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Complementary variational principles and variational–iterative principles

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Abstract. Complementary variational principles for the solution of certain linear equations are developed. It is shown that these may be used iteratively for the solution of nonlinear equations. Examples are presented with applications in particle theory, electromagnetic theory, communication theory and the Thomas–Fermi statistical theory for atoms.

1. Introduction

In previous papers (Burrows and Perks 1977, 1979) complementary variational principles for the equation

$$T\phi = f \tag{1.1}$$

in a suitably chosen real complete Hilbert space H have been introduced where T is a completely continuous, self-adjoint linear operator and f is some function belonging to H. These principles provide upper and lower bounds for

$$\langle \phi | f \rangle \tag{1.2}$$

where $\langle\ \rangle$ denotes the inner product of H and the theory has been applied to quantum mechanical scattering problems. This theory is described in § 2 of this paper and is applied to the solution of an integral equation which arises in the Kirkwood–Riseman theory of intrinsic viscosities and diffusion constants (Kirkwood and Riseman 1948).

The main purpose of this paper is to extend these calculations to deal with equations of the form

$$T\phi = f(\phi) \tag{1.3}$$

where f may be a nonlinear function of ϕ or more generally

$$T\phi = f(\phi) - L\phi \tag{1.4}$$

where L is a linear operator. Complementary variational principles for the solution of equation (1.3) have been introduced by Arthurs *et al* (see Arthurs 1970, Arthurs and Robinson 1969a,b, Arthurs and Anderson 1977, Arthurs and Coles 1977) providing upper and lower bounds to a functional when certain conditions are satisfied, one of which is

$$\mathrm{d}f/\mathrm{d}\phi < 0. \tag{1.5}$$

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In this paper we use a variational–iterative scheme to deal with the problems provided by equation (1.3) or (1.4) so that the simpler linear theory described in § 2 is applied to a sequence of equations, the solutions of which converge to the solution of equation (1.3) or (1.4). The theory is described in § 3 and applied to three examples. For two of the examples the original problem is rewritten so that it has the form of equation (1.3) or (1.4) where the self-adjoint operator T has a discrete spectrum. This condition is necessary for the application of the linear theory described in § 2.

2. The linear theory

Consider the functional

$$J(\Delta, \Phi) = \langle \Phi | T\Phi \rangle - 2\langle \Phi | f \rangle + \Delta \langle T\Phi - f | T\Phi - f \rangle \tag{2.1}$$

where Δ is a real constant. The first variation of $J(\Delta, \Phi)$ leads to

$$\delta J = 2(\langle \delta\Phi | T\Phi - f \rangle + \Delta \langle T\delta\Phi | T\Phi - f \rangle) \tag{2.2}$$

since T is a linear self-adjoint operator. This shows that J is stationary (i.e. $\delta J = 0$) at $\Phi = \phi$ the exact solution of equation (1.1). Further, the stationary values of J are found from

$$T\Phi - f + \Delta T(T\Phi - f) = 0. \tag{2.3}$$

Writing $T\Phi - f = u$ this becomes

$$\Delta Tu = -u. \tag{2.4}$$

If $\Delta = 0$ then ϕ is the unique stationary point. Also if $\Delta \neq 0$ and T does not have an eigenvalue $-1/\Delta$ then $u = 0$ and again ϕ is the unique stationary point. If, however, T has an eigenvalue $-1/\Delta$ ($\Delta \neq 0$) then it is easy to verify that $\psi = \phi + a\omega$ is a stationary point where a is real constant and ω is any eigenvector of T with eigenvalue $-1/\Delta$ and that

$$J(\Delta, \psi) = -\langle \phi | f \rangle. \tag{2.5}$$

In this analysis we assume that T does not have a zero eigenvalue so that T^{-1} exists and the solution of equation (1.1) is unique.

The second variation of J at any stationary point is given by

$$\delta^2 J = 2(\langle \delta\Phi | T\delta\Phi \rangle + \Delta \langle \delta\Phi | T^2 \delta\Phi \rangle). \tag{2.6}$$

If we now assume that T has a discrete spectrum so that we have the eigenvalue equation

$$T\omega_i = \lambda_i \omega_i \tag{2.7}$$

where the eigenvectors ω_i form a countably complete orthonormal set in the Hilbert space H. Thus for arbitrary $\delta\Phi$ in H we can write

$$\delta\Phi = \sum_i b_i \omega_i \tag{2.8}$$

and consequently

$$\delta^2 J = 2 \sum_i b_i^2 (\lambda_i + \Delta \lambda_i^2). \tag{2.9}$$

If we now choose Δ_1 so that

$$\Delta = \Delta_1 \geqslant -1/\lambda_i \tag{2.10}$$

for all λ_i then $J(\Delta, \Phi)$ becomes a minimum principle at the unique stationary point $\Phi = \phi$. Similarly a choice

$$\Delta = \Delta_2 \leqslant -1/\lambda_i \tag{2.11}$$

for all $\lambda_i \neq 0$ leads to a maximum principle. With these choices we have

$$J(\Delta_1, \Phi) \geqslant -\langle \phi | f \rangle \geqslant J(\Delta_2, \psi) \tag{2.12}$$

for all Φ, ψ belonging to H. In this paper most of the examples considered are such that T is a completely continuous operator (an operator which maps every set of bounded functions in H into a compact set and is also known as a compact operator (Pryce 1973)) so that it is bounded and possesses a discrete spectrum. In one example T is a Sturm–Liouville differential operator which has a discrete spectrum and is such that the extension of its Green function is completely continuous (see Pryce 1973).

As an example of the theory described consider the Kirkwood–Riseman integral equation

$$T\phi = \phi(x) - \lambda \int_{-1}^{1} \phi(t)|x-t|^{-\alpha}\, \mathrm{d}t = 1 \tag{2.13}$$

where $-1 \leqslant x \leqslant 1$, $0 < \alpha < 1$ and $\lambda < 0$. The Hilbert Space H for this example is the space of square-integrable real functions of x with inner product defined by

$$\langle \Phi | \Psi \rangle = \int_{-1}^{1} \Phi(x)\Psi(x)\, \mathrm{d}x. \tag{2.14}$$

We can write

$$T = I - \lambda \hat{K} \tag{2.15}$$

where I is the identity operator and $\hat{K}$ is the integral operator defined by

$$\hat{K}\Phi = \int_{-1}^{1} \Phi(t)|x-t|^{-\alpha}\, \mathrm{d}t, \qquad 0 < \alpha < 1. \tag{2.16}$$

Since the kernel of $\hat{K}$ is symmetric it follows that $\hat{K}$ is self-adjoint on H. It can be shown (Auer and Gardiner 1955) that the kernel of K may be represented by

$$|x-t|^{-\alpha} = \sum_{n=0}^{\infty} a_n P_n^{(\beta)}(x) P_n^{(\beta)}(t), \qquad \beta = \tfrac{1}{2}(\alpha - 1) \tag{2.17}$$

where $a_n > 0 \forall n$ and $\{P_n^{(\beta)}(x)\}$ is a set of Gegenbauer polynomials. These polynomials are orthogonal with respect to the weight function $(1-x^2)^{-\beta}$ so that

$$\int_{-1}^{1} (1-x^2)^{-\beta} P_n^{(\beta)}(x) P_m^{(\beta)}(x) = \delta_{nm} N(n, \beta), \tag{2.18}$$

where $N(n, \beta)$ is a numerical factor. From equations (2.17) and (2.18) we can show that K is positive definite with a discrete spectrum. Since $\lambda < 0$ this implies that the eigenvalues of T, λ_i are such that

$$\lambda_i \geqslant 1. \tag{2.19}$$

We can thus take $\Delta_1 = 0$ and $\Delta_2 = -1$ and these lead to

$$J(-1, \Psi) \leqslant \int_{-1}^{1} \phi(x)\, dx \leqslant J(0, \Phi) \tag{2.20}$$

$\forall \Phi$, Ψ belonging to H. Accurate trial functions can be obtained in the form

$$\Phi_N(x) = (1-x^2)^{-\beta} \sum_{n=0}^{N} b_n P_{2n}^{(\beta)}(x). \tag{2.21}$$

Using the trial functions of the form (2.21) enables us to use the relationship (2.18), thereby reducing the calculation. One- and two-parameter trial functions were used corresponding to $N = 0$ or 1. The results are given in tables 1 and 2 which contain the upper and lower bounds respectively and are compared with those obtained by Arthurs and Anderson (1977) using the same functionals but taking two-parameter approximations of the form $\Psi = Ax^2 + B$. There is qualitative agreement between the bounds obtained except for the case $\alpha = 0{\cdot}8, \lambda = -2$ where there seems to be a discrepancy. The bounds using trial functions of the form (2.21) seem to be better for larger values of $|\lambda|$. This is probably due to the fact that we have chosen more complicated trial functions which will be significant when for large $|\lambda|$ the contribution from the integral operator $\hat{K}$ becomes important.

3. Nonlinear theory

Consider now equation (1.3).

$$T\phi = f(\phi) \tag{3.1}$$

where in general $f(\phi)$ is a nonlinear function of ϕ. Consider also the related equations

$$T\psi_{n+1} = f(\Phi_n), \qquad n = 0, 1, 2 \ldots, \tag{3.2}$$

in a suitably chosen real complete Hilbert Space H where Φ_n is a variational approximation to ψ_n. Let ϕ denote the exact solution of (3.1); then

$$T(\phi - \psi_{n+1}) = f(\phi) - f(\Phi_n) = f'(v_n)\delta\Phi_n \tag{3.3}$$

where $\delta\Phi_n = \phi - \Phi_n$ and $v_n = t\phi + (1-t)\phi_n$ is some function belonging to the space and t is such that $0 < t < 1$. Here we have used Taylor's expansion of $f(\Phi_n)$ about ϕ. Assuming that T has non-zero eigenvalues, so that the solution of equation (3.3) is unique for fixed Φ_n, T^{-1} exists and is linear. Putting $\delta\psi_{n+1} = \phi - \psi_{n+1}$ we have

$$\delta\psi_{n+1} = T^{-1} f'(v_n)\delta\Phi_n. \tag{3.4}$$

Let Φ_{n+1} denote a variational approximation to ψ_{n+1}; then since ψ_{n+1}, Φ_{n+1}, Φ_n, ϕ and v_n all belong to H

$$\begin{aligned} \|\delta\Phi_{n+1}\| &= \|\phi - \Phi_{n+1}\| \\ &\leqslant \|\phi - \psi_{n+1}\| + \|\psi_{n+1} - \Phi_{n+1}\| \\ &\leqslant \|T^{-1}\| \|f'(v_n)\| \|\delta\Phi_n\| + \|\psi_{n+1} - \Phi_{n+1}\|. \end{aligned} \tag{3.5}$$

Here the norm $\|u\|$ for u belonging to H denotes $\langle u|u\rangle^{1/2}$ and we are assuming $\|f'(v_n)\|$ is

Table 1. $-n$ denotes $\times 10^{-n}$.

		One parameter		Two parameter			Anderson *et al* (1969)
α	$-\lambda$	$J(0, \Phi_0)$	a_0	$J(0, \Phi_1)$	a_0	a_1	$J(0, \Phi)$
0·2	2	−0·312 94	0·112 79	−0·338 35	0·129 5	0·754 67(−1)	−0·343 72
	32	10·256 98 (−1)	0·933 77 (−2)	−0·257 41 (−1)	0·927 77 (−2)	−0·154 57 (−2)	−0·257 72 (−1)
	1024	−0·819 6 (−3)	0·295 4 (−3)	−0·819 61 (−3)	0·295 41 (−3)	−0·19 (−5)	−0·816 56 (−3)
0·5	2	−0·235	0·980 7 (−1)	−0·235 75	0·983 81 (−1)	−0·145 35 (−1)	−0·235 98
	32	−0·167 01 (−1)	0·696 94 (−2)	−0·167 009 (−1)	0·695 51 (−1)	−0·934 (−1)	−0·166 39 (−1)
	1024	−0·526 5 (−3)	0·219 7 (−3)	−0·526 5 (−3)	0·219 7 (−3)	0	−0·524 36 (−3)
0·8	2	−0·997 09 (−1)	0·467 07 (−1)	−0·997 12 (−1)	0·467 09 (−1)	−0·587 5 (−3)	−0·996 18 (−1)
	32	−0·654 02 (−2)	0·306 37 (−2)	−0·654 02 (−2)	0·306 37 (−2)	−0·25 (−5)	−0·653 28 (−2)
	1024	−0·205 (−3)	0·96 (−4)	−0·205 0 (−3)	0·96 (−4)	0	−0·204 8 (−3)

Table 2.

		One parameter		Two parameter			Anderson *et al* (1969)
α	$-\lambda$	$J(-1, \Phi_0)$	a_0	$J(-1, \Phi_1)$	a_0	a_1	$J(-1, \Phi)$
0·2	2	−0·347 08	0·125 10	−0·346 36	0·124 84	−0·118 95 (−1)	−0·343 78
	32	−0·259 10 (−1)	0·933 7 (−2)	−0·259 01 (−1)	0·933 6 (−2)	−0·661 1 (−4)	−0·259 16 (−1)
	1024	−0·844 8 (−3)	0·295 5 (−3)	−0·844 8 (−3)	0·295 5 (−3)	−0·1 (−6)	−0·104 84 (−2)
0·5	2	−0·237 63	0·991 68	−0·236 65	0·987 58 (−1)	−0·111 63 (−1)	−0·236 6
	32	−0·167 2 (−1)	0·697 49 (−2)	−0·167 10 (−1)	0·697 21 (−2)	−0·686 (−4)	−0·176 63 (−1)
	1024	−0·332 81 (−3)	0·219 7 (−3)	−0·332 8 (−3)	0·219 7 (−3)	−0·1 (−6)	−0·158 93 (−2)
0·8	2	−0·997 54	0·467 29 (−1)	−0·997 24 (−1)	0·467 15 (−1)	−0·543 81 (−3)	−0·996 98 (−1)
	32	−0·654 08 (−2)	0·306 37 (−2)	−0·653 76 (−2)	0·306 37 (−2)	−0·24 (−5)	−0·663 38 (−2)
	1024	−0·307 9 (−3)	0·96 (−4)	−0·307 9 (−3)	0·96 (−4)	0	−0·367 38 (−3)

bounded. Further we assume T has a discrete set of eigenvalues $\lambda_i (\lambda_i \neq 0)$ and therefore

$$\|T^{-1}\| = \max_{\|u\| \neq 0} \frac{\|T^{-1}u\|}{\|u\|} \geqslant \frac{1}{|\lambda_i|} \tag{3.6}$$

for u belonging to H. Fixing Φ_n in equation (3.2) we can approximate the exact solution ψ_{n+1} to an arbitrary degree of accuracy using the linear variational techniques discussed in § 2. The complementary principles become in this case

$$J(\Delta, \Phi_{n+1}) = \langle \Phi_{n+1} | T\Phi_{n+1} \rangle - 2\langle \Phi_{n+1} | f(\Phi_n) \rangle + \Delta \langle T\Phi_{n+1} - f(\Phi_n) | T\Phi_{n+1} - f(\Phi_n) \rangle \tag{3.7}$$

and are such that

$$\begin{aligned} J(\Delta_2, \Phi_{n+1}) &\leqslant -\langle \psi_{n+1} | f(\Phi_n) \rangle \\ &\leqslant J(\Delta_1, \Phi_{n+1}) \end{aligned} \tag{3.8}$$

for suitably chosen Δ_1 and Δ_2. Thus we can make the quantity $\|\Phi_{n+1} - \psi_{n+1}\|$ as small as we please by increasing the flexibility of Φ_{n+1} and varying the parameters in Φ_{n+1}. The convergence of the sequence $\{\Phi_n\}$ to the exact solution of equation (3.1) will thus depend on

$$M = \|T^{-1}\| \|f'(v_n)\| = \frac{\|f'(v_n)\|}{|\lambda_0|} \tag{3.9}$$

where λ_0 is the eigenvalue of smallest modulus. If M is large we can rearrange equation (3.1) to

$$T\phi = T\phi + b(f(\phi) - T\phi) \tag{3.10}$$

where b is a real parameter. Equation (3.2) now becomes

$$T\psi_{n+1} = T\Phi_n + b(f(\Phi_n) - T\Phi_n) = F(\Phi_n). \tag{3.11}$$

In this case M is replaced by

$$M = \|(1-b)I + bT^{-1}f'(v_n)I\|, \tag{3.12}$$

I being the identity operator. Equation (3.5) thus becomes

$$\|\delta\Phi_{n+1}\| \leqslant M\|\delta\Phi_n\| + \|\psi_{n+1} - \Phi_{n+1}\|. \tag{3.13}$$

Increasing the number of parameters in Φ_{n+1} and varying these parameters we can make $\|\psi_{n+1} - \Phi_{n+1}\|$ as small as we please. We can therefore ensure

$$\|\psi_{n+1} - \Phi_{n+1}\| < \epsilon \|\delta\Phi_{n+1}\| \tag{3.14}$$

for arbitrary $\epsilon > 0$. Thus if

$$0 < M + \epsilon < 1 \tag{3.15}$$

is satisfied

$$\|\delta\Phi_{n+1}\| < \|\delta\Phi_n\| \tag{3.16}$$

and the process converges. There are many ways of forming the sequence $\{\Phi_n\}$. A procedure adopted in this paper is as follows. Let ω_{np} denote a trial function containing p variational parameters for each iterate $n = 0, 1, 2, \ldots$. At the nth iteration we choose the p parameters so that $J(\Delta_1, \omega_{n+1,p})$ is stationary where $f = f(\omega_{np})$. Denote by

$\epsilon_{n+1,p}$ the error in the trial function $\omega_{n+1,p}$ so that

$$\|\psi_{n+1} - \omega_{n+1,p}\| \leqslant \epsilon_{n+1,p}. \tag{3.17}$$

Thus we obtain

$$\|\delta\omega_{n+1,p}\| \leqslant \|(1-b)I + bT^{-1}f'(v_{np})I\| + \epsilon_{n+1,p}. \tag{3.18}$$

Fixing p in the trial functions ω_{np} and letting $n \to \infty$, then if the sequence $\{\omega_{np}\}$ has a limit ω_p (say), that is if convergence is attained we have

$$\|\delta\omega_p\| \leqslant \|(1-b)I + bT^{-1}f'(v_p)I\|\|\delta\omega_p\| + \epsilon_p \leqslant M_p\|\delta\omega_p\| + \epsilon_p. \tag{3.19}$$

Provided that b is chosen so that $M_p < 1$ we then have

$$\|\delta\omega_p\| < \epsilon_p/(1-M_p). \tag{3.20}$$

This procedure can be carried through using $J(\Delta_2, \psi)$ instead of $J(\Delta_1, \psi)$ but in the examples we shall consider $J(\Delta_1, \psi)$ is a simpler functional. We can now use $J(\Delta_2, \psi)$ with $f = f(\omega_p)$ to find bounds for ϵ_p. With this choice for f we have

$$J(\Delta_1, \omega_p) \geqslant -\langle\psi_p|f\rangle \geqslant J(\Delta_2, \psi), \tag{3.21}$$

where $\psi \in H$ and $T\psi_p = f(\omega_p) = f$. Thus

$$\begin{aligned} J(\Delta_1, \omega_p) - J(\Delta_2, \psi) &\geqslant \langle\psi_p|f\rangle + J(\Delta_1, \omega_p) \\ &= \langle\psi_p - \omega_p|(1+\Delta_1 T)T(\psi_p - \omega_p)\rangle \geqslant N\epsilon_p^2. \end{aligned} \tag{3.22}$$

Here

$$\begin{aligned} N &= \min_i(\lambda_i + \Delta_1\lambda_i^2) \\ &= \min(\lambda_0 + \Delta_1\lambda_0^2, \bar{\lambda}_0 + \Delta_1\bar{\lambda}_0^2) \end{aligned} \tag{3.23}$$

where λ_0 is the smallest positive eigenvalue of T and $\bar{\lambda}_0$ is the largest negative eigenvalue. Thus

$$\epsilon_p^2 \leqslant (J(\Delta_1, \omega_p) - J(\Delta_2, \psi))/N \tag{3.24}$$

and consequently

$$\epsilon_p^2 \leqslant (J(\Delta_1, \omega_p) - J(\Delta_2, \omega_p))/N. \tag{3.25}$$

In practice to use these bounds in (3.20) to obtain a bound for $\|\delta\omega_p\|$ we need to estimate M_p. One possibility is

$$M_p \approx \|(1-b)I + bT^{-1}f'(\omega_p)I\|. \tag{3.26}$$

The sequence $\{\Phi_n\}$ can now be continued by increasing p, the number of variational parameters, taking initially f to be $f(\omega_p)$. To start the procedure it is necessary to obtain a suitable Φ_0 so that in the first calculation $f = f(\Phi_0)$. From (3.24) and (3.20) we deduce that

$$\|\delta\omega_p\|^2 \leqslant CS \tag{3.27}$$

where C is a constant and

$$S = \min_{\psi \in H}(J(\Delta_1, \omega_p) - J(\Delta_2, \psi)). \tag{3.28}$$

In these calculations we shall use S or an upper bound for S, for example

$$J(\Delta_1, \omega_p) - J(\Delta_2, \omega_p) \tag{3.29}$$

as a measure of the convergence.

4. Example calculations

To illustrate the nonlinear theory we consider first the integral equation

$$\phi \hat{k} \phi = 1 \tag{4.1}$$

where

$$\hat{k}\Phi = \int_0^{\pi/2} \frac{\sin(x-y)}{\pi(x-y)} \Phi(y)\, dy \tag{4.2}$$

which arises in communication theory (Saltzberg 1965, Nowosad 1966). Here $\hat{k}$ is a self-adjoint positive definite operator and $f(\Phi) = 1/\Phi$. The Hilbert space H for this problem is taken to be the space of square integrable functions in $0 \leqslant x \leqslant \pi/2$ so that the inner product is

$$\langle u_1 | u_2 \rangle = \int_0^{\pi/2} u_1(x) u_2(x)\, dx. \tag{4.3}$$

Since

$$\int_0^{\pi/2} \int_0^{\pi/2} \frac{\sin^2(x-y)}{\pi^2 (x-y)^2}\, dx\, dy < \frac{1}{4} \tag{4.4}$$

then $\hat{k}$ is a completely continuous operator with a discrete spectrum $\{\lambda_i\}$. To obtain bounds for the smallest eigenvalue λ_0 we use

$$E - (D^2 - E^2)^{1/2} \leqslant \lambda_0 \leqslant E \tag{4.5}$$

where $E = \langle \Phi | \hat{k} \Phi \rangle$ and $D = \langle \hat{k}\Phi | \hat{k}\Phi \rangle$ (see Pauling and Bright Wilson 1935). By optimising Φ we obtain $\lambda_0 \geqslant 0{\cdot}0223$ so that $\Delta_1 = 0$ and $\Delta_2 = -45$ form acceptable choices of Δ for minimum and maximum principles respectively. As an initial approximation for the iterative process we use $\Phi_0 = a$ (a constant) and choose a so that

$$L(a) = \| \hat{k} a - 1/a \|^2 \tag{4.6}$$

is a minimum. This gives $a = a_0 = \omega_{01} = 1{\cdot}4627$. The sequence is then continued with $\Phi_n = \omega_{n1} = a_n$ (a constant) using $J(0, \omega_{n1})$ and taking $b = \frac{1}{2}$. This procedure leads to $\omega_1 = 1{\cdot}4628$ where $J(0, \omega_1) = -1{\cdot}5708$. In this case

$$S \leqslant J(0, \omega_1) - J(-45, x). \tag{4.7}$$

Taking $x = b_1$ (a constant) and choosing b_1 so that

$$dJ/db_1 = 0 \tag{4.8}$$

where $f = f(\omega_1)$, we obtain $S \leqslant 0{\cdot}0073$. We now continue the sequence using

$$\omega_{n2} = a_{n2} + c_{n2} x^2 \tag{4.9}$$

which leads to

$$\omega_2 = 1{\cdot}4518 + 0{\cdot}0141 x^2. \tag{4.10}$$

This may be compared with the approximations derived by Arthurs and Coles (1977) namely $1{\cdot}36+0{\cdot}06x^2$ and $1{\cdot}36+0{\cdot}08x^2$. As the measure of convergence we take $x=\omega_2$ for simplicity and obtain

$$S \leqslant 0{\cdot}0070. \tag{4.11}$$

We shall now consider the more difficult example

$$-\nabla^2\psi+\psi-\psi^3=0 \tag{4.12}$$

which has applications in elementary particle theory (Shiff 1962) and electromagnetic theory (Finkelstein *et al* 1951). It has also been used as an example of nonlinear variational theory by Robinson (1971). Three trivial solutions are 0, ± 1. It has been shown by Finkelstein using phase–plane analysis that in the spherically symmetric case there exists a countably discrete set of solutions. Denoting these by $\phi_N(r)$, $N=0, 1, \ldots$ with a discrete set of initial values $\phi_N(0)$ Finkelstein shows that

$$\phi_N'(0)=0 \tag{4.13}$$

and

$$\phi_N(r)\sim A\exp(-r)/r \qquad \text{as } r\to\infty \tag{4.14}$$

where A is a constant. If we only consider this set of solutions, then writing $P_N(r)=r\phi_N(r)$ it is easy to verify that (4.12) is equivalent to the integral equation

$$P_N(r)=-\int_0^\infty \min(r,s)\left(P_N(s)-\frac{P_N^3(s)}{s^2}\right)\mathrm{d}s. \tag{4.15}$$

If we put $P_N(r)=\exp(-r)q$ and rearrange (4.15), adding and subtracting $q(r)$, we obtain

$$\begin{aligned} Tq &= q(r)+\int_0^\infty \min(r,s)\exp(-s)q(s)\,\mathrm{d}s \\ &= (1-\exp(-r))q(r)+\int_0^\infty \min(r,s)\exp(-3s)/s^2\,\mathrm{d}s = f(q). \end{aligned} \tag{4.16}$$

We now consider the real Hilbert space of $\exp(-r)$ square integrable functions with the inner product

$$\langle u|v\rangle=\int_0^\infty \exp(-r)u(r)v(r)\,\mathrm{d}r. \tag{4.17}$$

In this space T is linear, self-adjoint and completely continuous so that we can apply the theory of § 3. $\Delta_1=0$ and $\Delta_2=-\frac{3}{2}$ are suitable choices for the minimum and maximum principles. Finkelstein also shows that $\phi_N(r)$ possesses N zeros in $0\leqslant r<\infty$. To find a variational approximation for $\phi_0(r)$ we may consider trial functions of the form

$$q=ar \tag{4.18}$$

(a being a constant). In order to find a zero-order approximation Φ_0 to ϕ_0 we take Φ_0 of the form (4.18) where a is chosen so that

$$L(a)=\|T(ar)-f(ar)\|^2 \tag{4.19}$$

is a minimum. This leads to $a=a_0=\omega_{01}=4{\cdot}5838$. The sequence is continued with $\omega_{n1}=a_n$ (a constant) taking $b=-1$ in equation (3.11). This leads to $\omega_1=4{\cdot}7683$ and

$J(0, \omega_1) = -73{\cdot}8948$. We now define $x = b_1 r$ and choose b_1 so that

$$(\mathrm{d}/\mathrm{d}b_1)J(-\tfrac{3}{2}, x) = 0 \tag{4.20}$$

where $F(\Phi_n) = F(\omega_1)$ in equation (3.11). This leads to

$$-74{\cdot}9633 = J(-\tfrac{3}{2}, x) \leqslant -\langle\psi_1|F(\omega_1)\rangle \leqslant J(0, \omega_1) = -73{\cdot}8949. \tag{4.21}$$

These are approximate bounds for

$$-\langle\psi|F(\psi)\rangle \tag{4.22}$$

where

$$T\psi = F(\psi) \tag{4.23}$$

and give the result

$$S \leqslant 1{\cdot}0685. \tag{4.24}$$

This clearly indicates that we need to use more complex trial functions. The calculations were now repeated with trial functions of the form

$$\omega_{n2} = a_n \exp[-(\alpha_n - 1)r] = aW(\alpha_n) \tag{4.25}$$

with $b = 1$ so that $F(\omega_{n2}) = f(\omega_{n2})$ and $\omega_{02} = \omega_1$. Choosing a_{n+1} and α_{n+1} to satisfy the stationary conditions

$$(\partial J(0, \omega_{n2})/\partial a_{n+1}) = (\partial J(0, \omega_{n2})/\partial \alpha_{n+1}) = 0 \tag{4.26}$$

we obtain the two nonlinear equations

$$a_{n+1}\langle W(\alpha_{n+1})|TW(\alpha_{n+1})\rangle - \langle W(\alpha_{n+1})|f(a_n W(\alpha_n))\rangle = 0 \tag{4.27}$$

and

$$a_{n+1}\langle W'(\alpha_{n+1})|TW(\alpha_{n+1})\rangle - \langle W'(\alpha_{n+1})|f(a_n W(\alpha_n))\rangle = 0 \tag{4.28}$$

(assuming $a_{n+1} \neq 0$). Solving these iteratively leads to $\omega_2 = 5{\cdot}3137\ W(1{\cdot}5656)$. Taking $x_2 = b_2 W(1{\cdot}5656)$ and optimising $J(-\frac{3}{2}, x_2)$ with $f = f(\omega_2)$ gives $b_2 = 5{\cdot}3155$,

$$-9{\cdot}5911 \leqslant -\langle\psi_2|f(\omega_2)\rangle \leqslant -9{\cdot}5872 \tag{4.29}$$

and

$$S \leqslant J(0, \omega_2) - J(-\tfrac{3}{2}, x_2) = 0{\cdot}039. \tag{4.30}$$

This indicates that the procedure is converging. In order to continue the sequence $\{\Phi_n\}$ we would now need to increase the complexity of the trial functions. Care is needed in this case since a function of the form $(a + br)\exp(\gamma r)$ for example may have a zero in $0 \leqslant r < \infty$ and consequently cause convergence to $\phi_1(r)$ instead of $\phi_0(r)$.

5. More general nonlinear equations

We now consider the more general equation

$$T\phi = f(\phi) - L\phi \tag{5.1}$$

where f is nonlinear and L is a linear operator not necessarily self-adjoint. Following

§ 3 we define ψ_{n+1} so that

$$T\psi_{n+1} = f(\Phi_n) - L\Phi_n \tag{5.2}$$

where Φ_n is a variational approximation to ψ_n. The analysis of § 3 can be carried through with $(f'(v_n) - L)\delta\Phi_n$ replacing $f'(v_n)\delta\Phi_n$ and $f(\Phi) - L\Phi$ replacing $f(\Phi)$.

As an example of the more general theory we consider the Thomas–Fermi equation for an atomic system with a nucleus of charge Z at the origin. The spherically symmetric equation which describes the normal state of the system is

$$\mathrm{d}^2\phi/\mathrm{d}x^2 = \phi^{3/2}/x^{1/2} \qquad 0 \leqslant x < \infty \tag{5.3}$$

where $\phi(0) = 1$, $\phi(x) \sim 0$ and $x\phi'(x) \sim 0$ as $x \to \infty$. We can rewrite equation (5.3) in the form

$$\begin{aligned} T\phi &= -x\,\mathrm{d}^2\phi/\mathrm{d}x^2 - (2-x)\,\mathrm{d}\phi/\mathrm{d}x + \phi \\ &= -\phi^{3/2}x^{1/2} - (2-x)\,\mathrm{d}\phi/\mathrm{d}x + \phi = f(\phi) - L\phi. \end{aligned} \tag{5.4}$$

We now consider the Hilbert space of $x\exp(-x)$ square integrable functions in $0 \leqslant x < \infty$. Thus

$$\langle u|v\rangle = \int_0^\infty u(x)v(x)x\,\exp(-x)\,\mathrm{d}x. \tag{5.5}$$

T is a self-adjoint Sturm–Liouville differential operator on this space with a discrete set of eigenvalues $\{\lambda_n\}$ and a corresponding complete set of eigenvectors ϕ_n. It can be shown that

$$\phi_n = \mathrm{d}L_n(x)/\mathrm{d}x \tag{5.6}$$

where $L_n(x)$ are the Laguerre polynomials and that $\lambda_n = n$, $n = 1, 2, 3, \ldots$. Thus $\lambda_n \geqslant 1$ and we may choose $\Delta_1 = 0$ and $\Delta_2 = -1$. The trial functions which we use in this calculation will have the simple form

$$q = \exp(-\alpha x). \tag{5.7}$$

To find an acceptable $\Phi_0 = \exp(-\alpha_0 x)$ we choose α_0 so that

$$L(\alpha) = \int_0^\infty \left(\frac{\mathrm{d}^2\Phi_0}{\mathrm{d}x^2} - \frac{\Phi_0^{3/2}}{x^{1/2}}\right)^2 x\,\mathrm{d}x \tag{5.8}$$

is a minimum which gives $\alpha_0 = 1{\cdot}046\,738$. The sequence is continued with $\Phi_n = \exp(-\alpha_n x)$ and the condition

$$\frac{\mathrm{d}}{\mathrm{d}\alpha_{n+1}} J(0, \Phi_{n+1}) = 0, \qquad f = f(\Phi_n) \tag{5.9}$$

leads to

$$g(\alpha_{n+1}, \alpha_n) = 0, \tag{5.10}$$

a nonlinear equation in α_{n+1} and α_n.

Solving $g(\beta, \beta) = 0$ numerically gives $\beta = 0{\cdot}731\,745$. Defining $\hat{q} = \exp(-\beta x)$ we then have

$$J(-1, \hat{q}) = 0{\cdot}099\,3428 \leqslant -\langle\hat{\psi}|f(\hat{q}) - L\hat{q}\rangle \leqslant J(0, \hat{q}) = 0{\cdot}113\,9443 \tag{5.11}$$

where

$$T\hat{\psi} = f(\hat{q}) - L\hat{q}. \tag{5.12}$$

Also the measure of convergence, S, is such that

$$S \leqslant J(0, \hat{q}) - J(-1, \hat{q}) = 0{\cdot}014\,6015 \qquad (f = f(\hat{q})) \tag{5.13}$$

compared with the bound

$$S \leqslant J(0, \Phi_0) - J(-1, \Phi_0) = 0{\cdot}070\,39 \qquad (f = f(\Phi_0)). \tag{5.14}$$

The total electron energy E for this model is related to the exact solution ϕ by

$$CE(\phi) = \int_0^\infty \left(\frac{1}{2}\left(\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)^2 + \frac{2}{5}\frac{\phi^{5/2}}{x^{1/2}}\right) = 0{\cdot}6806 \tag{5.15}$$

where C is a constant depending on Z. This value has been obtained by a numerical solution of equation (5.3) (Bush and Caldwell 1931, Kobayashi *et al* 1955). From the results in this paper

$$CE(\hat{q}) = 0{\cdot}7071. \tag{5.16}$$

Arthurs and Robinson (1969) have also considered the variational solution of equation (5.3) with trial functions of the form (5.7) and obtain values of $\alpha = 0{\cdot}93$ and $\alpha = 1{\cdot}383$ from functionals which provide upper and lower bounds for the total energy.

6. Conclusion

This paper shows that the linear variational theory introduced in the earlier papers and described in § 2 can be used as a variational–iterative procedure to solve nonlinear problems. The main purpose of this paper is to try to provide iterative schemes for the solution of such nonlinear equations which provide criteria for convergence. The real quantity S provides such a measure. In some cases bounds for $\langle\phi|f(\phi)\rangle$ are required where $T\phi = f(\phi)$ and these calculations also provide approximate bounds for this quantity.

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