Chapter 2

Geometrical optics

The material in this chapter is not needed for SAR or CT, but it is foundational for seismic imaging.

For simplicity, in this chapter we study the variable-wave speed wave equation (!)

$$\left(\frac{1}{c^2(x)} \frac{\partial^2}{\partial t^2} - \Delta \right) u = 0.$$

As explained earlier, this equation models either constant-density acoustics ($c^2(x)$ is then the bulk modulus), or optics ($c_{ref}/c(x)$ is then the index of refraction for some reference level $c_r ef$). It is a good exercise to generalize the constructions of this chapter in the case of wave equations with several physical parameters.

2.1 Traveltimes and Green's functions

In a uniform 3D medium, we have seen that the acoustic Green's function (propagator) is

$$G(x, y, t) = \frac{\delta(ct - |x-y|)}{4\pi c|x-y|}. \tag{2.1}$$

In a variable (smooth) medium $c(x)$, we can no longer expect an explicit formula for G. However, to good approximation, the Green's function can be expressed in terms of a progressing-wave expansion as

$$G(x, y, t) = a(x, y)\delta(t - \tau(x, y)) + R(x, y, t), \tag{2.2}$$

where a is some smooth amplitude function, τ is the so-called traveltime function, and R is a remainder which is not small, but *smoother* than a delta function.

The functions a and τ are determined by substituting the expression above in the wave equation

$$\left(\frac{1}{c^2(x)}\frac{\partial^2}{\partial t^2} - \Delta_x\right) G(x,y,t) = 0, \qquad x \neq y,$$

and equating terms that have the same order of smoothness. By this, we mean that a $\delta(x)$ is smoother than a $\delta'(x)$, but less smooth than a Heaviside step function $H(x)$. An application of the chain rule gives

$$\begin{aligned}\left(\frac{1}{c^2(x)}\frac{\partial^2}{\partial t^2} - \Delta_x\right) G = {} & a\left(\frac{1}{c^2(x)} - |\nabla_x \tau|^2\right)\delta''(t-\tau) \\ & + (2\nabla_x\tau\cdot\nabla_x a - a\Delta_x\tau)\,\delta'(t-\tau) \\ & + \Delta_x a\delta(t-\tau) + \left(\frac{1}{c^2(x)}\frac{\partial^2}{\partial t^2} - \Delta_x\right) R.\end{aligned}$$

The δ'' term vanishes if, and in the case $a \neq 0$, only if

$$|\nabla_x \tau(x,y)| = \frac{1}{c(x)}, \tag{2.3}$$

a very important relation called the *eikonal equation* for τ. It determines τ completely for x in some neighborhood of y. Notice that τ has the units of a time.

The δ' term vanishes if and only if

$$2\nabla_x\tau(x,y)\cdot\nabla_x a(x,y) - a(x,y)\Delta_x\tau(x,y) = 0, \tag{2.4}$$

a relation called the transport equation for a. It determines a up to a multiplicative scalar, for x in a neighborhood of y.

As for the term involving δ, it is a good exercise (see end of chapter) to check that the multiplicative scalar for the amplitude a can be chosen so that the solution R of

$$\Delta_x a(x,y)\delta(t-\tau(x,y)) + \left(\frac{1}{c^2(x)}\frac{\partial^2}{\partial t^2} - \Delta_x\right) R = \delta(x-y)\delta(t)$$

is smoother than G itself. A good reference for progressing wave expansions is the book "Methods of Mathematical Physics" by Courant and Hilbert (pp. 622 ff. in volume 2).

This type of expansion for solutions of the wave equation is sometimes derived in the frequency domain ω rather than the time domain t. In that case, it often takes on the name *geometrical optics*. Taking the Fourier transform of (2.2), we get the corresponding Ansatz in the ω domain:

$$\widehat{G}(x,y,\omega) = \int e^{i\omega t} G(x,y,t)\, dt = a(x,y) e^{i\omega\tau(x,y)} + \widehat{R}(x,y,\omega). \tag{2.5}$$

Because τ appears in a complex exponential, it is also often called a *phase*. The same exercise of determining a and τ can be done, by substituting this expression in the Helmholtz equation, with the exact same outcome as earlier. Instead of matching like derivatives of δ, we now match like powers of ω. The ω^2 term is zero when the eikonal equation is satisfied, the ω term is zero when the transport equation is satisfied, etc.

Doing the matching exercise in the frequency domain shows the true nature of the geometrical optics expression of the Green's function: it is a *high-frequency approximation*.

Let us now inspect the eikonal equation for τ and characterize its solutions. In a uniform medium $c(x) = c_0$, it is easy to check the following two simple solutions.

- With the condition $\tau(y,y) = 0$, the solution is the by-now familiar

  $$\tau(x,y) = \frac{|x-y|}{c_0},$$

  which defines a forward light cone, (or $-\frac{|x-y|}{c_0}$, which defines a backward light cone,) and which helps recover the phase of the usual Green's function (2.1) when plugged in either (2.2) or (2.5).

- This is however not the only solution. With the condition $\tau(x) = 0$ for $x_1 = 0$ (and no need for a parameter y), a solution is $\tau(x) = \frac{|x_1|}{c_0}$. Another one would be $\tau(x) = \frac{x_1}{c_0}$.

For more general boundary conditions of the form $\tau(x) = 0$ for x on some curve Γ, but still in a uniform medium $c(x) = c_0$, $\tau(x)$ takes on the interpretation of the *distance function* to the curve Γ.

Note that the distance function to a curve may develop kinks, i.e., gradient discontinuities. For instance, if the curve is a parabola $x_2 = x_1^2$, a kink is formed on the half-line $x_1 = 0$, $x_2 \geq \frac{1}{4}$ above the focus point. This complication originates from the fact that, for some points x, there exist several segments originating from x that meet the curve at a right angle. At the kinks, the gradient is not defined and the eikonal equation does not, strictly speaking, hold. For this reason, the eikonal equation is only *locally solvable* in a neighborhood of Γ. To nevertheless consider a generalized solution with kinks, mathematicians resort to the notion of viscosity solution, where the equation

$$\frac{1}{c^2(x)} = |\nabla_x \tau_\varepsilon|^2 + \varepsilon^2 \Delta_x \tau_\varepsilon$$

is solved globally, and the limit as $\varepsilon \to 0$ is taken. Note that in the case of nonuniform $c(x)$, the solution generically develops kinks even in the case when the boundary condition is $\tau(y, y) = 0$.

In view of how the traveltime function appears in the expression of the Green's function, whether in time or in frequency, it is clear that the level lines

$$\tau(x, y) = t$$

for various values of t are *wavefronts*. For a point disturbance at y at $t = 0$, the wavefront $\tau(x, y) = t$ is the surface where the wave is exactly supported (when $c(x) = c_0$ in odd spatial dimensions), or otherwise essentially supported (in the sense that the wavefield asymptotes there.) It is possible to prove that the wavefield $G(x, y, t)$ is exactly zero for $\tau(x, y) > t$, regardless of the smoothness of $c(x)$, expressing the idea that waves propagate no faster than with speed $c(x)$.

Finally, it should be noted that

$$\phi(x, t) = t - \tau(x, y)$$

is for each y (or regardless of the boundary condition on τ) a solution of the characteristic equation

$$\left(\frac{\partial \xi}{\partial t}\right)^2 = |\nabla_x \xi|^2,$$

called a Hamilton-Jacobi equation, and already encountered in chapter 1. Hence the wavefronts $t - \tau(x, y) = 0$ are nothing but characteristic surfaces for the wave equation. They are the space-time surfaces along which the waves propagate, in a sense that we will make precise in section 8.1.

2.2 Rays

We now give a general solution of the eikonal equation, albeit in a somewhat implicit form, in terms of *rays*. The rays are the characteristic curves for the eikonal equation. Since the eikonal equation was already itself characteristic for the wave equation (see the discussion at the end of the preceding section), the rays also go by the name *bicharacteristics*.

The rays are curves $X(t)$ along which the eikonal equation is simplified, in the sense that the total derivative of the traveltime has a simple expression. Fix y and remove it from the notations. We write

$$\frac{d}{dt}\tau(X(t)) = \dot{X}(t) \cdot \nabla\tau(X(t)). \tag{2.6}$$

This relation will simplify if we define the ray $X(t)$ such that

- the speed $|\dot{X}(t)|$ is $c(x)$, locally at $x = X(t)$;
- the direction of $\dot{X}(t)$ is perpendicular to the wavefronts, i.e., aligned with $\nabla\tau(x)$ locally at $x = X(t)$.

These conditions are satisfied if we specify the velocity vector as

$$\dot{X}(t) = c(X(t))\frac{\nabla\tau(X(t))}{|\nabla\tau(X(t))|}. \tag{2.7}$$

Since the eikonal equation is $|\nabla\tau(x)| = 1/c(x)$, we can also write

$$\dot{X}(t) = c^2(X(t))\nabla\tau(X(t)).$$

Using either expression of $\dot{X}(t)$ in (2.6), we have

$$\frac{d}{dt}\tau(X(t)) = 1,$$

which has for solution

$$\tau(X(t)) - \tau(X(t_0)) = t - t_0.$$

We now see that τ indeed has the interpretation of time. Provided we can solve for $X(t)$, the formula above solves the eikonal equation.

The differential equation (2.7) for $X(t)$ is however not expressed in closed form, because it still depends on τ. We cannot however expect closure from a single equation in $X(t)$. We need an auxiliary quantity that records the direction of the ray, such as

$$\xi(t) = \nabla\tau(X(t)).$$

Then (all the functions of x are evaluated at $X(t)$)

$$\begin{aligned}
\dot{\xi}(t) &= \nabla\nabla\tau \cdot \dot{X}(t) \\
&= \nabla\nabla\tau(X(t)) \cdot c^2 \nabla\tau \\
&= \frac{c^2}{2} \nabla|\nabla\tau|^2 \\
&= \frac{c^2}{2} \nabla c^{-2} \\
&= -\frac{c^{-2}}{2} \nabla c^2 \\
&= -\frac{|\nabla\tau|^2}{2} \nabla c^2 \\
&= -\frac{|\xi(t)|^2}{2} \nabla(c^2)(X(t)).
\end{aligned}$$

We are now in presence of a closed, stand-alone system for the rays of geometrical optics in the unknowns $X(t)$ and $\xi(t)$:

$$\begin{cases} \dot{X}(t) &= c^2(X(t))\, \xi(t), \qquad\qquad X(0) = x_0, \\ \dot{\xi}(t) &= -\frac{\nabla(c^2)}{2}(X(t))\, |\xi(t)|^2, \qquad \xi(0) = \xi_0. \end{cases}$$

The traveltime function $\tau(x)$ is equivalently determined as the solution of the eikonal equation (the Eulerian viewpoint), or as the time parameter for the ray equations (the Lagrangian viewpoint). While X is a space variable, together (X, ξ) are called *phase-space* variables. It is fine to speak of a curve $X(t)$ in space as a ray, although strictly speaking the ray is a curve $(X(t), \xi(t))$ in phase-space. Because of its units, ξ is in this context often called the slowness vector.

The system above is called *Hamiltonian* because it can be generated as

$$\begin{cases} \dot{X}(t) &= \nabla_\xi H(X(t), \xi(t)), \\ \dot{\xi}(t) &= -\nabla_x H(X(t), \xi(t)), \end{cases}$$

from the Hamiltonian

$$H(x, \xi) = \frac{1}{2} c^2(x) |\xi|^2.$$

This is the proper Hamiltonian for optics or acoustics; the reader is already aware that the Hamiltonian of mechanics is $H(x,p) = \frac{p^2}{2m} + V(x)$. Note that H is a conserved quantity along the rays[1]

It can be shown that the rays are extremal curves of the action functional (\$)

$$S(X) = \int_a^b \frac{1}{c(x)} d\ell = \int_0^1 \frac{1}{c(X(t))} |\dot{X}(t)| dt, \qquad \text{s.t.} \qquad X(0) = a,\ X(1) = b,$$

a result called the Fermat principle. For this reason, it can also be shown that the rays are geodesics curves in the metric (\$)

$$ds^2 = c^{-2}(x) dx^2, \qquad dx^2 = \sum_i dx_i \wedge dx_i.$$

The traveltime τ therefore has yet another interpretation, namely that of action in the variational Hamiltonian theory[2].

Inspection of the ray equations now gives another answer to the question of solvability of τ from the eikonal equation. There is no ambiguity in specifying τ from $|\nabla \tau(x,y)| = 1/c(x)$ and $\tau(y,y) = 0$ as long as there is a single ray linking y to x. When there are several such rays — a situation called multipathing — the traveltime function takes on multiple values $\tau_j(x,y)$ which each solve the eikonal equation locally. The function that records the "number of arrivals" from y to x has discontinuities along curves called *caustics*; the respective eikonal equations for the different branches τ_j hold away from caustics. The global viscosity solution of the eikonal equation only records the time of the first arrival.

2.3 Amplitudes

We can now return to the equation (2.4) for the amplitude, for short

$$2\nabla \tau \cdot \nabla a = -a \Delta \tau.$$

It is called a transport equation because it turns into an ODE in characteristic coordinates, i.e., along the rays. Again, all the functions of x should be

[1] So is the symplectic 2-form $dx \wedge d\xi$, hence areas are conserved as well.

[2] There is no useful notion of Lagrangian in optics, because the photon is massless. See the book on Mathematical methods of classical mechanics by Arnold and the treatise by Landau and Lifschitz for the fascinating analogy between the equations of optics and Lagrangian/Hamiltonian mechanics.

evaluated at $X(t)$ in the following string of equalities:

$$\begin{aligned}\frac{d}{dt}a(X(t)) &= \dot{X}(t)\cdot\nabla a\\ &= c^2\nabla\tau\cdot\nabla a\\ &= -\frac{c^2}{2}a\;\Delta\tau.\end{aligned}$$

If τ is assumed known, then this equation specifies $a(X(t))$ up to a multiplicative constant. If we wish to eliminate τ like we did earlier for the rays, then we need to express $\Delta\tau(X(t))$ not just in terms of $X(t)$ and $\xi(t)$, but also in terms of the first partials $\frac{\partial X}{\partial X_0}(t)$, $\frac{\partial X}{\partial \xi_0}(t)$, $\frac{\partial \xi}{\partial X_0}(t)$, $\frac{\partial \xi}{\partial \xi_0}(t)$ with respect to the initial conditions[3].

The transport equation can also be written in divergence form,

$$\nabla\cdot(a^2\nabla\tau) = 0,$$

which suggests that there exists an underlying conserved quantity, which integration will reveal. Assume for now that space is 3-dimensional. Consider a *ray tube* R, i.e, an open surface spanned by rays. Close this surface with two cross-sections S_+ and S_- normal to the rays. Apply the divergence theorem in the enclosed volume V. This gives

$$0 = \iiint_V \nabla\cdot(a^2\nabla\tau)dV = \oiint_{\partial V} a^2\nabla\tau\cdot n dS,$$

where n is the outward normal vector to the surface $\partial V = R\cup S_+\cup S_-$.

- For x on R, the normal vector n is by definition (of R) perpendicular to the ray at x, hence $\nabla\tau\cdot n = 0$.

- For x on $S_\pm$, the normal vector n is parallel to the ray at x, hence $\nabla\tau\cdot n = \pm|\nabla\tau|$.

As a result,

$$\int_{S_+} a^2|\nabla\tau|dS = \int_{S_-} a^2|\nabla\tau|dS,$$

[3]See for instance the 2006 paper by Candes and Ying on the phase-flow method for these equations.

thus

$$\int_{S_+} \frac{a^2}{c} dS = \int_{S_-} \frac{a^2}{c} dS.$$

This relation is an expression of conservation of energy. Passing to an infinitesimally thin ray tube linking x_0 to x, it becomes

$$a(x) = a(x_0) \sqrt{\frac{c(x_0)}{c(x)} \frac{dS}{dS_0}}.$$

It is again clear that the amplitude is determined up to a multiplicative scalar from this equation. A similar argument can be made in 2 space dimensions, and leads to the same conclusion with the ratio of line elements ds/ds_0 in place of the ratio of surface elements dS/dS_0.

Examples of solutions in a uniform medium in $\mathbb{R}^3$ include

- Plane waves, for which $dS/dS_0 = 1$ hence $a =$ constant,
- Cylindrical waves about $r = 0$, for which $dS/dS_0 = r/r_0$ hence $a \sim 1/\sqrt{r}$,
- Spherical waves about $r = 0$, for which $dS/dS_0 = (r/r_0)^2$ hence $a \sim 1/r$,
- A cylindrical focus or a caustic point at $r = a$ can generically be seen as a time-reversed cylindrical wave, hence $a \sim 1/\sqrt{r-a}$. A spherical focus is a geometrical exception; it would correspond to $a \sim 1/(r-a)$.

In the infinite-frequency geometrical optics approximation, the amplitude indeed becomes infinite at a focus point or caustic curve/surface. In reality, the amplitude at a caustic is an increasing function of the frequency ω of the underlying wave. The rate of growth is generically of the form $\omega^{1/6}$, as established by Keller in the 1950s.

Caustics and focus points give rise to bright spots in imaging datasets, although this information is probably never explicitly used in practice to improve imaging.

2.4 Caustics

For fixed t, and after a slight change of notation, the Hamiltonian system generates the so-called phase map $(x, \xi) \mapsto (y(x, \xi), \eta(x, \xi))$. Its differential is block partitioned as

$$\nabla_{(x,\xi)} \begin{pmatrix} y \\ \eta \end{pmatrix} = \begin{pmatrix} \frac{\partial y}{\partial x} & \frac{\partial y}{\partial \xi} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial \xi} \end{pmatrix}.$$

Besides having determinant 1, this Jacobian matrix has the property that

$$\delta_{kl} = \sum_j \frac{\partial \eta_j}{\partial \xi_l} \frac{\partial y_j}{\partial x_k} - \frac{\partial \eta_j}{\partial x_k} \frac{\partial y_j}{\partial \xi_l}. \tag{2.8}$$

This equation is conservation of the second symplectic form $d\eta \wedge dy = d\xi \wedge dx$ written in coordinates. It also follows from writing conservation of the first symplectic form $\xi \cdot dx = \eta \cdot dy$ as

$$\xi_j = \sum_i \eta_i \frac{\partial y_i}{\partial x_j}, \qquad 0 = \sum_i \eta_i \frac{\partial y_i}{\partial \xi_j},$$

and further combining these expressions. ($d\eta \wedge dy = d\xi \wedge dx$ also follows from $\xi \cdot dx = \eta \cdot dy$ by Cartan's formula). Equation (2.8) can also be justified directly, see the exercise section. Note in passing that it is not a Poisson bracket.

It is instructive to express (2.8) is ray coordinates. Without loss of generality choose the reference points $x_0 = 0$ and $\xi_0 = (1, 0)^T$. Let x_1 and ξ_1 be the coordinates of x and ξ along ξ_0, and x_2, ξ_2 along $\xi_0^\perp$. Consider (y_0, η_0) the image of (x_0, ξ_0) under the phase map. Let y_1 and y_2 be the coordinates of y and η along η_0, and x_2, ξ_2 along $\eta_0^\perp$. In other words, the coordinates labeled "1" are along the ray (longitudinal), and "2" across the ray (transversal).

In two spatial dimensions, only the coordinates across the ray give rise to a nontrivial relation in (2.8). One can check that the $k = l = 2$ element of (2.8) becomes

$$1 = \frac{\partial \eta_2}{\partial \xi_2} \frac{\partial y_2}{\partial x_2} - \frac{\partial \eta_2}{\partial x_2} \frac{\partial y_2}{\partial \xi_2}. \tag{2.9}$$

When either of the terms in this equation vanish, we say that (y, η) is on a *caustic*. Two regimes can be contrasted:

- If $\partial y_2 / \partial x_2 = 0$, we are in presence of a "x-caustic". This means that, as the initial point x is moved infinitesimally in a direction perpendicular to the take-off direction, the resulting location y does not move. A x-caustic is at the tip of a swallowtail pattern formed from an initial plane wavefront.

- If $\partial y_2/\partial \xi_2 = 0$, we are in presence of a "ξ-caustic". This means that, as the initial direction angle $\arg \xi$ changes infinitesimally, the resulting location y does not move. A ξ-caustic is at the tip of a swallowtail pattern formed from an initial point wavefront.

Equation (2.9) shows that these two scenarios cannot happen simultaneously. In fact, if the variation of y_2 with respect to x_2 is zero, then the variation of y_2 with respect to ξ_2 must be maximal to compensate for it; and vice-versa. When t is the first time at which either partial derivative vanishes, the caustic is a single point: we speak of a focus instead.

Notice that $\partial \eta_2/\partial x_2 = 0$ and $\partial \eta_2/\partial \xi_2 = 0$ are not necessarily caustic events; rather, they are inflection points in the wavefronts (respectively initially plane and initially point.)

2.5 Exercises

1. (Difficult) Show that the remainder R in the progressing wave expansion is smoother than the Green's function G itself.

2. In this exercise we compute the Fréchet derivative of traveltime with respect to the wave speed. For simplicity, let $n(x) = 1/c(x)$.

   (a) In one spatial dimension, we have already seen that $\tau(x) = \int_{x_0}^{x} n(x')dx'$. Find an expression for $\delta\tau(x)/\delta n(y)$ (or equivalently for the operator that it generates via $\langle \delta\tau(x)/\delta n, h\rangle$ for a test function h).

   (b) In several spatial dimensions, $\tau(x)$ obeys $|\nabla\tau(x)| = n(x)$ with $\tau(0) = 0$, say. First, show that $\delta\tau(x)/\delta n(y)$ obeys a transport equation along the rays. Then solve this equation. Provided there is one ray between 0 and x, argue that $\delta\tau(x)/\delta n(y)$, as a function of y, is concentrated along this ray.

   (c) What do your answers become when the derivative is taken with respect to $c(x)$ rather than $n(x)$?

   The function $\delta\tau(x)/\delta n(y)$ of y is often called *sensitivity kernel* (of τ with respect to n). It's a distribution, really.

3. Show that the Hamiltonian is conserved along the trajectories of a Hamiltonian system.

4. Show that the alternative Hamiltonian $H(x, \xi) = c(x)|\xi|$ generates an equivalent system of ODEs for the rays.

5. Show that the rays are circular in a linear wave velocity model, i.e., $c(\mathbf{x}) = z$ in the half-plane $z > 0$. Note: $\{z > 0\}$ endowed with $ds^2 = \frac{dx^2+dz^2}{z^2}$ is called the Poincaré half-plane, a very important object in mathematics.

6. Show that the traveltime τ is convex as a function of the underlying medium $c(x)$, by invoking the Fermat principle.

7. Prove (2.8).

   Hint. Show it holds at time zero, and use the Hamiltonian structure to show that the time derivative of the whole expression is zero.

8. Let $\{y(x, \xi), \eta(x, \xi)\}$ be the fixed-time phase map. Show that $\sum_i \frac{\partial \eta_i}{\partial \xi_k} \frac{\partial y_i}{\partial \xi_l}$ is symmetric.

   Hint. Same hint as above. Show that the time derivative of the difference of the matrix and its transpose vanishes.

9. Let $\tau(x, y)$ be the 2-point traveltime, and let $\{y(x, \xi), \eta(x, \xi)\}$ be the fixed-time phase map for the Hamiltonian of isotropic optics. Prove or disprove:

   (a)
   $$\sum_k \frac{\partial y_k}{\partial \xi_j} \frac{\partial \tau}{\partial y_k}(x, y(x, \xi)) = 0;$$

   (b)
   $$\sum_k \frac{\partial \eta_i}{\partial \xi_k} \frac{\partial^2 \tau}{\partial x_j \partial x_k}(x, y(x, \xi)) + \sum_k \frac{\partial y_k}{\partial x_j} \frac{\partial^2 \tau}{\partial y_i \partial y_k}(x, y(x, \xi)) = 0.$$