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SECOND WORKSHOP ON MATHEMATICS IN INDUSTRY

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"OPTIMAL CONTROL."

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BACKGROUND NOTES FOR A STUDY OF OPTIMISATION METHODS

IN THE CASE OF A CHEMICAL REACTION PROBLEM

COURSE ABSTRACT

A specific problem arising from the analysis of chemical reactions is considered and used as a vehicle for the application and comparison of various optimisation techniques. The example is interesting not the least for the fact that it is variously, under appropriate assumptions, an unconstrained or constrained, static or dynamic optimisation problem

1. A CHEMICAL REACTION PROBLEM:

A chemical reaction takes place in a tubular reactor packed with catalyst. The reaction scheme may be modelled as follows:

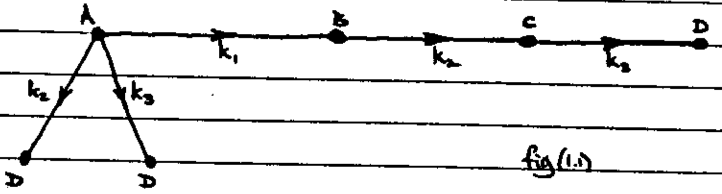

fig (1.1)

In the above scheme, A is the feed material, B is a transient intermediate product, C is the required "useful" product and D is "waste" material. The reactions are all assumed to be of first order with the rate constants k_i, $i = 1, 2, \ldots, 5$, obeying the law,

$$k_i = C_i \exp\left\{ -\frac{E_i}{R}\left(\frac{1}{T} - \frac{1}{658}\right)\right\} \qquad (1.1)$$

in which the C_i are frequency factors, the E_i are activation energies, R is the gas constant and T the absolute temperature. The values of the C_i and E_i may be determined experimentally as

	1	2	3	4	5
C_i	1.02	0.93	0.386	3.28	0.084
E_i	16,000	14,000	15,000	10,000	15,000

fig (1.2)

while the gas constant is

$$R = 1.9865 \qquad (1.2)$$

The problem is then to select a temperature profile in order that the yield of the useful product is maximised.

To obtain a mathematical formulation let the concentrations of the feed material A and the products B and C be denoted by x_1, x_2, x_3 respectively. The equations describing the reaction then become

$$\left.\begin{aligned} \frac{dx_1}{dt} &= -(k_1+k_2+k_3)\,x_1 && \triangleq f_1(x_1,x_2,x_3,T) \\ \frac{dx_2}{dt} &= k_1 x_1 - k_4 x_2 && \triangleq f_2(x_1,x_2,x_3,T) \\ \frac{dx_3}{dt} &= k_4 x_2 - k_5 x_3 && \triangleq f_3(x_1,x_2,x_3,T) \end{aligned}\right\} \quad (1.3)$$

If the reaction is assumed to start with one unit of A then the boundary conditions are

$$x_1(0) = 1 \; ; \; x_2(0) = 0 \; ; \; x_3(0) = 0 \qquad (1.4)$$

The problem is thus to determine the temperature profile $T(t)$ and the reaction time t_f so that the yield of the useful product $x_3(t_f)$ is a maximum.

There is one restriction however and that is that for the interest of catalyst stability the operating temperature must not exceed 550° C. Thus the constraint

$$0 \leq T(t) \leq 550° \qquad (1.5)$$

must at all times be obeyed.

Recall that the general problem of optimal control can be stated as follows

(1.6) : OPTIMAL CONTROL PROBLEM:

Determine the l-dimensional vector control function $u_0(t)$ for the system

$$\dot{x}(t) = f(x(t), u(t), t) \; , \; (x(t), \text{ an } n\text{-vector}) \qquad (1.7)$$

which transfers the initial event $(x^{(0)}, t_0)$ to ~~the~~ an event $(x(t_f), t_f)$ in the target set $S \subseteq \mathbb{R}^n \times [t_0, \infty)$ defined by algebraic relations

$$\psi(x(t), t) = 0 \; , \; (\psi(\cdot,\cdot), \text{ a } q\text{-vector}) \qquad (1.8)$$

in such a way that the performance index

$$J[x,u] = \phi(x(t_f), t_f) + \int_{t_0}^{t_f} F(x(\tau), u(\tau), \tau)\, d\tau \qquad (1.9)$$

is maximised.

It is apparent from this statement that the chemical reactor problem described above is a special case of this general optimal control problem in which $n = 3$, $l = 1$ and

$$\left.\begin{aligned} &\psi(\cdot\,,\cdot) \equiv 0 \quad \text{i.e. } S = \mathbb{R}^n \times [t_0, \infty) \\ &\phi(x(t_f), t_f) \equiv x(t_f) \; ; \; F(\cdot\,,\cdot\,,\cdot) \equiv 0 \end{aligned}\right\} \qquad (1.10)$$

Thus the chemical reaction problem we have described is a dynamic optimisation problem and in the sequel we will be concerned with the application and analysis of a number of techniques that may be utilised to solve this problem.

2: THE BEST ISOTHERMAL YIELD:

An interesting special case of the reaction problem occurs when only isothermal temperature profiles are implemented

$$\text{i.e.} \quad T(t) \equiv T, (\text{const}) \ \forall \ t \qquad (2.1)$$

In that event the kinetic equations (1.3) may be integrated analytically and the subsequent yield of the the useful product may be obtained as

$$x_3(t,T) = \frac{k_1 k_4 e^{-k_5 t}}{k-k_4} \left\{ \frac{1-e^{-(k_4-k_5)t}}{k_4-k_5} - \frac{1-e^{-(k-k_5)t}}{k-k_5} \right\} \qquad (2.2)$$

where

$$k \triangleq k_1 + k_2 + k_3 \qquad (2.3)$$

The best isothermal yield may then be found by maximising the expression (2.2) with respect to the two parameters t (the contact time) and T (the temperature). It is noted that the partial derivatives

$$\frac{\partial x_3}{\partial T}(t,T) \quad ; \quad \frac{\partial x_3}{\partial t}(t,T) \qquad (2.4)$$

can not be obtained analytically in any simple manner and so the majority of "gradient" methods of optimisation will not be feasible unless they incorporate a routine for numerical evaluation of the partial derivatives (2.4). The most natural way forward appear to be in terms of the "direct search" type of optimisation method and indeed the initial work on this problem (Rosenbrock and Storey, 1965) employed the Rosenbrock method (Rosenbrock, 1960). Their work indicates the optimal values shown in fig (2.1) in the cases of the unconstrained problem, obtained when the constraint (1.5) is ignored, and the constrained problem obtained when it is not.

OPTIMAL ISOTHERMAL VALUES

	T°C	t secs	x_3 %
unconstrained problem	710	0.076	42.3
constrained problem	650	0.26	41.6

fig (2.1)

Since this early work on the isothermal problem was performed the Rosenbrock method of optimisation has been superceded by other direct search methods. The application of several such methods to the chemical reaction problem will be considered and their performance analysed.

3: SOLUTION BY STATIC OPTIMISATION FORMULATION:

One obvious way to proceed in the case of the dynamic optimisation problem arising from the general chemical reaction problem described above, is to reduce the problem to a static optimisation one by some means or other and then use one of the existing static optimisation routines. There are various ways in which the given dynamic optimisation problem may be converted into a static one and we describe three such ways.

§(3.1): REDUCTION BY DISCRETE APPROXIMATION:

One way of reducing the dynamic optimisation problem presented by the general chemical reaction problem, to a static formulation is to write the kinetic equations (1.3) in finite difference form. In the case of (1.3) we obtain

$$\left.\begin{aligned} x_{1,r} - x_{1,r-1} &= -t_r(k_{1,r} + k_{2,r} + k_{3,r})x_{1,r} \\ x_{2,r} - x_{2,r-1} &= t_r(k_{1,r} x_{1,r} - k_{4,r} x_{2,r}) \\ x_{3,r} - x_{3,r-1} &= t_r(k_{4,r} x_{2,r} - k_{5,r} x_{3,r}) \\ r &= 1, 2, \ldots, n \end{aligned}\right\} \quad (3.1)$$

In equations (3.1),

$$k_{i,r} = C_i \exp\left\{-\frac{E_i}{R}\left(\frac{1}{T_r} - \frac{1}{658}\right)\right\} \quad (3.2)$$

$$i = 1, 2, \ldots, 5 \;;\; r = 1, 2, \ldots, n$$

The equations (3.1) are physically equivalent to approximating the tube by a series of n completely stirred tanks and they represent a material balance on the r^{th} tank (see fig (3.1))

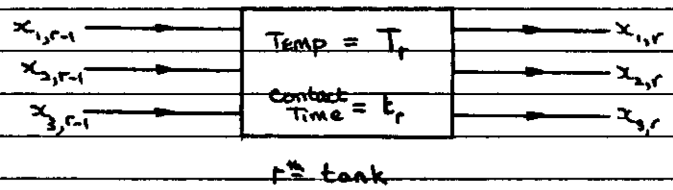

fig (3.1)

From the sets of algebraic equations (3.1) it is possible to obtain $x_3(t_f) \triangleq x_{2,n}$ (the yield of the desired product) by elimination. Thus $x_3(t_f)$ is obtained as a function of the 2n variables t_r, T_r $(r = 1, 2, \ldots, n)$ and this may be maximised directly by some appropriate optimisation procedure. In fact it again proves difficult to obtain the partial derivatives

$$\frac{\partial x_{3,n}}{\partial T_r} \;;\; \frac{\partial x_{3,n}}{\partial t_r} \quad (3.3)$$

$$r = 1, 2, \ldots, n$$

analytically and so a direct search technique suggests itself. Again early work (Rosenbrock and Storey, 1965) utilized the Rosenbrock method and the performance of this together with other more recent methods will be demonstrated and analysed.

In the case of the Rosenbrock method used to maximise the yield $x_{2,n}$ the following table showing the variation of $x_{2,n}$ with n (the number of tanks) was obtained

Nº of tanks	2	3	4	8
Best yield %	37.2	39.7	40.0	43.4

fig (3.2)

In the case of the approximation by 8 tanks the results giving rise to the best yield are given in fig (3.3) where the contact time t_r in each tank has been constrained to lie between 0 and 20 seconds.

TANK N°	1	2	3	4	5	6	7	8
TEMP: °C	550·0	550·0	550·0	426·9	386·2	353·6	267·5	190·0
HOLDING TIME: SECS	0·039	0·039	0·039	0·101	0·159	0·270	2·214	19·988

fig(3.3)

§(3.2): REDUCTION BY PARAMETRIC EXPANSION:

In this method a simple expression for the temperature profile is adopted which contains a number of adjustable parameters. On substitution of this into the kinetic equations (1.3) an appropriate numerical integration routine may be applied and the resulting $x_3(t_f)$ maximised with respect to the parameters occurring in the assumed temperature profile and t_f the final time.

If the trapezoidal rule is used in the integration stage of the above process then the finite difference equations take the form

$$\left.\begin{aligned} x_{1,r} &= x_{1,r-1}\frac{1-hk_{r-1}/2}{1+hk_{r}/2} \\ x_{2,r} &= x_{2,r-1}\frac{1-hk_{4,r-1}/2}{1+hk_{5,r}/2} + x_{1,r-1}\frac{hk_{1,r-1}/2}{1+hk_{4,r}/2} + x_{1,r}\frac{hk_{1,r}/2}{1+hk_{4,r}/2} \\ x_{3,r} &= x_{3,r-1}\frac{1-hk_{5,r-1}/2}{1+hk_{5,r}/2} + x_{2,r-1}\frac{hk_{4,r-1}/2}{1+hk_{5,r}/2} + x_{2,r}\frac{hk_{4,r}/2}{1+hk_{5,r}/2} \end{aligned}\right\} \quad (3.4)$$

where

$$k_r \triangleq k_{1,r} + k_{2,r} + k_{3,r} \qquad (3.5)$$

In the optimisation stage of this procedure a direct search technique is again an obvious candidate due to the difficulty in obtaining the appropriate gradient vector analytically. The results given below are the original results obtained by Rosenbrock and Storey (1965) using Rosenbrock's Method.

If a straight line relationship is adopted for the temperature profile

$$\text{i.e.} \quad T(°K) = a_1 - a_2 t \qquad (3.6)$$

and a final time $t_f = 0{\cdot}5$ secs is fixed then the results of fig (3.4) are obtained on using an integration step length $h = 0{\cdot}01$ in equations (3.4).

	a_1	a_2	$x_3(0{\cdot}5)\%$
START	527	500	34·8
END	550	312	42·87

fig(3.4)

For a quadratic temperature profile

$$\text{i.e.} \quad T(°K) = a_1 + a_2 t + a_3 t^2 \qquad (3.7)$$

and again $h = 0{\cdot}01$, $t_f = 0{\cdot}5$ the results of fig (3.5) may be obtained

	a_1	a_2	a_3	$x_3(0{\cdot}5)\%$
START	477	0	0	40·3
END	549·9	-288·3	-55·9	42·58

fig(3.5)

Another simple functional form that could be taken as a temperature profile in the kinetic equations (3.4) is the exponential

$$T(°K) = a_1 \exp(-a_2 t) \qquad (3.8)$$

with again the values of h and t_f taken as 0.01 and 0.5 secs respectively. The results of fig (3.6) are then obtained.

	a_1	a_2	$x_3(0.5)\%$
START	477	0	40.3
END	549.9	0.39	42.55

fig (3.6)

which gives a yield no better than the quadratic form of (3.7)

The results of the discrete approximation approach of §(3.1) indicate that first part of the temperature profile should be at the upper temperature limit and that the subsequent behaviour should be of a monotonic decreasing nature. A profile of the form shown in fig (3.7) might thus be reasonably used.

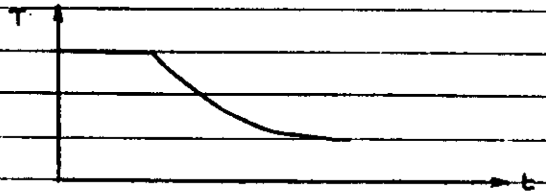

fig (3.7)

Fig (3.7) suggests that a hybrid construction of T from the simple functional forms (3.6), (3.7) and (3.8) be used. In the case of an approximation by two straight line segments the following expression results

$$T(°K) = \begin{cases} a_2 - a_1 t & ; \quad t \le a_4 \\ a_2 + a_4(a_3 - a_1) - a_3 t & ; \quad t > a_4 \end{cases} \qquad (3.9)$$

while a combination of linear and exponential forms gives rise to the expression

$$T(°K) = \begin{cases} a_2 - a_1 t & ; \quad t \le a_4 \\ (a_2 - a_4 a_1) \exp\{a_3(t - a_4)\} & ; \quad t > a_4 \end{cases} \qquad (3.10)$$

In the event the best form of (3.9) was achieved by the values of a_i $(i = 1, \dots, 4)$ given by (again with $h = 0.01$, $t_f = 0.5$)

$$a_1 = 310 \quad a_2 = 548 \quad a_3 = 294 \quad a_4 = 20 \qquad (3.11)$$

when a maximum yield of 42.81% is obtained. Interestingly the form (4.1) performs only marginally better with its best form producing 42.85% as the best yield.

An important aspect of the parametric expansion technique is that it can handle the case of a variable final time t_f quite easily. Indeed this method treats this simply as another parameter to be determined in the optimisation stage of the procedure. Thus for example if an upper limit of 10.0 secs on t_f is set and the functional form (3.9) (two straight lines) is used then the maximum yield improves to 44.46% as fig (3.8) demonstrates

	a_1	a_2	a_3	a_4	t_f	$x_3(t_f)\%$
START	310.0	548.0	294.0	20.0	0.5	42.81
END	434.2	549.9	47.5	10.5	10.00	44.46

fig (3.8)

In obtaining the results of fig (3.5) the starting values have been taken as the best values obtained for the form (3.9) when t_f was fixed at 0.5 secs.

§(3.3): REDUCTION BY THE RAYLEIGH-RITZ METHOD:

A brief description of this method is as follows. Suppose we are looking for a maximum of a functional $J[T(t)]$, $(x_3(t_f))^2$ in this case) over some set of competing functions Σ. Let

$$\phi_1(t),\ \phi_2(t),\ \ldots\ldots \qquad (3.12)$$

be an infinite set of basis functions for Σ (which satisfy any boundary conditions imposed). Let Σ_n be the n-dimensional subspace of Σ spanned by the first n of the functions (3.12) i.e. Σ_n is the set of all functions of the form

$$\alpha_1\phi_1(t) + \ldots + \alpha_n\phi_n(t) \qquad (3.13)$$

where $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$.

On each subspace Σ_n the functional $J[T]$ gives rise to a function

$$I(\alpha_1, \ldots, \alpha_n) \triangleq I[\alpha_1\phi_1 + \ldots + \alpha_n\phi_n] \qquad (3.14)$$

of the n parameters $\alpha_1, \ldots, \alpha_n$.

Now choose $\alpha_1, \ldots, \alpha_n$ to maximise (3.14) and let $\mu_n \triangleq \max J$ and $T_n \in \Sigma_n$ be the maximising function so obtained. Note that μ_n cannot decrease with n since

$$\Sigma_1 \subseteq \Sigma_2 \subset \ldots \subset \Sigma_n \subset \ldots\ldots \qquad (3.15)$$

Hence an increasing sequence

$$\mu_1 \leq \mu_2 \leq \ldots \leq \mu_n \leq \ldots\ldots$$

is obtained.

Under quite weak conditions it can be shown that the sequence of functions $\{T_n\}$ converges (under the norm of Σ) to the required maximising curve $T(t)$ of $J[T]$ over Σ. Thus again the dynamic optimisation problem is converted into a static optimisation formulation.

4: SOLUTION BY INDIRECT METHODS:

The solution methods discussed in the previous section are often referred to as "direct methods" because of way in which they directly approach the optimisation of the functional concerned. However as has been seen in previous talks the Pontryagin Maximum Principle provides the basis for the solution of the general problem of optimal control, and our chemical reaction problem is one such problem. Recall that in the case of the general problem (1.6) Pontryagin's Maximum Principle states

(4.1): THE MAXIMUM PRINCIPLE:

In order that $u_0(t)$ be optimal for the problem (1.6) it is necessary that there exist an n-vector function $\lambda(t)$ and a constant q-vector ν such that

(i) if $x_0(t)$ is the trajectory corresponding to $u_0(t)$ then

$$\left.\begin{aligned} \frac{dx_0(t)}{dt} &= \frac{\partial H}{\partial \lambda}(x_0(t), \lambda(t), u_0(t), t) \\ \frac{d\lambda(t)}{dt} &= -\frac{\partial H}{\partial x}(x_0(t), \lambda(t), u_0(t), t) \end{aligned}\right\} \qquad (4.2)$$

where the Hamiltonian H is defined as

$$H(x, \lambda, u, t) \triangleq F(x, u, t) + \lambda^T f(x, u, t) \qquad (4.3)$$

In conjunction with (4.2) the following boundary conditions must hold

$$x(t_0) = x^{(0)} \quad ; \quad \lambda(t_f) = \frac{\partial \Phi}{\partial x}(x_0(t_f), t_f) \qquad (4.4)$$

$$\frac{\partial \Phi}{\partial t}(x_0(t_f), t_f) + H(x(t_f), \lambda(t_f), u_0(t_f), t_f) = 0 \qquad (4.5)$$

where

$$\Phi(x, t) \triangleq \phi(x, t) + \nu^T \psi(x, t) \qquad (4.6)$$

- (ii) $u_0(t)$ must at all time maximise $H(x_0(t), \lambda(t), u, t)$

i.e. $$\max_u H(x_0(t), \lambda(t), u, t) = H(x_0(t), \lambda(t), u_0(t), t) \qquad (4.7)$$

It is noted that in any problem where the final time t_f is fixed then the condition (4.5) does not appear and

$$\phi(x, t) \equiv \phi(x) \quad ; \quad \psi(x, t) \equiv \phi(x) \qquad (4.8)$$

Numerical techniques for the solution of optimal control problems, which are based on the Maximum Principle are often referred to as "indirect methods" since they attempt to maximise the Hamiltonian rather than the performance index functional directly. We consider two such techniques

§(4.1): NEIGHBOURING EXTREMAL METHODS:

In the case of the chemical reaction problem

$$H(x, \lambda, T, t) \triangleq \sum_{i=1}^{3} \lambda_i f_i$$

$$= -(k_1 + k_2 + k_3)\lambda_1 x_1 + k_2 \lambda_2 x_1 - k_4(\lambda_2 - \lambda_3) x_3 - k_5 \lambda_3 x_3 \qquad (4.9)$$

and so the costate equations take the form,

$$\left.\begin{aligned}\frac{d\lambda_1}{dt} &= (k_1+k_2+k_3)\lambda_1 - k_1\lambda_2\\ \frac{d\lambda_2}{dt} &= k_4\lambda_2 - k_4\lambda_3\\ \frac{d\lambda_3}{dt} &= k_5\lambda_3\end{aligned}\right\} \quad (4.10)$$

With an assumed fixed operating time t_f the boundary conditions (4.4), (4.5) reduce to

$$\left.\begin{aligned}x_1(0) = 1 \;;\quad x_2(0) = 0 \;;\quad x_3(0) = 0\\ \lambda_1(t_f) = 0 \;;\quad \lambda_2(t_f) = 0 \;;\quad \lambda_3(t_f) = 1\end{aligned}\right\} \quad (4.11)$$

In accordance with (4.7) the optimal temperature profile T(t) is such that at all times it maximises H of (4.9). In fact since T(t) is constrained by the relationship

$$0 \leq T(t) \leq 550 \quad \forall t \in [0, t_f] \quad (4.12)$$

the optimal value of T(t) at any time t is either zero, 550 or a value of T which makes

$$\frac{\partial H}{\partial T}(x(t), \lambda(t), T, t) = 0 \quad (4.13)$$

It is noted that in (4.11) the boundary conditions for the kinetic equations (1.3) and the costate equations (4.10) are of a two-point nature with the values of the concentrations x_1, x_2, x_3 being given at the initial time $t = 0$, while the values of the costates $\lambda_1, \lambda_2, \lambda_3$ are given at the final time t_f. It is the solution of this two point boundary value problem that complicates the straightforward numerical application of the Maximum Principle as will now be seen.

The obvious way of applying the Maximum Principle numerically is to guess the values of the concentrations at the final time t_f. (Alternatively we may guess the initial values of the costate variables and proceed with obvious modifications) The kinetic equations (1.3) and the costate equations (4.10) may then be integrated backwards in time from $t = t_f$ to $t = 0$, using (4.7) to determine T(t) at each time point. The differences between the calculated concentrations x_1, x_2, x_3 at $t = 0$ and the desired values (4.11) may then be used to correct the guesses in $x_1(t_f), x_2(t_f), x_3(t_f)$. Thus neighbouring extremal methods are characterised by iterative algorithms for improving the guesses of the final time concentrations (alternatively, the initial values of the costates) so as to satisfy the given initial (alternatively, final time) conditions.

The main difficulty arising in this method as we have noted concerns the two point boundary value problem. Since the method proposes to integrate the state and costate equations in the same direction, then one set of equations, either the state or costate equations, will never be integrated in their naturally stable direction. Consequently the solutions $x(t)$, $\lambda(t)$ tend to become widely different in orders of magnitude as the integration proceeds. Thus, for example, small changes in the adopted values $x_1(t_f), x_2(t_f), x_3(t_f)$ can give rise to excessively large changes in $x_1(0), x_2(0), x_3(0)$. These observations are confirmed by the results of Rosenbrock and Storey (1965) which are summarised as follows (for an assumed fixed value of $t_f = 0.5$ secs).

FIRST RUN

t	Temp T	x_1	x_2	x_3	λ_1	λ_2	λ_3
0.50	381.5	0.004	0.016	0.425	0.000	0.000	1.00
0.00	550.0	0.048	0.104	0.354	0.253	0.536	0.942

fig (4.1)(a)

SECOND RUN

t	Temp. T	x_1	x_2	x_3	λ_1	λ_2	λ_3
0.50	346.5	0.002	0.013	0.430	0.000	0.000	1.00
0.00	352.2	0.004	0.036	0.415	0.078	0.643	0.979

fig(4.1)(b)

§(4.2): GRADIENT METHODS:

As was seen above any numerical method which attempts to integrate the state and costate equations (4.2) in the same direction can experience great numerical instability. To overcome this, methods have been suggested whereby each set of equations in (4.2) ~~are~~ is integrated in its naturally stable direction

One such method is the "gradient in function space" method which is the analogue of the steepest descent method in ordinary function optimisation. The method may briefly be described as follows

(4.14): GRADIENT METHOD IN FUNCTION SPACE:

(i) guess $u^{(0)}(t)$, a suitable approximation to $u^*(t)$ the optimal control e.g. the best straight line approximation to $u^*(t)$.

(ii) use $u^{(0)}(t)$ to integrate the state equations (1.7) from $t=t_0$ to $t=t_f$ (their naturally stable direction), storing the values of $x_i(t)$ $i=1,\dots,n$.

(iii) use $u^{(0)}(t)$ and $x(t)$ just found, to integrate the costate equations of (4.2) backwards from $t=t_f$ to $t=t_0$

(iv) at the same time as step (iii), compute the gradient vector $\partial H/\partial u$ using the values of $u^{(0)}(t)$, $\lambda(t)$ and the stored values of $x(t)$.

(v) Correct $u^{(0)}(t)$ to

$$u^{(1)}(t) = u^{(0)}(t) - \varepsilon \frac{\partial H}{\partial u}$$

where ε is some suitably chosen step length parameter

(vi) repeat.

The algorithm (4.14) is based closely on the steepest descent method of static optimisation and so not unexpectedly inherits its advantages and disadvantages (e.g. guaranteed reduction of the functional value on every iteration, slow convergence). The situation may be improved somewhat by the use of other static optimisation techniques within steps (iv) and (v) of the algorithm (4.14) (e.g. Newton's method, variable metric methods conjugate gradient techniques)

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