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Inverse diffraction, duality and optimal control

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Abstract. The reduced wave equation can describe a non-dynamical system having infinite dimensional state space and a control at the boundary. We define a generalised controllability property and show that it holds in a bounded domain. This property states that the linear subspace spanned by the trace of the system solution (i.e. the monochromatic scalar field) on a given boundary is dense in the corresponding Hilbert space as the boundary control is made to span an adequate Hilbert space. By duality, the 'controllability' property is shown to be equivalent to 'observability' of the adjoint system. The connection of this statement with the proof of uniqueness for inverse diffraction problems is discussed. The adjoint system solution is a Green function. The inverse problem is ill posed: it calls for a regularisation procedure related to minimising a real-valued convex functional which depends on complex variables. At this point Lions's theory of optimal control is applied to state the existence and uniqueness of the minimising control. Lagrangian theory is used to derive the explicit form of the functional gradient. The latter allows us to design a minimisation algorithm where primal and adjoint systems must be solved sequentially.

1. Introduction

In the last few years interest in inverse problems has grown among the optics community (see e.g. Baltes 1978, 1980). In the following we study some properties of the Helmholtz equation from a system theoretical point of view and their application to inverse problems. We do not discuss here the physical implications of modelling a diffraction phenomenon by the Helmholtz equation, such as evanescent waves, super-resolution problems, etc, although this would be an attractive subject. The system theoretical approach will bring about duality, which links control and observation. We shall see that some results originally stated for a 'direct' or 'control' problem can be easily translated into the language of 'estimation' or 'inverse' problems.

2. Distributed parameter system theory

Here we are not going to deal in detail with the formal setting of systems having infinite-dimensional state space, which are governed by partial differential equations. The interested reader may refer to Curtain and Pritchard (1978), Goodson *et al* (1967) or to Helton (1976). Basic system theory will be introduced gradually in the following, by making reference to our physical example. We shall restrict ourselves to the case of scalar diffraction in the stationary regime.

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Let us consider an open connected bounded set Ω of the three-dimensional Euclidean space R^3. The position vector in Ω is x. In Ω we define the complex scalar field $w(\cdot)$ with suppressed time dependence $\exp -j\omega t$. If w is known wherever it is defined, the physical phenomenon of stationary scalar diffraction is completely described. Hence we call w the 'system state'.

Usually w is not given directly but as the solution of the 'state equation' (SE). Let the properties of the medium inside Ω be represented by a potential function $V(x)$, then the SE for the interior problem we are considering reads

$$(\Delta+k^2)w = V(\cdot)w \qquad x\in\Omega\subset R^3. \tag{2.1}$$

k is the complex wavenumber. Equation (2.1) can be recast into

$$(\Delta+k^2n^2(x))w := Kw = 0. \tag{2.2}$$

$n(x)$ is the refractive index of the medium, which may take complex values.

In order to specify the system completely, we must add adequate boundary conditions (BC) and something else. The general theory of partial differential equations (PDE) states that the solution w must be sought for in a suitable Hilbert space W, which we shall study presently. The state space of a system governed by a PDE, also named a 'distributed parameter system' (DPS), is therefore infinite dimensional.

3. The interior problem

3.1. Problem statement and Sobolev space setting

The geometry of Ω is shown in figure 1. The boundary of Ω, $\partial\Omega$, consists of

$$\partial\Omega := \Gamma_1\cup\Gamma_2 \qquad \Gamma_1\cap\Gamma_2=\varnothing. \tag{3.1}$$

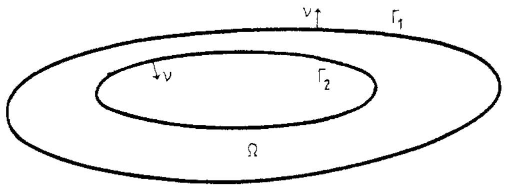

Figure 1. Two-dimensional sketch of domain geometry for the interior problem.

Both of the two-dimensional surfaces Γ_1 and Γ_2 are closed sets, i.e. Ω is not simply connected. Γ_1 and Γ_2 are regular surfaces, i.e. the position vector x on each of them is a continuously differentiable function of some parameters (see e.g. Ladyzhenskaia and Uraltseva 1968, p 6).

The BC we shall study are

$$w|_{\Gamma_1} = u\in U \qquad w|_{\Gamma_2}=0 \tag{3.2}$$

where U is a Hilbert space, the elements of which have Γ_1 as a support.

The spaces of interest to us are Sobolev's spaces $W^{m,2}(D)$, $D\subset R^n$ an open bounded set in R^n, which are introduced e.g. in § 3, ch 1 of Lions' (1971) textbook. Briefly stated $W^{m,2}(D)$, $m\geqslant 0$ integer, is the Hilbert space of functions $f\in L^2(D)$, the partial derivatives of which up to the mth are in $L^2(D)$. In particular $L^2(D) = W^{0,2}(D)$.

The inner product in $W^{m,2}(D)$, is defined by introducing the multi-index

$$q := (q_1, \dots, q_n) \tag{3.3}$$

$$|q| := \sum_{i=1}^{n} q_i. \tag{3.4}$$

The partial derivatives of f can be thus expressed by

$$D^q f := \partial^{|q|} hf / (\partial x_1^{q_1} \dots \partial x_n^{q_n}) \tag{3.5}$$

hence the inner product in $W^{m,2}$ is defined by

$$(g\,|\,f)_{W^{m,2}} := \sum_{|q| \leqslant m} (D^q g\,|\,D^q f)_{L^2}. \tag{3.6}$$

Example. Let $m = 1$, $n = 3$. Then

$$(g\,|\,f)_{W^{m,2}(D)} = (g\,|\,f)_{L^2(D)} + \sum_{i=1}^{3} \left(\frac{\partial g}{\partial x_i} \,\middle|\, \frac{\partial f}{\partial x_i}\right)_{L^2(D)} \tag{3.7}$$

Sobolev spaces $W^{s,2}(D)$ of arbitrary positive index s can also be defined by introducing the fractional derivative (Baiocchi and Capelo, 1978 p 113). Usually $W^{s,2}(D)$ is denoted by $H^s(D)$, which we shall do hereafter.

3.2. Existence and uniqueness of a solution

Given the topological relationship between Ω and Γ defined above, there exists a theorem relating Sobolev's spaces of functions defined respectively on Ω and Γ. This is the 'trace theorem', a simplified form of which reads: given $f \in H^m(\Omega)$, $m \geqslant 1$, integer, there exists a linear, continuous, surjective map

$$\begin{aligned} \gamma^0 : H^m(\Omega) &\twoheadrightarrow H^{m-1/2}(\Gamma) \\ f &\mapsto f|_\Gamma. \end{aligned} \tag{3.8}$$

γ^0 is a 'trace operator'. Every BC $f|_\Gamma$ is therefore the 'trace' on Γ of an element f. This applies to equation (3.2), where U is a proper subspace of $H^{m-1/2}(\Gamma)$. In fact

$$U \cong H^{m-1/2}(\Gamma_1) \times \{0_{\Gamma_2}\} \tag{3.9}$$

where the symbol $\cong$ stands for 'isomorphic to'.

From a system theoretical veiwpoint it would be attractive to study how u affects the state w, i.e. to find which hypotheses are needed for (2.2) and (3.2) to introduce a well defined 'input map' B

$$\begin{aligned} B : U &\to W \\ u &\mapsto w \end{aligned} \tag{3.10}$$

from the input space U to the state space W. B makes sense if the 'boundary control' u uniquely determines the solution $w(x; u)$, $x \in \Omega$. As physical intuition suggests to us, this holds if

$$-k^2 \notin \sigma_L \tag{3.11}$$

where σ_L is the spectrum of the operator $L(\cdot):=\Delta - V(\cdot)$. σ_L is found by solving

$$L(\cdot)w + k^2 w = 0 \qquad w|_{\partial\Omega} = 0. \tag{3.12}$$

Let $L(\cdot)$ be written as in § 3.4 of Ladyzhenskaia and Uraltseva (1968)

$$L(\cdot) = \sum_{i,j} \frac{\partial}{\partial x_i}\left(\delta_{ij}\frac{\partial}{\partial x_j}\right) - V(\cdot) \tag{3.13}$$

where δ_{ij} is Kronecker's symbol. Then L is strictly elliptic because there exist two positive constants m_1 and m_2 such that for all vectors y having real Cartesian components y_i, $i = 1, 2, 3$,

$$m_1 \sum_{i=1}^{3} y_i^2 \leq \sum_{i,j} \delta_{ij} y_i y_j \leq m_2 \sum_{i=1}^{3} y_i^2. \tag{3.14}$$

Moreover let the potential $V(\cdot)$ satisfy

$$\|V(\cdot)\|_{L^2(\Omega)} \leq m_2. \tag{3.15}$$

Then we can apply to system (2.1), (3.2) Fredholm's theorem on elliptic PDE (Ladyzhenskaia and Uraltseva 1968, § 3.5) dealing with existence, uniqueness and regularity of solutions and structure of σ_L. We have that the problem (2.2), (3.2), where u is in the sense of (3.8), (3.9) the trace of an element in $H^1(\Omega)$, admits a unique solution

$$w \in W = H^1(\Omega) \tag{3.16}$$

throughout the complex k^2 plane, except at a countable set of values k_n^2, $n = 1, 2, \ldots$. Hence σ_L is the countable set of eigenvalues. If $-k^2$ in (2.1) is not an eigenvalue, then the map B of (3.10) is well defined.

To complete the system theoretical picture we need to introduce an observation or 'output'-map C. One interesting choice is

$$C: W \to Y \qquad w \mapsto Cw := \left.\frac{\partial w}{\partial \nu}\right|_{\Gamma_2} \tag{3.17}$$

i.e. we observe the normal derivative on Γ_2; ν is the outward normal unit vector. The regularity of Cw can be evaluated from that of w through the trace theorem, which applies also to the normal derivative (Baiocchi and Capelo 1978, appendix 4). We conclude that

$$\left.\frac{\partial w}{\partial \nu}\right|_{\Gamma_2} \in H^{-1/2}(\Gamma_2) \tag{3.18}$$

provided a Sobolev's space with negative index is given a meaning. To this end let us introduce $H^{-m}(T)$, $m > 0$, where T is the boundary of the open bounded set $D \subset R^n$. Let $g \in H^m(T)$: we construct the continuous functional $\langle g|\cdot\rangle$. This is an element of the space $H^{-m}(T)$, dual to $H^m(T)$, where duality is represented by the $\langle\cdot|\cdot\rangle$ relationship (Lions and Magenes 1972, ch 1, § 7). Thus (3.18) makes sense.

3.3. *The maps B, C and a simple inverse problem*

The map γ^0 defined by (3.8) for an elliptic PDE is onto, but in geneal not invertible. In fact, Ker γ^0, i.e. the set of elements say u in $H^m(\Omega)$ which vanish on the boundary, is a subspace denoted by $H_0^m(\Omega)$. u is the solution of

$$\begin{aligned} Au &= f \in H^{m-2}(\Omega) \\ u|_\Gamma &= 0 \end{aligned} \tag{3.19}$$

where A is an elliptic operator and f is a 'distributed control' or 'source' term. In our system, $f=0$; moreover we have an eigenvalue problem; hence Ker γ^0 consists of eigensolutions defined by (3.12). If we assume $-k^2 \notin \sigma_L$, then Ker $\gamma^0 = \{0\}$, a sufficient condition for the linear map γ^0 to be invertible. By (3.8), γ^0 is related to B^{-1}. We restate (3.19) by

$$(\gamma^0)^{-1}\restriction_{\Gamma_1} = B. \tag{3.20}$$

Hence the requirement on eigenvalues affects both maps. After defining B, we now invoke some results on elliptic operators (Ladyzhenskaia and Uraltseva 1968, ch 3, § 8), related to the second fundamental inequality, to state that Im B is a proper subspace of $H^m(\Omega)$. As a consequence, not every element of $H^m(\Omega)$ can be obtained as a solution of a 'boundary control' system, such as (2.1) and (3.2). For a qualitative proof of this fact, let us compare u in (3.19) with w, the solution of (2.1), (3.2): there is no way of finding a sequence $\{w_n\}$ which converges towards u. The physical implication of this statement is well known in optics. Lohmann (1978) calls it 'the limit of three-dimensional display', i.e. the impossibility of achieving an arbitrary three-dimensional field amplitude distribution inside a volume by acting on the boundary alone. It is a typical feature of systems governed by PDE that solutions may span a proper closed subspace instead of the whole state space. In dynamical DPS, this originates the definitions of 'T-approximate controllability', when the range of the control map at time T is dense in some subspace, and of 'T-strict controllability', when the control map at time T is onto the state space (see e.g. Curtain and Pritchard 1978, Delfour and Mitter 1972). Finally we stress that nothing similar occurs in systems governed by ordinary differential equations, because their state space is finite dimensional.

The map C defined by (3.17) can be related to the trace operator γ^1, which yields the normal derivative at the boundary. We have:

$$C = \gamma^1\restriction_{\Gamma_2}. \tag{3.21}$$

We are interested in C^{-1}, which makes sense if Ker $C = \{0\}$. By taking (3.2) into account, we look for the solution w which vanishes on Γ_2 together with its normal derivative. Zero Cauchy data on the boundary or part of it imply (see e.g. Miranda 1970) that w vanishes everywhere in Ω. Hence in our particular case C is invertible.

After listing the properties of B and C, we can now define the composite linear map

$$\begin{aligned} M := C \bullet B &: H^{1/2}(\Gamma_1) \to H^{-1/2}(\Gamma_2) \\ v &\mapsto \left.\frac{\partial w}{\partial \nu}\right|_{\Gamma_2}. \end{aligned} \tag{3.22}$$

By combining the statements discussed above we find that

$$\operatorname{Ker} M = \{0\}. \tag{3.23}$$

From (3.23), normal derivative data on Γ_2 together with the SE (2.1), BC (3.2) and condition (3.11) are necessary and sufficient for the boundary control v to be identified uniquely. This is a particular inverse diffraction problem in a bounded domain, which is shown to have unique solution.

3.4. Extension to a general inverse problem in a bounded domain

If we replace the homogeneous BC on Γ_2 by

$$w|_{\Gamma_2} = h_1 \tag{3.24}$$

we still have well defined maps

$$\begin{aligned} B_1 &: H^{1/2}(\Gamma_1) \to H^1(\Omega) \\ &\quad v \mapsto w \end{aligned} \tag{3.25}$$

provided (3.11) holds, and

$$\begin{aligned} C_1 &: H^1(\Omega) \to H^{-1/2}(\Gamma_2) \\ &\quad w \mapsto \frac{\partial w}{\partial \nu}\bigg|_{\Gamma_2} = h_2. \end{aligned} \tag{3.26}$$

M_1, defined by

$$M_1 := C_1 \cdot B_1 \tag{3.27}$$

is a map from $H^{1/2}(\Gamma_1)$ to $H^{-1/2}(\Gamma_2)$. It is not linear because $v_1 = w|_{\Gamma_1}$ such that $h_2 = 0$, given $h_1 \neq 0$, is non-zero. M_1 is invertible: given the non-zero Cauchy data on Γ_2 $(h_1; h_2)$ the control v_1 at Γ_1 is uniquely identified. This can be proved *per absurdum* by assuming the existence of two distinct solutions w_1, w_2, having Γ_1 traces respectively v_1 and v_2. By solving the PDE system for $w_1 - w_2$ we are led to a Cauchy problem with zero data on Γ_2, which implies $w_1 \equiv w_2$ everywhere in $\bar{\Omega}$, hence $v_1 \equiv v_2$.

M_1 is an affine map, as can be proven by superposition. We shall write

$$\operatorname{Im} M_1 = M_1(0) + \operatorname{Im} M \tag{3.28}$$

where M is defined by (3.22) and we mean thereby that every element in the set $\operatorname{Im} M_1$ is obtained by translating the corresponding element in $\operatorname{Im} M$ by the vector $\partial w(v_1 = 0)/\partial\nu|_{\Gamma_2} = M_1(0)$. The latter depends on h_1.

We have thus shown the uniqueness of solution of an inverse problem (identification of boundary condition) when arbitrary Cauchy data are given.

3.5. 'Generalised controllability' and the adjoint system

For reasons which will be found in the next sections we now give a density statement for the map M. In the proof the role of duality will be stressed. By somehow arbitrarily extending the nomenclature used in dynamical system theory, we define the PDE system (2.1), (3.2), (3.17), subject to (3.11) to be '$\Gamma_1 \to \Gamma_2$ approximately controllable' in a generalised sense if

$$\overline{\operatorname{Im} M} = h^{-1/2}(\Gamma_2). \tag{3.29}$$

The physical meaning of (3.29) is that any element in $H^{-1/2}(\Gamma_2)$ can be approximated as closely as we wish with respect to the topology of $H^{-1/2}(\cdot)$, by adequately choosing the boundary control v. The proof of (3.29) will now follow. We notice that the indexes of trace spaces appearing e.g. in (3.22) are fractional. This fact is among the hypotheses of the trace theorem mentioned above for Sobolev spaces. A property similar to (3.29) is stated and proved in Lions (1971, p 78): however, it involves Sobolev spaces with integer indexes.

A density statement for a linear subspace $S \subseteq H$, i.e. $\bar{S} = H$, holds if the only element h orthogonal to S is $h = 0$. In our case $S = \operatorname{Im} M$; $H = H^{-1/2}(\Gamma_2)$. To state orthogonality we do not use the inner product in $H^{1/2}(\cdot)$, but we require the antilinear form defined below to vanish:

$$ {}_{H^{-1/2}(\Gamma_2)}\left\langle \frac{\partial w(v)}{\partial \nu}, h \right\rangle_{H^{1/2}(\Gamma_1)} = 0; \qquad \forall v \in H^{1/2}(\Gamma_1). \tag{3.30} $$

The subscripts remind us of the affiliations of the bra and the ket. As we shall see, (3.30) is a term appearing in Green's formula, the arguments of which belong to the above defined 'primal' PDE system and to an auxiliary system the 'adjoint', which is linked to the primal by duality rules. The adjoint system reads

$$ \begin{aligned} &L^+ p + \bar{k}^2 p := K^+ p = 0 \qquad x \in \Omega \\ &p|_{\Gamma_1} = 0 \\ &p|_{\Gamma_2} = h \in H^{1/2}(\Gamma_2). \end{aligned} \tag{3.31} $$

The rules for writing (2.31) are

(i) replace the state equation (2.1) with its adjoint; in general even if $k^2 n(x)^2$ is real, we do not know if $K = K^+$, unless we prove the domains $D(K)$, $D(K^+)$ are equal;

(ii) put a homogeneous Dirichlet BC where a control acted on the w-system;

(iii) put a control h on Γ_2 where we observe w. Moreover, as we are going to prove a density statement, the control h must satisfy (3.30). Its regularity is also known.

Fredholm's theorem also applies to (3.31), to state existence, uniqueness, regularity of solution $p(\cdot)$ and structure of σ_{L^+}. The results can be derived by analogy from those listed in § 3.2.

3.6. *The Green formula for the w and the p systems*

We have arrived at the adjoint system by rules (i) to (iii), which are based on system theoretical duality between control and observation (Delfour and Mitter 1972, Dolecki and Russel 1977). If we have two sets of operands which are dual to each other, we can at least formally apply the second Green formula (where the overbar denotes the complex conjugate):

$$ \int_\Omega \mathrm{d}\Omega\, (\bar{p} K w - \bar{K}^+ \bar{p} w) = \int_\Gamma \mathrm{d}\Gamma \left(\bar{p} \frac{\partial w}{\partial \nu} - \left(\frac{\partial \bar{p}}{\partial \nu} \right) w \right). \tag{3.32} $$

To stress the symmetry of the formula we shall introduce the following notation (Berzi 1976)

$$ \int_\Omega \mathrm{d}\Omega\, p \overleftrightarrow{K} w = \int_\Gamma \mathrm{d}\Gamma\, p \frac{\overleftrightarrow{\partial}}{\partial \nu} w \tag{3.33} $$

in close analogy to what is done in quantum field theory. All hypotheses for its weak form, listed in appendix 4 of Baiocchi and Capelo (1978) are satisfied by the non-zero operands in the primal and dual systems. The formula is a functional relationship between the state w of the controlled system and the state p of the observed one. p is a 'Green function'. Most readers may be familiar with the heuristic Green formula used in optics, where the Green function is the solution of a state equation having a 'delta function' source term and homogeneous BC. Actually the Green function, i.e. the dual system, is not assigned in a unique way: it depends on the task we want to solve. If we are interested in the field value at a point, then the appropriate source term is a delta function. If our task is an 'approximate controllability' proof, system (3.31) is needed. Later on we shall meet an optimal control problem: the dual state equation will have a distributed source term (see § 4).

Back to equation (3.32), from equations (2.1), (3.2), (3.30), (3.31) the only term left reads

$$\int_{\Gamma_1} \mathrm{d}\Gamma \frac{\partial \bar{p}}{\partial \nu} u = 0 \qquad \forall \in H^{1/2}(\Gamma_1) \tag{3.34}$$

hence $\partial p/\partial \nu|_{\Gamma_1} = 0$, which together with $p|_{\Gamma_1} = 0$ forms a Cauchy problem for the system (3.31) we have already met. In particular, it follows that $h = 0$ is the only element orthogonal to Im $C \cdot B$. Therefore property (3.29) holds.

3.7. Density statements and inverse diffraction

Given a linear operator M mapping a linear topological space U into another linear topological space Y, such that $\overline{\operatorname{Im} M} = Y$, and given the operator M^+ adjoint to M, which relates dual spaces, mapping Y' into U', it can be proved that:

$$\overline{\operatorname{Im} M} = Y \Leftrightarrow \operatorname{Ker} M^+ = \{0_{Y'}\} \tag{3.35}$$

Ker M^+ is the set of elements which are mapped into the null element of U'. Equation (3.25) is in many respects the relationship which originated research on system theoretical duality (Delfour and Mitter 1972, Dolecki and Russel 1977). If we identify U and Y respectively as the input and output spaces of the w (or primal) system and Y', U' as the input and output spaces of the p (or dual) system, then we can draw the following diagrams which synthesise some properties listed above:

$$U \xrightarrow{M} Y \qquad\qquad Y' \xrightarrow{M^+} U'$$

$$H^{1/2}(\Gamma_1) \to H^{-1/2}(\Gamma_2) \qquad\qquad H^{1/2}(\Gamma_2) \to H^{-1/2}(\Gamma_1)$$

$$u \mapsto \frac{\partial w}{\partial \nu}\bigg|\Gamma_2 \qquad\qquad h \mapsto \frac{\partial p}{\partial \nu}\bigg|\Gamma_1.$$

We can relate the input to the output by 'overriding' the state space and write:

$$\overline{\operatorname{Im} M} = Y. \tag{3.36}$$

Now we invoke (3.35) and conclude that in proving the 'approximate $\Gamma_1 \to \Gamma_2$ controllability' for the primal system, we implicitly showed that the linear map M^+ is one-to-one. The physical consequence is that given $p|_{\Gamma_1} = 0$, if we know $\partial p/\partial \nu|\Gamma_1$, we can reconstruct $p|_{\Gamma_2} = h$ unambigouously: the inverse problem or '$\Gamma_1 \to \Gamma_2$ observation' on the adjoint system has a unique solution.

This density statement is an alternative proof of uniqueness for the primal system inverse problem, because results are invariant with respect to duality. The structure of the second Green formula itself reminds us of this fact: this is nothing but a consequence of charge conservation by the scalar field (Roman 1968). With some additional calculations we can deal with arbitrary Dirichlet BC on Γ_2 for p: we remind the reader that duality easily extends to affine systems (Delfour and Mitter 1972).

Uniqueness holds for identification of boundary condition at Γ_1, if geometry is known, eigenvalues are excluded and Cauchy data on Γ_2 are available. If Γ_1 includes a measurable volume, we expect some sources to be located therein. The system studied here does not allow us to reconstruct that source distribution in a unique way. This is a well known result of inverse *scattering* theory, for which the reader is referrred to Arnett and Goedecke (1968), Bleistein and Cohen (1978).

4. Optimal control problems

4.1. An introductory example

Before discussing how to solve a practical inverse diffraction problem, i.e. given some measured Cauchy data on an adequate support, find the input which orginated them, we sketch some basic features of optimal control theory for elliptic PDE, although in the simplified form which fits our needs.

Let the DPS be described by

$$\begin{aligned} &Ay=0 \quad \text{in } \Omega \\ &y|_{\Gamma}=v\in U_{\mathrm{ad}}\subseteq U=H^{m-1/2}(\Gamma) \\ &Cy=y \quad \text{in } \Omega \end{aligned} \tag{4.1}$$

where A is an elliptic operator and y is a real valued function. We assume that existence, uniqueness and regularity of the solution $y(v)$ in a real Sobolev space are guaranteed by some adequate hypotheses. The map C here denotes distributed observation all over Ω.

Let the 'cost functional' be defined by

$$J(v):=\int_{\Omega}\mathrm{d}\Omega\,(y(v)-z_d)^2+c\|v\|_U^2:=P(v)+E(v) \qquad c>0 \tag{4.2}$$

where z_d is an arbitrary function defined in Ω. The 'physical' term $P(v)$ compares the solution $y(v)$ to the desired output z_d by a quadratic criterion. The 'economical' term $E(v)$ weights the cost of implementing the boundary control v, which must be chosen inside U_{ad}, a subset of the input space U.

A control $u\in U_{\mathrm{ad}}$ is defined 'optimal' if it minimises $J(\cdot)$:

$$J(u)=\inf_{v\in U_{\mathrm{ad}}} J(v). \tag{4.3}$$

The minimum of $J(\cdot)$ exists and is unique if (Lions 1971):

(i) U_{ad}, the admissible input set, is a closed subset of the Hilbert space U;

(ii) U_{ad} is convex, i.e.

$$\theta v_1+(1-\theta)v_2\in U_{\mathrm{ad}},\ \forall\theta,\ 0\leqslant\theta\leqslant 1,\ \forall v_1,\ v_2\in U_{\mathrm{ad}}; \tag{4.4}$$

(iii) $J(\cdot)$ is a continuous functional of v, satisfying

$$\lim_{\|v\|\to\infty} J(v)=+\infty; \tag{4.5}$$

(iv) $J(\cdot)$ is convex, i.e.

$$\forall v_1, v_2 \in U_{\mathrm{ad}}, \forall \gamma, 0 \leq \gamma \leq 1: J(\gamma v_1 + (1-\gamma)v_2) \leq \gamma J(v_1) + (1-\gamma)J(v_2). \tag{4.6}$$

It can be shown that J as defined by (4.2) satisfies all of these hypotheses, hence it attains its infimum value at u.

The optimal control problem we are interested in is stated by: (a1) the system (4.1) subject to (a2) condition (4.3). The latter can be converted into an inequality by invoking the general theory explained by Lions (1971, pp 9–17).

Given the real valued functional (4.2)

$$\begin{aligned} J\colon U_{\mathrm{ad}} &\mapsto R \\ v &\mapsto J(v) \end{aligned} \tag{4.7}$$

its Gateaux derivative (G-derivative) ∇J is defined as (Baiocchi and Capelo 1978, pp 38–52) the 'bra' vector such that

$$\lim_{\lambda\to 0} \frac{J(v+\lambda\delta v) - J(v)}{\lambda} = \underset{U'_{\mathrm{ad}}}{\langle} \nabla J(v), \delta v \underset{U_{\mathrm{ad}}}{\rangle} \qquad \lambda \geq 0; \forall\, \delta v \in U_{\mathrm{ad}} \tag{4.8}$$

where U'_{ad} is the dual of U_{ad} and δv is a variation of v allowed by the constraints, if any. If $U_{\mathrm{ad}} = U$, the problem is unconstrained.

By theorem (1.2) of Lions (1971, p 9), the minimising element u of (4.3) is characterised by the 'variational inequality'

$$\langle \nabla J(u), (v-u)\rangle \geq 0; \forall v \in U_{\mathrm{ad}} \tag{4.9}$$

where $(v-u)$ is the same as δu, or by

$$\langle \nabla J(v), v-u)\rangle \geq 0; \forall v \in U_{\mathrm{ad}}. \tag{4.10}$$

We are interested in determining the G-derivative, or gradient, explicitly. To this end we need the Lagrangian approach.

The solution of (4.1) can also be defined through the second Green formula. If there exists $y \in H^m(\Omega)$ such that

$$\int_\Omega \mathrm{d}\Omega\, p\overleftrightarrow{A} y = \int_\Gamma \mathrm{d}\Gamma\, p \frac{\overleftrightarrow{\partial}}{\partial \nu_A} y; \qquad \forall p \in H_0^m(\Omega) \tag{4.11}$$

We say y is the 'weak solution' of (4.1). $\partial/\partial\nu_A$ is the 'co-normal' derivative (Lions 1971, p 24), p plays the role of a Lagrangian multiplier. We denote the first and second integrals in (4.11) by $F(p; y)$ and $G(p; v)$ respectively.

The 'augmented cost functional' or problem Lagrangian is defined by

$$\boldsymbol{L}(y; v) := J(v) + F(p; y) - G(p; v) \tag{4.12}$$

where, due to (4.1) and (4.11),

$$F(p; y) = \int_\Omega \mathrm{d}\Omega\, A^+ py \tag{4.13}$$

$$G(p; v) = \int_\Gamma \mathrm{d}\Gamma \frac{\partial p}{\partial \nu_A} v. \tag{4.14}$$

The minimum of $\boldsymbol{L}$, which is unique because hypotheses (i) to (iv) above can be proved to hold, is characterised by $\delta\boldsymbol{L}(y(u); u) = 0$. As it is customary in Lagrangian theory, we take y and v as independent variables and write the first variation

$$\delta \boldsymbol{L} = \frac{\partial \boldsymbol{L}}{\partial y}\delta y + \frac{\partial \boldsymbol{L}}{\partial v}\delta v = 0. \tag{4.15}$$

We may well require

$$\frac{\partial \boldsymbol{L}}{\partial y}\delta y = 0 \qquad \forall\, \delta y \in H^m(\Omega) \tag{4.16}$$

which explicitly means

$$\int_\Omega \mathrm{d}\Omega\, [2(y - z_d) + A^+ p]\, \delta y = 0 \qquad \forall\, \delta y \in H^m(\Omega). \tag{4.17}$$

We are left with

$$\int_\Gamma \mathrm{d}\Gamma \frac{\partial p(v)}{\partial \nu_A}\delta v + 2c(v\,|\,\delta v)_U = 0 \qquad \forall\, \delta v \in U_{\mathrm{ad}}. \tag{4.18}$$

If $U = H^0(\Gamma)$, then the wanted gradient reads

$$\langle \nabla J(v), \cdot \rangle = \left(\frac{\partial p(v)}{\partial \nu_A} + 2cv\,|\,\cdot\right)_U. \tag{4.19}$$

We still have to characterise p uniquely. (4.17) and (4.11) define it as the solution of the 'adjoint system'

$$\begin{aligned} &A^+ p = -2[y(v) - z_d] \\ &p|_\Gamma = 0 \end{aligned} \tag{4.20}$$

for which existence, uniqueness and regularity theorems also apply.

Hence, instead of conditions (a1), (a2) above, in order to find the optimal control u we can use the following:

(b1) the primal system (4.1)
(b2) the adjoint system (4.20)
(b3) the variational inequality

$$\langle \partial p(v)/\partial \nu_A + 2cv,\, v - u \rangle \geqslant 0 \qquad \forall\, v \in U_{\mathrm{ad}}. \tag{4.21}$$

We notice that state equation (4.20) has the 'physical error' as a source term. This is related to the optimal control functional we must minimise. Finally, we stress that z_d has not been specified further: it need not be the solution of a given PDE, i.e. an input $v \in U_{\mathrm{ad}}$ such that $P(v) = 0$ may not exist. This fact is acceptable because we are dealing with optimal control, not controllability. In inverse problems often z_d results from interpolated experimental data; they can be represented by the sum of a deterministic function which is the solution of a PDE, and a stochastic process completely unrelated to the mathematical model of the physical phenomenon.

4.2. Cost functionals depending on complex variables

We must extend the results of § 4.1 to diffraction problems, where system states are complex quantities, i.e. scalar field amplitudes w, p, etc. the cost functional we need and the corresponding 'extended' Lagrangian, denoted respectively by J^e, $\boldsymbol{L}^e$, must take on real values, their physical meaning being related to energy. Sufficient conditions for this property to hold is that J^e, $\boldsymbol{L}^e$ be bilinear forms in $(w; \bar{w})$, etc, and/or contain terms like $|d|^2 . (w+\bar{w})$ etc, $d \in \mathbb{C}$. In order to satisfy these conditions we may have to add some terms to the old J, $\boldsymbol{L}$. The extension problem is also met and solved in Lagrangian field theory (see e.g. Roman 1968, part 1), where switching over from real to complex fields and possible addition of new terms in order to get say $\boldsymbol{L}^e$ is equivalent to doubling the system's degrees of freedom.

Let

$$
\begin{aligned}
w &= (w_r + i w_i)/2^{1/2} \\
\bar{w} &= (w_r - i w_i)/2^{1/2} \qquad (4.22) \\
w_r,\ w_i & \qquad \text{real.}
\end{aligned}
$$

Of course $\boldsymbol{L}^e(w; \bar{w}) = \boldsymbol{L}^e(w_r; w_i)$. We have a unitary transformation between fields, which enables us to perform calculations on $\boldsymbol{L}^e(w_r; w_i)$, a real functional of real independent variables. Equivalently $\delta \boldsymbol{L}^e$ is evaluated by varying w, $\bar{w}$ independently. If we refer to the example in § 4.1, we now let the state equation (4.1) hold for w; the extension rule brings in also the conjugate state equation for $\bar{w}$; the same holds for the dual system (4.20). Moreover

$$J^e := \int_\Omega \mathrm{d}\Omega\, (\bar{w} - \bar{z}_d)(w - z_d) + d\bar{d}(v\,|\,v)_U \qquad d \in \mathbb{C} \qquad (4.23)$$

and

$$\boldsymbol{L}^e(w; \bar{w}; v; \bar{v}) = J^e(w; \bar{w}; v; \bar{v}) + F(p; w) + F(\bar{p}; \bar{w}) - G(p; v) - G(\bar{p}; \bar{v}) \qquad (4.24)$$

which must be compared with (4.12), (4.13) and (4.14) for notations. By extending (4.18)

$$\frac{\partial \boldsymbol{L}^e}{\partial v}\,\delta v + \frac{\partial \boldsymbol{L}^e}{\partial \bar{v}}\,\delta \bar{v} = 0 \qquad (4.25)$$

we get the counterpart of (4.10)

$$\langle \nabla \boldsymbol{L}^e(\boldsymbol{v}), \boldsymbol{v} - \boldsymbol{u} \rangle \geqslant 0 \qquad \forall \boldsymbol{v} \in U_{\mathrm{ad}} \times U_{\mathrm{ad}} \qquad (4.26)$$

where

$$\nabla \boldsymbol{L}^e = \begin{bmatrix} \overline{\partial \boldsymbol{L}^e / \partial v} \\ \partial \boldsymbol{L}^e / \partial \bar{v} \end{bmatrix} \qquad \boldsymbol{v} - \boldsymbol{u} = \begin{bmatrix} v - u \\ \bar{v} - \bar{u} \end{bmatrix} \qquad (4.27)$$

(4.26) makes sense because in this case it relates to the real valued first variation of (4.24).

As we have seen the meaning of Lagrangians depending on complex field variables, we may apply these concepts to the density statement of §§ 3.5–3.7. The second Green formula (§ 3.6) then becomes part of a suitably defined problem Lagrangian. We do not go into further details, however. We just notice that a density statement can also be proved by a variational approach: a Lagrangian is written, its first variation evaluated and some terms thereof set in a seemingly arbitrary way equal to zero. The adjoint system is thus arrived at. Equivalently in § 3.5 we stated the duality rules in a seemingly arbitrary way in order to write the adjoint system just at the beginning of the proof. This remark should make the connection between the Green formula and the Lagrangian more clear, thus supporting the statement on charge conservation at the end of § 3.7.

4.3. The regularisation of the inverse diffraction interior problem

The Cauchy problem for an elliptic PDE is ill posed in the Hadamard sense (Miranda 1970, Ladyzhenskaia and Uraltseva 1968). The solution is unique but does not depend continuously on data. This lack of regularity becomes relevant when data are affected by measurement errors. To overcome ill posedness a regularisation procedure is used, which is borne by duality between control and estimation. The particular scheme we shall describe is suggested by a work by Bensoussan (1967), also described in Lions (1971, p 216ff), aiming at estimating the initial condition of a parabolic PDE.

Given the primal state equation (2.2) and given the measured data

$$w|_{\Gamma_2} = h_1, \qquad \left.\frac{\partial w}{\partial \nu}\right|_{\Gamma_2} = h_2$$

(the roles of Γ_1 and Γ_2 in figure 1 can be interchanged), we must reformulate the system in order to combine the suggestions listed in §§ 4.1 and 4.2.

Let

$$\begin{cases} Kw_1 = 0 \\ w_1|_{\Gamma_1} = v \\ w_1|_{\Gamma_2} = h_1 \\ Cw_1 = w_1 \quad \text{in } \Omega \end{cases} \qquad \begin{cases} Kw_2 = 0 \\ w_2|_{\Gamma_1} = v \\ \partial w_2/\partial \nu|_{\Gamma_2} = h_2 \\ Cw_2 = w_2 \quad \text{in } \Omega \end{cases} \tag{4.28}$$

both are subject to condition (3.11).

v is the boundary value to be identified. The w_1 system is of Dirichlet type; the w_2 system is a mixed boundary value (BV) problem. As Γ_1 and Γ_2 are closed and disjoint, both problems can be easily shown to admit unique solutions w_1, w_2 (Miranda 1970, Ladyzhenskaia and Uraltseva 1968); their regularity is linked to that of data as discussed in § 3.2.

Let us think of the direct problem for, say, the w_1 system. Given $(v; h_1)$ we get w_1; h_2 is then the normal derivative of w_1 at Γ_2. If we take exactly $(v: h_2)$ as a data for a mixed BV problem, we again find w_1, hence $w_1 = w_2$ i.e. in Ω.

$(h_1; h_2)$ as experimentally determined, are affected by noise, hence the values we assign to h_2 are no longer related to w_1 in a deterministic way. Yet it makes sense to equate h_2 to a normal derivative and therefore to write the w_2 system. These remarks help in relating the direct (control) to the inverse (identification of v) task. We shall write a physical term in the cost functional, which compares $w_1(v)$ with $w_2(v)$:

$$P^{e}(v) := \int_{\Omega} \mathrm{d}\Omega \, |w_1(v) - w_2(v)|^2. \tag{4.29}$$

If $J^{e}(\cdot)$ for this problem consisted of $P(\cdot)$ alone, J^{e} would not be stable†, a fact stemming from original ill posedness. In order to warrant existence uniqueness and stability of the minimising element we introduce

$$E^{e}(v) := \varepsilon \|v\|_U^2 \qquad \varepsilon > 0 \tag{4.30}$$

and set

$$J_{\varepsilon}(\cdot) := P^{e}(\cdot) + E^{e}(\cdot). \tag{4.31}$$

† i.e. its minimising element would not continuously depend on data $(h_1; h_2)$.

The inverse problem consists of finding u_ε such that

$$J_\varepsilon(u_\varepsilon) = \inf_{v \in U_{ad}} J_\varepsilon(v). \tag{4.32}$$

The regularity of the BC to be identified must be known *a priori.* For simplicity we set

$$U_{ad} = U = H^0(\Gamma_1). \tag{4.33}$$

If the counterpart of conditions (i) to (iv) in § 4.1 hold for J_ε then u_ε is unique. Moreover

$$\lim_{\varepsilon \to 0} u_\varepsilon = \hat{u} \tag{4.34}$$

where $\hat{u}$ is such that $P^e(\hat{u}) = 0$. The method presented here is also known as Tichonov's regularisation (Tichonov and Arsenin 1976). We want to characterise u_ε by the counterpart of conditions (b1) to (b3) in § 4.1. As a first step we define the conjugate primal system pair, having solution $[\bar{w}_1(\bar{v}); \bar{w}_2(\bar{v})]$; w_1, w_2, $\bar{w}_1$, $\bar{w}_2$ satisfy a suitable second Green formula analogous to (4.11), the only difference being caused by the mixed BV problem. We note in passing that normal and co-normal derivatives for the Laplacian coincide. By a procedure, which mostly duplicates the one given, described in § 4.1 and which is lengthened by the use of conjugate states, we arrive at the optimality set consisting of:

(c1) the primal system pair (4.28) and its conjugate

(c2) the adjoint system pair

$$\begin{array}{ll} K^+ p_1 = w_1 - w_2 & K^+ p_2 = w_1 - w_2 \\ p_1|_{\Gamma_1} = 0 & p_2|_{\Gamma_1} = 0 \\ p_1|_{\Gamma_1} = 0 & \partial p_2/\partial\nu|_{\Gamma_2} = 0 \end{array} \tag{4.35}$$

and its conjugate;

(c3) the variational inequality

$$\int_{\Gamma_1} d\Gamma_1 \left(\frac{\partial}{\partial\nu}[\bar{p}_1(\bar{v}) - \bar{p}_2(\bar{v})] + \varepsilon\bar{v}\right)(v - u_\varepsilon) + \int_{\Gamma_1} d\Gamma_1 \left(\frac{\partial}{\partial\nu}[p_1(v) - p_2(v)] + \varepsilon v\right)(\bar{v} - \bar{u}_\varepsilon) \geqslant 0$$

$$\forall\, (v; \bar{v}) \in H^0(\Gamma_1) \times H^0(\Gamma_1) \tag{4.36}$$

which explicitly contains the regularising parameter ε. The practical relevance of (4.36) will be discussed further in the next section.

4.4. *The structure of a data inversion algorithm*

In § 4.3 we have related near field reconstruction to minimisation of a functional. This connection which is brought about by the variational approach to solutions of PDE, also play a basic role in suggesting how an algorithm should be designed. For an extensive treatment of the theoretical approach and its practical consequences in parameter identification, we refer the reader to Chavent's (1971, 1977) fundamental work and to the literature mentioned therein.

The inequality (4.26) must be inserted into the iterative algorithm, sketched by the flow chart of figure 2, where v_0, the initial estimate of v is somewhat arbitrary.

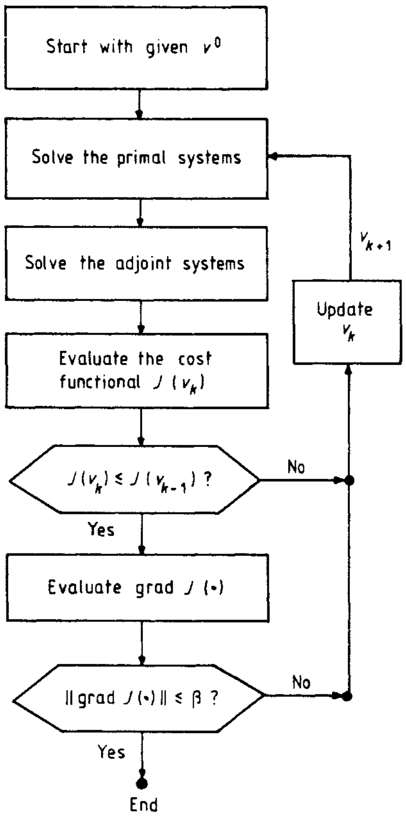

Figure 2. Simplified flow chart for the data inversion algorithm.

Primal and adjoint systems are solved by some standard techniques.

The cost functional and its gradient are evaluated. Then we need an updating law to relate the gradient at the kth iteration to the $(k+1)$th estimate of v. This law is the basic feature of steepest descent algorithms (see e.g. Chavent 1977). The target is to minise $\|\nabla J_\varepsilon\|$; the inequality

$$J_\varepsilon^{(k+1)} \leqslant J_\varepsilon^{(k)} \tag{4.37}$$

must also hold for any result to make sense. The stopping test is given by:

$$\|\nabla J_\varepsilon\| \leqslant \beta \qquad \beta > 0, \text{ given.} \tag{4.38}$$

The gradient is yielded by (4.36)

5. Conclusion

We have tried to show how some system theoretical concepts such as duality, controllability, observability, optimal control can be relevant in the theory of inverse diffraction and lead to the design of a functional minimisation algorithm.

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