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The development of bivariational principles for the calculation of upper and lower bounds

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THE PAPER shows how complementary bivariational principles for the calculation of upper and lower bounds to inner products involving the solution of equations of the type $Tf = f_0$ may be developed from simple basic ideas. These are illustrated in detail for the case when T is a linear self-adjoint operator in a real Hilbert space, and the method of extension of the ideas to non-self-adjoint and, finally, to nonlinear operators is shown, with examples of formulae at present available for practical use.

Pokazano w jaki sposób z prostych pojęć podstawowych wyprowadzić można uzupełniające zasady biwariacyjne dla obliczania kresów górnych i dolnych iloczynów skalarnych rozwiazań równań typu $Tf = f_0$. Procedurę tę ilustruje szczegółowo przypadek, gdy T jest samosprzężonym operatorem w rzeczywistej przestrzeni Hilberta; pokazano również sposób rozszerzenia tej metody na przypadki operatorów niesamosprzężonych a także nieliniowych, wraz z przykładami wzorów nadających się do praktycznego zastosowania.

Показан способ вывода — из простых основных понятий — дополнения к бивариационным принципам для расчета верхних и нижних пределов скалярных произведений решений уравнений типа $Tf = f_0$ Эта процедура иллюстрируется подробно для случая, если T — самосопряженный оператор в действительном пространстве Гильберта; показан также способ распространения этого метода на случаи несопряженных операторов и нелинейных, вместе с формулами пригодными для практического использования.

1. Introduction

VARIATIONAL principles have been studied for a long time. There are many books and many, many more papers on the subject. Much of the mathematical work has been concerned with finding approximate values of the solution of an equation, perhaps a differential or an integral equation, by minimising or maximising some "action functional". The functional provides a means to an end and is not necessarily of interest for its own sake. In many problems of importance in engineering and physics, on the other hand, what is sought is the value of a functional involving the solution, and often in the form of an inner product, while the solution itself is only of secondary interest. Typically, if f is the unknown solution of some equation and g_0 a given function, what is sought is an evaluation of the inner product $\langle f, g_0\rangle$ defined over some vector space. Over the years several variational principles have been derived to give upper and/or lower bounds for $\langle f, f_0\rangle$, where

$$Tf = f_0$$

and (for example) $T: \mathscr{H} \to \mathscr{H}$ is a self-adjoint linear operator in a real Hilbert space with $f_0 \in \mathscr{H}$. These principles involve the approximation of f in some suitable way and have been much used. For the more general product $\langle f, g_0 \rangle$ BARNSLEY and ROBINSON (1974) and COLE and PACK (1974, 1975) independently suggested the use of *two* approximating functions, one for f and one for a function *associated* with g_0, in order to obtain what Barnsley and Robinson named *complementary bivariational principles* (bi — to indicate the dual approximations, complementary in the sense that they would yield both upper and lower bounds). COLE and PACK (1975) showed how to produce *families* of bounds, upper and lower, and were able to make some comparisons between the methods adopted and the accuracy of the results.

The author had the honour and privilege of lecturing on these studies in Warsaw University in 1977 at the invitation of Professor FISZDON, and will lay out in this paper the basic ideas and the considerable advances that have since been presented, permitting the approximate calculation of inner products for wide classes of problems, including nonlinear ones, under certain conditions.

2. Variational principles for self-adjoint linear operators

The most famous and commonly-used variational principle yielding an approximation to an inner product is the one given in COURANT and HILBERT (1953): Corresponding to

$$Tf = f_0, \tag{2.1}$$

where $T: \mathscr{H} \to \mathscr{H}$ is a self-adjoint linear operator in a real Hilbert space with an inner product $\langle .,. \rangle$ and f_0 is a real function $\in \mathscr{H}$, the functional

$$\begin{aligned} G(\phi) &= \langle \phi, 2f_0 - T\phi \rangle \\ &= L_0(\phi), \quad \text{say, with} \quad \phi \in \mathscr{H}, \end{aligned} \tag{2.2}$$

has a stationary value when $\phi = f$ and provides either a lower or an upper bound for the functional $\langle f, f_0 \rangle = G(f)$ according, respectively, as the operator T is positive or negative definite.

Cole and Pack generalised this by seeking families of functionals bounding $\langle f, f_0 \rangle$ from both above and below starting from the expression

$$\begin{aligned} G(\phi) &= \langle f, f_0 \rangle - \langle \phi - f, H'(\phi - f) \rangle \\ &= \langle f, f_0 \rangle - \langle \delta f, H' \delta f \rangle, \quad \text{say} \end{aligned} \tag{2.3}$$

and specifying that H' should be a self-adjoint linear operator of definite sign. To fix ideas, T is taken to be positive definite and is required to satisfy the conditions

$$0 < m\langle \phi, \phi \rangle \leqslant \langle \phi, T\phi \rangle \leqslant M \langle \phi, \phi \rangle, \tag{2.4}$$

where m, M are real (positive) constants, $\forall \phi \in \mathscr{H}$. The authors looked for H' in such a form that Eq. (2.3) could be manipulated into an expression that would eliminate the unknown function f. Clearly, such a procedure would yield lower or upper bounds for $\langle f, f_0 \rangle$ depending on the sign of H'. The approximations would become better, the closer ϕ happened to approximate to f.

It was found that the choice

(2.5)(1) $$H' = T - THT$$

(which ensures that H' is self-adjoint if H is) enabled Eq. (2.3) to be expressed as

(2.6) $$G(\phi) = \langle \phi, 2f_0 - T\phi \rangle + \langle f_0 - T\phi, H(f_0 - T\phi) \rangle,$$

eliminating f as required.

We see at once that the functional (2.2) corresponds to $H = 0$ and provides a lower bound to $\langle f, f_0 \rangle$ for $T > 0$ since $H' > 0$ in that case. A closer lower bound is given by

(2.7) $$G(\phi) = L_0(\phi) + \frac{1}{M} \langle f_0 - T\phi, f_0 - T\phi \rangle.$$

Examples of upper bounds (for positive T) are:

(2.8) $$G(\phi) = L_0(\phi) + \frac{1}{m} \langle f_0 - T\phi, f_0 - T\phi \rangle$$

or, better,

(2.9) $$G(\phi) = L_0(\phi) + \langle f_0 - T\phi, \tau^{-1}(f_0 - T\phi) \rangle,$$

where $\tau^{-1} = (T1)^{-1} I$.

For multi-dimensional linear Fredholm integral equations of the type

$$T_{ij}(s, s') f_j = (f_0)_i \quad (i, j = 1, 2, \ldots, r)$$

with the (possibly vector) independent variable s, τ is to be interpreted as the diagonal matrix

$$\tau_{ij} = \tau_i \delta_{ij}$$

with $\tau_i(s) = T_{ij}(s, s') l_j(s')$; $l(s')$ being a vector function with components equal to unity everywhere. The constant m in Eq. (2.8) is here min inf $\tau_i(s)$ over the domain of s.

These results have been applied to a number of problems involving Fredholm integral equations of the second kind: the so-called Clausing problem — the conductance of a circular pipe linking a large reservoir with a vacuum, when the flow through the pipe is steady and free molecular (COLE, 1977); the conductance of a rectangular duct under the same circumstances (here the operator is a 2×2 matrix) (COLE, 1979); the shearing stress in plane Couette flow in rarefied gas dynamics based on the BGK model of the Boltzmann equation (COLE and PACK, 1979). The accuracy achieved in the calculation is very high in every case, the upper and lower bounds rarely differing by more than a fraction of a percent of their mean.

3. Bivariational principles for self-adjoint linear operators

All the formulae derived from the expression (2.3) establish variational principles involving one approximating function and yield bounds to $\langle f, f_0 \rangle$, f_0 being the non-

(1) There are sign changes from the notation used in COLE and PACK (1975) in Eqs. (2.3), (2.5) and (4.2).

homogeneous term in the operator equation for the unknown f. Bivariational principles are called into play to find approximations to more general inner products of type $\langle f, g_0\rangle$. The basic idea is to associate with the unknown function f another unknown function, g, satisfying an auxiliary equation, which, for self-adjoint linear operators, is

$$Tg = g_0. \tag{3.1}$$

BARNSLEY and ROBINSON (1974) used the identity

$$\langle f, g_0\rangle \equiv \frac{1}{2}\langle \gamma f+\gamma^{-1}g, \gamma f_0+\gamma^{-1}g_0\rangle - \frac{1}{2}\gamma^2\langle f, f_0\rangle - \frac{1}{2}\gamma^{-2}\langle g, g_0\rangle, \tag{3.2}$$

where γ is a real parameter, and then used functionals of the type appropriate to ensure an upper or lower bound (as desired) for the whole, for each of the three inner products occurring on the right-hand side. Their results and those of COLE and PACK (1975) together with later extensions by ROBINSON and BARNSLEY (1979) and COLE (1980) are best considered in the light of functionals in the form

$$\begin{aligned} G(\phi, \psi) = \langle \alpha f, \beta g_0\rangle - \frac{1}{2}\{&\langle \alpha\delta f, A'\alpha\delta f\rangle + \langle \alpha\delta f, B'\beta\delta g\rangle + \langle D'\alpha\delta f, \beta\delta g\rangle \\ &+\langle \beta\delta g, C'\beta\delta g\rangle\} = \langle \alpha f, \beta g_0\rangle - \frac{1}{2}\left\langle [\alpha\delta f\ \beta\delta g], \begin{bmatrix} A' & B' \\ D' & C'\end{bmatrix}\begin{bmatrix}\alpha\delta f \\ \beta\delta g\end{bmatrix}\right\rangle, \end{aligned} \tag{3.3}$$

where $\delta f = \phi - f$ and $\delta g = \psi - g$, ϕ and ψ are approximations to f and g respectively, α and β are numbers or operators that commute with T, and A', B', C', D' are self-adjoint linear operators such that the expression in curly brackets shall be either positive or negative definite for all δf, δg. The inner product $\langle \alpha f, \beta g_0\rangle$ may be expressed as a sum of multiples of the (four) inner products $\langle \alpha f, \alpha f_0\rangle$, $\langle \beta g, \beta g_0\rangle$, $\langle \alpha f \pm \beta g, \alpha f_0 \pm \beta g_0\rangle$, any three of which are linearly independent under the properties assigned to α, β and T (which make $\langle \alpha f, \beta g_0\rangle = \langle \alpha f_0, \beta g\rangle$). Write q, $w = \alpha f \pm \beta g$ and q_0, $w_0 = \alpha f_0 \pm \beta g_0$, respectively. We find that

$$\begin{aligned} \langle \alpha f, \beta g_0\rangle &\equiv \frac{1}{2}[\langle \alpha f, \alpha f_0\rangle + \langle \beta g, \beta g_0\rangle - \langle w, w_0\rangle] \\ &\equiv \frac{1}{2}[\langle q, q_0\rangle - \langle \alpha f, \alpha f_0\rangle - \langle \beta g, \beta g_0\rangle] \\ &\equiv \frac{1}{4}[\langle q, q_0\rangle - \langle w, w_0\rangle]. \end{aligned} \tag{3.4}$$

Let δq, $\delta w = \alpha(\phi - f) \pm \beta(\psi - g)$, respectively. Then, to utilise the results of Sect. 2, we must seek re-arrangements of the second-order terms in Eq. $(3.3)_2$ to combine with the inner products (in one of Eq. (3.4)) so as to produce pairs of terms like the expression (2.3). We find that for Eq. $(3.4)_3$ we require $A' = C'$ and $B' = D'$. On the other hand, error terms suitable for Eqs. $(3.4)_1$ and $(3.4)_2$ require only that $B' = D'$. If we write

$$G(\phi, \psi) = \langle \alpha f, \beta g_0\rangle + \langle \mathbf{\delta e}, E'\mathbf{\delta e}\rangle, \tag{3.5}$$

where $\mathbf{\delta e} = [\alpha\delta f\, \beta\delta g]$ is the error vector, then the forms corresponding to Eqs. (3.4) are respectively

$$(3.6)(^2) \quad \langle \mathbf{\delta e}, E'\mathbf{\delta e}\rangle = \frac{1}{2}[+\langle \delta w, B'\delta w\rangle - \langle \alpha\delta f, (B'+A')\alpha\delta f\rangle - \langle \beta\delta g, (B'+C')\beta\delta g\rangle]$$

$$= \frac{1}{2}[-\langle \delta q, B'\delta q\rangle + \langle \alpha\delta f, (B'-A')\alpha\delta f\rangle + \langle \beta\delta g, (B'-C')\beta\delta g\rangle]$$

$$= \frac{1}{4}[-\langle \delta q, (B'+A')\delta q\rangle + \langle \delta w, (B'-A')\delta w\rangle].$$

Bivariational bounds are now obtained by applying the method of Sect. 2 to the sum of Eqs. (3.4) and (3.6), three times for the $(3.6)_1$ or $(3.6)_2$ versions and twice for the $(3.6)_3$ version, with appropriate choice of sign for the operators occurring in the second-order terms to ensure the required type of bound. In every case the operators with dashes are replaced by means of formulae such as

$$A' = T - TAT$$

and the final results produce bounds for the form

$$(3.7) \qquad G(\phi, \psi) = J_\alpha(\phi, \psi) + \langle \mathbf{c}, K\mathbf{c}\rangle,$$

with

$$(3.8) \qquad J_\alpha(\phi, \psi) = \langle \alpha\phi, \beta g_0\rangle + \langle \alpha f_0, \beta\psi\rangle - \langle \beta\psi, T\alpha\phi\rangle,$$

and

$$(3.9) \qquad \mathbf{c} = [\alpha(f_0 - T\phi)\beta(g_0 - T\psi)].$$

The matrix operator K can most succinctly be written as

$$(3.10) \qquad \begin{bmatrix} \tilde{A} & B \\ B & \tilde{C} \end{bmatrix}$$

when (formally) $\tilde{A} = A - T^{-1}$, $\tilde{C} = C - T^{-1}$ $(\rightarrow A' = -T\tilde{A}T, C' = -T\tilde{C}T$: $\tilde{A} = \tilde{C}$ in using Eq. $(3.6)_3)$. The choices of $\tilde{A}$, B, $\tilde{C}$ are free apart from the conditions on the signs of the operators occurring in Eqs. (3.6) to produce the desired type of bound. Knowledge of T^{-1} is, of course, not required.

For $\alpha = \dfrac{1}{\beta}$, pure numbers, Cole has found some improved bounds by optimising with respect to α after setting $\tilde{A} = \tilde{C} = \mp\dfrac{1}{2m}$, $B' = \dfrac{1}{m}TT - T = T_0$ (positive definite for $T > 0$). In this case we write

$$(3.11) \qquad J\langle \phi, \psi\rangle = \langle \phi, g_0\rangle + \langle f_0, \psi\rangle - \langle \psi, T\phi\rangle,$$

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(2) Identification with the results given by COLE (1980, p. 118) follows by putting:
in $(3.3)_1$, $B' = W'$, $B'+A' = F'$, $B'+C' = G'$,
in $(3.3)_2$, $B' = Q'$, $B'-A' = F'$, $B'-C' = G'$,
in $(3.3)_3$, $2B' = Q'+W$, $2A' = Q'-W'$.

which we shall call the *basic functional*. The bounds are then

$$G_{\pm}(\phi, \psi) = J(\phi, \psi) + \frac{1}{2m} [\langle f_0 - T\phi, g_0 - T\psi\rangle \pm || f_0 - T\phi|| \, ||g_0 - T\psi||], \tag{3.12}$$

where m has the meaning assigned in the conditions (2.4) and $||\cdot||$ denotes the norm associated with $\langle .,.\rangle$. These bounds are essentially equivalent to bounds derived by ROBINSON (1978) and by ROBINSON and BARNSLEY (1979) from ideas based on the identity (3.2). Tables of bounds on $\langle f, g_0\rangle$ with comments on their computation and relative simplicity to use are given in COLE (1980).

4. Some observations on the principles for $T = T^*$

With the choice $B' = T$, $A' = 0$ in Eq. $(3.6)_3$,

$$G(\phi, \psi) = J_\alpha(\phi, \psi) \tag{4.1}$$

and then Eq. $(3.3)_1$ shows at once that

$$J_\alpha(\phi, \psi) = \langle \alpha f, \beta g_0\rangle - \langle \alpha\delta f, T\beta\delta g\rangle. \tag{4.2}$$

This functional provides the generalisation of the classical variational principle (2.2), but whereas the latter has an error of definite sign (yielding a lower bound for $T > 0$), functional $J_\alpha(\phi, \psi)$ — as Eq. (4.2) illustrates clearly — gives an approximation with an error of indefinite sign. Bivariational functionals of this kind are called *saddle-point functionals* by COLE and PACK (1975).

COLE (1978) has shown the correspondence between the results obtained from an appropriate application of the Bubnov-Galerkin (projection) process and results derived by the method of Sect. 3, and with SPIGA (1979) he has compared the computability and accuracy of results for Fredholm integral equations obtained by approximations based on this process, using a suitable system of orthonormal coordinate functions. Applications to Couette, Poiseuille and thermal creep flows are described in detail.

ROBINSON and BARNSLEY (1979) have shown how these ideas may be used to obtain point-wise approximations to the solution of a Fredholm integral equation (³) of the type

$$f(x) - \lambda \int_a^b k(x, y) f(y) dy = f_0(x) \qquad (a \leqslant x \leqslant b), \tag{4.3}$$

where $k(x, y)$ is real and symmetric, $f_0(x)$ a real function and λ small enough to permit the inversion of $T = I - \lambda K$. For $f \in \mathscr{H}$ and suitable restrictions on k, we can use

$$\langle f, k(x, y)\rangle = \int_a^b k(x, y) f(y) dy = \frac{1}{\lambda}\{f(x) - f_0\}. \tag{4.4}$$

(³) For a more general setting to the use of these ideas for point-wise approximation, see ROACH (1977).

The bivariational principles applied to the left-hand side will provide upper and lower bounds for $f(x)$. Since the auxiliary equation for g is

$$g(x, x') - \lambda \int_a^b k(x, y) g(y, x') dx' = k(x, x'),$$

we see that the function g to which ψ approximates is, in fact, the resolvent kernel of the Fredholm equation.

5. Non-self-adjoint operators

The method may be extended to non-self-adjoint operators by converting $Tf = f_0$ to

(5.1) $$T^*Tf = T^*f_0,$$

where T^* is the adjoint of T with respect to the inner product in $\mathscr{H}$. Since T^*T is self-adjoint, the auxiliary equation is

(5.2) $$T^*Th = g_0.$$

Provided that $g_0 \in D(T^*)$ and α, β commute with both T and T^* (and so, also, with TT^*) the formulae of Sect. 3 may be used with ϕ approximating to f and, say, χ approximating to h. We see that Eq. (3.7) becomes

$$G(\phi, \chi) = J_\alpha(\phi, \chi) + \langle \tilde{\mathbf{c}}, K\tilde{\mathbf{c}} \rangle$$

with

$$\tilde{\mathbf{c}} = [\alpha(T^*f_0 - T^*T\phi)\beta(g_0 - T^*T\chi)]$$
$$= \begin{bmatrix} T^* & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \alpha(f_0 - T\phi) \\ \beta(g_0 - T^*T\chi) \end{bmatrix} = S^* \begin{bmatrix} \alpha(f_0 - T\phi) \\ \beta(g_0 - T^*\psi) \end{bmatrix}$$

with

$$T\chi = \psi$$

and, consequently,

$$T^*\psi = g_0$$

and

$$\langle \tilde{\mathbf{c}}, K\tilde{\mathbf{c}} \rangle = \langle S^*\mathbf{c}, KS^*\mathbf{c} \rangle = \langle \mathbf{c}, SKS^*\mathbf{c} \rangle$$

with

$$\mathbf{c} = [\alpha(f_0 - T\phi), \beta(g_0 - T^*\psi)].$$

Here $K = \begin{bmatrix} \tilde{A} & B \\ B & \tilde{C} \end{bmatrix}$ with $\tilde{A} = A - (T^*T)^{-1}$, etc. and dashed operators are found from, for example,

$$B' = T^*T - T^*TBT^*T.$$

Since

$$\begin{aligned} J_\alpha(\phi, \chi) &= \langle \alpha\phi, \beta g_0 \rangle + \langle \beta\chi, \alpha T^* f_0 \rangle - \langle B\chi, T^*T\alpha\phi \rangle \\ &= \langle \alpha\phi, \beta g_0 \rangle + \langle \beta T\chi, \alpha f_0 \rangle - \langle \beta T\chi, T\alpha\phi \rangle \\ &= \langle \alpha\phi, \beta g_0 \rangle + \langle \beta\psi, \alpha f_0 \rangle - \langle \beta\psi, T\alpha\phi \rangle \\ &= J_\alpha(\phi, \psi), \end{aligned}$$

we see that we can base bivariational bounds on the formulae

$$Tf = f_0, \quad T^*\psi = g_0, \tag{5.3}$$

and

$$G(\phi, \psi) = J_\alpha(\phi, \psi) + \langle \mathbf{c}, SKS^*\mathbf{c}\rangle. \tag{5.4}$$

The inequalities required of the operator T^*T, namely, that $\langle\phi, T^*T\phi\rangle/\langle\phi,\phi\rangle$ should be bounded both below and above, becomes a requirement on $\langle T\phi, T\phi\rangle/\langle\phi,\phi\rangle$:

$$M\|\phi\| \geqslant \|T\phi\| \geqslant m\|\phi\|, \tag{5.5}$$

$J_\alpha(\phi, \psi)$ is a saddle-point functional as before. For $\alpha = \beta = 1$, $J\langle\phi, \psi\rangle = \langle\phi, g_0\rangle + \langle\psi, f_0\rangle - \langle\psi, T\phi\rangle$ is, in fact, the inhomogeneous Rayleigh–Ritz stationary approximation quoted by STAKGOLD (1968).

Formulae for $G(\phi, \psi)$ giving complementary bounds for $\langle f, g_0\rangle$ for non-self-adjoint operators are tabulated in COLE (1980), with comparisons of the computability of the bounds based on three as against two groupings of inner products (*vide* Eqs. (3.6) above). There are more economical bounds obtainable from three, which are developed from formulae given by BARNSLEY and ROBINSON (1976), where the original extensions were displayed. The reader is referred to the above papers for details of the bounds.

6. Bounds for nonlinear problems

The further generalisation of the method to make it applicable to certain nonlinear operators is due to BARNSLEY and ROBINSON (1977). Let $Ff = 0$ be an operator equation in a real Hilbert space $\mathscr{H}$ with the inner product $\langle .,.\rangle$ and let $g_0 \in \mathscr{H}$ be an arbitrary vector in that space, as before. Since F is no longer required to be linear, any nonhomogeneous term f_0 is absorbed into F. Here $F: D(F) \subset \mathscr{H} \to \mathscr{H}$ with $D(F)$ a linear subspace dense in $\mathscr{H}$. The basic condition imposed on F, corresponding to the inequality (5.5), is

$$\|F\phi_1 - F\phi_2\| \geqslant m\|\phi_1 - \phi_2\|, \tag{6.1}$$

at least for a suitable subset $\mathfrak{S}$ of $D(F)$, with a constant $m > 0$ and $\forall\, \phi_1, \phi_2, \in \mathfrak{S}$. The condition implies that if there is a solution of $Ff = 0$ in $\mathfrak{S}$, then it is unique.

We associate with

$$Ff = 0 \tag{6.2$_1$}$$

the auxiliary equation

$$F_f'^* g = g_0, \tag{6.2$_2$}$$

where $F_f'^*$ represents the adjoint of the Gateaux derivative of F at f. Equation $(6.2)_2$ reduces to $F^*g = g_0$ for a *linear* non-self-adjoint operator, and is itself linear in g at a fixed f. The form $J(\phi, \psi)$ occurring in the bivariational principles now reads

$$J(\phi, \psi) = \langle\phi, g_0\rangle - \langle\psi, F\phi\rangle \tag{6.3}$$

with ϕ, ψ as approximations for f and g, respectively, chosen from $\mathfrak{S}$. That this expression has a stationary value at (f, g_0) under Eqs. $(6.2)_{1,2}$ is most simply demonstrated by introducing the approximations

$$\phi(t) = f+t(\phi-f), \tag{6.4}$$

where t is a real parameter in [0, 1]. This is an interpolation along a ray between the solution f and the approximating function ϕ. The Gateaux derivative of F at *any* f in $D(F)$ is defined by F'_f such that for each $\phi, f \in D(F)$,

$$F\phi(t) = Ff+F'_f[\phi(t)-f]+\nu\big((f, \phi(t)\big) \tag{6.5}$$

with

$$\|\nu\big(f, \phi(t)\big)\| \to o(t) \quad \text{as} \quad t \to 0. \tag{6.6}$$

We shall assume that F'_f is a linear mapping, but it may be unbounded. It is also assumed to possess a closed extension, so that F'^*_f is a closed linear mapping with $D(F'^*_f)$ dense in $\mathscr{H}$.

The nature of the approximation to $\langle f, g_0\rangle$ provided by $J(\phi, \psi)$, considered as an operator over a domain $\subset \mathscr{H}\times\mathscr{H}$, is indicated by the fact that

$$\begin{aligned} J\big(\phi(t), \psi(t)\big)-\langle f, g_0\rangle &= \langle g_0, \phi(t)-f\rangle-\langle\psi(t), F\phi(t)\rangle \\ &= \langle g_0, \phi(t)-f\rangle-\langle\psi(t), F'_f[\phi(t)-f]\rangle-\langle\psi(t), \nu\rangle \\ &= \langle g_0, \phi(t)-f\rangle-\langle F'^*_f\psi(t), \phi(t)-f\rangle-\langle\psi(t), \nu\rangle \\ &= \langle g_0-F'^*_f\psi(t), \phi(t)-f\rangle-\langle\psi(t), \nu\rangle. \end{aligned}$$

With no more required than that $\psi(t) \to g$ as $t \to 0$, $J\big(\phi(t), \psi(t)\big) \to \langle f, g_0\rangle$ as $t \to 0$. If we write $\psi(t) = g+t(\psi-g)$, then we see at once that

$$J\big(f, \psi(t)\big)-J(f, g) \equiv 0$$
$$\Rightarrow \frac{\partial J}{\partial\psi} \equiv 0 \quad \text{at} \quad (f, g);$$

also, since

$$J\big(\phi(t), g\big)-J(f, g) = \langle g_0, \phi(t)-f\rangle-\langle g, F\phi(t)\rangle = \langle g_0-F'^*_f g, \phi(t)-f\rangle-\langle g, \nu\rangle, \tag{6.7}$$

where the first inner product on the right-hand side vanishes and

$$\|\langle g, \nu\rangle\| \leqslant \|g\|\,\|\nu\| \to o(t) \quad \text{as} \quad t \to 0 \quad \text{by Eq. (6.6)},$$

it follows that $\dfrac{\partial J}{\partial\phi} = 0$ at (f, g) in the Gateaux sense of the partial derivative. Thus $J(\phi, \psi)$ provides a stationary approximation to $\langle f, g_0\rangle$, albeit of the saddle-point type as described in Sect. 4.

An interesting special case of the use of J is afforded by algebraic equations, where, for $Ff = 0$, $f \in \mathscr{R}$, $f > 0$, with the inner product defined by ordinary multiplication and $\|\cdot\|$ by $|\cdot|$, and with $g_0 = 1$, $J(\phi, \psi)$ becomes an approximation to $\langle g_0, f\rangle = f$, the required root of the equation. The auxiliary equation here is $F'_f\psi = 1$ with F'_f the Frechet derivative of F in this particular context, providing the value $\psi = 1/F'_f(\phi)$ to be inserted in J. The formula for J is easily seen to yield Newton's approximation to the root of an equation.

In general, when $Ff = 0$ is posed on a Hilbert space, the approximation $J(\phi, \psi)$ provides a generalisation of Newton's approximation, with the advantage that it does not require knowledge of the inverse of the Gateaux derivative $F'_f(\phi)$. In order to obtain genuine upper and lower bounds it is clearly essential to add and subtract terms to the basic functional $J(\phi, \psi)$. To achieve this a further condition requires to be placed on the operator, so that there are inequalities corresponding to both of those previously introduced in (2.4).

A suitable condition is

$$(6.8) \qquad ||F\phi_1 - F\phi_2 - F'_{\phi_1}(\phi_1-\phi_2)|| \leqslant \frac{1}{2}k||\phi_1-\phi_2|| \quad (k \geqslant 0).$$

Barnsley and Robinson show that, given

$$(6.9) \qquad \begin{aligned} C(\phi, \psi) &= \frac{1}{c}||F'^*_\phi\psi - g_0||\,||F\phi|| + \frac{k}{2c^2}||\psi||\,||F\phi||^2, \\ &\psi \in D(F'^*_\phi), \\ &\phi \in \mathfrak{S}, \end{aligned}$$

where $\mathfrak{S}$ is a subset of $D(F)$ in which the solution f lies, then

$$(6.10) \qquad J(\phi, \psi) - C(\phi, \psi) \leqslant \langle g_0, f\rangle \leqslant J(\phi, \psi) + C(\phi, \psi).$$

As a special case we may note that if we write $Ff \equiv Af - f_0$, where A is a *linear* mapping (but F, of course, is not!), then $k = 0$ and the "correcting" functional reproduces bounds already derived for non-self-adjoint operators in earlier papers (BARNSLEY and ROBINSON (1976)), namely

$$(6.11) \qquad \begin{aligned} C(\phi, \psi) &= \frac{1}{m}|A^*\psi - g_0||\,||A\phi - f_0||, \\ &\psi \in D(A^*), \\ &\phi \in D(A). \end{aligned}$$

Other conditions on F lead to other bounds. For example, if

$$(6.12) \qquad |F\phi_1 - F\phi_2 - F'_{\phi_1}(\phi_1-\phi_2)| \leqslant \frac{1}{2}k|\phi_1-\phi_2|^2, \quad \forall \phi_1, \phi_2 \in \mathfrak{S},$$

we can write

$$(6.13) \qquad C(\phi, \psi) = \frac{1}{c}||F'^*_\phi\psi - g_0||\,||F\phi|| + \frac{k}{2c^2}|\psi|_{\sup}||F\phi||^2.$$

As examples, the authors give bounds on a transmission signal, a problem arising in communication theory and involving a nonlinear integral equation, and bounds on the heat contained in a bar, involving a nonlinear diffusion equation with boundary conditions. In each case simple approximations to the solution and to the subject of the auxiliary equation lead to close bounds on the quantities sought.

7. Conclusion

The developments outlined above provide formulae for upper and lower bounds to inner products involving the solution to an equation posed in Hilbert space. The progression from self-adjoint linear operators to nonlinear operators is shown with an indication of the choices available at present. It would seem that there is scope for further refinement of the functionals, with clearer understanding of what is required to produce families of closer bounds. The applications of these results to problems in physics and engineering have only just begun and many uses of them will be found, as inner products of the kind studied are closely associated with ideas of flux of important physical quantities.

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