QUARTERLY OF APPLIED MATHEMATICS
APRIL, 1977

DUAL EXTREMUM PRINCIPLES FOR A NONLINEAR DIFFUSION PROBLEM

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Abstract. Maximum and minimum principles for a nonlinear boundary value problem in diffusion with concentration-dependent coefficient $D(c)$ are derived in a unified manner from the theory of dual extremum principles. The results are illustrated by a calculation in the case $D(c) = \exp c$.

The purpose of this note is to give a new variational formulation of the nonlinear boundary value problem described by the equation

$$-\frac{d}{dz}\left(D(c)\frac{dc}{dz}\right) = \frac{1}{2}z\frac{dc}{dz}, \qquad 0 < z < \infty, \tag{1}$$

$$c(0) = 1, \qquad c(\infty) = 0. \tag{2}$$

This problem arises in the study of diffusion into a semi-infinite medium, where the diffusion coefficient D is a function of the concentration c. The associated flux is given by

$$f(z) = D(c)\,dc/dz, \qquad f \leq 0, \tag{3}$$

and we shall suppose that $D(c) \in C^1[0, 1]$ and that $D(c) > 0$ for $c > 0$. Shampine [1] has shown that this kind of problem possesses a unique solution and has discussed in [2] some aspects of an approximate solution due to Macey [3]. This latter work formulates the solution c implicitly via an expression for $z(c)$. That is, the dependent and independent variables are interchanged.

If we adopt this approach, the problem in (1) to (3) may be written as [2]

$$dz/dc = D(c)/f, \qquad z(1) = 0, \tag{4}$$

$$-df/dc = \tfrac{1}{2}z, \qquad 0 < c < 1, \qquad f(0) = 0. \tag{5}$$

Here z and f are regarded as functions of the independent variable c.

To give a variational formulation of the problem we now observe that (4) and (5) are examples of the canonical equations

$$dz/dc = \partial H/\partial f, \tag{6}$$

$$-df/dc = \partial H/\partial z, \tag{7}$$

with the Hamiltonian $H(f, z)$ given by

$$H(f, z) = D(c)\ln|f| + \tfrac{1}{4}z^2. \tag{8}$$

We note that

$$\partial^2 H/\partial f^2 = -D(c)/f^2, \qquad \partial^2 H/\partial z^2 = \tfrac{1}{2}. \tag{9}$$

Since $D(c) \geq 0$, H is concave in f and convex definite in z, which in turn means that we can obtain dual extremum principles [see 4, 5].

Following the general procedure for canonical equations [see 4] we introduce the action functional

$$I(f, z) = \int_0^1 \left\{ f \frac{dz}{dc} - H(f, z) \right\} dc - (fz)_{c=1} , \tag{10a}$$

$$= \int_0^1 \left\{ -\frac{df}{dc} z - H(f, z) \right\} dc - (fz)_{c=0} . \tag{10b}$$

The integral I is stationary at the solution (f, z) of (4) and (5).

Now we define two sets of functions

$$\Omega_1 = \left\{ (f, z): \frac{dz}{dc} = \frac{D(c)}{f} , z(1) = 0 \right\} , \tag{11}$$

$$\Omega_2 = \left\{ (f, z): -\frac{df}{dc} = \frac{1}{2} z, 0 < c < 1, f(0) = 0 \right\}. \tag{12}$$

These sets intersect at the exact solution (f, z) of the problem, and they play a basic role in our procedure for obtaining dual extremum principles. Thus, we define a functional J by

$$J(z_1) = I(f_1 , z_1) \quad \text{via} \quad (10a), \quad \text{with} \quad (f_1 , z_1) \quad \text{in} \quad \Omega_1 . \tag{13}$$

This gives

$$J(z_1) = \int_0^1 \{ D(c) - D(c) \ln |D(c)/z_1'| - \tfrac{1}{4} z_1^2 \} \, dc, \tag{14}$$

with

$$z_1(1) = 0. \tag{15}$$

Also, we define a functional G by

$$G(f_2) = I(f_2 , z_2) \quad \text{via} \quad (10b), \quad \text{with} \quad (f_2 , z_2) \quad \text{in} \quad \Omega_2 . \tag{16}$$

This gives

$$G(f_2) = \int_0^1 \{ (f_2')^2 - D(c) \ln |f_2| \} \, dc, \tag{17}$$

with

$$f_2(0) = 0. \tag{18}$$

From their definitions, these functionals J and G are stationary at the exact functions z and f respectively. In addition, the global dual extremum principles

$$J(z_1) \le J(z) = G(f) \le G(f_2) \tag{19}$$

hold, equality arising when $z_1 = z$ and $f_2 = f$. These dual principles for the transformed problem (4) and (5) appear to be new, and they are much simpler than those corresponding to the original problem (1) and (2) which can be obtained from the results in [6].

To illustrate the use of these dual extremum principles we have performed calculations of the dual functionals for the case

$$D(c) = \exp c. \tag{20}$$

As trial functions we took

$$z_1 = c^{-k}(1 - c) \sum_{n=2}^{6} a_n c^{n-2}, \tag{21}$$

which satisfies $z_1(1) = 0$, and

$$f_2 = -\sum_{n=1}^{6} b_n c^n, \tag{22}$$

which satisfies $f_2(0) = 0$. The parameters a_n, b_n and k were found by optimizing J and G. The results are given in Table 1.

TABLE 1. Variational parameters.

$k =$	0.1165	$b_1 =$	1.8396
$a_2 =$	2.4374	$b_2 =$	−1.5638
$a_3 =$	0.3344	$b_3 =$	0.3580
$a_4 =$	0.1068	$b_4 =$	0.4896
$a_5 =$	0.8816	$b_5 =$	0.2152
$a_6 =$	−0.3044	$b_6 =$	−0.1220
$J =$	1.9743	$G =$	1.9772

We see from Table 1 that the functional J is within 0.003 of the exact metric for the problem, and hence in global terms the function $z_1(c)$ in (21) is an accurate variational solution. The inverse of (21) therefore provides an accurate estimate of the concentration $c(z_1)$. Numerical values of this can be read from Table 2, along with values of the flux $f(c)$. For this problem we estimate the initial flux $f(z_1 = 0) \equiv f(c = 1)$ to be −0.7862.

TABLE 2. Variational solutions $z_1(c)$ and $f_2(c)$.

c	$z_1(c)$	c	$f_2(c)$
0	∞	0.0	0
0.00001	9.3255	0.1	−0.1687
0.0001	7.1300	0.2	−0.3089
0.001	5.4476	0.3	−0.4242
0.01	4.1329	0.4	−0.5184
0.1	2.9105	0.5	−0.5956
0.3	2.0689	0.6	−0.6591
0.5	1.4758	0.7	−0.7113
0.7	0.9235	0.8	−0.7522
0.8	0.6363	0.9	−0.7793
0.9	0.3308	1.0	−0.7862
0.95	0.1690		
1.0	0		

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