4. Bildschirmdialog mit LEINET

Im Rahmen des LEINET-Dialog lassen sich zunächst die einzelnen Netze relativ rasch auf den aktuellen Stand bringen. Gleichzeitig lassen sich nach jeden Optimierungsbaustein(also speziell auch nach RF oder RL) ein Dialog führen,wo die Ergebnisse der Berechnungen analysiert werden können und die praktische Brauchbarkeit der Lösung untersucht wird.Man kann sich auf diese Weise leicht über die Güte von Lösungen informieren,gegebenenfalls können Neurechnungen vom Bildschirm aus angestoßen werden.

Die wichtigsten Möglichkeiten,sich über eine Lösung ein Bild zu verschaffen sind im LEINET gegeben:

Dies ist möglich durch

- Darstellen von Vorgangsumgebungen
- Darstellung von Brigadeplänen $\mathfrak{Z}^j$
- Anzeigen von speziellen Entfernungen E_{kl}
- Darstellen von Gesamtaufwendungen von Ressourcen
- Anzeigen des kritischen Weges in $\mathcal{N}^*$
- Darstellen von Ressourcenbelastungen auch für nichtbilanzierte Ressourcen

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REMARKS ON THE NUMERICAL TREATMENT OF OPTIMAL CONTROL PROBLEMS

1. Introduction

In lots of practical applications the numerical treatment of optimal control problems with ordinary differential equations (ODE) is necessary. We mention here the optimization of chemical reactions, electronic circuits, the guidance of a spaceship, energetic processes and mechanical systems. Typical for many of such problems are nonlinearities in the ODE and control and state constraints, too.

In chapter 2 we formulate a general problem of optimal control and discuss special cases. This problem is quite similar to that in [15]; in [7] we show that also a relatively complicate model for the optimization of a suspension polymerization may be formulated in this way.

In this paper we suggest as an approach to the numerical treatment the application of discretization methods and of descent methods for the arising finite-dimensional optimization problems This approach has the advantage that cost-profitable controls may be expected after a short calculation time. In chapter 3 we go into a "proper" and problem- oriented discretization of control and state variables. Especially it is referred to the consequences of applying software packages to the automatical integration of the state equation. One consequence is a problem-dependent choice of the state-discretization, a further one the appropriate computation of the gradient. The latter is demonstrated with the case of variable one-step methods and specially of the implicit Euler method.

In chapter 5 concrete variants of methods are suggested and hints to the related literature are given. In case there only occur vectorial control parameters, a variable metric method for constrained optimization is applied, and in the other case an adaptive scheme of discretization-, conditional gradient-, and penalty-shifting methods is used.

2. Formulation of the problem

We consider the following general problem of optimal control, where the system is described by an ODE for the state variables

(1) $\dot{x}(t)=f(t,v(t),p,x(t))$, $t\in[t_o,t_e]$, $x(t_o)=x_o(p)$,

the controls are functions v(.) and parameters p, which satify the constraints of the set of admissible controls

(2) $C:=\{u\in C_1 \mid g_j(x(t_e),p)\leq 0$, $j=1,\ldots,d\}$

(3) $C_1:=\{u=[v,p]\in L_2^r(t_o,t_e)\times R^s \mid a^v\leq v(t)\leq b^v$ a.e. in (t_o,t_e) , $a^p\leq p\leq b^p\}$

and where the system performance is measured in terms of the functional

(4) $J(u):=g_o(x(t_e),p)$, $u=[v,p]\in C$.

Now the problem (P) is to minimize J(u) subject to $u\in C$.

The subset C_1 of C contains all simple linear control constraints and C is completed by terminal state constraints.

For the further consideration we assume:

g_j: $R^n\times R^s\longrightarrow R^1$, $j=1,\ldots,d$;

$f:[t_o,t_e]\times R^r\times R^s\times R^n\longrightarrow R^n$, x_o: $R^s\longrightarrow R^n$;

$t_o,t_e\in R^1$; r,s,n,d are natural numbers;

$a^v,b^v\in R^r$, $a^p,b^p\in R^s$;

let g_j, $j=0,\ldots,d$, f, x_o be continuously differentiable functions of x,v,p and let (1) be uniquely solvable for all occuring initial values $x_o(p)$.

Remark 1:

a) Further problems of optimal control, e.g. problems where the objective is an integral functional, problems with more general constraints to v,p and with state path constraints may be transformed into a problem of the above type (P) by introducing suitable new state variables x_j, $j=n+1,\ldots$. We succeed in doing the same for problems with free initial and final time t_o,t_e by transforming the problem to a fixed interval and involving t_o,t_e in the vector of the control parameter p (see [15], [16], [7]).

b) In practical applications it sometimes occurs that some or all admissible control functions may be characterized by a finite number of parameters, e.g. by a fixed number of possible points of discontinuity and the respective function values in the case of piecewise constant controls (comp. also [15], [16]) These parameters can then be added to p and the control function can be formulated in the form v(t,p). If it is only minimized with respect to the control parameter p (i.e. r=0), then (P) represents a nonlinear programming problem in R^s and can be numerically treated respectively effectively (see chapt.5).

c) In the present paper existence results for (P) are of no interest. But we note that C_1 is weakly compact in the Hilbert space $H:=L_2^r(t_o,t_e)\times R^s$ and that C is also weakly compact and J weakly continuous if the mapping $S: C\longrightarrow R^n$ $S(u):=x(t_e)$ is weakly continuous (according to our above assumption the functions g_j, $j=0,\ldots,d$, are continuous). [3] contains e.g. a theorem on the weak continuity of S (under certain conditions).

3. Discretization of control and state variables

If we aim at developing a computational method in optimal control, then a discretization of control and state variables is necessary in any case.

For the discretization of controls we consider a grid $G:=\{t_o=\tilde{t}_o<\tilde{t}_1<\ldots<\tilde{t}_M=t_e\}$ on $[t_o,t_e]$ and use the following finite-dimensional approximation of C:

(5) $C_G:=\{u=[v,p]\in C \mid v(.)$ is piecewise constant, left-continuous and has jumps at $\tilde{t}_j$, $j=1,\ldots,M-1\}$.

We want to restrict ourselves to this simple version for the discretization of C, although essentially more general variants are imaginable (see [15], [16]).

Now, in order to minimize the functional J on C_G it is often necessary to solve (1) by an ODE code. Thereby an available standard code will be chosen, or a method will be applied that takes into account certain properties of the problem (1), e.g. stiffness, smoothness. In most cases the used code chooses at each step the particular integration procedure and the stepsize on the basis of a tolerance parameter δ and the local behaviour of the ODE (see [19]). As a result we obtain a variable multistep method (see [10]).

But, we want to restrict ourselves here to the case of variable one-step methods (e.g. variable step, variable formula Runge-Kutta methods) and for the more general case we refer to [7]. We consider the following method:

(6) $x_l = x_{l-1} + h_l \varphi_l(p, r_G v; x_l, x_{l-1})$
$l=1,\ldots,N,\ x_o = x_o(p),$

where $h_l = t_l - t_{l-1}$, $l=1,\ldots,N$, $t_N = t_e$, is the used sequence of stepsizes and $\varphi_l: R^s x R^{Mr} x R^n x R^n \longrightarrow R^n$, $l=1,\ldots,N$, shall be differentiable with respect to all variables;
$r_G v := (v(\tilde{\tau}_1),\ldots,v(\tilde{\tau}_M))^T$ contains all information about v.

First we note that in general the stepsizes h_l, φ_l and N depend on $u=[v,p]$, but we want to assume that, with only small perturbations of u, the used ODE code leaves h_l, φ_l, $l=1,\ldots,N$, unchanged.

After having performed the discretization of the control and state variables we get a discrete optimal control problem, where the functional J_D depends on the grid G and the tolerance parameter δ:

(P_D) $J_D(u) := g_o(x_N, p) \longrightarrow$ Min! subject to $u \in C_G$, where x_N is determined by (6) and $x(t_e)$ is replaced by x_N.

Remark 2:

We assume that it holds for (6) that:

$$\max_{l=1,\ldots,N} |x_l - x(t_l)| \xrightarrow[\delta\to 0]{} 0 .$$

Here δ mostly represents a bound or estimate for the local discretization error.

If we have, moreover, the denotation $\tilde{h} := \max_{1\le j\le M} |\tilde{\tau}_j - \tilde{\tau}_{j-1}|$, then it would be desirable if it was valid that:

$$(*) \quad \inf_{u\in C_G} J_D(u) \xrightarrow[\substack{\tilde{h}\to 0\\ \delta\to 0}]{} \inf_{u\in C} J(u)$$

Special statements of the type (*) were proved for the case of the explicit Euler method with the same grids for control and state variables (the tolerance δ is dropped) in [1],[8].

Yet, for practical applications it seems to be better to choose the grid for the state variables in dependence on the problem and automatically (by an ODE code for a tolerance δ) and to fix (for the present) the grid for the control variables.

The general results of [8],[9] about perturbations of optimization problems, especially continuity results for the extremal value function, seem to be applicable to the more general problem, too.

4. Computation of the gradient

An essential consequence after the discretization of the problem (P) is the adjustment of the gradient to the discretization, i.e. the computation of the gradient of J_D. Thereby we want to assume that $J_D: C_G \longrightarrow R^1$ is differentiable and that consequently the gradient $J_D' = [J_{D,v}', J_{D,p}']: C_G \longrightarrow L_2^r(t_o,t_e) x R^s$ can be computed according to the formula:

$$\frac{d}{d\alpha} J(u+\alpha\bar{u})\Big|_{\alpha=0} = (J_{D,v}'(u),\bar{v})_{L_2^r} + (J_{D,p}'(u),\bar{p})_{R^s}$$

As a special case of a more general result in [7] we obtain:

$$(7) \quad J_{D,v}'(u)(t) = (\tilde{\tau}_j - \tilde{\tau}_{j-1})^{-1} \sum_{l=1}^{N} h_l \left(\frac{\partial\tilde{\varphi}_l}{\partial v_j}\right)^T z_l$$
$$t \in (\tilde{\tau}_{j-1}, \tilde{\tau}_j],\ j=1,\ldots,M;$$

$$(8) \quad J_{D,p}'(u) = \sum_{l=1}^{N} h_l \left(\frac{\partial\tilde{\varphi}_l}{\partial p}\right)^T z_l + \left(\frac{\partial x_o}{\partial p}(p)\right)^T z_o + \left(\frac{\partial g_o}{\partial p}(x_N,p)\right)^T$$

$$\left(I - h_N \left(\frac{\partial\tilde{\varphi}_N}{\partial x_N}\right)^T\right) z_N = \left(\frac{\partial g_o}{\partial x}(x_N,p)\right)^T$$

$$(9) \quad \left(I - h_l \left(\frac{\partial\tilde{\varphi}_l}{\partial x_l}\right)^T\right) z_l = \left(I + h_{l+1}\left(\frac{\partial\tilde{\varphi}_{l+1}}{\partial x_l}\right)^T\right) z_{l+1}$$
$$(l=N-1,\ldots,1)$$
$$z_o = \left(I + h_1\left(\frac{\partial\tilde{\varphi}_1}{\partial x_o}\right)^T\right) z_1$$

($\sim$ denotes that the functions are considered at $(p, r_G v;\ x_l, x_{l-1})$).

For the special case of the implicit Euler method instead of (6) we have

$$\varphi_l(p, r_G v;\ x_l, x_{l-1}) = f(t_l, v(t_l), p, x_l) =: f|_l$$
$$= f(t_l, v(\tilde{\tau}_j), p, x_l)\ ,\ \text{if } t_l \in (\tilde{\tau}_{j-1}, \tilde{\tau}_j]\ .$$

Thus we obtain:

$$J'_{D,v}(u)(t) = (\tilde{\tau}_j - \tilde{\tau}_{j-1})^{-1} \sum_{\substack{l=1 \\ t_l \in (\tilde{\tau}_{j-1}, \tilde{\tau}_j]}}^{N} h_l \left(\frac{\partial f}{\partial v}\Big|_l\right)^T z_l$$

$$(t \in (\tilde{\tau}_{j-1}, \tilde{\tau}_j]\ ,\ j=1,\dots,M)$$

$$J'_{D,p}(u) = \sum_{l=1}^{N} h_l \left(\frac{\partial f}{\partial p}\Big|_l\right)^T z_l + \left(\frac{\partial x_o}{\partial p}(p)\right)^T z_o + \left(\frac{\partial g_o}{\partial p}(x_N, p)\right)^T$$

$$\left(I - h_N \left(\frac{\partial f}{\partial x}\Big|_N\right)^T\right) z_N = \left(\frac{\partial g_o}{\partial x}(x_N, p)\right)^T$$

$$\left(I - h_l \left(\frac{\partial f}{\partial x}\Big|_l\right)^T\right) z_l = z_{l+1}\ ,\ l=N-1,\dots,1,$$

$$z_o = z_1$$

Remark 3:

These formulas for the computation of the gradient yield the necessity to store x_l, h_l, φ_l, $l=1,\dots,N$, when performing (6), in order to be able to compute the gradient by means of (7),(8),(9) in a suitable and simple way. In a certain sense (9) represents an induced discretization of the so-called costate equation (see also [6]) For detailed investigations we refer to [7].

5. Some remarks on the numerical treatment

Let us start with some remarks on numerical methods for the discrete problems (P_D) (for the present let δ and G be fixed). (P_D) represents an optimization problem of the dimension s+M, where M may be "great" in dependence on G. This is the reason why different methods are used for the cases r=0 (i.e. there do not occur any control functions v, thus M=0) and $r \geq 1$.

Case 1 (r=0):

The nonlinear optimization problem (P_D) is iteratively solved by a variable metric method for nonlinear constraints according to Powell[13]. This method is based on the successive minimization of a quadratic objective function subject to linear constraints, where the matrix of the quadratic function is suitably updated. As in [14] the implementation is carried out by using the sub-programme QUAPRO from [5].

In extensive tests of comparison with the most important other codes for solving nonlinear optimization problems this method has proved its outstanding efficiency (especially with respect to the number of function- and gradient-calls) and reliability (see [18]).

The necessary gradients of the objective and the constraint functions are computed as in chapter 4. The method is adaptively implemented (in the sense of [11],p.283) with the discretization (6), i.e. the tolerance δ.

Case 2 ($r \geq 1$):

(P_D) is treated with a penalty shifting method by Fletcher/Powell ([4],[2]), where an auxiliary function

$$T(u;y,r) := J_D(u) + \frac{1}{2} \sum_{j=1}^{d} r_j \max{}^2\{0,\ y_j + g_j(x_N, p)\}\ ,\ y, r \in R^d,$$

is successively minimized subject to $u \in C_{1D}$ (discretization of C_1). Here the shifting and penalty parameters y, are changed iteratively as in [2], chapt.4.

To treat the minimization problems on C_{1D} we use the method of conditional gradient (e.g. see[20]). For this purpose methods with a higher speed of convergence should be used, as e.g. a method of conjugate gradients modified for the case of simple linear constraints.

Finally an adaptive scheme guarantees that the total algorithm independently changes its parameters (tolerance δ, maximum grid-stepsize $\tilde{h}$, shifting and penalty parameter), depending on the success of the convergence (see [11]).

In the present implementation we use the implicit Euler method in (6) in order to meet the case of stiff ODEs (1), too. For this purpose we use a general concept of Shampine [17]. We did without higher order ODE methods (for the present) because the controls entering into the right hand side of the ODE are discontinuous and hence no higher order than that of the Euler method can be expected in general.

There will be reports on numerical experiences and results on the conference.

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