# Waves and Imaging
# Class notes - 18.325

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# Preface

In the margins of this text we use

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

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

These notes are accompanied by computer exercises in Python, that show how to code the adjoint-state method in 1D, in a step-by-step fashion, from scratch. They are provided by Russell Hewett, as part of our software platform, the Python Seismic Imaging Toolbox (PySIT), available at http://pysit.org.

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# Chapter 1

# Wave equations

## 1.1 Physical models

### 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 $\rho_0$ and $\kappa_0$ 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 $\rho$ 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 $p_1, \rho_1, v_1$. Consider a medium at rest (\$): $p_0, \rho_0$ 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 $\rho_0$ 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 $\rho_1$ 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 $\rho_0$ 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 $\rho_0$ and $\kappa_0$ 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
$$\varepsilon = \frac{1}{2}(\nabla u + (\nabla u)^T),$$
a symmetric time-dependent tensor field.
- The stress tensor $\sigma$, also a symmetric time-dependent tensor field.

For elastic waves, the density $\rho$ 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 $\rho$, $\lambda$, and $\mu$ 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,

$$\sigma = C : \varepsilon,$$

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

These equations form a closed system when they are complemented by

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

which holds by definition of $\varepsilon$.

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

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

with

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

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

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

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 $\lambda$ and $\mu$ are also called Lamé parameters:

- $\lambda$ corresponds to longitudinal waves, also known as compressional, pressure waves (P).
- $\mu$ 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

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

and the energy inner product is

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

The elastic wave equation looks like an acoustic wave equation with "2 terms, hence 2 waves". To make this observation more precise, assume that $\lambda$ and $\mu$ 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 $\phi$ and $\psi$:

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

where $\phi$ is a scalar field and$\psi$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 $\psi'$ 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 $\psi'$, 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 $\phi$, $\psi$ 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

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

Take the divergence of this equation to conclude that (with the same decay condition at infinity as earlier), "something" is harmonic, hence zero. Therefore, each potential $\phi$ and $\psi$ solve their own scalar wave equation: one for the longitudinal waves ($\phi$) and one for the transverse waves ($\psi$). 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 $\lambda$ 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 $\lambda$ and $\mu$ are constant is a very strong one: there is a lot of physics in the coupling of $\phi$ and $\psi$ 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 $\varepsilon$ and the magnetic permeability $\mu$,
- Forcings: electric currents $j$ and electric charges $\rho$.

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

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

Maxwell's equations in a medium with possible space-varying parameters $\varepsilon$ and $\mu$ 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 $\varepsilon$ and $\mu$ 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 $\varepsilon = \varepsilon_0$, $\mu = \mu_0$. 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

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

provided

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

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

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

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

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

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

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

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

We now see that in a uniform medium, $\varepsilon$ and $\mu$ are constant and the last two terms drop, revealing a wave equation with speed

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

[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 $c_0 = 1/\sqrt{\varepsilon_0 \mu_0}$. Even when $\varepsilon$ and $\mu$ 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 $\rho_S$ for surface currents and surface charges respectively. If the two dielectrics correspond to finite parameters $\varepsilon_1, \varepsilon_2$ and $\mu_1, \mu_2$, 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 $\varepsilon = \varepsilon' + i\sigma/\omega$, where $\sigma$ is called the conductivity. All these quantities could be frequency-dependent. It is the ratio $\sigma/\varepsilon'$ that tends to infinity when the conductor is "perfect". Materials for which $\varepsilon$ 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 $\sigma/\omega$, and not just $\sigma$, 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 $\omega$ 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 $\omega$. 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 $\omega$ 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 $\lambda$ 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 $f_\omega$ 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 $\omega$ 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 $\omega$ 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 $f_\omega$ 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 $f_\omega$ 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 $\omega$ 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 $\lambda_j$ 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 $\xi$ 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

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

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 characteristic.

- 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 $\xi$ and $\eta$, here expressed in terms of $\xi$:

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

[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 $\xi$ 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 $\xi$ 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 $\xi$ differentiation. We get $u_\eta$ from $v_1$, as well as $u_{\eta\xi}, u_{\eta\xi\xi}, \ldots$ by further $\xi$ 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 $\eta$ 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 $(r, \theta, \phi)$, 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,

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}(ru) = \frac{\partial^2}{\partial r^2}(ru).$$

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[7]

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

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 $t \leq 0$.

[7]Note that the argument of $\delta$ has derivative 1 in the radial variable, hence no Jacobian is needed. We could alternatively have written an integral over the unit sphere, such as

$$u(x,t) = ct \int_{S^2} \psi(x + ct\xi) dS_\xi.$$

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, called Kirchhoff's formula[8], 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 heterogeneous 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[9] 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 heterogeneous media, explicit formulas are usually not available.

[8]Though credited to Poisson.

[9]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.

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[10] through (1.16), even as $x \in \mathbb{R}^n$ and $c$ is a function of $x$.

**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*

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

*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

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

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

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 $\Gamma$, 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 $\Gamma$.

### 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:

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

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

$$-\left[\omega^2 + c^2(x)\Delta\right] \widehat{G}(x,y;\omega) = \delta(x-y). \tag{1.19}$$

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

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

The Helmholtz Green's function is an outgoing spherical wave generated by a "point source" at $x = y$.

In the literature, the constant-medium Green's function is often encountered in the form $\frac{e^{ik\|x-y\|}}{4\pi\|x-y\|}$, without the $c^2$ in the denominator. This version of $\widehat{G}$ originates instead from the equation $-[\frac{\omega^2}{c^2} + \Delta]\widehat{G}(x,y;\omega) = \delta(x-y)$, which differs from (1.19) by an overall $c^2$ factor.

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[11]

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 $\frac{e^{\pm ik\|x-y\|}}{4\pi\|x-y\|}$ which have the same modulus and obey the same equation (1.19). 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 ($r = \|x\|$)

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

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

$$\widehat{G}(x,y,\omega) = \frac{i}{4}H_0^{(1)}(k|x-y|), \qquad k = \omega/c.$$

where $H_0^{(1)} = J_0 + iY_0$ is the Hankel function of order zero.

### 1.2.5 Reflected waves

Spatial variability in the physical parameters ($\rho, \kappa; \varepsilon, \mu; \lambda, \mu$, 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-$C^\infty$ singularities, which generate reflected waves alongside transmitted waves.

[11] 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. Their rationale for this choice is that $e^{ikx}$, in conjunction with the time convention $e^{-i\omega t}$, is a right-going wave. 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.

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

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

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

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 $\rho_1, \rho_2$ 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 $\omega$ 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

$$u(x,t) = f(x - c_1 t) + Rf(-x - c_1 t), \qquad x < 0, \tag{1.20}$$

$$u(x,t) = Tf(\frac{c_1}{c_2}(x - c_2 t)), \qquad x > 0. \tag{1.21}$$

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. One can derive the expression of $Z$ from the time-harmonic regime. The first equation (1.1) in the acoustic system reads, in the $(k,\omega)$ 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:

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

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

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

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 refraction. To obtain the $R$ and $T$ coefficients in the optical case, the procedure is as follows:

- Consider Ampère'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 $D = \varepsilon E$.

- 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 $n = \frac{c_{ref}}{c} = c_{ref}\sqrt{\varepsilon\mu}$. 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. Derive from first principles the wave equation for waves on a taut string, i.e., a string subjected to pulling tension. [Hint: assume that the tension is a vector field $T(x)$ tangent to the string. Assume that the mass density and the scalar tension (the norm of the tension vector) are both constant along the string. Consider the string as vibrating in two, not three spatial dimensions. Write conservation of momentum on an infinitesimally small piece of string. You should obtain a nonlinear PDE: finish by linearizing it with respect to the spatial derivative of the displacement.]

2. 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 $c^2(x) = \frac{\partial f}{\partial \rho}(\rho_0(x), s_0(x))$.]

3. In a 2011 episode of the TV show Mythbusters, the team tested the myth that you can better survive an underwater explosion by floating on your back than by treading water. The myth was confirmed, with data showing that the pressure resulting from a 10lb TNT explosion is much smaller at shallower depths.

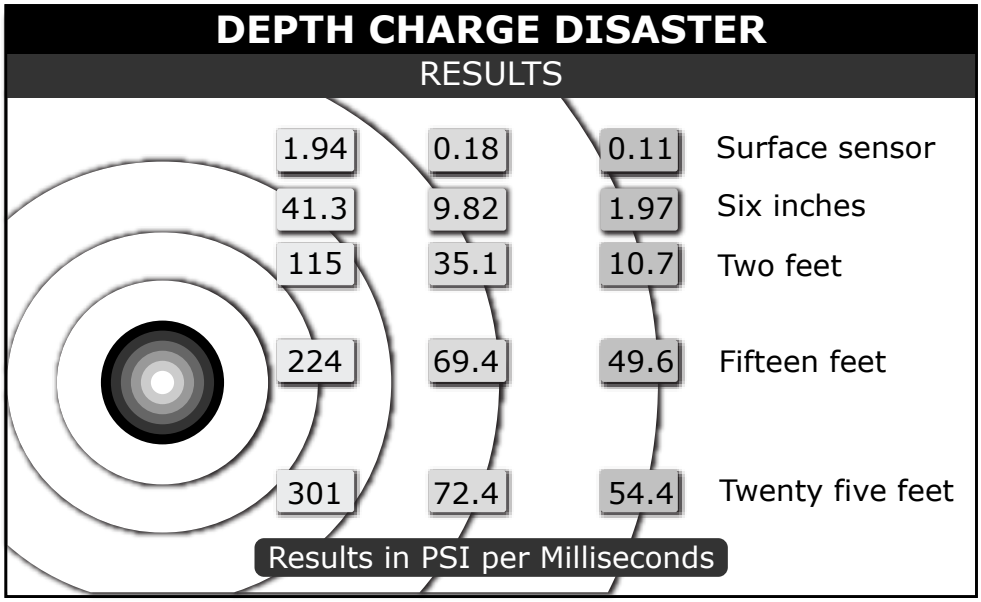


Image by MIT OpenCourseWare.

Explain this observation theoretically. [Hint: "boundary condition"]

4. 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.

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

6. Predict that elastic waves can only propagate at speeds $c_P$ or $c_S$, by studying plane wave solutions of the form $\mathbf{r}e^{i(k \cdot x - \omega t)}$ (for some fixed vector $\mathbf{r} \in \mathbb{R}^3$), for the elastic equation (1.5) with constant parameters $\rho, \lambda, \mu$.

7. 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 $f_\omega$ is a solution of the homogeneous Helmholtz equation (1.10) with constant $c$, and simplify the expres-

sion of $f_\omega$ by means of a Bessel function. [Hint: show first that $f_\omega$ is radially symmetric.]

8. 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*.

9. Consider a characteristic curve as the level set $\xi(x,t)$ =const., where $\xi$ 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 $c(x)$.

10. 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.

11. We have seen the expression of the wave equation's Green function in the $(x,t)$ and $(x,\omega)$ domains. Find the expression of the wave equation's Green function in the $(\xi,t)$ and $(\xi,\omega)$ domains, where $\xi$ is dual to $x$ and $\omega$ 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.]

12. 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.]

13. 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 (1.20, 1.21) of a wavefield scattering at a jump interface in one spatial dimension.]

14. 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.

15. 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 ($c_{ref}/c(x)$ is then the index of refraction for some reference level $c_ref$). It is a good exercise to generalize the constructions of this chapter in the case of wave equations with several physical parameters.

## 2.1 Traveltimes and Green's functions

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

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

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

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

where $a$ is some smooth amplitude function, $\tau$ 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 $\tau$ 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 $\delta''$ 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 $\tau$. It determines $\tau$ completely for $x$ in some neighborhood of $y$. Notice that $\tau$ has the units of a time.

The $\delta'$ 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 $\delta$, 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 $\omega$ 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 $\omega$ 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 $\tau$ appears in a complex exponential, it is also often called a *phase*. The same exercise of determining $a$ and $\tau$ can be done, by substituting this expression in the Helmholtz equation, with the exact same outcome as earlier. Instead of matching like derivatives of $\delta$, we now match like powers of $\omega$. The $\omega^2$ term is zero when the eikonal equation is satisfied, the $\omega$ 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 $\tau$ 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 $\Gamma$, but still in a uniform medium $c(x) = c_0$, $\tau(x)$ takes on the interpretation of the *distance function* to the curve $\Gamma$.

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 $\Gamma$. To nevertheless consider a generalized solution with kinks, mathematicians resort to the notion of viscosity solution, where the equation

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

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

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

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

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

Finally, it should be noted that

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

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

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

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

## 2.2 Rays

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

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

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

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

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

These conditions are satisfied if we specify the velocity vector as

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

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

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

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

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

which has for solution

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

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

The differential equation (2.7) for $X(t)$ is however not expressed in closed form, because it still depends on $\tau$. 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 $(X, \xi)$ are called *phase-space* variables. It is fine to speak of a curve $X(t)$ in space as a ray, although strictly speaking the ray is a curve $(X(t), \xi(t))$ in phase-space. Because of its units, $\xi$ is in this context often called the slowness vector.

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

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

from the Hamiltonian

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

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

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

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

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

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

The traveltime $\tau$ 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 $\tau$ from the eikonal equation. There is no ambiguity in specifying $\tau$ 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 $\tau_j$ 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 $\tau$ is assumed known, then this equation specifies $a(X(t))$ up to a multiplicative constant. If we wish to eliminate $\tau$ 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 $\omega$ of the underlying wave. The rate of growth is generically of the form $\omega^{1/6}$, as established by Keller in the 1950s.

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

## 2.4 Caustics

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

is block partitioned as

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

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

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

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

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

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

It is instructive to express (2.8) is ray coordinates. Without loss of generality choose the reference points $x_0 = 0$ and $\xi_0 = (1, 0)^T$. Let $x_1$ and $\xi_1$ be the coordinates of $x$ and $\xi$ along $\xi_0$, and $x_2, \xi_2$ along $\xi_0^\perp$. Consider $(y_0, \eta_0)$ the image of $(x_0, \xi_0)$ under the phase map. Let $y_1$ and $y_2$ be the coordinates of $y$ and $\eta$ along $\eta_0$, and $x_2, \xi_2$ along $\eta_0^\perp$. In other words, the coordinates labeled "1" are along the ray (longitudinal), and "2" across the ray (transversal).

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

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

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

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

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

Equation (2.9) shows that these two scenarios cannot happen simultaneously. In fact, if the variation of $y_2$ with respect to $x_2$ is zero, then the variation of $y_2$ with respect to $\xi_2$ must be maximal to compensate for it; and vice-versa. When $t$ is the first time at which either partial derivative vanishes, the caustic is a single point: we speak of a focus instead.

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

## 2.5 Exercises

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

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

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

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

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

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

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

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

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

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

7. Prove (2.8).

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

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

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

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

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

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

# 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 $\varepsilon$,

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

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

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

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):

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

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:

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

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

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

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

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

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

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

This is called a *Born series*. The proof of convergence, based on the "weak scattering" condition $\varepsilon \| G\, m_1\, \frac{\partial^2}{\partial t^2} \|_* < 1$, 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,

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

[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

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

where $\varepsilon u_1$ represent single scattering, $\varepsilon^2 u_2$ 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

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

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 $\varepsilon$ 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

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

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

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

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 $u_1 = -G m_1 \frac{\partial^2 u_0}{\partial t^2}$.

## 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 2013, 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 $M = M_0 + \varepsilon M_1$. Let $w = w_0 + \varepsilon w_1 + \ldots$ Calculations very similar to those of the previous section (a good exercise) show that

- The Lippmann-Schwinger equation is

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

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

- The Neumann series of interest is

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

  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

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

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

Notice that the condition $\varepsilon\|w_1\|_* < \|w_0\|_*$ is precisely one of weak scattering, i.e., that the primary reflected wave $\varepsilon w_1$ 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] *$\Omega$. Consider these fields for $t \in [0, T]$. Then the weak scattering condition $\varepsilon\|w_1\|_* < \|w_0\|_*$ is satisfied, hence the Born series converges, as soon as*

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

*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 $\Omega$ when its Fourier transform, as a function of $\omega$, is supported in $[-\Omega, \Omega]$.

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

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

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 $\|f'\|_\infty \le \Omega\|f\|_\infty$ for all $\Omega$-bandlimited $f$. Then

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

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

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

□

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 $\varepsilon\|w_1\|_* < \|w_0\|_*$ encodes the idea that the primary reflected field $\varepsilon w_1$ is small compared to the incident field $w_0$. It is satisfied when $\varepsilon$ is small, and when $w_1$ is not so large that it would undo the smallness of $\varepsilon$ (via the factors $\Omega T$, for instance). It turns out that

- the full scattered field $w_{sc} = w - w_0$ is also on the order of $\varepsilon\Omega T\|M_1\|_\infty$ — 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 $1 \le p \le \infty$.

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

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 $w_{sc} - \varepsilon w_1$ on the order of $\varepsilon^2$) precisely when scattering is weak ($\varepsilon w_1$ and $w_{sc}$ on the order of $\varepsilon$.)

## 3.3 Convergence of the Born series (physics)

Let us explain why the criterion $\varepsilon\Omega T < 1$ (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 $c = c_0 + \varepsilon c_1 = 1 + \varepsilon$. In one spatial dimension, $u(x,T) = f(x - cT)$. As a Taylor series in $\varepsilon$, this is

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

  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 $\Omega$, i.e., wavelength $2\pi/\Omega$. The Born approximation

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

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

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

  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 $\varepsilon\Omega T < 1$ 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 (1.20) and (1.21). The transmitted wave will undergo a shift as in the previous example, so we expect $\varepsilon\Omega T < 1$ to be sharp for it. The full reflected wave, on the other hand, is

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

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

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

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

- 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 negligible.

The Born approximation is often satisfied in the low-frequency regime (small $\Omega$), by virtue of the fact that cycle skipping is not as much of an issue. In the high-frequency regime, the heuristics for validity of the Born approximation are 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).

The second requirement is the most important one: it prohibits transmitted waves from propagating in the wrong velocity for too long. 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 chapter on seismic imaging).

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 small-wavenumber components of $m(x)$ (model velocity estimation), or when dealing with multiple scattering (internal multiples). However, note that multiple reflections from features already present in the modeling (such as ghosts due to reflections at the ocean-air interface) do not count as non-linearities.

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.

The very prevalent *least-squares* framework formulate the inverse problem as finding $m$ as the solution of the minimization problem

$$\min_m J[m], \qquad \text{where} \qquad J[m] = \frac{1}{2}\|d - \mathcal{F}[m]\|_2^2, \tag{3.10}$$

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.

In the sequel we consider iterative schemes based on the variations of $J$ at a base point $m_0$, namely the functional gradient $\frac{\delta J}{\delta m}[m_0]$, a linear functional in $m$ space; and the functional Hessian $\frac{\delta^2 J}{\delta m^2}[m_0]$, also called wave-equation Hessian, an operator (or bilinear form) in $m$ space. The appendix contains a primer on functional calculus.

Two extreme scenarios cause problems when trying to solve for $m$ as the minimizer of a functional $J$:

- The inverse problem is called *ill-posed* when there exist directions $m_1$ in which $J(m)$ has a zero curvature, or a very small curvature, in the vicinity of the solution $m^*$. Examples of such directions are the eigenvectors of the Hessian of $J$ associated to *small* eigenvalues. The curvature is then twice the eigenvalue, i.e., twice the second directional derivative in the eigen-direction. Small perturbations of the data, or of the model $\mathcal{F}$, induce modifications of $J$ that may result in large movements of its global minimum in problematic directions in the "near-nullspace" of the Hessian of $J$.

- Conversely, the inverse problem may suffer from severe non-convexity when the abundance of local minima, or local "valleys", hinders the search for the global minimum. This happens when the Hessian of $J$ alternates between having *large* positive and negative curvatures in some direction $m_1$.

Many inversion problems in high-frequency imaging suffer from some (not overwhelming) amount of ill-posedness, and can be quite non-convex. These topics will be further discussed in chapter 9.

The gradient descent method[5] applied to $J$ is simply

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

The choice of $\alpha$ is a balance between stability and speed of convergence – see two exercises at the end of the chapter. In practice, a line search for $\alpha$ is often a good idea.

The usual rules of functional calculus give the expression of $\frac{\delta J}{\delta m}$, also known as the "sensitivity kernel" of $J$ with respect to $m$.

[5] Also called Landweber iteration in this nonlinear context.

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

With some care, calculations involving functional derivatives are more efficiently done using the usual rules of calculus in $\mathbb{R}^n$. For instance, the result above is more concisely justified from

$$\begin{aligned} \langle \frac{\delta}{\delta m}\left(\frac{1}{2}\langle \mathcal{F}[m] - d, \mathcal{F}[m] - d\rangle\right), m_1\rangle &= \langle Fm_1, \mathcal{F}[m] - d\rangle \\ &= \langle F^*(\mathcal{F}[m] - d), m_1\rangle. \end{aligned}$$

The reader may still wish to use a precise system for bookkeeping the various free and dummy variables for longer calculations – see the appendix for such a system.

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

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

$$m^{(k+1)} = m^{(k)} - \left(\frac{\delta^2 J}{\delta m^2}[m^{(k)}]\right)^{-1} \frac{\delta J}{\delta m}[m^{(k)}]. \tag{3.12}$$

Here $\left(\frac{\delta^2 J}{\delta m^2}[m^{(k)}]\right)^{-1}$ is an operator: it is the inverse of the functional Hessian of $J$.

Any iterative scheme based on a local descent direction may converge to a wrong local minimum when $J$ is nonconvex. Gradient descent typically converges slowly – a significant impediment for large-scale problems. The

Gauss-Newton iteration converges faster than gradient descent in the neighborhood of a local minimum, when the Hessian of $J$ is (close to being) positive semi-definite, but may otherwise result in wrong update directions. It is in general much more complicated to set up Gauss-Newton than a gradient descent since the wave-equation Hessian is a large matrix, costly to store and costly to invert. Good practical alternatives include quasi-Newton methods such as LBFGS, which attempt to partially invert the wave-equation Hessian.

## 3.5 Exercises

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

2. Derive Born series with a multiscale expansion: write $m = m_0 + \varepsilon m_1$, $u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \ldots$, substitute in the wave equation, and equate like powers of $\varepsilon$. 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 in two different directions $m_1$, $m_1'$ to find the equation for the Hessian $\frac{\delta^2 \mathcal{F}}{\delta m_1 \delta m_1'}$, as a bilinear form of two functions $m_1$ and $m_1'$. Check that (up to a factor 2) your answer reduces to the equation for $u_2$ obtained in exercise 2 when $m_1 = m_1'$. The Hessian of $\mathcal{F}$ reappears in the next chapter as we describe accelerated descent methods for the inversion problem.

   **Solution.** A first derivative with respect to $m_1$ gives

$$\frac{\delta m}{\delta m_1} \frac{\partial^2 \mathcal{F}(m)}{\partial t^2} + \left( m \frac{\partial^2}{\partial t^2} - \Delta \right) \frac{\delta \mathcal{F}(m)}{\delta m_1} = 0.$$

   The notation $\frac{\delta m}{\delta m_1}$ means the linear form that takes a function $m_1$ and returns the operator of multiplication by $m_1$. We may also write it as

the identity $I_{m_1}$ "expecting" a trial function $m_1$. A second derivative with respect to $m_1'$ gives

$$\frac{\delta m}{\delta m_1}\frac{\partial^2}{\partial t^2}\frac{\delta \mathcal{F}(m)}{\delta m_1'} + \frac{\delta m}{\delta m_1'}\frac{\partial^2}{\partial t^2}\frac{\delta \mathcal{F}(m)}{\delta m_1} + \left(m\frac{\partial^2}{\partial t^2} - \Delta\right)\frac{\delta^2 \mathcal{F}(m)}{\delta m_1 \delta m_1'} = 0.$$

We now evaluate the result at the base point $m = m_0$, and perform the pairing with two trial functions $m_1$ and $m_1'$. Denote

$$v = \langle \frac{\delta^2 \mathcal{F}(m_0)}{\delta m_1 \delta m_1'} m_1, m_1' \rangle.$$

Then the equation for $v$ is

$$\left(m_0\frac{\partial^2}{\partial t^2} - \Delta\right) v = -m_1\frac{\partial^2 u_1'}{\partial t^2} - m_1'\frac{\partial^2 u_1}{\partial t^2},$$

where $u_1$, $u_1'$ are the respective linearized reflection fields generated by $m_1$, $m_1'$. In this formulation, the computation of $v$ requires solving four wave equations, for $v$, $u_1$, $u_1'$, and $u_0$ (which appears in the equations for $u_1$ and $u_1'$). Notice that $v = 2u_2$ when $m_1 = m_1'$.

5. Compute $\frac{\delta^2 \mathcal{F}}{\delta m^2}$ in an alternative way by polarization: find the equations for the second-order field $u_2$ when the respective model perturbations are $m_1 + m_1'$ and $m_1 - m_1'$, and take a combination of those two fields.

6. 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 $M_0 + \varepsilon M_1$). Prove the following energy estimate for the solution of (3.8):

$$E(t) \leq \left(\int_0^t \|f\|(s)\, ds\right)^2, \tag{3.13}$$

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.]

7. 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 $w - w_0 = O(\varepsilon)$, and that $w - w_0 - w_1 = O(\varepsilon^2)$.

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

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

[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

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

8. Consider the gradient descent method applied to the linear least-squares problem $\min_x \|Ax - b\|_2$. Show that

$$\alpha = \frac{1}{\|A^* A\|}$$

is a safe choice in the sense that the resulting gradient step is a contraction, i.e., the distance between successive iterates decreases monotonically.

9. Consider $J(m)$ any smooth, locally convex function of $m$.

(a) Show that the specific choice

$$\alpha = \frac{\langle \frac{\delta J}{\delta m}[m^{(k)}], \frac{\delta J}{\delta m}[m^{(k)}] \rangle}{\langle \frac{\delta J}{\delta m}[m^{(k)}], \frac{\delta J^2}{\delta m^2}[m^{(k)}] \frac{\delta J}{\delta m}[m^{(k)}] \rangle}$$

for the gradient descent method results from approximating $J$ by a quadratic function *in the direction of* $\delta J/\delta m$, near $m^{(k)}$, and finding the minimum of that quadratic function.

(b) Show that the Gauss-Newton iteration (3.12) results from approximating $J$ by a quadratic near $m^{(k)}$, and finding the minimum of that quadratic function.

10. Prove the following formula for the wave-equation Hessian $\frac{\delta^2 J}{\delta m_1 \delta m_1'}$ in terms of $F$ and its functional derivatives:

$$\frac{\delta^2 J}{\delta m_1 \delta m_1'} = F^* F + \langle \frac{\delta^2 \mathcal{F}}{\delta m_1 \delta m_1'}, \mathcal{F}[m] - d \rangle. \tag{3.14}$$

Note: $F^*F$ is called the normal operator.

**Solution.** To compute Hessians, it is important to expand the notation to keep track of the different variables, i.e., we compute $\frac{\delta^2 J}{\delta m_1 \delta m_1'}$. A first derivative gives

$$\frac{\delta J}{\delta m_1} = \langle \frac{\delta \mathcal{F}(m)}{\delta m_1}, \mathcal{F}(m) - d \rangle,$$

where the inner product bears on $\mathcal{F}$ in each factor. A second derivative gives

$$\frac{\delta^2 J}{\delta m_1 \delta m_1'} = \langle \frac{\delta \mathcal{F}(m)}{\delta m_1}, \frac{\delta \mathcal{F}(m)}{\delta m_1'} \rangle + \langle \frac{\delta^2 \mathcal{F}(m)}{\delta m_1 \delta m_1'}, \mathcal{F}(m) - d \rangle.$$

This result is then evaluated at the base point $m = m_0$, where $\frac{\delta \mathcal{F}(m_0)}{\delta m_1} = F$. The second term in the right-hand side already has the desired form. The first term in the right-hand-side, when paired with $m_1$ and $m_1'$, gives

$$\langle F m_1, F m_1' \rangle = \langle F^* F m_1, m_1' \rangle,$$

hence it can be seen as $F^*F$, turned into a bilinear form by application to $m_1$ and inner product with $m_1'$. Notice that, if we pair the whole equation with $m_1$ and $m_1'$, and evaluate at $m = m_0$, we arrive at the elegant expression.

$$\langle \frac{\delta^2 J}{\delta m_1 \delta m_1'} m_1, m_1' \rangle = \langle u_1, u_1' \rangle + \langle v, u_0 - d \rangle, \tag{3.15}$$

where $v$ was defined in the solution of an earlier exercise as

$$v = \langle \frac{\delta^2 \mathcal{F}(m_0)}{\delta m_1 \delta m_1'} m_1, m_1' \rangle.$$

11. 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 $m$, and when there is a sufficiently large number of receivers and/or sources, 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 $\varepsilon m_1$). 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 8.1.

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, resulting in what is 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 two arbitrary 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

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

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

The boundary terms over $\partial V$ 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

$$q|_{t=T}=\frac{\partial q}{\partial t}|_{t=T}=0. \tag{4.2}$$

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* in general the physical field run backward in time (because of the limited sampling at the receivers), instead, it is introduced purely out of computational convenience.

The analysis needs to be modified when boundary conditions are present. Typically, homogeneous Dirichlet and Neumann boundary conditions should the same for $u_0$ and for $q$ – a choice which will manifestly allow to cancel out the boundary terms in the reasoning above – but absorbing boundary conditions involving time derivatives need to be properly time-reversed as well. A systematic, painless way of solving the adjoint problem is to follow

the following sequence of three steps: (i) time-reverse the data $d_{\text{ext}}$ at each receiver, (ii) solve the wave equation forward in time with this new right-hand-side, and (iii) time-reverse the result at each point $x$.

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

$$(F^*d)(x) = -\int_0^T q(x,t)\frac{\partial^2 u_0}{\partial t^2}\,dt. \tag{4.3}$$

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 $d_{\text{ext}}$;

2. Use $d_{\text{ext}}$ 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 measured data, then $I_m$ is not the model $m$ that gave rise to $d$. In seismology, the imaging condition (4.3) 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 (4.3) called backprojection.

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,

$$(F^* d)(x) = -\sum_s \int_0^T q_s(x,t) \frac{\partial^2 u_{0,s}}{\partial t^2}(x,t)\, dt, \tag{4.4}$$

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

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

The sum over $s$ in the new imaging condition (4.4) 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.

## 4.2 The imaging condition in the frequency domain

We now modify the exposition to express both the adjoint-state equation and the imaging condition in the frequency ($\omega$) domain. The nugget in this section is that complex conjugation in $\omega$ 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,

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

The complex conjugate is important, now that we are in the frequency domain – though since the overall quantity is real, it does not matter which of the two integrand's factors it is placed on. As previously, we pass to the extended dataset

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

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

$$\widehat{(Fm)}(x_r,\omega) = \int \widehat{G}(x,y;\omega)m(y)\omega^2\widehat{u_0}(y,\omega)\,dy. \tag{4.5}$$

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

$$\widehat{q}(x,\omega) = \int \overline{\widehat{G}(y,x;\omega)}\widehat{d_{\text{ext}}}(y,\omega)\,dy. \tag{4.6}$$

(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

$$F^*d(y) = 2\pi\int_{\mathbb{R}} \widehat{q}(y,\omega)\omega^2\overline{\widehat{u_0}(y,\omega)}\,d\omega. \tag{4.7}$$

This equation is the same as (4.3), by Parseval's identity. Equation (4.6) is the integral version of (4.1) in the frequency domain. The complex conjugation of $\widehat{G}$ in (4.6) is the expression in the frequency domain of the fact that the adjoint equation is solved backwards in time[1]. We can alternatively interpret $\widehat{q} = \overline{G} d_{\text{ext}}$ by applying an extra conjugate, namely $\overline{\widehat{q}} = G\overline{d_{\text{ext}}}$, which can be read as the sequence of operations: (i) time-reverse $d_{\text{ext}}$, (ii) propagate it forward in time, and (iii) time-reverse the result. This is the same prescription as in the time-domain case, and offers the added advantage of not having to rethink the boundary condition for the backward equation.

The integral in $t$ in (4.3) is over $[0, T]$ because such is the support of $q\frac{\partial^2 u_0}{\partial t^2}$. The integral in $\omega$ in (4.7) 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 $\omega$.

Equation (4.7) is valuable for a few different reasons:

- It can be further simplified to highlight its geometrical content as an approximate curvilinear integral, such as explained in the next chapter;
- The integral over $\omega$ 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 9.

## 4.3 The general adjoint-state method

In this section we explain how to use the adjoint-state method to compute the first and second variations of an objective function $J[u(m)]$ in a parameter $m$, when $u$ is constrained by the equation $L(m)u = f$, where $L(m)$ is a linear operator that depends on $m$.

[1]Time reversal of any real-valued function becomes conjugation in the Fourier domain:

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

We refer to "$u$ space", "$m$ space", and "$f$ space" for the respective $L^2$ spaces containing $u$, $m$, and $f$. The first variation of $J$ is simply

$$\frac{\delta J}{\delta m} = \langle \frac{\delta J}{\delta u}, \frac{\delta u}{\delta m} \rangle_u, \tag{4.8}$$

where the inner product pairs $\delta u$ in each equation, hence acts in $u$ space. Notice that $\delta u/\delta m$ is an operator acting in $m$ space and returning a function in $u$ space[2].

If we were interested in computing the directional derivative of $J$ in some direction $m$, namely $\langle \frac{\delta J}{\delta m}, m \rangle$, then we would simply swap the $m$-space inner product with the $u$-space inner product from (4.8), and recognize that $u = \frac{\delta u}{\delta m} m$ is easily accessible by solving the linearized version of the equation $L(m)u = f$. This result is straightforward to obtain, and the adjoint-state method is not necessary.

The interesting problem is that of computing $\frac{\delta J}{\delta m}$ as a function in $m$-space. In principle, equation (4.8) is all that is needed for this purpose, except that explicitly computing the full kernel of the operator $\frac{\delta u}{\delta m}$ can be highly inefficient in comparison to the complexity of specifying the function $\frac{\delta J}{\delta m}$.

The adjoint-state method is a very good way of eliminating $\frac{\delta u}{\delta m}$ so that $\frac{\delta J}{\delta m}$ can be computed in more favorable complexity. In order to achieve this, differentiate the "state equation" $L(m)u = f$ with respect to $m$ to get

$$\frac{\delta L}{\delta m} u + L \frac{\delta u}{\delta m} = 0.$$

We see that $\frac{\delta u}{\delta m}$ can be eliminated by composition with $L$ on the left. The main idea of the adjoint-state method is that a copy of $L$ can materialize in (4.8) provided the other factor, $\frac{\delta J}{\delta u}$, is seen as the *adjoint* of $L$ applied to some field $q$,

$$L^* q = \frac{\delta J}{\delta u}, \qquad \text{(adjoint-state equation)} \tag{4.9}$$

with $q$ naturally called the adjoint field. Then,

$$\begin{aligned} \frac{\delta J}{\delta m} &= \langle L^* q, \frac{\delta u}{\delta m} \rangle_u = \langle q, L \frac{\delta u}{\delta m} \rangle_f \\ &= -\langle q, \frac{\delta L}{\delta m} u \rangle_f \qquad \text{(imaging condition)} \end{aligned} \tag{4.10}$$

[2]It relates to what we called $F = \delta\mathcal{F}/\delta m$ earlier by the operator $S$ of sampling at the receivers, via $\mathcal{F} = Su$ or $\delta\mathcal{F}/\delta m = S\delta u/\delta m$.

This latter expression is often much easier to compute than (4.8).

**Example 1.** *In the setting of section 4.1, $m$ is a function of $x$; $u$ and $f$ are functions of $(x,t)$. The state equation $L(m)u = f$ is the forward wave equation $m\partial_t^2 u - \Delta u = f$ with zero initial conditions. When we evaluate all our quantites at $m_0$, then $u$ becomes $u_0$, the incident field. The adjoint-state equation $L^*q = \frac{\delta J}{\delta u}$ is the backward wave equation $m\partial_t^2 q - \Delta q = \frac{\delta J}{\delta u}$ with zero final conditions. The least-squares cost function is $J[u] = \frac{1}{2}\|Su - d\|_2^2$ with $S$ the operator of sampling at the receivers, so that the adjoint source $\frac{\delta J}{\delta u} = S^*(Su - d)$ is the data residual extended to a function of $x$ and $t$.*

*The quantity $\frac{\delta L}{\delta m}u$ is a multiplication operator from $m$-space to $f$-space (which takes the function $m$ to the function $m\partial_t^2 u$), expressed in coordinates as*

$$(\frac{\delta L}{\delta m(y)}u)(x,t) = \delta(x-y)\,\partial_t^2 u(x,t), \qquad (x \in R^3, y \in \mathbb{R}^3.)$$

*Using the formula above, $-\langle q, \frac{\delta L}{\delta m}u\rangle_f$ becomes the usual imaging condition $-\int q(x,t)\partial_t^2 u(x,t)\,dt$.*

The adjoint-state method also allows to compute second variations. We readily compute the functional Hessian of $J$ as

$$\frac{\delta^2 J}{\delta m \delta m'} = \langle \frac{\delta u}{\delta m}, \frac{\delta^2 J}{\delta u \delta u'}\frac{\delta u'}{\delta m'}\rangle_u + \langle \frac{\delta J}{\delta u}, \frac{\delta^2 u}{\delta m \delta m'}\rangle_u,$$

where the u-space inner product pairs the $\delta u$ factors in each expression.

This Hessian is an object with two free variables[3] $m$ and $m'$. If we wish to view it as a bilinear form, and compute its action $\langle m, \frac{\delta^2 J}{\delta m \delta m'}m'\rangle_m$ on two functions $m$ and $m'$, then it suffices to pass those functions inside the $u$-space inner product to get

$$\langle u, \frac{\delta^2 J}{\delta u \delta u'}u'\rangle_u + \langle \frac{\delta J}{\delta u}, v\rangle_u.$$

The three functions $u = \frac{\delta u}{\delta m}m$, $u' = \frac{\delta u'}{\delta m'}m'$, and $v = \langle m, \frac{\delta^2 u}{\delta m \delta m'}m'\rangle$ can be computed by solving simple (linearized) equations derived from the state equation $L(m)u = f$. (See a few exercises at the end of this chapter.) The

[3]Here $m$ and $m'$ are functions, hence can be seen as independent variables, i.e., points, in a function space. Free, or unpaired variables are to functional calculus what free indices are to vector calculus: they are "open slots" available to be filled by pairing with a function/vector in an inner product.

adjoint-state method is not needed for evaluating the Hessian as a bilinear form.

On the other hand, we are generally not interested in computing the full matrix representation of $\frac{\delta^2 J}{\delta m \delta m'}$ with row index $m$ and column index $m'$ either: this object is too large to store.

The most interesting question is the computation of the action of the Hessian as an operator on a function, say $m'$. While $m'$ is paired, the variable $m$ remains free, hence the result is a function in $m$-space. This problem can be solved by the second-order adjoint-state method, which we now explain.

As earlier, we can pass $m'$ inside the $u$-space inner product to get

$$\frac{\delta^2 J}{\delta m \delta m'} m' = \langle \frac{\delta u}{\delta m}, \frac{\delta^2 J}{\delta u \delta u'} u' \rangle + \langle \frac{\delta J}{\delta u}, \frac{\delta^2 u}{\delta m \delta m'} m' \rangle, \tag{4.11}$$

with $u' = \frac{\delta u'}{\delta m'} m'$ easily computed. However, two quantities are not immediately accessible:

1. the remaining $\frac{\delta u}{\delta m}$ factor with the un-paired $m$ variable, and
2. the second-order $\frac{\delta^2 u}{\delta m \delta m'} m'$ factor.

Both quantities have two free variables $u$ and $m$, hence are too large to store, let alone compute.

The second-order factor can be handled as follows. The second variation of the equation $L(m)u = f$ is

$$\frac{\delta^2 L}{\delta m \delta m'} u + \frac{\delta L}{\delta m} \frac{\delta u}{\delta m'} + \frac{\delta L}{\delta m'} \frac{\delta u}{\delta m} + L \frac{\delta^2 u}{\delta m \delta m'} = 0.$$

We see that the factor $\frac{\delta^2 u}{\delta m \delta m'}$ can be eliminated provided $L$ is applied to it on the left. We follow the same prescription as in the first-order case, and define a *first adjoint field* $q_1$ such that

$$L^* q_1 = \frac{\delta J}{\delta u}. \qquad \text{(1st adjoint-state equation)} \tag{4.12}$$

A substitution in (4.11) reveals

$$\begin{aligned} \frac{\delta^2 J}{\delta m \delta m'} m' = \langle \frac{\delta u}{\delta m}, \frac{\delta^2 J}{\delta u \delta u'} u' \rangle_u - \langle q_1, \left( \frac{\delta L}{\delta m'} m' \right) \frac{\delta u}{\delta m} \rangle_f \\ - \langle q_1, \left( \frac{\delta^2 L}{\delta m \delta m'} m' \right) u + \frac{\delta L}{\delta m} u' \rangle_f, \end{aligned}$$

with $u' = \frac{\delta u}{\delta m'} m'$, as earlier. The term on the last row can be computed as is; all the quantities it involves are accessible. The two terms in the right-hand-side of the first row can be rewritten to isolate $\delta u/\delta m$, as

$$\langle \frac{\delta^2 J}{\delta u \delta u'} u' - \left( \frac{\delta L}{\delta m'} m' \right)^* q_1, \, \frac{\delta u}{\delta m} \rangle_u.$$

In order to eliminate $\frac{\delta u}{\delta m}$ by composing it with $L$ on the left, we are led to defining a *second adjoint-state field* $q_2$ via

$$L^* q_2 = \frac{\delta^2 J}{\delta u \delta u'} u' - \left( \frac{\delta L}{\delta m'} m' \right)^* q_1. \qquad \text{(2nd adjoint-state equation)} \quad (4.13)$$

All the quantities in the right-hand side are available. It follows that

$$\langle L^* q_2, \frac{\delta u}{\delta m} \rangle_u = \langle q_2, L \frac{\delta u}{\delta m} \rangle = -\langle q_2, \frac{\delta L}{\delta m} u \rangle_f.$$

Gathering all the terms, we have

$$\frac{\delta^2 J}{\delta m \delta m'} m' = -\langle q_2, \frac{\delta L}{\delta m} u \rangle_f - \langle q_1, \left( \frac{\delta^2 L}{\delta m \delta m'} m' \right) u + \frac{\delta L}{\delta m} u' \rangle_f,$$

with $q_1$ obeying (4.12) and $q_2$ obeying (4.13).

**Example 2.** *In the setting of section 4.1, call the base model $m = m_0$ and the model perturbation $m' = m_1$, so that $u' = \frac{\delta u}{\delta m}[m_0]m'$ is the solution $u_1$ of the linearized wave equation $m_0 \partial_t^2 u_1 - \Delta u_1 = -m_1 \partial_t^2 u_0$ with $u_0 = L(m_0)u_0 = f$ as previously. The first variation $\frac{\delta L}{\delta m}$ is the same as explained earlier, while the second variation $\frac{\delta^2 L}{\delta m \delta m'}$ vanishes since the wave equation is linear in $m$. Thus if we let $H = \frac{\delta^2 J}{\delta m \delta m'}$ for the Hessian of $J$ as an operator in $m$-space, we get*

$$H m_1 = -\int q_2(x,t) \partial_t^2 u_0(x,t) \, dt - \int q_1(x,t) \partial_t^2 u_1(x,t) \, dt.$$

*The first adjoint field is the same as in the previous example, namely $q_1$ solves the backward wave equation*

$$m_0 \partial_t^2 q_1 - \Delta q_1 = S^*(S u_0 - d), \qquad \textit{zero f.c.}$$

*To get the equation for $q_2$, notice that $\frac{\delta^2 J}{\delta u \delta u'} = S^* S$ and $\left( \frac{\delta L}{\delta m'} m_1 \right)^* = \frac{\delta L}{\delta m'} m_1 = m_1 \partial_t^2$. Hence $q_2$ solves the backward wave equation*

$$m_0 \partial_t^2 q_2 - \Delta q_2 = S^* S u_1 - m_1 \partial_t^2 q_1, \qquad \textit{zero f.c.}$$

*Note that the formulas (3.14) (3.15) for $H$ that we derived in an exercise in the previous chapter are still valid, but they do not directly allow the computation of $H$ as an operator acting in $m$-space. The approximation $H \simeq F^*F$ obtained by neglecting the last term in (3.14) is recovered in the context of second-order adjoints by letting $q_1 = 0$.*

## 4.4 The adjoint state as a Lagrange multiplier

The adjoint field $q$ was introduced in a somewhat opportunistic and artificial way in earlier sections. 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 the constraint. The problem is the same as in the previous section, namely to compute the functional gradient of $J[u(m)]$ with respect to $m$ – and the resulting expression is the same as previously – but we show how the Lagrangian construction offers a new way of interpreting it.

Instead of considering $J[u(m)]$ as a functional to minimize on $m$, we now view $J$ as a function of $u$ only, and accommodate the constraint $L(m)u = f$ by pairing it with a function $q$ in $f$-space in order to form the so-called Lagrangian[4]

$$\mathcal{L}[u, m, q] = J[u] - \langle q, L(m)u - f \rangle_f.$$

The function $q$ is called Lagrange multiplier in this context, and is arbitrary for the time being. 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 the desired quantity, namely

$$\frac{d}{dm} J[u(m)] = \langle \frac{\delta \mathcal{L}}{\delta u}, \frac{\delta u}{\delta m} \rangle + \frac{\delta \mathcal{L}}{\delta m}. \tag{4.14}$$

The partials of $\mathcal{L}$ are computed as

- $\frac{\delta \mathcal{L}}{\delta u} = \frac{\delta J}{\delta u} - L^*q$, since $\langle q, Lu \rangle_f = \langle L^*q, u \rangle_u$,
- $\frac{\delta \mathcal{L}}{\delta m} = -\langle q, \frac{\delta L}{\delta m} u \rangle_f$,
- $\frac{\delta \mathcal{L}}{\delta q} = L(m)u - f$.

[4] We reserve the letter $\mathcal{L}$ for the Lagrangian and $L$ for the state equation.

In convex optimization, the traditional role of the Lagrangian is that putting to zero its partials[5] is convenient way of deriving the optimality conditions that hold at critical points, both for the primal and the dual problems. In particular, if the partials of $\mathcal{L}$ are zero at $(u, m, q)$, then $m$ is a critical point of $J[u(m)]$.

The way we make use of the Lagrangian in this section is different, because we aim to derive the expression of $\frac{d}{dm}J[u(m)]$ *away from critical points*. In particular, we are not going to require $\frac{\delta\mathcal{L}}{\delta m}$ to be zero. Still, we find it advantageous to put $\frac{\delta\mathcal{L}}{\delta u} = 0$ as a convenient choice to help simplify the expression of the gradient of $J$. Indeed, in that case we recover the imaging condition (4.10) from

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

It is always possible to achieve $\frac{\delta\mathcal{L}}{\delta u} = 0$, by defining $q$ to be the solution of $L^*q = \frac{\delta J}{\delta u}$, the adjoint-state equation (4.9). Note that putting $\frac{\delta\mathcal{L}}{\delta q} = 0$ recovers the state equation $L(m)u = f$.

## 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 $d - u_0 \simeq \varepsilon u_1$. Invert for $m_1$ by solving the system $u_1 = Fm_1$, i.e., $m_1 = F^{-1}u_1$. Then form $m = m_0 + \varepsilon m_1$.*

2. Consider the forward wave equation for $u_0$ in one spatial dimension with an absorbing boundary condition of the form $(\frac{1}{c(0)}\partial_t - \partial_x)u(0) = 0$ at the left endpoint $x = 0$ of the interval $[0, 1]$. Assume that $c(x)$ is locally uniform and equal to $c(0)$ in a neighborhood of $x = 0$.

[5] Or letting 0 be a subgradient of $\mathcal{L}$ in the non-smooth case.

(a) Argue why this choice of boundary condition accommodates left-going waves, but not right-going waves.

(b) Find the corresponding boundary condition for the adjoint-state equation on the backwards field $q$.

3. *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-hand side.]

4. *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 $S^*$. Note that when the linearized forward model $F$ has $S$ as its last operation, then the imaging operator $F^*$ has $S^*$ as its first operation. 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.

5. Repeat the general adjoint-state theory by assuming a possibly nonlinear state equation of the form $L(m, u) = f$.

# 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 $\varepsilon u_1$, and $u_1 = Fm_1$. This disregards multiple scattering. In the sequel we will write $\varepsilon = 1$ 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 $m(x) = m_0(x) + \varepsilon m_1(x)$ is *constant in time*, with $m_0$ *constant in time and space*. This disregards moving scatterers. As mentioned earlier, we put $\varepsilon = 1$. 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 occasionally made for convenience, but can easily be removed if necessary:

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.

7. *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.

8. *Flat topography*: the scatterers are located at elevation $z = 0$.

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 $\omega_0$ is the *carrier frequency* and $\Delta\omega$ is the *bandwidth*. We speak of *wideband* acquisition when $\Delta\omega$ is a large fraction of $\omega_0$. As usual, $\omega = 2\pi\nu$ where $\nu$ 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 $\omega$ 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 (4.5), 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

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

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 (!)

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

In the sequel we assume $h = 0$ for simplicity. We also abuse notations slightly (!) and write $A(x,s,\omega)$ for the amplitude.

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 $\omega$ 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

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

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 $(s,\omega)$ rather than the model variable $x$.

[1]It could be handy to introduce a multiplicative factor $2\pi$ 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

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

Assume for the moment that $p(t) = \delta(t)$; 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 $t$. In practice $p$ is 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, as we will see.

The phase $-2ik|x-\gamma(s)|$ needs no modification: it is already "kinematically correct" (for deep reasons that will be expanded on at length in the chapter on microlocal analysis). 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

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

[2] $B$ for filtered Backprojection, or for Gregory Beylkin, who was the first to propose it in 1984.

with

$$K(x,y) = \iint_{\mathcal{M}} e^{-2ik|x-\gamma(s)|+2ik|y-\gamma(s)|} Q(x,s,\omega) A(y,s,\omega)\, ds d\omega. \tag{5.3}$$

The integral runs over the so-called data manifold $\mathcal{M}$. We wish to choose $Q$ so that $BF$ is as close to the identity as possible, i.e.,

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

This can be done by reducing the oscillatory integral in (5.3) to an integral of the form

$$\frac{1}{(2\pi)^2} \int e^{i(x-y)\cdot\xi}\, d\xi,$$

which, as we know, equals $\delta(y-x)$ if the integral is taken over $\mathbb{R}^2$. The integral will turn out to be over a bounded set, the characterization of which is linked to the question of resolution as explained in the next section, but the heuristic that we want to approach $\delta(y-x)$ remains relevant.

As the integral in (5.3) is in data space $(s,\omega)$, we define $\xi \in \mathbb{R}^2$ as the result of an as-yet undetermined change of variables

$$(s,\omega) \mapsto \xi = \Xi(s,\omega;x).$$

($\xi$ is xi, $\Xi$ is capital xi.) The additional dependence on $x$ indicates that the change of variables will be different for each $x$.

To find $\Xi$, we need to introduce some notations. We follow Borden-Cheney [**?**] closely. Denote the range vector by

$$R_{y,s} = \gamma(s) - y_T$$

For reference, its partials are

$$\frac{\partial R_{y,s}}{\partial s} = \dot\gamma(s),$$

$$\nabla_y R_{y,s} = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} = -P_2.$$

We understand both $R_{y,s}$ and $\frac{\partial R_{y,s}}{\partial s}$ a column 3-vectors in a matrix context. The modification to deal with a nonzero elevation $h(x_1,x_2)$ in $x_T$ is simple. Then

$$\frac{\partial}{\partial s}|R_{y,s}| = \left(\frac{\partial R_{y,s}}{\partial s}\right)^T \frac{R_{y,s}}{|R_{y,s}|} = \dot\gamma(s)\cdot\widehat{R_{y,s}},$$

$$\nabla_y |R_{y,s}| = \left( \frac{\partial R_{y,s}}{\partial y} \right)^T \frac{R_{y,s}}{|R_{y,s}|} = P_2^T \widehat{R_{y,s}},$$

where $\widehat{R_{y,s}}$ is the unit range vector. The operation of pre-multiplying a column 3-vector by $P_2^T$ corresponds to extraction of the first two components of the vector. (Recall that $x$ and $y$ are coordinates in two dimensions, while their physical realizations $x_T$ and $y_T$ have a zero third component.)

With the partial derivatives in hand we can now apply the principle of stationary phase (see appendix C) to the integral (5.3). The coordinates $x$ and $y$ are fixed when considering the phase

$$\phi(s, \omega) = 2k(|R_{y,s}| - |R_{x.s}|).$$

We can introduce a large parameter $\alpha$ in the phase by normalizing frequencies as $\omega = \alpha\omega'$ (recall $k = \omega/c$); the higher the frequency band of the pulse the better the approximation from stationary phase asymptotics. The critical points occur when

$$\frac{\partial \phi}{\partial \omega} = \frac{2}{c}(|R_{y,s}| - |R_{x.s}|) = 0,$$

$$\frac{\partial \phi}{\partial s} = 2k\, \dot{\gamma}(s) \cdot (\widehat{R_{y,s}} - \widehat{R_{x,s}}) = 0.$$

The Hessian matrix is singular, which seemingly precludes a direct application of lemma 5 in appendix 4, but the second example following the lemma shows the trick needed to remedy the situation: use a trial function $f(y)$ and extend the integration variables to also include $y$. Henceforth we denote the phase as $\phi(s, \omega, y)$ to stress the extra dependence on $y$.

The critical points occur when 1) the *ranges* are equal, and 2) the *down-range velocities* are equal. For fixed $x$, the first condition can be visualized in three-dimensional $y_T$-space as a sphere centered about $\gamma(s)$, and passing through $x_T$. The second condition corresponds to a cone with symmetry axis along the tangent vector $\dot{\gamma}(s)$ to the trajectory, and with the precise opening angle that ensures that $x_T$ belongs to the cone. Thirdly, we have $y_T = (y_1, y_2, 0)$, so an additional intersection with the horizontal plane $z = 0$ should be taken. The intersection of the sphere, the cone, and the plane, consists of two points: $y_T = x_T$, and $y_T = x_{T,\text{mirr}}$, the mirror image of $x_T$ about the local flight plane (the vertical plane containing $\dot{\gamma}(s)$). In practice, the antenna beam pattern "looks to one side", so that $A(x, s, \omega) \simeq 0$ for $x$ on the "uninteresting" side of the flight path, therefore the presence of $x_{T,\text{mirr}}$

can be ignored. (If not, the consequence would be that SAR images would be symmetric about the flight plane.)

With the critical point essentially unique and at $y = x$, we can invoke stationary phase to claim that the main contribution to the integral is due (!) to points $y$ near $x$. This allows to simplify the integral (5.3) in two ways: 1) the amplitude $A(y, s, \omega)$ is smooth enough in $y$ that we can approximate it by $A(x, s, \omega)$, and 2) the phase factor can be approximated as locally linear in $y - x$, as

$$\phi(s, \omega, y) = 2k(|R_{y,s}| - |R_{x.s}|) \simeq (y - x) \cdot \xi.$$

A multivariable Taylor expansion reveals that $\xi$ can be chosen as the $y$-gradient of the phase, evaluated at $x$:

$$\xi = \Xi(x, \omega; x) = \nabla_y \phi(s, \omega, y)|_{y=x} = 2kP_2^T \widehat{R_{x,s}}.$$

We have therefore reduced the expression of $K(y, x)$ to

$$K(x, y) \simeq \int_{\mathcal{M}} e^{i(y-x)\cdot \Xi(s,\omega;x)} Q(x, s, \omega) A(x, s, \omega)\, ds d\omega.$$

Changing from $(s, \omega)$ to $\xi$ variables, and with a reasonable abuse of notation in the arguments of the amplitudes, we get

$$K(x, y) \simeq \int e^{i(y-x)\cdot \xi} Q(x, \xi) A(x, \xi)\, |\frac{\partial(s, \omega)}{\partial \xi}|\, d\xi.$$

The Jacobian $J = |\frac{\partial(s,\omega)}{\partial \xi}|$ of the change of variables goes by the name *Beylkin determinant*.

The proper choise of $Q$ that will make this integral close to $\int e^{i(y-x)\cdot\xi}\, d\xi$ is now clear: we should take

$$Q(x, \xi) = \frac{1}{A(x, \xi)|\frac{\partial(s,\omega)}{\partial \xi}|} \chi(x, \xi), \tag{5.4}$$

(!) for some adequate cutoff $\chi(x, \xi)$ to prevent division by small numbers. The presence of $\chi$ owes partly to the fact that $A$ can be small, but also partly (and mostly) to the fact that the data variables $(s, \omega)$ are limited to the data manifold $\mathcal{M}$. The image of $\mathcal{M}$ in the $\xi$ domain is now an $x$-dependent set that we may denote $\Xi(\mathcal{M}; x)$. The cutoff $\chi(x, \xi)$ essentially indicates this set in the $\xi$ variable, in a smooth way so as to avoid unwanted ringing artifacts.

The conclusion is that, when $Q$ is given by (5.4), the filtered backprojection operator $B$ acts as an approximate inverse of $F$, and the kernel of $BF$ is well modeled by the approximate identity

$$K(x,y) \simeq \int_{\Xi(\mathcal{M};x)} e^{i(y-x)\cdot\xi}\, d\xi.$$

## 5.4 Resolution

See Borden-Cheney chapter 9.

(...)

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

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

## 5.5 Exercises

1. Prove (5.2) in an alternative fashion by substituting in the far-field approximation of $G$ in the imaging condition (4.7).

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 $\theta$ (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 $\theta$ 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 $\omega$.)

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

- Take a Fourier transform to pass from $t$ to $\omega$;
- Multiply by $\omega$;
- Take an inverse Fourier transform from $\omega$ 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.)

[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.

## 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 $\theta$ and dependent variable $t$, and wavelength $2\pi$.)

2. In this problem set we will form an image from a fan-beam CT dataset. (Courtesy Frank Natterer)

   Download the data set at `http://math.mit.edu/icg/ct.mat`

   and load it in MATLAB® with `load ct.mat`

   The array $g$ is a sinogram. It has 513 rows, corresponding to uniformly sampled offsets $t$, and 360 columns, corresponding to uniform, all-around angular sampling with 1-degree steps in $\theta$. The acquisition is fan-beam: a transformation is needed to recover the parallel-beam geometry. The fan-beam geometry manifests itself in that the angle depends on the offset $t$ in a linear fashion. Instead of being just $\theta$, it is ($1 \leq t \leq 513$ is the row index)

   $$\theta + \frac{t - 257}{256}\alpha,$$

   with

   $$\sin\alpha = \frac{1}{2.87}.$$

   Imaging from a parallel-beam sinogram is done by filtered backprojection. Filtering is multiplication by $\omega$ in the $\omega$ domain dual to the offset $t$. Backprojection of a sinogram $g(t, \theta)$ is

   $$I(x) = \sum_{\theta} g(x \cdot \mathbf{e}_\theta, \theta),$$

   where $\mathbf{e}_\theta$ is $(\cos\theta, \sin\theta)^T$. Form the image on a grid which has at least 100 by 100 grid points (preferably 200 by 200). You will need an interpolation routine since $x \cdot \mathbf{e}_\theta$ may not be an integer; piecewise linear interpolation is accurate enough (`interp1` in MATLAB).

   In your writeup, show your best image, your code, and write no more than one page to explain your choices.

# 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. They call the sum over $s$ in $F^* d = \sum_s F_s^* d_s$ a postmigration stack (not 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 also 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 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. We assume constant-density (single-parameter) acoustics.

3. 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.

4. 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.)

5. Data are assumed to be point samples of the solution of the wave equation, rather than filtered versions thereof (both in space and time).

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

Typically, filtered versions of pressure disturbances are measured by microphones.

6. 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.).

## 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 $\tau$, 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 Depth extrapolation

## 7.4 Extended modeling

## 7.5 Exercises

1. Show the formula for Kirchhoff migration directly from the imaging condition (4.3) and the geometrical optics approximation of the Green's function.

2. Predict the recorded arrival time, for fixed $x_s$ and as a function of $x_r$ at the surface, of the wave that undergoes a single reflction off a horizontal reflector at depth $z$. Assume a constant background speed $c_0$.

# Chapter 8

# Microlocal analysis of imaging

In this chapter we consider that the receiver and source positions $(x_r, x_s)$ are restricted to a vector subspace $\Omega \subset \mathbb{R}^6$, such as $\mathbb{R}^2 \times \mathbb{R}^2$ in the simple case when $x_{r,3} = x_{s,3} = 0$. We otherwise let $x_r$ and $x_s$ range over a continuum of values within $\Omega$, which allows us to take Fourier transforms of distributions of $x_r$ and $x_s$ within $\Omega$. We call $\Omega$ the *acquisition manifold*, though in the sequel it will be a vector subspace for simplicity[1]. (!)

## 8.1 Preservation of the wavefront set

In this section we show that, in simple situations, the operators $F$ and $F^*$ defined earlier have inverse kinematic behaviors, in the sense that the respective mappings of singularities that they induce are inverses of one another.

The microlocal analysis of $F$ and $F^*$ hinges on the mathematical notion of wavefront set that we now introduce. We start by describing the characterization of functions with (or without) singularities.

Nonsingular functions are infinitely differentiable, hence have Fourier transforms that decay "super-algebraically".

**Lemma 1.** *Let $u \in C_0^\infty(\mathbb{R}^n)$. Then, for all $N > 0$,*

$$|\widehat{u}(k)| \leq C_N (1 + |k|^2)^{-N}.$$

[1]The Fourier transform can still be defined for functions on general manifolds, but this involves patches, a partition of unity, and many distractions that we prefer to avoid here. The microlocal theory presented here carries over mostly unchanged to the manifold setting.

*Proof.* In the Fourier integral defining $\widehat{u}(k)$, insert $N$ copies of the differential operator $L = \frac{I-\Delta_x}{1+|k|^2}$ by means of the identity $e^{ix\cdot k} = L^N e^{ix\cdot k}$. Integrate by parts, pull out the $(1+|k|^2)^{-N}$ factor, and conclude by boundedness of $u(x)$ and all its derivatives. □

A singularity occurs whenever the function is not locally $C^\infty$.

**Definition 2.** *Let $u \in \mathcal{S}'(\mathbb{R}^n)$, the space of tempered distributions on $\mathbb{R}^n$. We define the singular support of $u$ as*

$$\textit{sing supp}(u) = \{x \in \mathbb{R}^n : \textit{there does not exist an open}$$

$$\textit{neighborhood } V \textit{ of } x \textit{ such that } u \in C^\infty(V)\}.$$

In addition to recording where the function is singular, we also want to record the *direction* in which it is singular. This idea gives rise to the notion of wavefront set, that we now build up to.

"Direction of singularity" is associated to lack of decay of the Fourier transform in the same direction. For this purpose it is useful to consider sets invariant under rescaling, i.e., cones.

**Definition 3.** *A set $X$ is said to be a conic neighborhood of a set $Y \subset \mathbb{R}^n$ if*

- *$X$ is open;*
- *$Y \subset X$;*
- *$\xi \in X$ implies $\lambda\xi \in X$ for all $\lambda > 0$.*

**Definition 4.** *The singular cone of a tempered distribution $u \in \mathcal{S}'(\mathbb{R}^n)$ is the set*

$$\Gamma(u) = \{\eta \in \mathbb{R}^n \backslash \{0\} : \textit{there does not exist a conic}$$

$$\textit{neighborhood } W \textit{ of } \eta \textit{ such that for } \xi \in W,$$

$$|\widehat{u}(k)| \leq C_N(1+|k|^2)^{-N}, \qquad \textit{for all } N > 0.\}$$

The intuition is that $\Gamma(u)$ records the set of directions $\xi$ in which the Fourier transform of $u$ decays slowly. The reason for formulating the definition in negative terms is that we want the resulting cone to be closed, i.e., isolated directions in which the Fourier transform would accidentally decay quickly, while decay is otherwise slow along an open set of nearby directions, do not count.

The construction of $\Gamma(u)$ is global – a direction is labeled singular without regard to the locations $x$ where there are singularities that may have contributed to the direction being labeled singular. To go further we need to localize the construction.

**Lemma 2.** *Let $\phi \in C_0^\infty(\mathbb{R}^n)$ and $u \in \mathcal{S}'(\mathbb{R}^n)$. Then $\Gamma(\phi u) \subset \Gamma(u)$.*

**Definition 5.** *Let $x \in X \subset \mathbb{R}^n$. We call singular fiber at $x$ the set*

$$\Gamma_x(u) = \{\bigcap_\phi \Gamma(\phi u) : \phi \in C_0^\infty(X), \phi(x) \neq 0\}.$$

The idea of this definition is that we localize $u$ by means of multiplication with a smooth function $\phi$ of arbitrarily small support, then consider the smallest resulting singular cone. The definition can equivalently be formulated by means of a family of smooth indicators whose support converges toward the singleton $\{x\}$ in the sense of sets:

$$\Gamma_x(u) = \{\lim_{j\to\infty} \Gamma(\phi_j u) : \phi_j \in C_0^\infty(X), \phi_j(x) \neq 0, \operatorname{supp}\phi_j \to \{x\}\}.$$

Note that $\Gamma_x(u)$ is empty if $u$ is smooth ($C^\infty$) at $x$.

The wavefront set then consists of the union of the singular cones, taken as fibers over the singular support.

**Definition 6.** *Let $u \in \mathcal{S}'(\mathbb{R}^n)$. The wavefront set of $u$ is the set*

$$WF(u) = \{(x,\xi) \in \mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\}) : \xi \in \Gamma_x(u)\}.$$

*The set $\mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\})$ is also abbreviated as $T^*\mathbb{R}^n\backslash 0$.*

Because this definition localizes the singularites of $u$ both in position and in direction, it is the basis for *microlocal* analysis.

In this context, the product $\mathbb{R}^n \times \mathbb{R}^n$ is the cotangent bundle of $\mathbb{R}^n$, and denoted $T^*\mathbb{R}^n$. The reason for viewing each singular cones (each fiber) as a subset of the cotangent space at $x$ rather than the tangent space at $x$ will be apparent in the sequel as we study the behavior of $WF(u)$ under change of variables.

Notice that the projection of $WF(u)$ on the first $\mathbb{R}^n$ (relative to $x$) is the singular support sing supp$(u)$, while the projection of $WF(u)$ on the second $\mathbb{R}^n$ (relative to $\xi$) is the singular cone $\Gamma(u)$.

In the context of imaging, we will use the same notation as introduced above and let $\xi$ be the wave-vector variable, dual to position $x \in \mathbb{R}^n$ in model space. Usually, $n = 3$. Data space is indexed by the base variables $(x_s, x_r, t) \in \Omega \times \mathbb{R} \equiv \mathbb{R}^{n_d}$, usually with $n_d = 5$. We denote by $(\xi_r, \xi_s, \omega)$ the corresponding dual variables, i.e., the independent variables of the Fourier transform of a function of $(x_s, x_r, t)$. The wavefront set of a distribution $d(x_r, x_s, t)$ in $\mathbb{R}^{n_d}$ is then

$$WF(d) = \{(x_r, x_s, t; \xi_r, \xi_s, \omega) \in T^*\mathbb{R}^{n_d} \backslash 0 : (\xi_r, \xi_s, \omega) \in \Gamma_{(x_r, x_s, t)}(d)\}.$$

We will also consider wavefront sets of functions in the product space $\mathbb{R}^n \times \mathbb{R}^{n_d} = \mathbb{R}^{n+n_d}$ of model space and data space, such as the distributional integral kernel $K$ of $F$. We have

$$WF(K) = \{(x_r, x_s, t, x; \xi_r, \xi_s, \omega, \xi) \in T^*\mathbb{R}^{n+n_d} \backslash 0 : (\xi_r, \xi_s, \omega, \xi) \in \Gamma_{(x_r, x_s, t, x)}(K)\}. \tag{8.1}$$

In a product space, a wavefront set has the additional interpretation of being a *relation*. The role of $WF(K)$, where $K$ is the kernel of $F$, is that it provides a way of predicting $WF(Fm_1)$ from $WF(m_1)$ using a simple composition rule.

In order to see $WF(K)$ as a relation, however, two minor modifications need to be made to the definition (8.1). First, the variables first need to be re-arranged as $((x, \xi), (x_r, x_s, t; \xi_r, \xi_s, \omega))$, in order to be seen as elements of the product space $T^*\mathbb{R}^n \times T^*\mathbb{R}^{n_d}$. Second, the sign of the first co-variable $\xi$ needs to be flipped, so that we instead consider the "wavefront prime" $WF'(K)$. In short,

$$((x, -\xi), (x_r, x_s, t; \xi_r, \xi_s, \omega)) \in WF'(k) \quad \Leftrightarrow \quad (x_r, x_s, t, x; \xi_r, \xi_s, \omega, \xi) \in WF(K)$$

We call $WF'(K)$ the wavefront relation of the operator whose kernel is $K$.

More generally, the operations that define relations are as follows.

- The composition of a relation $C \subset X \times Y$ and a set $S \subset X$ is the set

$$C \circ S = \{y \in Y : \text{ there exists } x \in S \text{ such that } (x, y) \in C\}.$$

- The composition of two relations $C \subset X \times Y$ and $C' \in Y \times Z$ is the relation

$$C \circ C' = \{(x, z) \in X \times Z : \text{ there exists } y \in Y$$
$$\text{such that } (x, y) \in C, (y, z) \in C'\}.$$

- The transposition of a relation $C$ is the relation

$$C^T = \{(y, x) \in Y \times X : (x, y) \in C\}.$$

We call identity relation on $X$ the set $I = \{(x, x) : x \in X\}$. Note that all our relations are "canonical" in the sense that they preserve areas in a generalized sense[2]. We will not purse this topic further here.

The high-level idea is that we would like to write $WF(Fm_1) \subset WF'(K) \circ WF(m_1)$, but this identity is not always true. The obstruction is that elements of $WF'(K)$ are in $T^*\mathbb{R}^{n \times n_d} \backslash 0$, which is in general a larger set than $(T^*\mathbb{R}^n \backslash 0) \times (T^*\mathbb{R}^{n_d} \backslash 0)$. Hence the interpretation of $WF'(K)$ as a relation runs into trouble with those elements such that either $\xi = 0$ but $(\xi_s, \xi_r, \omega) \neq 0$; or conversely $(\xi_s, \xi_r, \omega) = 0$ but $\xi \neq 0$. We say such elements are part of the *zero sections* of $WF'(K)$. In the sequel, we simply treat the case when those zero sections are empty.

The proper way of composing wavefront sets is the following celebrated theorem, due to Hörmander.

**Theorem 5.** *Let $K$ be the distributional kernel of an operator $F$, with wavefront set (8.1). Assume that the elements of $WF'(K)$ obey*

$$\xi = 0 \quad \Leftrightarrow \quad (\xi_s, \xi_r, \omega) = 0,$$

*i.e., $WF'(K)$ does not have zero sections. Then, for all $m_1$ in the domain of $F$,*

$$WF(Fm_1) \subset WF'(K) \circ WF(m_1).$$

The physical significance of the zero sections will be made clear below when we compute $WF(K)$ for the imaging problem.

We can now consider the microlocal properties of the imaging operator $F^*$. Its kernel is simply $K^T$, the transpose of the kernel $K$ of $F$. In turn, the relation $WF'(K^T)$ is simply the transpose of $WF'(K)$ seen as a relation in the product space $T^*\mathbb{R}^n \times T^*\mathbb{R}^{n_d}$,

$$WF'(K^T) = (WF'(K))^T.$$

[2]Namely, they are Lagrangian manifolds: the second fundamental symplectic form vanishes when restricted to canonical relations. The precaution of flipping the sign of the first covariable $\xi$ in the definition of $WF'(K)$ translates into the fact that, in variables $((x, \xi), (y, \eta))$, it is $dx \wedge d\xi - dy \wedge d\eta$ that vanishes when restricted to the relation, and not $dx \wedge d\xi + dy \wedge d\eta$.

Our interest is in whether the normal operator $F^*F$ preserves the singularities of the function $m_1$ it is applied to, i.e., whether imaging "places" singularities of the model perturbation at the right location from the knowledge of the linearized data $Fm_1$. To study the mapping of singularities of the normal operator $F^*F$, we are led to the composition

$$WF(F^*Fm_1) \subset (WF'(K))^T \circ WF'(K) \circ WF(m_1).$$

up to the same precaution involving zero-sections as above. The question is now whether the transpose relation can be considered an inverse, i.e., whether $(WF'(K))^T \circ WF'(K)$ is a subset of the identity on $T^*\mathbb{R}^n$. A simple condition of injectivity is necessary and sufficient for this to be the case.

**Definition 7.** *We say a relation $C \subset X \times Y$ is injective if*

$$(x_1, y) \in C, (x_2, y) \in C \quad \Rightarrow \quad x_1 = x_2.$$

As a map from $X$ to $Y$, an injective relation may be multivalued, but as a map from $Y$ to $X$, the transpose relation is a graph.

**Lemma 3.** *A relation $C$ is injective if and only if $C^T \circ C \subset I$.*

*Proof.* Assume that $C \subset X \times Y$ is injective, and let $S \subset X$. By contradiction, if $C^T \circ C$ were not a subset of $I$, then there would exist an element $x$ of $X$, for which there exists an element $x'$ of $C^T \circ C \circ x$ such that $x' \neq x$. By definition of $C^T \circ C$, this means that there exists $y \in Y$ such that $(y, x') \in C^T$ and $(x, y) \in C$. By definition of transpose relation, we have $(x', y) \in C$. Injectivity of $C$ implies $x = x'$, a contradiction.

By contraposition, assume that $C \subset X \times Y$ is not injective, i.e., there exist two elements $(x, y)$ and $(x', y)$ of $C$ for which $x \neq x'$. Then $(y, x') \in C^T$ by definition of transpose, and $(x, x') \in C^T \circ C$ by definition of composition. Since $x \neq x'$, $C^T \circ C$ is not contained in the identity relation $I = \{(x, x) : x \in X\}$. □

We have all the pieces to gather the main result on preservation of singularities.

**Theorem 6.** *Let $K$ be the distributional kernel of an operator $F$, with wavefront set (8.1). Assume that the elements of $WF'(K)$ obey*

$$\xi = 0 \quad \Leftrightarrow \quad (\xi_s, \xi_r, \omega) = 0,$$

*i.e., $WF(K)$ does not have zero sections. Further assume that $WF'(K)$ is injective as a relation in $(T^*\mathbb{R}^n\backslash 0) \times (T^*\mathbb{R}^{n_d}\backslash 0)$. Then, for all $m_1$ in the domain of $F$,*

$$WF(F^*Fm_1) \subset WF(m_1).$$

*Proof.* Notice that the zero sections of $(WF'(K))^T$ are the same as those of $WF'(K)$, hence Hörmander's theorem can be applied twice. We get

$$WF(F^*Fm_1) \subset (WF'(K))^T \circ WF'(K) \circ WF(m_1).$$

Under the injectivity assumption, lemma 3 allows to conclude. □

The assumptions of the theorem are tight:

- If zero sections are present, the composition law is different and adds elements away from the diagonal, as shown in the general formulation of Hörmander's theorem in [**?**].
- If injectivity does not hold, lemma 3 shows that the composition of two relations $C^T \circ C$ must have non-diagonal components.

## 8.2 Characterization of the wavefront set

In this section we construct the wavefront relation $WF'(K)$ explicitly in the simple scenario of section 7.2.

Recall that the setting of section 7.2 is one in which the background model $m_0(x)$ is heterogeneous and smooth, and enjoys no multipathing in the zone of interest. The source wavelet $w(t)$ (entering the right-hand side of the wave equation) still needs to be an impulse $\delta(t)$ in order to create propagating singularities. If instead the wavelet is essentially bandlimited, then so will the wavefields, but there are still remnants of the microlocal theory in the magnitude and locality of the propagating "wiggles"[3].

(!) (!)

The distributional kernel of GRT migration is then

$$K(x; x_r, x_s, t) = a(x, x_r, x_s)\delta''(t - \tau(x_r, x, x_s)),$$

where $\tau(x_r, x, x_s) = \tau(x_r, x) + \tau(x, x_s)$ is the three-point traveltime, and $a$ is a smooth amplitude, except for a singularity at $x = x_r$ and $x = x_s$.

[3]Microlocal theory can be expressed scale-by-scale, with wave packet decompositions and/or the so-called FBI transform. We leave out this topic.

The singular support of $K$ is the same as its support as a measure, namely

$$\text{sing supp}(K) = \{(x, x_r, x_s, t) : t = \tau(x_r, x, x_s)\}.$$

In what follows we keep in mind that, for $(x, x_r, x_s, t)$ to be a candidate base point in the wavefront relation of $K$, i.e., with a non-empty fiber, it is necessary that $t = \tau(x_r, x, x_s)$.

To find this wavefront relation, we first localize $K$ around some reference point $(x_0, x_{r,0}, x_{s,0}, t_0)$ by multiplication with increasingly sharper cutoff functions, such as

$$\chi(\|x - x_0\|)\ \chi(\|x_r - x_{r,0}\|)\ \chi(\|x_s - x_{s,0}\|)\ \chi(|t - t_0|),$$

where $\chi$ is a $C_0^\infty$ function compactly supported in the ball $B_\epsilon(0)$ for some $\epsilon$ that tends to zero. To keep notations manageable in the sequel, we introduce the symbol $[\,\chi\,]$ to refer to *any* $C_0^\infty$ function of $(x, x_r, x_s, t)$ (or any subset of those variables) with support in the ball of radius $\epsilon$ centered at $(x_0, x_{r,0}, x_{s,0}, t_0)$ (or any subset of those variables, resp.).

We then take a Fourier transform in every variable, and let

$$I(\xi, \xi_r, \xi_s, \omega) = \iiiint e^{i(x\cdot\xi - x_r\cdot\xi_r - x_s\cdot\xi_s - \omega t)} K(x; x_r, x_s, t)[\,\chi\,]dx\, dx_r\, dx_s\, dt. \tag{8.2}$$

According to the definition in the previous section, the test of membership in $WF'(K)$ involves the behavior of $I$ under rescaling $(\xi, \xi_r, \xi_s, \omega) \to (\alpha\xi, \alpha\xi_r, \alpha\xi_s, \alpha\omega)$ by a single number $\alpha > 0$. Namely,

$$((x_0; \xi), (x_{r,0}, x_{s,0}, t_0; \xi_r, \xi_s, \omega)) \notin WF'(K)$$

provided there exists a sufficiently small $\epsilon > 0$ (determining the support of $[\,\chi\,]$) such that

$$I(\alpha\xi, \alpha\xi_r, \alpha\xi_s, \alpha\omega) \le C_m \alpha^{-m} \quad \text{for all } m > 0.$$

Notice that the Fourier transform in (8.2) is taken with a minus sign in the $\xi$ variable (hence $e^{ix\cdot\xi}$ instead of $e^{-ix\cdot\xi}$) because $WF'(K)$ – the one useful for relations – precisely differs from $WF(K)$ by a minus sign in the $\xi$ variable.

Before we simplify the quantity in (8.2), notice that it has a wave packet interpretation: we may let

$$\varphi(x) = e^{-ix\cdot\xi}\chi(\|x - x_0\|),$$

$$\psi(x_r, x_s.t) = e^{-i(x_r\cdot\xi_r + x_s\cdot\xi_s + \omega t)}\chi(\|x_r - x_{r,0}\|)\ \chi(\|x_s - x_{s,0}\|)\ \chi(|t - t_0|),$$

and view

$$I(\xi, \xi_r, \xi_s, \omega) = \langle \psi, F\varphi\rangle_{(x_r, x_s, t)},$$

with the complex conjugate over the second argument. The quantity $I(\xi, \xi_r, \xi_s, \omega)$ will be "large" (slow decay in $\alpha$ when the argument is scaled as earlier) provided the wave packet $\psi$ in data space "matches", both in terms of location and oscillation content, the image of the wave packet $\varphi$ in model space under the forward map $F$.

The $t$ integral can be handled by performing two integrations by parts, namely

$$\int e^{-i\omega t}\delta''(t - \tau(x, x_r, x_s))\chi(\|t - t_0\|)\, dt = e^{-i\omega\tau(x, x_r, x_s)}\widetilde{\chi}_\omega(\tau(x, x_r, x_s)),$$

for some smooth function $\widetilde{\chi}_\omega(t) = e^{i\omega t}(e^{-i\omega t}\chi(|t-t_0|))''$ involving a (harmless) dependence on $\omega^0$, $\omega^1$ and $\omega^2$. After absorbing the $\widetilde{\chi}_\omega(\tau(x, x_r, x_s))$ factor in a new cutoff function of $(x, x_r, x_s)$ still called $[\,\chi\,]$, the result is

$$I(\xi, \xi_r, \xi_s, \omega) = \iiint e^{i(x\cdot\xi - x_r\cdot\xi_r - x_s\cdot\xi_s - \omega\tau(x, x_r, x_s))}a(x; x_r, x_s)[\,\chi\,]dx\, dx_r\, dx_s. \tag{8.3}$$

First, consider the case when $x_0 = x_{r,0}$ or $x_0 = x_{s,0}$. In that case, no matter how small $\epsilon > 0$, the cutoff function $[\,\chi\,]$ never avoids the singularity of the amplitude. As a result, the Fourier transform is expected to decay slowly in some directions. The ampltude's singularity is not the most interesting from a geometrical viewpoint, so for the sake of simplicity, we just brace for every possible $(\xi, \xi_r, \xi_s, \omega)$ to be part of the fiber relative $(x_0, x_{r,0}, x_{s,0}, t_0)$ where either $x_0 = x_{r,0}$ or $x_0 = x_{s,0}$. It is a good exercise to characterize these fibers in more details; see for instance the analysis in [**?**].

Assume now that $x_0 \neq x_{r,0}$ and $x_0 \neq x_{s,0}$. There exists a sufficiently small $\epsilon$ for which $a(x, x_r, x_s)$ is nonsingular and smooth on the support of $[\,\chi\,]$. We may therefore remove $a$ from (8.3) by absorbing it in $[\,\chi\,]$:

$$I(\xi, \xi_r, \xi_s, \omega) = \iiint e^{i(x\cdot\xi - x_r\cdot\xi_r - x_s\cdot\xi_s - \omega\tau(x, x_r, x_s))}[\,\chi\,]dx\, dx_r\, dx_s. \tag{8.4}$$

What is left is an integral that can be estimated by the *stationary phase* lemma, or more precisely, the simplest version of such a result when the phase is nonstationary: see lemma 4 in appendix C.

The phase in (8.4) is $\phi(x, x_r, x_s) = x\cdot\xi - x_r\cdot\xi_r - x_s\cdot\xi_s - \omega\tau(x, x_r, x_s)$. Notice that $\phi$ involves the co-variables in a linear manner, hence is homogenenous of degree 1 in $\alpha$, as needed in lemma 4. Its gradients are

$$\nabla_x\phi = \xi - \omega\nabla_x\tau(x, x_r, x_s),$$

$$\nabla_{x_r}\phi = -\xi_r - \omega\nabla_{x_r}\tau(x, x_r, x_s),$$

$$\nabla_{x_s}\phi = -\xi_s - \omega\nabla_{x_s}\tau(x, x_r, x_s).$$

If either of these gradients is nonzero at $(x_0, x_{r,0}, x_{s,0})$, then it will also be zero in a small neighborhood of that point, i.e., over the support of $[\chi]$ for $\epsilon$ small enough. In that case, lemma 4 applies, and it follows that the decay of the Fourier transform is fast no matter the (nonzero) direction $(\xi, \xi_r, \xi_s, \omega)$. Hence, if either of the gradients is nonzero, the point $((x_0, \xi), (x_{r,0}, x_{s,0}, t_0; \xi_r, \xi_s, \omega))$ is *not* in $WF'(K)$.

Hence $((x_0, \xi), (x_{r,0}, x_{s,0}, t_0; \xi_r, \xi_s, \omega))$ may be an element in $WF'(K)$ only if the phase has a critical point at $(x_0, x_{r,0}, x_{s,0})$:

$$\xi = \omega\nabla_x\tau(x_0, x_{r,0}, x_{s,0}), \tag{8.5}$$

$$\xi_r = -\omega\nabla_{x_r}\tau(x_0, x_{r,0}, x_{s,0}), \tag{8.6}$$

$$\xi_s = -\omega\nabla_{x_s}\tau(x_0, x_{r,0}, x_{s,0}). \tag{8.7}$$

Additionally, recall that $t_0 = \tau(x_0, x_{r,0}, x_{s,0})$. We gather the result as follows:

$$WF'(K) \subset \{\, ((x, \xi), (x_r, x_s, t; \xi_r, \xi_s, \omega)) \in (T^*\mathbb{R}^n \times T^*\mathbb{R}^{n_d})\backslash 0 :$$

$$t = \tau(x, x_r, x_s),\ \omega \neq 0,\ \text{and, either } x = x_r,\ \text{or } x = x_s,$$

$$\text{or (8.5, 8.6, 8.7) hold at } (x, x_r, x_s)\ \}.$$

Whether the inclusion is a proper inclusion, or an equality, (at least away from $x = x_r$ and $x = x_s$) depends on whether the amplitude factor in (8.4) vanishes in an open set or not.

Notice that $\omega \neq 0$ for the elements in $WF'(K)$, otherwise (8.5, 8.6, 8.7) would imply that the other covariables are zero as well, which is not allowed in the definition of $WF'(K)$. In the sequel, we may then divide by $\omega$ at will.

The relations (8.5, 8.6, 8.7) have an important physical meaning. Recall that $t = \tau(x, x_r, x_s)$ is called isochrone curve/surface when it is considered in model $x$-space, and moveout curve/surface when considered in data $(x_r, x_s, t)$-space.

- The relation $\xi = \omega \nabla_x \tau(x, x_r, x_s)$ indicates that $\xi$ is *normal to the isochrone* passing through $x$, with level set $t = \tau(x, x_r, x_s)$. In terms of two-point traveltimes, we may write

$$\frac{\xi}{\omega} = \nabla_x \tau(x, x_r) + \nabla_x \tau(x, x_s).$$

  Observe that $\nabla_x \tau(x, x_r)$ is tangent at $x$ to the ray from $x_r$ to $x$, and $\nabla_x \tau(x, x_s)$ is tangent at $x$ to the ray from $x_s$ to $x$, hence $\xi$ is the bisector direction for those two rays. The (co)vector $\xi$ may be understood as the (co)normal to a "localized mirror" about which the incident wave reflects in a specular manner to create the scattered wave. The equation above is then the vector expression of *Snell's law of reflection*, that the angle of incidence $\angle(\nabla_x \tau(x, x_s), \xi)$ equals the angle of reflection $\angle(\nabla_x \tau(x, x_r), \xi)$.

- The special case $\xi = 0$ is equally important from a physical viewpoint. Since $\omega \neq 0$, it corresponds to

$$\nabla_x \tau(x, x_r) = -\nabla_x \tau(x, x_s),$$

  i.e., the tangents to the incident and reflected rays are collinear and opposite in signs. This happens when $x$ is a point on the direct, unbroken ray linking $x_r$ to $x_s$. We may call this situation forward scattering: it corresponds to *transmitted waves* rather than reflected waves. The reader can check that it is the only way in which a zero section is created in the wavefront relation (see the previous section for an explanation of zero sections and how they impede the interpretation of $WF'(K)$ as a relation.)

- Consider now (8.6) and (8.7). Pick any $\eta = (\eta_r, \eta_s)$, form the combination $\eta_r \cdot$ (8.6) + $\eta_s \cdot$ (8.7) = 0, and rearrange the terms to get

$$\begin{pmatrix} \xi_r \\ \xi_s \\ \omega \end{pmatrix} \cdot \begin{pmatrix} \eta_r \\ \eta_s \\ \eta_r \cdot \nabla_{x_r} \tau + \eta_s \cdot \nabla_{x_s} \tau \end{pmatrix} = 0,$$

  with both $\tau$ evaluated at $(x, x_r, x_s)$. The second vector in the dot product is an arbitrary vector tangent to the moveout surface $t = \tau(x, x_r, x_s)$ in $(x_r, x_s, t)$-data space. Thus $(\xi_r, \xi_s, \omega)$ is *normal to the moveout surface.*

(!) We are now ready to interpret $WF'(K)$ in terms of the mapping of singularities that it generates. Assume that no forward scattering is taking place, i.e., we are only dealing with reflected rather than transmitted waves. From a singularity in model space at a point $x$ and in the direction $\xi$ – a local mirror placed at $x$ with conormal $\xi$ – the wavefront relation predicts that there may be singularities in data space, with location(s) $(x_r, x_s, t)$ and corresponding conormal direction(s) $(\xi_r, \xi_s, \omega)$ determined as follows.

Fix a couple $(x, \xi)$.

1. For each $x_s$, find the unique ray that links $x_s$ to $x$.

2. At $x$, find the direction of the incoming ray as $\nabla_x \tau(x, x_s)$.

3. Determine $\nabla_x \tau(x, x_r)$ as the vector with magnitude $1/c(x)$ (from the eikonal equation), and direction so that (8.5) holds for some $\omega$. This can be done by computing the reflection of $\nabla_x \tau(x, x_s)$ about the axis generated by $\xi$,

$$\nabla_x \tau(x, x_r) = \nabla_x \tau(x, x_s) - 2 \frac{\nabla_x \tau(x, x_s) \cdot \xi}{\xi \cdot \xi} \, \xi.$$

4. Trace the ray from $x$ and take-off direction $-\nabla_x \tau(x, x_r)$:

   - If the ray is closed or exits the domain before reaching a receiver, discard $x_s$. This particular $x_s$ does not give rise to any singularity (relative to this particular couple $(x, \xi)$.)
   - If the ray reaches a receiver $x_r$, let $t = \tau(x, x_s) + \tau(x, x_r)$. Some singularity may appear at the point $(x_s, x_r, t)$ in data space.

5. Determine $\omega = \|\xi\| / \|\nabla_x \tau(x, x_r) + \nabla_x \tau(x, x_s)\|$. The normalization of $\xi$ starts as arbitrary, and is undone by division by $\omega$.

6. Determine $\xi_r$ and $\xi_s$ directly from (8.6) and (8.7). Then the covector conormal to the singularity at $(x_r, x_s, t)$ is $(\xi_r, \xi_s, \omega)$ (as well as all its positive multiples.)

Notice that both the data variables $(x_r, x_s, t)$ and the covariables $(\xi_r, \xi_s, \omega)$ are determined uniquely from $x$ and $\xi$ in this situation, hence the singularity mapping induced by the wavefront relation is one-to-one.

If we make the additional two assumptions that the receivers surround the domain of interest (which would require us to give up the assumption that the acquisition manifold $\Omega$ is a vector subspace), and that there is no trapped (closed) ray , then the test in point 4 above always succeeds. In (!) that case, the wavefront relation is onto, hence bijective, and can be inverted by a sequence of steps with a similar geometrical content as earlier. See an exercise at the end of this chapter.

## 8.3 Pseudodifferential theory

## 8.4 Exercises

1. Compute the wavefront set of the following functions/distributions of two variables: (1) the indicator function $H(x_1)$ (where $H$ is the Heaviside function) of the half-plane $x_1 > 0$, (2) the indicator function of the unit disk, (3) the indicator function of the square $[-1, 1]^2$, (4) the Dirac delta $\delta(x)$.

2. Find conditions on the acquisition manifold under which forward scattering is the only situation in which a zero section can be created in $WF'(K)$. [Hint: transversality with the rays from $x$ to $x_r$, and from $x$ to $x_s$.]

3. Perform the geometrical construction of $(WF'(K))^T$ for migration, analogous to the geometrical construction of $WF'(K)$ for Born modeling done in section 8.2. Assume: 1) $\tau$ single-valued, 2) no forward scattering, 3) full aperture of receivers, 4) no trapped rays, and 5) the acquisition manifold $\Omega$ is a vector subspace equal to the Cartesian product of two copies of the same subspace of codimension 1 in $\mathbb{R}^3$ (one for $x_r$ and one for $x_s$). In other words, you may assume that both $x_r$ and $x_s$ lie on the "surface" $z = 0$.

   **Solution.** Fix $(x_r, x_s, t)$ and $(\xi_r, \xi_s, \omega) \neq 0$. We aim to determine a unique $(x, \xi)$ so that $((x, \xi), (x_r, x_s, t; \xi_r, \xi_s, \omega)) \in WF'(K)$.

   Starting with (8.6), notice first that $\nabla_{x_r}\tau(x, x_r)$ is a partial gradient: it is the projection to the acquisition manifold $\Omega$ at $x_r$ of the three-dimensional gradient of $\tau$ in its second argument, say $\nabla_y\tau(x, y)|_{y=(x_r,0)}$, in coordinates $y = (x_r, z)$ so that $\Omega$ is represented by $z = 0$. A similar

observation holds for $\nabla_{x_s}\tau(x, x_s)$. Since the norm of each partial gradient is less than the norm of the full gradient, and since the eikonal equation determines this latter norm, $\xi_r$ and $\xi_s$ must obey the geometric compatibility relations

$$|\xi_r| \leq \frac{\omega}{c(x_r)}, \qquad |\xi_s| \leq \frac{\omega}{c(x_s)}.$$

The coordinate $z$ is one-dimensional from our assumption on the acquisition manifold, so we can now assemble the full gradient of $\tau$ at $x_r$. With the help of (8.6) we obtain

$$\nabla_y \tau(x, y)|_{y=(x_r,0)} = \left( -\frac{\xi_r}{\omega}, \pm\sqrt{\frac{1}{c^2(x_r)} - \frac{|\xi_r|^2}{\omega^2}} \right).$$

(The sign is determined on geometrical grounds, so that $\nabla_y\tau$ points outside the domain of interest.) Minus the direction of $\nabla_y\tau$ is also the take-off direction of a ray from $x_r$. We obtain $\nabla_y\tau(x, y)|_{y=(x_s,0)}$ in the same fashion from (8.7), which determines the take-off direction of a ray from $x_s$. These rays meet at a single point that we call $x$. We may alternatively intersect either of these rays with the isochrone $t = \tau(x, x_r, x_s)$ to obtain $x$; this piece of information is redundant in the wavefront relation[4]. Finally, we determine $\xi = \omega\nabla_x\tau(x, x_r, x_s)$.

[4]Only because we have assumed that the acquisition manifold has low codimension.

# Chapter 9

# Optimization

## 9.1 Regularization and sparsity

## 9.2 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

$$I_m(x) = -\sum_j \int_0^T \frac{\partial^2 \widetilde{u}_{0,j}}{\partial t^2}(x,t)\, \widetilde{q}_j(x,t)\, dt. \tag{9.1}$$

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 (9.1).

# 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* $\phi$ 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 $\phi$ 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 $\phi$ at $f$, and we denote it as

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

It is also called the *first variation* of $\phi$. 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 $\phi$ 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

# Finite difference methods for wave equations

Many types of numerical methods exist for computing solutions to wave equations – finite differences are the simplest, though often not the most accurate ones.

Consider for illustration the 1D time-dependent problem

$$m(x)\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + f(x,t), \qquad x \in [0,1],$$

with smooth $f(x,t)$, and, say, zero initial conditions. The simplest finite difference scheme for this equation is set up as follows:

- Space is discretized over $N+1$ points as $x_j = j\Delta x$ with $\Delta x = \frac{1}{N}$ and $j = 0, \ldots, N$.

- Time is discretized as $t_n = n\Delta t$ with $n = 0, 1, 2, \ldots$. Call $u_j^n$ the computed approximation to $u(x_j, t_n)$. (In this appendix, $n$ is a superscript.)

- The centered finite difference formula for the second-order spatial derivative is

  $$\frac{\partial^2 u}{\partial x^2}(x_j, t_n) = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} + O((\Delta x)^2),$$

  provided $u$ is sufficiently smooth – the $O(\cdot)$ notation hides a multiplicative constant proportional to $\partial^4 u/\partial x^4$.

- Similarly, the centered finite difference formula for the second-order time derivative is

$$\frac{\partial^2 u}{\partial t^2}(x_j, t_n) = \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{(\Delta t)^2} + O((\Delta t)^2),$$

  provided $u$ is sufficiently smooth.

- Multiplication by $m(x)$ is realized by multiplication on the grid by $m(x_j)$. Gather all the discrete operators to get the discrete wave equation.

- The wave equation is then solved by marching: assume that the values of $u_j^{n-1}$ and $u_j^n$ are known for all $j$, then isolate $u_j^{n+1}$ in the expression of the discrete wave equation.

Dirichlet boundary conditions are implemented by fixing. e.g., $u_0 = a$. Neumann conditions involve a finite difference, such as $\frac{u_1 - u_0}{\Delta x} = a$. The more accurate, centered difference approximation $\frac{u_1 - u_{-1}}{2\Delta x} = a$ with a ghost node at $u_{-1}$ can also be used, provided the discrete wave equation is evaluated one more time at $x_0$ to close the resulting system. In 1D the absorbing boundary condition has the explicit form $\frac{1}{c}\partial_t u \pm \partial_x u = 0$ for left (-) and right-going (+) waves respectively, and can be implemented with adequate differences (such as upwind in space and forward in time).

The grid spacing $\Delta x$ is typically chosen as a small fraction of the representative wavelength in the solution. The time step $\Delta t$ is limited by the CFL condition $\Delta t \leq \Delta x \,/\, \max_x c(x)$, and is typically taken to be a fraction thereof.

In two spatial dimensions, the simplest discrete Laplacian is the 5-point stencil which combines the two 3-point centered schemes in $x$ and in $y$. Its accuracy is also $O(\max\{\Delta x)^2, (\Delta y)^2\})$. Designing good absorbing boundary conditions is a somewhat difficult problem that has a long history. The currently most popular solution to this problem is to slightly expand the computational domain using an absorbing, perfectly-matched layer (PML).

More accurate schemes can be obtained from higher-order finite differences. Low-order schemes such as the one explained above typically suffer from unacceptable numerical dispersion at large times. If accuracy is a big concern, spectral methods (spectral elements, Chebyshev polynomials, etc.) are by far the best way to solve wave equations numerically with a controlled, small number of points per wavelength.

# Appendix C

# Stationary phase

See Stein's book *Harmonic analysis* [**?**], chapter 8, as a reference on stationary phase and for proofs of the claims below.

If an integrand has a phase factor with no stationary points, and the amplitude is otherwise smooth, then the integral has a very small value because the positive parts cancel out the negative parts. The following result makes this heuristic precise as an asymptotic bound on the value of the integral when the phase has a large prefactor.

**Lemma 4.** *(The non-stationary phase lemma.) Let* $\chi \in C_0^\infty(\mathbb{R}^n)$*,* $\phi \in C^\infty(\overline{supp\,\chi})$*, and let*

$$I_\alpha = \int_{\mathbb{R}^n} e^{i\alpha\phi(x)}\chi(x)dx.$$

*If* $\nabla\phi(x) \neq 0$ *for all* $x \in supp\,\chi$*, then*

$$|I_\alpha| \leq C_m\alpha^{-m}, \qquad \text{for all } m > 0.$$

*Proof.* Integrate by parts after inserting an $m$-th power of the differential operator

$$L = \frac{I - \Delta_x}{1 + \alpha^2|\nabla_x\phi(x)|^2},$$

which leaves the exponential factor unchanged. A fortiori, $1+\alpha^2|\nabla_x\phi(x)|^2 > C\alpha^2$ for some number $C > 0$. Deal with the odd values of $m$ by interpolation (geometric mean) from the $m-1$ and $m+1$ cases. □

If the phase otherwise has critical points, then the value of the integral is mostly determined by the behavior of the integrand near those critical points.

**Lemma 5.** *Consider the same setting as earlier, but consider the presence of a point $x^*$ such that*

$$\nabla\phi(x^*) = 0, \qquad D^2\phi(x^*) \text{ invertible},$$

*where $D^2\phi$ denotes the Hessian matrix of $\phi$. Assume that $\nabla\phi(x) \neq 0$ for $x \neq x^*$. Then, as $\alpha \to \infty$,*

$$I_\alpha = \left(\frac{2\pi}{\alpha}\right)^{n/2} \chi(x^*) e^{i\alpha\phi(x^*)} \frac{e^{i\frac{\pi}{4}sgn(D^2\phi(x^*))}}{\sqrt{\det(D^2\phi(x^*))}} + O(\alpha^{-\frac{n}{2}-1}),$$

*where sgn denotes the signature of a matrix (the number of positive eigenvalues minus the number of negative eigenvalues.)*

See [**?**] for a proof. More generally, if there exists a point $x^*$ where all the partials of $\phi$ of order less than or equal to $\ell$ vanish, but $\partial^\ell\phi(x^*)/\partial x_1^\ell \neq 0$ in some direction $x_1$, then it is possible to show that $I_\alpha = O(\alpha^{-1/\ell})$.

Here are a few examples.

- A good example for the above lemma is

$$\int_{-\infty}^{\infty} e^{i\alpha x^2}\, dx \sim \frac{1}{\sqrt{\alpha}}.$$

  The real part of the integrand, $\cos(\alpha x^2)$, is non-oscillatory at the origin, but develops significant oscillations as soon as $x$ is on the order of $\pm 1/\sqrt{\alpha}$. The extent of the range over which the integrand essentially does not oscillate (e.g., as measured from the length of the first half period) determines the order of magnitude of the value of the integral.

- An important case not immediately handled by any of the previous lemmas is the stationary phase explanation of the often-invoked fact that[1]

$$\int_{\mathbb{R}^n} \left( \int_{\mathbb{R}^n} e^{i(y-x)\cdot\xi} d\xi \right) f(x) dx \sim f(y).$$

  The large factor $\alpha$ of the stationary phase lemmas can be placed in the exponent as $i\alpha(y-x)\cdot\xi$. The rescaling $\xi' = \alpha\xi$ quickly helps to get

[1] The actual value of the integral is $(2\pi)^n f(y)$. The function $f$ is only required to be continuous with some decay at infinity for this relation to make sense pointwise. Fourier analysis makes all of this precise, of course.

rid of it by turning it into a multiplicative $1/\alpha^n$ factor for the integral above. Hence the equivalent, stationary-phase-friendly formulation of the relation above is really

$$\int_{\mathbb{R}^n} \left( \int_{\mathbb{R}^n} e^{i\alpha(y-x)\cdot\xi} d\xi \right) f(x) dx \sim \frac{f(y)}{\alpha^n}.$$

As a function of $\xi$ alone, the phase $\phi(\xi) = (y-x)\cdot\xi$ has a critical point when $x = y$ , but the Hessian is degenerate: $\phi''(\xi) = 0$. We cannot apply any of the stationary phase lemmas to the integral on $\xi$ alone.

The solution is to consider the double integral over $x$ and $\xi$: the phase $\phi(x,\xi) = (y-x)\cdot\xi$ is still critical when $x = y$, and now $\xi = 0$, but the Hessian matrix is

$$D^2\phi = \begin{pmatrix} \nabla_x\nabla_x\phi & \nabla_x\nabla_\xi\phi \\ \nabla_\xi\nabla_x\phi & \nabla_\xi\nabla_\xi\phi \end{pmatrix} = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix},$$

which is invertible independently of the base point $(x^*, \xi^*)$. Hence lemma 5 applies in $2n$ dimensions, and actually predicts the exact value of the integral, namely $(2\pi/\alpha)^n f(y)$. The condition $y = x$ signifies that, of all the values of $f(x)$, only that at $x = y$ matters for the result of the integral. The condition $\xi = 0$ is a manifestation of the fact that $f(x)$ was assumed to be minimially smooth (hence it is $\widehat{f}(0)$ when $\xi = 0$ that matters). The function $f$ may have oscillatory factors like $e^{i\,100\,\psi(x)}$ for some other phase $\psi$, but no factors of the form $e^{i\alpha\psi(x)}$ involving $\alpha$ explcitly.

- Another interesting example is the integral

$$\int_{\mathbb{R}^n} \left( \int_{\mathbb{R}^n} e^{i(y-x)\cdot\xi} d\xi \right) \int e^{ix\cdot\eta} F(\eta) d\eta\, dx$$

which often appears in Fourier analysis. It can be seen as the composition of an inverse Fourier transform of $F$, from $\eta$ to $x$, followed by a Fourier transform, from $x$ to $\xi$, followed by an inverse Fourier transform, from $\xi$ to $y$. Indeed, the integral reduces to (an unimportant multiple of $2\pi$ times) $\check{F}(y)$. For fixed $\eta$ we can still see the phase as having two arguments, namely $\phi(x,\xi) = (y-x)\cdot\xi + x\cdot\eta$, but the equations for the critical points now look more symmetric:

$$\frac{\partial\phi}{\partial x} = \eta - x = 0, \qquad \frac{\partial\phi}{\partial\xi} = y - x = 0,$$

and $D^2\phi$ is the same as previously. We now have $x^* = y$ and $\xi^* = \eta$, so $\phi(x^*, \xi^*) = y \cdot \eta$. Stationary phase over the inner $(x, \xi)$ variables then reduces the outer $\eta$ integral to (a constant times) $\int e^{iy\cdot\eta} F(\eta) d\eta$, as needed.

The relation $\eta = \xi$ indicates that, in the course of the first two Fourier transforms taking $\eta$ to $x$, then to $\xi$, it is only the value of $F$ at $\eta = \xi$ which matters to determine the result $F(\xi)$. The relation $x = y$ indicates that, from the result $f(x)$ of having done the first Fourier transform from $\eta$ to $x$, it is only the value $f(y)$ at $x = y$ which matters to determine the end result $f(y) = \check{F}(y)$.

The set of equations

$$x = y, \qquad \xi = \eta$$

is a simple example of a so-called canonical relation in phase-space, the space made of all the quadruples $(x, \xi; y, \eta)$. In particular, it is precisely the relation corresponding to the identity map from $(x, \xi)$ to $(y, \eta)$. The adjective "canonical" refers to the fact that the map is symplectic, i.e., preserves areas, which is instantiated in our context by the fact that $|\det D^2\phi| = 1$. Phase-space relations are introduced and used in chapter 8.

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