} - \mathbf{x}')] = \mathbf{p} \cdot \nabla' [-\nabla^2 G_0(\mathbf{x}, \mathbf{x}')] = -\nabla^2 [\mathbf{p} \cdot \nabla' G_0(\mathbf{x}, \mathbf{x}')],$$

and hence

$$D_{\mathbf{p}}(\mathbf{x}, \mathbf{x}') = \mathbf{p} \cdot \nabla' G_0(\mathbf{x}, \mathbf{x}') = \mathbf{p} \cdot \frac{\mathbf{x} - \mathbf{x}'}{4\pi|\mathbf{x} - \mathbf{x}'|^3}.$$

In electrostatics, ths would be the potential of a dipole. Note that this falls off as $\sim 1/|\mathbf{x} - \mathbf{x}'|^2$, whereas G_0 falls off as $\sim 1/|\mathbf{x} - \mathbf{x}'|$.

Given this solution, we can now interpret the scattered part of the solution (5) above: **a small inhomogeneity gives an effective dipole source p** at $\mathbf{x}_1$, where

$$\mathbf{p} = -\ln(c_2/c_1) \frac{(\mathbf{x}_1 - \mathbf{x}_0)}{4\pi|\mathbf{x}_1 - \mathbf{x}_0|^3} \text{ volume}(V).$$

In electrostatics, for a typical case where V is a small piece of matter in vacuum, $c_2 < c_1$, so $\mathbf{p}$ is parallel to $\mathbf{x}_1 - \mathbf{x}_0$. Physically, a positive point charge induces a dipole moment $\mathbf{p}$ *pointed away* from the charge, because a "+" charge at $\mathbf{x}_0$ pushes "+" charges in V *away* from it, as shown below.
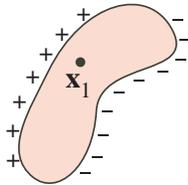
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