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EXTENDED VARIATIONAL FORMULATION

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The paper shows how to transform a given problem, linear or nonlinear, into another that has the same solution and that admits a variational formulation with a (true) minimum. For a given problem there exists an infinity of equivalent problems, each with minimality property. The method uses integral transforms whose kernels must satisfy appropriate conditions. A general procedure is described that permits to generate kernels for initial or boundary value problems with arbitrary domains. The use of degenerate kernels permits us to obtain a numerical solution for problems defined on complicated domains.

1. Notation

The term *equation* refers to differential, integral, integro-differential, algebraic or operator equation of whatever kind; it may be a single equation or a system of equations. The functions appearing in an equation may depend on one or more variables. These functions may be scalar, vector, tensor, matrix–valued, functions, etc. The term *additional conditions* refers to initial, boundary, asymptotic, periodic conditions, etc. and the functional class, say $C^2(\Omega)$, $L^2(\Omega)$, etc.

The term *problem* means the set formed by an equation and additional conditions. A problem will be denoted as

$$N(u) = f \text{ equivalent to } \begin{cases} \mathcal{N}(u) = f \text{ (equation)} \\ \text{additional conditions on } u. \end{cases} \tag{1}$$

We call N the *operator* of the problem and $\mathcal{N}$ the *formal operator* [12].

We use the symbol N to denote a nonlinear operator and $v = N(u)$ to denote the correspondence between two variables, putting the argument u in round brackets like in a function $y = f(x)$ while a linear operator will be denoted Lu without brackets like in the linear function $y = fx$. An operator depending on two arguments will be denoted $w = P(u, v)$ just like a function of two variables is denoted $z = f(x, y)$. If it is linear on v, we shall write $w = P(u)v$ or also $w = P_u v$. The *domain* of the operator is understood to be the set of functions that satisfy the given additional conditions. $\mathcal{N}$ denotes the formal operator.

We shall say that two problems, or two equations, are *equivalent* when they have the same solution set.

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2. The meanings of the variational formulation

The term *inverse problem* of the calculus of variations stands for the search of a variational formulation for a given problem. It has four different interpretation as describes in the sequel.

2.1. The formal variational formulation

The classical variational formulation can be stated as follows: [2].

> Given an *equation* $\mathcal{N}(u) = f$, find a functional $F[u] = \int_\Omega \mathcal{F}(u) d\Omega$, if it exists, whose Euler-Lagrange equation coincides with the given equation.

The attention is normally focused on the equation while the additional conditions are neglected. Since only the formal operator $\mathcal{N}$ is involved, we shall call this a *formal* variational formulation.[3]

This is the usual meaning given to the expression "inverse problem" in theoretical physics. The functional that gives the field equations is called the *action* of the field. The assertion that the action is stationary with respect to the solution is known as the principle of stationary action. It must be remarked that even if it is often called the principle of *minimal action* the action is only stationary [7, p.66].

In the above context *the main interest is to characterize the structure of the field equation*, and not to look for the solutions by using the direct method as for example, the Ritz method. The spirit is well described by the famous statement by Sir Arthur Eddington: "From its first introduction, action has always been looked upon as something whose sole *raison d'être* is to be varied — and, moreover, *varied in such a way as to defy the laws of nature!*" [10, p.137].

This means that the variational formulation, understood in this sense, does not goes beyond the derivation of the Euler-Lagrange equations, i.e., field equations or equations of motion. The solution of the equation is performed by the traditional integration methods for ordinary or partial differential equations in which the existence of the functional play no role.

This formulation become more attractive after the discovery by Noether that there is a link between invariance and conservation laws that may easily be inferred from the invariance of the functional.

The prototype of this variational formulation is the Hamilton principle for evolution equations. The various field actions used in field theories are generalizations of the same principle. The Hamilton principle and its generalization cannot be used to find the solution of problem of Eq.(1) in the case of time dependent fields. The reason is that in order to find the stationary value of the functional, it is necessary to consider functions that vanish at initial and final instants of a given time interval. Since in a time dependent field, the field at the *final* instant is not known, it is impossible to utilize the direct methods of the calculus of variations. This because the base functions used in such a method should satisfy a final condition that is not known a priori (with the obvious exception of periodic boundary conditions in time).

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[2] [8, p.778], [9, p.63], [18, p.10], [6, p.159], [17, p.75], [5, p.781].

[3] Dedecker [9, 1950, p.63] use the adjective *formal*. See also [22] for a short history of the inverse problem.

2.2. The operatorial variational formulation

A completely different situation arises in time independent problems such as those of electrostatics, magnetostatics, elastostatics, stationary heat conduction, etc. In these cases we have only boundary conditions and the stationarity is searched among the functions satisfying the boundary condition. Here direct methods can be utilized and are commonly used: among them the Ritz method which is used today mainly in the connection with the finite elements method. In these problems we often have a minimum of the functional, contrary to the variational formulation for time dependent fields where the functional is only stationary and does not have a maximum or minimum. Typical is the case of the deformed configuration of a deformable body under the action of conservative forces that attain the minimum of the total potential energy.

The peculiar difference between time-variable fields and statical (or stationary) fields is that in time variable fields the functions used to detect the stationary value of the functional do not satisfy the given initial conditions. In statical (or stationary) fields the functions used in the functional are exactly those that satisfy the given boundary conditions. In the first case, the domain of the functional is different from that of the operator while in the second case the two domains coincide.

This leads to another meaning of the inverse problem:

> Given a problem $N(u) = f$, we ask if there exists a functional F whose Euler-Lagrange equation coincides with the equation of the problem and whose domain coincides with the one of the problem.

This means that the stationary value must be searched *among the functions that satisfy the additional conditions of the problem*. We shall call this the *operatorial* variational formulation. The difference between the formal and the operatorial formulations is illustrated in Fig. (1).

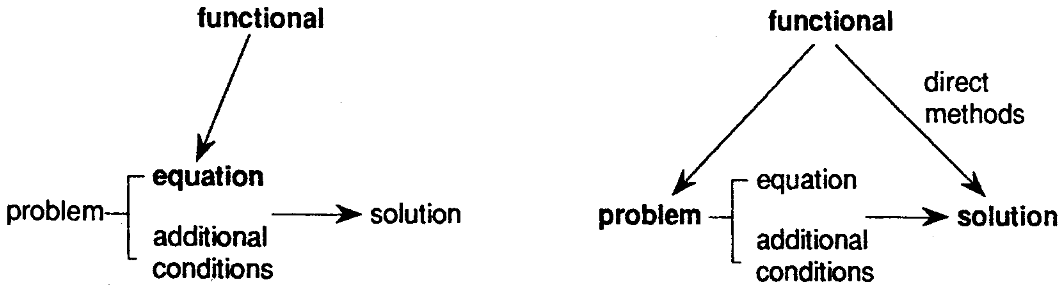

Fig. 1.
The difference between the formal variational formulation (left) and the operatorial variational formulation (right).

2.3. The extended variational formulation

What is to be done when a variational formulation either in the formal or the operatorial sense does not exist? One may try to transform the equation or the whole problem in another equation or problem that is equivalent and admits a variational formulation.

There are many ways to obtain an equivalent *equation*. The simplest way is to multiply the equation by a non-vanishing function $\mu(x)$ called the *integrating factor*

$$\mu[\mathcal{N}(u) - f] = 0. \tag{2}$$

One may generalize the integrating factor to a function containing u and its derivatives, say $\mu(x; u(x), u'(x))$, with the obvious requirement that no new solutions be introduced. In the case of a system of equations one may apply a matrix or simply rearrange the equations. Sometime the equivalence may be obtained by a change of the function $u = f(\phi)$.

To obtain an equivalent *problem* one may apply an operator P on the left with the condition that the operator be invertible. The problem

$$P[N(u) - f] = 0 \tag{3}$$

has the same set of solutions as those of Eq.(1). In particular the operator may be linear and may depend on u:

$$L[N(u) - f] = 0 \quad \text{or} \quad L_u[N(u) - f] = 0 \tag{4}$$

and the problems $Lv = 0$ and $L_u v = 0$ must have only the null solution, $v = 0$ for every u.

Another possibility is to perform an operatorial transform

$$N(Q(\phi)) - f = 0 \quad \text{with} \quad u = Q(\phi). \tag{5}$$

We shall call procedures in Eq.(3) and Eq.(5) left- and right-multiplications, respectively. The prototype of the left-multiplication is used to transform the Cauchy problem into an equivalent integral problem. The prototype of a right-multiplication is the one used in the transformation of the problem $Lu - f = 0$, that has no variational formulation, in the problem $LL^*\phi - f = 0$ which admits a variational formulation.

If, for a given problem, there are other problems equivalent to it, then one of these may admit a variational formulation in the formal or operatorial sense. In this case we shall say that the original problem admits a variational formulation in the *extended* sense. Extended, because, even if the domain of the functional coincides with the domain of the given problem, its Euler-Lagrange equation is not the given equation but that of an equivalent problem.

Then we are lead to a third and fourth interpretations of the inverse problem in the formal and operatorial sense[4]

Given an *equation* $\mathcal{N}(u) = f$, is there an equivalent *equation* that admits a variational formulation in the formal sense?

Given a *problem* $N(u) = f$, is there an equivalent *problem* that admits a variational formulation in the operatorial sense?

[4] Filippov used the term *quasiclassical* formulation [11, p.5]

3. Conservative operators

The conditions to be satisfied by an operator in order to be the gradient of a functional can be found starting from the observation that a mapping $v = N(u)$ with $u \in \mathcal{U}$ and $v \in V$ may be viewed as a *vector field* on the space $\mathcal{U}$ [20].

This is a beautiful and astonishing interpretation! It simplifies the search for criteria for the operatorial variational formulation. It permits us to extend the notion of circulation of a vector field along a line once the notion of a line and a scalar product are introduced. Let us suppose that on the two real normed spaces $\mathcal{U}$ and $\mathcal{V}$ is defined a real nondegenerate bilinear form and that their topologies make the bilinear form continuous: such topologies are called *duality compatible* [19]. Such a bilinear form will be called a *scalar product*.

Let us introduce the notion of line in $\mathcal{U}$ as a continuous mapping $\eta : [0,1] \to \mathcal{U}$. In particular, a straight line from u_0 to u is defined by $\eta(\lambda) = u_0 + \lambda(u - u_0)$.

Let us assume that the domain $\mathcal{D}(N)$ is convex, that the map $\lambda \to \langle N(u+\lambda\phi), \phi\rangle$ is continuous. One may define the *circulation* of the vector $N(u)$ along the line $\eta(\lambda)$ from the point $u_0 = \eta(0)$ to the point $u = \eta(1)$.

$$C \stackrel{\text{def}}{=} \int_{\lambda=0}^{\lambda=1} \langle N(\eta(\lambda)), \delta\eta(\lambda)\rangle = \int_{\lambda=0}^{\lambda=1} \langle N(\eta(\lambda)), \frac{d\eta(\lambda)}{d\lambda}\rangle d\lambda. \tag{6}$$

If this circulation does not depend on the line connecting the two *points* u_0 and u, one may call the vector field, i.e. the operator N, *conservative*.[5] When this happens, one may assign a *potential* to every point of the domain $\mathcal{D}(N)$ given by

$$F[u] \stackrel{\text{def}}{=} F[u_0] + \int_{\lambda=0}^{\lambda=1} \langle N(\eta(\lambda)), \delta\eta(\lambda)\rangle. \tag{7}$$

This potential is the functional we are searching for. In fact it can be shown that

$$\delta F[u] = \langle N(u), \delta u\rangle \tag{8}$$

and then, if the δu form a dense subset of $\mathcal{U}$, the critical points of the functional, i.e. those points for which $\delta F[u] = 0$, are the solutions of the problem $N(u) = 0$. The operator N is called the *gradient* of F. What is the condition of independence of the circulation from the line?

The method used in ordinary vector fields consists of choosing any closed line and verifying that the circulation along this line vanishes. Taking two vectors, i.e. two functions ϕ and ψ, one may write

$$\langle N(u), \lambda\phi\rangle + \langle N(u+\lambda\phi), \mu\psi\rangle = \langle N(u), \mu\psi\rangle + \langle N(u+\mu\psi), \lambda\phi\rangle + \varepsilon(\lambda,\mu). \tag{9}$$

Given some weak continuity assumptions on the derivative N'_u [23, p.56], the path independence requires that $\lim \frac{\varepsilon(\lambda,\mu)}{\lambda\mu} = 0$ for $\lambda \to 0$ and $\mu \to 0$. By dividing both sides for $\lambda\mu$ and taking the limit one obtains

[5] Usually one say "potential" operator in the sense that the operator admits a potential. We think that the name "conservative", reminiscent of the vector fields in $\mathbb{R}^n$, is perfectly legitimate, as are the names "monotone", "symmetric", "continuous", etc.

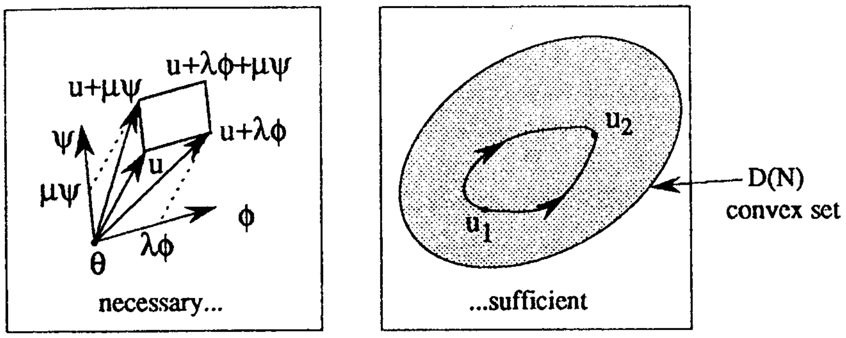

Fig. 2.
The necessary and sufficient conditions for the existence of the potential of an operator.

$$\lim_{\lambda,\mu\to 0}\left[\left\langle\frac{N(u+\lambda\phi)-N(u)}{\lambda},\psi\right\rangle-\left\langle\frac{N(u+\mu\psi)-N(u)}{\mu},\phi\right\rangle\right]=0. \tag{10}$$

If we denote by N'_u the Gâteaux derivative, which is a linear operator, this condition becomes

$$\langle N'_u\phi,\psi\rangle=\langle N'_u\psi,\phi\rangle \quad \text{for every } \phi,\psi\in\mathcal{D}(N'_u),\ u\in\mathcal{D}(N). \tag{11}$$

This means that the derivative of the operator must be symmetric. When the domain is convex, this condition becomes sufficient. Since linear operators have a linear domain and many nonlinear ones have a convex domain (non–homogeneous linear boundary or initial conditions form such a domain) then this condition is sufficient for these operators.

We remember that for a given a linear operator $P:\mathcal{D}(P)\subseteq\mathcal{U}\to\mathcal{V}$, all operators $Q:\mathcal{D}(Q)\subseteq\mathcal{U}\to\mathcal{V}$ satisfying

$$\langle P,\phi,\psi\rangle=\langle Q\psi,\phi\rangle \quad \text{for every } \phi\in\mathcal{D}(P) \text{ and } \psi\in\mathcal{D}(Q) \tag{12}$$

are said to be ***adjoint*** to P [13, p.167]. The operator Q with the largest domain is called *the* adjoint of P and is denoted by P^*. Its domain is the set of *all* elements ψ for which the relation Eq. (12) holds for every $\phi\in\mathcal{D}(P)$. This shows that there are in general many operators that are adjoint to a given one: all of them are *restrictions* of the adjoint P^*, i.e. $Q\subseteq P$. These may be obtained from P^* adding supplementary boundary conditions or, that is more common, restricting the functional class.

When the operator $Q=P$ in Eq.(12), then P is said *symmetric* while when $P^*=P$, the operator P is said *self-adjoint*.

Summarizing one may say that the necessary condition for the existence of a variational formulation is the symmetry of the derivative of the operator. Since this condition was discovered by Volterra,[6] we shall call this the *Volterra symmetry condition*.

[6] See Volterra [25, p.104], [26, p.47], [27]. Kerner quoted Volterra [14, p.572] and Vainberg quoted Kerner [23, p.313]. See also [21] for a detailed exposition of this point.

4. Extended variational formulation

Given a problem that does not satisfy the criteria for the existence of a variational formulation, we shall explore the possibility of finding a general procedure to obtain an equivalent problem using the left-multiplication by an operator. We shall show that, under weak conditions on the operator N, it is possible to generate an infinity of equivalent problems all of which admit a variational formulation.[7] We remark that, in the context of the formal variation formulation, there is not a general procedure to obtain explicitly an integrating factor for an arbitrarily given equation. Much of the early history of the inverse problem of the Calculus of Variations was devoted to the search for integrating factors of special classes of equations [22].

On the contrary, a constructive procedure to find explicitly *integrating operators* in the operatorial formulation has been found [21]. To explain the method used, we shall start with simple considerations on algebraic systems of equations. Let us consider three systems of algebraic equations

$$\begin{cases} +x - 3y = -2 \\ +4x + y = +5 \end{cases}; \quad \begin{cases} +4x + y = +5 \\ -x + 3y = +2 \end{cases}; \quad \begin{cases} +4x + y = +5 \\ +x - 3y = -2. \end{cases} \tag{13}$$

One immediately realizes that they have the same solution $x = y = 1$.

Since the first two matrices are not symmetric, the corresponding systems do not have a variational formulation. To make the matrices symmetric it is enough to change the order of the equations in the first case and to change the sign of the second one. The change of the order of the equation or of the sign of an equation is equivalent to a left-multiplication of the third system by the matrices

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad A = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{14}$$

These matrices are invertible. Performing the product in both cases one obtains a symmetric matrix that gives rise to a system equivalent to the systems Eq. (13). The search of symmetrizing matrices, as we have done now, is based on trial and error method.

This raises the following question: Given a nonsymmetric matrix, does a systematic way to generate symmetrizing matrices exist? The answer is affirmative.

Theorem 1. Given an invertible matrix L (then L^* is also invertible), for every symmetrical and invertible matrix K, the matrix $A = L^*K$ is a symmetrizing matrix. Inversely, for every symmetrizing matrix A there exists an invertible and symmetric matrix K such that $A = L^*K$.

Proof. If K is a symmetric and invertible matrix, putting $A = L^*K$, we see that $AL = L^*KL = (L^*KL)^* = (AL)^*$, then A is a symmetrizing matrix. Inversely, if A is a symmetrizing matrix, then matrix $K = (L^*)^{-1}A$ is also symmetric. In fact, $L^*KL = AL = (AL)^* = (L^*KL)^* = L^*K^*L$ and therefore $K^* = K$. (qed) □

This simple result is significant because, not only it permits to generate in a systematic way *all* symmetrizing matrices, but it way also be extended to other linear operators, such as differential, integral or integro-differential operators. Furthermore, and this is surprising, it can be extended to nonlinear operators. It then gives us the

[7] An analogous result for the right-multiplication in terms of operators seems to be an open problem.

possibility to pass from a search of the integrating *factor* to the *explicit generation* of an infinity of integrating *operators*.

We shall show that it is possible to transform a problem, generally nonlinear, into an equivalent one that satisfies the following three requirements: [11, p.2] (A) the order of the derivatives in the functional must be lower than the one in the equation; (B) the functional is bounded from below; (C) the set of *critical points* of the functional, i.e. the set of elements $u \in \mathcal{U}$ for which $\delta F[u] = 0$ coincides with the set of solutions of the problem.

We shall see in a moment that these requirements can be easily satisfied. The problem of giving an extended variational formulation is solved by the following [21]

Theorem 2. Let $\mathcal{U}$ and $\mathcal{V}$, be two real normed vector spaces and let $\langle v, u\rangle$ be a scalar product that put the two spaces in duality. Given a problem

$$N(u) = f \tag{15}$$

with $N : \mathcal{D}(N) \subseteq \mathcal{U} \mapsto \mathcal{R}(N) \subseteq \mathcal{V}$, let us assume that N satisfies the four conditions

N1) has a convex domain;

N2) admits a (linear) Gâteaux derivative for all $u \in \mathcal{D}(N)$;

N3) the domain of N'_u is dense in $\mathcal{U}$;

N4) for every $u \in \mathcal{D}(N)$ there exists an invertible adjoint of the derivative N'_u which we shall denote by N'^*_u;

Let $K : \mathcal{V} \to \mathcal{U}$ be a *linear* and *continuous* operator that satisfies the four conditions

K1) Symmetry, i.e. $K \subseteq K^*$;

K2) Positive definitess, i.e. $\langle v, Kv\rangle > 0$ for $v \neq 0$[8] on $\mathcal{D}(K)$;

K3) $\mathcal{D}(K) \supseteq \mathcal{R}(N)$ i.e., its domain contains the range of N; and $f \in \mathcal{D}(K)$;

K4) $\mathcal{D}(N'^*_u) \supseteq \mathcal{R}(K)$ i.e. the range is contained in the domain of N'^*_u for every $u \in \mathcal{D}(N)$, i.e.

Under these hypotheses the problem

$$N'^*_u K[N(u) - f] = 0 \tag{16}$$

has the following properties

A1) $\mathcal{D}(N'^*_u KN) = \mathcal{D}(N)$;

A2) is equivalent to Eq. (15);

A3) $N'^*_u KN$ is conservative and the potential is given by

$$F[u] = \frac{1}{2}\langle N(u) - f, K[N(u) - f]\rangle \tag{17}$$

with $\mathcal{D}(F) = \mathcal{D}(N)$. Moreover the critical points of F coincide with the solutions of problem Eq.(15);

A4) if u_0 is a solution of problem Eq.(15) then $F[u] \geq F[u_0]$ and if the solution is unique it is $F[u] > F[u_0]$.

Proof. For property (K3) the operator KN has the same domain of N. For property (N2) the Gâteaux derivative N'_u exists and it is linear; for (K4) the operator $N'^*_u KN$ has the same domain of KN and therefore of N. Then property (A1) is proved.

[8] We follow the notation of Mikhlin [16, p.31].

Every solution of problem Eq. (15) is also a solution of problem Eq. (16). Vice versa, since for (K2) the operator K is invertible and for (N4) $N_u'^*$ is also invertible, then it follows that $N_u'^* K$ is invertible. Then the solutions of the problem Eq.(16) are also solutions of problem Eq.(15) and property (A2) is proved.

Property $\mathcal{D}(F) = \mathcal{D}(N)$ follows from a direct inspection of Eq.(17). Since

$$\begin{aligned} \delta F[u] &= \langle \delta N(u), K[N(u) - f] \rangle = \langle N_u' \, \delta u, K[N(u) - f] \rangle = \\ &= \langle N_u'^* K[N(u) - f], \delta u \rangle, \end{aligned} \tag{18}$$

where we used the symmetry of K given in (Kl), the continuity of K and the continuity of the scalar product. From (N3) the condition $\delta F[u] = 0$ implies by Eq.(18) that $N_u'^* K[N(u) - f] = 0$. The property (A3) is proved.

From (K2) it follows that $F[u]$ is positive. If u_0 is a solution of problem Eq.(15) then $F[u_0] = 0$ and for property (K2) is $F[u] \geq F[u_0]$. If the solution is unique it is $F[u] > F[u_0]$ and then property (A4) is proved. (qed) □

It is remarkable that the solution of whatever problem, linear or nonlinear, with differential or integral equations, with boundary or initial conditions both homogeneous and nonhomogeneous, may be considered as giving the minimum of a functional and, moreover to an infinity of functionals. The extended variational formulation may be utilized also for initial value problems, something that was not possible in the classical calculus of variations because operators connected with initial conditions cannot satisfy the symmetry requirement. From a numerical point of view this theorem permits to use finite elements also in a time domain instead of using finite differences in a time domain and finite elements in a space domain.

5. How to find the operator K

When N is a differential operator the operator K may be of integral kind, e.g.

$$v(s) = \int_{\Omega_x} k(s,x) u(x) d\Omega \tag{19}$$

with $k(s,x) = k(x,s)$. Generally speaking conditions (Kl) and (K3) of Th.(2) are easily satisfied. The fact that K is an integral operator implies the possibility of lowering the order of the derivatives in the functional, as in the case of classical variational formulation. It follows that the requirements (A),(B),(C) stated earlier are satisfied.

It seems difficult to satisfy the conditions (K2) and (K4). In principle every Green function of a symmetric operator with domain Ω that satisfies the same boundary conditions of the given operator may be a useful kernel. But for domains Ω of arbitrary shape this is impracticable because we do not have an explicit form of the Green function. This difficulty has been stressed by Filippov [11, p.6; p.157].

We now present a method to overcome this difficulty. It consists in the use of kernels of the kind

$$k(s,x) = \beta(x)\beta(s)h(s,x), \tag{20}$$

where $h(s,x)$ is a function symmetric in its arguments s, x such that the corresponding integral operator H be positive definite and the function $\beta(x)$ satisfies the homogeneous boundary conditions of $N_u'^*$. Let $\Omega \subseteq \mathbb{R}$ be a bounded domain and let

$\mathcal{U} = \mathcal{L}^p(\Omega)$ and $\mathcal{V} = L^q(\Omega)$ with $p, q > 1$ and $\frac{1}{p} + \frac{1}{q} = 1$ and $\langle v, u \rangle = \int_\Omega v(x)u(x)d\Omega$.
Suppose that $\beta \in L^\infty(\Omega)$ and $h \in L^\infty(\Omega \times \Omega)$

Theorem 3. If the kernel $h(s,x)$ is symmetric and gives rise to a positive definite operator $H : \mathcal{U} \to \mathcal{V}$; if the function $\beta(x)$ vanishes at most on a set of null measure, then the kernel $k(s,x)$ in Eq.(20) gives rise to a positive definite operator $K : \mathcal{V} \to \mathcal{U}$.

Proof. Note that

$$\begin{aligned} \langle v, Kv \rangle &= \int_{\Omega_s}\int_{\Omega_x} h(s,x)\,[\beta(s)v(s)]\,[\beta(x)v(x)]\,dxds = \\ &= \int_{\Omega_s}\int_{\Omega_x} h(s,x)\bar{v}(s)\bar{v}(x)dxds = \langle \bar{v}, H\bar{v} \rangle, \end{aligned} \tag{21}$$

where we set $\bar{v}(x) = v(x)\beta(x)$. Since we have requested that the function $\beta(x)$ may vanish at most on a set of null measure, the condition $v(x) \neq 0$ implies that $\bar{v}(x) \neq 0$. Since $\langle \bar{v}, H\bar{v} \rangle > 0$, it follows that $\langle v, Kv \rangle > 0$. (qed) □

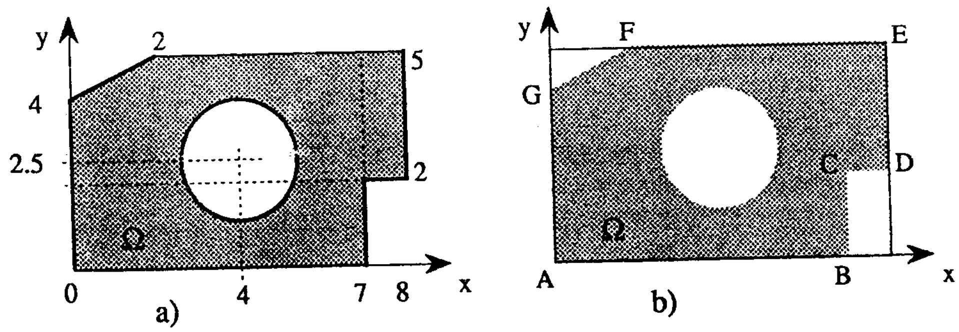

Fig. 3.
An example of complex domain.

In particular in the one dimensional problem the function $\beta(x)$ may vanish at most in a discrete number of points and in the two–dimensional case it must vanish on a finite number of lines.

This kernel decomposition allows us to distribute the two factors with separate functions. Since $h(s,x)$ is positive definite, the operator K is also positive definite and therefore invertible as required by (K2). The boundary conditions (K4) are satisfied by the function $\beta(x)$ and then by the kernel $k(s,x)$. This decomposition leads to a remarkable simplification in the generation of operators K for domains Ω of arbitrary shape.

5.1. How to find a kernel $h(s,x)$

We shall show how to find a kernel $h(s,x)$ which gives rise to a symmetric, positive definite operator H

One way is to use an analytic function whose Taylor series has positive coefficients and is uniformly convergent. A simple example is that of the function $\exp(sx)$. In fact if $v \in L^2[0,1]$

$$\begin{aligned}\langle v, Hv\rangle &= \int_0^1\int_0^1 \exp(sx)v(s)\,v(x)dsdx = \int_0^1\int_0^1 \sum_{k=0}^{\infty}\frac{(sx)^k}{k!}v(s)v(x)dsdx = \\ &= \sum_{k=0}^{\infty}\frac{1}{k!}\int_0^1 s^k v(s)ds\int_0^1 x^k v(x)dx = \sum_{k=0}^{\infty}\frac{1}{k!}(p_k)^2 > 0.\end{aligned} \tag{22}$$

Let us observe that the only function $v \in L^2[0,1]$ with all p_k equal to zero is the zero function.

To give a variational formulation with (true) minimum of the initial value problem

$$-u''(x) = f(x), \quad u(0) = p, \quad u'(0) = q, \quad u \in C^2[0,1] \tag{23}$$

we observe that

$$\begin{aligned} N &= \{-D^2, \quad u(0) = p, \quad u'(0) = q, \quad u \in C^2[0,1]\}, \\ N'_u &= \{-D^2, \quad \phi(0) = 0, \quad \phi'(0) = 0, \quad \phi \in C^2[0,1]\}, \\ N'^*_u &= \{-D^2, \quad \psi(1) = 0, \quad \psi'(1) = 0, \quad \psi \in C^2[0,1]\}, \end{aligned} \tag{24}$$

where we have taken one of the possible adjoints. A possible kernel is

$$k(s,x) = \exp(sx)(1-s)^2(1-x)^2, \tag{25}$$

because it satisfies the boundary conditions of N'^*_u i.e. $k(s,1) = 0$ and $\partial_x K(s,x)\big|_{x=1} = 0$. We remark that initial value problems had always been lacking a variational formulation with a true minimum.

A second way to find an integral operator H that is symmetric and positive definite is the following. Let us consider a region Ω of $\mathbb{R}^2$ with an irregular shape as in Fig.(3a). Let us insert the region Ω in a rectangle $\mathcal{R}$, e.g., the one shown in Fig.(3b). The Green function of any symmetric linear differential operator on $\mathcal{R}$ gives rise to a symmetric and positive definite operator $\overline{H}$ on $L^2(R)$ and defines H as the restriction of $\overline{H}$ to $L^2(\Omega)$. Green functions of some differential operators for a rectangle are known in closed form.

5.2. How to find a function $\beta(x)$

Let us consider, as an example, the time dependent problem of the Fourier equation considered in the region $\Omega \subseteq \mathbb{R}^2$ of Fig.(3) with mixed boundary conditions on $\partial\Omega = L_1 \cup L_2$ and in the time interval $[0,T]$ (see [15])[9]

$$\begin{cases} -\Delta u(x,y,t) + \partial_t u(x,y,t) = f(x,y,t) \\ u|_{L_1} = p, \ \frac{\partial u}{\partial n}\big|_{L_2} = q, \ u|_{t=0} = r, u \in W_2^{2,1}(\Omega \times [0,T]) \end{cases} \tag{26}$$

with p, q and r assigned functions. Since the operator is nonlinear (inhomogeneous boundary conditions do not constitute a linear domain) we must perform the derivative. We obtain

[9] $u \in W_2^{2,1}(\Omega \times [0,T])$ means that $u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}, u_t \in L^2(\Omega \times [0,T])$.

$$N'_u = \Big\{-\Delta + \partial_t, \phi|_{L_1} = 0, \frac{\partial \phi}{\partial n}\Big|_{L_2} = 0, \phi|_{t=0} = 0, \quad u \in W_2^{2,1}(\Omega \times [0,T])\Big\}. \tag{27}$$

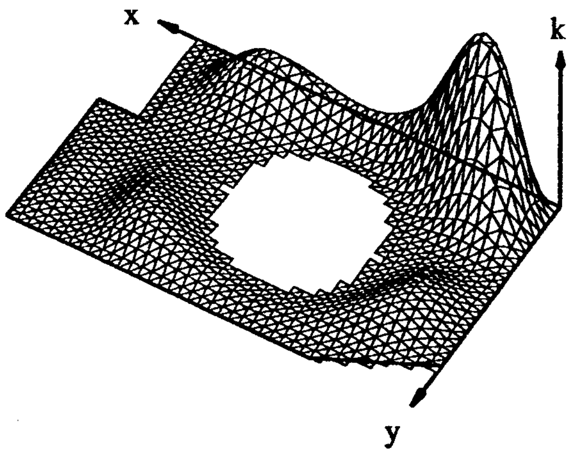

Fig. 4.
An example of function $\beta(x)$ that satisfies the boundary conditions of Fig. 3a.

To obtain an adjoint we must consider the relation

$$\int_0^T \int_\Omega \psi[-\Delta\phi + \partial_t\phi] d\Omega dt = \\ = \int_0^T \int_\Omega \phi[-\Delta\psi + \partial_t\psi] d\Omega dt + \int_0^T \oint_{\partial\Omega} \left[\psi \frac{\partial \phi}{\partial n} - \phi \frac{\partial \psi}{\partial n}\right] dS dt + \int_\Omega [\psi\phi]_0^T d\Omega. \tag{28}$$

A possible adjoint is

$$N'^*_u = \Big\{-\Delta - \partial_t, \psi|_{L_1} = 0, \frac{\partial \psi}{\partial n}\Big|_{L_2} = 0, \psi|_{t=T} = 0, \quad \psi \in W_2^{2,1}(\Omega \times [0,T])\Big\}. \tag{29}$$

The boundary conditions that the kernel $k(s,x)$ must satisfy are those of the domain of the operator N'^*_u. These are homogeneous boundary conditions. To simplify the form of the functional we may impose supplementary conditions on β not required by Th.(2), in order to guarantee that all boundary terms, arising from the integration by parts, vanish. This leads us to require that the function $\beta(s,x)$, as well as its normal derivative, vanishes on the whole boundary.

Since the kernel k must satisfy the homogeneous boundary conditions of ψ, these conditions will be imposed on the function β. Then

$$\beta(x,y,t)|_{L_1}=0, \quad \frac{\partial}{\partial n}\beta(x,y,t)\bigg|_{L_2}=0, \quad \beta(x,y,t)|_{t=T}=0. \tag{30}$$

With reference to Fig.(3) the equations that define the boundary are

$$\begin{aligned}
&\text{side } AB \quad && a(x,y)\stackrel{\text{def}}{=} y=0,\\
&\text{side } BC \quad && b(x,y)\stackrel{\text{def}}{=} x-7=0,\\
&\text{side } CD \quad && c(x,y)\stackrel{\text{def}}{=} y-2=0,\\
&\text{side } DE \quad && d(x,y)\stackrel{\text{def}}{=} x-8=0,\\
&\text{side } EF \quad && e(x,y)\stackrel{\text{def}}{=} y-5=0,\\
&\text{side } FG \quad && f(x,y)\stackrel{\text{def}}{=} 4+\frac{x}{2}-y=0,\\
&\text{side } GA \quad && g(x,y)\stackrel{\text{def}}{=} x=0,\\
&\text{circumference } && h(x,y)=(x-4)^2+(y-2.5)^2-(1.5)^2.
\end{aligned} \tag{31}$$

To obtain the function β we perform the product of the functions giving the sides of the region raising every equation to the square

$$\beta(x,y,t)=a^2b^2c^2d^2e^2f^2g^2h^2(T-t). \tag{32}$$

One may easily see that this function and its normal derivative vanish at the boundary of the spatial domain while the function vanishes at the final instant.

Let us consider, for example, the function $\beta(x,y,t)=a^2g^2(T-t)$. Since

$$\nabla\beta=(2ag^2\nabla a+2ga^2\nabla g)(T-t), \tag{33}$$

we obtain

$$\frac{\partial\beta}{\partial n}=\mathbf{n}\cdot\nabla\beta=\left(2ag^2\frac{\partial a}{\partial n}+2ga^2\frac{\partial g}{\partial n}\right)(T-t). \tag{34}$$

It vanishes on the whole boundary.

If the domain is not convex this function vanishes also along lines passing in the region Ω as shown in Fig.(4). This is of no consequence because the measure of the set is null. The kernel may be

$$k(r,s,\tau;x,y,t)=\exp(rxsyt\tau)\beta(x,y,t)\beta(r,s,\tau). \tag{35}$$

6. The choice of degenerate kernels

The numerical solution of a problem using the extended variational formulation is complicated by the presence of the integral transform that doubles the number of integrations. A problem in a three dimensional domain leads to six integrations! For one dimensional problems the doubling may be acceptable [24].

This obstacle can be bypassed if one chooses degenerate kernels because in this case the number of integrations remains equal to the dimensionality of the domain. A degenerate kernel, also called separable kernel, is one of the form

$$k(s,x) = \beta(x)\beta(s)\sum_{i,j=1}^{m} h_{ij}\alpha_i(s)\alpha_j(x), \tag{36}$$

where the functions $\alpha_i(x)$ may be selected according to some appropriate criteria. The coefficients h_{ij} may be assigned directly taking them as elements of a symmetric, positive definite matrix H.

The functional given in Eq.(17) may be approximated as follows: introducing the m quantities

$$N_i[u] \stackrel{\text{def}}{=} \int_{\Omega} \alpha_i(x)\beta(x)N(u(x))dx, \quad f_i \stackrel{\text{def}}{=} \int_{\Omega} \alpha_i(x)\beta(x)f(x)dx, \tag{37}$$

the functional $F[u]$ is approximated by

$$\begin{aligned} F_{prox}[u] &= \frac{1}{2}\int_{\Omega} [N(u(s)) - f(s)] \times \\ &\times \int_{\Omega} \left[\sum_{i,j=1}^{m} h_{ij}\alpha_i(s)\alpha_j(x)\beta(s)\beta(x)\right] [N(u(x)) - f(x)]dsdx = \\ &= \frac{1}{2}\sum_{i,j=1}^{m} h_{ij}N_i[u]N_j[u] - \sum_{i,j=1}^{m} h_{ij}N_i[u]f_j + \frac{1}{2}\sum_{i,j=1}^{m} h_{ij}f_i f_j. \end{aligned} \tag{38}$$

This quadratic expression is useful for numerical calculations.

The use of degenerate kernels, and then of non-invertible operators, is admissible in an appoximate method of solution. This requires that the functions $\alpha_j(x)$ be member of a complete set of functions. The degenerate kernels in the extended variational formulation, without the introduction of the function $\beta(x)$, has been used to find the equilibrium configuration of large deformations of an elastic beam subjected to a follower force by finite element methods: see [1] [2] [3] [4].

The use of the function β and of degenerate kernels to solve problems with arbitrary domains may open a new way in numerical problem solving, taking into account that this is made possible also for time-dependent problems. Finite elements, or, in general Ritz method, may now be utilized in time domain.

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Расширенная вариационная задача

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Используя интегральные преобразования, излагается метод приведения заданной задачи к новой задаче, допускающей вариационную формулировку.