### 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.

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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*.

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#### 5.2. FORWARD MODEL

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  $\hat{x} = \frac{x}{|x|}$ ,

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

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  $\hat{p}(\omega)$  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  $\hat{x}$ , 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

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

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  $m_1$ )

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

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

$$\widehat{d}(s,\omega) = \int \frac{e^{ik|x-\gamma(s)|}}{4\pi|x-\gamma(s)|} \omega^2 \widehat{u}_0(x,\omega) m(x)\widehat{w}^{(1)}(k(x-\gamma(s)),\omega).$$

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:

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

with amplitude

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

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

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

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

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

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  $A(x, s, \omega) = \omega^2 \hat{p}(\omega)$  to its leading  $\omega$  dependence. Then

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

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<sup>1</sup>

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

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

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

This means that

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

<sup>&</sup>lt;sup>1</sup>It could be handy to introduce a multiplicative factor  $2\pi$  in case the Parseval identity were to be used later.

#### 5.3. FILTERED BACKPROJECTION

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, xlinked 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<sup>2</sup> B to replace  $F^*$ :

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

By composing B with F, we obtain

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

 $<sup>^2</sup>B$  for filtered Back projection, or for Gregory Beylkin, who was the first to propose it in 1984.

with

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

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

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$$\nabla_{y}|R_{y,s}| = \left(\frac{\partial R_{y,s}}{\partial y}\right)^{T} \frac{R_{y,s}}{|R_{y,s}|} = P_{2}^{T} \widehat{R_{y,s}}$$

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 downrange 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  $\gamma(s)$  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 = 0should 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*:

$$\xi = \Xi(x,\omega;x) = \nabla_y \phi(s,\omega,y)|_{y=x} = 2k P_2^T \widehat{R_{x,s}}$$

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

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

The Jacobian  $J = \left|\frac{\partial(s,\omega)}{\partial\xi}\right|$  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

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

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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.

(...)

$$\Delta x_1 = \frac{c}{\Delta \omega \sin \psi}$$
$$\Delta x_2 = \frac{L}{2}, \qquad L \ge \lambda$$

### 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.

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## 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 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:

•  $\phi(f) = \langle g, f \rangle$ ,  $\frac{\delta \phi}{\delta f}[f] = g$ ,  $\frac{\delta \phi}{\delta f}[f](h) = \langle g, h \rangle$ 

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).

• 
$$\phi(f) = f(x_0),$$

$$\frac{\delta\phi}{\delta f}[f] = \delta(x - x_0),$$
 (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  $\frac{\delta \mathcal{F}_i}{\delta f_i}$ , 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

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

*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

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

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<sup>1</sup>

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

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

<sup>&</sup>lt;sup>1</sup>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  $\hat{f}(0)$  when  $\xi = 0$ that matters). The function f may have oscillatory factors like  $e^{i100\psi(x)}$ for some other phase  $\psi$ , but no factors of the form  $e^{i\alpha\psi(x)}$  involving  $\alpha$ explicitly.

• 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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