# DYNAMIC PROGRAMMING, INVARIANT IMBEDDING AND TWO-POINT BOUNDARY VALUE PROBLEMS

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SUMMARY

Ordinary and partial differential equations involving conditions at various points, or at several boundaries, arise naturally from the calculus of variations, the domain of mathematical physics, and from mixtures of both disciplines. As is well-known, problems of this nature are of greater analytic complexity, and present many more obstacles in the way of computational solution, than those whose solutions are determined by initial values.

The object of this paper is to show how certain uniform techniques based upon functional equations can be used to provide new analytic approaches to questions of this type, and to furnish computational algorithms which are far better adapted to modern day computers than those of classical analysis. Our aim is to replace multi-point boundary value problems by initial value problems.

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## I. DYNAMIC PROGRAMMING

### 1. Introduction

Ordinary and partial differential equations involving conditions at various points, or at several boundaries, arise naturally from the calculus of variations, the domain of mathematical physics, and from mixtures of both disciplines. As is well-known, problems of this nature are of greater analytic complexity, and present many more obstacles in the way of computational solution, than those whose solutions are determined by initial values.

The object of this paper is to show how certain uniform techniques based upon functional equations can be used to provide new analytic approaches to questions of this type, and to furnish computational algorithms which are far better adapted to modern day computers than those of classical analysis. Our aim is to replace multi-point boundary value problems by initial value problems.

To treat those problems originating in the calculus of variations, or equivalent to questions with this origin, we employ the theory of dynamic programming, [1]. For various classes of problems emanating from the field of mathematical physics, we invoke the theory of invariant imbedding, [2], [21].

Both theories utilize the fundamental concept of semi-groups of transformations, a subject discussed in great detail and with many applications in [3]. Our applicationsof this basic idea are, however, quite different from those in the cited reference. We allow as semi-group variables, not only time, but length, radius, area, volume, and so on. In the theory of branching processes, [4], [5], [6], where functional equations play a key role, space and energy semi-group variables are also employed, together with the classic time variable.

## 2. Two-point Boundary-value Problems

Although the methods we employ can be, and have been, [7], utilized to some extent for the study of partial differential equations, we shall restrict ourselves in this part of the paper to the case of ordinary differential equations. The second part of the paper will be more closely connected with partial differential equations, of the type stemming from the Boltzmann equation.

Consider an n-th order differential equation of the form

$$(1) \qquad u^{(n)} = g(u,u',\ldots,u^{(n-1)}).$$

If we take initial conditions of the form

$$(2) \qquad u(0) = c_0, u'(0) = c_1, \ldots, u^{(n-1)}(0) = c_{n-1},$$

and impose various reasonable conditions on the function $g$, as, for example, given in [8], we can assert the existence and uniqueness of a function $u(t)$, satisfying (1) over some interval $[0,t_0]$, and the conditions of (2) at $t = 0$.

With this type of initial information, digital computers, and occasionally analogue computers, can be utilized in a number of very efficient ways to obtain the numerical solution.

For the case of initial value problems of the foregoing kind, both the existence and uniqueness of the solution are plausible, and not particularly difficult to establish. The situation, however, changes radically when we impose not the conditions of (2), but conditions of the form

$$u(0) = c_0, u'(0) = c_1, \ldots, u^{(k)}(0) = c_k, \tag{3}$$

$$u(t_0) = b_0, u'(0) = b_1, \ldots, u^{(n-2-k)}(0) = b_{n-k-2},$$

or, more generally, $n$ mixed conditions of the form

$$g_i(u(0), \ldots, u^{(n-1)}(0); u(t_0), \ldots, u^{(n-1)}(t_0)) = 0, \tag{4}$$

$i = 1,2,\ldots,n$.

Since solutions are constrained at two points, $t = 0$ and $t = t_0$, problems of this type are called <u>two-point boundary value</u> problems. It is no longer clear that solutions satisfying these conditions exist, nor that there is any uniqueness.

Frequently, by means of various analytic artifices, such as successive approximations or fixed-point theorems, existence, and even uniqueness, of solution can be established. However, as is often the case, these tools, so valuable for laying the foundations, are not powerful enough to yield efficient algorithms leading to a numerical solution.

The adjective "efficient," as used here, is strongly time-dependent. A quarter of a century ago, the criterion of an algorithm was bound to pencil and paper calculations, carried out perhaps by a team of computers. A few years later, many additional algorithms were admitted as feasible with the appearance of the desk computer. With the entry of the modern digital computer, we can think in terms of algorithms which formerly would have been unthinkable.

The algorithms we present below, derived from dynamic programming and invariant imbedding, are definitely predicated upon the use of a digital computer, although occasionally they do yield results susceptible to hand methods.

One of the pleasures associated with the field of the numerical solutions of differential equations, and indeed of equations of all types, is that we are engaged in a never-ending game. We get to first base when we devise any method, using currently available devices, which will yield an accurate numerical solution. We advance around the bases as we cut down on the time and the memory requirements. Finally, when we have reduced the computational solution to a hand computation, or to the use of simple tables, we have won an inning.

To begin the discussion, let us fasten our attention upon the second order equation

$$(5) \qquad u'' = g(u,u'), \quad 0 \leq t \leq T,$$

with two-point boundary conditions of the form

$$(6) \qquad u(0) = c_1, \quad k(u(T),u'(T)) = 0.$$

To make things interesting, we naturally take the function $g$ to be non-linear.

A straightforward numerical solution via digital computer requires the values of $u$ and $u'$ at $t = 0$ or $t = T$. Given information of the type appearing in (6), the usual approach to these problems involves a search process which zeroes in on the solution. An initial guess of $u'(0)$ is made, and the numerical solution of (5) is obtained, using this hypothesized value and the given value of $u(0)$. Using this solution, the quantity $k(u(T),u'(T))$ is calculated. If this compares favorably with the value zero, we accept this approximate solution; if not, we guess another value, and so on.

This is clearly a rather uninspired and pedestrian approach, with a number of disadvantages. For a large and significant class of problems of the foregoing type, we wish to present another approach which yields an exact solution in terms of initial value problems--although, in different variables.

This approach, an application of the theory of dynamic programming, can be utilized to treat many types of variational processes which resist the classical techniques. In the second part of the paper, we will discuss another class of equations, which can be treated by means of invariant imbedding.

## 3. Connection with Calculus of Variations

Our first approach to questions of this type is by means of the connection which exists between the equation in (2.5) and the Euler equation associated with the functional

(1) $$J(u) = \int_0^T h(u,u')dt.$$

In many cases, the variational problem is the original source of the differential equation.

Consider the problem of minimizing the functional $J(u)$ subject only to the initial condition

(2) $$u(0) = c_1.$$

Under appropriate conditions on $h(u,u')$, the minimizing function $u$ is determined as a solution of the equation

(3) $$\frac{\partial h}{\partial u} - \frac{d}{dt}\frac{\partial h}{\partial u'} = 0,$$

the Euler equation. An additional constraint,

(4) $$\left.\frac{\partial h}{\partial u'}\right|_{t=T} = 0$$

is obtained from the variational procedure.

It is interesting to note that even when the original variational problem does not initially contain a two point boundary value condition, the variational procedure automatically yields one.

If $h(u,u')$ is quadratic in $u$ and $u'$, the Euler equation is linear, in which case the two-point problem is very much simpler. Otherwise, the equation in (3) is non-linear.

Let us now assume that (2.5) is precisely the equation that one obtains from (3) after dividing through by $h_{u'u'}$, assumed uniformly non-zero. We shall then resolve the two-point boundary value problem of (2.5) and (2.6) by presenting a direct solution of the variational problem in (1), based upon an initial value equation.

## 4. Dynamic Programming

Let us briefly sketch the dynamic programming approach to variational equations of the type described in the foregoing section. What follows will be completely formal. Further details, and some rigorous justification, will be found in [1]; see also Dreyfus, [9], Osborn, [10].

We begin with the observation that the minimum of $J(u)$ depends upon the initial value $c$, and the length of the interval, $T$. Hence, we write

(1) $$f(c,T) = \underset{u}{\text{Min}}\ J(u).$$

This function is defined for $T \geq 0$, $-\infty < c < \infty$.

To derive a functional equation for $f(c,T)$, we can use the principle of optimality, [1], or, once we know what we want to obtain, we can proceed directly as follows. Write

(2) $$\begin{aligned} f(c,T) &= \underset{u[0,T]}{\text{Min}} \int_0^T h(u,u')dt \\ &= \underset{u[0,S]}{\text{Min}}\ \underset{u[S,T]}{\text{Min}} \left[\int_0^S h(u,u')dt + \int_S^T h(u,u')dt\right] \\ &= \underset{u[0,S]}{\text{Min}} \left[\int_0^S h(u,u')dt + \underset{u[S,T]}{\text{Min}} \int_S^T h(u,u')dt\right] \\ &= \underset{u[0,S]}{\text{Min}} \left[\int_0^S h(u,u')dt + f(u(S),T-S)\right]. \end{aligned}$$

In order to obtain a functional equation of conventional type, we regard $S$ as an infinitesimal. Then, to terms in $S^2$, we have

(3) $$u(S) = c + vS,$$

$$\int_0^S h(u,u')dt = h(c,v)S,$$

where we have set

(4) $$v \equiv u'(0) \equiv v(c,T).$$

Furthermore, as $S \longrightarrow 0$, minimization over all functions defined over $[0,S]$ becomes equivalent to minimization over all initial slopes. Thus, (2) becomes

$$(5)\qquad f(c,T) = \min_{v} \left[h(c,v)S + f(c + vS, T - S)\right] + O(S^2).$$

Still proceeding formally, this becomes

$$(6)\qquad f(c,T) = \min_{v} \left[h(c,v)S + f(c,T) + Svf_c - Sf_T\right] + O(S^2),$$

which reduces to

$$(7)\qquad f_T = \min_{v} \left[h(c,v) + vf_c\right].$$

This equation, together with the <u>initial</u> condition

$$(8)\qquad f(c,0) \equiv 0 \quad \text{for all} \quad c,$$

determines the function $f(c,T)$.

For the connection between (7) and the Euler variational equation, see Dreyfus, [9], Osborn, [10], or [1].

## 5. An Example

As an illustration, consider the problem of minimizing the integral

$$(1)\qquad J(u) = \int_0^T (u'^2 + g(u))dt,$$

over all functions $u$ satisfying the initial condition $u(0) = c$. Writing

$$(2)\qquad f(c,T) = \min_{u} J(u),$$

we have, from (4.7), the equation

$$f_T = \operatorname*{Min}_{v} \left[ v^2 + g(c) + v f_c \right], \tag{3}$$

or

$$f_T = g(c) - \frac{f_c^2}{4}\ . \tag{4}$$

The solution of this equation then leads to the solution of the two-point boundary value problem

$$u'' - \frac{g'(u)}{2} = 0, \tag{5}$$

$$u(0) = c, \quad u'(T) = 0.$$

Similar explicit results can be obtained for variational problems of the form

$$\operatorname*{Min}_{u_i} \int_0^T \left[ \sum_{i,j=1}^{M} a_{ij} u_i' u_j' + g(u_1, u_2, \ldots, u_M) \right] dt. \tag{6}$$

A greater variety of nonlinear differential equations may be obtained by starting with the problem of minimizing

$$J(y) = \int_0^T g(x,y)\,dt \tag{7}$$

over all $y$ where $x$ and $y$ are related by

$$\frac{dx}{dt} = h(x,y), \quad x(0) = c. \tag{8}$$

## 6. Discussion

Let us stop a moment and observe the basic device we have utilized. In place of considering an isolated variational problem for fixed initial value $c$ and fixed interval $[0,T]$, we have treated the whole class of problems arising from any initial value and any $T > 0$.

We have thus imbedded the original variational problem within a family of variational problems. To solve the original variational problem, we derive relations connecting neighboring problems. The equation in (4.7) expresses the way the solution changes as the parameters $c$ and $T$ change.

Precisely the same conceptual trick will be employed in dealing with the transport processes discussed in the second part of the paper.

## 7. Computational Aspects

To obtain the numerical solution of (4.7), we can follow the usual approach and replace it by a difference scheme such as

$$\frac{f(c,T+\Delta) - f(c,T)}{\Delta} = \underset{v}{\mathrm{Min}} \left[ h(c,v) + v\left(\frac{f(c+\delta,T) - f(c,T)}{\delta}\right) \right]. \tag{1}$$

We found, however, that it was better to use an approximation to (4.5) such as

$$f(c,T) = \underset{v}{\mathrm{Min}} \left[ h(c,v)\Delta + f(c + \Delta s, T - \Delta) \right], \tag{2}$$

where $T = 0, \Delta, 2\Delta, \ldots$ .

One advantage of this approach is that no ratio of small quantities, $\Delta/\delta$, is involved.

Those interested in the computational solutions of particular problems along these lines may refer to Cartaino-Dreyfus, [11], and Bellman-Dreyfus, [12].

The success of this approach suggests that similar techniques may be applicable to other types of partial differential equations. For a treatment of the equation

$$(3) \qquad u_t = uu_x,$$

and similar equations, see Bellman-Cherry-Wing, [13].

## 8. Convergence of Discrete Process to Continuous Process

As soon as we employ a formula such as (7.2), the question arises as to the convergence of the function obtained from (7.2) to the solution of (4.7). This can be approached in several ways, using the connection with the classical calculus of variations, cf. the treatment by Fleming in [14], or directly from (7.2) without any previous foundation of the calculus of variations; see [15].

## 9. Dimensionality

Let us now point out what prevents us from applying these methods in a <u>routine</u> fashion to the solution of a large class of current problems of significance. If we apply these methods to the determination of the minimum of the functional

(1) $$J(u_1,\dots,u_k) = \int_0^T g(u_1,u_2,\dots,u_k;u_1',u_2',\dots,u_k')dt,$$

with constraints $u_i(0) = c_i$, $i = 1,2,\dots,k$, we encounter functions of $k$ variables. These can be used for computational purposes with current digital computers if $k = 1,2$, with the case $k = 3$ soon to be feasible. For general $k$, the memory requirements become excessive. We must then have recourse to various types of approximations; cf. [16], [17].

## 10. Three-point Boundary Value Problems

Precisely the same approach can be used in the study of three-point boundary-value problems. Thus, if the fourth order equation

(1) $$u^{(4)} = h(u,u',u^{(2)},u^{(3)})$$

is derived from a variational problem associated with

(2) $$J(u) = \int_0^T g(u,u',u^{(2)})dt,$$

we can treat a boundary value problem such as

(3) $$u(0) = c_1, \quad u'(0) = c_2, \quad u(t_1) = c_3, \quad u(T) = c_4,$$

$0 < t_1 < T$, by introducing the function

(4) $$f(c_1,c_2,T) = \text{Min } J(u).$$

## 11. Implicit Variational Problems

In many interesting situations, the variational problem may not involve an explicit analytic functional. These are akin to free boundary problems in hydrodynamics in the sense that the solution itself determines some of the points where boundary conditions are applied. For example, one may wish to minimize the time required to restore a physical system to equilibrium; see [18], [19], or one may wish to minimize the terminal velocity when a desired terminal state is attained; see [20].

# II. NEUTRON TRANSPORT PROCESSES

## 12. Introduction

In this part of the paper, we wish to illustrate the application of the functional equation approach to the study of various types of two point boundary value problems that arise from mathematical physics. To show how equations of this type arise, we shall formulate some problems in the field of neutron transport theory, first in classical terms and then by means of the theory of invariant imbedding, [21], [22].

Once again, we obtain both a new analytic, and a new computational, approach. First, we shall treat the physical model giving rise to a linear form of the Boltzmann equation, where we have a choice of one approach or the other, and then we shall treat a particular collision process, where the classical approach leads to a nonlinear system of differential equations with two-point boundary values.

## 13. A Neutron Process for a One-dimensional Rod

Let us now describe a simple mathematical version of a neutron fission process. By a "rod," we shall mean the interval $[x,0]$, where to be consistent with notation in other papers we invert the usual direction. By a "neutron," we shall mean a particle which possesses the following property: when entering the sub-interval $[y + \Delta, y]$, from the right, there is a probability $p_1(y)\Delta$ that it divides into two particles of precisely the same nature, one going to the right and one to the left, and a probability $1 - p_1(y)\Delta$ that it traverses the interval with no interaction; when entering from the left, we have a similar situation with $p_1(y)$ replaced by $p_2(y)$. Here $\Delta$ is considered to be an infinitesimal, and all expressions are considered exact to terms of order $\Delta^2$.

On the basis of a model of this type, we would like to be able to predict the existence of a critical length. To attain this end, we begin by asking for the reflected and transmitted flux resulting from unit flux per unit time entering the rod at $x$.

By the terms reflected flux and transmitted flux, we mean the expected number of neutrons per unit time leaving $x$ to the left and the expected number of neutrons leaving $0$ to the right per unit time.

## 14. Classical Approach

The usual approach to these problems is by way of the determination of the internal fluxes. Let $y$ be a point inside the interval $[x,0]$, and define

(1) $u(y)$ = the flux to the right at $y$, per unit time,

$v(y)$ = the flux to the left at $y$, per unit time.

Once again, the term "flux" is used as a synonym for expected number. For a rigorous formulation of processes of this nature, see the forthcoming monograph by T. E. Harris, [6].

An "input-output" analysis yields the following relations, correct to terms in $\Delta^2$,

(2) $$u(y) = u(y + \Delta)(1 - p_1(y)\Delta) + p_1(y)\Delta u(y) + p_2(y)\Delta v(y).$$

Passing to the limit as $\Delta \to 0$, we obtain the differential equation

(3) $$u'(y) = - p_2(y)v(y).$$

A similar analysis leads to the complementary relation

(4) $$v'(y) = p_1(y)u(y).$$

The boundary conditions which fix the solution of this system of linear equations are

(5) $$u(x) = 1,$$
$$v(0) = 0,$$

which express the known facts that we have unit input from the left at $x$ and none from the right at $0$.

Eliminating $v(y)$, we obtain a single second order differential equation

(6) $$(u'(y)/p_2(y))' = - p_1(y)u(y),$$

with the two-point boundary conditions

(7) $u(x) = 1, \quad u'(0) = 0.$

What we wish to point out is that the physical setting automatically leads to a two-point boundary condition. A similar situation occurs in the study of transmission lines, where equivalent equations and conditions hold; cf. [23], [24].

## 15. Invariant Imbedding Approach

Let us now introduce functional equations. As in the first part of the paper, we imbed the particular process under discussion within a family of processes of the same general nature. In place of regarding $x$ as a fixed constant, we consider it to be a parameter which assumes all positive values.

We then introduce the two functions

(1) $f(x)$ = the reflected flux from $[x,0]$ due to unit incident flux at $x$,

$g(x)$ = the transmitted flux at $0$ due to unit incident flux at $x$.

To derive equations for $f(x)$ and $g(x)$, we proceed in very much the same fashion as before. As the flux proceeds through the sub-interval $[x, x - \Delta]$, part of it interacts and part of it proceeds through unaffected. In either case, the flux reflected from the interval $[x - \Delta, 0]$ can be expressed in terms of the function $f(x - \Delta)$. As this reflected flux traverses the interval $[x - \Delta, x]$, part of it interacts and results in a further reflection from $[x - \Delta, 0]$. Since all other processes contribute terms of order $\Delta^2$, we need merely take account of these to obtain our desired relation.

The analytic result is

$$(2) \qquad f(x) = p_1(x)\Delta + p_1(x)f(x)\Delta + (1 - p_1(x)\Delta)(f(x) - \Delta f'(x))\Big[(1 - p_2(x)\Delta) + p_2(x)\Delta + p_2(x)\Delta f(x)\Big],$$

to terms in $\Delta^2$.

Taking the limit as $\Delta \rightarrow 0$, we obtain the equation

$$(3) \qquad f'(x) = p_1(x) + p_2(x)f^2(x),$$

with the initial value $f(0) = 0$.

Similarly, we can obtain an equation for $g(x)$, which will involve $f(x)$. Further details may be found in [21], [22].

## 16. Energy Dependence

A more interesting situation is that where we take the energy of the particle into account. To avoid partial differential equations, the usual practice is to divide the energy range up into a number of different levels or groups.

In this way, there arises what is currently called "multi-group theory."

Assume that there are $N$ different energy levels, $i = 1,2,\ldots,N$, and introduce the following functions:

(1) $f_{ij}(x)$ = the reflected flux in state $j$ (energy level $j$) due to unit incident flux in state $i$ at $x$.

In place of the functions $p_1(x)$ and $p_2(x)$, we have functions

(2) $p_{ijk}(x)\Delta$ = the probability that in $[x, x - \Delta]$ a particle in state $i$ will fission into two particles, one in state $j$ and one in state $k$, where the $j$-particle goes to the left and the $k$-particle to the right.

For the sake of simplicity, assume that there is no directional effect.

As in the simple case, the classical approach yields a set of $2N$ linear differential equations with two-point boundary values, for the interval fluxes, while the invariant imbedding approach yields $N^2$ nonlinear differential equations with initial value constraints.

From the computational point of view, one has to compare the solution of linear differential equations of order $2N$ plus linear algebraic equations of order $N$ versus the solution of $N^2$ nonlinear differential equations. For $N = 10$, it would seem preferable to use the system of 100 nonlinear differential equations. From the standpoint of the determination of critical length, the nonlinear differential equations seem preferable.

For further discussion, and other geometries, see [21], [22], [25].

## 17. Collision Processes

In the preceding cases, we possessed explicit analytic solutions of the two-point boundary value problem. Let us now consider some physical processes which lead to nonlinear transport equations with two-point boundary value problems. These are collision processes where we face the full force of the Boltzmann equation.

In this case, the conventional approach leads to great difficulties, even from the standpoint of existence and uniqueness of solutions; cf. Carleman, [26], while the invariant imbedding approach appears to offer definite advantages.

Let us define the collision process, now assumed purely deterministic, by means of the function

(1) $\phi(u,v,y)\Delta$ = the diminution in intensity of a flux of strength $u$ entering $[y + \Delta, y]$ from the left when a flux of strength $v$ enters from the right.

With $u(y)$ and $v(y)$ defined as before, left- and right-hand fluxes at $y$, we obtain the equations

$$(2) \qquad u(y) = u(y + \Delta)(1 - p(y)\Delta)(1 - \phi(u,v,y)\Delta/u) + p(y)u(y)\Delta + v(y)p(y)\Delta,$$

or

$$(3) \qquad u'(y) = p(y)v(y) - \phi(u,v,y).$$

Similarly,

$$(4) \qquad v'(y) = - p(y)u(y) - \phi(u,v,y).$$

The boundary conditions, as before, are

$$(5) \qquad u(x) = 1, \quad v(0) = 0.$$

Due to the nonlinearity, we face a problem of some computational difficulty.

## 18. Functional Equation Approach

Let us now apply invariant imbedding techniques. Let

(1) $f(u,x)$ = the reflected flux from $x$ when the incident flux has intensity $u$.

Then, we have, to terms in $O(\Delta^2)$,

$$(2)\qquad f(u,x) = p(x)\Delta + p(x)f(u,x)\Delta + \left[1 - \phi(u,f(u,x),x)\Delta/f(u,x)\right]\left[f(u + f(u,x)p(x)\Delta - p(x)u\Delta - \phi(u,f(u,x),x)\Delta, x - \Delta)\right],$$

leading to the partial differential equation

$$(3)\qquad \frac{\partial f}{\partial x} = p(x) + p(x)f(u,x) - \phi(u,f(u,x),x) + \left[f(u,x)p(x) - p(x)u - \phi(u,f(u,x),x)\right]\frac{\partial f}{\partial u},$$

with the initial value

$$(4)\qquad f(u,0) = 0, \quad u \geq 0.$$

This yields a feasible computational approach. Further details may be found in [27].

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