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EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

THE MAXIMUM PRINCIPLE, ITS COMPUTATIONAL ASPECTS AND ITS RELATIONS TO OTHER OPTIMIZATION TECHNIQUES

by

W. DE BACKER

1964

Joint Nuclear Research Center
Ispra Establishment - Italy

Scientific Data Processing Center - CETIS

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INTRODUCTION

This report is the text of an introductory seminar on optimal control held by the author for EURATOM personnel at CETIS in April 1963.

After the first IFAC-Congress held in Moscow in 1960, a growing interest in optimal control has been noticed throughout the world. Many contributions in this field originated in some very important papers presented at the congress, especially those by Pontryagin, Bellman and their respective co-authors.

In this report we are concerned with the mathematical theory developed by the Pontryagin team and which is better known as the Maximum Principle.

As an introduction we tried to give a synthetic statement of the theorems on the Maximum Principle and to discuss its relations to other optimization techniques (chapters 1 and 3). Our main point of interest however is the synthesis of optimal control and particularly its computational aspects. As, as yet this is an unsolved problem we tried to give a general outline of present possibilities and future hopes (chapters 2, 3 and 5). Some original work of the author on penalty functions and generalized gradient techniques has been included (cfr. chapter 3 and 4).

However, since progress is very quick in this field new important developments have been published after April 1963. This was particularly the case at the second IFAC-Congress held in Basle in September 1963, where optimal control was the main topic in the theoretical section. Some problems we referred to in this report are already solved now, for instance the synthesis of linear optimal control and some theoretical difficulties in connection with penalty functions.

On the other hand new experience concerning the computational aspects of optimal control in general and some applications in nuclear reactor control in particular, have been obtained in CETIS. Results will be published as soon as possible. Most specialists in optimal control now agree that progress in computer synthesis is intimately related to progress in technology of hybrid computation.

CHAPTER 1 THE MAXIMUM PRINCIPLE

1.1. Statement of the fundamental Problem

We consider $x(t)$ to be the state vector $x(t) = (x^1(t), \ldots, x^i(t), \ldots, x^n(t))$, belonging to a region G of the n-dimensional state space and whose evolution is described by a system of differential equations

$$\frac{dx(t)}{dt} = f\left[x(t), u(t)\right] \qquad (1)$$

with $f = (f^1, \ldots, f^n)$. In this system $u(t) = (u^1(t), \ldots, u^r(t))$ is a control vector whose range is in a subset U of the r-dimensional control space. The subset U is usually defined by

$$q^l(u) \lesseqgtr 0 \qquad l = 1, \ldots, s \qquad (2)$$

and the region G is usually defined by

$$g^j(x) \lesseqgtr 0 \qquad j = 1, \ldots, m \qquad (3)$$

In relations (2) and (3) the inequality sign is optional.

The initial condition $x(t_o) = x_o$ and the final condition $x(t_1) = x_1$ of the system belong respectively to the sets S_o and S_1 which are smooth manifolds in G of arbitrary dimension (but less than n).

Among all admissible controls $u \in U$ which transfer the point x from $x_o \in S_o$ to $x_1 \in S_1$, it is asked to find one for which the functional

$$J = \int_{t_o}^{t_1} f^o\left[x(t), u(t)\right] dt \qquad (4)$$

takes on the least possible value.

1.2. Discussion

We propose to comment on the general aspects and the restrictions of the problem as stated in § 1.1., in order to evaluate the power of the mathematical optimization theory proposed by the Pontryagin team.

1.2.1. The system of dynamical constraints

The set of equations (1) covers a very general class of dynamical systems and probably is the most general one which is possible to program on an analog computer. It consists of n different first order differential equations of the type

$$\frac{dx^i}{dt} = f^i\,(x^1, x^2, \ldots, x^i, \ldots, x^n, u^1, \ldots, u^r)$$

It can easily be shown that an n-order differential equation can be written as a set of n first order differential equations.

Example: $\ddot{x} + 2\zeta\omega_o\dot{x} + \omega_o^2 x = c$ is equivalent to

$$\frac{dx^2}{dt} = c - 2\zeta\omega_o x^2 - \omega_o^2 x^1$$

$$\frac{dx^1}{dt} = x^2$$

with $x^2 = \dot{x}$ and $x^1 = x$

It should be remembered that even a partial differential equation corresponds to the formulation (1), but then with $n = \infty$. The approximation by finite differences however, which is a common technique for solving partial differential equations on analog and digital computers, automatically fits in with (1) since n has been given a finite number.

The vector equation (1) itself may be the subject of a finite difference approximation with respect to time

$$x\,(t + \Delta t) = x\,(t) + f\left[x\,(t), u\,(t)\right]\Delta t \qquad (5)$$

or

$$x^i_{j+1} = x^i_j + f^i\,(x^1_j, \ldots, x^n_j, u^1_j, \ldots, u^r_j)\,\delta \qquad (5')$$

with $\delta = \Delta t$

$i = 1, \ldots, n$

$j = 1, \ldots, N$

This formulation is useful for digital computers and for iterative techniques with analog computers.

The set (1) generally represents the model of a dynamical system such as a space engine, a nuclear reactor or a power generating system. We would draw attention to the importance of the simplicity and validity of such a model with respect to the physical system. Without simplicity and especially without a reasonably low number of equations the optimization, even with large electronic computers, becomes a heavy, risky and even an impossible task. On the other hand a lack of knowledge about the validity and the regions of validity of a simplified model may lead to solutions which are completely unrealistic from a physical point of view.

1.2.2. The control variables

The essential difference between the state variables and the control variables is that the latter are completely free from dynamical constraints. At every instant they can be chosen anywhere in the control region U.

If some variable, subject of a dynamical constraint were considered as a control variable, the optimization would take place ignoring that constraint. This generally gives rise to surprising and very unrealistic results. It may be dangerous, for instance, to ignore the inertia and the transfer function of the control system itself, even if at first sight its quality would suggest their unimportance. This again points out the problem of the validity of the dynamical model.

For the mathematical statement of the problem, U could be an arbitrary set, but in technical problems U is always a closed set. Some particular types of control regions are

- the hypercube $q^i(u) = |u^i| - 1 \leq 0$ (6)

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

- the hypersphere $q(u) = \sum_{i=1}^{n} (u^i)^2 - 1 = (u, u) - 1 \leq 0$ [+]) (7)

The number of control variables r, especially when compared with n, is evidently a very important characteristic of the control possibilities of the system.

[+]) By (a, b) we mean the scalar product of the vectors a and b.

In some problems time appears explicitly in f^i (x, u, t), f^o (x, u, t) or g^j (x, t), making the whole system non-autonomous. In such a case we consider time as a new state variable $x^{n+1} = t$ wherever it appears explicitly, while a new differential equation $dx^{n+1}/dt = 1$ is added to the system. In this way we obviously satisfy once more the general definition of (1).

Algebraic relations between state variables of the type $\varphi(x) = 0$ are more difficult to handle. In most cases $\varphi(x) = 0$ can be solved for one state variable as a function of the others $x^\alpha = \Theta\,(x^1, \ldots, x^{\alpha-1}, x^{\alpha+1}, \ldots, x^n)$, which can be introduced in all f^i wherever x^α appears. Such a substition is surely the "cleanest" method. Sometimes however this technique is not desirable because of programming difficulties. This is particularly true if several nonlinear algebraic relations have to be treated. Therefore a second possibility is to consider $\varphi(x) = 0$ as a relation of type (3), for which Lagrange multipliers have to be introduced, as will be shown by the theorems of Pontryagin.

Sometimes no system of dynamical constraints has been given, but the time derivative $\dot{x}$ of the state variable x has to be chosen in order to minimize the given functional. In this case it should not be forgotten that system (1) takes the form

$$\frac{dx^i}{dt} = u^i \qquad\qquad i = 1, \ldots, n$$

Although equations of the type

$$\frac{dx}{dt} = f\left[x(t),\ x(t-\tau_1),\ x(t-\tau_2),\ \ldots,\ u(t)\right]$$

are not accepted by the definition of system (1) some generalizations of the theorems of Pontryagin are possible, enabling them to be included (cfr. ref. [1], ch. IV, § 27).

1.2.3. Restricted state variables

The control vector $u \in U$ has to be chosen such that x stays in the interior of G. We already know from (3) that G may be defined by inequality or equality constraints. We also noticed that the last case offers the possibility of introducing algebraic relations of the type $\varphi(x) = 0$.

Sometimes additional equations of type (1) are necessary for the definition of G. We take the example of integral constraints:

$$\int_{t_o}^{t} \rho(x,u)\, dt' \leq A$$

Then we introduce the additional equation

$$\frac{dx^{n+1}}{dt} = f^{n+1}(x, u) = \rho(x, u)$$

such that G can be defined by $x^{n+1} - A \leq 0$.

According to the application, g (x) may be the maximum altitude of an aircraft, a mechanical stop in a servomechanism, the maximum operating temperature of an electric motor, a given disposable income budget or an integral constraint such as the charge of an accumulator or an available quantity of fuel.

1.2.4. The functional J

Introducing the definition

$$\frac{dx^o(t)}{dt} = f^o\left[x(t), u(t)\right] \quad \text{with } x^o(t_o) = x_o^o \qquad (8)$$

we see that $J = x_1^o - x_o^o$ and the problem reduces to finding u (t) such that $x^o(t_1)$ takes on the least possible value. Every maximal problem can be changed into a minimal problem by inverting the sign of $f^o(x, u)$. Equation (8) can be added to the set of equations (1) increasing the order of the system by one. It has to be observed, however, that none of the functions f or f^o contains the variable x^o.

Some special cases are of particular interest. Taking $f^o(x, u) = 1$ we have $J = t_1 - t_o$, representing a time-optimal problem. This already shows that neither t_o nor t_1 necessarily has to be given by the problem. They can be part of the solution. It may equally happen that $J = F(x_1) - F(x_o)$ is a function only of the initial and final conditions of the state variables, which implies $f^o(x, u) = dF/dt = (\partial F/\partial x, f)$. Both cases will be studied later (cfr. § 1.7. and chapter 4).

Some authors prefer the expression $f^o(x, \dot{x}, t)$. It can easily be shown that this is a special case of our definition $f^o(x, u)$. We only have to consider t as a new state variable (cfr. § 1.2.1.) and to substitute all $\dot{x}$ by the corresponding $f(x, u)$ of the equations (1).

The right definition of the optimization criterion is of course the crucial point of the problem. It can be the mean square error in a servomechanism, the consumption of fuel of a missile or an aircraft, some maximal distance, minimal time, minimal cost in a production process, minimal xenon poisoning during the shutdown of a nuclear reactor, etc.

Finally, it may happen that the function $f^o(x, u)$ is not given explicitly, but has to be measured while optimizing. This new restriction imposes special techniques, which will not be discussed.

1.2.5. Initial and final conditions

The fact that S_o and S_1 are sets implies that x_o and x_1 are not necessarily given points. Their choice as elements of S_o and S_1 is indeed a part of the solution of the problem.

In a time-optimal problem for instance, t_1 is not given and the same is true for some, or all, the components of x_1 in a maximum distance problem.

An interesting case is where every instant t is considered as a t_o of an optimization process ending at $t_1 = t + T$. After having solved the problem for $t \leqslant t' \leqslant t + T$, the initial decision u (t) is taken and this brings the system to the time $t + \Delta t$ where the whole optimization process has to be repeated for $t_o = t + \Delta t$. In this way we have a continuous sequence of optimization processes of which the initial decisions describe a time trajectory. Some aspects of this problem are studied in chapter 4.

1.3. The Maximum Principle and the Theorems of the Pontryagin Team

We shall restrict ourselves to a very condensed statement of the theorems concerning the maximum principle. For more mathematical details as well as rigorous demonstrations we refer to ref. [1]. Three cases have to be distinguished.

1.3.1. The optimal trajectory lies in the interior of G

We assume the functions f^i (x, u) (i = 0, 1, ..., n) to be defined and continuous together with their partial derivatives $\partial f^i / \partial x^\alpha$, $\alpha = 1, \ldots, n$, on G x U. Admissible controls $u(t) \in U$ have to be piecewise continuous.

In order to formulate the maximum principle we consider in addition to the system (1) another set of differential equations in the continuous non-zero variables $\psi_0, \psi_1, \ldots, \psi_n$, called the adjoint system.

$$\frac{d\psi_i}{dt} = -\sum_{\alpha=0}^{n} \frac{\partial f^\alpha (x, u)}{\partial x^i} \psi_\alpha \qquad (9)$$

$$i = 0, 1, \ldots, n$$

Introducing the definition

$$\mathcal{H}(\psi, x, u) = \sum_{\alpha=0}^{n} \psi_\alpha f^\alpha (x, u) \qquad (10)$$

system (1) and (9) can be rewritten as a Hamiltonian system.

$$\frac{dx^i}{dt} = \frac{\partial \mathcal{H}}{\partial \psi_i} \qquad i = 0, 1, \ldots, n \qquad (11)$$

$$\frac{d\psi_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x^i} \qquad i = 0, 1, \ldots, n \qquad (12)$$

Theorem:

Necessary conditions for optimality of the problem stated in § 1.1., with the above mentioned restrictions and definitions, are

1. Maximum condition

   At every instant t, u(t) has to be chosen such that $\mathcal{H}$ attains its least upper bound

$$\mathfrak{M}(\psi, x) = \sup_{u \in U} \mathcal{H}(\psi, x, u) \qquad (13)$$

2. Terminal conditions

$$\psi_0(t_1) \leq 0 \qquad \mathfrak{M}[\psi(t_1), x(t_1)] = 0 \qquad (14)$$

3. Transversality conditions

   $\psi(t_0)$ has to be orthogonal to a tangent plane of S_0 in the point $x_0 \in S_0$.

   $\psi(t_1)$ has to be orthogonal to a tangent plane of S_1 in the point $x_1 \in S_1$.

If these three conditions are satisfied it results that ψ_0 is constant and $\mathfrak{M}(\psi, x) = 0$ at any time t, $t_0 \leq t \leq t_1$, and not just at t_1.

Whenever ψ_0 is different from zero, which is true for nearly all possible applications, we can take $\psi_0 = -1$, since the adjoint system (9) is homogeneous in ψ.

1.3.2. The optimal trajectory lies on the boundary of G

Necessary conditions are piecewise smooth boundaries for U and G, while u(t) itself has to be a piecewise smooth time function.

We shall formulate the optimizing conditions for G and U defined respectively by $g(x) \leqslant 0$ and $q(u) \leqslant 0$ instead of the set of relations (2) and (3). The theorems, however, can easily be generalized for values of m and l bigger than one.

Let us introduce the notations

$$p(x, u) = \left(\frac{\partial g(x)}{\partial x}, f(x, u)\right) \qquad (15)$$

$$= \sum_{\alpha=1}^{n} \frac{\partial g(x)}{\partial x^{\alpha}} f^{\alpha}(x, u)$$

For an optimal trajectory lying entirely on the boundary $g(x)$ it is obviously necessary and sufficient that $g(x_o) = 0$ and $p(x, u) = 0$ for $t_o \leqslant t \leqslant t_1$.

The approach is now to introduce Lagrange multipliers $\lambda(t)$ and $\nu(t)$ for $g(x)$ and $q(u)$ and to apply the maximum principle as stated in § 1.2.1. Because of the Lagrange multipliers the maximization of $\mathcal{H}$ then has to be changed into relation (18), linked to additional conditions indicated below.

Theorem [+])

Necessary conditions for optimality of the problem stated in § 1.1. with the restrictions of § 3.2.1. and § 3.2.2. and with the definitions (10), (11) and (15) are:

$$\frac{d\psi_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x^i} + \lambda \frac{\partial p}{\partial x^i} \qquad i = 0, 1, \ldots, n \qquad (16)$$

[+]) The theorem is only true for "regular" optimal trajectories. The rigorous definition and the discussion of this requirement would lead us too far from a synthetic statement of the theorem. For more details we refer to ref. [1] ch. VI p. 265.

$$p(x,u) = 0 \qquad \text{and} \qquad g(x_0) = 0 \tag{17}$$

$$\frac{\partial \mathcal{H}}{\partial u^j} = \lambda \frac{\partial p}{\partial u^j} + \nu \frac{\partial q}{\partial u^j} \qquad j = 1, \ldots, r \tag{18}$$

$$\mathcal{M}(\psi, x) = \mathcal{H}(\psi, x, u) = 0 \tag{19}$$

$$\psi_0(t) = \text{constant} \leq 0 \tag{20}$$

$\psi(t_0)$ is different from zero and a tangent to the boundary $g(x)$, which generally means

$$\left[\psi(t_0), \text{ grad } g(x)\right] = 0 \tag{21}$$

This condition is only necessary in order to eliminate trivial solutions of the type $\psi + \nu$ grad g (ν is arbitrary)

if $d\lambda/dt$ exists, $(d\lambda/dt)$ grad $g(x)$ is directed towards the interior of G or else in zero. (22)

1.3.3. The optimal trajectory partly lies in the interior of G and partly on the boundary of G

For parts of the optimal trajectory in the interior of G the conditions of § 1.3.1. are valid. For parts of the optimal trajectory on the boundary of G, the conditions of § 1.3.2. have to be applied. As yet missing is a junction condition, which every pair of adjoining sections satisfies. This condition is called a jump condition for the vector $\psi(t)$ at the junction time τ.

Without going into details we point out two important possibilities:

a) The trajectory reaches and then follows the boundary of G. The vector $\psi(t)$ changes discontinuously with an amount μ grad $g(x)$ such that (21) can be satisfied.

b) The trajectory lies on the boundary of G and leaves it for the interior. No change is imposed on $\psi(\tau)$.

In both cases the optimal trajectory remains smooth at the junction points.

1.3.4. Remarks

The theorems of Pontryagin only give necessary conditions for optimal control. Nothing is said about the existence and the uniqueness of the solution.

A straightforward application of the theorems can give serious computational complications in connection with the calculation of the Lagrange multipliers and the criterion indicating the instant when the trajectory has to leave the boundary for the interior.

For this reason we refer to the technique of implicit computing of Lagrange multipliers. This technique only approximates to the solution of the problem, but has the advantage of bypassing a lot of complications which for this reason have not even been mentioned in the preceding paragraphs. The technique of implicit computing of Lagrange multipliers is related to the theory of the penalty functions which will be discussed in chapter 3.

1.4. The Principle of Optimality and its Relation to the Maximum Principle

It is our aim to show in a formal way how the maximum principle could be deduced from the principle of optimality of Bellman (cfr. [3] pp. 56 - 59 and [1] pp. 69 - 73).

1.4.1. The principle of optimality

"An optimal policy has the property that whatever the initial state and the initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision" (Bellman).

This means that whatever be the initial state (all x and not only x_o) the first decision (u (t) and not only u (t_o)) can be determined only if we know the optimal trajectories (and the corresponding returns) starting from all the states which could be reached by our first decision (cfr. Fig. 1.1.).

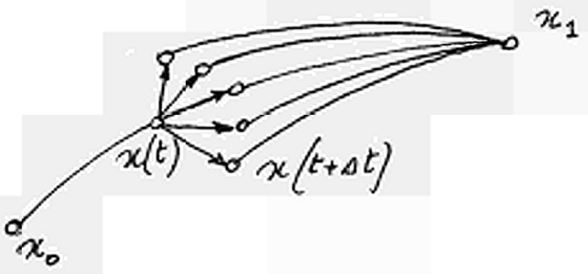

Fig. 1.1.

The principle of optimality has been given a discrete-time formulation and applying it to our problem of § 1.1. we have to take the finite difference version of the time derivatives (cfr. relation (5))

$$J(x) = \underset{u \in U}{\text{Max}} \left[-f^0(x, u)\Delta t + J(x + f(x, u)\Delta t) \right] \qquad (23)$$

In this mathematical formulation of the principle of optimality $J(x)$ has the meaning of the minimal value of (4), corresponding to the solution of the problem of § 1.1. for a trajectory starting at $x(t)$ at time t with a decision $u(t)$ and ending at time t_1 at the point $x_1 \in S_1$.

1.4.2. The continuous version of the principle of optimality

In order to derive a continuous version of (23) by a limit operation, we develop $J(x + f(x, u)\Delta t)$ by a time series.

$$J\left[x + f(x, u)\Delta t\right] = J(x) + \sum_{\alpha=1}^{n} \left[\frac{\partial J}{\partial x^\alpha} f^\alpha\right]\Delta t + O\left[(\Delta t)^2\right] \qquad (24)$$

This operation obviously requires the existence of the partial derivatives of J with respect to all x^α. Introducing (24) into (23), cancelling $J(x)$ in both members, deviding all terms by Δt and passing through the limit, we obtain

$$0 = \underset{u \in U}{\text{Max}} \left[-f^0(x, u) + \sum_{\alpha=1}^{n} \frac{\partial J}{\partial x^\alpha} f^\alpha(x, u) \right] \qquad (25)$$

Remarking that we have by definition

$$\frac{\partial J(x)}{\partial x^0} = \frac{\partial \left[x^0(t_1) - x^0(t) \right]}{\partial x^0(t)} = -1$$

it is possible to write (25) as follows

$$\underset{u \in U}{\text{Max}} \left[\frac{\partial J}{\partial x^\alpha} f^\alpha(x, u) \right] = 0 \qquad (26)$$

Relation (26) coincides with the maximum principle and the relations (10), (13) and (14). The only point which should be cleared up is the equivalence of $\partial J / \partial x^\alpha$ and ψ^α. In other words we want to know if $\partial J / \partial x^\alpha$ as well satisfies the Hamiltonian system.

1.4.3. The Hamiltonian system

We introduce the notations

$$\underset{u \in U}{\text{Max}} \left(\sum_{\alpha=1}^{n} \frac{\partial J}{\partial x^\alpha} f^\alpha \right) = M\left[\frac{\partial J}{\partial x}(x), x \right] = \beta(x) = 0 \qquad (27)$$

We mean that at every instant of the optimal trajectory the maximization gives a $u\left[x(t)\right]$, such that $f^\alpha(x, u)$ becomes $f^\alpha\left[x, u(x)\right] = f'^\alpha(x)$ (synthesis problem). It is in this sense that the partial derivatives $\partial f'^\alpha / \partial x^i$ have to be understood in this paragraph.

Calculating $\partial \beta(x) / \partial x^i = 0$ we have

$$\sum_{\alpha=0}^{n} \frac{\partial^2 J}{\partial x^\alpha \partial x^i} f'^\alpha = -\sum_{\alpha=0}^{n} \frac{\partial J}{\partial x^\alpha} \frac{\partial f'^\alpha}{\partial x^i}$$

which is the same as:

$$\frac{d}{dt}\left(\frac{\partial J}{\partial x^i}\right) = -\frac{\partial M\left(\frac{\partial J}{\partial x}, x\right)}{\partial x^i} \qquad (28)$$

At the same time we see that

$$\frac{d}{dt}\left(x^i\right) = \frac{\partial M\left(\frac{\partial J}{\partial x}, x\right)}{\partial \left(\frac{\partial J}{\partial x^i}\right)} \qquad (29)$$

Equations (28) and (29) clearly constitute the Hamiltonian system we were looking for. Moreover we identified $\partial J/\partial x^i$ as the variables ψ_i of the adjoint system.

1.4.4. Remarks

1. We showed how some relations of Pontryagin could be deduced from the principle of optimality of Bellman. We should not forget however that the principle of Bellman is valid for a much more general class of problems than the one we defined in § 1.1.

2. On the other hand the deduction of relation (26) was only possible on condition that $J(x)$ was twice differentiable. This restriction is not necessary for the theorems of Pontryagin and is not even realized for the first derivative, $\partial J/\partial x^i$, in many current applications, particularly bang-bang problems.

3. The Hamiltonian system (28) - (29) has been formulated for the already maximized H-function. This obviously makes the system unpractical for optimizing purposes since it considers $u(x)$ as a known function.

4. The given deductions from the principle of optimality are interesting for a good understanding of the more general maximum principle. We have to keep in mind that if $\partial J/\partial x^i$ exists it is the same as the ψ_i variable of the adjoint system.

1.5. The Calculus of Variations and its Relations to the Maximum Principle

1.5.1. Survey

The problem of the calculus of variations is a particular case of the problem stated in § 1.1. The problem of Lagrange for instance is equivalent to the latter if the control region U is an open set of the r-dimensional control space E^r. It generally coincides with E^r. For this reason the maximum condition can be satisfied by relations of the type $\partial \mathcal{H}/\partial u^i = 0$ and the Weierstrass

criterion, following equally from the maximum principle for U being an open set. When U is a closed set the Weierstrass condition is false (cfr. [1] p. 256).

A still more special case is the elementary problem of Euler in the calculus of variations, corresponding to the problem of § 1.1. if $f^i = u^i$, G and U coinciding with the n-dimensional state-space and an n-dimensional control space (r = n). The well-known Euler equations and the Legendre condition immediately follow from the maximum principle.

This short survey points out the importance of the maximum principle as a generalization of the classical problem of variations. This more general theory is indispensable for the very important class of applications where the optimal trajectory corresponds to control variables partly or completely lying on the boundary of the closed control region.

1.5.2. An example - Analytical mechanics as an optimal process

We want to derive the basic equations of mechanics in the form of an optimal trajectory for a Lagrange mechanical system. This problem could be solved by the calculus of variations, but we shall apply the maximum principle in order to illustrate the method. [4]

For one physical point with mass m in a potential field $U(x^1, x^2, x^3)$ the problem is characterized by

$$dx^i/dt = f^i = u^i \qquad i = 1, 2, 3 \qquad (30)$$

$$f^o = \sum_{i=1}^{3} \frac{m\,(\dot{x}^i)^2}{2} - U(x^1, x^2, x^3) \qquad (31)$$

It immediately follows that

$$\mathcal{H} = \sum_{i=1}^{3} \psi_i u^i - \sum_{i=1}^{3} \frac{m\,(u^i)^2}{2} + U(x^1, x^2, x^3) \qquad (32)$$

Maximization of $\mathcal{H}$ gives

$$\frac{\partial \mathcal{H}}{\partial u^i} = \psi_i - m u^i = 0 \quad \text{or} \quad \psi_i = m \frac{dx^i}{dt} \qquad (33)$$

Relation (12) gives

$$\frac{d\psi_i}{dt} = -\frac{\partial U}{\partial x^i} \qquad (34)$$

Combining (33) and (34) we have

$$m\,\frac{d^2x^i}{dt^2} = -\frac{\partial U}{\partial x^i} \qquad (35)$$

which is nothing else than the Newton equations for a potential field.

Finally, we want to draw attention to the meaning of $\mathcal{L} = 0$ for $\psi = \partial J/\partial x$ in variational calculus and especially in theoretical physics. Indeed this partial differential equation corresponds to the Hamilton-Jacobi equation and is connected by the Heisenberg uncertainty relations to the well-known Schrödinger equation.

It is the custom to write the partial derivative $\partial J/\partial t$ explicitly in the Hamilton-Jacobi, the Schrödinger and even in the Bellman equation (25). As we considered time appearing explicitly as a state variable our relations (13), (14), (26) are general as well (cfr. § 1.2.1.).

1.6. An illustrative Exercise

We take the example examined in ref. [1] , p. 23, which because of its simplicity will be useful for later discussion of the computational aspects.

We consider the equation $d^2x/dt^2 = u$ which can be rewritten in the form of the following system ($x^1 = x$ and $x^2 = \dot{x}$)

$$\frac{dx^1}{dt} = x^2 \qquad (36)$$

$$\frac{dx^2}{dt} = u \qquad (37)$$

The control variable u is constrained by the condition $|u| \leq 1$ while G coincides with the two-dimensional state space.

The problem consists of getting to the origin (0, 0) from a given initial state $x_o = (x_o^1, x_o^2)$ in the shortest time.

The function $\mathcal{H}$ has the form

$$\mathcal{H} = \psi_1 x^2 + \psi_2 u - 1 \qquad (38)$$

The adjoint system is given by the equation (12)

$$\frac{d\psi_1}{dt} = 0 \qquad \frac{d\psi_2}{dt} = -\psi_1 \qquad (39)$$

of which the solution is given by $\psi_1(t) = \psi_1(t_o)$ and $\psi_2(t) = \psi_2(t_o) - t\psi_1(t_o)$

The maximization of the $\mathcal{H}$-function gives

$$u = \text{sign } \psi_2(t) \qquad (40)$$

It follows that the control variable is a piecewise constant function taking the values + 1 or - 1. Since ψ_2 is a linear time function u changes its sign only once.

Introducing relation (40) in the combined system of original and adjoint differential equations, the solution of the system still depends upon the initial conditions $\psi_1(t_o)$ and $\psi_2(t_o)$ of the adjoint system. Considering them as parameters we have a family of optimal trajectories, from which we have to pick out the one which ends in the point ($x_1^1 = 0$, $x_1^2 = 0$). We do this by choosing the appropriate values of $\psi_1(t_o)$ and $\psi_2(t_o)$. This is the essence of the so-called two-point boundary problem.

Having solved the maximization problem and the two-point boundary problem for all possible values of x_o we can represent the solutions by Fig. 1.2.

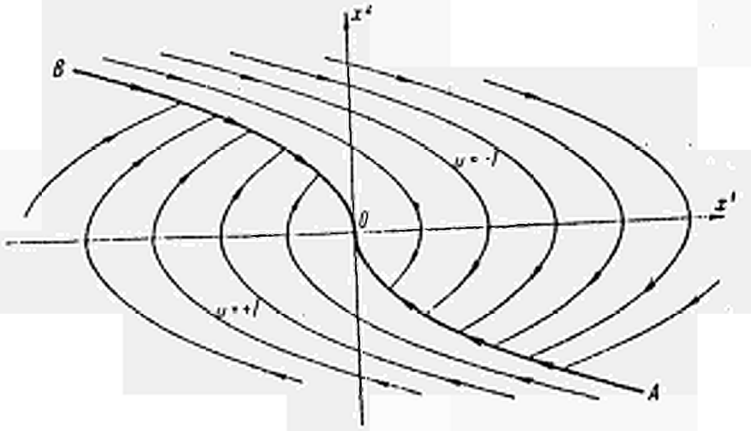

Fig. 1.2.

The optimal trajectories are composed of parts of parabolas belonging either to the family u = + 1 or the family u = - 1. Both families are separated by the switching line AOB.

1.7. Linear time-optimal Processes

The linear time-optimal problem is defined by the following equations, the meaning of which is easily understood by the discussion of the fundamental problem of § 1.1.

$$\frac{dx}{dt} = Ax + Bu \qquad (40)$$

A and B are linear operators defined, in terms of the coordinates $x^1, \ldots, x^n$ and $u^1, \ldots, u^r$, by the matrices (a^i_j) and (b^i_k) respectively $(i = 1, \ldots, n;\ j = 1, \ldots, n;\ k = 1, \ldots, r)$.

For the time optimality we have

$$J = \int_{t_0}^{t_1} 1 \cdot dt = t_1 - t_0 \qquad (41)$$

Further, we shall assume the control region U to be a convex, closed polyhedron.

In this case $\mathcal{H}(\psi, x, u)$ has the form

$$\mathcal{H} = (\psi, Ax) + (\psi, Bu) - 1 \qquad (42)$$

and the adjoint system is given by

$$\frac{d\psi}{dt} = - A^{+} \psi \qquad (43)$$

where A^{+} is the transpose of A.

Obviously, $\mathcal{H}$ attains its maximum simultaniously with (ψ, Bu). This implies, and it can be demonstrated, that u is piecewise constant and that its values are vertices of U.

It can be demonstrated also (ref. [1] pp. 123 - 135) that the solution of the linear time-optimal problem exists and is unique. Up to now, such theorems have not been demonstrated for the fundamental problem of § 1.1.

An interesting special case is where the control region U is an r-dimensional cube

$$|u^k| \leq 1 \qquad k = 1, \ldots, r \qquad (44)$$

Then we have that the maximization of

$$(\psi, Bu) = \sum_{k=1}^{r} \sum_{i=1}^{n} \psi_i b_k^i u^k \qquad (45)$$

reduces to the maximization of each of the terms

$$\sum_{i=1}^{n} \psi_i b_k^i u^k \qquad k = 1, \ldots, r \qquad (46)$$

Hence we obtain

$$u^k = \operatorname{sign} \sum_{i=1}^{n} \psi_i b_k^i \qquad k = 1, \ldots, r \qquad (47)$$

These results have been formulated also by La Salle [5] and Feldbaum [6] and they are known as the "bang-bang principle".

It follows, for instance, that if all the eigenvalues of the matrix A are real, u has not more than n - 1 switchings, where n is the order of system.

As can be verified, this confirms the results of the example of § 1.6. Indeed, for this second order system we have one switching line. Only if x_o is on this switching line is there no sign inversion

of u. For a third order system it would be possible to have two switching surfaces, and so on.

The construction of switching (hyper-) surfaces implies that the synthesis problem has been solved. This, as we know already, is impossible without solving the corresponding two-point boundary problem.

Chapter 2 COMPUTATIONAL ASPECTS OF THE MAXIMUM PRINCIPLE

2.1. General Computing Diagram

One of the most important advantages of the maximum principle is that the particularities and special characteristics of a given optimization problem can be handled in such a way that considerable simplification is possible with respect to the general and fundamental problem of § 1.1.

As a consequence, several kinds of techniques, depending on the nature of the problem, can be introduced in the general optimization scheme of the Pontryagin team's theorems. Very often analytical simplifications are possible and sometimes even the solution can be found analytically. This was the case, for instance, for the example of § 1.5.2. If we are not so fortunate, computer techniques have to be tried. It is this aspect which is the object of our main interest.

In order to organize our discussion about the possible simplifications and the corresponding computing techniques, we have to consider the general computing diagram (Fig. 2.1.) as it is imposed by the maximum principle.

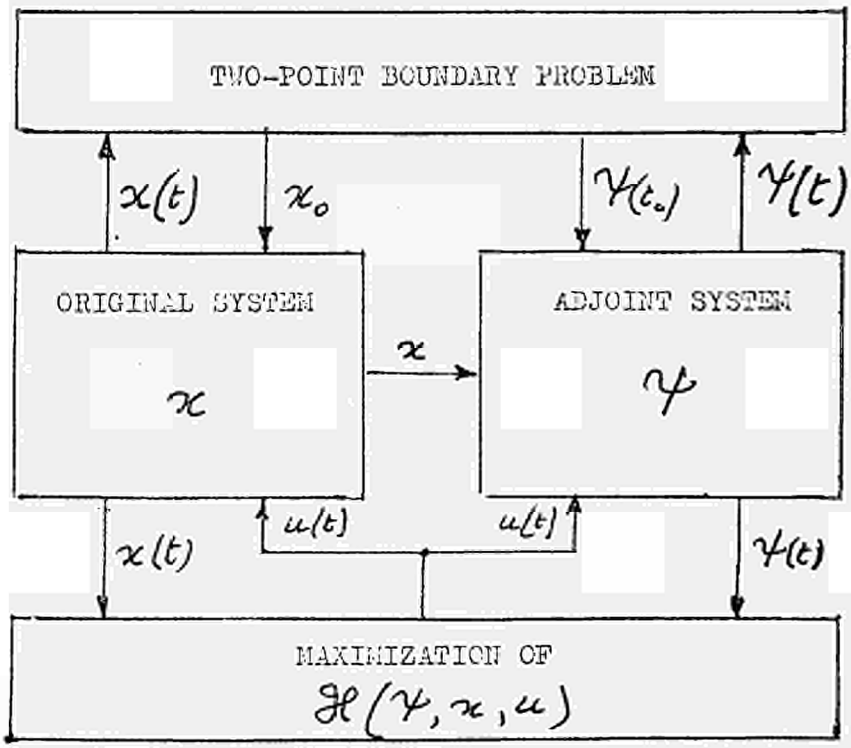

Fig. 2.1.

The diagram comprises the original set of differential equations of the state vector x (t), the set of differential equations of the adjoint variable $\psi(t)$, a system furnishing a control vector u (t) to the systems x and ψ such that at every instant $\mathcal{H}(\psi, x, u)$ has its maximum value, and finally a system which is solving the two-point boundary problem and gives the appropriate initial conditions for the x - ψ model.

The computational aspects of these systems will be discussed in the paragraphs following. We must not forget however that analytical simplifications can sometimes even lead to the complete elimination of one of the parts of Fig. 2.1.

2.2. The Illustrative Exercise of § 1.6.

As an illustration we could try to define the diagram of Fig. 2.1. for the optimization problem of § 1.6., simulated on an analog computer.

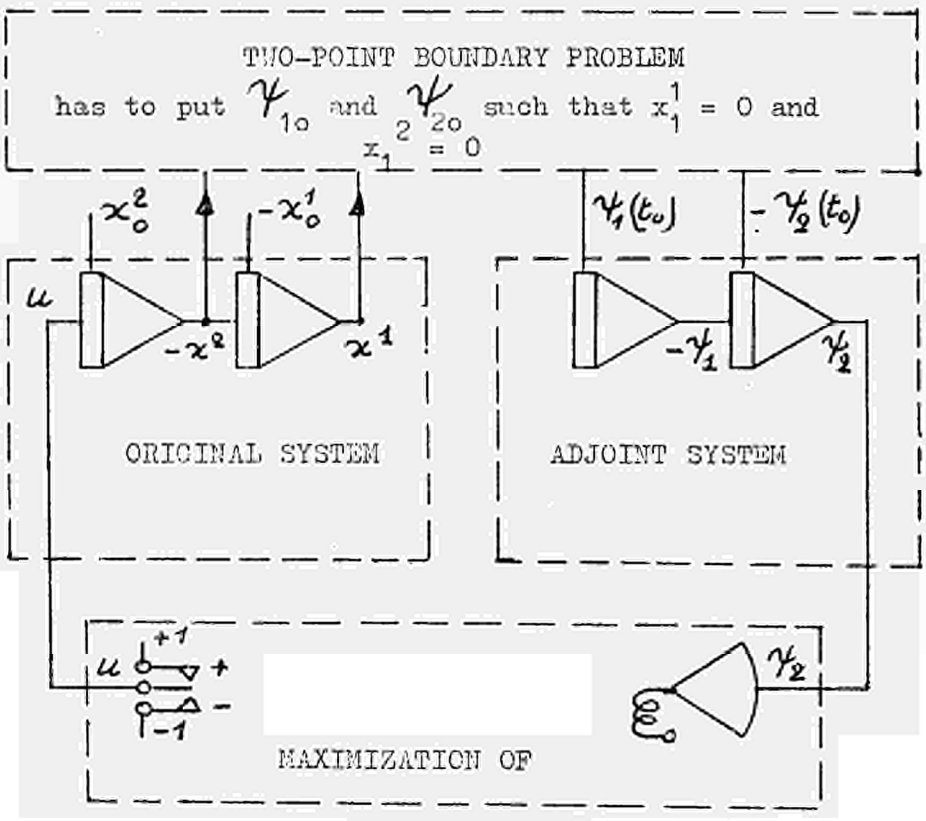

Fig. 2.2.

As we know by relation (1.40) the maximization of $\mathcal{H}$ can be simulated by a simple relay feeding the constant values + 1 or - 1 to the x-model, depending upon the sign of ψ_2. The simple second order x-model has given initial conditions x_o^2 and x_o^1, while the initial conditions ψ_{10} and ψ_{20} of the second order adjoint system have to be calculated by the two-point boundary problem solver. Up to now the theorems of Pontryagin give no ready information about the structure of this last system. Pontryagin himself suggests (ref. [1] p. 181) a trial and error approach.

Of course, in the simple case of our example it is also possible to find the solutions $x(t)$, $x^2(t)$, $\psi_1(t)$ and $\psi_2(t)$ analytically, and for that reason the two-point boundary problem can be solved analytically as well. The result is the synthetizing diagram of Fig. 1.2. Consequently, the computing diagram of Fig. 2.2. should be considered only as an illustration and not as the best method for the particular case we have taken as an example.

2.3. The Original and Adjoint Systems

The computer representation of the combined x - ψ- model poses no new difficulties. Indeed, it consists of a set of ordinary differential equations with $u = (u^1, \ldots, u^r)$ as input variables and with initial conditions which are partially given and partially determined by the two-point boundary problem solver.

The x-model is not influenced by the ψ- variables. In general, the reverse is not true. The adjoint system is independent of the original system only if the partial derivatives $\partial f^i / \partial x^\alpha$ do not contain x any more. This if the case where all f^i are linear expressions of x.

For solving ordinary differential equations analog computers are indicated. For digital computers a discrete representation is necessary (cfr. (1.5)).

2.4. The Lagrange Multipliers

The presence of constraints on the state variables seriously complicates the computing diagram.

We know by the theorems and the discussions of § 1.3.2. and § 1.3.3. that whenever the optimal trajectory reaches the boundary of G the $\mathcal{Y}$- model has to be replaced by a new one which comprises the Lagrange multipliers for that boundary. These Lagrange multipliers have to be calculated continuously such that the trajectory moves along the boundary. The Lagrange multipliers influence as well the maximization of $\mathcal{H}$, since the trajectory has to be optimal with the given boundary conditions.

On the other hand one has to observe whether at some instant the optimal trajectory has to leave the boundary for the interior of G. At that instant the $\mathcal{Y}$- model has to be modified once more. At every junction point new initial conditions for the next $\mathcal{Y}$- model have to be introduced in order to satisfy the jump conditions of § 1.3.3.

It is obvious that the straightforward application of the theorems of Pontryagin for restricted state variables requires a logically complicated computer set-up. For this reason we attach great value to the technique of implicit computing of Lagrange multipliers, by which the mentioned computational difficulties are bypassed. This technique is mathematically related to the concept of "penalty function".

The concept of penalty function is not new (cfr. ref [7] p. 213). Yet no computational experience and even no rigorous mathematical treatment in connection with the fundamental problem of Pontryagin exists. A more detailed discussion will be found in Chapter 3.

2.5. The Maximization of $\mathcal{H}$

The maximization of $\mathcal{H}(\mathcal{Y}, x, u)$ corresponds to a new optimization problem for which the variables $\mathcal{Y}$ and x have to be considered as parameters, while the control vector u becomes the new state vector. In fact, $\mathcal{H}$ becomes an object function of the type F (x'), with constraints in state-space which are given by the definition of U.

This kind of problem belongs to the well-known domain of nonlinear, or if we are fortunate, linear programming. In both cases analog and digital techniques exist and are competitive.

If for some reason it is necessary to put the x - $\mathcal{Y}$ - model on an analog computer while a digital computer maximizes $\mathcal{H}$, some kind of linkage between the two computers has to be provided. In this case the computing time for the maximization of $\mathcal{H}$ becomes an important point. Indeed, since the maximization process has to be accomplished at every instant, the computing time must be negligible or else the analog computer has to be put to HCLD at discrete time intervals.

Taking account of the fact that the computing time of analog techniques for the optimization of F (x') can be made very small, it seems to be advisable to solve the fundamental problem entirely on the analog computer whenever it is possible.

A fruitful idea is to consider the maximization problem of $\mathcal{H}$ itself as a particular case of the fundamental problem of Pontryagin. A feasible formulation of this new problem in terms of § 1.1. would be as follows:

1. Consider the control vector u as a new state vector x', such that $\mathcal{H}$ can be written in the form $\left[- F (x')\right]$.

2. The optimization criterion is defined by

$$J (x') = F\left[x' (t + \Delta t)\right] - F\left[x' (t)\right] = \int_t^{t+\Delta t} f^{o} (x', u')\, dt'$$

with

$$f^{o} (x', u') = \sum_{\alpha=1}^{n} \frac{\partial F (x')}{\partial x'^{\alpha}}\, f^{\alpha} (x', u')$$

and Δt arbitrarily small.

3. The control region U of the original problem corresponds to G in the new problem.

4. The new dynamical constraints are defined by

$$\frac{dx'^{i}}{dt} = u'^{i} \qquad i = 1, \ldots, r$$

where u' is the control vector of the new problem with a new control region U' defined by the relation

$$q (u') = \sum_{i=1}^{r} (u'^{i})^2 - R \leqslant 0$$

representing a hypersphere with radius R. R can be chosen in order to make the computing time of the optimization process small.

The complete discussion of this problem is referred to chapter 4. It will be shown that it corresponds to the well-known gradient technique. Of course, this method has the disadvantage that the optimization process may stop at a local maximum of $\mathcal{H}$ as well as at a global one. This is not so serious as it might appear, because the global maximum of $\mathcal{H}$ is zero and so it can always be distinguished from a local optimum.

Finally, we should not forget that general discussion about $\mathcal{H}$ is interesting only for a very small proportion of real problems. In most cases the maximization of $\mathcal{H}$ reduces to a very simple and sometimes a trivial process. Let us consider some special cases.

In control problems, for instance, the number of control variables is generally very small with respect to the number of state variables. They intervene in very few equations and very often in a simple, sometimes linear way. In addition the control region U can have some simple geometrical definition such as a hyperparallelopiped. All this means that in a considerable number of applications the control variables only switch between constant values depending upon the sign of some function. Our exercise of § 1.6. and § 2.2. is a good illustration of what happens in this case. It results that very often the maximization can be done by a simple combination of relays on the analog computer.

Other simplifications are possible when U coincides completely with the r-dimensional control space. Then it is possible to write (cfr. § 1.5.2.)

$$\frac{\partial \mathcal{H}}{\partial u^i} = 0 \qquad \text{for } i = 1, \ldots, r$$

In this way the maximization of $\mathcal{H}$ reduces to the solution of a set of algebraic equations. Sometimes this set can be solved immediately, sometimes matrix theory is helpful.

2.6. The Two-Point Boundary Problem

Obviously, for this problem a solution by trial and error is possible only if very few initial conditions (maximum three) have to be handled. In a more general way the problem can be solved by iteration or some

kind of invariant imbedding. The last method is only applicable in connection with the dynamic programming approach to the fundamental problem (cfr. § 2.7.).

The iteration method is the best adapted to be used with the maximum principle technique. Chapter 5 will discuss the method in detail. The essence is that the two-point boundary problem can be formulated once more as a special case of our fundamental problem of § 1.1. The result is an iterative version of a gradient technique.

2.7. Dynamic Programming

The dynamic programming technique introduced by Bellman (ref. [2] and [3]) is based upon the principle of optimality written as a recurrence relation (cfr. § 1.4.1.). When applied to our fundamental problem of § 1.1. this recurrence relation takes the form of equation (1. 23.). In this way dynamic programming, as well as the maximum principle technique, is able to solve the fundamental problem. The computational aspects however are essentially different.

It would lead us too far to expose the dynamic programming technique in detail (cfr. ref. [2] and ref. [3], ch. V), but some remarks and comparisons are useful.

Because of the structure of the recurrence relation, requiring the logical organization of a large memory, dynamic programming refers essentially to the digital computer.

The basic idea is not to regard the fundamental problem as an isolated problem for given initial and final conditions, but instead to imbed it within a family of optimization processes, corresponding to a large set of possible initial and final conditions. Dynamic programming only needs the recurrence relation and the discrete version of the dynamic constraints, which are both handled in a simple and standard way, whatever may be the special characteristics of the given problem.

The advantages of such an overall standard technique are obvious. The two-point boundary problem, for instance, is completely bypassed. We have only to choose the solution with the right initial and final conditions as a member of the family. At the same time we have for this

solution a complete sensitivity analysis with the boundary conditions as parameters. If dynamic programming guarantees the global optimum it is interesting to note that the same technique can be used to obtain the second, third, etc. best solution, if they correspond to local optima. Non-analycity imposes no difficulties for dynamic programming and paradoxically, constraints simplify the computational part. Indeed, constraints make the family of solutions smaller and for this reason call for a smaller memory.

The unique but severe difficulty with dynamic programming is the dimensionality of the problem, requiring large memories and long computing times for the digital computer. Bellman himself states (ref. [3] p. 100):

"..., control problems involving one state variable can be treated in a very simple fashion and require a negligible time. Questions involving two state variables are within the power of modern digital computers but can require computing times of the order of magnitude of ten or twenty hours. Questions involving three state variables can be treated on a few machines now available, and will be amenable to a number of machines that are now in the planning or production stage, but may require even longer amounts of time.

Barring any unforeseen developments of a radical nature, we must, however, acknowledge the fact that at no time in the foreseeable future do we expect to possess machines that will handle problems involving ten or twenty state variables in any prosaic fashion".

2.8. Conclusions

We can conclude that the weakness of dynamic programming coincides with the strength of the maximum principle. Just because of the standard organization of dynamic programming it is difficult to exploit the particularities of a given problem. With the maximum principle this is possible because of the rather complicated analytical structure of the theorems of Pontryagin. There is no standard technique, but a family of special techniques, corresponding to the possible simplifications of the problem. In this way it should be possible to solve problems, even if the number of state variables exceeds twenty.

On the other hand our discussions have illustrated the possibilities of analog computers in solving optimization problems. The consequence is a considerable reduction in computing time due to the simpler treatment of differential equations on the analog computer.

However, it would be too early to conclude that maximum principle techniques refer principally to analog computers. More experience with practical problems should indicate up to what point some kind of linkage with the digital computer would be useful.

Chapter 3 PENALTY FUNCTIONS

3.1. Introduction

The theory of penalty functions gives the possibility of by-passing the fundamental complications which are connected to a straightforward application of the theorems of Pontryagin for restricted state variables. Some essential difficulties concerning this subject have been mentioned already in § 2.4.

The basic idea of the theory of penalty functions is to approximate to the fundamental problem with restricted state variables with a modified problem without restricted state variables, called the penalty problem.

The modification consists principally of the definition of a new $f^o(x, u)$, which is called the penalty function f_p^o for the original problem. The definition of $f_p^o(x, u)$ is such that some penalty has to be added to $f^o(x, u)$ whenever the state constraints are violated. We expect that the optimization process itself will keep these penalties small, forcing the optimal trajectory to stay in the interior of G.

Although it is not always necessary, the same can be done with respect to the constraints of the control region U.

The concept of penalty function is not new. It has already been studied by Courant and Moser (ref. [7] p. 213, ref. [8] , ref. [9]) for ordinary minimum problems with object functions of the type $F(x)$ and constraints of the type $g^1(x) \leq 0$. What we shall try to do is to generalize the method for the fundamental problem of Pontryagin (cfr. § 1.1.).

3.2. Statement of the Penalty Problem

We consider again $x(t)$ to be the state vector $x(t) = (x^1(t), \ldots, x^i(t), \ldots, x^n(t))$, belonging to the n-dimensional state space and whose evolution is described by a system of differential equations

$$\frac{dx(t)}{dt} = f\left[x(t), u(t)\right] \qquad (1)$$

with $f = (f^1, \ldots, f^n)$. In this system $u(t) = (u^1(t), \ldots, u^r(t))$ is a control vector whose range is in the r-dimensional control space.

The initial condition $x(t_o) = x_o$ and the final condition $x(t_1) = x_1$ of the system belong respectively to the sets S_o and S_1 which are smooth manifolds of arbitrary dimension (but less than n).

Among all admissible controls u which transfer the point x from $x_o \in S_o$ to $x_1 \in S_1$, it is asked to find one for which the functional

$$J_p = \int_{t_o}^{t_1} f_P^o \left[x(t), u(t) \right] dt \qquad (2)$$

takes on the least possible value.

The function $f_P^o \left[x(t), u(t) \right]$ called "penalty function" takes the form

$$f_P^o(x, u) = f^o(x, u) + \frac{1}{2} k \left[p(x, u) \right]^2 + \frac{1}{2} l \left[q(u) \right]^2 \qquad (3)$$

$$\text{with} \qquad p(x, u) = \sum_{\alpha=1}^{n} \frac{\partial g(x)}{\partial x^\alpha} f^\alpha(x, u) \qquad (4)$$

and

$$\begin{aligned} k &= 0 && \text{for } g(x) \leq 0 \\ k &= \text{large and positive} && \text{for } g(x) > 0 \end{aligned} \qquad (5)$$

$$\begin{aligned} l &= 0 && \text{for } q(u) \leq 0 \\ l &= \text{large and positive} && \text{for } q(u) > 0 \end{aligned} \qquad (6)$$

It is essential that $g(x)$ and $q(u)$ have the same meaning as in § 1.1. (relations (1.2.) and (1.3.)).

The fact that the penalty problem has been defined for only one $g(x)$ and one $q(u)$ is not restrictive. The introduction of more constraints of type (1.2.) and (1.3.) with $l = 1, \ldots, n$ and $j = 1, \ldots, m$ is always possible.

3.3. Formal Application of the Maximum Principle to the Penalty Problem

Since no closed control region U and no closed state region G exists, a straightforward application of the maximum principle gives the following relations:

$$\mathcal{H}_p(\psi, x, u) = \sum_{\alpha=0}^{n} \psi_\alpha f^\alpha + \frac{1}{2}\psi_0 \left[k(p)^2 + l(q)^2\right] \qquad (7)$$

For $\psi_0 = -1$ and $\mathcal{H}(\psi, x, u) = \sum_{\alpha=0}^{n} \psi_\alpha f^\alpha$

we have

$$\mathcal{H}_p = \mathcal{H} - \frac{1}{2}\left[k(p)^2 + l(q)^2\right] \qquad (8)$$

We suppose that the maximization of $\mathcal{H}_p$ is guaranteed by the conditions

$$\frac{\partial \mathcal{H}_p}{\partial u^j} = 0 \qquad j = 1, \ldots, r$$

So we have

$$\frac{\partial \mathcal{H}}{\partial u^j} = \lambda \frac{\partial p}{\partial u^j} + \gamma \frac{\partial q}{\partial u^j} \qquad j = 1, \ldots, r \qquad (9)$$

with $\lambda = k\, p(x, u)$ (10)

$\gamma = l\, q(u)$ (11)

The Hamiltonian system is given by

$$\frac{dx^i}{dt} = \frac{\partial \mathcal{H}_p}{\partial \psi^i} = f^i(x, u) \qquad (12)$$

$$\frac{d\psi_i}{dt} = -\frac{\partial \mathcal{H}_p}{\partial x^i} = -\frac{\partial \mathcal{H}}{\partial x^i} + \lambda \frac{\partial p}{\partial x^i} \qquad (13)$$

This formal development immediately shows the correspondence between the fundamental problem and the penalty problem, especially in connection with the relations (9) and (13) (cfr. § 1.3.2. relations (1.18) and (1.16)).

3.4. A second Version of the Penalty Problem

A second possible version of the penalty problem would be where no penalties for the control constraints are introduced.

$$f_p^o(x, u) = f^o(x, u) + \frac{1}{2} k \left[p(x, u)\right]^2 \qquad (3')$$

In this case the original definition of admissible controls $u \in U$ has to be maintained.

The $\mathcal{H}_p$-function

$$\mathcal{H}_p = \mathcal{H} - \frac{1}{2} k (p)^2 \qquad (8')$$

has to be maximized for $u \in U$, taking account of the functions $q^1(u) \leqslant 0$. This implies that relation (9) is no longer true. In the case however where $\mathcal{H}_p$ is maximized by some gradient technique the terms $\partial \mathcal{H} / \partial u^j$ and $\lambda \partial p / \partial u^j$ would appear again when using this technique (cfr. § 3.7.).

3.5. Discussion

First of all we want to mention some positive points in favour of the formal application of § 3.3.

Indeed, for parts of the optimal trajectory lying in the interior of G ($k = 0$ imposing $\lambda = 0$ - cfr. (10)) the solution of the penalty problem is identical with the solution of the fundamental problem (cfr. § 1.3.1.). If the optimal control u belongs to the interior of the control region U ($q(u) < 0$), we have $l = 0$ which includes $\nu = 0$ (cfr. (11)). In this case the condition $\partial \mathcal{H} / \partial u^j = 0$ is obviously necessary for the maximum principle. However, if for some reason u leaves the interior U, a penalty ($\frac{1}{2} l q^2 dt$) has to be paid. We expect that by the optimization process this penalty will be minimized together with $f^o(x, u)$. This means that if u leaves U it will be kept near the boundary $q(u) = 0$ and that the larger we take the value of l, the smaller will be the constraint violations $q(u) = \nu / l > 0$. In this way ν itself is an approximation by implicit computing to the Lagrange multiplier for the boundary of U. This proves to be all right since equation (9) (with $\lambda = 0$) corresponds exactly to the necessary condition for u lying on $q(u) = 0$.

If now, in the described conditions, the optimal trajectory itself violates the state constraint, $g(x) \leqslant 0$, a new penalty ($\frac{1}{2} k p^2 dt$) has to be paid. Once more the optimization system will keep the constraint violations small by approximating implicitly the Lagrange multiplier λ for the boundary of G. Again relation (9) corresponds to relation (1.16) of § 1.3.2. while relation (10) shows how p tends to zero for increasing k, which is exactly what is required by relation (1.17) of § 1.3.2. For the discontinuous change of k from zero to a

large value when the state constraint is violated, jump conditions, which are different from those mentioned in § 1.3.3., have to be satisfied (see ref.[1] p.302 and p.311).

In addition to this rather intuitive description of the proposed technique we can state that as far as our experience goes the computational results (see also § 3.6. and § 3.7.) confirm the validity of the arguments.

However, we should not pass over some mathematical objections of cruxial importance. The fact that the final equations proved to be in agreement with the general theory is not at all convincing. Indeed, this correspondence can be demonstrated only for the limit case of the penalty problem for all l and k increasing to infinity, and we do not know anything about the convergence of the approximation of the solution for that limit case. Finally, for the jump conditions, it is not clear how they become identical with those of § 1.3.3.

As far as the stability and the existence of the solution are concerned, aspects which have not had a rigorous discussion even for the fundamental problem, analysis of them become still more embarrassing because of the functions k and l taking alternatively large and zero values. Even if the proposed technique proved to be legitimate these difficulties can make some applications impracticable.

3.6. Computational Aspects

The computational difficulties of the penalty function technique are intimately related to the theoretical ones. The implicit computing of Lagrange multipliers by definition requires closed loop computing circuits. Those loops have essentially a high gain character due to the large values of the k's and l's, and nonlinear aspects due to the discontinuous change to zero values of those variables.

Let us consider the consequences for analog computers. The strongly accentuated high-gain and nonlinear aspects make immediately apparent the high-frequency errors of the computing elements and the imperfections of diode circuits. In particular the putting of a mechanical relay in series with high-gain amplifiers causes a difficult problem.

At the present moment, experience in the development and use of the technologically best computing circuits is extremely limited. New research has to be started in order to compare the possible alternatives for the computing diagram, the optimal values for the k's and l's, the best time scale, etc. Introducing additional damping forces for $g(x) > 0$ or nonlinear functions instead of constant k's for $g(x) > 0$ may be very useful, but their influence upon the accuracy of the optimal trajectory still has to be examined carefully.

Generally the modified statement of the penalty problem discussed in § 3.4. gives less technological complications. Indeed, since $u(t)$ can move in U without friction and without inertia the stability problems for the Lagrange multipliers $\gamma = lq(u)$ are very difficult. For this reason a straightforward simulation of U by limiters, eliminating the l's, may be very practical. This is especially true if U is a parallelopiped.

In spite of all the computational difficulties mentioned, the technique of penalty functions proves to be relatively simple and well adapted for programming on analog computers because of the continuous representation of variables on the computer.

For digital computers it seems that the convergence problems of the solution due to the finite difference representations of the variables are much more complicated than the stability problems due to high-frequency errors in analog computers. Yet, it is not excluded that even for digital computers the implicit computing technique of the penalty functions still has advantages with respect to the direct computation of the Lagrange multipliers by the Pontryagin theorems for restricted state variables.

3.7. Example

We take again the example of § 1.6., adding a constraint for the state variables x^1 and x^2

$$g\,(x^1,\ x^2) = x^1 - x^2 - 1 \leqslant 0 \qquad (14)$$

The problem will be solved on an analog computer.

Applying the technique of the penalty functions, we have

$$\mathcal{H}_p = \psi_1 x^2 + \psi_2 u - 1 - \frac{1}{2}\,k\,(p)^2 \qquad (15)$$

with

$$p\,(x,\ u) = +\,x^2 - u \qquad (16)$$

The adjoint variables are now given by

$$\frac{d\psi_1}{dt} = 0 \qquad \psi_1\,(t) = \psi_1\,(t_o) \qquad (17)$$

$$\frac{d\psi_2}{dt} = -\,\psi_1 + k\,(+\,x^2 - u) \qquad (18)$$

Suppose we maximize $\mathcal{H}_p$ by a gradient technique (cfr. chapter 4) than we have

$$\frac{du}{dt'} = K\frac{\partial \mathcal{H}_p}{\partial u} = K\left[\,\psi_2 + k\,(+\,x^2 - u)\right] \qquad (19)$$

Since this maximization process has to be finished theoretically at every instant t, its computing time must be negligibly small with respect to the time constants of the original dynamical system (relations (1.36.) and (1.37.)). This can be done by taking K very large (high-gain amplifier). On the other hand u has to be kept within the region $[-1,\ +1]$. We do this by connecting a limiter to the amplifier representing u.

The complete computing diagram of the problem will be found on Fig. 3.1. Curves made by the computer for several different initial conditions of $x = (x^1,\ x^2)$ and the corresponding values $\psi_1\,(t_o)$ and $\psi_2\,(t_o)$, satisfying the two-point boundary conditions, are

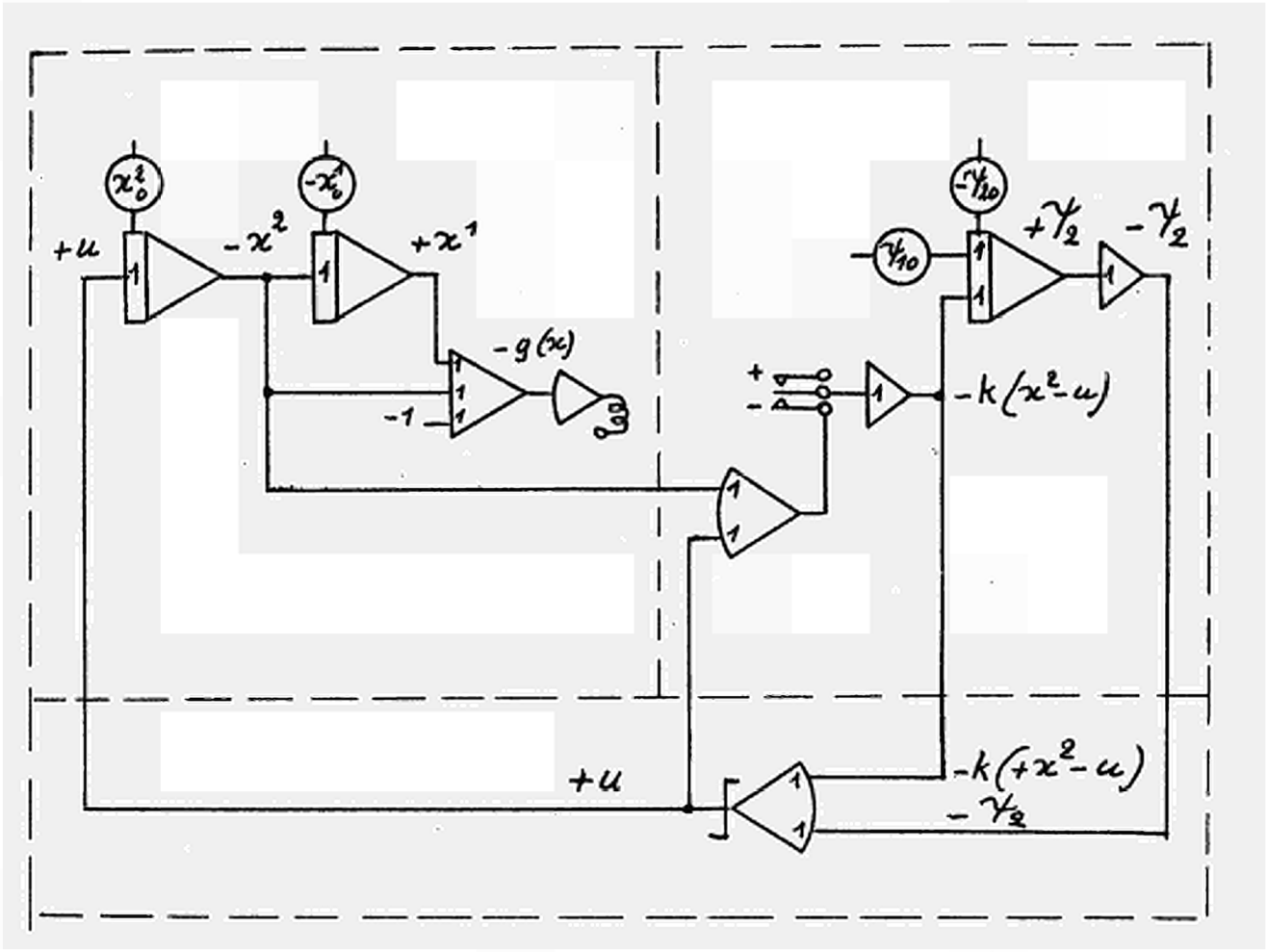

Fig. 3.1.

shown in Fig! 3.2. The plot is identical with Fig. 1.2., except for the region where $g(x^1,x^2) > 0$, but we do not know anything about the validity of the trajectories which are not tangent to the boundary at their junction points.

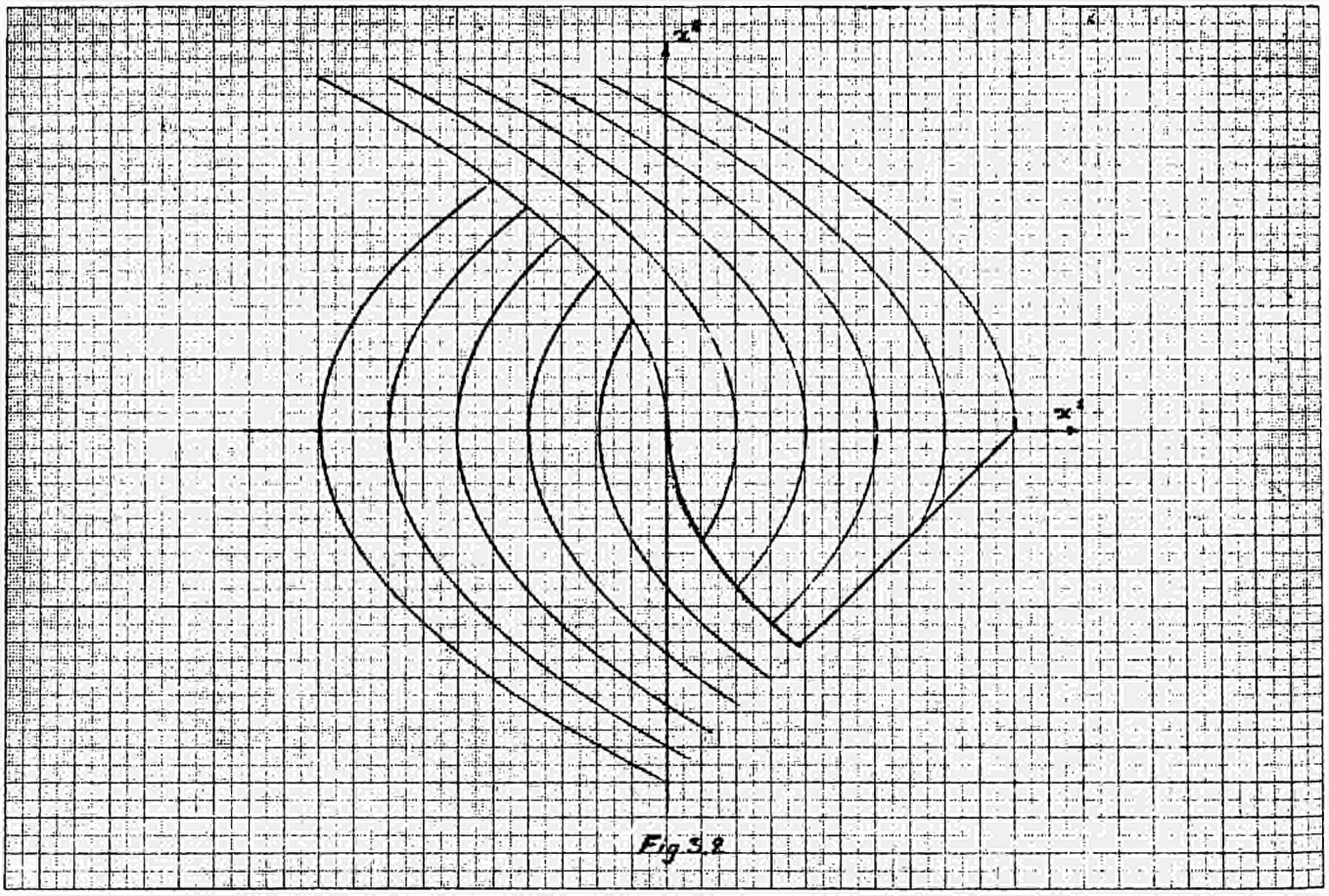

Fig 3.2

3.8. Conclusions

The technique of penalty functions surely is a very promising one but a lot of mathematical and computational difficulties still have to be studied. Research in this field requires at the same time a good mathematical background, experience in programming and sufficient knowledge of computer technology.

CHAPTER 4 - The Generalized Gradient

4.1. Introduction

We consider the problem of minimizing a given function $F(x^1, \ldots, x^i, \ldots, x^n)$ where the variables x^i are subject to constraints of the form:

$$g^j(x^1, \ldots, x^i, \ldots, x^n) \leqslant 0 \qquad j = 1, \ldots, m$$

One possible technique for this kind of problem is based upon the construction of a set of differential equations of the steepest descent type for the variables x^i. Pyne [10] has done this for linear programming problems on the analog computer, but his method is equally valid for nonlinear objective functions and constraints. Representing the whole set of variables x^i by the vector $x = (x^1, \ldots, x^i, \ldots, x^n)$ the steepest descent equations can be written as

$$\frac{dx}{dt} = -k\left[\text{grad } F(x) + \sum_{j=1}^{m} k_j\, g^j(x)\, \text{grad } g^j(x)\right] \qquad (1)$$

with $k_j = 0$ if $g^j(x) \leqslant 0$

k_j = large and positive if $g^j(x) > 0$ (2)

An additional aspect of these equations is the implicit computation of the functions $k_j\, g^j(x)$ as approximations of the Lagrange multipliers for $g^j(x) = 0$. This is related to the theory of the penalty functions studied in chapter 3. Indeed, relation (1) could have been written as

$$\frac{dx}{dt} = -k \text{ grad } P(x) \qquad (3)$$

where $P(x)$ is a penalty function,

$$P(x) = F(x) + \frac{1}{2}\sum_{j=1}^{m} k_j \left[g^j(x)\right]^2 \qquad (4)$$

which has to be minimized without additional constraints. The approximation is the better the more k_j tends to infinity for $g^j(x) > 0$.

It is obvious that the set of equations (1) and (2) or (3), (4) and (2) is not the only possible one describing trajectories of x (t) ending at (at least a local) minimum of F (x). This means that additional constraints and even additional criteria with respect to the optimal trajectory could be satisfied before it is uniquely determined. These latent degrees of freedom make some generalizations possible. The maximum principle and other theorems of the Pontryagin team [1] will permit us to analyse a related but more general problem and to define the concept of generalized gradient.

4.2. Statement of the Problem

$F(x^1, \ldots, x^i, \ldots, x^n)$ is a given function which has to be guided to its (local) minimum at some time τ, taking account of following system of constraints.

We consider x (t) to be a state vector $x = (x^1, \ldots, x^i, \ldots, x^n)$, belonging to a closed subset G of the n-dimensional state space and whose evolution is described by a system of ordinary differential equations

$$\frac{dx(t)}{dt} = f\left[x(t), u(t)\right] \qquad (5)$$

with $f = (f^1, \ldots, f^i, \ldots, f^n)$. In this system the control vector $u = (u^1, \ldots, u^r)$ has to be chosen as an element of the closed subset U of the r-dimensional control space. The subset G is defined by

$$g^j(x) \leqslant 0 \qquad j = 1, \ldots, m \qquad (6)$$

and the subset U is defined by

$$q^l(u) \leqslant 0 \qquad l = 1, \ldots, s \qquad (7)$$

We shall show that the minimizing F (x) by generalized gradient corresponds to minimizing the functional

$$J(x) = F\left[x(t+T)\right] - F\left[x(t)\right] = \int_t^{t+T} f^0(x, u)\, dt' \qquad (8)$$

with

$$f^0(x, u) = \sum_{\alpha=1}^{n} \frac{\partial F(x)}{\partial x^\alpha} f^\alpha(x, u) \qquad (9)$$

The initial condition x_o of the optimal trajectory reduces to one point. At every instant $x_o = x(t)$. The final condition $x_1 = x(t+T)$ belongs to the set of all possible x, reachable at the time T after t, with admissible $u \in U$. We call this set $R_T(t)$ and its boundary $\rho[x(t+T)] = 0$.

4.3. The Generalized Gradient as a Special Case of the Maximum Principle

4.3.1. The optimal trajectory completely lies in the interior of G

Requiring that u (t) is piecewise continuous and that all f^i and all $\partial f / \partial x^i$ are defined and continuous on G X U together with their partial derivatives, we can apply the maximum principle for the problem defined in § 4.2. By definition we have

$$\mathcal{H} = \sum_{i=o}^{n} \psi_i f^i = \sum_{i=1}^{n} \left(\psi_i + \psi_o \frac{\partial F}{\partial x^i} \right) f^i \qquad (10)$$

The vector function $\psi = (\psi_o, \psi_1, \ldots, \psi_n)$ of the adjoint system is given by the Hamiltonian system

$$\frac{d\psi_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x^i} = -\psi_o \frac{d}{dt} \left(\frac{\partial F}{\partial x^i} \right) - \sum_{\alpha=1}^{n} \left(\psi_\alpha + \psi_o \frac{\partial F}{\partial x^\alpha} \right) \frac{\partial f^\alpha}{\partial x^i}$$

Knowing that ψ_o is negative and constant this relation can be reduced to

$$\frac{d}{dt} \left(\psi_i + \psi_o \frac{\partial F}{\partial x^i} \right) = -\sum_{\alpha=1}^{n} \left(\psi_\alpha + \psi_o \frac{\partial F}{\partial x^\alpha} \right) \frac{\partial f^\alpha}{\partial x^i}$$

Calling $\psi_i + \psi_o \frac{\partial F}{\partial x^i} = \psi_i'$ we can write the Hamiltonian system as follows

$$\mathcal{H} = \sum_{i=1}^{n} \psi_i' f^i$$

$$\frac{dx^i}{dt} = \frac{\partial \mathcal{H}}{\partial \psi_i'} = f^i$$

$$\frac{d\psi_i'}{dt} = -\frac{\partial \mathcal{H}}{\partial x^i} = -\sum_{\alpha=1}^{n} \psi_\alpha' \frac{\partial f^\alpha}{\partial x^i}$$

This formulation obviously corresponds to another problem, which has the same $f^i(x, u)$ as the original one of § 4.2., but with a different adjoint system ($\psi_i \neq \psi_i'$) and with $f'^o = 0$. Such a problem has a trivial solution. All admissible $u \in U$ satisfying the boundary conditions are optimal. This is possible if $\mathcal{H} \equiv 0$, by taking $\psi_i' = 0$, independantly of U, initial or final conditions. For this reason we can take

$$\psi_i = \frac{\partial F}{\partial x^i} \qquad \psi_o = -1 \qquad \mathcal{H} \equiv 0 \qquad (11)$$

In contrast to most other applications, the control variable is not determined by the maximum principle.

4.3.2. <u>The trajectory partly lies in the interior of G and partly on the boundary of G</u>

Introducing the Lagrange multipliers for the boundary of G and the jump conditions for ψ at the junction points where the optimal trajectory reaches or leaves the boundary of G, we apply the maximum principle for restricted state coordinates. A reasoning similar to that of § 4.3.1. leads to the relations (12) and (13). For simplicity we took m = 1 in relation (6).

$$\psi_i = \frac{\partial F}{\partial x^i} + \lambda \frac{\partial g}{\partial x^i} \qquad \psi_o = -1 \qquad \mathcal{H} \equiv 0 \qquad (12)$$

$$\lambda = 0 \qquad \text{for } g(x) < 0 \qquad (13\,a)$$

$$\lambda = -\frac{\sum_{i=1}^{n} \frac{\partial F}{\partial x^i} \cdot \frac{\partial g}{\partial x^i}}{\sum_{i=1}^{n} \left(\frac{\partial g}{\partial x^i}\right)^2} \qquad \text{for } g(x) = 0 \qquad (13\,b)$$

Relation (13 b) satisfies the boundary condition $(\psi, \text{grad } g) = 0$ for $g(x) = 0$.

4.3.3. The transversality conditions

Since $\mathcal{H} \equiv 0$ it finally results that the optimal control u has to be determined by the transversality conditions of the theorems of Pontryagin, stating that $\psi(t_1)$, which corresponds in our problem to $\psi(t + T)$, has to be orthogonal to the set $R_T(t)$ of the final events $x_1 = x(t_1) = x(t + T)$. Two possibilities have to be considered. They are illustrated in Fig. 4.1.

a) $x(t + T)$ lies in the interior of $R_T(t)$. In this case the orthogonality condition can only be satisfied by

$$\psi_i(t + T) = \left(\frac{\partial F}{\partial x^i} + \lambda \frac{\partial g}{\partial x^i}\right)_{x(t+T)} = 0 \qquad (14)$$

This is true whatever be the value of T.

b) $x(t + T)$ lies on the boundary $\rho[x(t + T)] = 0$ of $R_T(t)$.

Now we have

$$\psi_i(t + T) = \left(\frac{\partial F}{\partial x^i} + \lambda \frac{\partial g}{\partial x^i}\right)_{x(t+T)} = \mu \left(\frac{\partial \rho}{\partial x^i}\right)_{x(t+T)} \qquad (15)$$

a b

Fig. 4.1.

4.3.4. Conclusions

1. With the generalized gradient it is no longer true that $dx/dt = f(x, u)$ moves along the steepest descent, but the vector ψ of the adjoint system takes over the same function.

2. Since the Hamiltonian is identically zero, the optimal control can only be determined by the transversality conditions and not necessarily in a unique way.

3. If the optimal trajectory $x(t)$ stops somewhere ($dx/dt = 0$) at a time τ in a point $x(\tau)$, it necessarily stops inside $R_T(\tau)$. This means (cfr (14)) that this point is a (local) optimum of $F(x)$. The fact that the trajectory stops implies u = constant, but not necessarily $u = 0$.

4. The optimal trajectory does not necessarily stop anywhere, even at a (local) optimum of $F(x)$. Indeed, the imposed system of constraints (cfr. (5), (6), (7)) may very well be of such a kind that it is completely impossible to keep the system at the optimum of $F(x)$. This is not at all in contradiction with the optimality of the trajectory. Fig. 4.2. illustrates this phenomenon.

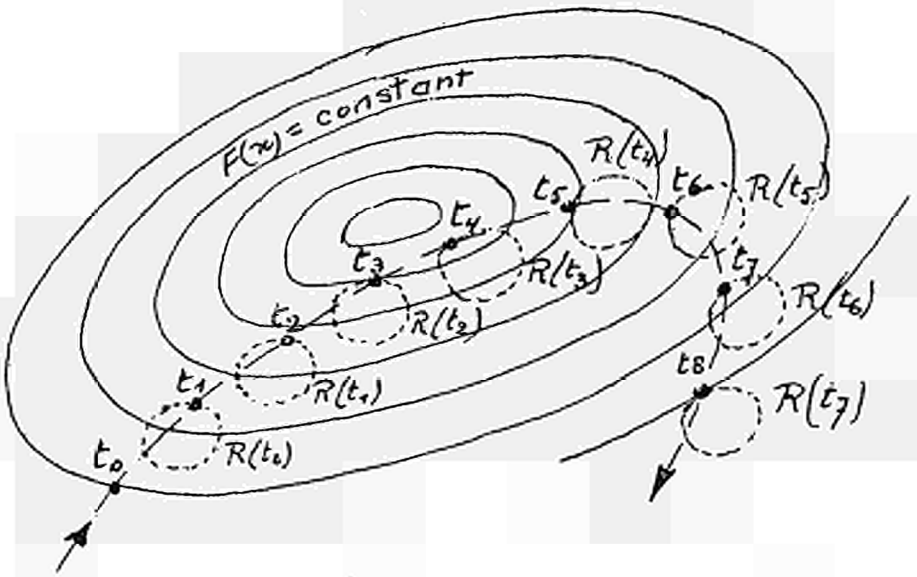

Fig. 4.2.

5. Whenever x (t + T) lies on the boundary $\rho = 0$ of R_T (t), the trajectory can be determined by (15), the definition of $\rho = 0$ and the equations (7) giving the boundary of U. Indeed these relations determine u (t) and μ. Examples will be given in § 4.4. and § 4.6.

6. Whenever x (t + T) lies in the interior of R_T (t) the trajectory is not uniquely determined unless $T = \Delta t$ is arbitrarily small. Indeed, the trajectory is composed of a sequence of initial conditions x (t) of an optimization problem for $t \leq t' \leq t + T$ of which only the final condition is given by our optimization criterion (8). In this case we propose a new optimization criterion.

$$J = \int_t^{t+T} F(x)\, dt' \qquad (16)$$

The problem will be subject of further study. Meanwhile the difficulty will be bypassed by taking T arbitrarily small, which eliminates the optimization between t and t + T.

7. It should be noticed that the evolution of the system only takes account of the direction of the vector (grad F + λ grad g) and not of its magnitude. The speed of evolution is more closely related to the system of dynamical constraints (5) and the boundary of U (7).

8. While optimizing we have to take account of the values of F (x) only for x in the interior of R_T (t). Outside this region F (x) is completely ignored. It looks as if the optimizing system has a limited "horizon" of information around the moving point x (t) and which is defined by R_T (t). If the trajectory stops at a local optimum, the optimizer never finds a possibly higher optimum if this lies outside its horizon. The probability of staying at a local optimum obviously grows with decreasing T and becomes a certainty for T arbitrarily small. The concept of the horizon of an optimizing system seems to be realistic. Indeed, the ability of predicting and interpreting all possible events within some time period T is linked to a degree of complexity which is limited for most technologically realizable optimizing systems.

4.4. The Steepest Descent as a Special Case of the Generalized Gradient

We consider the problem of § 4.2. with the following restrictions:

$T = \Delta t$ = arbitrarily small

$$f^i = u^i \qquad i = 1, \ldots, n \qquad (17)$$

$$q(u) = \sum_{i=1}^{n} (u^i)^2 - 1 \leq 0 \qquad (18)$$

By (18) U is represented by a unit hypersphere in the n-dimensional state-space. It follows immediately that $R_{\Delta t}(t)$ too is a hypersphere with radius Δt and that for $x(t + \Delta t)$ on the boundary $\rho = 0$ we have

$$\left(\frac{\partial F}{\partial x^i} + \lambda \frac{\partial g}{\partial x^i}\right)_{x(t+\Delta t)} = \mu \left(\frac{\partial \rho}{\partial x^i}\right)_{x(t+\Delta t)} = 2\mu \left[x^i(t + \Delta t) - x^i(t)\right]$$

$$= (2\mu \Delta t)\, u^i$$

Knowing that for $x(t + \Delta t)$ on $\rho = 0$, u is on $q(u) = 0$ we can calculate

$$2\mu \Delta t = \sum_{i=1}^{n} u^i \left(\frac{\partial F}{\partial x^i} + \lambda \frac{\partial g}{\partial x^i}\right)$$

Since μ is negative for a minimizing problem we have the following final solution:

$$\frac{dx}{dt} = 0 \quad \text{for} \quad \text{grad } F + \lambda \text{ grad } g = 0 \qquad (19)$$

$$\frac{dx}{dt} = -k (\text{grad } F + \lambda \text{ grad } g) \qquad (20)$$

with $\lambda =$ (13 a) and (13 b)

$$k = \frac{1}{2\mu \Delta t} = \left[\sum_{i=1}^{n} \left(\frac{\partial F}{\partial x^i} + \lambda \frac{\partial g}{\partial x^i}\right)^2\right]^{-1/2} \qquad (21)$$

Relations (19) and (20) obviously are equivalent to (1) for m = 1. The only points meriting some comment are k and λ. As stated already in the introduction $k_j\, g^j(x)$ $(j = 1)$ is nothing but an approximation of the Lagrange multiplier λ, generated by implicit computing. As far as k is concerned, in relation (20) it has been taken for the highest possible speed of x up to the endpoint. At the

endpoint however, (19) is necessary since (20) becomes undetermined. In relation (1) k has not yet been specified. The only important restriction on k is that it is a scalar, which is the case in (1) as well as in (20).

To resume, it has been shown that for the steepest descent not only ψ_i but also dx^i/dt is directed along (grad F + λ grad g). This is true because T = Δ t and $\rho\left[x\ (t + \Delta\ t)\right] = 0$ is a hypersphere.

4.5. Computational Aspects of the Generalized Gradient

On condition that grad F (x) and grad g (x) have sufficiently simple analytical expressions (or some simple analytical approximation, preferably linear, quadratic or third order polynomials) the equations (1) can be programmed without difficulty for analog and digital computers. In most cases the same is true for the generalized gradient if we take T = Δ t. Especially when the set of equations (5) constitutes a complicated, high order, non-linear dynamical system the choice of an analog computer is indicated.

Whenever grad F (x) and grad g (x) have no simple analytical expression all hope should not be lost. Modern perturbation techniques and sensitivity analysis are often very useful and easily programmable tools for estimating complicated gradients. This is especially the case for iteration procedures of the gradient type for solving two point boundary problems and parameter optimizations (cfr. chapter 5).

We draw special attention to the implicit computing of the Lagrange multipliers or the technique of the penalty functions, whose computational aspects have been discussed in § 3.6.

Time-dependant optimizing functions and constraints, making the whole system non-autonomous, do not affect the generality of the proposed techniques. As stated in § 1.2.1. it is sufficient to consider time, wherever it appears explicitly, as a new state variable $x^{n+1} = t$ and to add a new equation of type (5): $dx^{n+1}/dt = 1$.

4.6. Example of a Generalized Gradient Application

In terms of the statement of the problem of § 4.2. we take

$$dx^i/dt = h^i x^i \qquad i = 1, \ldots, n \qquad (22)$$

$$g(x) \leqslant 0$$

$$q^i(u) = -u^i - A^i \leqslant 0$$

$$q^{i+n}(u) = +u^i - B^i \leqslant 0$$

$$T = \Delta t$$

The boundary of the set of possible events $\rho[x(t + \Delta t)] = 0$ takes the form of

$$x^i(t + \Delta t) = (-A^i \Delta t)\, x^i(t)$$
$$x^i(t + \Delta t) = (+B^i \Delta t)\, x^i(t) \qquad \text{for } i = 1, \ldots, n \qquad (23)$$

Fig. 4.3. clearly shows the structure of the solution, which can very well be approximated by the equations (24), taking full advantage of the implicit computing technique.

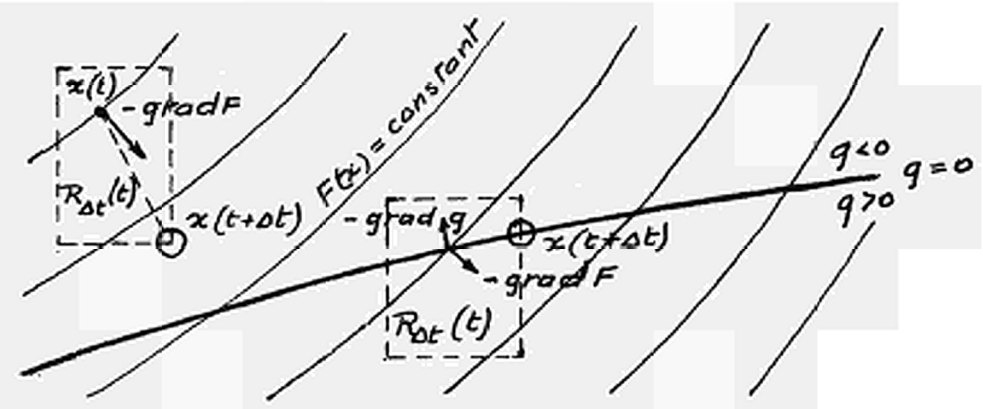

Fig. 4.3.

$$\frac{dx}{dt} = - k\, x \left[\text{grad } F\,(x) + k_1\, g\,(x)\, \text{grad } g\,(x) \right] \qquad (24)$$

with: $- Ax \leqslant dx/dt \leqslant Bx$

k and k_1 large and positive, but $k_1 = 0$ for $g\,(x) \leqslant 0$.

A and B are constant vectors with coordinates A^i and B^i, representing the edges of the hyperparallelopiped U.

The larger k and k_1 the better the accuracy, but the more critical the stability of dx/dt whenever it lies between - Ax and Bx. This particularly happens on the boundary $g\,(x) = 0$ (see Fig. 4.3.).

The analog computing diagram takes the form of Fig. 4.4.

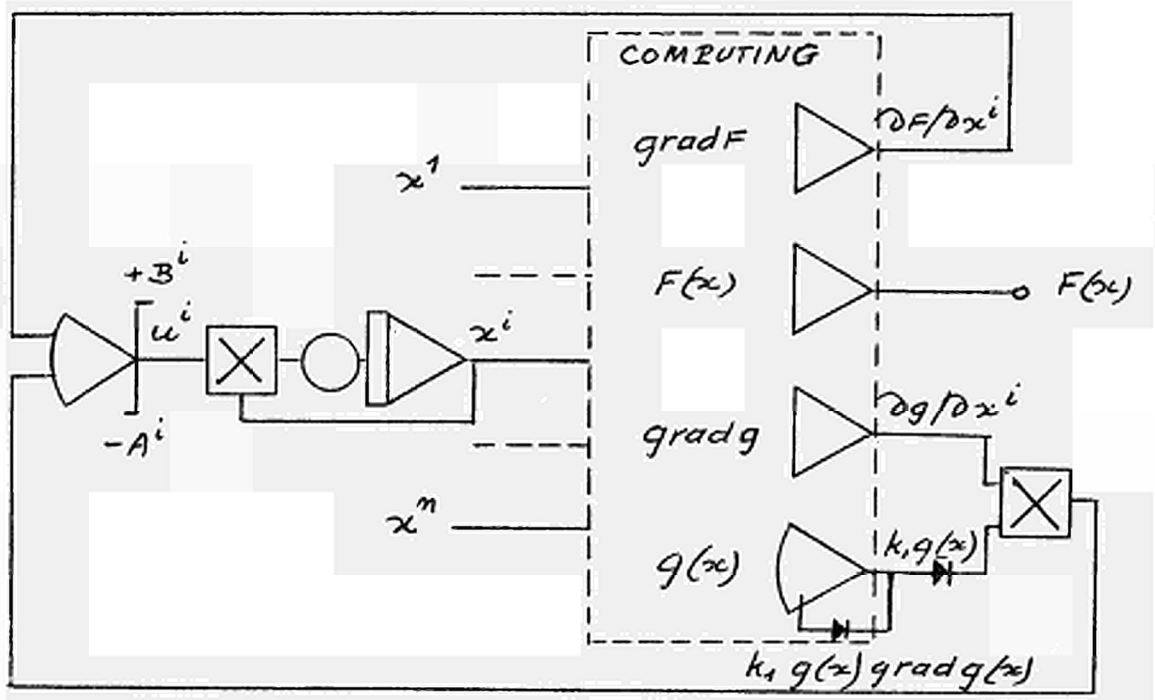

Fig. 4.4.

4.7. Application Fields

The most important class of engineering applications probably is the optimization of industrial production processes for which the slow variation of the properties of the process constitutes a system of dynamical constraints of type (5), and for which a certain profit function corresponding to the quality of the final product, the production costs or some other criterion can be fixed [11].

Another interesting field would be the study of macro-economic structures. Indeed, the generalized gradient opens the possibility of integrating the laws of economic growth and economic optimization in one model.

Chapter 5 TWO-POINT BOUNDARY PROBLEMS AND PARAMETER OPTIMIZATION

5.1. Introduction

Refering to chapter 2 and particularly to § 2.6., we want to comment on the general computing diagram of § 2.1. in connection with the initial conditions of the x-ψ-system.

The fact that the transversality conditions of § 1.3.1. give some boundary conditions for $t = t_o$ and others for $t = t_1$, while the computing diagram for the x-ψ-system requires the complete set of initial conditions, constitutes the essential difficulty of what generally is called the two-point boundary problem.

We propose to solve this sub-problem of the fundamental problem of Pontryagin by an iterative version of a gradient technique, which itself can be considered as a special application of the maximum principle (cfr. chapter 4).

The two-point boundary problem not only occurs in connection with our fundamental optimization problem but concerns a much more general class of problems. In addition, parameter optimization problems have the same fundamental structure. For this reason we prefer to state the problem with a terminology independant of the one introduced in chapter 1, such that the same symbols can have a different meaning in both chapters. The original x-, ψ- and u-variables, for instance, will be considered all as state variables x with respect to the two-point boundary problem.

5.2. The Two-Point Boundary Problem as an Optimization Problem

We consider $x(t, x_o)$ to be the state vector

$$x(t, x_o) = \left[x^1(t, x_o), \ldots, x^i(t, x_o), \ldots, x^n(t, x_o)\right]$$

belonging to the n-dimensional state space and whose evolution is described by a system of differential equations

$$\frac{\partial x(t, x_o)}{\partial t} = f\left[x(t, x_o)\right] \qquad (1)$$

with $f = [f^1, \ldots, f^n]$, and by a point of the n-dimensional initial condition space

$$x_o = x\,(t_o, x_o) = (x_o^1, \ldots, x_o^i, \ldots, x_o^n)$$

By definition the final value of $x\,(t, x_o)$ is given by

$$x_1 = x\,(t_1, x_o) = (x_1^1, \ldots, x_1^i, \ldots, x_1^n)$$

Suppose that a set of final conditions of the type

$$\theta^q\,(x_1) = 0 \qquad q = 1, \ldots, r \qquad (2)$$

has to be satisfied, then it will be asked to find some x_o for which the function

$$F\,(x_1) = \sum_{q=1}^{r} \left[\theta^q\,(x_1)\right]^2 \qquad (3)$$

takes on the least possible value. Obviously, this minimum has to be zero.

Stated in this way the problem is of the same type as the one defined in § 4.2. and it can be solved by the corresponding gradient techniques. A steepest descent version, for instance, would describe a trajectory as a function of a new independant variable T, ending at the optimal value of x_o (cfr. § 4.4. and relation (4.20) with $\lambda = 0$).

$$\frac{dx_o^j}{d\tau} = -k\,\frac{\partial F\,(x_1)}{\partial x_o^j} \qquad j = 1, \ldots, n \qquad (4)$$

It has to be noticed that $F\,(x_1)$ does not depend on t. Nevertheless it is true that, if t is represented by real time on an analog computer, some finite computation time $t_1 - t_o$ is necessary before $F\left[x\,(t_1, x_o)\right]$ can be evaluated as a function of x_o. Therefore, only a discrete version of relation (4) is practicable. A fortiori, this discrete version is necessary when applied with a digital computer. Consequently, the method takes the form of an iterative technique.

$$(x_o^j)^{\nu+1} = (x_o^j)^{\nu} - (k.\Delta\tau)\left[\frac{\partial F\left[x\,(t_1, x_o)\right]}{\partial x_o^j}\right]^{\nu} \qquad (5)$$

$$\nu = 1, 2, 3, \ldots$$

$$j = 1, \ldots, n$$

Steepest descent iteration has a very simple logic and iterative analog computers (cfr. ref. [16]) are indicated for this job. The only difficulty is the calculation of the gradient of F with respect to the initial conditions x_o^j.

We can write

$$\frac{\partial F(x_1)}{\partial x_o^j} = \sum_{i=1}^{n} \frac{\partial F(x_1)}{\partial x_1^i} \frac{\partial x^i(t_1, x_o)}{\partial x_o^j} \qquad (6)$$

$\partial F / \partial x_1^i$ can be found immediately by differenciating definition (3) of $F(x_1)$. The quantities $\partial x_1^i / \partial x_o^j$, however, have to be computed as the final values of the time dependant initial condition influence coefficients.

$$s^{ij}(t) = \frac{\partial x^i(t, x_o)}{\partial x_o^j} \qquad (7)$$

$$s_1^{ij} = s^{ij}(t_1) = \frac{\partial x^i_1}{\partial x_o^j} \qquad (8)$$

These variables $s^{ij}(t)$ are the solutions of the so-called sensitivity equations.

5.3. Sensitivity Equations

Considering the definition (7) of the initial condition influence coefficients $s^{ij}(t)$ and the system of differential equations of relation (1), the sensitivity equations for a given x_o necessarily take the form

$$\frac{ds^{ij}(t)}{dt} = \sum_{\alpha=1}^{n} \frac{\partial f^i(x)}{\partial x^\alpha} s^{\alpha j}(t) \qquad (9)$$

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

$$j = 1, \ldots, n$$

By definition the initial conditions of the sensitivity equations are

$$s_o^{ij} = s^{ij}(t_o) = 0 \quad \text{if} \quad i \neq j$$

$$s_o^{ij} = s^{ij}(t_o) = 1 \quad \text{if} \quad i = j \qquad (10)$$

It would lead us too far to discuss the theory of sensitivity equations and we refer to the literature available on that subject (cfr. ref.: [13] , [14] , [15] , [17] , [18] , [19] , [20])

A few remarks however are important for the applications in which we are interested.

First of all we would draw attention to the similarity between the sensitivity equations and the adjoint system of Pontryagin.

$$\frac{ds^i(j)}{dt} = \sum_{\alpha=1}^{n} \frac{\partial f^i}{\partial x^\alpha} \, s^\alpha(j)$$

$$\frac{d\psi_i}{dt} = -\sum_{\alpha=1}^{n} \frac{\partial f^\alpha}{\partial x^i} \psi_\alpha$$

They have a related structure, but we should not forget that the same symbols refer to different objects. Indeed, the adjoint system follows from the dynamical constraints of the original state vector, while the sensitivity equations for the two-point boundary problem apply simultaneously to the original state vector x and the adjoint vector ψ, linked together by the control vector u. This means, for instance, that if the original state vector is n-dimensional, (2n) different sensitivity equations are necessary, each of them having (2n) different sets of initial conditions, such that in total $(2n)^2$ initial condition influence parameters are available for the two-point boundary optimization.

The definition of the sensitivity equations requires the differentiability with respect to all x^i of the functions $f^\alpha(x)$ of system (1). In connection with the fundamental optimization problem of § 1.1. this requirement very often gives rise to complications due to discontinuities in the functions $f^\alpha(x)$, as applied to the x-ψ-u-model.

These difficulties may originate in the special characteristics of the maximization process of $\mathcal{H}(\psi, x, u)$, very often behaving like a switching circuit, or in the fundamental discontinuities of the penalty functions (cfr. chapter 3).

At the present moment neither a rigorous discussion of the mathematical consequences of this problem, nor a general method for handling it, is available. In particular cases however, as will be shown in §§ 5.5.2. and 5.6., some special tricks may give satisfactory computational results.

5.4. Parameter Optimization

We consider x (t, p) to be the state vector

$$x\ (t,\ p) = \left[\ x^1\ (t,\ p),\ \ldots,\ x^i\ (t,\ p),\ \ldots\ x^n\ (t,\ p)\right]$$

belonging to the n-dimensional state space and whose evolution is described by a system of differential equations

$$\frac{\partial x\ (t,\ p)}{\partial t} = f\left[\ x\ (t,\ p)\right] \qquad (\ 11\ )$$

with $f = (f^1, \ldots, f^n)$ and by a point of the r-dimensional parameter space $p = (p^1, \ldots, p^r)$. The initial conditions of system (11) constitute a given set of n numerical values.

$$x_o = x\ (t_o,\ p) = (x_o{}^1, \ldots, x_o{}^n)$$

By definition the final value of x (t, p) is given by

$$x_1 = x\ (t_1,\ p) = \left[\ x^1\ (t_1,\ p),\ \ldots,\ x^n\ (t_1,\ p)\ \right]$$

It is asked to find a point p in parameter space such that some given function $F\ (x_1)$ takes on the least possible value.

Obviously, this problem is essentially identical with the two-point boundary problem, as it was solved in § 5.2. To eliminate any possible doubt, it would be sufficient to introduce r new equations of the type

$$\frac{dx_p^i}{dt} = 0 \qquad (\ 12\ )$$

with initial condition

$$x_p\ (t_o) = p \qquad (\ 13\ )$$

and to add these r equations to the system (1). In this way any possible parameter optimization problem can be converted into an initial condition problem.

Of course, some differences may occur between the particular definitions of the object function $F\ (x_1)$. With the two-point boundary problem some given final conditions have to be satisfied by minimizing relation (3). For parameter optimization a much more general class of possible criteria exists, but many of them can be written in one

way or another as some least squares error minimization, where the error ε by a suitable definition is considered as a function of the state variables $\varepsilon[x(t, p)]$. Then we have

$$F = \int_{t_0}^{t_1} (\varepsilon)^2 \, dt \qquad (14)$$

and the parameter iteration takes the form

$$(p^j)^{\nu+1} = (p^j)^{\nu} - (k.\Delta\sigma) \left(\frac{\partial F}{\partial p^j}\right)^{\nu} \qquad (15)$$

with

$$\frac{\partial F}{\partial p^j} = 2 \int_{t_0}^{t_1} \varepsilon[x(t, p)] \left[\sum_{i=1}^{n} \frac{\partial \varepsilon(x)}{\partial x^i} \frac{\partial x^i(t, p)}{\partial p^j} \right] dt \qquad (16)$$

where the parameter influence coefficients $s^{ij} = \partial x^i / \partial p^j$ are one more given by the sensitivity equations (9).

Automatic mean squares error minimization is of great importance in adaptive control studies and we refer to the literature available on that subject. Ref. [13], for instance, discusses in detail the technique of which we have given only a general outline in this paragraph.

5.5. General Discussion and Computational Aspects

5.5.1. Convergence Problems

Strictly speaking, no convergence problems would exist if relation (4) could be used instead of the discrete version (5). The larger we take the finite intervals $\Delta\sigma$, the quicker the iteration process goes, but the more we risk having convergence difficulties. Indeed, taking finite steps we ignore the finer structure of $F[x(t_1, x_o)]$ between two subsequent values of x_o and this may lead even to divergent series of larger and larger steps taking x_o away from the optimum.

The difficulty is that the convergence not only depends upon the value of $\Delta\sigma$, but also upon the characteristics of the problem and the way the factor k has been defined. As we know already by § 4.4., k can be chosen in order to assure a constant speed of iteration (cfr. relations (4.17), (4.18) and (4.20) with $\lambda = 0$), but this is generally not the best solution

for a rapid and safe convergence. Taking k constant and considering ($k.\Delta\sigma$) as one coefficient is already a better proposal, but it should not exclude other solutions to be studied in the future.

Finally, we should not forget that the steepest descent approach we are discussing now, is not the only gradient technique which is able to solve the problem. Of course, since we are interested only in the final result, no particular dynamical constraints for the iteration process are given, and in these conditions the steepest descent equations (cfr. § 4.4. equation (4.18)) are the simplest we could imagine. However, nobody knows if for some problems other iterative constraints have better convergence characteristics. Then perhaps the generalized gradient technique may be helpful.

It may happen with a parameter optimization (rarely with a two-point boundary problem) that the parameters (respectively initial conditions) have to belong to some given set P. This restriction does not complicate the theoretical solution. The condition $p \in P$ is completely equivalent to $x \in G$ in terms of the statements of § 4.2. Consequently the Lagrange multipliers for the boundary of P have to be introduced. For the steepest descent the relations have been deduced in § 4.4. (cfr. equations (4.2C), (4.13 a), (4.13 b) and (4.21)). Just as before the convergence problems are linked to the discrete version of these relations and now the difficulties are particularly important because of the discontinuous change of the Lagrange multipliers on the boundary of P.

5.5.2. Local and global optima

Another embarrassing point is the choice of the first value of the series of initial conditions iterating to the solution of the two-point boundary problem.

We know that the global minimum of $F(x_1)$ is zero (cfr. relation (3)), but as steepest descent techniques can never distinguish global from local minima, the success of the iteration process entirely depends on the initial value of x_o.

Sometimes common sense indicates which values will be successful. In many other cases only a limited number of alternatives has to be tried. Intuitively one would expect that the general solution of the problem has to be found by some logical decision process, but at the present moment no systematic approach has been formulated. Everything still has to be done in this field.

5.5.3. Sensitivity and discontinuity problems

In connection with what already has been said about this problem in § 5.3., we want to indicate a possible solution for particular cases.

A frequently used discontinuous relation, resulting from the maximization of $\mathcal{H}$ (cfr. § 2.5.) is of the type

$$u = \text{sign}\ \varphi \qquad (17)$$

where u is one of the control variables to be fed to the x-system and φ is some function of the state variables x and the adjoint variables ψ. Deriving the sensitivity equations, relation (17) has to be differentiated with respect to some initial condition or some parameter, which we shall call μ.

$$\frac{\partial u}{\partial \mu} = \frac{d\ (\text{sign}\ \varphi)}{d\varphi} \frac{\partial \varphi}{\partial \mu} \qquad (18)$$

This immediately poses the problem of the existence of what we formally called $d\ (\text{sign}\ \varphi)/d\varphi$. Even considering it to be a Dirac-function $\delta(\varphi)$, we are still left with the difficulty of representing this function on a computer.

One way out is the direct integration of the sensitivity equations having $\partial u/\partial \mu$ as input. Suppose that these equations are of the type

$$\frac{d}{dt}\left(\frac{\partial x}{\partial \mu}\right) = f\left(\frac{\partial x}{\partial \mu}, \frac{\partial u}{\partial \mu}\right) \qquad (19)$$

where f $(\partial x/\partial\mu , \partial u/\partial\mu)$ is a linear function of $\partial u/\partial\mu$. Then the following system would be programmed.

1° for $\varphi \neq 0$ solve the equation

$$\frac{d}{dt}\left(\frac{\partial x}{\partial \mu}\right) = f\left(\frac{\partial x}{\partial \mu}, 0\right) \qquad (20)$$

2° for $\varphi = 0$ add the instantaneous value of the linear part of f $(\partial x/\partial\mu , \partial\varphi/\partial\mu)$ to the variable $\partial x/\partial\mu$.

The exercise of § 5.6. gives an illustration of this possibility.

In the cases where f $(\partial x/\partial\mu , \partial u/\partial\mu)$ is non-linear, perhaps some other particularities make a similar trick possible. However, more investigation concerning the validity and the restrictions of the method, the necessary conditions for the influence coefficients of the type $\partial\varphi/\partial\mu$ (continuity etc.) and in general a rigorous mathematical background is strongly recommended.

5.5.4. Iterative analog computers

The technique exposed in this chapter can easily be programmed on an analog computer, on condition that some digital control logic is provided. Indeed, the automization of the iteration process is only possible using some special kind of hybrid computer which is already known in literature as the iterative analog computer.

In fact, what we need is that the modes of the computer, INITIAL CONDITION, HOLD and OPERATE can be changed automatically by the computing diagram itself and that the initial conditions for each run are automatically imposed by some function of the final values of the preceeding run. This is possible with the so-called complementary integrators used as memories. Complementary integrators are in the OPERATE mode when the normal integrators are in the INITIAL CONDITION mode, and vice-versa. For more details we refer to ref. [16],

where one of the possible technical realizations of such an iterative computer is discussed. Most constructors of analog computers have their own slightly different systems, and even classic analog computers are not so difficult to modify so that they have some primitive but very useful iterative control possibilities. It is in this way that the problem of § 5.6. has been programmed and that technological research on the system is continued in our laboratories (ref. [21]).

5.6. The Illustrative Exercise of § 1.6. and § 2.2.

Considering once more the very simple problem of § 1.6. we want to illustrate the iterative technique for the two-point boundary problem by completing the computing diagram of Fig. 2.2. (§ 2.2.).

After all, the application is nearly a trivial one. By the structure of the equations (cfr. relations (1.39 .) and (1.40) of § 1.6.) it is obvious that only one of the two initial conditions $\psi_1(t_o)$ and $\psi_2(t_o)$ has to be optimized, since the right instant at which $\psi_2(t)$ has to change its sign depends only on the ratio $\psi_2(t_o)/\psi_1(t_o)$. For this reason, the proposed technique is of little interest in such a simple case, where trial and error gives the solution as well and probably in less time. However, we consider it as a good example of how the method works.

Taking $\psi_1(t_o) = \psi_{10}$ constant we have to optimize $\psi_2(t_o) = \psi_{20}$ such that at some time t_1 the function

$$F(x) = (x^1)^2 + (x^2)^2 \qquad (21)$$

will take on its least possible value, which is zero and which corresponds to the final conditions $x_1^1 = 0$ and $x_1^2 = 0$.

The recurrence relation for ψ_{20} is given by

$$\psi_{20}^{\nu+1} = \psi_{20}^{\nu} - \left(\frac{\partial F(x_1)}{\partial \psi_{20}}\right)^{\nu} \Delta \qquad (22)$$

The constant value Δ has to be sufficiently small to avoid convergence difficulties (cfr. § 5.5.1.).

At the same time we have

$$\frac{\partial F}{\partial \psi_{20}} = 2 \left(x^1 \frac{\partial x^1}{\partial \psi_{20}} + x^2 \cdot \frac{\partial x^2}{\partial \psi_{20}} \right) \qquad (23)$$

where the initial condition influence coefficients $\partial x^1 / \partial \psi_{20}$ and $\partial x^2 / \partial \psi_{20}$ are given by the sensitivity equations

$$\frac{d}{dt} \left(\frac{\partial x^1}{\partial \psi_{20}} \right) = \frac{\partial x^2}{\partial \psi_{20}} \qquad \frac{\partial x_o^1}{\partial \psi_{20}} = 0 \qquad (24)$$

$$\frac{d}{dt} \left(\frac{\partial x^2}{\partial \psi_{20}} \right) = \frac{\partial u}{\partial \psi_{20}} \qquad \frac{\partial x_o^2}{\partial \psi_{20}} = 0 \qquad (25)$$

$$\frac{\partial u}{\partial \psi_{20}} = \delta (\psi_2) \frac{\partial \psi_2}{\partial \psi_{20}} \qquad (26)$$

$$\frac{d}{dt} \left(\frac{\partial \psi_2}{\partial \psi_{20}} \right) = - \frac{\partial \psi_1}{\partial \psi_{20}} = 0 \qquad \frac{\partial \psi_{20}}{\partial \psi_{20}} = 1 \qquad (27)$$

According to the remarks of § 5.5.3. equations (25), (26) and (27) can be rearranged as follows:

$$\frac{\partial x^2}{\partial \psi_{20}} = 0 \quad \text{before sign inversion of } \psi_2 \qquad (28)$$

$$\frac{\partial x^2}{\partial \psi_{20}} = 1 \quad \text{after sign inversion of } \psi_2 \qquad (29)$$

Another difficulty consists in the fact that for every iterate $\partial F / \partial \psi_{20}$ has to be computed for a time instant t_1, which is unknown up to now and which has to correspond to the minimal time $t_1 - t_o$ after having solved the problem. By common sense it has been decided to consider t_1 for every iterate as the point where $F \left[x (t) \right]$ arrives at a minimum after the first switching. For this reason we have to compute

$$\frac{dF}{dt} = 2 \left(x^1 \frac{dx^1}{dt} + x^2 \frac{dx^2}{dt} \right) = 2 x^2 (x^1 + u) \qquad (30)$$

The complete computing diagram (Fig. 5.1.) has been made for the case where the starting point x_o of the trajectory lies on the right of the switching line (cfr. Fig. 1.2.). This specification is connected to the choice of the first value of ψ_{20}^{ν} ($\nu = 0$) and the difficulties discussed in § 5.5.2. When dF/dt goes from a negative to a positive value after the switching of u from - 1 to + 1, a mechanical relay stops the computer run, and the quantity $(\partial F/\partial \psi_{20})\Delta$ is added to the value ψ_{20}^{ν}, which was put into a memory M during the run ν. The sum $\psi_{20}^{\nu+1}$ is memorized by the complementary memory $\bar{M}$ and imposed as the initial condition of ψ_2 for the next computer run, which starts automatically at this moment. The first value of ψ_{20}^{ν} ($\nu = 0$) comes from a potentiometer to be switched off immediately after the start of the iteration process. Fig. 5.2. gives two families of curves, A and B, corresponding to iterations with two different first values of ψ_{20}.

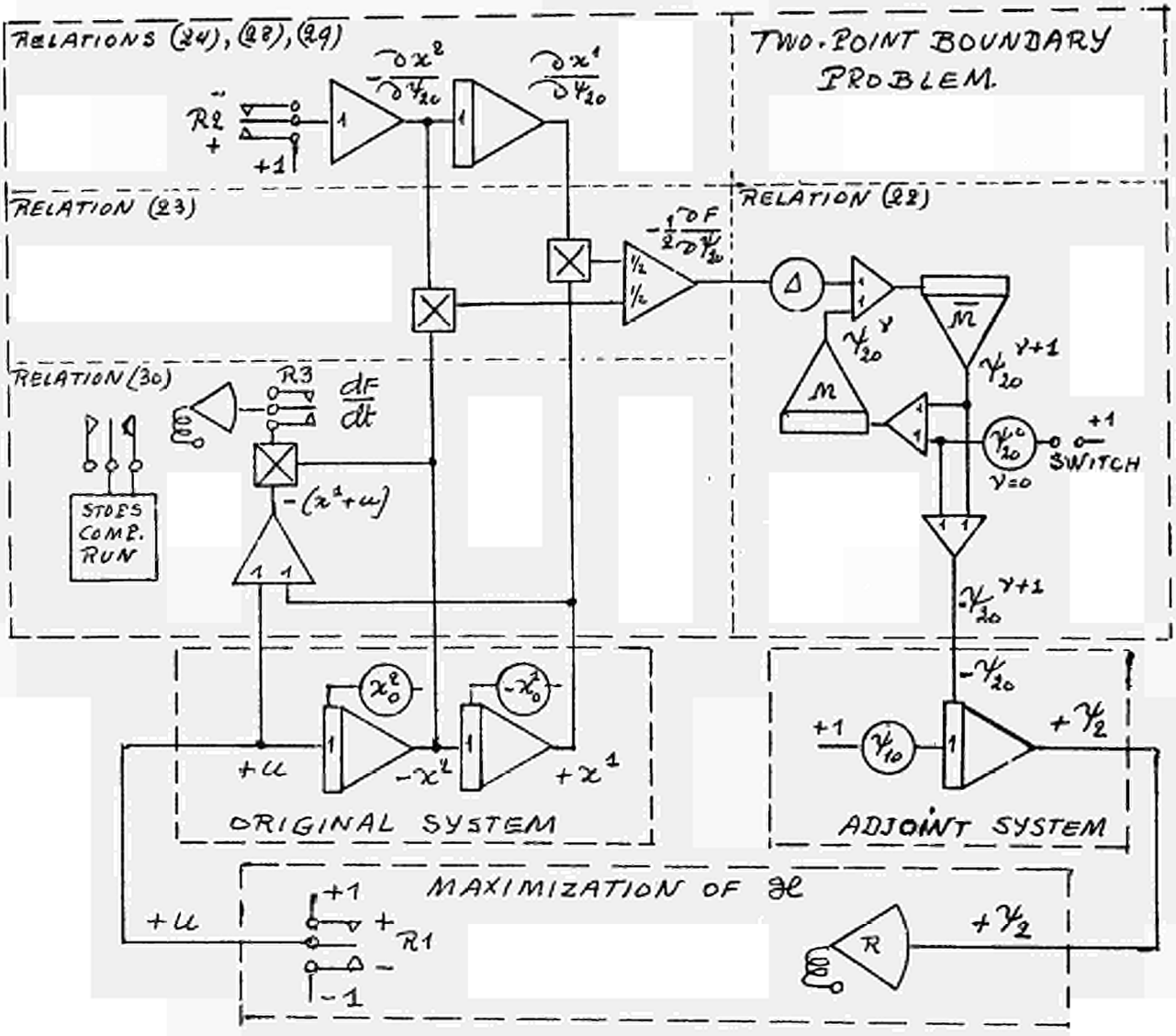
RELATIONS (24), (28), (29)
TWO-POINT BOUNDARY PROBLEM
RELATION (23)
RELATION (22)
RELATION (30)
R2
+1
R3
STOES COMP. RUN
SWITCH
ORIGINAL SYSTEM
ADJOINT SYSTEM
MAXIMIZATION OF
R1
R

Fig 5.1.

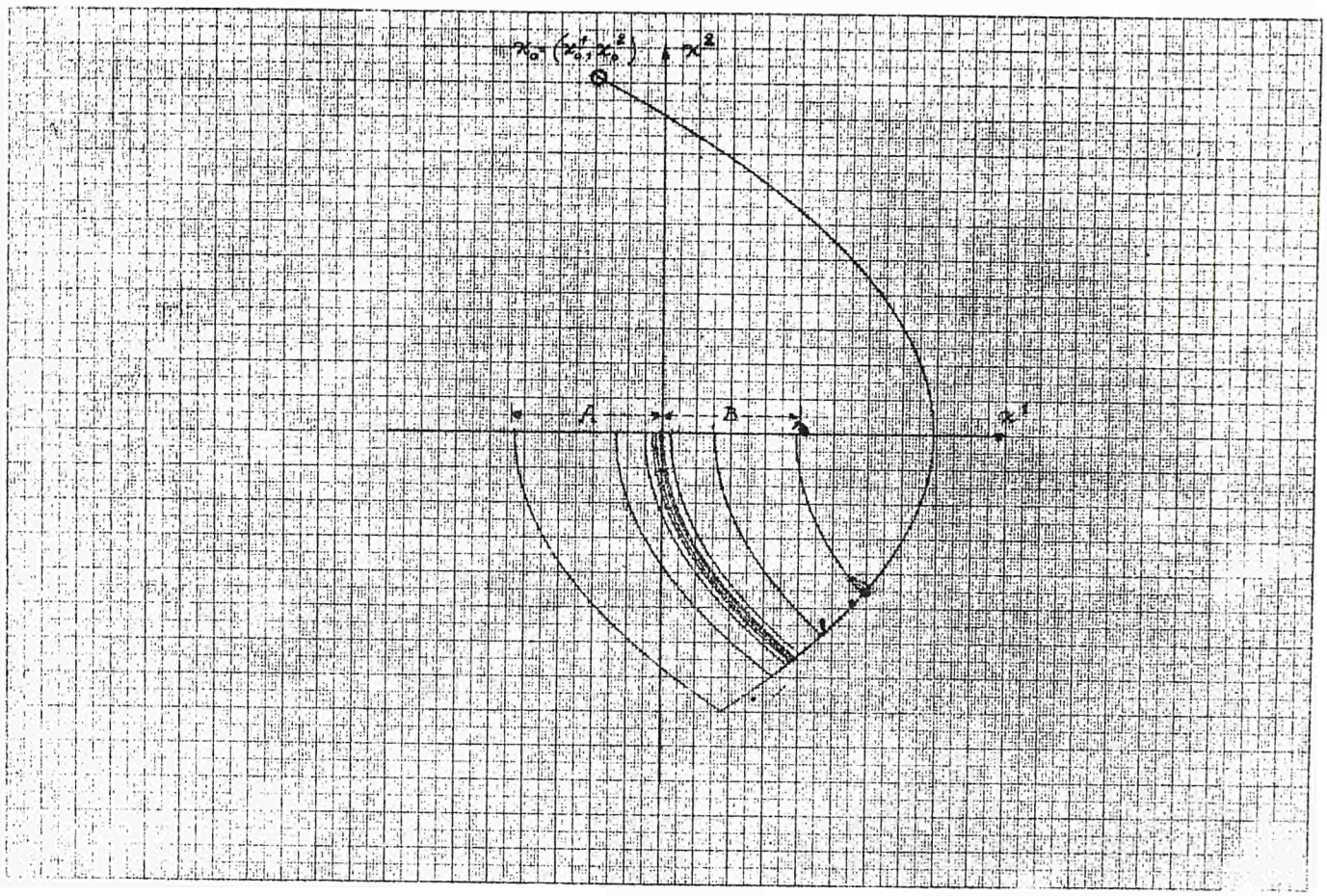

Fig 5.2

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