18.325 - Waves and Imaging
Fall 2012 - Class notes

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Preface

In the margins of this text we use

- the symbol (!) to draw attention every time a physical assumption or simplification is made; and
- the symbol ($) to draw attention every time a mathematical fact is stated without proof.

Thanks are extended to the following people for discussions, suggestions, and early drafts: Thibaut Lienart, Nicholas Maxwell, Pierre-David Letourneau, Russell Hewett, and Vincent Jugnon.

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1.1.1 Acoustic waves

Acoustic waves are propagating pressure disturbances in a gas or liquid. With $p(x,t)$ the pressure fluctuation (a time-dependent scalar field) and $v(x,t)$ the particle velocity (a time-dependent vector field), the acoustic wave equations read

$$\frac{\partial v}{\partial t} = -\frac{1}{\rho_0}\nabla p, \tag{1.1}$$

$$\frac{\partial p}{\partial t} = -\kappa_0 \nabla \cdot v. \tag{1.2}$$

The two quantities ρ_0 and κ_0 are the mass density and the bulk modulus, respectively. They are linked to the wave speed c through $\kappa_0 = \rho_0 c^2$. Initial conditions on p and v must be supplied. A forcing term may be added to the dynamic balance equation (1.1) when external forces (rather than initial conditions) create the waves.

Let us now explain how these equations are obtained from a linearization of Euler's gas dynamics equations in a uniform background medium ($). Consider the mass density ρ as a scalar field. In the inviscid case ($), conservation of momentum and mass respectively read

$$\rho(\frac{\partial v}{\partial t} + v \cdot \nabla v) = -\nabla p, \qquad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0.$$

An additional equation, called constitutive relation, must be added to close the system. It typically relates the pressure and the density in an algebraic way, and encodes a thermodynamic assumption about compression and dilation. For instance if the gas is assumed to be ideal, and if the compression-dilation process occurring in the wave is adiabatic reversible (no heat transfer), then $p \sim \rho^\gamma,\ \gamma = 1.4$, where $\sim$ indicates equality up to a dimensional constant. More generally, assume for the moment that the constitutive relation takes the form

$$p = f(\rho)$$

for some scalar function f, which we assume differentiable and strictly increasing ($f'(\rho) > 0$ for all $\rho > 0$).

Consider small disturbances off of an equilibrium state:

$$p = p_0 + p_1, \qquad \rho = \rho_0 + \rho_1, \qquad v = v_0 + v_1.$$

In what follows, neglect quadratic quantities of p_1, ρ_1, v_1. Consider a medium at rest (\$): p_0, ρ_0 independent of t, and $v_0 = 0$. After some algebraic simplification the conservation of momentum becomes

$$\rho_0 \frac{\partial v_1}{\partial t} = -\nabla p_0 - \nabla p_1.$$

To zero-th order (i.e., at equilibrium, $p_1 = \rho_1 = v_1 = 0$,) we have

$$\nabla p_0 = 0 \qquad \Rightarrow \qquad p_0 \text{ constant in } x.$$

To first order, we get

$$\rho_0 \frac{\partial v_1}{\partial t} = -\nabla p_1,$$

which is exactly (1.1) after renaming $v_1 \to v$, $p_1 \to p$. The constitutive relation must hold at equilibrium, hence p_0 constant in x implies that ρ_0 is also constant in x (uniform). Conservation of mass becomes

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \nabla \cdot v_1 = 0.$$

Differentiate the constitutive relation to obtain $p_1 = f'(\rho_0)\rho_1$. Call $f'(\rho_0) = c^2$, a number that we assume positive. Then we can eliminate ρ_1 to get

$$\frac{\partial p_1}{\partial t} + \rho_0 c^2 \nabla \cdot v_1 = 0.$$

This is exactly (1.2) with $\kappa_0 = \rho_0 c^2$.

Conveniently, the equations for acoustic waves in a variable medium $\rho_0(x)$, $\kappa_0(x)$ are obvious modifications of (1.1), (1.2):

$$\frac{\partial v}{\partial t} = -\frac{1}{\rho_0(x)} \nabla p, \tag{1.3}$$

$$\frac{\partial p}{\partial t} = -\kappa_0(x) \nabla \cdot v. \tag{1.4}$$

A different argument is needed to justify these equations, however. The previous reasoning does not leave room for variable $\rho_0(x)$ or $\kappa_0(x)$. Instead, it is necessary to introduce a more realistic constitutive relation

$$p = f(\rho, s),$$

where s is the entropy. An additional equation for conservation of entropy needs to be considered. The new constitutive relation allows ρ_0 and s_0 to be functions of x in tandem, although p_0 is still (necessarily) uniform in x. The reasoning leading to (1.3), (1.4) is the subject of an exercise in section 1.3.

Acoustic waves can take the form of a first-order system of equations, or else a second-order scalar equation. Combining (1.3), (1.4), we get

$$\frac{\partial^2 p}{\partial t^2} = \kappa_0(x) \nabla \cdot (\frac{1}{\rho_0(x)} \nabla p).$$

Initial conditions on both p and $\partial p / \partial t$ must be supplied. This equation may come with a right-hand side $f(x,t)$ that indicates forcing. When ρ_0 and κ_0 are constant, the scalar wave equation reduces to

$$\frac{\partial^2 p}{\partial t^2} = c_0^2 \, \Delta p.$$

Waves governed by (1.3), (1.4) belong in the category of hyperbolic waves because they obey conservation of energy. Define

$$w = \begin{pmatrix} v \\ p \end{pmatrix}, \qquad L = \begin{pmatrix} 0 & -\frac{1}{\rho_0} \nabla \\ -\kappa_0 \nabla \cdot & 0 \end{pmatrix}.$$

Then the acoustic system simply reads

$$\frac{\partial w}{\partial t} = Lw.$$

L is called the generator of the evolution.

Definition 1. *The system $\frac{\partial w}{\partial t} = Lw$ is said to be hyperbolic if L is a matrix of first-order differential operators, and there exists an inner product $\langle w, w' \rangle$ with respect to which $L^* = -L$, i.e., L is anti-self-adjoint.*

An adjoint operator such as L^* is defined through the equation[1]

$$\langle Lw, w' \rangle = \langle w, L^* w' \rangle, \qquad \text{for all } w, w'.$$

For instance, in the case of the acoustic system, the proper notion of inner product is (the factor $1/2$ is optional)

$$\langle w, w' \rangle = \frac{1}{2} \int (\rho_0 v \cdot v' + \frac{1}{\kappa_0} p p') \, dx.$$

It is an exercise in section 1.3 to show that $\langle Lw, w' \rangle = \langle w, L^* w' \rangle$ for that inner product, for all w, w'.

Theorem 1. *If $\frac{\partial w}{\partial t} = Lw$ is a hyperbolic system, then $E = \langle w, w \rangle$ is conserved in time.*

Proof.

$$\begin{aligned} \frac{d}{dt} \langle w, w \rangle &= \langle \frac{\partial w}{\partial t}, w \rangle + \langle w, \frac{\partial w}{\partial t} \rangle \\ &= 2 \langle \frac{\partial w}{\partial t}, w \rangle \\ &= 2 \langle Lw, w \rangle \\ &= 2 \langle w, L^* w \rangle \\ &= 2 \langle w, (-L) w \rangle \\ &= -2 \langle Lw, w \rangle. \end{aligned}$$

A quantity is equal to minus itself if and only if it is zero. □

In the case of acoustic waves,

$$E = \frac{1}{2} \int (\rho_0 v^2 + \frac{p^2}{\kappa}) \, dx,$$

[1]The existence of L^* can be traced back to the Riesz representation theorem once $\langle Lw, w' \rangle$ is shown to be a continuous functional of w in some adequate Hilbert space norm.

which can be understood as kinetic plus potential energy. We now see that the factor $1/2$ was chosen to be consistent with the physicists' convention for energy.

In the presence of external forcings the hyperbolic system reads $\partial w/\partial t = Lw + f$: in that case the rate of change of energy is determined by f.

For reference, common boundary conditions for acoustic waves include

- Sound soft boundary condition: Dirichlet for the pressure, $p = 0$.
- Sound-hard boundary condition: Neumann for the pressure, $\frac{\partial p}{\partial n} = 0$, or equivalently $v \cdot n = 0$.

Another important physical quantity is related to acoustic waves: the acoustic impedance $Z = \sqrt{\rho_0 \kappa_0}$. We will see later that impedance jumps determine reflection and transmission coefficients at medium discontinuities.

1.1.2 Elastic waves

Elastic waves are propagating pressure disturbances in solids. The interesting physical variables are

- The displacement $u(x,t)$, a time-dependent vector field. In terms of u, the particle velocity is $v = \frac{\partial u}{\partial t}$.
- The strain tensor
$$\epsilon = \frac{1}{2}(\nabla u + (\nabla u)^T),$$
a symmetric time-dependent tensor field.
- The stress tensor σ, also a symmetric time-dependent tensor field.

For elastic waves, the density ρ is very often assumed independent of t along particle trajectories, namely $\rho_0(x,0) = \rho_0(x + u(x,t), t)$.

The equation of elastic waves in an isotropic medium (where all the waves travel at the same speed regardless of the direction in which they propagate) ($) reads

$$\rho \frac{\partial^2 u}{\partial t^2} = \nabla(\lambda \nabla \cdot u) + \nabla \cdot (\mu(\nabla u + (\nabla u)^T)). \tag{1.5}$$

where ρ, λ, and μ may possibly depend on x. As for acoustic waves, a forcing term is added to this equation when waves are generated from external forces.

To justify this equation, start by considering the equation of conservation of momentum ("$F = ma$"),

$$\rho \frac{\partial v}{\partial t} = \nabla \cdot \sigma,$$

possibly with an additional term $f(x,t)$ modeling external forces. The notation $\nabla\cdot$ indicates tensor divergence, namely $(\nabla \cdot \sigma)_i = \sum_j \frac{\partial \sigma_{ij}}{\partial x_j}$. Stress and strain are linked by a constitutive relation called Hooke's law,

$$\sigma = C : \epsilon,$$

where C is the 4-index elastic tensor. In three spatial dimensions, C has 81 components. The colon indicates tensor contraction, so that $(C : \epsilon)_{ij} = \sum_{k\ell} C_{ijk\ell}\epsilon_{k\ell}$.

These equations form a closed system when they are complemented by

$$\frac{\partial \epsilon}{\partial t} = \frac{1}{2}(\nabla v + (\nabla v)^T),$$

which holds by definition of ϵ.

At this point we can check that the first-order system for v and ϵ defined by the equations above is hyperbolic. Define

$$w = \begin{pmatrix} v \\ \epsilon \end{pmatrix}, \qquad L = \begin{pmatrix} 0 & L_2 \\ L_1 & 0 \end{pmatrix},$$

with

$$L_1 v = \frac{1}{2}(\nabla v + (\nabla v)^T), \qquad L_2 \epsilon = \frac{1}{\rho_0} \nabla \cdot (C : \epsilon).$$

Then, as previously, $\frac{\partial w}{\partial t} = Lw$. An exercise in section 1.3 asks to show that the matrix operator L is anti-selfadjoint with respect to the inner product

$$\langle w, w' \rangle = \frac{1}{2} \int (\rho v \cdot v' + \epsilon : C : \epsilon)\, dx.$$

The corresponding conserved elastic energy is $E = \langle w, w \rangle$.

Isotropic elasticity is obtained where C takes a special form with 2 degrees of freedom rather than 81, namely

$$C_{ijk\ell} = \lambda \delta_{ij}\delta_{kl} + \mu(\delta_{i\ell}\delta_{jk} + \delta_{ik}\delta_{j\ell}).$$

We are not delving into the justification of this equation. The two elastic parameters λ and μ are also called Lamé parameters:

- λ corresponds to longitudinal waves, also known as compressional, pressure waves (P).
- μ corresponds to transverse waves, also known as shear waves (S).

Originally, the denominations P and S come from "primary" and "secondary", as P waves tend to propagate faster, hence arrive earlier, than S waves.

With this parametrization of C, it is easy to check that the elastic system reduces to the single equation (1.5). In index notation, it reads

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \partial_i(\lambda \partial_j u_j) + \partial_j(\mu(\partial_i u_j + \partial_j u_i)).$$

For reference, the hyperbolic propagator L_2 reduces to

$$L_2 \epsilon = \frac{1}{\rho}(\nabla(\lambda \operatorname{tr} \epsilon) + 2\, \nabla \cdot (\mu \epsilon)), \qquad \operatorname{tr} \epsilon = \sum_i \epsilon_{ii},$$

and the energy inner product is

$$\langle w, w' \rangle = \frac{1}{2} \int (\rho v \cdot v' + 2\, \mu \operatorname{tr}(\epsilon^T \epsilon') + \lambda (\operatorname{tr} \epsilon)(\operatorname{tr} \epsilon'))\, dx.$$

The elastic wave equation looks like an acoustic wave equation with "2 terms, hence 2 waves". To make this observation more precise, assume that λ and μ are constant (\$). Use some vector identities[2] to reduce (1.5) to

$$\begin{aligned} \rho \frac{\partial^2 u}{\partial t^2} &= (\lambda + \mu) \nabla(\nabla \cdot u) + \mu \Delta u, \\ &= (\lambda + 2\mu) \nabla(\nabla \cdot u) - \mu \nabla \times \nabla \times u. \end{aligned}$$

Perform the Helmholtz (a.k.a. Hodge) decomposition of u in terms of potentials ϕ and ψ:

$$u = \nabla \phi + \nabla \times \psi,$$

where ϕ is a scalar field and ψ is a vector field[3]. These two potentials are determined up to a gauge choice, namely

$$\phi' = \phi + C, \qquad \psi' = \psi + \nabla f.$$

[2] In this section, we make use of $\nabla \times \nabla \times u = \nabla(\nabla \cdot u) - \Delta u$, $\nabla \cdot \nabla \times \psi = 0$, and $\nabla \times \nabla \psi = 0$.

[3] Normally the Helmholtz decomposition comes with a third term h which obeys $\Delta h = 0$, i.e., h is harmonic, but under suitable assumptions of decay at infinity the only solution to $\Delta h = 0$ is $h = 0$.

Choose f such that ψ' has zero divergence:

$$\nabla \cdot \psi' = 0 \qquad \Rightarrow \qquad \Delta f = -\nabla \cdot \psi.$$

This is a well-posed Poisson equation for f. With this choice of ψ', it holds that

$$\nabla \cdot u = \Delta\phi, \qquad \nabla \times u = \nabla \times \nabla \times u = -\Delta\psi.$$

The elastic wave equation can then be rewritten in terms of ϕ, ψ as

$$\nabla \left[\rho \frac{\partial^2 \phi}{\partial t^2} - (\lambda + 2\mu)\Delta\phi \right] + \nabla \times \left[\rho \frac{\partial^2 \psi}{\partial t^2} - \mu \Delta\psi \right] = 0.$$

Take the gradient of this equation to conclude that (with a suitable decay condition at infinity)

$$\rho \frac{\partial^2 \phi}{\partial t^2} - (\lambda + 2\mu)\Delta\phi = \text{ harmonic } = 0.$$

Now that the first term is zero, we get (with a suitable decay condition at infinity)

$$\rho \frac{\partial^2 \psi}{\partial t^2} - \mu \Delta\psi = \nabla(\text{something}) = 0.$$

Hence each potential ϕ and ψ solve their own scalar wave equation: one for the longitudinal waves (ϕ) and one for the transverse waves (ϕ). They obey a superposition principle. The two corresponding wave speeds are

$$c_P = \sqrt{\frac{\lambda + 2\mu}{\rho_0}}, \qquad c_S = \sqrt{\frac{\mu}{\rho_0}}.$$

In the limit $\mu \to 0$, we see that only the longitudinal wave remains, and λ reduces to the bulk modulus. In all cases, since $\lambda \geq 0$ we always have $c_P \geq \sqrt{2} c_S$: the P waves are indeed always faster (by a factor at least $\sqrt{2}$) than the S waves.

The assumption that λ and μ are constant is a very strong one: there is a lot of physics in the coupling of ϕ and ψ that the reasoning above does not capture. Most important is mode conversion as a result of wave reflection at discontinuity interfaces of $\lambda(x)$ and/or $\mu(x)$.

1.1.3 Electromagnetic waves

The quantities of interest for electromagnetic waves are:

- Physical fields: the electric field E, and the magnetic field H,
- Medium parameters: the electric permittivity ϵ and the magnetic permeability μ,
- Forcings: electric currents j and electric charges ρ.

The electric displacement field D and the magnetic induction field B are also considered. In the linearized regime (\$), they are assumed to be linked to the usual fields E and H by the constitutive relations

$$D = \epsilon E, \qquad B = \mu H.$$

Maxwell's equations in a medium with possible space-varying parameters ϵ and μ read

$$\nabla \times E = -\frac{\partial B}{\partial t} \qquad \text{(Faraday's law)} \tag{1.6}$$

$$\nabla \times H = \frac{\partial D}{\partial t} + j \qquad \text{(Ampère's law with Maxwell's correction)} \tag{1.7}$$

$$\nabla \cdot D = \rho \qquad \text{(Gauss's law for the electric field)} \tag{1.8}$$

$$\nabla \cdot B = 0 \qquad \text{(Gauss's law for the magnetic field)} \tag{1.9}$$

The integral forms of these equations are obtained by a volume integral, followed by a reduction to surface equations by Stokes's theorem for (1.6), (1.7) and the divergence (Gauss's) theorem for (1.8), (1.9). The integral equations are valid when ϵ and μ are discontinuous, whereas the differential equations strictly speaking are not.

The total charge in a volume V is $\int_V \rho dV$, while the total current through a surface S is $\int_S j \cdot dS$. Conservation of charge follows by taking the divergence of (1.7) and using (1.8):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot j = 0.$$

In vacuum, or dry air, the parameters are constant and denoted $\epsilon = \epsilon_0$, $\mu = \mu_0$. They have specific numerical values in adequate units.

We now take the viewpoint that (1.6) and (1.7) are evolution equations for E and H (or D and B) that fully determine the fields when they are solved

forward (or backward) in time. In that setting, the other two equations (1.8) and (1.9) are simply constraints on the initial (or final) condition at $t = 0$. As previously, we may write Maxwell's equations in the more concise hyperbolic form

$$\frac{\partial w}{\partial t} = Lw + \begin{pmatrix} -j/\epsilon \\ 0 \end{pmatrix}, \qquad \text{with } w = \begin{pmatrix} E \\ H \end{pmatrix},$$

provided

$$L = \begin{pmatrix} 0 & \frac{1}{\epsilon}\nabla\times \\ -\frac{1}{\mu}\nabla\times & 0 \end{pmatrix}.$$

The "physical" inner product that makes $L^* = -L$ is

$$\langle w, w' \rangle = \frac{1}{2}\int (\epsilon E E' + \mu H H')\, dx.$$

The electromagnetic energy $E = \langle w, w \rangle$ is conserved when $j = 0$.

It is the balanced coupling of E and H through (1.6) and (1.7) that creates wave-like solutions to Maxwell's equations (and prompts calling the physical phenomenon electromagnetism rather than just electricity and magnetism.) Combining both equations, we obtain

$$\frac{\partial^2 E}{\partial t^2} = -\frac{1}{\epsilon}\nabla \times (\frac{1}{\mu}\nabla \times E),$$

$$\frac{\partial^2 H}{\partial t^2} = -\frac{1}{\mu}\nabla \times (\frac{1}{\epsilon}\nabla \times H).$$

These wave equations may be stand-alone but E and H are still subject to essential couplings.

A bit of algebra[4] reveals the more familiar form

$$\Delta E - \epsilon\mu\frac{\partial^2 E}{\partial t^2} + \frac{\nabla\mu}{\mu} \times (\nabla \times E) + \nabla(E \cdot \frac{\nabla\epsilon}{\epsilon}) = 0.$$

We now see that in a uniform medium, ϵ and μ are constant and the last two terms drop, revealing a wave equation with speed

$$c = \frac{1}{\sqrt{\epsilon\mu}}.$$

[4]Using the relations $\nabla \times \nabla \times F = \nabla(\nabla \cdot F) - \Delta F$ again, as well as $\nabla \cdot (F \times G) = G \cdot (\nabla \times F) - F \cdot (\nabla \times G)$.

The speed of light is $c_0 = 1/\sqrt{\epsilon_0 \mu_0}$. Even when ϵ and μ vary in x, the last two terms are kinematically much less important than the first two because they involve lower-order derivatives of E. They would not, for instance, change the path of the "light rays", a concept that we'll make clear later.

For reference, we now list the jump conditions that the electric and magnetic fields obey at a dielectric interface. These relations can be obtained from the integral form of Maxwell's equations, posed over a thin volume straddling the interface. Let n be the vector normal to a dielectric interface.

$$n \times E_1 = n \times E_2 \qquad \text{(continuous tangential components)}$$

$$n \times H_1 = n \times H_2 + j_S$$

$$n \cdot D_1 = n \cdot D_2 + \rho_S$$

$$n \cdot H_1 = n \cdot H_2 \qquad \text{(continuous normal component)}$$

We have used j_S and ρ_S for surface currents and surface charges respectively. If the two dielectrics correspond to finite parameters ϵ_1, ϵ_2 and μ_1, μ_2, then these currents are zero. If material 2 is a perfect electric conductor however, then these currents are not zero, but the fields E_2, H_2, D_2 and H_2 are zero. This results in the conditions $n \times E = 0$ (E perpendicular to the interface) and $n \times H = 0$ (H parallel to the interface) in the vicinity of a perfect conductor.

Materials conducting current are best described by a complex electric permittivity $\epsilon = \epsilon' + i\sigma/\omega$, where σ is called the conductivity. All these quantities could be frequency-dependent. It is the ratio σ/ϵ' that tends to infinity when the conductor is "perfect". Materials for which ϵ is real are called "perfect dielectrics": no conduction occurs and the material behaves like a capacitor. We will only consider perfect dielectrics in this class. When conduction is present, loss is also present, and electromagnetic waves tend to be inhibited. Notice that the imaginary part of the permittivity is σ/ω, and not just σ, because we want Ampère's law to reduce to $j = \sigma E$ (the differential version of Ohm's law) in the time-harmonic case and when $B = 0$.

1.2 Special solutions

1.2.1 Plane waves, dispersion relations

In this section we study special solutions of wave equations that depend on x like e^{ikx}. These solutions are obtained if we assume that the time dependence

is harmonic, namely if the unknown is $w(x,t)$, then we assume (\$)

$$w(x,t) = e^{-i\omega t} f_\omega(x), \qquad \omega \in \mathbb{R}.$$

The number ω is called angular frequency, or simply frequency. Choosing $e^{+i\omega t}$ instead makes no difference down the road. Under the time-harmonic assumption, the evolution problem $\frac{\partial w}{\partial t} = Lw$ becomes an eigenvalue problem:

$$-i\omega f_\omega = L f_\omega.$$

Not all solutions are time-harmonic, but all solutions are *superpositions* of harmonic waves at different frequencies ω. Indeed, if $w(x,t)$ is a solution, consider it as the inverse Fourier transform of some $\widehat{w}(x,\omega)$:

$$w(x,t) = \frac{1}{2\pi} \int e^{-i\omega t} \widehat{w}(x,\omega) d\omega.$$

Then each $\widehat{w}(x,\omega)$ is what we called $f_\omega(x)$ above. Hence there is no loss of generality in considering time-harmonic solutions.

Consider the following examples.

- The one-way, one-dimensional wave equation

  $$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \qquad x \in \mathbb{R}.$$

  Time harmonic solutions $u(x,t) = e^{-i\omega t} f_\omega(x)$ obey

  $$i\frac{\omega}{c} f_\omega = f'_\omega, \qquad x \in \mathbb{R}.$$

  The solution to this equation is

  $$f_\omega(x) = e^{ikx}, \qquad k = \frac{\omega}{c} \in \mathbb{R}.$$

  Evanescent waves corresponding to decaying exponentials in x and t are also solutions over a half-line, say, but they are ruled out by our assumption (\$) that $\omega \in \mathbb{R}$.

  While ω is the angular frequency (equal to $2\pi/T$ where T is the period), k is called the wave number (equal to $2\pi/\lambda$ where λ is the wavelength.) It is like a "spatial frequency", though it is prudent to reserve the word

frequency for the variable dual to time. The quantity measured in Hertz [1/s] and also called frequency is $\nu = \omega/(2\pi)$.

The full solution then takes the form

$$u(x,t) = e^{i(kx-\omega t)} = e^{ik(x-ct)},$$

manifestly a right-going wave at speed c. If the equation had been $\frac{\partial u}{\partial t} - c\frac{\partial u}{\partial x} = 0$ instead, the wave would have been left-going: $u(x,t) = e^{ik(x+ct)}$.

- The n-dimensional wave equation in a uniform medium,

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta u, \qquad x \in \mathbb{R}^n.$$

When $u(x,t) = e^{-i\omega t} f_\omega(x)$, the eigenvalue problem is called the (homogeneous) Helmholtz equation. It is

$$-\omega^2 f_\omega(x) = \Delta f_\omega(x), \qquad x \in \mathbb{R}^n. \tag{1.10}$$

Again, plane waves are solutions to this equation:

$$f_\omega(x) = e^{ik\cdot x},$$

provided $\omega^2 = |k|^2 c^2$, i.e., $\omega = \pm|k|c$. Hence f_ω is a function that oscillates in the direction parallel to k. The full solution is

$$u(x,t) = e^{i(k\cdot x - \omega t)},$$

which are plane waves traveling with speed c, along the direction k. We call k the *wave vector* and $|k|$ the *wave number*. The wavelength is still $2\pi/|k|$. The relation $\omega^2 = |k|^2 c^2$ linking ω and k, and encoding the fact that the waves travel with velocity c, is called the *dispersion relation* of the wave equation.

Note that $e^{ik\cdot x}$ are not the only (non-growing) solutions of the Helmholtz equation in free space; so is any linear combination of $e^{ik\cdot x}$ that share the same wave number $|k|$. This superposition can be a discrete sum or a continuous integral. An exercise in section 1.3 deals with the continuous superposition with constant weight of all the plane waves with same wave number $|k|$.

Consider now the general case of a hyperbolic system $\frac{\partial w}{\partial t} = Lw$, with $L^* = -L$. The eigenvalue problem is $-i\omega f_\omega = Lf_\omega$. It is fine to assume ω real: since L is antiselfadjoint, iL is selfadjoint (Hermitian), hence all the eigenvalues of L are purely imaginary. This is sometimes how hyperbolic systems are defined — by assuming that the eigenvalues of the generator L are purely imaginary.

We still look for eigenfunctions with a $e^{ik\cdot x}$ dependence, but since w and f_ω may now be vectors with m components, we should make sure to consider

$$f_\omega(x) = e^{ik\cdot x} r, \qquad r \in \mathbb{R}^m.$$

However, such f_ω cannot in general expected to be eigenvectors of L. It is only when the equation is *translation-invariant* that they will be. This means that the generator L is a matrix of differential operators with constant coefficients – no variability as a function of x is allowed. In this translation-invariant setting, and only in this setting, L is written as a multiplication by some matrix $P(k)$ in the Fourier domain. Say that f has m components $(f_1, \dots f_m)$; then

$$Lf(x) = \frac{1}{(2\pi)^n} \int e^{ik\cdot x} P(k) \widehat{f}(k) dk,$$

where $P(k)$ is an m-by-m matrix for each k. Here $P(k)$ is called the dispersion matrix. We refer to operators such as L as *diagonal* in the Fourier domain, with respect to the k variable, because they act like a "diagonal matrix" on vectors of the continuous index k — although for each k the small matrix $P(k)$ is not in general diagonal[5]. In pure math, $P(k)$ is called the multiplier, and L is said to be a multiplication operator in the Fourier domain.

For illustration, let us specialize our equations to the 2D acoustic system with $\rho_0 = \kappa_0 = c = 1$, where

$$w = \begin{pmatrix} v \\ p \end{pmatrix}, \qquad L = \begin{pmatrix} 0 & 0 & -\frac{\partial}{\partial x_1} \\ 0 & 0 & -\frac{\partial}{\partial x_2} \\ -\frac{\partial}{\partial x_1} & -\frac{\partial}{\partial x_2} & 0 \end{pmatrix}.$$

[5]Non-diagonal, translation-variant operators would require yet another integral over a k' variable, and would read $Lf(x) = \frac{1}{(2\pi)^n} \int\int e^{ik\cdot x} Q(k,k') \widehat{f}(k') dk'$, for some more complicated object $Q(k,k') \in \mathbb{R}^{m\times m}$. The name "diagonal" comes from the fact that $Q(k,k')$ simplifies as $P(k)\delta(k-k')$ in the translation-invariant case. You can think of $P(k)\delta(k-k')$ as the continuous analogue of $d_i\delta_{ij}$: it is a "diagonal continuous matrix" as a function of k (continuous row index) and k' (continuous column index).

It can be readily checked that

$$P(k) = \begin{pmatrix} 0 & 0 & -ik_1 \\ 0 & 0 & -ik_2 \\ & & \\ -ik_1 & -ik_2 & 0 \end{pmatrix},$$

from which it is apparent that $P(k)$ is a skew-Hermitian matrix: $P^*(k) = -P(k)$.

We can now study the conditions under which $-i\omega f_\omega = Lf_\omega$: we compute (recall that r is a fixed vector)

$$\begin{aligned} L(e^{ik\cdot x}r) &= \frac{1}{(2\pi)^n}\int e^{ik'\cdot x}P(k')\widehat{[e^{ik\cdot x}r]}(k')dk', \\ &= \frac{1}{(2\pi)^n}\int e^{ik'\cdot x}P(k')(2\pi)^n\delta(k-k')rdk', \qquad = e^{ik\cdot x}P(k)r. \end{aligned}$$

In order for this quantity to equal $-i\omega e^{ik\cdot x}r$ for all x, we require (at $x = 0$)

$$P(k)\, r = -i\omega\, r.$$

This is just the condition that $-i\omega$ is an eigenvalue of $P(k)$, with eigenvector r. We should expect both ω and r to depend on k. For instance, in the 2D acoustic case, the eigen-decomposition of $P(k)$ is

$$\lambda_0(k) = -i\omega_0(k) = 0, \qquad r_0(k) = \begin{pmatrix} k_2 \\ -k_1 \\ 0 \end{pmatrix}$$

and

$$\lambda_\pm(k) = -i\omega_\pm(k) = -i|k|, \qquad r_\pm(k) = \begin{pmatrix} \pm k_1/|k| \\ \pm k_2/|k| \\ |k| \end{pmatrix}.$$

Only the last two eigenvalues correspond to physical waves: they lead to the usual dispersion relations $\omega(k) = \pm|k|$ in the case $c = 1$. Recall that the first two components of r are particle velocity components: the form of the eigenvector indicates that those components are aligned with the direction k of the wave, i.e., acoustic waves can only be longitudinal.

The general definition of dispersion relation follows this line of reasoning: there exists one dispersion relation for each eigenvalue λ_j of $P(k)$, and $-i\omega_j(k) = \lambda_j(k)$; for short

$$\det\left[i\omega I + P(k)\right] = 0.$$

1.2.2 Traveling waves, characteristic equations

We now consider a few examples that build up to the notion of characteristic curve/surface.

- Let us give a complete solution to the one-way wave equation of one space variable in a uniform medium:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \qquad u(x,0) = u_0(x). \tag{1.11}$$

The study of plane wave solutions in the previous section suggests that the variable $x - ct$ may play a role. Let us perform the change of variables

$$\xi = x - ct, \qquad \eta = x + ct.$$

It inverts as

$$x = \frac{\xi + \eta}{2}, \qquad t = \frac{\eta - \xi}{2c}.$$

By the chain rule, e.g.,

$$\frac{\partial}{\partial \xi} = \frac{\partial x}{\partial \xi}\frac{\partial}{\partial x} + \frac{\partial t}{\partial \xi}\frac{\partial}{\partial t},$$

we get

$$-2c\frac{\partial}{\partial \xi} = \frac{\partial}{\partial t} - c\frac{\partial}{\partial x}, \qquad 2c\frac{\partial}{\partial \eta} = \frac{\partial}{\partial t} + c\frac{\partial}{\partial x}.$$

With $U(\xi, \eta) = u(x,t)$, the wave equation simply becomes

$$\frac{\partial U}{\partial \eta} = 0,$$

whose general solution is $U(\xi,\eta) = F(\xi)$ for some differentiable function F. Hence $u(x,t) = F(x - ct)$. In view of the initial condition, this is

$$u(x,t) = u_0(x - ct).$$

The solutions to (1.11) are all the right-going waves with speed c, and nothing else.

The wave propagate along the lines $\xi(x,t) = x - ct =$const. in the (x,t) plane. For this reason, we call ξ the *characteristic coordinate*, and we call the lines $\xi(x,t) =$ const. *characteristic curves*.

Notice that imposing a boundary condition $u(0,t) = v_0(t)$ rather than an initial condition is also fine, and would result in a solution $u(x,t) = v_0(t - x/c)$. Other choices are possible; they are called Cauchy data. However, a problem occurs if we try to specify Cauchy data along a characteristic curve $\xi =$ constant, as $v_0(\eta)$:

1. this choice is not in general compatible with the property that the solution should be constant along the characteristic curves; and furthermore
2. it fails to determine the solution away from the characteristic curve.

In other words, there is a problem with both existence and uniqueness when we try to prescribe Cauchy data on a characteristic curve. This fact will be used in the sequel to define these curves when their geometric intuition becomes less clear.

- Using similar ideas, let us describe the full solution of the (two-way) wave equation in one space dimension,

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0, \qquad u(x,0) = u_0(x), \qquad \frac{\partial u}{\partial t}(x,0) = u_1(x).$$

The same change of variables leads to the equation

$$\frac{\partial U}{\partial \xi \partial \eta} = 0,$$

which is solved via

$$\frac{\partial U}{\partial \eta}(\xi,\eta) = f(\xi), \qquad U(\xi,\eta) = \int^{\xi} f(\xi')d\xi' + G(\eta) = F(\xi) + G(\eta).$$

The resulting general solution is a superposition of a left-going wave and a right-going wave:

$$u(x,t) = F(x - ct) + G(x + ct).$$

Matching the initial conditions yields d'Alembert's formula (1746):

$$u(x,t) = \frac{1}{2}(u_0(x - ct) + u_0(x + ct)) + \frac{1}{2c}\int_{x-ct}^{x+ct} u_1(y)dy.$$

It is the complete solution to the 1D wave equation in a uniform wave speed c. Notice that we now have two families of criss-crossing characteristic curves, given by $\xi(x,t) = \text{const.}$ and $\eta(x,t) = \text{const.}$ Cauchy data cannot be prescribed on either type of characteristics.

- Consider now the wave equation in a variable medium $c(x)$ (technically, acoustic waves on an infinite string with variable bulk modulus):

$$\frac{\partial^2 u}{\partial t^2} - c^2(x)\frac{\partial^2 u}{\partial x^2} = 0, \qquad u(x,0) = u_0(x), \qquad \frac{\partial u}{\partial t}(x,0) = u_1(x).$$

We will no longer be able to give an explicit solution to this problem, but the notion of characteristic curve remains very relevant. Consider an as-yet-undetermined change of coordinates $(x,t) \mapsto (\xi,\eta)$, which generically changes the wave equation into

$$\alpha(x)\frac{\partial^2 U}{\partial \xi^2} + \frac{\partial^2 U}{\partial \xi \partial \eta} + \beta(x)\frac{\partial^2 U}{\partial \eta^2} + \left[p(x)\frac{\partial U}{\partial \xi} + q(x)\frac{\partial U}{\partial \eta} + r(x)U\right] = 0,$$

with

$$\alpha(x) = \left(\frac{\partial \xi}{\partial t}\right)^2 - c^2(x)\left(\frac{\partial \xi}{\partial x}\right)^2,$$
$$\beta(x) = \left(\frac{\partial \eta}{\partial t}\right)^2 - c^2(x)\left(\frac{\partial \eta}{\partial x}\right)^2.$$

The lower-order terms in the square brackets are kinematically less important than the first three terms[6]. We wish to define characteristic coordinates as those along which

$$U(\xi,\eta) \simeq F(\xi) + G(\eta),$$

i.e., "directions in which the waves travel" in space-time. It is in general impossible to turn this approximate equality into an actual equality (because of the terms in the square brackets), but it is certainly possible to choose the characteristic coordinates so that the $\frac{\partial^2 U}{\partial \xi^2}$ and $\frac{\partial^2 U}{\partial \eta^2}$ vanish. Choosing $\alpha(x) = \beta(x) = 0$ yields the same equation for both ξ and η, here expressed in terms of ξ:

$$\left(\frac{\partial \xi}{\partial t}\right)^2 - c^2(x)\left(\frac{\partial \xi}{\partial x}\right)^2 = 0. \tag{1.12}$$

[6]In a sense that we are not yet ready to make precise. Qualitatively, they affect the shape of the wave, but not the character that the waves travel with local speed $c(x)$.

This relation is called the *characteristic equation*. Notice that $\xi = x - ct$ and $\eta = x + ct$ are both solutions to this equation in the case when $c(x) = c$ is a constant. But it can be checked that $\xi = x \pm c(x)t$ is otherwise not a solution of (1.12). Instead, refer to the exercise section for a class of solutions to (1.12).

- Consider now the n dimensional wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2(x)\Delta u = 0, \qquad u(x,0) = u_0(x), \qquad \frac{\partial u}{\partial t}(x,0) = u_1(x).$$

A change of variables would now read $(x_1, \ldots, x_n, t) \mapsto (\xi, \eta_1, \ldots, \eta_n)$. The variable ξ is called characteristic when the coefficient of the leading term $\frac{\partial^2 U}{\partial \xi^2}$ vanishes in the expression of the equation in the new coordinates. This condition leads to the n-dimensional version of the characteristic equation

$$\left(\frac{\partial \xi}{\partial t}\right)^2 - c^2(x)|\nabla_x \xi|^2 = 0. \tag{1.13}$$

The same relations should hold for the other coordinates $\eta_1, \ldots, \eta_n$ if they are to be characteristic as well. Equation (1.13) is called a *Hamilton-Jacobi* equation. We now speak of characteristic surfaces $\xi(x,t) = \text{const.}$, rather than curves.

The set of solutions to (1.13) is very large. In the case of constant c, we can check that possible solutions are

$$\xi(x,t) = x \cdot k \pm \omega t, \qquad \omega = |k|c,$$

corresponding to more general plane waves $u(x,t) = F(x \cdot k \pm \omega t)$ (which the reader can check are indeed solutions of the n-dimensional wave equation for smooth F), and

$$\xi(x,t) = \|x - y\| \pm ct, \qquad \text{for some fixed } y, \text{ and } x \neq y,$$

corresponding to concentric spherical waves originating from y. We describe spherical waves in more details in the next section. Notice that both formulas for ξ reduce in some sense to $x \pm ct$ in the one-dimensional case.

The choice of characteristic coordinates led to the reduced equation

$$\frac{\partial^2 U}{\partial \xi \partial \eta} + \text{ lower order terms } = 0,$$

sometimes called "first fundamental form" of the wave equation, on the intuitive basis that solutions (approximately) of the form $F(\xi) + G(\eta)$ should travel along the curves $\xi = \text{const.}$ and $\eta = \text{const.}$ Let us now motivate this choice of the reduced equation in more precise terms, by linking it to the idea that *Cauchy data cannot be prescribed on a characteristic curve.*

Consider $u_{tt} = c^2 u_{xx}$. Prescribing initial conditions $u(x,0) = u_0$, $u_t(x,0) = u_1$ is perfectly acceptable, as this completely and uniquely determines all the partial derivatives of u at $t = 0$. Indeed, u is specified through u_0, and all its x-partials $u_x, u_{xx}, u_{xxx}, \ldots$ are obtained from the x-partials of u_0. The first time derivative u_t at $t = 0$ is obtained from u_1, and so are $u_{tx}, u_{txx}, \ldots$ by further x-differentiation. As for the second derivative u_{tt} at $t = 0$, we obtain it from the wave equation as $c^2 u_{xx} = c^2 (u_0)_{xx}$. Again, this also determines $u_{ttx}, u_{ttxx}, \ldots$ The third derivative u_{ttt} is simply $c^2 u_{txx} = c^2 (u_1)_{xx}$. For the fourth derivative u_{tttt}, apply the wave equation twice and get it as $c^4 (u_0)_{xxxx}$. And so on. Once the partial derivatives are known, so is u itself in a neighborhood of $t = 0$ by a Taylor expansion — this is the original argument behind the Cauchy-Kowalevsky theorem.

The same argument fails in characteristic coordinates. Indeed, assume that the equation is $u_{\xi\eta} + p u_\xi + q u_\eta + r u = 0$, and that the Cauchy data is $u(\xi, 0) = v_0(\xi)$, $u_\eta(\xi, 0) = v_1(\eta)$. Are the partial derivatives of u all determined in a unique manner at $\eta = 0$? We get u from v_0, as well as $u_\xi, u_{\xi\xi}, u_{\xi\xi\xi}, \ldots$ by further ξ differentiation. We get u_η from v_1, as well as $u_{\eta\xi}, u_{\eta\xi\xi}, \ldots$ by further ξ differentiation. To make progress, we now need to consider the equation $u_{\xi\eta} + (\text{l.o.t.}) = 0$, but two problems arise:

- First, all the derivatives appearing in the equation have already been determined in terms of v_0 and v_1, and there is no reason to believe that this choice is compatible with the equation. In general, it isn't. There is a problem of existence.

- Second, there is no way to determine $u_{\eta\eta}$ from the equation, as this term does not appear. Hence additional data would be needed to determine this partial derivative. There is a problem of uniqueness.

The only way to redeem this existence-uniqueness argument is by making sure that the equation contains a $u_{\eta\eta}$ term, i.e., by making sure that η is *non*-characteristic.

Please refer to the exercise section for a link between characteristic equations, and the notions of traveltime and (light, sound) ray. We will return to such topics in the scope of geometrical optics, in chapter 7.

1.2.3 Spherical waves, Green's functions

Consider $x \in \mathbb{R}^3$ and c constant. We will only be dealing with solutions in 3 spatial dimensions for now. We seek radially symmetric solutions of the wave equation. In spherical coordinate (r, θ, ϕ), the Laplacian reads

$$\Delta u = \frac{1}{r}\frac{\partial^2}{\partial r^2}(ru) + \text{ angular terms.}$$

For radially symmetric solutions of the wave equation, therefore,

$$\frac{\partial^2}{\partial t^2}(ru) = \frac{\partial^2}{\partial r^2}(ru).$$

This is a one-dimensional wave equation in the r variable, whose solution we derived earlier:

$$ru(r,t) = F(r-ct) + G(r+ct) \qquad \Rightarrow \qquad u(r,t) = \frac{F(r-ct)}{r} + \frac{G(r+ct)}{r}.$$

Spherical waves corresponding to the F term are called *outgoing*, while waves corresponding to the G term are called *incoming*. More generally, spherical waves can be outgoing/incoming with respect to any point $y \in \mathbb{R}^3$, for instance

$$u(x,t) = \frac{F(\|x-y\| - ct)}{\|x-y\|}.$$

Notice that we had already seen that $\|x-y\| \pm ct$ is a characteristic variable for the wave equation, in the previous section. The surfaces $\|x-y\| = ct+$ const. are often called *light cones* in the setting of electromagnetic waves.

In what follows we will be interested in the special case $F(r) = \delta(r)$, the Dirac delta, for which the wave equation is only satisfied in a distributional sense. Superpositions of such spherical waves are still solutions of the wave equation.

It turns out that *any* solution of the wave equation in $\mathbb{R}^3$, with constant c, can be written as a superposition of such spherical waves. Let us consider a quantity which is not quite the most general yet:

$$u(x,t) = \int_{\mathbb{R}^3} \frac{\delta(\|x-y\| - ct)}{\|x-y\|} \psi(y) dy. \tag{1.14}$$

Since $\|x-y\| = ct$ on the support of the delta function, the denominator can be written ct. Denoting by $B_x(ct)$ the ball centered at x and with radius ct, we can rewrite

$$u(x,t) = \frac{1}{ct} \int_{\partial B_x(ct)} \psi(y) dy.$$

hence the name spherical means (note that the argument of δ has derivative 1 in the radial variable — no Jacobian is needed.) The interesting question is that of matching $u(x,t)$ given by such a formula, with the initial conditions. By the mean value theorem,

$$u(x,t) \sim 4\pi ct\psi(x), \qquad t \to 0,$$

which tends to zero as $t \to 0$. On the other hand, an application of the Reynolds transport theorem (or a non-rigorous yet correct derivative in time of the equation above) yields

$$\lim_{t\to 0} \frac{\partial u}{\partial t}(x,t) = 4\pi c\psi(x).$$

We are therefore in presence of initial conditions $u_0 = 0$, and arbitrary $u_1 = 4\pi c\psi(x)$ arbitrary. In that case, *the* solution of the constant-c wave equation in $\mathbb{R}^3$ is

$$u(x,t) = \int G(x,y;t) u_1(y)\, dy,$$

with the so-called *Green's function*

$$G(x,y;t) = \frac{\delta(\|x-y\| - ct)}{4\pi c^2 t}, \qquad t > 0, \tag{1.15}$$

and zero when $t \leq 0$.

Let us now describe the general solution for the other situation when $u_1 = 0$, but $u_0 \neq 0$. The trick is to define $v(x,t)$ by the same formula (1.14), and consider $u(x,t) = \frac{\partial v}{\partial t}$, which also solves the wave equation:

$$\left[\frac{\partial^2}{\partial t^2} - c^2\Delta\right] \frac{\partial v}{\partial t} = \frac{\partial}{\partial t}\left[\frac{\partial^2}{\partial t^2} - c^2\Delta\right] v = 0.$$

The limits are now

$$\lim_{t\to 0} u(x,t) = 4\pi c\psi(x),$$

and

$$\frac{\partial u}{\partial t} = \frac{\partial^2 v}{\partial t^2} = c^2\Delta v, \qquad \lim_{t\to 0} c^2\Delta v(x,t) = c^2\Delta \lim_{t\to 0} v(x,t) = 0$$

(limit and derivative are interchangeable when the function is smooth enough.) The time derivative trick is all that is needed to generate the solution in the case $u_1 = 0$:

$$u(x,t) = \int \frac{\partial G}{\partial t}(x,y;t)u_0(y)\,dy.$$

The general solution is obtained by superposition of these two special cases:

$$u(x,t) = \int \left[\frac{\partial G}{\partial t}(x,y;t)u_0(y) + G(x,y;t)u_1(y)\right] dy. \tag{1.16}$$

The concept of Green' function G is much more general than suggested by the derivation above. Equation (1.16), for instance, holds in arbitrary dimension and for variable media, albeit with a different Green's function — a claim that we do not prove here. In two dimensions and constant c for instance, it can be shown[7] that

$$G(x,y;t) = \frac{1}{2\pi c\sqrt{c^2t^2 - \|x-y\|^2}}, \qquad \text{when } t > 0,$$

and zero otherwise. In variable media, explicit formulas are usually not available.

In the wider context of linear PDE, Green's functions are more often introduced as linking a right-hand-side forcing f to the solution u upon integration. For a linear PDE $\mathcal{L}u = f$, Green's functions are to the differential operator $\mathcal{L}$ what the inverse matrix A^{-1} is to a matrix A. Accordingly, the Green's function describes the solution of the wave equation with a right-hand side forcing — a setting more often encountered in imaging than initial-value problems. The premise of the proposition below is that G is defined[8] through (1.16), even as $x \in \mathbb{R}^n$ and c is a function of x.

[7] By the so called "method of descent". See the book *Introduction to PDE* by Gerald Folland for a wonderful explanation of wave equations in constant media.

[8] The tables could be turned, and G could instead be defined by (1.17). In that case (1.16) would be a proposition.

Proposition 2. *(Duhamel principle) For $x \in \mathbb{R}^n$, and $t > 0$, the solution of the inhomogeneous problem*

$$\left[\frac{\partial^2}{\partial t^2} - c^2(x)\Delta\right] u(x,t) = f(x,t), \qquad u(x,0) = \frac{\partial u}{\partial t}(x,0) = 0.$$

is

$$u(x,t) = \int_0^t \int G(x,y;t-s) f(y,s)\, dy ds. \tag{1.17}$$

Proof. Let us check that the wave equation holds.

For each $s > 0$, consider the auxiliary problem

$$\left[\frac{\partial^2}{\partial t^2} - c^2(x)\Delta\right] v_s(x,t) = f(x,t), \qquad v_s(x,0) = 0, \qquad \frac{\partial v_s}{\partial t}(x,0) = f(x,s).$$

Then

$$v_s(x,t) = \int G(x,y;t) f(y,s)\, dy.$$

The candidate formula for u is

$$u(x,t) = \int_0^t v_s(x,t-s)\, ds.$$

Let us now check that this u solves the wave equation. For one, $u(x,0) = 0$ because the integral is over an interval of length zero. We compute

$$\frac{\partial u}{\partial t}(x,t) = v_s(x,t-s)|_{s=t} + \int_0^t \frac{\partial v_s}{\partial t}(x,t-s)\, ds = \int_0^t \frac{\partial v_s}{\partial t}(x,t-s)\, ds.$$

For the same reason as previously, $\frac{\partial u}{\partial t}(x,0) = 0$. Next,

$$\begin{aligned}
\frac{\partial^2 u}{\partial t^2}(x,t) &= \frac{\partial v_s}{\partial t}(x,t-s)|_{s=t} + \int_0^t \frac{\partial^2 v_s}{\partial t^2}(x,t-s)\, ds \\
&= f(x,t) + \int_0^t c^2(x)\Delta v_s(x,t-s)\, ds \\
&= f(x,t) + c^2(x)\Delta \int_0^t v_s(x,t-s)\, ds \\
&= f(x,t) + c^2(x)\Delta u(x,t).
\end{aligned}$$

Since the solution of the wave equation is unique, the formula is general. □

Because the Green's function plays such a special role in the description of the solutions of the wave equation, it also goes by *fundamental solution*. We may specialize (1.17) to the case $f(x,t) = \delta(x-y)\delta(t)$ to obtain the equation that the Green's function itself satsfies,

$$\left[\frac{\partial^2}{\partial t^2} - c^2(x)\Delta_x\right] G(x,y;t) = \delta(x-y)\delta(t).$$

In the spatial-translation-invariant case, G is a function of $x-y$, and we may write $G(x,y;t) = g(x-y,t)$. In that case, the general solution of the wave equation with a right-hand side $f(x,t)$ is the space-time convolution of f with g.

A spatial dependence in the right-hand-side such as $\delta(x-y)$ may be a mathematical idealization, but the idea of a point disturbance is nevertheless a very handy one. In radar imaging for instance, antennas are commonly assumed to be point-like, whether on arrays or mounted on a plane/satellite. In exploration seismology, sources are often modeled as point disturbances as well (shots), both on land and for marine surveys.

The physical interpretation of the concentration of the Green's function along the cone $\|x-y\| = ct$ is called the *Huygens principle*. Starting from an initial condition at $t=0$ supported along (say) a curve Γ, this principle says that the solution of the wave equation is mostly supported on the envelope of the circles of radii ct centered at all the points on Γ.

1.2.4 The Helmholtz equation

It is often convenient to use a formulation of the wave equation in the frequency domain. If

$$\widehat{u}(x,\omega) = \int e^{i\omega t} u(x,t)\, dt,$$

and if $\left[\frac{\partial^2}{\partial t^2} - c^2(x)\Delta_x\right] u = f$, then it is immediate to check that the (inhomogeneous) *Helmholtz equation* holds:

$$-\left[\omega^2 + c^2(x)\Delta\right] \widehat{u}(x,\omega) = \widehat{f}(x,\omega).$$

The notion of Green's function is also very useful for the Helmholtz equation: it is the function $\widehat{G}(x,y;\omega)$ such that

$$\widehat{u}(x,\omega) = \int \widehat{G}(x,y;\omega)\widehat{f}(y,\omega)\, dy.$$

It is a good exercise to check that $\widehat{G}(x, y; \omega)$ is indeed the Fourier transform of $G(x, y; t)$ in t, by Fourier-transforming (1.17) and applying the convolution theorem. By specializing the Helmholtz equation to the right-hand side $\widehat{f}(x, \omega) = \delta(x)$, we see that the Green's function itself obeys

$$-\left[\omega^2 + c^2(x)\Delta\right] \widehat{G}(x, y; \omega) = \delta(x). \tag{1.18}$$

In particular, for $x \in \mathbb{R}^3$ and constant c, we get $(x \neq y)$

$$\begin{aligned}
\widehat{G}(x, y; \omega) &= \int_0^\infty e^{i\omega t} \frac{\delta(\|x - y\| - ct)}{4\pi c^2 t}\, dt \\
&= \int_0^\infty e^{i\omega t} \frac{\delta(\|x - y\| - ct)}{4\pi c \|x - y\|}\, dt \\
&= \int_0^\infty e^{i\frac{\omega}{c}t'} \frac{\delta(\|x - y\| - t')}{4\pi \|x - y\|}\, dt' \\
&= \frac{e^{ik\|x-y\|}}{4\pi\|x - y\|}, \qquad k = \omega/c.
\end{aligned}$$

We will often use this form of the Green's function in the sequel. It is an outgoing spherical wave generated by a "point source" at $x = y$.

Note that $\omega \to -\omega$ corresponds to time reversal: $\frac{e^{-ik\|x-y\|}}{4\pi\|x-y\|}$ is also a solution of the Helmholtz equation for $x \neq y$, but it is an incoming rather than outgoing wave. The sign in the exponent depends on the choice of convention for the Fourier transform[9]

Some mathematical care should be exercised when posing the Helmholtz equation in free space. Uniqueness, in particular, is not as easy to guarantee as for the time-dependent wave equation. "Sufficient decay as $\|x\| \to \infty$" is not a good criterion for uniqueness, since we've just seen an example of two waves $\frac{e^{\pm i\omega\|x-y\|/c}}{4\pi\|x-y\|}$ which have the same modulus and obey the same equation (1.18). Instead, it is customary to require the wave to be *outgoing* in order to have a well-posed problem in constant c. We say that $\widehat{u}(x, \omega)$ obeys the *Sommerfeld radiation condition* in $\mathbb{R}^3$ if $(r = \|x\|)$

$$\left(\frac{\partial}{\partial r} - ik\right) \widehat{u}(x, \omega) = o(\frac{1}{|x|}),$$

[9]We choose $e^{i\omega t}$ for the direct transform, and $e^{-i\omega t}$ for the inverse transform, in accordance with practice in signal processing, radar imaging, and seismic imaging. For the spatial Fourier transforms, however, we adopt the opposite convention $e^{-ik\cdot x}$ for the direct transform, and $e^{ik\cdot x}$ for the inverse transform.

i.e., $\lim_{|x|\to\infty} |x| \left(\frac{\partial}{\partial r} - ik\right) \widehat{u}(x,\omega) = 0$. It is a good exercise to check that $\widehat{G}(x,y;\omega)$ obeys this radiation conditions, while $\widehat{G}(x,y;-\omega)$ does not.

For reference, the expression of the Green's function in two spatial dimensions, in a uniform medium $c(x) = c$, is

$$\widehat{G}(x,y,\omega) = (...)H_0^{(1)}(k|x-y|), \qquad k = \omega/c.$$

where $H_0^{(1)} = J_0 + iY_0$ is called a Hankel function.

1.2.5 Reflected waves

Spatial variability in the physical parameters ($\rho, \kappa; \epsilon, \mu; \lambda, \mu$, etc.) entering the wave equation generate wave scattering, i.e., changes of the direction of propagation of the waves. Of particular interest are discontinuities, or other non-C^∞ singularities, which generate reflected waves alongside transmitted waves.

Let us study reflection and transmission in the 1D, variable-density acoustics equation

$$\frac{\partial^2 u}{\partial t^2} = \kappa(x) \frac{\partial}{\partial x} \left(\frac{1}{\rho(x)} \frac{\partial u}{\partial x} \right).$$

Consider a step discontinuity at $x = 0$, with $\rho(x) = \rho_1$ and $\kappa(x) = \kappa_1$ in $x < 0$, and $\rho(x) = \rho_2$ and $\kappa(x) = \kappa_2$ in $x > 0$. Assume an incident plane wave $u_i(x,t) = e^{i(k_1 x - \omega t)}$ in $x < 0$; we are interested in finding the reflection coefficient R and the transmission coefficient T so the solution reads

$$u_i(x,t) + u_r(x,t) = e^{i(k_1 x - \omega t)} + Re^{i(k_1 x + \omega t)}, \qquad x < 0.$$

$$u_t(x,t) = Te^{i(k_2 x - \omega t)}, \qquad x > 0.$$

The connection conditions are the continuity of u and $\frac{1}{\rho}\frac{\partial u}{\partial x}$. To justify this, remember that u is in fact a pressure disturbance in the acoustic case, while $\frac{1}{\rho}\frac{\partial u}{\partial x}$ is minus the time derivative of particle velocity, and these two quantities are continuous on physical grounds. There is also a mathematical justification for the continuity of $\frac{1}{\rho}\frac{\partial u}{\partial x}$: if it weren't, then $\frac{\partial}{\partial x}\left(\frac{1}{\rho(x)}\frac{\partial u}{\partial x}\right)$ would have a point mass (Dirac atom) at $x = 0$, which would pose a problem both for the multiplication by a discontinuous $\kappa(x)$, and because $\frac{\partial^2 u}{\partial t^2}$ is supposed to be a finite function, not a distribution.

At $x = 0$, the connection conditions give

$$1 + R = T,$$

$$\frac{1}{\rho_1}(-ik_1 - ik_1 R) = \frac{1}{\rho_2}(ik_2 T).$$

Eliminate k_1 and k_2 by expressing them as a function of ρ_1, ρ_2 only; for instance

$$\frac{k_1}{\rho_1} = \frac{\omega}{\rho_1 c_1} = \frac{\omega}{\sqrt{\rho_1 \kappa_1}},$$

and similarly for $\frac{k_2}{\rho_2}$. Note that ω is fixed throughout and does not depend on x. The quantity in the denominator is physically very important: it is $Z = \rho c = \sqrt{\kappa\rho}$, the *acoustic impedance*. The R and T coefficients can then be solved for as

$$R = \frac{Z_2 - Z_1}{Z_2 + Z_1}, \qquad T = \frac{2Z_2}{Z_2 + Z_1}.$$

It is the *impedance jump* $Z_2 - Z_1$ which mostly determines the magnitude of the reflected wave.$R = 0$ corresponds to an impedance match, even in the case when the wave speeds differ in medium 1 and in medium 2.

The same analysis could have been carried out for a more general incoming wave $f(x - c_1 t)$, would have given rise to the same R and T coefficients, and to the complete solution

$$u(x,t) = f(x - c_1 t) + Rf(-x - c_1 t), \qquad x < 0, \tag{1.19}$$

$$u(x,t) = Tf(\frac{c_1}{c_2}(x - c_2 t)), \qquad x > 0. \tag{1.20}$$

The reader can check the relation

$$1 = R^2 + \frac{Z_1}{Z_2} T^2,$$

which corresponds to conservation of energy. An exercise in section 1.3 aims to establish this link. Note that $\mathcal{R} = R^2$ and $\mathcal{T} = \frac{Z_1}{Z_2} T^2$ are sometimes referred to as reflection and transmission coefficients, though they measure intensities rather than amplitudes. The intensity coefficients are even denoted as R and T in place of $\mathcal{R}$ and $\mathcal{T}$ in some texts.

Physically, the acoustic impedance Z is the proportionality constant between the pressure amplitude and the velocity amplitude of an acoustic wave.

We do not have direct access to Z in the acoustic equations however, as $p(x,t) \neq Zv(x,t)$ pointwise – only combinations of partial derivatives match. So Z is in some sense an "averaged quantity" over at least a wavelength. On can derive the expression of Z from the time-harmonic regime. The first equation (1.1) in the acoustic system reads, in the (k,ω) domain (in one spatial dimension),

$$i\omega\widehat{v}(k,\omega) = -\frac{1}{\rho_0} ik\widehat{p}(k,\omega),$$

or, if we simplify further,

$$|\widehat{p}| = Z|\widehat{v}|, \qquad Z = \rho_0 c = \sqrt{\rho_0 \kappa_0}.$$

The same relation would have been obtained from (1.2). The larger Z, the more difficult to move particle from a pressure disturbance, i.e., the smaller the corresponding particle velocity.

The definition of acoustic impedance is intuitively in line with the traditional notion of electrical impedance for electrical circuits. To describe the latter, consider Ampère's law in the absence of a magnetic field:

$$\frac{\partial D}{\partial t} = -j \qquad \Rightarrow \qquad \epsilon \frac{\partial E}{\partial t} = -j.$$

In the time-harmonic setting (AC current), $i\omega\epsilon\widehat{E} = -\widehat{j}$. Consider a conducting material, for which the permittivity reduces to the conductivity:

$$\epsilon = i\frac{\sigma}{\omega}$$

It results that $\widehat{E} = Z\widehat{j}$ with the resistivity $Z = 1/\sigma$. This is the differential version of Ohm's law. The (differential) impedance is exactly the resistivity in the real case, and can accommodate capacitors and inductions in the complex case. Notice that the roles of E (or V) and j (or I) in an electrical circuit are quite analogous to p and v in the acoustic case.

There are no waves in the conductive regime we just described, so it is out of the question to seek to write R and T coefficients, but reflections and transmissions of waves do occur at the interface between two dielectric materials. Such is the case of light propagating in a medium with variable index of reflection. To obtain the R and T coefficients in the optical case, the procedure is as follows:

- Consider Amp‘ere's law again, but this time with a magnetic field H (because it is needed to describe waves) but no current (because we are dealing with dielectrics):

$$\frac{\partial D}{\partial t} = \nabla \times H.$$

  Use $D = \epsilon E$.

- Assume plane waves with complex exponentials, or in the form $E(k \cdot x - \omega t)$ and $H(k \cdot x - \omega t)$.

- Use continuity of $n \times E$ and $n \times H$ at the interface (tangential components).

- Assume no magnetism: $\mu = \text{const}$.

The quantity of interest is not the impedance, but the index of refraction $n = \frac{1}{c} = \sqrt{\epsilon\mu}$. Further assuming that the waves are normally incident to the interface, we have

$$R = \frac{n_2 - n_1}{n_2 + n_1}, \qquad T = \frac{2n_2}{n_2 + n_1}.$$

These relations become more complicated when the angle of incidence is not zero. In that case R and T also depend on the polarization of the light. The corresponding equations for R and T are then called Fresnel's equations. Their expression and derivation can be found in “Principles of optics” by Born and Wolf.

1.3 Exercises

1. Continue the reasoning in section 1.1.1 with the entropy to justify the equations of variable-density acoustics. [Hints: conservation of entropy reads $\frac{\partial s}{\partial t} + v \cdot \nabla s = 0$. Continue assuming that the background velocity field is $v_0 = 0$. Assume a fixed, variable background density $\rho_0(x)$. The new constitutive relation is $p = f(\rho, s)$. Consider defining $c^2(x) = \frac{\partial f}{\partial \rho}(\rho_0(x), s_0(x))$.]

2. First, show the multivariable rule of integration by parts $\int \nabla f \cdot g = -\int f \nabla \cdot g$, when f and g are smooth and decay fast at infinity, by invoking the divergence theorem. Second, use this result to show that $L^* = -L$ for variable-density acoustics (section 1.1.1), i.e., show that $\langle Lw, w' \rangle = -\langle w, Lw' \rangle$ for all reasonable functions w and w', and where $\langle \cdot, \cdot \rangle$ is the adequate notion of inner product seen in section 1.1.1.

3. Show that $\langle Lw, w' \rangle = -\langle w, Lw' \rangle$ for general elastic waves.

4. In $\mathbb{R}^2$, consider

$$f_\omega(x) = \int_0^{2\pi} e^{ik_\theta \cdot x} d\theta, \qquad k_\theta = |k| \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix},$$

with $|k| = \omega/c$. Show that f_ω is a solution of the homogeneous Helmholtz equation (1.10) with constant c, and simplify the expression of f_ω by means of a Bessel function. [Hint: show first that f_ω is radially symmetric.]

5. Find all the functions $\tau(x)$ for which

$$\xi(x,t) = \tau(x) - t$$

is a solution of (1.12) in the case $x \in \mathbb{R}$.

The function $\tau(x)$ has the interpretation of a *traveltime*.

6. Consider a characteristic curve as the level set $\xi(x,t) =$const., where ξ is a characteristic coordinate obeying (1.12). Express this curve parametrically as $(X(t), t)$, and find a differential equation for $X(t)$ of the form $\dot{X}(t) = \ldots$ How do you relate this $X(t)$ to the traveltime function $\tau(x)$ of the previous exercise? Justify your answer.

Such functions $X(t)$ are exactly the *rays* — light rays or sound rays. They encode the idea that waves propagate with local speed $c(x)$.

7. Give a complete solution to the wave equation in $\mathbb{R}^n$,

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta u, \qquad u(x,0) = u_0(x), \qquad \frac{\partial u}{\partial t}(x,0) = u_1(x),$$

by Fourier-transforming $u(x,t)$ in the x-variable, solving the resulting ODE to obtain the $e^{\pm i|k|/ct}$ time dependencies, matching the initial conditions, and finishing with an inverse Fourier transform. The resulting formula is a generalization of d'Alembert's formula.

8. We have seen the expression of the wave equation's Green function in the (x,t) and (x,ω) domains. Find the expression of the wave equation's Green function in the (ξ,t) and (ξ,ω) domains, where ξ is dual to x and ω is dual to t. [Hint: it helps to consider the expressions of the wave equation in the respective domains, and solve these equations, rather than take a Fourier transform.]

9. Show that the Green's function of the Poisson or Helmholtz equation in a bounded domain with homogeneous Dirichlet or Neumann boundary condition is symmetric: $G(x,y) = G(y,x)$. [Hint: consider $G(x,y)\Delta_x G(x,z) - G(x,z)\Delta_x G(x,y)$. Show that this quantity is the divergence of some function. Integrate it over the domain, and show that the boundary terms drop.]

10. Check that the relation $1 = R^2 + \frac{Z_1}{Z_2}T^2$ for the reflection and transmission coefficiets follows from conservation of energy for acoustic waves. [Hint: use the definition of energy given in section 1.1.1, and the general form (1.19, 1.20) of a wavefield scattering at a jump interface in one spatial dimension.]

11. The wave equation (3.2) can be written as a first-order system

$$M\frac{\partial w}{\partial t} - Lw = \widetilde{f},$$

with

$$w = \begin{pmatrix} \partial u/\partial t \\ \nabla u \end{pmatrix}, \qquad M = \begin{pmatrix} m & 0 \\ 0 & 1 \end{pmatrix}, \qquad L = \begin{pmatrix} 0 & \nabla\cdot \\ \nabla & 0 \end{pmatrix}, \qquad \widetilde{f} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

First, check that $L^* = -L$ for the L^2 inner product $\langle w, w'\rangle = \int (w_1 w_1' + w_2 \cdot w_2')\, dx$ where $w = (w_1, w_2)^T$. Then, check that $E = \langle w, Mw\rangle$ is a conserved quantity.

12. Another way to write the wave equation (3.2) as a first-order system is

$$M\frac{\partial w}{\partial t} - Lw = \widetilde{f},$$

with

$$w = \begin{pmatrix} u \\ v \end{pmatrix}, \qquad M = \begin{pmatrix} m & 0 \\ 0 & 1 \end{pmatrix}, \qquad L = \begin{pmatrix} 0 & I \\ \Delta & 0 \end{pmatrix}, \qquad \widetilde{f} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

First, check that $L^* = -L$ for the inner product $\langle w, w' \rangle = \int (\nabla u \cdot \nabla u' + vv')\, dx$. Then, check that $E = \langle w, Mw \rangle$ is a conserved quantity.

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 ($1/c(x)$ is then the index of refraction). 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 seem 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

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

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

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

is solved globally, and the limit as $\epsilon \to 0$ 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 7.3.

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.

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 $\xi(t)$:

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

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.

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 ($)

$$ds^2 = c^{-2}(x) dx^2.$$

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

2.5 Exercises

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

Chapter 3

Scattering series

In this chapter we describe the nonlinearity of the map $c \mapsto u$ in terms of a perturbation (Taylor) series. To first order, the linearization of this map is called the Born approximation. Linearization and scattering series are the basis of most inversion methods, both direct and iterative.

The idea of perturbation permeates imaging for physical reasons as well. In radar imaging for instance, the background velocity is $c_0 = 1$ (speed of light), and the *reflectivity* of scatterers is viewed as a deviation in $c(x)$. The assumption that $c(x)$ does not depend on t is a strong one in radar: it means that the scatterers do not move. In seismology, it is common to consider a smooth background velocity $c_0(x)$ (rarely well known), and explain the scattered waves as reflections due to a "rough" (singular/oscillatory) perturbations to this background. In both cases, we will write

$$\frac{1}{c^2(x)} = m(x), \qquad \frac{1}{c_0^2(x)} = m_0(x), \qquad m \text{ for "model"},$$

and, for some small number ϵ,

$$m(x) = m_0(x) + \epsilon m_1(x). \tag{3.1}$$

Note that, when perturbing $c(x)$ instead of $m(x)$, an additional Taylor approximation is necessary:

$$c(x) = c_0(x) + \epsilon c_1(x) \qquad \Rightarrow \qquad \frac{1}{c^2(x)} \simeq \frac{1}{c_0^2(x)} - 2\epsilon \frac{c_1(x)}{c_0^3(x)}.$$

While the above is common in seismology, we avoid making unnecessary assumptions by choosing to perturb $m(x) = 1/c^2(x)$ instead.

Perturbations are of course not limited to the wave equation with a single parameter c. The developments in this chapter clearly extend to more general wave equations.

3.1 Perturbations and Born series

Let

$$m(x)\frac{\partial^2 u}{\partial t^2} - \Delta u = f(x,t), \tag{3.2}$$

with zero initial conditions and $x \in \mathbb{R}^n$. Perturb $m(x)$ as in (3.1). The wavefield u correspondingly splits into

$$u(x) = u_0(x) + u_{sc}(x),$$

where u_0 solves the wave equation in the undisturbed medium m_0,

$$m_0(x)\frac{\partial^2 u_0}{\partial t^2} - \Delta u_0 = f(x,t). \tag{3.3}$$

We say u is the total field, u_0 is the incident field[1], and u_{sc} is the scattered field, i.e., anything but the incident field.

We get the equation for u_{sc} by subtracting (3.3) from (3.2), and using (3.1):

$$m_0(x)\frac{\partial^2 u_{sc}}{\partial t^2} - \Delta u_{sc} = -\epsilon\, m_1(x)\frac{\partial^2 u}{\partial t^2}. \tag{3.4}$$

This equation is implicit in the sense that the right-hand side still depends on u_{sc} through u. We can nevertheless reformulate it as an implicit integral relation by means of the Green's function:

$$u_{sc}(x,t) = -\epsilon \int_0^t\!\!\int_{\mathbb{R}^n} G(x,y;t-s) m_1(y) \frac{\partial^2 u}{\partial t^2}(y,s)\, dyds.$$

Abuse notations slightly, but improve conciseness greatly, by letting

- G for the operator of space-time integration against the Green's function, and

[1]Here and in the sequel, u_0 is not the initial condition. It is so prevalent to introduce the source as a right-hand side f in imaging that it is advantageous to free the notation u_0 and reserve it for the incident wave.

- m_1 for the operator of multiplication by m_1.

Then $u_{sc} = -\epsilon\, G\, m_1\, \frac{\partial^2 u}{\partial t^2}$. In terms of u, we have the implicit relation

$$u = u_0 - \epsilon\, G\, m_1\, \frac{\partial^2 u}{\partial t^2},$$

called a *Lippmann-Schwinger* equation. The field u can be formally[2] expressed in terms of u_0 by writing

$$u = \left[I + \epsilon\, G\, m_1\, \frac{\partial^2}{\partial t^2} \right]^{-1} u_0. \tag{3.5}$$

While this equation is equivalent to the original PDE, it shines a different light on the underlying physics. It makes explicit the link between u_0 and u, as if u_0 "generated" u via scattering through the medium perturbation m_1.

Writing $[I + A]^{-1}$ for some operator A invites a solution in the form of a Neumann series $I - A + A^2 - A^3 + \ldots$, provided $\|A\| < 1$ in some norm. In our case, we write

$$u = u_0 - \epsilon \left(G\, m_1\, \frac{\partial^2}{\partial t^2} \right) u_0 + \epsilon^2 \left(G\, m_1\, \frac{\partial^2}{\partial t^2} \right) \left(G\, m_1\, \frac{\partial^2}{\partial t^2} \right) u_0 + \ldots$$

This is called a *Born series*. The proof of convergence, based on the "weak scattering" condition $\epsilon \| G\, m_1\, \frac{\partial^2}{\partial t^2} \|_* < 1$, in some norm to be determined, will be covered in the next section. It retroactively justifies why one can write (3.5) in the first place.

The Born series carries the physics of *multiple scattering*. Explicitly,

$$\begin{aligned}
u &= u_0 \qquad\qquad\qquad \text{(incident wave)} \\
&- \epsilon \int_0^t \int_{\mathbb{R}^n} G(x, y; t-s) m_1(y) \frac{\partial^2 u_0}{\partial t^2}(y, s)\, dy ds \\
&\qquad\qquad \text{(single scattering)} \\
&+ \epsilon^2 \int_0^t \int_{\mathbb{R}^n} G(x, y_2; t-s_2) m_1(y_2) \frac{\partial^2}{\partial s_2^2} \left[\int_0^{s_2} \int_{\mathbb{R}^n} G(y_2, y_1; s_2 - s_1) m_1(y_1) \frac{\partial^2 u_0}{\partial t^2}(y_1, s_1)\, dy_1 ds_1 \right] dy_2 ds_2 \\
&\qquad\qquad \text{(double scattering)} \\
&+ \ldots
\end{aligned}$$

[2]For mathematicians, "formally" means that we are a step ahead of the rigorous exposition: we are only interested in inspecting the *form* of the result before we go about proving it. That's the intended meaning here. For non-mathematicians, "formally" often means rigorous, i.e., the opposite of "informally"!

We will naturally summarize this expansion as

$$u = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots \tag{3.6}$$

where ϵu_1 represent single scattering, $\epsilon^2 u_2$ double scattering, etc. For instance, the expression of u_1 can be physically read as "the incident wave initiates from the source at time $t = 0$, propagates to y where it scatters due to $m(y)$ at time $t = s$, then further propagates to reach x at time t." The expression of u_2 can be read as "the incident wave initiates from the source at $t = 0$, propagates to y_1 where it first scatters at time $t = s_1$, them propagates to y_2 where it scatters a second time at time $t = s_2$, then propagates to x at time t, where it is observed." Since scatterings are not a priori prescribed to occur at fixed points in space and time, integrals must be taken to account for all physically acceptable scattering scenarios.

The approximation

$$u_{sc}(x) \simeq \epsilon u_1(x)$$

is called the *Born approximation*. From $u_1 = -Gm_1 \frac{\partial^2 u_0}{\partial t^2}$, we can return to the PDE and obtain the equation for the primary reflections:

$$m_0(x)\frac{\partial^2 u_1}{\partial t^2} - \Delta u_1 = -m_1(x)\frac{\partial^2 u_0}{\partial t^2}. \tag{3.7}$$

The only difference with (3.4) is the presence of u_0 in place of u in the right-hand side (and ϵ is gone, by choice of normalization of u_1). Unlike (3.4), equation (3.7) is explicit: it maps m_1 to u_1 in a linear way. The incident field u_0 is determined from m_0 alone, hence "fixed" for the purpose of determining the scattered fields.

It is informative to make explicit the dependence of $u_1, u_2, \dots$ on m_1. To that end, the Born series can be seen as a Taylor series of the *forward map*

$$u = \mathcal{F}[m],$$

in the sense of the calculus of variations. Denote by $\frac{\delta \mathcal{F}}{\delta m}[m_0]$ the "functional gradient" of $\mathcal{F}$ with respect to m, evaluated at m_0. It is an operator acting from model space (m) to data space (u). Denote by $\frac{\delta^2 \mathcal{F}}{\delta m^2}[m_0]$ the "functional Hessian" of $\mathcal{F}$ with respect to m, evaluated at m_0. It is a bilinear form from model space to data space. See the appendix for background on functional derivatives. Then the functional version of the Taylor expansion enables to express (3.6) in terms of the various derivatives of $\mathcal{F}$ as

$$u = u_0 + \epsilon \frac{\delta \mathcal{F}}{\delta m}[m_0]\, m_1 + \frac{\epsilon^2}{2}\langle \frac{\delta^2 \mathcal{F}}{\delta m^2}[m_0]\, m_1, m_1\rangle + \dots$$

It is convenient to denote the *linearized forward map* by (print) F:

$$F = \frac{\delta \mathcal{F}}{\delta m}[m_0],$$

or, for short, $F = \frac{\partial u}{\partial m}$. It is a linear operator. The point of F is that it makes explicit the linear link between m_1 and u_1:

$$u_1 = F m_1.$$

While $\mathcal{F}$ is supposed to completely model data (up to measurement errors), F would properly explain data only in the regime of the Born approximation.

Let us show that the two concepts of linearized scattered field coincide, namely

$$u_1 = \frac{\delta \mathcal{F}}{\delta m}[m_0]\, m_1 = -G m_1 \frac{\partial u_0}{\partial t^2}.$$

This will justify the first term in the Taylor expansion above. For this purpose, let us take the $\frac{\delta}{\delta m}$ derivative of (3.2). As previously, write $u = \mathcal{F}(m)$ and $F = \frac{\delta \mathcal{F}}{\delta m}[m]$. We get the operator-valued equation

$$\frac{\partial^2 u}{\partial t^2} I + m \frac{\partial^2}{\partial t^2} F - \Delta F = 0.$$

Evaluate the functional derivatives at the base point m_0, so that $u = u_0$. Applying each term as an operator to the function m_1, and defining $u_1 = F m_1$, we obtain

$$m_1 \frac{\partial^2 u_0}{\partial t^2} + m_0 \frac{\partial^2 u_1}{\partial t^2} - \Delta u_1 = 0,$$

which is exactly (3.7). Applying G on both sides, we obtain the desired conclusion that $u_1 = -G m_1 \frac{\partial u_0}{\partial t^2}$.

3.2 Convergence of the Born series (math)

We are faced with two very interrelated questions: justifying convergence of the Born series, and showing that the Born approximation is accurate when the Born series converges. The answers can either take the form of mathematical theorems (this section), or physical explanations (next section). As of 2012, the community's mathematical understanding is not yet up to par with the physical intuition!

Let us describe what is known mathematically about convergence of Born series in a simple setting. To keep the notations concise, it is more convenient to treat the wave equation in first-order hyperbolic form

$$M\frac{\partial w}{\partial t} - Lw = f, \qquad L^* = -L, \tag{3.8}$$

for some inner product $\langle w, w' \rangle$. The conserved energy is then $E = \langle w, Mw \rangle$. See one of the exercises at the end of chapter 1 to illustrate how the wave equation can be put in precisely this form, with $\langle w, w' \rangle$ the usual L^2 inner product and M a positive diagonal matrix.

Consider a background medium M_0, so that $M = M_0 + \epsilon M_1$. Let $w = w_0 + \epsilon w_1 + \ldots$ Calculations very similar to those of the previous section (a good exercise) show that

- The Lippmann-Schwinger equation is

  $$w = w_0 - \epsilon G M_1 \frac{\partial w}{\partial t},$$

  with the Green's function $G = (M_0 \frac{\partial}{\partial t} - L)^{-1}$.

- The Neumann series of interest is

  $$w = w_0 - \epsilon G M_1 \frac{\partial w_0}{\partial t} + \epsilon^2 G M_1 \frac{\partial}{\partial t} G M_1 \frac{\partial w_0}{\partial t} + \ldots$$

  We identify $w_1 = -G M_1 \frac{\partial w_0}{\partial t}$.

- In differential form, the equations for the incident field w_0 and the primary scattered field w_1 are

  $$M_0\frac{\partial w_0}{\partial t} - Lw_0 = f, \qquad M_0\frac{\partial w_1}{\partial t} - Lw_1 = -M_1\frac{\partial w_0}{\partial t}, \tag{3.9}$$

- Convergence of the Born series occurs when

  $$\epsilon \| G M_1 \frac{\partial}{\partial t} \|_* < 1,$$

  in some induced operator norm, i.e., when $\epsilon \|w_1\|_* < \|w_0\|_*$ for arbitrary w_0, and $w_1 = -G M_1 \frac{\partial w_0}{\partial t}$, for some norm $\| \cdot \|_*$.

Notice that the condition $\epsilon\|w_1\|_* < \|w_0\|_*$ is precisely one of weak scattering, i.e., that the primary reflected wave ϵw_1 is weaker than the incident wave w_0.

While any induced norm over space and time in principle works for the proof of convergence of the Neumann series, it is convenient to use

$$\|w\|_* = \max_{0\le t\le T} \sqrt{\langle w, M_0 w\rangle} = \max_{0\le t\le T} \|\sqrt{M_0} w\|.$$

Note that it is a norm in space *and* time, unlike $\|w\| = \sqrt{\langle w, w\rangle}$, which is only a norm in space.

Theorem 3. *(Convergence of the Born series) Assume that the fields w, w_0, w_1 are bandlimited with bandlimit[3] Ω. Consider these fields for $t \in [0, T]$. Then the weak scattering condition $\epsilon\|w_1\|_* < \|w_0\|_*$ is satisfied, hence the Born series converges, as soon as*

$$\epsilon\, \Omega T\, \|\frac{M_1}{M_0}\|_\infty < 1.$$

Proof. We compute

$$\begin{aligned}
\frac{d}{dt}\langle w_1, M_0 w_1\rangle &= 2\langle w_1, M_0 \frac{\partial w_1}{\partial t}\rangle \\
&= 2\langle w_1, L w_1 - M_1 \frac{\partial w_0}{\partial t}\rangle \\
&= -2\langle w_1, M_1 \frac{\partial w_0}{\partial t}\rangle \qquad \text{because } L^* = -L \\
&= -2\langle \sqrt{M_0} w_1, \frac{M_1}{\sqrt{M_0}} \frac{\partial w_0}{\partial t}\rangle.
\end{aligned}$$

Square roots and fractions of positive diagonal matrices are legitimate operations. The left-hand-side is also $\frac{d}{dt}\langle w_1, M_0 w_1\rangle = 2\|\sqrt{M_0} w_1\|_2 \frac{d}{dt}\|\sqrt{M_0} w_1\|_2$. By Cauchy-Schwarz, the right-hand-side is majorized by

$$2\|\sqrt{M_0} w_1\|_2\, \|\frac{M_1}{\sqrt{M_0}} \frac{\partial w_0}{\partial t}\|_2.$$

Hence

$$\frac{d}{dt}\|\sqrt{M_0} w_1\|_2 \le \|\frac{M_1}{\sqrt{M_0}} \frac{\partial w_0}{\partial t}\|_2.$$

[3] A function of time has bandlimit Ω when its Fourier transform, as a function of ω, is supported in $[-\Omega, \Omega]$.

$$\|\sqrt{M_0}w_1\|_2 \leq \int_0^t \|\frac{M_1}{\sqrt{M_0}}\frac{\partial w_0}{\partial t}\|_2(s)\,ds.$$

$$\begin{aligned}\|w_1\|_* = \max_{0\leq t\leq T}\|\sqrt{M_0}w_1\|_2 &\leq T\max_{0\leq t\leq T}\|\frac{M_1}{\sqrt{M_0}}\frac{\partial w_0}{\partial t}\|_2 \\ &\leq T\|\frac{M_1}{M_0}\|_\infty \max_{0\leq t\leq T}\|\sqrt{M_0}\frac{\partial w_0}{\partial t}\|_2.\end{aligned}$$

This last inequality is almost, but not quite, what we need. The right-hand side involves $\frac{\partial w_0}{\partial t}$ instead of w_0. Because time derivatives can grow arbitrarily large in the high-frequency regime, this is where the bandlimited assumption needs to be used. We can invoke a classical result known as Bernstein's inequality[4], which says that $\|f'\|_\infty \leq \Omega\|f\|_\infty$ for all Ω-bandlimited f. Then

$$\|w_1\|_* \leq \Omega T\|\frac{M_1}{M_0}\|_\infty\|w_0\|_*.$$

In view of our request that $\epsilon\|w_1\|_* < \|w_0\|_*$, it suffices to require

$$\epsilon\,\Omega T\,\|\frac{M_1}{M_0}\|_\infty < 1.$$

□

See the book Inverse Acoustic and Electromagnetic Scattering Theory by Colton and Kress for a different analysis that takes into account the size of the support of M_1.

Note that the beginning of the argument, up to the Cauchy-Scwharz inequality, is called an *energy estimate* in math. See an exercise at the end of this chapter. It is a prevalent method to control the size of the solution of many initial-value PDE, including nonlinear ones.

The weak scattering condition $\epsilon\|w_1\|_* < \|w_0\|_*$ encodes the idea that the primary reflected field ϵw_1 is small compared to the incident field w_0. It is satisfied when ϵ is small, and when w_1 is not so large that it would undo the smallness of ϵ (via the factors ΩT, for instance). It turns out that

- the full scattered field $w_{sc} = w - w_0$ is also on the order of $\epsilon\Omega T\|M_1\|_\infty$ — namely the high-order terms don't compromise the weak scattering situation; and

[4]The same inequality holds with the L^p norm for all $1 \leq p \leq \infty$.

- the remainder $w_{sc}-\epsilon w_1 = w-w_0-\epsilon w_1$ is on the order of $\epsilon^2(\Omega T\|M_1\|_\infty)^2$.

Both claims are the subject of an exercise at the end of the chapter. The second claim is the mathematical expression that the Born approximation is accurate (small $w_{sc} - \epsilon w_1$ on the order of ϵ^2) precisely when scattering is weak (ϵw_1 and w_{sc} on the order of ϵ.)

3.3 Convergence of the Born series (physics)

Let us explain why the criterion $\epsilon\Omega T < 1$ (assuming the normalization $\|M_1/M_0\|_\infty = 1$) is adequate in some cases, and why it is grossly pessimistic in others.

- Instead of m or M, consider the wave speed $c_0 = 1$. Consider a constant perturbation $c_1 = 1$, so that $c = c_0 + \epsilon c_1 = 1 + \epsilon$. In one spatial dimension, $u(x,T) = f(x - cT)$. As a Taylor series in ϵ, this is

$$u(x,T) = f(x-(1+\epsilon)T) = f(x-T)-\epsilon T f'(x-T)+\frac{\epsilon^2}{2}T^2 f''(x-T)+\dots$$

  We identify $u_0(x,T) = f(x-T)$ and $u_1(x,T) = -Tf'(x-T)$. Assume now that f is a waveform with bandlimit Ω, i.e., wavelength $2\pi/\Omega$. The Born approximation

$$f(x-(1+\epsilon)T) - f(x-T) \simeq -\epsilon T f'(x-T)$$

  is only good when the translation step ϵT between the two waveforms on the left is a small fraction of a wavelength $2\pi/\Omega$, otherwise the subtraction $f(x-(1+\epsilon)T)-f(x-T)$ will be out of phase and will not give rise to values on the order of ϵ. The requirement is $\epsilon T \ll 2\pi/\Omega$, i.e.,

$$\epsilon\Omega T \ll 2\pi,$$

  which is exactly what theorem 3 is requiring. We could have reached the same conclusion by requiring either the first or the second term of the Taylor expansion to be $o(1)$, after noticing that $|f'| = O(\Omega)$ or $|f''| = O(\Omega^2)$. In the case of a constant perturbation $c_1 = 1$, the waves undergo a shift which quickly becomes nonlinear in the perturbation. This is the worst case: the requirement $\epsilon\Omega T < 1$ is sharp.

- As a second example, consider $c_0 = 1$ and $c_1(x) = H(x)$. The profile of reflected and transmitted waves was studied in equations (1.19) and (1.20). The transmitted wave will undergo a shift as in the previous example, so we expect $\epsilon\Omega T < 1$ to be sharp for it. The full reflected wave, on the other hand, is

$$u_r(x,T) = R_\epsilon f(-x-T), \qquad R_\epsilon = \frac{\epsilon}{2+\epsilon}.$$

  Notice that ϵ only appears in the reflection coefficient R_ϵ, not in the waveform itself. As $\epsilon \to 0$, u_r expands as

$$u_r(x,T) = \frac{\epsilon}{2} f(-x-T) - \frac{\epsilon^2}{4} f(-x-T) + \dots$$

  We recognize $u_1 = \frac{1}{2} f(-x-T)$. The condition for weak scattering and accuracy of the Born approximation is now simply $\epsilon < 1$, which is in general much weaker than $\epsilon\Omega T < 1$.

- In the case when $c_0 = 1$ and c_1 is the indicator function of a thin slab in one dimension, or a few isolated scatterers in several dimensions, the Born approximation is often very good. That's when the interpretation of the Born series in terms of multiple scattering is the most relevant. Such is the case of small isolated objects in synthetic aperture radar: double scattering from one object to another is often completely negligible.

The heuristic for validity of the Born approximation (even when $\epsilon\Omega T$ is not small) is that

1. c_0 or m_0 should be *smooth*
2. c_1 or m_1 should be *localized*, or better yet, localized and oscillatory (zero mean).

We do not yet have a way to turn these empirical criteria and claims into rigorous mathematical results. Seismologists typically try to operate in the regime of this heuristic when performing imaging with migration (see next chapter).

Conversely, there are a few settings in which the Born approximation is clearly violated: (i) in radar, when waves bounce multiple times before being

recorded (e.g. on the ground and on the face of a building, or in cavities such as airplane engines), (ii) in seismology, when trying to optimize over the low-frequency components of $m(x)$ (model velocity estimation), or when dealing with multiple scattering (internal multiples, multiples resulting from acoustic wave-guide reflections in shallow waters, or ghosts due to reflections at the ocean-air interface.)

Scattered waves that do not satisfy the Born approximation have long been considered a nuisance in imaging, but have recently become the subject of some research activity.

3.4 A first look at optimization

In the language of the previous sections, the forward map is denoted

$$d = \mathcal{F}[m], \qquad d = \text{data}, \qquad m = \text{model},$$

where $d_{r,s}(t) = u_s(x_r, t)$,

- x_r is the position of receiver r,
- s indexes the source,
- and t is time.

The inverse problem of imaging is that of solving for m in the system of nonlinear equations $d = \mathcal{F}[m]$. No single method will convincingly solve such a system of nonlinear equations efficiently and in all regimes.

A basic, yet quite prolific idea is to view m as the solution of the minimization problem

$$\min_m J[m], \qquad \text{where} \qquad J[m] = \frac{1}{2}\|d - \mathcal{F}[m]\|_2^2,$$

where $\|d\|_2^2 = \sum_{r,s} \int_0^T |d_{r,s}(t)|^2$ is the L^2 norm squared in the space of vectors indexed by r, s (discrete) and t (continuous, say). J is called the *output least-squares* criterion, or objective, or cost.

The *Landweber iteration* is the gradient descent method applied to J:

$$m^{(k+1)} = m^{(k)} - \alpha \frac{\delta J}{\delta m}[m^{(k)}]. \tag{3.10}$$

The choice of α is a balance between stability and speed of convergence (see one exercise at the end of the chapter.) The usual rules of functional calculus give the expression of $\frac{\delta J}{\delta m}$.

Proposition 4. *Put* $F = \frac{\delta F}{\delta m}[m]$. *Then*

$$\frac{\delta J}{\delta m}[m] = F^*(\mathcal{F}[m] - d).$$

Proof. Since $\mathcal{F}[m+h] = \mathcal{F}[m] + Fh + O(\|h\|^2)$, we have

$$\langle \mathcal{F}[m+h]-d, \mathcal{F}[m+h]-d\rangle = \langle \mathcal{F}[m]-d, \mathcal{F}[m]-d\rangle + 2\langle Fh, \mathcal{F}[m]-d\rangle + O(\|h\|^2).$$

Therefore

$$\begin{aligned} J[m+h] - J[m] &= \frac{1}{2} 2\langle Fh, \mathcal{F}[m]-d\rangle + O(\|h\|^2) \\ &= \langle h, F^*(\mathcal{F}[m]-d)\rangle + O(\|h\|^2). \end{aligned}$$

We conclude by invoking (A.1). □

The problem of computing F^* will be completely addressed in the next chapter.

The *Gauss-Newton iteration* is Newton's method applied to J:

$$m^{(k+1)} = m^{(k)} - \left(\frac{\delta^2 J}{\delta m^2}[m^{(k)}]\right)^{-1} \frac{\delta J}{\delta m}[m^{(k)}]. \tag{3.11}$$

The operator $\left(\frac{\delta^2 J}{\delta m^2}[m^{(k)}]\right)^{-1}$ is the inverse of the functional Hessian of J (also called wave-equation Hessian).

The Landweber iteration typically converges slowly, or could converge to a wrong local minimum when J is nonconvex. This topic will be further discussed in chapter 8. The Gauss-Newton iteration converges faster than gradient descent in the neighborhood of a (local) minimum, but may otherwise result in wrong update directions. It is in general much more complicated to set up than gradient descent since the wave-equation Hessian is a large matrix, costly to store and costly to invert.

3.5 Exercises

1. Repeat the development of section (3.1) in the frequency domain (ω) rather than in time.

2. Derive Born series with a multiscale expansion: write $m = m_0 + \epsilon m_1$, $u = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \ldots$, substitute in the wave equation, and equate like powers of ϵ. Find the first few equations for u_0, u_1, and u_2.

3. Write the Born series for the acoustic system, i.e., find the linearized equations that the first few terms obey. [Hint: repeat the reasoning of section 3.1 for the acoustic system, or equivalently expand on the first few three bullet points in section 3.2.]

4. At the end of section 3.1 we found the equation that u_1 obeys by differentiating (3.2) with respect to m. Now, differentiate (3.2) twice with respect to m to obtain the PDE that the Hessian of u with respect to m satisfies. We may denote the Hessian $\delta^2\mathcal{F}/\delta m \delta m'$. As a corollary, find an expression for u_2 as the solution of a new linearized wave equation with u_1 in the right-hand side. (Your answer should match that of exercise 2.) This expression of the Hessian is important later on as we describe accelerated descent methods for the inversion problem.

5. Consider the setting of section 3.2 in the case $M = I$. No perturbation will be needed for this exercise (no decomposition of M into $M_0 + \epsilon M_1$). Prove the following energy estimate for the solution of (3.8):

$$E(t) \leq \left(\int_0^t \|f\|(s)\, ds \right)^2, \tag{3.12}$$

   where $E(t) = \langle w, Mw \rangle$ and $\|f\|^2 = \langle f, f \rangle$. [Hint: repeat and adapt the beginning of the proof of theorem 3.]

6. Consider (3.8) and (3.9) in the special case when $M_0 = I$. Let $\|w\| = \sqrt{\langle w, w \rangle}$ and $\|w\|_* = \max_{0 \leq t \leq T} \|w\|$. In this exercise we show that $w - w_0 = O(\epsilon)$, and that $w - w_0 - w_1 = O(\epsilon^2)$.

   (a) Find an equation for $w - w_0$. Prove that

$$\|w - w_0\|_* \leq \epsilon \, \|M_1\|_\infty \, \Omega T \, \|w\|_*$$

   [Hint: repeat and adapt the proof of theorem 3.]

(b) Find a similar inequality to control the time derivative of $w - w_0$.

(c) Find an equation for $w - w_0 - w_1$. Prove that

$$\|w - w_0 - w_1\|_* \leq \left(\epsilon \|M_1\|_\infty \Omega T\right)^2 \|w\|_*$$

7. For the Landweber iteration (3.10), and $J[m]$ the output least-squares criterion, consider

$$\alpha = \frac{1}{\|\delta J/\delta m\|_2^2},$$

where $\|\cdot\|_2$ is the usual L^2 norm of functions of x. Show that this choice of α is safe in the sense that the Landweber iteration becomes a contraction when $\mathcal{F}$ is linear.

8. Show that the Gauss-Newton iteration (3.11) results from approximating J by a quadratic near $m^{(k)}$, and finding the minimum of that quadratic function.

9. Prove the following formula for the wave-equation Hessian $\frac{\delta^2 J}{\delta m^2}$ in terms of F and its functional derivatives:

$$\frac{\delta^2 J}{\delta m^2} = F^* F + \langle \frac{\delta^2 \mathcal{F}}{\delta m^2}, \mathcal{F}[m] - d \rangle.$$

(F^*F is called normal operator.)

10. Show that the spectral radius of the Hessian operator $\frac{\delta^2 J}{\delta m^2}$, when data are (essentially) limited by $t \leq T$ and $\omega \leq \Omega$, is bounded by a constant times $(\Omega T)^2$.

Chapter 4

Adjoint-state methods

As explained in section (3.4), the adjoint F^* of the linearized forward (modeling) operator F plays an important role in the formula of the functional gradient $\frac{\delta J}{\delta m}$ of the least-squares cost function J:

$$\frac{\delta J}{\delta m}[m] = F^*(\mathcal{F}[m] - d).$$

While F is the basic linear map from model space to data space, F^* is the basic linear map from data space to model space. F^* is not only the building block of iterative optimization schemes, but the mere application of F^* to data is the simplest form of "imaging". For instance, when the initial guess $m^{(0)} = m_0$ is a smooth background model reasonably close to the true solution m, the first iteration of gradient descent,

$$m^{(1)} = \alpha F^*(d - \mathcal{F}[m_0]),$$

often gives a good "image" of the scatterers (somewhat close to the actual ϵm_1). For this reason, F^* is often called the *imaging operator*.

It should also be noted that F^* behaves not entirely unlike F^{-1}, i.e., F is somewhat close to being unitary. This statement does not have a rigorous formulation of the form $\|F^*F - I\| \leq (\ldots)$, but rather of the form "F^*F does not move singularities around like F or F^* do". More details on the microlocal aspects of this question will be given in chapter 7.

Forming the full matrix $F = \frac{\delta \mathcal{F}}{\delta m}$ and transposing it is not a practical way to compute F^*. The adjoint-state method provides an elegant solution to this problem, called the "imaging condition".

4.1 The imaging condition

For any $d_r(t)$ function of the receiver index r and time t, and $m(x)$ function of position x (here m and d are any two functions, not necessarily linked to one another by the forward model), we have

$$\langle d, Fm \rangle = \langle F^* d, m \rangle.$$

The inner product on the left is in data space,

$$\langle d, Fm \rangle = \sum_r \int_0^T d_r(t) u(x_r, t)\, dt, \qquad u = Fm,$$

while the inner product on the right is in model space.

$$\langle F^* d, m \rangle = \int_{\mathbb{R}^n} (F^* d)(x) m(x)\, dx.$$

The relation $u = Fm$ is implicitly encoded by the two equations

$$\left(m_0 \frac{\partial^2}{\partial t^2} - \Delta \right) u = -m \frac{\partial^2 u_0}{\partial t^2},$$

$$\left(m_0 \frac{\partial^2}{\partial t^2} - \Delta \right) u_0 = f.$$

Note that a single right-hand side generates u_0, and that we have omitted the source subscript s in this section; we will return to multiples sources shortly.

The argument that isolates and makes explicit the contribution of m in $\sum_r \int_0^T d_r(t) u(x_r, t)\, dt$ is one of integration by parts. In order to integrate by parts in x, we need to turn the sum over receivers into an integral. This can be achieved by considering a distributional extended dataset where each measurement $d_r(t)$ is accompanied by a Dirac delta located at x_r:

$$d_{\text{ext}}(x, t) = \sum_r d_r(t) \delta(x - x_r).$$

We then have

$$\langle d, Fm \rangle = \int_{\mathbb{R}^n} \int_0^T d_{\text{ext}}(x, t) u(x, t)\, dx dt.$$

In order to use the wave equation for u, a copy of the differential operator $\left(m_0 \frac{\partial^2}{\partial t^2} - \Delta \right)$ needs to materialize. This is done by considering an auxiliary

field $q(x,t)$ that solves the same wave equation with $d_{\text{ext}}(x,t)$ as a right-hand side:

$$\left(m_0\frac{\partial^2}{\partial t^2}-\Delta\right)q(x,t)=d_{\text{ext}}(x,t),\qquad x\in\mathbb{R}^n, \tag{4.1}$$

with as-yet unspecified "boundary conditions" in time. Substituting this expression for $d_{\text{ext}}(x,t)$, and integrating by parts both in space and in time reveals

$$\begin{aligned}\langle d,Fm\rangle &= \int_V\int_0^T q(x,t)\left(m_0\frac{\partial^2}{\partial t^2}-\Delta\right)u(x,t)\,dxdt\\ &+\int_V m_0\frac{\partial q}{\partial t}u|_0^T\,dx-\int_V m_0 q\frac{\partial u}{\partial t}|_0^T\,dx\\ &+\int_{\partial V}\int_0^T\frac{\partial q}{\partial n}u\,dS_x dt-\int_{\partial V}\int_0^T q\frac{\partial u}{\partial n}\,dS_x dt,\end{aligned}$$

where V is a volume that extends to the whole of $\mathbb{R}^n$, and ∂V is the boundary of V — the equality then holds in the limit of $V=\mathbb{R}^n$.

The boundary terms over ∂V vanish in the limit of large V by virtue of the fact that they involve u – a wavefield created by localized functions f,m,u_0 and which does not have time to travel arbitrarily far within a time $[0,T]$. The boundary terms at $t=0$ vanish due to $u|_{t=0}=\frac{\partial u}{\partial t}|_{t=0}=0$. As for the boundary terms at $t=T$, they only vanish if we impose

$$q|_{t=T}=\frac{\partial q}{\partial t}|_{t=T}=0.$$

Since we are only interested in the values of $q(x,t)$ for $0\le t\le T$, the above are *final conditions* rather than initial conditions, and the equation (4.1) is run *backward in time*. The wavefield q is called *adjoint* field, or adjoint state. The equation (4.1) is itself called adjoint equation. Note that q is *not* the physical field run backward in time (because of the limited sampling at the receivers), instead, it is introduced purely out of mathematical convenience.

We can now return to the simplification of the left-hand-side,

$$\begin{aligned}\langle d,Fm\rangle &= \int_{\mathbb{R}^n}\int_0^T q(x,t)\left(m_0\frac{\partial^2}{\partial t^2}-\Delta\right)u(x,t)\,dxdt\\ &=-\int_{\mathbb{R}^n}\int_0^T q(x,t)m(x)\frac{\partial^2 u_0}{\partial t^2}\,dxdt\end{aligned}$$

This quantity is also supposed to be $\langle m, F^*d\rangle$, regardless of m, so we conclude

$$(F^*d)(x) = -\int_0^T q(x,t)\frac{\partial^2 u_0}{\partial t^2}\,dt. \tag{4.2}$$

This equation is called the *imaging condition*: it expresses the action of F^* on d as the succession of the following steps:

1. Place data $d_r(t)$ at the location of the receivers with point masses to get d_{ext};

2. Use d_{ext} as the right-hand side in the adjoint wave equation to get the adjoint, backward field q;

3. Simulate the incident, forward field u_0; and finally

4. Take the time integral of the product of the forward field u_0 (differentiated twice in t), and the backward field q, for each x independently.

The result is a function of x which sometimes serves the purpose of image, and may sometimes be called $I_m(x)$. Note that we have not performed a full inversion; if d are measuered data, then I_m is not the model m that gave rise to d. In seismology, the imaging condition (4.2) is called reverse-time migration, or simply *migration*. In radar, the imaging condition does not have a particular name, but in the next chapter we will encounter a simplification of (4.2) called backprojection.

4.2 Stacks and gathers

If we now restore the presence of multiple sources, the wavefields u, u_0, and u_1 will depend on the source index s. The source term f_s — typically of the form $w(t)\delta(x - x_s)$ — is in the right-hand side of the wave equations for u_0 and u, while u_1 implicitly depends on f_s through u_0. For a fixed source s, we denote

$$u_s = \mathcal{F}_s[m], \qquad u_{0,s} = \mathcal{F}_s[m_0], \qquad u_{1,s} = F_s m_1,$$

while we continue to denote $u = \mathcal{F}[m]$, $u_0 = \mathcal{F}[m_0]$ and $u_1 = Fm_1$ for the *collection* of such wavefields over s.

The data inner-product now has an additional sum over s, namely

$$\langle d, Fm\rangle = \sum_s \sum_r \int_0^T d_{r,s}(t) u_s(x_r, t)\, dt.$$

The formula for F^* can be obtained by taking adjoints one s at a time, namely

$$\begin{aligned}\langle F^* d, m\rangle = \langle d, Fm\rangle &= \sum_s \langle d_s, F_s m\rangle \\ &= \sum_s \langle F_s^* d_s, m\rangle \\ &= \langle \sum_s F_s^* d_s, m\rangle,\end{aligned}$$

hence

$$F^* = \sum_s F_s^*.$$

More explicitly, in terms of the imaging condition,

$$(F^* d)(x) = -\sum_s \int_0^T q_s(x,t) \frac{\partial^2 u_{0,s}}{\partial t^2}(x,t)\, dt, \tag{4.3}$$

where the adjoint field q_s is relative to the source s:

$$\left(m_0 \frac{\partial^2}{\partial t^2} - \Delta\right) q_s(x,t) = d_{\mathrm{ext},s}(x,t).$$

The sum over s in the new imaging condition (4.3) is sometimes called a *stack*. It is often the case that particular images $F_s^* d$ are not very informative on their own, but a stack uses the redundancy in the data to bring out the information and reveal more details.

The mathematical tidbit underlying stacks is that the operation of creating a vector $(x, x, \ldots, x)$ out of a single number x has for adjoint the operation of summing the components of a vector.

The set of $F_s^* d_s$ indexed by s is called *prestack migration*, or prestack depth migration (PSDM) by geophysicists. Tellingly, they call $F^* d = \sum_s F_s^* d_s$ poststack migration. They also call the source s a *shot*. When the dataset d_s is indexed by shot s, it is called a *shot gather*, or common shot gather

(CSG). Alternatively, a dataset can be organized by midpoint $x_m = \frac{x_s+x_r}{2}$ vs. half-offset $h = \frac{x_s-x_r}{2}$ — in that case it is called common midpoint gather (CMP). Since the midpoint does not generally fall on a grid, doing a CMP requires binning[1].

4.3 The adjoint state as a Lagrange multiplier

The adjoint field q was introduced in a somewhat opportunistic and artificial way in section 4.1. In this section, we show that it has the interpretation of a Lagrange multiplier in a constrained optimization framework, where the wave equation serves as a constraints for an otherwise bare least-squares cost function.

Specifically consider the least-squares objective as a function of u rather than m,

$$J[u] = \frac{1}{2}\|d-u\|_2^2,$$

where u is the wavefield prediction and d are the observed data. The model m only appears implicitly through the constraint that u needs to satisfy, namely

$$\left(m\frac{\partial^2}{\partial t^2} - \Delta\right) u = f.$$

Critical points are those for which the total derivative of $J[u(m)]$ with respect to m is zero. Normally one would have to access $\delta u/\delta m$ to compute this total derivative, because by the chain rule[2]

$$\frac{d}{dm}J[u(m)] = \langle \frac{\delta J}{\delta u}, \frac{\delta u}{\delta m}\rangle = \langle u-d, \frac{\delta u}{\delta m}\rangle.$$

A more computationally favorable formula for $\frac{d}{dm}J[u(m)]$ can be derived by considering a traditional concept in constrained optimization: the Lagrangian

$$\mathcal{L}[u,m,q] = J[u] - \langle q, \left(m\frac{\partial^2}{\partial t^2} - \Delta\right) u - f\rangle.$$

[1]Which can be a very inaccurate operation from a numerical viewpoint, i.e., as inaccurate as its adjoint, nearest-neighbor interpolation.

[2]This equation contains a space-time inner product of $u-d$ vs. u differentiated. It is not the application of $\frac{\delta u}{\delta m}$ as an operator F to $u-d$. Recall that F acts in model space anyway.

Here q is the Lagrange multiplier, itself a function of x and t, and the inner product is over x and t. Notice that $\mathcal{L}[u(m), m, q] = J[u(m)]$ regardless of q when $u = u(m)$, i.e., when the constraint is satisfied. This expression can be differentiated to give

$$\frac{d}{dm}J[u(m)] = \langle \frac{\delta \mathcal{L}}{\delta u}, \frac{\delta u}{\delta m} \rangle + \frac{\delta \mathcal{L}}{\delta m}.$$

After a short exercise of integration by parts identical to the one in the previous section, and provided $q|_{t=T} = \frac{\partial q}{\partial t}|_{t=T} = 0$, the partial $\frac{\delta \mathcal{L}}{\delta u}$ evaluated at some point $u_0 = u(m_0)$ is

$$\frac{\delta \mathcal{L}}{\delta u} = u_0 - d - \left(m_0 \frac{\partial^2}{\partial t^2} - \Delta \right) q$$

The other partials evaluated at $u_0 = u[m_0]$ are immediate:

$$\frac{\delta \mathcal{L}}{\delta m} = -\int_0^T q \frac{\partial^2 u_0}{\partial t^2}\, dt,$$

$$\frac{\delta \mathcal{L}}{\delta q} = \left(m_0 \frac{\partial^2}{\partial t^2} - \Delta \right) u_0 - f.$$

Putting $\frac{\delta \mathcal{L}}{\delta q} = 0$ results in the *state equation*

$$\left(m_0 \frac{\partial^2}{\partial t^2} - \Delta \right) u_0 = f,$$

satisfied as soon as we consider a feasible $u_0 = u(m_0)$. Putting $\frac{\delta \mathcal{L}}{\delta u} = 0$ results in the *adjoint-state equation*

$$\left(m_0 \frac{\partial^2}{\partial t^2} - \Delta \right) q = u_0 - d. \tag{4.4}$$

We choose to impose $\frac{\delta \mathcal{L}}{\delta u} = 0$, hence q to satisfy the adjoint-state equation, precisely so that the gradient of J reduces to

$$\frac{d}{dm}J[u(m_0)] = \frac{\delta \mathcal{L}}{\delta m} = -\int_0^T q \frac{\partial^2 u_0}{\partial t^2}\, dt. \tag{4.5}$$

This recovers the imaging condition obtained earlier. The formula is in agreement with our previous characterization of J, namely (back when J depended explicitly on m),

$$\frac{\delta J}{\delta m}[m_0] = F^*(\mathcal{F}[m_0] - d).$$

Indeed, we have seen that F^* is realized via an imaging condition involving an adjoint state, and $\mathcal{F}[m_0] - d = u_0 - d$ is the right-hand side in (4.4).

It should be noted that the traditional role of the Lagrangian is to give optimality conditions on (u, m, q) that describe the critical points of J. This is done by putting all the partials of $\mathcal{L}$ to zero[3]. What we did earlier was different: we considered the Lagrangian at points that are not critical, and only put its partial $\frac{\delta \mathcal{L}}{\delta u}$ to zero as a device to simplify the expression of the gradient of J. In our setting, away from critical points, the partial $\frac{\delta \mathcal{L}}{\delta m} = dJ/dm$ is in general nonzero.

4.4 The imaging condition in the frequency domain

We now return to the setting of section 4.1, and modify the exposition to express both the adjoint-state equation and the imaging condition in the frequency (ω) domain. The nugget in this section is that complex conjugation in ω corresponds to time reversal. We assume a single source for simplicity.

We are again interested in finding F^* such that $\langle d, Fm\rangle = \langle F^*d, m\rangle$ for all generic d and m. The data inner product $\langle d, Fm\rangle$ can be expressed in the frequency domain by means of the Parseval formula,

$$\langle d, Fm\rangle = 2\pi \sum_r \int_{\mathbb{R}} \overline{\widehat{d_r}(\omega)}\widehat{(Fm)}(x_r, \omega)d\omega = \sum_r \int d_r(t)(Fm)(x_r, t)dt.$$

The complex conjugate is important, now that we are in the frequency domain. As previously, we pass to the extended dataset

$$\widehat{d_{\text{ext}}}(x, \omega) = \sum_r \widehat{d_r}(\omega)\delta(x - x_r),$$

[3]When $\mathcal{L}$ and J are smooth — otherwise one should consider that zero belongs in the subdifferential of $\mathcal{L}$.

and turn the sum over r into an integral over x. The linearized scattered field is

$$\widehat{(Fm)}(x_r,\omega) = \int \widehat{G}(x,y;\omega)m(y)\omega^2\widehat{u_0}(y,\omega)\,dy. \tag{4.6}$$

To simplify the resulting expression of $\langle d, Fm\rangle$, we let

$$\widehat{q}(x,\omega) = \int \overline{\widehat{G}(y,x;\omega)}\widehat{d_{\text{ext}}}(y,\omega)\,dy. \tag{4.7}$$

(Note that Green's functions are always symmetric under the swap of x and y, as we saw in a special case in one of the exercises in chapter 1.) It follows that

$$\langle d, Fm\rangle = \int m(y)\left[2\pi\int_{\mathbb{R}} \widehat{q}(y,\omega)\omega^2\overline{\widehat{u_0}(y,\omega)}\,d\omega\right]\,dy,$$

hence

$$F^*d(y) = 2\pi\int_{\mathbb{R}} \widehat{q}(y,\omega)\omega^2\overline{\widehat{u_0}(y,\omega)}\,d\omega. \tag{4.8}$$

This equation is the same as (4.2), by Parseval's identity. Equation (4.7) is the integral version of (4.1) in the frequency domain. The complex conjugation of $\widehat{G}$ in (4.7) expresses *time reversal*; such is the case for any Fourier transform of a real function:

$$\overline{\widehat{f}(\omega)} = \overline{\int e^{i\omega t}f(t)\,dt} = \int e^{-i\omega t}f(t)dt = \int e^{i\omega t}f(-t)\,dt.$$

The integral in t in (4.2) is over $[0,T]$ because such is the support of $q\frac{\partial^2 u_0}{\partial t^2}$. The integral in ω in (4.8) is over $\mathbb{R}$. It is tempting to truncate this integral to "the frequencies that have been measured" — but that is strictly speaking incompatible with the limits on t (for the same reason that a function compactly supported in time cannot also be compactly supported in frequency.) Careful consideration of cutoffs is needed to control the accuracy of a truncation in ω.

Equation (4.8) is valuable for a few different reasons:

- It can be further simplified in some situations, such as in the next chapter;
- The integral over ω can be deliberately restricted in the scope of descent iterations, so as to create sweeps over frequencies. This is sometimes important to deal with the lack of convexity of full inversion; see chapter 8.

4.5 Exercises

1. Starting from an initial guess model m_0, a known source function f, and further assuming that the Born approximation is valid, explain how the inverse problem $d = \mathcal{F}[m]$ can be completely solved by means of F^{-1}, the inverse of the linearized forward operator (provided F is invertible). The intermediate step consisting in inverting F is called the *linearized inverse problem*.

   Solution. *Form the incident field as $u_0 = Gf$. Subtract from observed data to get $d - u_0$. Since the Born approximation is assumed valid, we have $d - u_0 \simeq \epsilon u_1$. Invert for m_1 by solving the system $u_1 = Fm_1$, i.e., $m_1 = F^{-1}u_1$. Then form $m = m_0 + \epsilon m_1$.*

2. *Snapshot migration.* The treatment of reverse-time migration seen earlier involves data $u(x_r, t)$ for an interval in time t, and at fixed receiver points x_r. Consider instead the snapshot setup, where t is fixed, and there are receivers everywhere in the domain of interest. (So we have full knowledge of the wavefield at some time t.) Repeat the analysis of the imaging operator, adjoint to the forward operator that forms snapshot data from singly scattered waves. In particular, find what the adjoint-state wave equation becomes in this case. [Hint: it involves nonzero final data, and a zero right-had side.]

3. *Sampling.* Call S the linear operator that maps a function $f(x)$ to the vector of point samples $\{f(x_r)\}_r$. Find a formula for S^*. When the linearized forward model is written as SF, the imaging operator is F^*S^*; the presence of S^* explains why we passed from $d_r(t)$ to $d_{\text{ext}}(x, t)$ in the first step of the derivation of the imaging operator.

Chapter 5

Synthetic-aperture radar

The object of synthetic aperture radar imaging (SAR) is to infer reflectivity profiles from measurement of scattered electromagnetic waves. The word "aperture" refers to the perceived angular resolution from the viewpoint of the sensor (antenna). The expression "synthetic aperture" refers to the fact that the aperture is created not from a very directional antenna, or array of antennas (as in ultrasound), but results from a computational process of triangulation, implicit in the handling of data with a backprojection formula.

The goal of the chapter is to gain an understanding of the geometry underlying the operators F and F^* arising in SAR. Our reference for this chapter is the book "Fundamentals of radar imaging" by Cheney and Borden.

5.1 Assumptions and vocabulary

We will make the following basic assumptions: (!)

1. *Scalar fields* obeying the wave equation, rather than vector fields obeying Maxwell's equation. This disregards polarization (though processing polarization is a sometimes a simple process of addition of images.) The reflectivity of the scatterers is then encoded via $m(x)$ as usual, rather than by specifying the shape of the boundary $\partial\Omega$ and the type of boundary conditions for the exterior Maxwell problem.

2. *The Born approximation*, so that data d are proportional to ϵu_1, and $u_1 = Fm_1$. This disregards multiple scattering. In the sequel we will write $\epsilon = 1$ for simplicity.

3. *No dispersion*, so that all waves travel at the same speed regardless of frequency, as in the wave equation. Dispersion happens for radio waves in the ionosphere.

4. The reflectivity $m(x) = m_0(x) + \epsilon m_1(x)$ is *constant in time*, with m_0 *constant in time and space*. This disregards moving scatterers. As mentioned earlier, we put $\epsilon = 1$. For convenience, we will also drop the subscript 1 from m_1, so that *in this chapter, m stands for the perturbation* in squared slowness $1/c^2$.

A few other "working" assumptions are made for convenience, but can
(!) easily be removed later:

5. *The far field assumption*: spherical wavefronts are assumed to be locally planar, for waves at the scatterer originating from the antenna (or vice-versa).

6. *Monostatic SAR*: the same antenna is used for transmission and reception. It is not difficult to treat the bistatic/multistatic case where different antennas play different roles.

6. *Start-stop approximation*: in the time it takes for the pulse to travel back and forth from the antenna to the scatterers, the antenna is assumed not to have moved.

SAR typically operates with radio waves or microwaves, with wavelengths on the order of meters to centimeters. Moving antennas are typically carried by planes or satellites. A variant of SAR is to use arrays of fixed antennas, a situation called MIMO (multiple input, multiple output.) If the frequency band is of the form $[\omega_0 - \Delta\omega/2, \omega_0 + \Delta\omega/2]$, we say ω_0 is the *carrier frequency* and $\Delta\omega$ is the *bandwidth*. We speak of *wideband* acquisition when $\Delta\omega$ is a large fraction of ω_0. As usual, $\omega = 2\pi\nu$ where ν is in Hertz.

The direction parallel to the trajectory of the antenna is called *along-track*. The vector from the antenna to the scatterer is called *range vector*, its direction is the *range direction*, and the direction perpendicular to the range direction is called *cross-range*. The distance from the antenna to the scatterer is also called *range*. The length of the horizontal projection of the range vector is the *downrange*.

We will not deal with the very interesting topic of Doppler imaging, where
(!) frequency shifts are used to infer velocities of scatterers. We will also not

cover the important topic of interferometric SAR (InSAR) where the objective is to create difference images from time-lapse datasets.

We finish this section by describing the nature of the far-field approximation in more details, and its consequence for the expression of the Green's function $\frac{e^{ik|x-y|}}{4\pi|x-y|}$. Consider an antenna located near the origin. We will assume that a scatterer at x is "far" from a point y on the antenna in the sense that

$$|y| \ll |x|, \qquad k|y|^2 \ll |x|.$$

Then, if we let $\widehat{x} = \frac{x}{|x|}$,

$$\begin{aligned} |x-y| &= \sqrt{|x|^2 - 2x\cdot y + |y|^2} \\ &= |x|\sqrt{1 - 2\frac{\widehat{x}\cdot y}{|x|} + \frac{|y|^2}{|x|^2}} \\ &\simeq |x|\left(1 - \frac{\widehat{x}\cdot y}{|x|} + \frac{1}{2}\frac{|y|^2}{|x|^2} + \dots\right) \\ &= |x| - \widehat{x}\cdot y + \frac{1}{2}\frac{|y|^2}{|x|} + \dots \end{aligned}$$

We therefore have

$$e^{ik|x-y|} = e^{ik|x|}e^{-ik\widehat{x}\cdot y}\left(1 + O\left(\frac{k|y|^2}{|x|}\right)\right),$$

$$\frac{1}{|x-y|} = \frac{1}{|x|}\left(1 + O\left(\frac{|y|}{|x|}\right)\right).$$

As a result, in the far field,

$$\frac{e^{ik|x-y|}}{4\pi|x-y|} \simeq \frac{e^{ik|x|}}{4\pi|x|}e^{-ik\widehat{x}\cdot y}.$$

This simplification will cause the y integrals to become Fourier transforms.

5.2 Forward model

We can now inspect the *radiation field* created by the antenna at the transmission side. The $\simeq$ sign will be dropped for $=$, although it is understood

that the approximation is only accurate in the far field. Call $j(x,\omega)$ the scalar analogue of the vector forcing generated by currents at the antenna, called current density vector. (The dependence on ω is secondary.) Call $\widehat{p}(\omega)$ the Fourier transform of the user-specified pulse $p(t)$. Then

$$\widehat{u_0}(x,\omega) = \int \frac{e^{ik|x|}}{4\pi|x|} e^{-ik\widehat{x}\cdot y} j(y,\omega)\widehat{p}(\omega)\, dy.$$

This reduces to a spatial Fourier transform of j in its first argument,

$$\widehat{u_0}(x,\omega) = \frac{e^{ik|x|}}{4\pi|x|}\widehat{j}^{(1)}(k\widehat{x},\omega)\widehat{p}(\omega).$$

For short, we let

$$J(\widehat{x},\omega) = \widehat{j}^{(1)}(k\widehat{x},\omega),$$

and call it the *radiation beam pattern*. It is determined by the shape of the antenna. As a function of $\widehat{x}$, the radiation beam pattern is often quite broad (not concentrated).

For an antenna centered at position $\gamma(s)$, parametrized by s (called slow time), the radiation field is therefore

$$\widehat{u_{0,s}}(x,\omega) = \frac{e^{ik|x-\gamma(s)|}}{4\pi|x-\gamma(s)|} \widehat{J(x-\gamma(s),\omega)}\widehat{p}(\omega).$$

The scattered field $u_1(x,\omega)$ is not directly observed. Instead, the recorded data are the linear functionals

$$\widehat{d}(s,\omega) = \int_{A_s} u_1(y,\omega) w(y,\omega)\, dy$$

against some window function $w(x,\omega)$, and where the integral is over the antenna A_s centered at $\gamma(s)$. Recall that u_1 obeys (4.6), hence (with m standing for what we used to call m_1)

$$\widehat{d}(s,\omega) = \int_{A_s}\int \frac{e^{ik|x-y|}}{4\pi|x-y|}\omega^2 \widehat{u_0}(x,\omega) m(x) w(y,\omega)\, dydx.$$

In the regime of the the far-field approximation for an antenna at $\gamma(s)$, we get instead (still using an equality sign)

$$\widehat{d}(s,\omega) = \int \frac{e^{ik|x-\gamma(s)|}}{4\pi|x-\gamma(s)|}\omega^2 \widehat{u_0}(x,\omega) m(x) \widehat{w}^{(1)}(k\widehat{(x-\gamma(s))},\omega).$$

The start-stop approximation results in the same $\gamma(s)$ used at transmission and at reception. For short, we let

$$W(\widehat{x},\omega) = \widehat{w}^{(1)}(k\widehat{x},\omega),$$

and call it the *reception beam pattern*. For a perfectly conducting antenna, the two beam patterns are equal by reciprocity: ($)

$$J(\widehat{x},\omega) = W(\widehat{x},\omega).$$

We can now carry through the substitutions and obtain the expression of the linearized forward model F:

$$\widehat{d}(s,\omega) = \widehat{Fm}(s,\omega) = \int e^{2ik|x-\gamma(s)|} A(x,s,\omega) m(x)\, dx, \tag{5.1}$$

with amplitude

$$A(x,s,\omega) = \omega^2\, \widehat{p}(\omega)\, \frac{J(\widehat{x-\gamma(s)},\omega) W(\widehat{x-\gamma(s)},\omega)}{16\pi^2 |x-\gamma(s)|^2}.$$

So far we have assumed that $x = (x_1, x_2, x_3)$, and that dx a volume element. We could alternatively assume a two-dimensional reflectivity profile at a known elevation $x_3 = h(x_1, x_2)$. In that case we write

$$x_T = (x_1, x_2, h(x_1, x_2)),$$

assume a reflectivity of the form $m(x) = \delta(x_3 - h(x_1, x_2))V(x_1, x_2)$, and get (!)

$$\widehat{d}(s,\omega) = \int e^{2ik|x_T-\gamma(s)|} A(x_T,s,\omega) V(x_1,x_2)\, dx_1 dx_2.$$

The geometry of the formula for F is apparent if we return to the time variable. For illustration, reduce $A(x,s,\omega) = \omega^2 \widehat{p}(\omega)$ to its leading ω dependence. Then

$$\begin{aligned} d(s,t) &= \frac{1}{2\pi} \int e^{-i\omega t} \widehat{d}(s,\omega)\, d\omega \\ &= -\frac{1}{2\pi} \int p''\left(t - 2\frac{|x-\gamma(s)|}{c_0}\right) m(x)\, dx. \end{aligned}$$

We have used the fact that $k = \omega/c_0$ to help reduce the phase to the simple expression

$$t - 2\frac{|x - \gamma(s)|}{c}$$

Its physical significance is clear: the time taken for the waves to travel to the scatterer and back is twice the distance $|x - \gamma(s)|$ divided by the light speed c_0. Further assuming $p(t) = \delta(t)$, then there will be signal in the data $d(s,t)$ only at a time $t = 2\frac{|x-\gamma(s)|}{c}$ compatible with the kinematics of wave propagation. The locus of possible scatterers giving rise to data $d(s,t)$ is then a sphere of radius $ct/2$, centered at the antenna $\gamma(s)$. It is a good exercise to modify these conclusions in case $p(t)$ is a narrow pulse (oscillatory bump) supported near $t = 0$, or even when the amplitude is returned to its original form with beam patterns.

In SAR, s is called slow time, t is the fast time, and as we mentioned earlier, $|x - \gamma(s)|$ is called range.

5.3 Filtered backprojection

In the setting of the assumptions of section 5.1, the imaging operator F^* is called *backprojection* in SAR. Consider the data inner product[1]

$$\langle d, Fm\rangle = \int \widehat{d}(s,\omega)\overline{\widehat{Fm}(s,\omega)}\, ds d\omega.$$

As usual, we wish to isolate the dependence on m to identify $\langle d, Fm\rangle$ as $\langle F^*d, m\rangle$. After using (5.1), we get

$$\langle d, Fm\rangle = \int m(x) \iint e^{-2ik|x-\gamma(s)|}\overline{A(x,s,\omega)}\widehat{d}(s,\omega)\, ds d\omega.$$

This means that

$$(F^*d)(x) = \iint e^{-2ik|x-\gamma(s)|}\overline{A(x,s,\omega)}\widehat{d}(s,\omega)\, ds d\omega. \tag{5.2}$$

Notice that the kernel of F^* is the *conjugate* of that of F, and that the integration is over the data variables (s,ω) rather than the model variable x.

[1]It could be handy to introduce a multiplicative factor 2π in case the Parseval identity were to be used later.

The physical interpretation is clear if we pass to the t variable, by using $\widehat{d}(s,\omega) = \int e^{i\omega t} d(s,t)\, dt$ in (5.2). Again, assume $A(x,s,\omega) = \omega^2 \widehat{p}(\omega)$. We then have

$$(F^* d)(x) = -\frac{1}{2\pi} \int p'' \left(t - 2\frac{|x-\gamma(s)|}{c_0} \right) d(s,t)\, ds dt.$$

Further assume $p(t) = \delta(t)$. Then F^* places a contribution to the reflectivity at x if and only if there is signal in the data $d(s,t)$ for s,t,x linked by the same kinematic relation as earlier, namely $t = 2\frac{|x-\gamma(s)|}{c}$. In other words, it "spreads" the data $d(s,t)$ along a sphere of radius $ct/2$, centered at $\gamma(s)$, and adds up those contributions over s and t. Notice that p is in practice a narrow pulse, not a delta, hence those spheres become thin shells. Strictly speaking, "backprojection" refers to the amplitude-free formulation A =constant, i.e., in the case when $p''(t) = \delta(t)$. But we will use the word quite liberally, and still refer to the more general formula (5.2) as backprojection. So do many references in the literature.

Backprojection can also be written in the case when the reflectivity profile is located at elevation $h(x_1, x_2)$. It suffices to evaluate (5.2) at $x_T = (x_1, x_2, h(x_1, x_2))$.

We now turn to the problem of modifying backprojection to give a formula approximating F^{-1} rather than F^*. Hence the name *filtered backprojection*. It will only be an approximation of F^{-1} because of sampling issues that will be studied in detail in the sequel.

The phase $-2ik|x-\gamma(s)|$ needs no modification: it is already "kinematically correct". Only the amplitude needs to be changed, to yield a new operator[2] B to replace F^*:

$$(Bd)(x) = \iint e^{-2ik|x-\gamma(s)|} Q(x,s,\omega) \widehat{d}(s,\omega)\, ds d\omega.$$

By composing B with F, we obtain

$$(BFm)(x) = \int K(x,y) m(y)\, dy,$$

with

$$K(y,x) = \iint e^{-2ik|x-\gamma(s)|+2ik|y-\gamma(s)|} Q(x,s,\omega) A(y,s,\omega)\, ds d\omega.$$

[2] B for filtered Backprojection, or for Beylkin. See why shortly.

We wish to choose Q so that BF is as close to the identity as possible, i.e.,

$$K(x, y) \simeq \delta(x - y).$$

(...)

5.4 Resolution

(...)

$$\Delta x_1 = \frac{c}{\Delta\omega \ \sin\psi}$$

$$\Delta x_2 = \frac{L}{2}, \qquad L \geq \lambda$$

5.5 Exercises

1. Prove (5.2) in an alternative fashion by substituting in the far-field approximation of G in the imaging condition (4.8).

2. *Bistatic SAR*: repeat and modify the derivation of (5.1) in the case of an antenna $\gamma_1(s)$ for transmission and another antenna $\gamma_2(s)$ for reception.

Chapter 6

Computerized tomography

6.1 Assumptions and vocabulary

(...)

Computerized tomography (CT scans, as well as PET scans) imaging involves inversion of a Radon or X-ray transform. It is primarily used for medical imaging.

In two spatial dimensions, the variables in the Radon domain are t (offset) and θ (angle). Data in the form $d(t, \theta)$ corresponds to the *parallel beam* geometry. More often, data follow the *fan-beam* geometry, where for a given value of θ the rays intersect at a point (the source of X-rays), and t indexes rays within the fan. The transformation to go from parallel-beam to fan-beam and back is

$$d_{\text{fan}}(t, \theta) = d_{\text{para}}(t, \theta + (at + b)),$$

for some numbers a and b that depend on the acquisition geometry. Datasets in the Radon domain are in practice called *sinograms*, because the Radon transform of a Dirac mass is a sine wave[1].

6.2 The Radon transform and its inverse

Radon transform:

$$(Rf)(t, \theta) = \int \delta(t - x \cdot e_\theta) f(x)\, dx,$$

[1]More precisely, a distribution supported on the graph of a sine wave, see an exercise at the end of the chapter.

with $e_\theta = (\cos\theta, \sin\theta)^T$.

Fourier transform in t / Fourier-slice theorem[2]:

$$\widehat{Rf}(\omega, \theta) = \int e^{-i\omega x \cdot e_\theta} f(x)\, dx.$$

Adjoint Radon transform / (unfiltered) backprojection:

$$\begin{aligned} R^* d(x) &= \int e^{i\omega x \cdot e_\theta} \widehat{d}(\omega, \theta)\, d\omega d\theta \\ &= \int \delta(t - x \cdot e_\theta) d(t, \theta)\, dt d\theta \\ &= \int d(x \cdot \theta, \theta)\, d\theta \end{aligned}$$

Inverse Radon transform / filtered backprojection in the case of two spatial dimensions:

$$R^{-1} d(x) = \frac{1}{(2\pi)^n} \int e^{i\omega x \cdot e_\theta} \widehat{d}(\omega, \theta)\, \omega\, d\omega d\theta.$$

(notice the factor ω.)

Filtered backprojection can be computed by the following sequence of steps:

- Take a Fourier transform to pass from t to ω;
- Multiply by ω;
- Take an inverse Fourier transform from ω back to t, call $D(t, \theta)$ the result;
- Compute $\int d(x \cdot \theta, \theta)\, d\theta$ by quadrature and interpolation (piecewise linear interpolation is often accurate enough.)

6.3 Exercises

1. Compute the Radon transform of a Dirac mass, and show that it is nonzero along a sinusoidal curve (with independent variable θ and dependent variable t, and wavelength 2π.)

[2]The direct Fourier transform comes with $e^{-i\omega t}$. Here t is offset, not time, so we use the usual convention for the FT.

Chapter 7

Seismic imaging

Much of the imaging procedure was already described in the previous chapters. An image, or a gradient update, is formed from the imaging condition by means of the incident and adjoint fields. This operation is called migration rather than backprojection in the seismic setting. The two wave equations are solved by a numerical method such as finite differences.

In this chapter, we expand on the structure of the Green's function in variable media. This helps us understand the structure of the forward operator F, as well as migration F^*, in terms of a 2-point traveltime function $\tau(x, y)$. This function embodies the variable-media generalization of the idea that time equals total distance over wave speed, an aspect that was crucial in the expression of backprojection for SAR. Traveltimes are important for "traveltime tomography", or matching of traveltimes for inverting a wave speed profile. Historically, they have also been the basis for Kirchhoff migration, a simplification of (reverse-time) migration.

7.1 Assumptions and vocabulary

In seismic imaging, the forward operator F is called *Born modeling*, and the adjoint/imaging operator F^* is called *migration*. F is sometimes also called *demigration*. We will see in a later section that F^* "undoes" most of F in a kinematic sense. The set of $F_s^* d_s$ indexed by the source s is called *prestack migration*, or prestack depth migration (PSDM) by geophysicists. Tellingly, they call $F^* d = \sum_s F_s^* d_s$ poststack migration.

A point x inside the Earth is said to be in the *subsurface*. Usually $x =$

(x', z) where x' are the horizontal coordinates, and z is depth. Data space is indexed by $(x_r, , x_s, t)$ where x_r, x_s are usually (but not always) at $z = 0$. Datasets are called *seismograms*. Time is usually depicted as a vertical axis, pointing *down*.

They also call the source s a *shot*. When the dataset d_s is indexed by shot s, it is called a *shot gather*, or common shot gather (CSG). Alternatively, a dataset can be organized by midpoint $x_m = \frac{x_s+x_r}{2}$ vs. half-offset $h = \frac{x_s-x_r}{2}$ — in that case it is called common midpoint gather (CMP). Since the midpoint does not generally fall on a grid, doing a CMP requires binning[1].

(!) Many physical assumptions are made to keep the algebra simple in this chapter. They are as follows:

1. We use a wave equation that models acoustic waves, rather than (visco-)elastic waves. All the waves are treated like P waves, hence mistakes will be made with the S waves, as well as mode conversion. Another consequence of using the acoustic simplification is that the medium is assumed to be isotropic, i.e., the waves do not travel at different speeds depending on the direction in which they travel. Laminated rocks are usually anisotropic. Finally, we do not model the (frequency-dependent) dissipation of energy, and dispersion, of the seismic waves.

2. Boundary conditions are omitted, corresponding to the situation of non-reflecting boundaries. This can be inaccurate in the presence of water-air or rock-air interfaces, better modeled by a Neumann condition (see chapter 1). Free boundaries corresponding to topography (or bathymetry) can be particularly hard to model properly.

3. We assume the source is known, and of the form $f_s(x, t) = \delta(x - x_s)w(t)$. In practice the source needs to be determined or calibrated, usually from a direct arrival. The assumption that the source is a scalar function of x and t in an acoustic wave equation is itself not necessarily accurate (such as in earthquakes, for instance.)

4. We do not deal with the issue of acquisition noise in data (malfunctioning detectors, ambient seismic noise, incoherent scattering off of structure that are not to be imaged, etc.).

[1] Which can be a very inaccurate operation from a numerical viewpoint, i.e., as inaccurate as its adjoint, nearest-neighbor interpolation.

7.2 Kirchhoff modeling and migration

Consider a single, fixed source at location x_s. (If there are several sources, they are handled as in the earlier section on "stacks".) We have already seen how migration F^* is computed with the so-called imaging condition in chapter 4. In that case, F^* is called *reverse-time migration*.

The "Kirchhoff" version of the forward and adjoint operators F and F^* are obtained by using the geometrical optics approximation of the Green's function, from chapter 2. Starting from the Born approximation, we obtain Kirchhoff modeling after a few lines of algebra:

$$(Fm)(x_r, t) = \int a(x_s, x)a(x, x_r)\delta''(t - \tau(x_r, x, x_s))m(x)\, dx,$$

where $\tau(x_r, x, x_s) = \tau(x_r, x) + \tau(x, x_s)$ is the three-point traveltime. The curve/surface $t = \tau(x_r, x, x_s)$ traced in x-space (model space) is called *isochrone*. It is an ellipse/ellipsoid when the background wave speed is uniform.

Passing to the adjoint in a now-familiar manner by equating $\langle d, Fm\rangle = \langle F^*d, m\rangle$, we obtain Kirchhoff migration as

$$(F^*d)(m) = \iint a(x_s, x)a(x, x_r)\delta''(t - \tau(x_r, x, x_s))d(x_r, t)\, dx_r dt.$$

The curve/surface $t = \tau(x_r, x, x_s)$ traced in (x_r, t) space (data space) is called *moveout curve/surface*. It is a hyperbola/hyperboloid when the background wave speed is uniform. Certain references call Kirchhoff migration any backprojection-style formula where either the amplitudes $a(x_s, x)$, $a(x, x_r)$ or the derivatives on the Dirac delta are absent, or both. Both F and F^*, in their "Kirchhoff" version, are generalized Radon transforms.

Historically, Kirchhoff migration (KM) has been very important because it is an explicit formula that requires solving ODEs (for τ, mostly), not PDE. Hence it is computationally much more attractive than reverse-time migration (RTM). KM is still used in optimization schemes where cheap inexact iterations are useful.

7.3 Microlocal analysis of migration

7.4 Oscillatory integrals

7.5 Exercises

1. Show the formula for Kirchhoff migration directly from the imaging condition (4.2) and the geometrical optics approximation of the Green's function.

2. Consider the imaging condition (4.8). Substitute in the geometrical optics approximation of the Green's function, and perform a stationary phase argument to justify the following two heuristics:

   - When q is generated from data u_0 (incident field only), the model update is concentrated near points x corresponding to *forward scattering*:
   $$\nabla_x \tau(x, x_r) + \nabla_x \tau(x, x_s) = 0.$$
   - When q is generated from data u_1 (primary reflections only), the model update is concentrated near points x corresponding to *specular scattering*:
   $$\nabla_x \tau(x, x_r) + \nabla_x \tau(x, x_s) \text{ conormal to the isochrone at } x.$$

   The second situation corresponds to the idea that migration "images the reflectors".

Chapter 8

Optimization

8.1 Regularization and sparsity

8.2 Dimensionality reduction techniques

One way to reduce the dimensionality of a dataset is to scramble data as $\widetilde{d} = Cd$, where

$$\widetilde{d}_{j,r}(t) = \sum_s c_{j,s} d_{r,s}(t - b_{j,s}).$$

The numbers $c_{j,s}$ and $b_{j,s}$ may be random, for instance. The point is that using fewer values of j than s may result in computational savings — a strategy sometimes called source encoding. By linearity of the wave equation, the scrambled data $\widetilde{d}$ can be seen as originating from scrambled shots, or *supershots* $\widetilde{f} = Cf$, for

$$\widetilde{f}_j(x,t) = \sum_s c_{j,s} f_s(x, t - b_{j,s}).$$

Scrambled data may be all that's available in practice, in acquisition scenarios known as simultaneous sourcing.

The adjoint operation C^* results in twice-scrambled data $D = C^*\widetilde{d}$, where

$$D_{r,s}(t) = \sum_j c_{j,s} \widetilde{d}_{j,r}(t + b_{j,s}).$$

The linearized forward model with scrambling is $\widetilde{d} = CFm$. The basic imaging operator is still the adjoint, $I_m = F^*C^*\widetilde{d}$. In addition to the

traditional incident and adjoint fields

$$u_{0,s} = Gf_s, \qquad q_s = \overline{G}d_s,$$

where G is the Green's function in the unperturbed medium, and $\overline{G}$ the time-reversed Green's function, we define the scrambled fields

$$\widetilde{u}_{0,j} = G\widetilde{f}_j, \qquad \widetilde{q}_j = G\widetilde{d}_j.$$

Also define the twice-scrambled adjoint field

$$Q_s = G(C^*\widetilde{d})_s.$$

Then

$$I_m(x) = (F^*C^*\widetilde{d})(x) = -\sum_s \int_0^T \frac{\partial^2 u_{0,s}}{\partial t^2}(x,t)\, Q_s(x,t)\, dt.$$

Another formula involving j instead of s (hence computationally more favorable) is

$$I_m(x) = -\sum_j \int_0^T \frac{\partial^2 \widetilde{u}_{0,j}}{\partial t^2}(x,t)\, \widetilde{q}_j(x,t)\, dt. \tag{8.1}$$

To show this latter formula, use $Q = C^*\widetilde{q}$, pass C^* to the rest of the integrand with $\sum_s v_s(C^*w)_s = \sum_j (Cv_j)w_j$, and combine $Cu_0 = \widetilde{u}_0$.

Scrambled data can also be used as the basis of a least-squares misfit, such as

$$\widetilde{J}(m) = \frac{1}{2}\|\widetilde{d} - C\mathcal{F}(m)\|_2^2.$$

The gradient of $\widetilde{J}$ is F^*C^* applied to the residual, hence can be computed with (8.1).

8.3 Velocity estimation and autofocus

Appendix A

Calculus of variations, functional derivatives

The calculus of variations is to multivariable calculus what functions are to vectors. It answers the question of how to differentiate with respect to functions, i.e., objects with an uncountable, infinite number of degrees of freedom. Functional calculus is used to formulate linearized forward models for imaging, as well as higher-order terms in Born series. It is also useful for finding stationary-point conditions of Lagrangians, and gradient descent directions in optimization.

Let X, Y be two function spaces endowed with norms and inner products (technically, Hilbert spaces). A *functional* ϕ is a map from X to $\mathbb{R}$. We denote its action on a function f as $\phi(f)$. An *operator* F is a map from X to Y. We denote its action on a function f as Ff.

We say that a functional ϕ is Fréchet differentiable at $f \in X$ when there exists a linear functional $A : X \mapsto \mathbb{R}$ such that

$$\lim_{h \to 0} \frac{|\phi(f+h) - \phi(f) - A(h)|}{\|h\|} = 0.$$

If this relation holds, we say that A is the *functional derivative*, or Fréchet derivative, of ϕ at f, and we denote it as

$$A = \frac{\delta \phi}{\delta f}[f].$$

It is also called the *first variation* of ϕ. It is the equivalent of the gradient in multivariable calculus. The fact that A is a map from X to $\mathbb{R}$ corresponds

to the idea that a gradient maps vectors to scalars when paired with the dot product, to form directional derivatives. If $X = \mathbb{R}^n$ and $f = (f_1, \ldots, f_n)$, we have

$$\frac{\delta\phi}{\delta f}[f](h) = \nabla\phi(f) \cdot h.$$

For this reason, it is is also fine to write $A(h) = \langle A, h\rangle$.

The differential ratio formula for $\frac{\delta\phi}{\delta f}$ is called Gâteaux derivative,

$$\frac{\delta\phi}{\delta f}[f](h) = \lim_{t\to 0} \frac{\phi(f+th) - \phi(f)}{t}, \tag{A.1}$$

which corresponds to the idea of the directional derivative in $\mathbb{R}^n$.

Examples of functional derivatives:

- $\phi(f) = \langle g, f\rangle$,
$$\frac{\delta\phi}{\delta f}[f] = g, \qquad \frac{\delta\phi}{\delta f}[f](h) = \langle g, h\rangle$$
Because ϕ is linear, $\frac{\delta\phi}{\delta f} = \phi$. Proof: $\phi(f+th) - \phi(f) = \langle g, f+th\rangle - \langle g, f\rangle = t\langle g, h\rangle$, then use (A.1).

- $\phi(f) = f(x_0)$,
$$\frac{\delta\phi}{\delta f}[f] = \delta(x - x_0), \qquad \text{(Dirac delta)}.$$
This is the special case when $g(x) = \delta(x - x_0)$. Again, $\frac{\delta\phi}{\delta f} = \phi$.

- $\phi(f) = \langle g, f^2\rangle$,
$$\frac{\delta\phi}{\delta f}[f] = 2fg.$$
Proof: $\phi(f+th) - \phi(f) = \langle g, (f+th)^2\rangle - \langle g, f\rangle = t\langle g, 2fh\rangle + O(t^2) = t\langle 2fg, h\rangle + O(t^2)$, then use (A.1).

Nonlinear operators $\mathcal{F}[f]$ can also be differentiated with respect to their input function. We say $\mathcal{F} : X \to Y$ is Fréchet differentiable when there exists a linear operator $F : X \to Y$

$$\lim_{h\to 0} \frac{\|\mathcal{F}[f+h] - \mathcal{F}[f] - Fh\|}{\|h\|} = 0.$$

F is the functional derivative of $\mathcal{F}$, and we write

$$F = \frac{\delta \mathcal{F}}{\delta f}[f].$$

We still have the difference formula

$$\frac{\delta \mathcal{F}}{\delta f}[f]h = \lim_{t \to 0} \frac{\mathcal{F}[f + th] - \mathcal{F}[f]}{t}.$$

Examples:

- $\mathcal{F}[f] = f$. Then
$$\frac{\delta \mathcal{F}}{\delta f}[f] = I,$$
the identity. Proof: $\mathcal{F}$ is linear hence equals its functional derivative. Alternatively, apply the difference formula to get $\frac{\delta \mathcal{F}}{\delta f}[f]h = h$.

- $\mathcal{F}[f] = f^2$. Then
$$\frac{\delta \mathcal{F}}{\delta f}[f] = 2f,$$
the operator of multiplication by $2f$.

Under a suitable smoothness assumption, the Fréchet Hessian of an operator F can also be defined: it takes two functions as input, and returns a function in a linear manner ("bilinear operator"). It is defined through a similar finite-difference formula

$$\langle \frac{\delta^2 \mathcal{F}}{\delta f^2}[f]h_1, h_2 \rangle = \lim_{t \to 0} \frac{\mathcal{F}[f + t(h_2 + h_1)] - \mathcal{F}[f + th_2] - \mathcal{F}[f + th_1] + \mathcal{F}[f]}{t^2}.$$

The Hessian is also called second variation of $\mathcal{F}$. For practical calculations of the Hessian, the notation $\frac{\delta^2 \mathcal{F}}{\delta f^2}$ is too cavalier. Instead, it is useful to view the Hessian as the double directional derivative

$$\frac{\delta^2 \mathcal{F}}{\delta f \delta f'}$$

in two directions f and f', and compute those derivatives one at a time. This formula is the equivalent of the mixed partial $\frac{\partial^2 f}{\partial x_i \partial x_j}$ when the two directions are x_i and x_j in n dimensions.

Functional derivatives obey all the properties of multivariable calculus, such as chain rule and derivative of a product (when all the parties are sufficiently differentiable).

Whenever in doubt when faced with calculations involving functional derivatives, keep track of free variables vs. integration variables — the equivalent of "free indices" and "summation indices" in vector calculus. For instance,

- $\frac{\delta \mathcal{F}}{\delta f}$ is like $\frac{\delta \mathcal{F}_i}{\delta f_j}$, with two free indices i and j;
- $\frac{\delta \mathcal{F}}{\delta f} h$ is like $\sum_j \frac{\delta \mathcal{F}_i}{\delta f_j} h_j$, with one free index i and one summation index j.
- $\frac{\delta^2 \mathcal{F}}{\delta f^2}$ is like $\frac{\delta^2 \mathcal{F}_i}{\delta f_j \delta f_k}$, with three free indices i, j, k.
- $\langle \frac{\delta^2 \mathcal{F}}{\delta f^2} h_1, h_2 \rangle$ is like $\sum_{j,k} \frac{\delta^2 \mathcal{F}_i}{\delta f_j \delta f_k} (h_1)_j (h_2)_k$, with one free index i and two summation indices j and k.

No free index indicates a scalar, one free index indicates a function (or a functional), two free indices indicate an operator, three indices indicate an "object that takes in two functions and returns one", etc.

Appendix B

Convex optimization: duality and certification

Let $A \in \mathbb{R}^{m \times n}$ with $m < n$, and assume that A has full row rank. Consider the primal problem

$$\min_x f(x) \quad \text{s.t.} \quad Ax = b. \qquad (P)$$

Assume that $f(x)$ is convex, and that all quantities are real. Set constraints or inequality constraints can be taken into account in this framework, with the notion of set indicator, equal to zero on the set and infinity otherwise. "Primal feasibility" refers to x obeying $Ax = b$ and $f(x) < \infty$.

Consider first the case of a smooth f. At the minimizer $x^\sharp$, the set $\{x : Ax = b\}$ should be tangent to the level lines of f, i.e., the gradient $\nabla f(x^\sharp)$ should be orthogonal to $\{x : Ax = b\}$, i.e., there should exist λ such that $A^T\lambda = \nabla f(x^\sharp)$. When f is nonsmooth, we are instead led to consider the subdifferential

$$\partial f(x) = \{\eta : f(y) \geq f(x) + \langle \eta, y - x \rangle, \forall y \in \mathbb{R}^n\}.$$

The elements of the subdifferential are called subgradients. When f is smooth, $\partial f(x)$ reduces to a single point, the gradient. The optimality condition then takes the following form.

Theorem 5. *(Generalized KKT) The point $x^\sharp$ is a minimizer of (P) if and only if there exists λ such that*

$$A^T\lambda \in \partial f(x^\sharp),$$

in other words, such that $A^T\lambda$ is a subgradient at $x^\sharp$.

Proof. The subdifferential of the indicator function of $\{x : Ax = b\}$ is $\mathrm{Ran}(A^T)$, hence the condition $0 \in \partial f(x) + \partial 1_{Ax=b}$ reduces to the existence of some $A^T\lambda$ in $\partial f(x)$. □

We call $\eta = A^T\lambda$ a certificate: its existence certifies that $x^\sharp$ is a minimizer.

The Lagrangian framework is a convenient and elegant formalism to generate such optimality conditions automatically. We call λ a Lagrangian multiplier, and form the Lagrangian as

$$\mathcal{L}(x, \lambda) = f(x) + \langle \lambda, b - Ax \rangle = f(x) - \langle \eta, x \rangle + \langle \lambda, b \rangle,$$

with $\eta = A^T\lambda$. If one can find a pair (x, λ) such that "all the partials of $\mathcal{L}$ are zero", then x is a minimizer of the primal problem. Indeed,

- $\mathcal{L}$ is smooth in λ, and $\nabla_\lambda \mathcal{L}(x, \lambda) = Ax - b$, which vanishes when the equality constraint is obeyed;
- $\partial_x \mathcal{L}(x, \lambda) = \partial_x f(x) - A^T\lambda$. Requiring that zero be in the subdifferential of $\mathcal{L}$ in x recovers the condition of the theorem.

Any λ completing the pair $(x^\sharp, \lambda)$ at optimum is itself solution of a problem called the dual. For this reason, λ is also called a dual variable and η is called a dual certificate. The dual problem helps find all the values of $\eta = A^T\lambda$ that certify $x^\sharp$ without having to solve the primal problem (P). For each λ, consider the (convex, unconstrained) problem

$$g(\lambda) = \min_x \mathcal{L}(x, \lambda).$$

It can be seen that $g(\lambda) \leq f(x^\sharp)$, and that g is concave[1]. The dual problem consists in maximizing $g(\lambda)$. To express it in terms of f, consider the convex conjugate (Legendre-Fenchel transform)

$$f^*(\eta) = \max_x \langle \eta, x \rangle - f(x) = -\min_x f(x) - \langle \eta, x \rangle.$$

[1] To show the inequality, consider that $f(x) \geq f(x) + \langle \lambda, b - Ax \rangle$ for all feasible x, since the second term vanishes. This inequality is still true when x is fixed in the left-hand side, and an unqualified minimum over x is take in the right-hand side. Hence $f(x) \geq g(\lambda)$ for all feasible x. Conclude by taking a minimum over x in the left-hand side. Next, g is concave because it is the infimum of a family of affine functions of λ. Note that $g(\lambda)$ is concave even when $f(x)$ is not convex.

Then the dual problem is

$$\max_{\lambda} -f^*(A^T\lambda) + \langle \lambda, b\rangle \qquad (D)$$

"Dual feasibility" refers to $f^*(\eta) < \infty$, so that $g(\lambda) > -\infty$. In most situations of practical interest, strong duality holds[2]: the maximum value of $g(\lambda)$ is exactly $f(x^\sharp)$. As a result, the duality gap $f(x) - g(\lambda)$ is zero at optimum.

The set of all $A^T\lambda$ such that λ is dual-optimal is exactly the set of dual certificates. This observation follows from the fact that, by definition of f^*,

$$f(x) + f^*(\eta) \geq \langle \eta, x\rangle, \qquad \text{(Fenchel's inequality).} \qquad (B.1)$$

Equality above is the statement that the duality gap is zero, which happens if and only if x is primal-optimal and η is dual-optimal[3].

Note that the set of dual certificates is in general rather large, and it is in bijection with the set of dual-optimal λ since we have assumed that A has full row rank.

Some interesting geometry underlies the equation $\eta \in \partial f(x_0)$. The vector η defines a codimension-1 hyperplane P_η of equation $\langle \eta, x - x_0\rangle = 0$. Two observations can be made about this hyperplane.

1. In the half-space $\langle \eta, x - x_0\rangle \geq 0$ we have $f(x) \geq f(x_0)$. Hence the hyperplane P_η is subtangent to (or, supporting) the level set $\{x : f(x) \leq f(x_0)\}$.

2. Since $\eta \in \mathrm{Ran}(A^T)$, we have $\langle \eta, x - x_0\rangle = 0$ as soon as x obeys the constraint $Ax = Ax_0$. Hence the hyperplane P_η contains the affine subspace $\{x : Ax = Ax_0\}$.

[2]The primal can be seen as constrained by $f(x) < \infty$. If the interior of the set of feasible x for that constraint intersects $\{x : Ax = b\}$, then we say that the constraint $f(x) < \infty$ is qualified in the sense of Slater. In that case, strong duality holds.

[3]The proof of the observation goes as follows. Assume first that λ is dual optimal, and let $\eta = A^T\lambda$. Because there is no duality gap, (B.1) holds with equality when $x = x^\sharp$. Apply the definition of convex conjugate one more time, with a new variable x:

$$f(x^\sharp) \leq f(x) - \langle \eta, x\rangle + \langle \lambda, b\rangle, \qquad \text{for all } x \in \mathbb{R}^n. \qquad (B.2)$$

Conclude $\eta \in \partial f(x^\sharp)$ by noticing that $b = Ax^\sharp$, and rearranging the terms. Conversely, assume that $\eta = A^T\lambda \in \partial f(x^\sharp)$, which implies (B.2). The inequality is still true upon taking a minimum in x, which yields $f(x^\sharp) \leq -f^*(\eta) + \langle \lambda, b\rangle = g(\lambda)$. Since $f(x^\sharp) \geq g(\lambda)$, we have equality, hence λ is an argument of $\max g(\lambda)$.

As a result, the hyperplane P_η separates the two convex sets $\{x : f(x) \leq f(x_0)\}$ and $\{x : Ax = Ax_0\}$. Since x_0 is a point in that intersection, we now also have a geometrical proof that x_0 is a minimizer.