

SLOVAK UNIVERSITY OF TECHNOLOGY IN BRATISLAVA
FACULTY OF CHEMICAL AND FOOD TECHNOLOGY

**GLOBAL AND DYNAMIC OPTIMIZATION OF
PROCESSES**

DIPLOMA WORK

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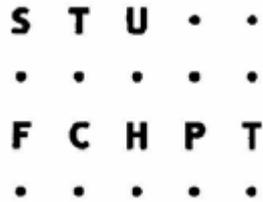
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Čestné prehlásenie

Čestne prehlasujem, že som diplomovú prácu vypracovala samostatne, podľa pokynov vedúceho práce a s použitím zdrojov uvedených v literatúre.

V Bratislave, 20. mája 2010

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Podpis

Abstract

The objective of this work is solving problems of dynamic, global and global dynamic optimization. The first chapter deals with dynamic optimization. It consists of the problem formulation and description of two analytical methods of its solution – the calculus of variations and Pontryagin’s minimum principle. These methods are used to solve the time-optimal control problem of a car with and without constraints on velocity. The second chapter deals with static and dynamic global optimization. One of the spatial branch-and-bound methods, used for solving of nonconvex problems, is described here. Two illustrative examples are solved using these methods which are based on convex relaxation.

Keywords: dynamic optimization, calculus of variations, minimum principle, global optimization, nonconvex optimization problem, convex relaxation

Abstrakt

Cieľom tejto práce je riešenie problémov dynamickej, globálnej a globálnej dynamickej optimalizácie. Prvú časť sa zaoberá dynamickou optimalizáciou. Tvorí ju formulácia optimalizačného problému a opis dvoch analytických metód jeho riešenia – variačného počtu a Pontrjaginovho princípu minima. Ďalej je predstavené použitie týchto metód na riešenie problému časovo optimálneho riadenia auta bez a s obmedzením na rýchlosť. Druhá časť pojednáva o statickej a dynamickej globálnej optimalizácii. Podstatu tejto práce predstavuje opis jednej z priestorových metód vetiev a hraníc, ktorá sa používa na nájdenie riešenia nekonvexných problémov. Za pomoci konvexnej relaxácie, na ktorej sú tejto metódy založené, boli vyriešené dva vzorové príklady.

Kľúčové slová: dynamická optimalizácia, variačný počet, princíp minima, globálna optimalizácia, nekonvexný optimalizačný problém, konvexná relaxácia

Content

Introduction	10
1 Dynamic Optimization	12
1.1 Problem Formulation	12
1.1.1 Mathematical Model	12
1.1.2 Constraints.....	13
1.1.3 Objective Function	14
1.2 Analytical Methods of Dynamic Optimization	15
1.2.1 Calculus of variations.....	15
1.2.2 Pontryagin’s Minimum Principle	20
1.3 Example of a Minimum-Time Problem	22
1.3.1 Time-Optimal Control of a Car.....	23
1.3.2 Time-Optimal Control of a Car with Constraints on Velocity.....	27
2 Global Optimization	32
2.1 Spatial Branch-and-Bound method	32
2.1.1 NLP Problem Formulation	32
2.1.2 The α BB Algorithm	33
2.1.3 Convex Relaxation	33
2.1.4 Calculation of Parameter α	37
2.1.5 Branching Strategies	39
2.2 Example.....	39
3 Global Dynamic Optimization	44
3.1 Dynamic Optimization Problem	44
3.2 Bounding the Solutions of Parameter Dependent ODEs	45
3.3 Formulation of the Convex Relaxation	46
3.4 Bounds on Variables	47
3.5 Convex Relaxation of the Set of Equality Constraints.....	47
3.6 Convex Relaxation of the NLP	49
3.7 Example.....	50
Conclusion	53
Bibliography	55

List of Figures

Fig. 1: Time profile of the control u for the unconstrained problem	26
Fig. 2: Time profile of the traveled distance x_1 for the unconstrained problem.....	26
Fig. 3: Time profile of the velocity x_2 for the unconstrained problem.....	27
Fig. 4: Time profile of the control u for the constrained problem	30
Fig. 5: Time profile of the traveled distance x_1 for the constrained problem.....	30
Fig. 6: Time profile of the velocity x_2 for the constrained problem.....	31
Fig. 7: Objective function $J(x)$ for $x \in [-1, 0]$	40
Fig. 8: Objective function $J(x)$ and the overall underestimator $L(x)$ for $x \in [-1, 0]$	41
Fig. 9: Objective function and its convex underestimators for each iteration	42-43
Fig. 10: Trajectories of the state variable for different values of parameter including parameter independent bounds on the state variable.....	46

Introduction

One of the most basic things in this world is the search for optimality. Even in our everyday life we encounter situations where there are multiple solutions for a problem available and naturally we want to choose the best possible one. The optimal control theory, which plays an important role in designing of modern systems, can for example serve the purpose in maximization of profits from (or minimization of expenses for) the operation of physical, social or economic processes.

Optimization problems are ever-present in the mathematical modeling of real systems. Differential and algebraic equations, which describe the processes, can be optimized using different analytical and numerical methods of dynamic optimization. The most important analytical methods include dynamic programming, Pontryagin's minimum principle and the calculus of variations. Numerical methods can be divided into direct (e.g., sequential and simultaneous methods) and indirect (such as boundary condition iteration and control vector iteration). Each of these methods has its advantages and disadvantages and which one is used depends on the type of the problem being solved.

In a large number of optimization problems, which are currently solved using algorithms of nonlinear programming (NLP), we often encounter nonconvexities in some functions that participate in these problems. These nonconvexities can cause that these problems yield several local extrema. This means that standard optimization methods often provide suboptimal solutions, what led to the development of global optimization.

Methods of global optimization can be basically divided into deterministic (such as generalized Benders decomposition, branch and bound, interval analysis) and stochastic (e.g., multistart, variable neighborhood search and genetic algorithms) methods. This work is focused on deterministic methods, since they guarantee ε -convergence to a global solution. One of the most used and most appropriate methods to solve global optimization problems is the deterministic branch-and-bound method (BB). An extension of the classical BB method is the spatial branch-and-bound method (sBB).

Section 1 of this work deals with dynamic optimization. It starts with the problem formulation and with introducing the notation and nomenclature to be used in other parts of the work. Later, two analytical methods for solving optimization problems

are described. The use of these methods is shown on concrete examples, meaning the problem of time-optimal control of a car with and without constraints on velocity.

Section 2 deals with static and dynamic global optimization. We describe the α BB method, which belongs to the sBB methods and is based on the principle of convex relaxation of the original nonconvex problem. This method's algorithm is then used to solve two illustrative examples. The first one represents static optimization because the optimized variables are time independent and in the second one they depend on time and also parameters, what makes it a dynamic optimization problem.

1 Dynamic Optimization

The goal of dynamic optimization (open-loop optimal control) is to determine a set of profiles of time dependent input (control) variables for dynamic systems that optimize a given objective function (cost functional or optimization criterion) in regard to specified constraints. Best profiles in closed-loop determine the optimal control.

1.1 Problem Formulation

This section deals with important aspects of problem formulation and introduction of the notation and nomenclature to be used in other parts of this work.

The optimal control problem formulation requires:

- Mathematical description (e.g. model) of the process to be controlled
- Definition of constraints
- Determination of the objective function

1.1.1 Mathematical Model

The modeling of the process is very important for any control problem. The objective is to obtain the simplest mathematical model that adequately describes the responses of the physical system to all assumed inputs. The process model is usually formed by a set of equations. These equations combine the inputs, properties and variables that describe the behavior and outputs of the process. This work will deal only with processes described by ordinary differential equations (ODEs)

$$\dot{x}(t) = f(x(t), u(t), t) \quad x(t_0) = x_0 \quad \forall t \in [t_0, t_f], \quad (1.1.1)$$

where

t – represents time as an independent variable

$x(t) = [x_1(t), x_2(t), \dots, x_n(t)]^T$ – represents the n-dimensional vector of state variables

$\dot{x}(t) = [\dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t)]^T$ – represents their derivatives with respect to time

$u(t) = [u_1(t), u_2(t), \dots, u_m(t)]^T$ – represents m-dimensional vector of control variables

$f(t) = [f_1(t), f_2(t), \dots, f_n(t)]^T$ – represents the n-dimensional vector function that describes the process

$x(t_0) = [x_1(t_0), x_2(t_0), \dots, x_n(t_0)]^T$ – represents the initial conditions (conditions in time t_0)

1.1.2 Constraints

Constraints are functions that determine the domain of admissible values of variables participating in the process. There are different types of constraints:

- Equality constraints

Point constraints

$$h(x(t), u(t), t) = 0 \quad (1.1.2)$$

Differential equation constraints

$$h(x(t), \dot{x}(t), u(t), t) = 0 \quad (1.1.3)$$

- Inequality constraints

$$g(x(t), u(t), t) \leq 0 \quad (1.1.4)$$

- Isoperimetric constraints

$$\int_{t_0}^{t_f} e(x(t), \dot{x}(t), u(t), t) dt \leq c \quad (1.1.5)$$

These constraints can be transformed into differential equation constraints by introducing of the new variables

$$z(t) = \int_{t_0}^{t_f} e(x(t), \dot{x}(t), u(t), t) dt \quad (1.1.6)$$

Boundary conditions for these additional variables are $z(t_0) = 0$ and $z(t_f) = c$. Differentiating equation (1.1.5) with respect to time gives

$$\dot{z}(t) = e(x(t), \dot{x}(t), u(t), t), \quad (1.1.7)$$

or,

$$\dot{z}(t) - e(x(t), \dot{x}(t), u(t), t) = 0 \quad (1.1.8)$$

1.1.3 Objective Function

A functional (objective function) J is a rule of correspondence that assigns to each function $x(t)$ in a certain class Ω a unique real number (a unique value). Simply said, a functional is actually a „function of a function“. In general it can be written in one of these three forms:

- Bolza form

$$J(u(t)) = G(x(t_f), t_f) + \int_{t_0}^{t_f} F(x(t), u(t), t) dt \quad (1.1.9)$$

- Lagrange form

$$J(u(t)) = \int_{t_0}^{t_f} F(x(t), u(t), t) dt \quad (1.1.10)$$

- Mayer form

$$J(u(t)) = G(x(t_f), t_f) \quad (1.1.11)$$

where

J – represents the optimization criterion

G – represents the component of the objective function evaluated at final conditions

$\int_{t_0}^{t_f} F dt$ – represents the component of the objective function evaluated over a time interval.

Note that all the three forms of the functional are interchangeable and can be derived one from another.

1.2 Analytical Methods of Dynamic Optimization

There exist a lot of various analytical methods for solving an optimal control problem. From all of the analytical methods these three are the most important:

- Dynamic Programming
- Calculus of Variations
- Pontryagin's Minimum (Maximum) Principle

In this section calculus of variations (Kirk, 1970) and Pontryagin's minimum (Pontryagin et al., 1962) principle will be introduced.

1.2.1 Calculus of variations

In Section 1.1.3 the definition of functional was given. Now in order to consider extreme values of functionals the increment of a functional J will be introduced. In general it can be defined as

$$\Delta J = J(u + \delta u) - J(u) \tag{1.2.1}$$

It can be denoted by $\Delta J(u, \delta u)$ as to emphasize that it depends on the functions u and δu . Function δu is called the variation of the function u . Another way of notation is

$$\Delta J(u, \delta u) = \delta J(u, \delta u) + g(u, \delta u) \cdot \|\delta u\|, \tag{1.2.2}$$

where δJ is the variation of the functional J . It is a part of the increment that is linear in the variation δu . The fundamental theorem of the calculus of variations says that if $u^*(t)$ is an extremal then the necessary condition for the extreme of a functional is

$$\delta J(u^*, \delta u) = 0 \quad \text{for all admissible } \delta u. \quad (1.2.3)$$

The way to derive more concrete conditions will be shown by solving a problem with free final time t_f and free end point x_f .

The objective is to find the necessary conditions that the extreme $u^*(t)$ must satisfy for the functional in Lagrange form

$$J(u(t)) = \int_{t_0}^{t_f} F(x(t), u(t), t) dt ; \quad (1.2.4)$$

t_0 and $x(t_0) = x_0$ are specified, t_f and $x(t_f) = x_f$ are free. Moreover, the conditions given by the differential equation constraints that represent the state equations must also be satisfied

$$0 = f(x(t), u(t), t) - \dot{x}(t). \quad (1.2.5)$$

If we add constraints (1.2.5) into the functional (1.2.4) we can form the augmented functional

$$J_a(u(t)) = \int_{t_0}^{t_f} F(x(t), u(t), t) + \lambda^T(t) [f(x(t), u(t), t) - \dot{x}(t)] dt, \quad (1.2.6)$$

where $\lambda(t) = [\lambda_1(t), \lambda_2(t), \dots, \lambda_n(t)]^T$ is the vector of Lagrange multipliers, also called adjoint variables. It can be clearly seen that if the constraints are satisfied then $J_a = J$ for any $\lambda(t)$. For further simplification we define

$$F_a(x(t), \dot{x}(t), u(t), \lambda(t), t) = F(x(t), u(t), t) + \lambda^T(t) [f(x(t), u(t), t) - \dot{x}(t)] \quad (1.2.7)$$

such that

$$J_a(u(t)) = \int_{t_0}^{t_f} F_a(x(t), \dot{x}(t), u(t), \lambda(t), t) dt. \quad (1.2.8)$$

In order to enable the use of the fundamental theorem we must at first determine the variation by forming the increment

$$\begin{aligned} \Delta J_a = & \left[\frac{\partial F_a}{\partial \dot{x}}(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \right]^T \delta x(t_f) \\ & + \left[F_a(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \right] \delta t_f \\ & + \int_{t_0}^{t_f} \left\{ \left[\frac{\partial F_a}{\partial x}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \right. \\ & - \frac{d}{dt} \left[\frac{\partial F_a}{\partial \dot{x}}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \delta x(t) \\ & + \left[\frac{\partial F_a}{\partial u}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \delta u(t) \\ & \left. + \left[\frac{\partial F_a}{\partial \lambda}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \delta \lambda(t) \right\} dt + o(\cdot), \end{aligned} \quad (1.2.9)$$

where $o(\cdot)$ denotes terms of higher than first order.

Next, we must relate $\delta x(t_f)$ to δt_f and δx_f :

$$\delta x_f = \delta x(t_f) + \dot{x}^*(t_f) \delta t_f, \quad (1.2.10)$$

or

$$\delta x(t_f) = \delta x_f - \dot{x}^*(t_f) \delta t_f. \quad (1.2.11)$$

Substituting this in equation (1.2.9) and collecting the linear terms we obtain the variation

$$\begin{aligned}
\delta J_a(u^*) = 0 = & \left[\frac{\partial F_a}{\partial \dot{x}}(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \right]^T \delta x_f \\
& + \left[F_a(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \right. \\
& \left. - \left[\frac{\partial F_a}{\partial \dot{x}}(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \right]^T \dot{x}^*(t_f) \right] \delta t_f \\
& + \int_{t_0}^{t_f} \left\{ \left[\frac{\partial F_a}{\partial x}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \right. \\
& \left. - \frac{d}{dt} \left[\frac{\partial F_a}{\partial \dot{x}}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \right\} \delta x(t) \\
& + \left[\frac{\partial F_a}{\partial u}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \delta u(t) \\
& + \left[\frac{\partial F_a}{\partial \lambda}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right]^T \delta \lambda(t) \Big\} dt.
\end{aligned} \tag{1.2.12}$$

From the non-integral terms in equation (1.2.12) the conditions (1.2.13) can be formed and the conditions (1.2.14) are formed from the integral terms. Equation (1.2.14a) is also known as the Euler equation.

$$\begin{aligned}
0 &= \frac{\partial F_a}{\partial \dot{x}}(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \\
0 &= \lambda^*(t_f)
\end{aligned} \tag{1.2.13a}$$

$$\begin{aligned}
0 &= F_a(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \\
& - \left[\frac{\partial F_a}{\partial \dot{x}}(x^*(t_f), \dot{x}^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \right]^T \dot{x}^*(t_f) \\
0 &= F(x^*(t_f), u^*(t_f), t_f) + \lambda^{*T}(t_f) [f(x^*(t_f), u^*(t_f), t_f)]
\end{aligned} \tag{1.2.13b}$$

$$0 = \frac{\partial F_a}{\partial x}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) - \frac{d}{dt} \left[\frac{\partial F_a}{\partial \dot{x}}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \right] \quad (1.2.14a)$$

$$\dot{\lambda}^*(t) = -\frac{\partial F}{\partial x}(x^*(t), u^*(t), t) - \left[\frac{\partial f}{\partial x}(x^*(t), u^*(t), t) \right]^T \lambda^*(t)$$

$$0 = \frac{\partial F_a}{\partial u}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \quad (1.2.14b)$$

$$0 = \frac{\partial F}{\partial u}(x^*(t), u^*(t), t) + \left[\frac{\partial f}{\partial u}(x^*(t), u^*(t), t) \right]^T \lambda^*(t)$$

$$0 = \frac{\partial F_a}{\partial \lambda}(x^*(t), \dot{x}^*(t), u^*(t), \lambda^*(t), t) \quad (1.2.14c)$$

$$\dot{x}^*(t) = f(x^*(t), u^*(t), t).$$

In order to simplify the notation the Hamilton function H can be used, it is also called the Hamiltonian and is defined as follows

$$H(x(t), u(t), \lambda(t), t) = F(x(t), u(t), t) + \lambda^T(t) [f(x(t), u(t), t)]. \quad (1.2.15)$$

Now the necessary conditions can be written as

$$0 = \lambda^*(t_f) \quad (1.2.16a)$$

$$0 = H(x^*(t_f), u^*(t_f), \lambda^*(t_f), t_f) \quad (1.2.16b)$$

and

$$\dot{x}^*(t) = \frac{\partial H}{\partial \lambda}(x^*(t), u^*(t), \lambda^*(t), t) \quad (1.2.17a)$$

$$\dot{\lambda}^*(t) = -\frac{\partial H}{\partial x}(x^*(t), u^*(t), \lambda^*(t), t) \quad (1.2.17b)$$

$$0 = \frac{\partial H}{\partial u}(x^*(t), u^*(t), \lambda^*(t), t) \quad (1.2.17c)$$

for all $t \in \langle t_0, t_f \rangle$.

1.2.2 Pontryagin's Minimum Principle

This method is used for searching of the best possible control, so that the dynamic system can change from one state to another while considering the constraints on the control variables.

By definition, the control u^* causes that the functional J has a relative minimum if

$$J(u) - J(u^*) = \Delta J \geq 0 \quad (1.2.18)$$

for all admissible controls sufficiently close to u^* . If $u = u^* + \delta u$, then the increment can be expressed as

$$\Delta J(u^*, \delta u) = \delta J(u^*, \delta u) + o(.) \quad (1.2.19)$$

δJ is linear in δu and the higher-order terms $o(.)$ approach zero as the norm of δu approaches zero. Necessary conditions for the control problem are

$$\delta J(u^*, \delta u) \geq 0 \quad (1.2.20)$$

if u^* lies on the boundary during any portion of the time interval $t \in \langle t_0, t_f \rangle$, and

$$\delta J(u^*, \delta u) = 0 \quad (1.2.21)$$

if u^* lies within the boundary during the entire time interval $t \in \langle t_0, t_f \rangle$.

If we assume that the state equations are satisfied, $\lambda^*(t)$ is selected so that the coefficient of δx in the integral is equal to zero and the boundary conditions for final time are also satisfied, we can write the equation of the increment (1.2.9) as

$$\Delta J(u^*, \delta u) = \int_{t_0}^{t_f} \left[\frac{\partial H}{\partial u}(x^*(t), u^*(t), \lambda^*(t), t) \right]^T \delta u(t) dt + o(.) \quad (1.2.22)$$

The integrand is the first-order approximation to the change in H caused by a change in u , therefore

$$\Delta J(u^*, \delta u) = \int_{t_0}^{t_f} \left[H(x^*(t), u^*(t) + \delta u(t), \lambda^*(t), t) - H(x^*(t), u^*(t), \lambda^*(t), t) \right] dt + o(.) \quad (1.2.23)$$

If $u^*(t) + \delta u(t)$ lies in a sufficiently small neighborhood of u^* ($\|\delta u\| < \beta$) then the higher-order terms $o(\cdot)$ are small. Thus, for u^* to be a minimizing (optimal) control it is necessary that

$$\int_{t_0}^{t_f} [H(x^*(t), u^*(t) + \delta u(t), \lambda^*(t), t) - H(x^*(t), u^*(t), \lambda^*(t), t)] dt \geq 0 \quad (1.2.24)$$

for all admissible δu , such that $\|\delta u\| < \beta$.

In order for equation (1.2.24) to be satisfied for all admissible δu in the specified neighborhood, the following inequality must be satisfied

$$H(x^*(t), u^*(t) + \delta u(t), \lambda^*(t), t) \geq H(x^*(t), u^*(t), \lambda^*(t), t) \quad (1.2.25)$$

for all admissible $\delta u(t)$ and for all $t \in \langle t_0, t_f \rangle$. If that is the case then let us consider the following control

$$\begin{aligned} u(t) &= u^*(t); & t \notin \langle t_1, t_2 \rangle \\ u(t) &= u^*(t) + \delta u(t); & t \in \langle t_1, t_2 \rangle, \end{aligned} \quad (1.2.26)$$

where $\langle t_1, t_2 \rangle$ is an arbitrarily small, but nonzero, time interval and $\delta u(t)$ is a variation of an admissible control that satisfies the condition $\|\delta u\| < \beta$. Let us suppose that inequality (1.2.25) is not satisfied for the control described in equations (1.2.26), then in the interval $\langle t_1, t_2 \rangle$ the inequality changes to

$$H(x^*(t), u(t), \lambda^*(t), t) < H(x^*(t), u^*(t), \lambda^*(t), t) \quad (1.2.27)$$

and, therefore

$$\begin{aligned} & \int_{t_0}^{t_f} [H(x^*(t), u(t), \lambda^*(t), t) - H(x^*(t), u^*(t), \lambda^*(t), t)] dt \\ &= \int_{t_1}^{t_2} [H(x^*(t), u(t), \lambda^*(t), t) - H(x^*(t), u^*(t), \lambda^*(t), t)] dt < 0. \end{aligned} \quad (1.2.28)$$

Since the interval $\langle t_1, t_2 \rangle$ can be anywhere in the interval $\langle t_0, t_f \rangle$, it is clear that if inequality (1.2.27) is satisfied for any $t \in \langle t_0, t_f \rangle$ then it is always possible to form an admissible control as in equation (1.2.26), which makes $\Delta J < 0$, thus contradicting the optimality of the control u^* . Therefore we assume that the necessary condition for u^* to minimize functional J is

$$H(x^*(t), u^*(t), \lambda^*(t), t) \leq H(x^*(t), u(t), \lambda^*(t), t) \quad (1.2.29)$$

for all $t \in \langle t_0, t_f \rangle$ and for all admissible controls. Equation (1.2.29), which implies that an optimal control must minimize the Hamiltonian, is called Pontryagin's minimum principle.

Although the minimum principle was derived for controls with values in a closed and bounded region, it can be applied to problems in which the admissible controls are not bounded. This can be done by viewing the unbounded control region as having arbitrarily large bounds, thus ensuring that the optimal control will not be constrained by the boundaries. In this case, the necessary condition for minimizing the Hamiltonian is that

$$\frac{\partial H}{\partial u}(x^*(t), u^*(t), \lambda^*(t), t) = 0. \quad (1.2.30)$$

If the equality (1.2.30) is satisfied and the matrix

$$\frac{\partial^2 H}{\partial u^2}(x^*(t), u^*(t), \lambda^*(t), t)$$

is positive definite then we can consider condition (1.2.30) to be sufficient.

1.3 Example of a Minimum-Time Problem

In this section the use of the analytical methods will be shown on concrete examples, while searching for a time-optimal control of a car with and without constraints on velocity. These examples can be found in Kirk (1970) and Fikar (2007).

1.3.1 Time-Optimal Control of a Car

The objective is to drive the car from point O to point e in the shortest possible time. To simplify the model, let us approximate the car by a unit point mass described by its position (traveled distance), velocity $x_2(t) = v(t) = \dot{d}(t)$ and acceleration $u(t) = a(t) = \dot{v}(t)$. The process then takes the form of following state equations

$$\dot{x}_1(t) = x_2(t) \quad (1.3.1)$$

$$\dot{x}_2(t) = u(t) \quad (1.3.2)$$

The objective function for minimization of time is

$$J = \int_{t_0}^{t_f} 1 \, dt = t_f \quad (1.3.3)$$

where t_0 is the time of leaving O and we consider it being zero, and t_f is the time of arrival at e .

The car starts from rest and stops upon reaching point e . In this case initial and terminal constraints can be expressed as follows

$$\begin{aligned} x_1(0) &= 0 & x_1(t_f) &= e = 300 \\ x_2(0) &= 0 & x_2(t_f) &= 0 \end{aligned} \quad (1.3.4)$$

Constraints on acceleration (deceleration) are given by inequality $-1 \leq u(t) \leq 2$.

The first step is the composition of the Hamilton function according to the equation (1.2.15)

$$H(x(t), u(t), \lambda(t), t) = 1 + \lambda_1(t)x_2(t) + \lambda_2(t)u(t) \quad (1.3.5)$$

According to the minimum principle, the optimal control $u^*(t)$ must satisfy the condition

$$1 + \lambda_1^*(t_f)x_2^*(t_f) + \lambda_2^*(t_f)u^*(t_f) \leq 1 + \lambda_1^*(t_f)x_2^*(t_f) + \lambda_2^*(t_f)u(t_f) \quad (1.3.6)$$

By differentiating the Hamiltonian with respect to $u(t)$ we get the condition

$$\lambda_2^*(t) = 0 \quad (1.3.7)$$

However, if there exists a time interval where $\lambda_2^*(t) = 0$ then the equation (1.3.6) provides no information on the relation between $u^*(t)$, $x^*(t)$ and $\lambda^*(t)$.

From equation (1.2.17b) we obtain auxiliary differential equations

$$\begin{aligned} \dot{\lambda}_1^*(t) &= 0 \\ \dot{\lambda}_2^*(t) &= -\lambda_1^*(t), \end{aligned} \quad (1.3.8)$$

whose solution can be written as

$$\begin{aligned} \lambda_1^*(t) &= c_1 \\ \lambda_2^*(t) &= -c_1 t + c_2 \end{aligned} \quad (1.3.9)$$

In order to satisfy the condition (1.3.7) the constants of integration c_1 and c_2 must be equal to zero and by substituting these values in the Hamiltonian we obtain

$$H(x^*(t), u^*(t), \lambda^*(t), t) = 1 \quad \forall t \in \langle t_0, t_f \rangle. \quad (1.3.10)$$

But since the final time is free, the equation (1.3.10) violates the necessary condition that

$$H(x^*(t), u^*(t), \lambda^*(t), t) = 0 \quad \forall t \in \langle t_0, t_f \rangle. \quad (1.3.11)$$

We conclude that $\lambda_2^*(t)$ cannot be zero during a finite time interval. Isolated times when $\lambda_2^*(t)$ passes through zero indicate a switching of the control. Thus, the form of the optimal control given by the equation (1.3.6) is

$$u^*(t) = \begin{cases} -1, & \text{for } \lambda_2^*(t) > 0 \\ +2, & \text{for } \lambda_2^*(t) < 0 \end{cases} \quad (1.3.12)$$

Equation (1.3.9) indicates that switching of the control will occur at most once since it is a linear equation. From a physical point of view it is obvious that at the beginning, the

control has the value 2 (the car is accelerating) and then switches to the value -1 (the car is decelerating), because the car starts from rest. An opposite combination would not make sense.

Next, the conditions given by the state equations must be satisfied

$$\begin{aligned}\dot{x}_1^*(t) &= x_2^*(t) \\ \dot{x}_2^*(t) &= u^*(t)\end{aligned}\tag{1.3.13}$$

The general solution of the state equations for $u^*(t) = 2$ and $u^*(t) = -1$ is

$$x_1^*(t) = t^2 + c_3 t + c_4, \quad x_2^*(t) = 2t + c_3, \quad \text{for } t \in \langle 0, t_s \rangle \tag{1.3.14}$$

$$x_1^*(t) = -\frac{1}{2}t^2 + c_3 t + c_4, \quad x_2^*(t) = -t + c_3, \quad \text{for } t \in \langle t_s, t_f \rangle \tag{1.3.15}$$

where c_3 and c_4 are constants of integration and t_s represents the switching time. By solving equations (1.3.14) for the initial conditions we obtain $c_3 = c_4 = 0$ and by solving equations (1.3.15) for the terminal conditions we obtain $c_3 = 0$ and $c_4 = e = 300$. Then the solution of the state equations is

$$x_1^*(t) = t^2, \quad x_2^*(t) = 2t, \quad \text{for } t \in \langle 0, t_s \rangle \tag{1.3.16}$$

$$x_1^*(t) = -\frac{1}{2}t^2 + e, \quad x_2^*(t) = -t, \quad \text{for } t \in \langle t_s, t_f \rangle \tag{1.3.17}$$

At the switching time $x_1^*(t)$ is continuous, therefore

$$t_s^2 = -\frac{1}{2}(t_f - t_s)^2 + e \tag{1.3.18}$$

The final time can be then expressed as a function of the switching time

$$t_f = t_s + \sqrt{2e - 2t_s^2} \tag{1.3.19}$$

We can obtain the minimum final time by differentiating equation (1.3.19) with respect to t_s and consider it being equal to zero. This way we can define the equation for calculation of t_s

$$t_s = \sqrt{\frac{e}{3}} = \sqrt{\frac{300}{3}} = 10 \quad (1.3.20)$$

The time profile of the control u is shown in Fig. 1. We can clearly see that it really switches from acceleration to deceleration after 10 seconds.

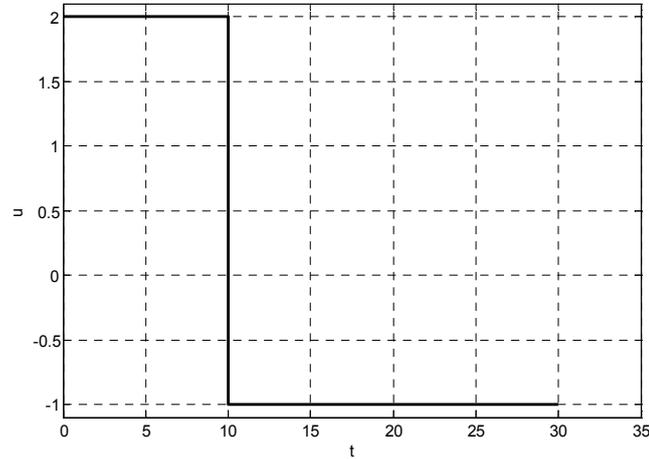


Fig. 1: Time profile of the control u for the unconstrained problem

By substituting the equation (1.3.20) into (1.3.19), we can evaluate t_f

$$t_f = 3\sqrt{\frac{e}{3}} = 3\sqrt{\frac{300}{3}} = 30 \quad (1.3.21)$$

The total time needed can be displayed through the time profile of the traveled distance which is shown in Fig. 2

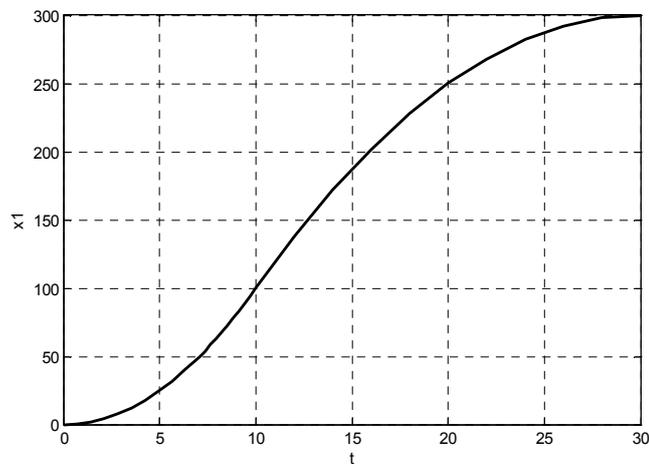


Fig. 2: Time profile of the traveled distance x_l for the unconstrained problem

The maximum achieved velocity is calculated as

$$x_{2,\max}^* = 2t_s = -(t_s - t_f) = 20 \quad (1.3.22)$$

How the velocity changes in time is shown in Fig. 3

Thus, the optimal control is given by the situation where the car is driven with maximum acceleration for the first 100 meters (this represents one third of the total time) and for the next 200 meters with maximum deceleration (which represents the remaining two thirds of the total time).

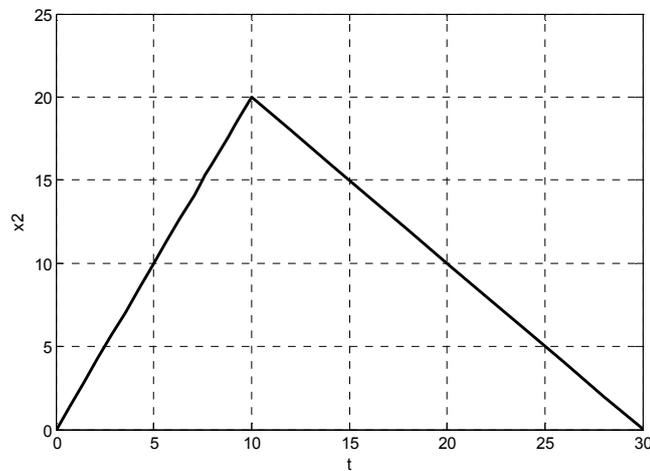


Fig. 3: Time profile of the velocity x_2 for the unconstrained problem

1.3.2 Time-Optimal Control of a Car with Constraints on Velocity

Now, let us consider the same example as before, but furthermore we add in the constraint on velocity, which can be expressed by the condition

$$|x_2(t)| \leq 10 \quad (1.3.23)$$

For this problem we create a new Hamilton function

$$H(x(t), u(t), \lambda(t), \mu(t), t) = 1 + \lambda_1(t)x_2(t) + \lambda_2(t)u(t) + \mu(t)(x_2^2(t) - 10^2), \quad (1.3.24)$$

where μ is another auxiliary variable and based on the Kuhn-Tucker optimality conditions (Kuhn and Tucker, 1951) can be defined as

$$\mu(t) \begin{cases} = 0 & \text{if } x_2^2(t) - 10^2 < 0 \\ \geq 0 & \text{if } x_2^2(t) - 10^2 = 0 \end{cases} \quad (1.3.25)$$

From equation (1.2.17b) we obtain auxiliary differential equations

$$\begin{aligned} \dot{\lambda}_1^*(t) &= 0 \\ \dot{\lambda}_2^*(t) &= -\lambda_1^*(t) + 2\mu^*(t)x_2^*(t) \end{aligned} \quad (1.3.26)$$

In this case, the switching of the control can occur at most twice, which means that there can be two switching times t_{S1} and t_{S2} . The state equations then take this form

$$x_1^*(t) = t^2 + c_3t + c_4, \quad x_2^*(t) = 2t + c_3, \quad \text{for } t \in \langle 0, t_{S1} \rangle \quad (1.3.27)$$

$$x_1^*(t) = c_3t + c_4, \quad x_2^*(t) = c_3, \quad \text{for } t \in \langle t_{S1}, t_{S2} \rangle \quad (1.3.28)$$

$$x_1^*(t) = -\frac{1}{2}t^2 + c_3t + c_4, \quad x_2^*(t) = -t + c_3, \quad \text{for } t \in \langle t_{S2}, t_f \rangle \quad (1.3.29)$$

where on the first interval $u^*(t) = 2$, on the second $u^*(t) = 0$ and on the third $u^*(t) = -1$. The values for the constants of integration c_3 and c_4 can be obtained by solving these equations for the boundary conditions

$$\begin{aligned} c_3 &= 0, & c_4 &= 0, & \text{for } t \in \langle 0, t_{S1} \rangle \\ c_3 &= 2t_{S1}, & c_4 &= t_{S1}^2, & \text{for } t \in \langle t_{S1}, t_{S2} \rangle \\ c_3 &= 0, & c_4 &= e = 300, & \text{for } t \in \langle t_{S2}, t_f \rangle \end{aligned}$$

The solution to the state equations is then

$$x_1^*(t) = t^2, \quad x_2^*(t) = 2t, \quad \text{for } t \in \langle 0, t_{S1} \rangle \quad (1.3.30)$$

$$x_1^*(t) = t_{S1}^2 + 2t_{S1}t, \quad x_2^*(t) = 2t_{S1}, \quad \text{for } t \in \langle t_{S1}, t_{S2} \rangle \quad (1.3.31)$$

$$x_1^*(t) = -\frac{1}{2}t^2 + e, \quad x_2^*(t) = -t, \quad \text{for } t \in \langle t_{S2}, t_f \rangle \quad (1.3.32)$$

The first switching time t_{S1} can be now evaluated directly from the equation (1.3.31) if we assume that in this case $u^*(t) = 0$ and the velocity is on its boundary value given by the constraint (1.3.23)

$$x_2^*(t) = 2t_{S1} = 10, \quad t_{S1} = 5$$

Then again $x_I^*(t)$ is continuous in the switching times. Because we already know the value of t_{S1} , we can calculate the other time t_{S2} by comparing of equations (1.3.31) and (1.3.32)

$$t_{S1}^2 + 2t_{S1}(t_{S2} - t_{S1}) = -\frac{1}{2}(t_f - t_{S2})^2 + e \quad (1.3.33)$$

The final time can be then expressed as a function of the switching time t_{S2} from equation (1.3.33)

$$t_f = t_{S2} + \sqrt{2e - 4t_{S1}t_{S2} + 2t_{S1}^2} \quad (1.3.34)$$

The minimum final time t_f can be obtained by differentiating equation (1.3.34) with respect to t_{S2} and consider it being equal with zero. This way we can define the equation from which t_{S2} is going to be calculated

$$t_{S2} = \frac{e - t_{S1}^2}{2t_{S1}} = \frac{300 - 25}{10} = 27,5 \quad (1.3.35)$$

The time profile of the control u is shown in Fig. 4. Now we can see that the acceleration stops after 5 seconds and the deceleration starts after 27,5 seconds.

By substituting the equation (1.3.35) and the value of t_{S1} into (1.3.34), we can evaluate t_f

$$t_f = \frac{e - t_{S1}^2}{2t_{S1}} + 2t_{S1} = \frac{300 - 25}{10} + 10 = 37,5 \quad (1.3.36)$$

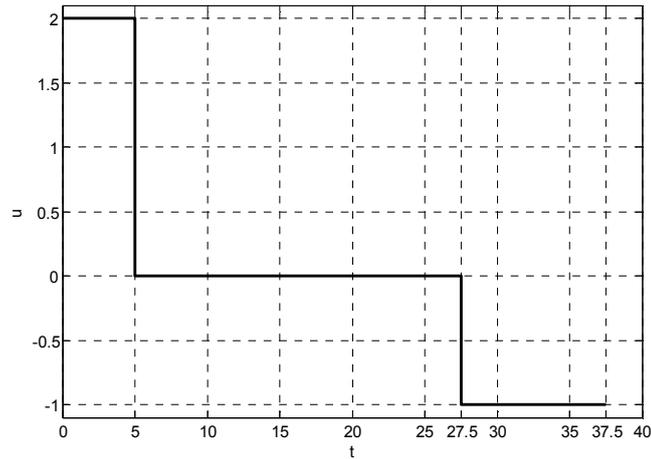


Fig. 4: Time profile of the control u for the constrained problem

The total time needed can be again displayed through the time profile of the traveled distance which is shown in Fig. 5

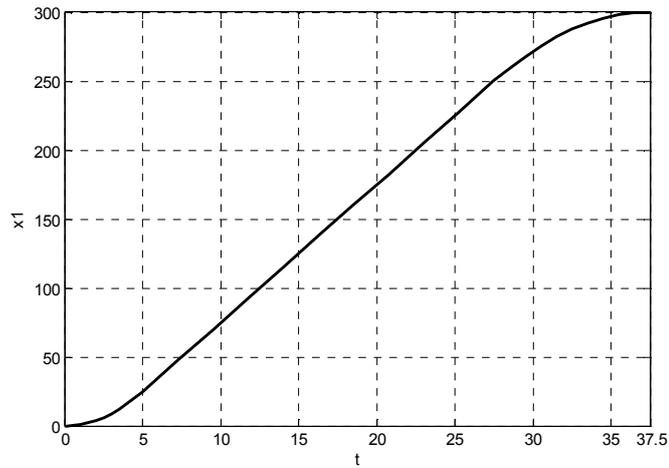


Fig. 5: Time profile of the traveled distance x_1 for the constrained problem

The maximum velocity which can be achieved is clearly the velocity on the boundary (shown in Fig. 6)

$$x_{2,\max}^* = 2t_{S1} = -(t_{S2} - t_f) = 10 \quad (1.3.37)$$

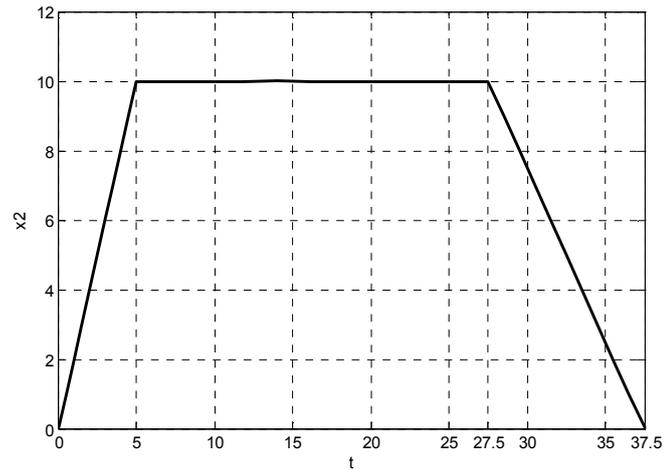


Fig. 6: Time profile of the velocity x_2 for the constrained problem

The optimal control for this example is given by the situation where the car is driven with maximum acceleration for the first 25 meters, then the next 225 meters it is moving with constant speed (the car is neither accelerating nor decelerating) and the last 50 meters it is maximally decelerating. The final time is naturally longer than the one obtained in the first example seeing that the maximum achieved velocity is reduced by a half.

2 Global Optimization

Global optimization methods were developed in order to solve nonconvex optimization problems, i.e. problems which have several local extrema. It is clear that standard optimization methods can not be used to solve nonconvex problems because they would often lead only to suboptimal results.

In this Section the deterministic Spatial Branch-and-Bound method (sBB) will be introduced. Specifically, the α BB method (Adjiman et al., 1998), which belongs to the sBB methods, will be described.

2.1 Spatial Branch-and-Bound method

This method is called “spatial” because it gradually divides the Euclidean space where the problem is defined into smaller and smaller regions and then solved recursively by generating converging sequences of upper and lower bounds of the value of the objective function.

2.1.1 NLP Problem Formulation

The NLP problem is given by the formulation:

$$\min_x J(x) \tag{2.1.1a}$$

$$h(x) = 0 \tag{2.1.1b}$$

$$g(x) \leq 0 \tag{2.1.1c}$$

where $x \in C \subseteq R^n$ is a vector of optimized parameters of size n . Function $J(x)$ represents the optimization criterion, $h(x)$ is a set of equality constraints and $g(x)$ represents a set of inequality constraints. These functions belong to C^2 , the set of continuously twice-differentiable functions.

2.1.2 The α BB Algorithm

The α BB algorithm is designed to solve nonconvex minimization problems of the type (2.1.1). Its theoretical properties guarantee the finding of the global optimum of such a problem with finite ε -convergence.

The branch and bound algorithm starts with the relaxation of the original nonconvex problem, whereby we acquire a new convex problem. By solving the relaxed problem we obtain the lower bound of the solution of the problem given which is in some way easier than solving the original problem. The relaxed problem is actually a convex optimization problem whose objective function underestimates the nonconvex objective function on a certain interval. Because each local minimum of such a problem is at the same time a global minimum, standard NLP algorithms designed to search for local extrema are able to find this lower bound reliably. The upper bound is obtained as a local solution of the original nonconvex problem on a given interval.

If these bounds are not within some ε tolerance then the interval is divided using one of the branching strategies. This way we obtain two new subproblems. For each one of them the relaxation is constructed again and new upper and lower bounds are computed. If some lower bound is greater than current best upper bound on any subinterval then global optimum cannot exist on this interval, hence this interval is excluded from further calculations. Such an operation is called *fathoming*.

This whole process of branching and bounding is repeated until the lower bound on all active intervals is within the ε tolerance of the current best upper bound.

2.1.3 Convex Relaxation

As mentioned before, BB algorithms are based on the principle of convex relaxation. A determining step is the decomposition of the objective function into a sum of nonconvex terms of special type (STNT) and nonconvex terms of arbitrary type (ATNT). Based on this classification of the terms, the objective function $J(x)$ can be written as:

$$J(x) = STNT(x) + ATNT(x) \quad (2.1.2a)$$

s.t.

$$\begin{aligned}
STNT(x) = & LT(x) + CT(x) + \sum_{i=1}^{n_{BT}} b_i x_{BTi,1} x_{BTi,2} + \sum_{i=1}^{n_{TT}} t_i x_{TTi,1} x_{TTi,2} x_{TTi,3} \\
& + \sum_{i=1}^{n_{FT}} f_i \frac{x_{FTi,1}}{x_{FTi,2}} + \sum_{i=1}^{n_{FTT}} ft_i \frac{x_{FTTi,1} x_{FTTi,2}}{x_{FTTi,3}} + \sum_{i=1}^{n_{UT}} UT_i(x_{UTi})
\end{aligned} \tag{2.1.2b}$$

$$ATNT(x) = \sum_{i=1}^{n_{NT}} NT_i(x) \tag{2.1.2c}$$

where $LT(x)$ represents a linear term; $CT(x)$ represents a convex term; n_{BT} stands for the number of bilinear terms, $x_{BTi,1}$ and $x_{BTi,2}$ denote the two variables that participate in the i -th bilinear term and b_i is its coefficient; n_{TT} stands for the number of trilinear terms, $x_{TTi,1}$, $x_{TTi,2}$ and $x_{TTi,3}$ denote the three variables that participate in the i -th trilinear term and t_i is its coefficient; n_{FT} stands for the number of fractional terms, $x_{FTi,1}$ and $x_{FTi,2}$ denote the two variables that participate in the i -th fractional term and f_i is its coefficient; n_{FTT} stands for the number of fractional trilinear terms, $x_{FTTi,1}$, $x_{FTTi,2}$ and $x_{FTTi,3}$ denote the three variables that participate in the i -th fractional trilinear term and ft_i is its coefficient; n_{UT} stands for the number of univariate concave terms, $UT_i(x_{UTi})$ represents the i -th univariate concave term and x_{UTi} denotes the variable that participates in it; n_{NT} stands for the number of nonconvex terms of arbitrary type, $NT_i(x)$ represents the i -th nonconvex term of arbitrary type.

Convex underestimators are constructed for these terms, with the exception of linear and convex terms which do not need to be convexified.

Underestimation of Bilinear Terms

In case of a bilinear term xy , the convex lower bound over the domain $[x^L, x^U] \times [y^L, y^U]$ can be obtained by introducing of a new variable w_{BT} which replaces every occurrence of xy in the problem and by adding following four linear inequality constraints:

$$w_{BT} \geq x^L y + xy^L - x^L y^L \tag{2.1.3a}$$

$$w_{BT} \geq x^U y + xy^U - x^U y^U \tag{2.1.3b}$$

$$w_{BT} \leq x^L y + xy^U - x^L y^U \tag{2.1.3c}$$

$$w_{BT} \leq x^U y + xy^L - x^U y^L \tag{2.1.3d}$$

where x^L is the lower bound and x^U is the upper bound of the variable x . The same goes for variable y .

Underestimation of Trilinear Terms

The trilinear term of the form xyz can be underestimated over the domain $[x^L, x^U] \times [y^L, y^U] \times [z^L, z^U]$ by introducing of a new variable w_{TT} and by adding following eight linear inequality constraints:

$$w_{TT} \geq xy^Lz^L + x^Ly^Lz^L - 2x^Ly^Lz^L \quad (2.1.4a)$$

$$w_{TT} \geq xy^Uz^U + x^Uy^Uz^U - x^Uy^Uz^U \quad (2.1.4b)$$

$$w_{TT} \geq xy^Lz^L + x^Ly^Lz^U - x^Ly^Lz^L - x^Ly^Lz^U \quad (2.1.4c)$$

$$w_{TT} \geq xy^Uz^L + x^Uy^Uz^L - x^Uy^Uz^L - x^Uy^Uz^U \quad (2.1.4d)$$

$$w_{TT} \geq xy^Lz^U + x^Ly^Lz^U - x^Ly^Lz^L - x^Ly^Lz^U \quad (2.1.4e)$$

$$w_{TT} \geq xy^Lz^U + x^Ly^Lz^U - x^Ly^Lz^L - x^Ly^Lz^U \quad (2.1.4f)$$

$$w_{TT} \geq xy^Uz^L + x^Uy^Uz^L - x^Uy^Uz^L - x^Uy^Uz^U \quad (2.1.4g)$$

$$w_{TT} \geq xy^Uz^U + x^Uy^Uz^U - 2x^Uy^Uz^U \quad (2.1.4h)$$

Underestimation of Fractional Terms

For fractional terms x/y one new variable w_{FT} is introduced and two inequality constraints which depend on the sign of the bounds on the variable x are added:

$$w_{FT} \geq \begin{cases} \frac{x^L}{y} + \frac{x}{y^U} - \frac{x^L}{y^U} & \text{if } x^L \geq 0 \\ \frac{x}{y^U} - \frac{x^L y}{y^L y^U} + \frac{x^L}{y^L} & \text{if } x^L < 0 \end{cases} \quad (2.1.5a)$$

$$w_{FT} \geq \begin{cases} \frac{x^U}{y} + \frac{x}{y^L} - \frac{x^U}{y^L} & \text{if } x^U \geq 0 \\ \frac{x}{y^L} - \frac{x^U y}{y^L y^U} + \frac{x^U}{y^U} & \text{if } x^U < 0 \end{cases} \quad (2.1.5b)$$

Underestimation of Fractional Trilinear Terms

Fractional trilinear terms of the form xy/z are underestimated by introducing one new variable w_{FTT} and inequality constraints for $x^L, y^L, z^L \geq 0$:

$$w_{FTT} \geq \frac{xy^L}{z^U} + \frac{x^L y}{z^U} + \frac{x^L y^L}{z} - 2 \frac{x^L y^L}{z^U} \quad (2.1.6a)$$

$$w_{FTT} \geq \frac{xy^L}{z^U} + \frac{x^L y}{z^L} + \frac{x^L y^U}{z} - \frac{x^L y^U}{z^L} - \frac{x^L y^L}{z^U} \quad (2.1.6b)$$

$$w_{FTT} \geq \frac{xy^U}{z^L} + \frac{x^U y}{z^U} + \frac{x^U y^L}{z} - \frac{x^U y^L}{z^U} - \frac{x^U y^U}{z^L} \quad (2.1.6c)$$

$$w_{FTT} \geq \frac{xy^U}{z^U} + \frac{x^U y}{z^L} + \frac{x^L y^U}{z} - \frac{x^L y^U}{z^U} - \frac{x^U y^U}{z^L} \quad (2.1.6d)$$

$$w_{FTT} \geq \frac{xy^L}{z^U} + \frac{x^L y}{z^L} + \frac{x^U y^L}{z} - \frac{x^U y^L}{z^L} - \frac{x^L y^L}{z^U} \quad (2.1.6e)$$

$$w_{FTT} \geq \frac{xy^U}{z^U} + \frac{x^U y}{z^L} + \frac{x^L y}{z} - \frac{x^L y^U}{z^U} - \frac{x^U y^U}{z^L} \quad (2.1.6f)$$

$$w_{FTT} \geq \frac{xy^L}{z^U} + \frac{x^L y}{z^L} + \frac{x^U y^L}{z} - \frac{x^U y^L}{z^L} - \frac{x^L y^L}{z^U} \quad (2.1.6g)$$

$$w_{FTT} \geq \frac{xy^U}{z^L} + \frac{x^U y}{z^L} + \frac{x^U y^U}{z} - 2 \frac{x^U y^U}{z^L} \quad (2.1.6h)$$

Underestimation of Univariate Concave Terms

Univariate concave terms are usually underestimated by their linearization at the lower bound of the variable. This way no new variables or constraints are needed. The underestimator of the concave function $UT(x)$ over $[x^L, x^U]$ then takes the form of a linear function of the variable x

$$UT(x^L) + \frac{UT(x^U) - UT(x^L)}{x^U - x^L} (x - x^L) \quad (2.1.7)$$

Underestimation of Arbitrary Type of Nonconvex Terms

The nonconvex terms of arbitrary type are underestimated over the whole domain $[x^L, x^U]$ by the function $L_\alpha(x)$ which is defined as

$$L_\alpha(x) = J(x) + \sum_{j=1}^{n_{NT}} \alpha_j (x_j^U - x_j)(x_j^L - x_j) \quad (2.1.8)$$

where $\alpha_j \geq 0$ corresponds to the terms $j= 1, \dots, n_{NT}$. All nonconvexities in the original function $J(x)$ can be overpowered by the convex quadratic term, given sufficiently large values of the α_j parameters. Since the sum in equation (2.1.8) is negative over the whole domain $[x^L, x^U]$, $L_\alpha(x)$ is a valid underestimator of the function $J(x)$.

Overall Convex Underestimator

Given the decomposition of the objective function $J(x)$ in the equation (2.1.2) and the underestimation of individual terms, then the final underestimator $L(x)$ to the function $J(x)$ can be written as

$$\begin{aligned} L(x) = & LT(x) + CT(x) + \sum_{i=1}^{n_{BT}} b_i w_{BTi} + \sum_{i=1}^{n_{TT}} t_i w_{TTi} + \sum_{i=1}^{n_{FT}} f_i w_{FTi} + \sum_{i=1}^{n_{FTT}} ft_i w_{FTTi} \\ & + \sum_{i=1}^{n_{UT}} \left[UT_i(x_{UTi}^L) + \frac{UT_i(x_{UTi}^U) - UT_i(x_{UTi}^L)}{x_{UTi}^U - x_{UTi}^L} (x_i - x_{UTi}^L) \right] \\ & + \sum_{i=1}^{n_{NT}} \left[NT_i(x) + \sum_{j=1}^n \alpha_{ij} (x_j^U - x_j)(x_j^L - x_j) \right] \end{aligned} \quad (2.1.9)$$

where α_{ij} corresponds to the i -th nonconvex terms of arbitrary type and the j -th variable and variables w_{BTi} , w_{TTi} , w_{FTi} , w_{FTTi} must satisfy their respective constraints.

2.1.4 Calculation of Parameter α

Since $L(x)$ in equation (2.1.9) is a convex function, its Hessian matrix $H_L(x)$ is positive semi-definite. Moreover, matrix $H_L(x)$ is related to the Hessian matrix $H_J(x)$ of the function $J(x)$ by:

$$H_L(x) = H_J(x) + 2\Delta \quad (2.1.10)$$

where Δ is a diagonal shift matrix whose diagonal elements are the parameters α_i . In order to derive a valid convex underestimator, the set of α parameters must satisfy the following theorem:

Theorem: The function $L(x)$ given by the equation (2.1.9) is convex if $H_L(x) = H_J(x) + 2\Delta = H_J(x) + 2\text{diag}(\alpha_i)$ is a positive semi-definite for all $x \in [x^L, x^U]$.

To identify a valid diagonal shift matrix, the underestimator is re-formulated using a single α value:

$$L(x, \alpha) = J(x) + \alpha \sum_{j=1}^n (x_j^U - x_j)(x_j^L - x_j) \quad (2.1.11)$$

All non-zero elements of Δ are then equal to the parameter α . It can be shown that $L(x)$ is a valid convex underestimator of the objective function $J(x)$ if:

$$\alpha \geq \max\left(0, -\frac{1}{2} \min_{i, x^L \leq x \leq x^U} \lambda_i(x)\right) \quad (2.1.12)$$

where λ_i are the eigenvalues of matrix $H_J(x)$.

If $J(x)$ is convex then all eigenvalues of matrix $H_J(x)$ are non-negative for any $x \in [x^L, x^U]$. Then according to equation (2.1.12) $\alpha = 0$ and the original function does not change. On the other hand: the more nonconvex the function $J(x)$, the smaller its minimum eigenvalue and the larger the parameter α .

If we consider an interval Hessian matrix $[H_J] \subseteq \{ H_J(x), x \in [x^L, x^U] \}$ then a sufficient condition for convexity is given as:

$$\alpha \geq \max\left(0, -\frac{1}{2} \lambda_{\min}([H_J])\right) \quad (2.1.13)$$

where $\lambda_{\min}([H_J])$ is the minimum eigenvalue of the interval matrix family $[H_J]$.

2.1.5 Branching Strategies

The process of branching in BB algorithms has a significant effect on the rate of convergence, especially in α BB algorithms since the quality of the underestimator depends on the variable bounds. For example, if a variable participates only in linear terms of the problem, branching on it will not have any effect on the accuracy of the convex underestimators. While considering this and also other observations, to implement the α BB algorithm we can choose one of four branching strategies that are currently available:

1. Strategy: Use a k -section on all or some of the variables.
2. Strategy: Use measure of the quality of each term's underestimator, based on the maximum separation distance between term and underestimator.
3. Strategy: Use a measure of the quality of each term's underestimator, based on the separation distance at the optimum point.
4. Strategy: Use a measure of the overall influence of each variable on the quality of the lower bounding problem.

2.2 Example

Let us illustrate the α BB algorithm by solving the nonconvex optimization problem (2.2.1) with a global minimum $x = -1.0009$ and two local minima $x = [-0.7325, -1.0009]$

$$\min_x J(x) = \cos(14.5x - 0.3) + x^2 + 0.2x \quad (2.2.1)$$

such that

$$-1 \leq x \leq 0.$$

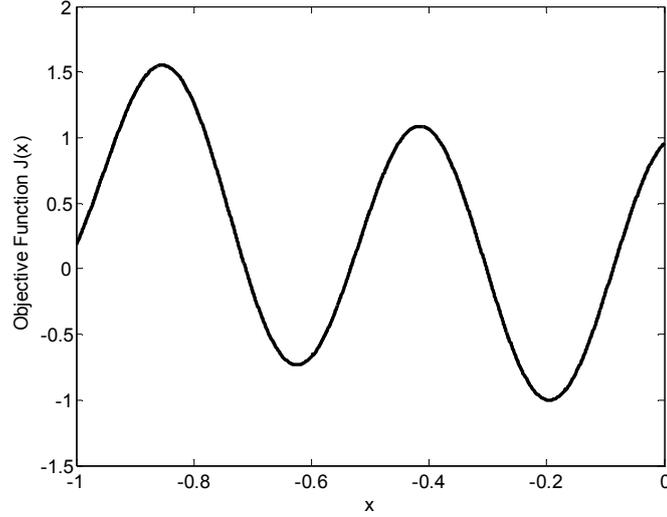


Fig. 7: Objective function $J(x)$ for $x \in [-1, 0]$

The first step is the decomposition of the objective function and the classification of individual terms:

$\cos(14.5x - 0.3)$	- nonconvex term of arbitrary type (ATNT)
x^2	- convex term (CT)
$0.2x$	- linear term (LT)

It is apparent that only the first term of the objective function needs to be underestimated, the others remain unchanged. The underestimator of the nonconvex term is formed based on the equation (2.1.8):

$$\begin{aligned}
 L_{\alpha}(x) &= ATNT(x) + \alpha(x^U - x)(x^L - x) \\
 &= \cos(14.5x - 0.3) + \alpha(x^U - x)(x^L - x) \\
 &= \cos(14.5x - 0.3) + \alpha(0 - x)(-1 - x) \\
 &= \cos(14.5x - 0.3) + \alpha(x + x^2)
 \end{aligned} \tag{2.2.2}$$

Then the overall underestimator from equation (2.1.9) can be written as:

$$\begin{aligned}
 L(x) &= L_{\alpha}(x) + CT(x) + LT(x) \\
 &= \cos(14.5x - 0.3) + \alpha(x^U - x)(x^L - x) + x^2 + 0.2x \\
 &= \cos(14.5x - 0.3) + \alpha(x + x^2) + x^2 + 0.2x
 \end{aligned} \tag{2.2.3}$$

In order to calculate the parameter α , we need to know the Hessian $H_J(x)$ of $J(x)$:

$$\begin{aligned} H_J(x) = J''(x) &= -14.5 * 14.5 \cos(14.5x - 0.3) + 2 \\ &= -210.25 \cos(14.5x - 0.3) + 2 \end{aligned} \quad (2.2.4)$$

The value of the parameter α for the interval $x \in \langle -1, 0 \rangle$ can be now easily computed using the equation (2.1.13):

$$\begin{aligned} \alpha &\geq \max\left(0, -\frac{1}{2} \lambda_{\min}([H_J])\right) \\ \alpha &\geq \max\left(0; -\frac{1}{2}(-208.25)\right) = \max(0; 104.125) \\ \alpha &\geq 104.125 \end{aligned} \quad (2.2.5)$$

After substituting it into (2.2.3) we obtain the final equation for the overall underestimator of the function $J(x)$ for $x \in [-1, 0]$ (shown in Fig. 8):

$$L(x) = \cos(14.5x - 0.3) + 104.125(x + x^2) + x^2 + 0.2x \quad (2.2.6)$$

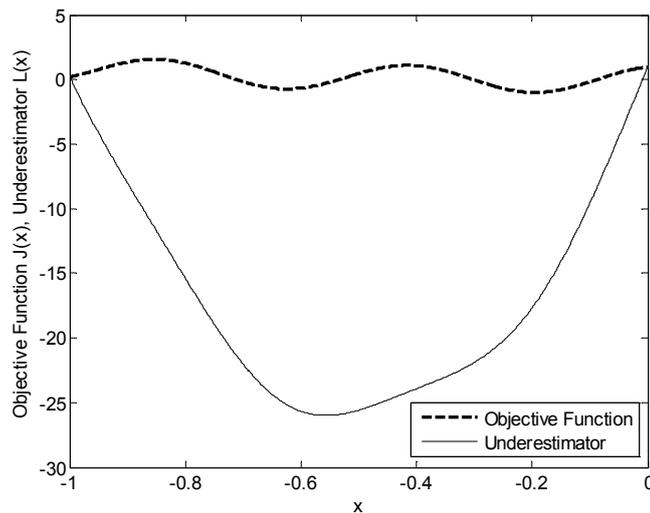


Fig. 8: Objective function $J(x)$ and the overall underestimator $L(x)$ for $x \in [-1, 0]$

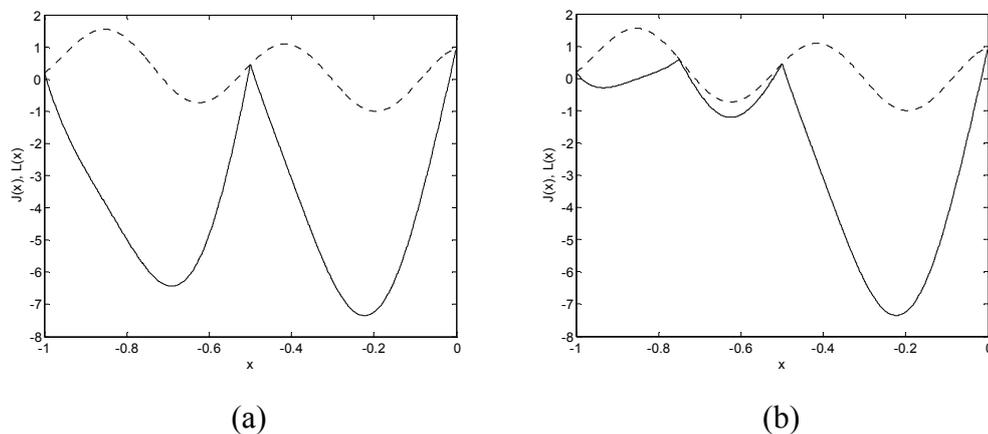
The next step is to determine the lower and upper bound on the solution of the problem. The lower bound is given by the minimum of the function $L(x)$ and the upper bound by the minimum of $J(x)$:

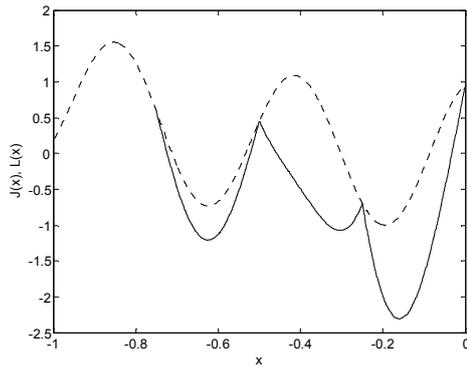
$$\min(L) = -25.9932$$

$$\min(J) = -1.0009$$

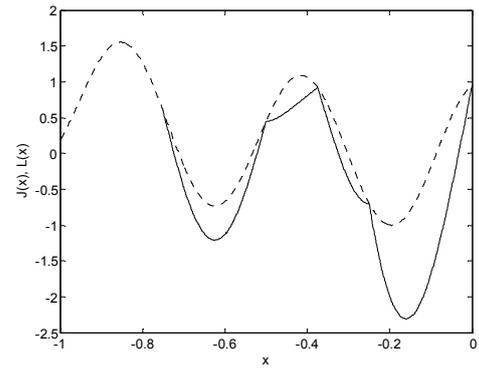
With this we already found one of the local extrema, but evidently, there is a considerable distance between the bounds. In order to find the solution with the tolerance $\varepsilon = 0.001$, the original problem must be divided into two smaller problems and these will be solved the same way as the original. For branching on the intervals the first branching strategy is used. Specifically, the method used will be a bisection (the interval will be cut in halves). We continue this way until we obtain the solution with the required tolerance ε .

The global optimum has been identified in six iterations. The objective function and its underestimators for each iteration are plotted in Fig. 9.

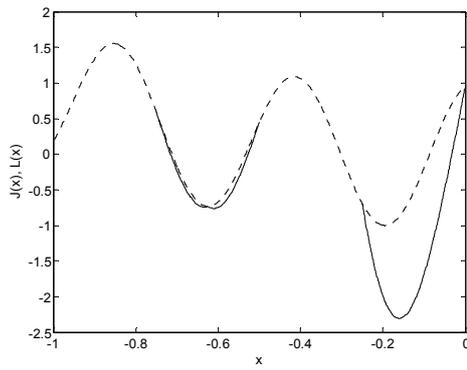




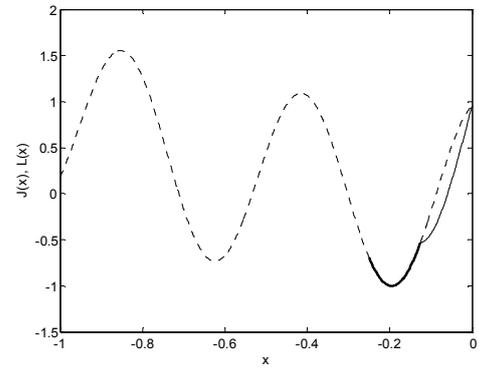
(c)



(d)



(e)



(f)

Fig. 9: Objective function and its convex underestimators for each iteration

3 Global Dynamic Optimization

In the previous Section static global optimization was introduced where the optimized variables were time independent. Now, let us show how the process of convex relaxation and bounding of variables change if we consider the optimized variables to be time and parameter dependent (Paramichail and Adjiman, 2002; Paramichail and Adjiman, 2004).

3.1 Dynamic Optimization Problem

The formulation of the dynamic optimization problem studied is given by:

$$\begin{aligned}
 & \min_p J(x(t_i, p), p) \quad ; \quad i = 0, 1, \dots, NP \\
 \text{s.t.} & \\
 & \dot{x} = f(t, x, p) \quad \forall t \in [t_0, t_{NP}] \\
 & x(t_0, p) = x_0(p) \\
 & g_i(x(t_i, p), p) \leq 0, \quad i = 0, 1, \dots, NP \\
 & p^L \leq p \leq p^U
 \end{aligned} \tag{3.1.1}$$

where J is the objective function, t represents time as the independent variable, t_0 and t_{NP} are the initial and final time, NP is the number of points considered additionally to the initial point, x and \dot{x} are state variables and their time derivatives, p are time-invariant parameters, p^L and p^U are bounds on the parameters, x_0 denote the initial conditions and g_i represent inequality constraints.

The sequential approach is used for the solution of this NLP problem and provides an upper bound for the global optimum solution. Given values for the parameters p , the system can be integrated from t_0 to t_{NP} . After reaching t_{NP} , the objective function and the constraints can be evaluated. The evaluation of their gradients requires the solution of the sensitivity equations, which are derived by differentiating the differential equations with respect to the parameters p :

$$\dot{x}_p(t, p) = \frac{\partial f}{\partial x} x_p(t, p) + \frac{\partial f}{\partial p} \quad \forall t \in [t_0, t_{NP}] \tag{3.1.2}$$

where

$$x_p(t, p) = \frac{\partial x}{\partial p} \quad (3.1.3)$$

and

$$\dot{x}_p(t, p) = \frac{\partial}{\partial t} \left(\frac{\partial x}{\partial p} \right). \quad (3.1.4)$$

The initial condition for the sensitivity equations is found by differentiating the initial condition of the original system with respect to the parameters p :

$$x_p(t_0, p) = \frac{\partial x_0}{\partial p}. \quad (3.1.5)$$

3.2 Bounding the Solutions of Parameter Dependent ODEs

The dependence of convex relaxations on variable bounds is a common feature of deterministic global optimization algorithms. Since the state variables appear in the nonconvex objective function and constraints, a method for the derivation of rigorous bounds on these variables at point t_i ($i = 0, 1, \dots, NP$) is needed. This issue can be resolved by generating bounds on the solution space of the dynamic system. The following ODE is studied:

$$\dot{x}(t) = f(t, x(t), p) \quad \forall t \in [t_0, t_{NP}] \quad (3.2.1)$$

$$x(t_0) = x_0(p) \quad (3.2.2)$$

where $x(t)$ and $\dot{x}(t) \in R^n$, f is a function of parameters $p \in [p^L, p^U]$, and can be considered as a set of functions. The same is true for the initial value x_0 which is usually a function of p and is considered as a set. The lower bounds (subfunctions) $\underline{x}(t)$ and upper bounds (superfunctions) $\bar{x}(t)$, such that $\underline{x}(t) \leq x(t, p) \leq \bar{x}(t)$, $\forall p \in [p^L, p^U]$, $\forall t \in I$, must be determined for the solution of this ODE, $x(t)$. If f is continuous and satisfies a uniqueness condition on $I_0 \times R^n \times [p^L, p^U]$ then $\underline{x}(t)$ and $\bar{x}(t)$ are given as the solution of the following ODE system

$$\begin{aligned}
\dot{\underline{x}}_k(t) &= \inf_{p \in [p^L, p^U]} f_k \left(t, \underline{x}_k(t), [\underline{x}_{k-1}(t), \bar{x}_{k-1}(t)] \right) \\
\dot{\bar{x}}_k(t) &= \sup_{p \in [p^L, p^U]} f_k \left(t, \bar{x}_k(t), [\underline{x}_{k-1}(t), \bar{x}_{k-1}(t)] \right) \\
\forall t \in I_0 \quad \text{and} \quad k &= 1, 2, \dots, n
\end{aligned} \tag{3.2.3}$$

$$\begin{aligned}
\underline{x}(t_0) &= \inf_{p \in [p^L, p^U]} x_0(p) \\
\bar{x}(t_0) &= \sup_{p \in [p^L, p^U]} x_0(p)
\end{aligned} \tag{3.2.4}$$

The system described by (3.2.3) and (3.2.4) provides a practical procedure to construct bounding trajectories for any ODE system which satisfies the appropriate continuity and uniqueness conditions.

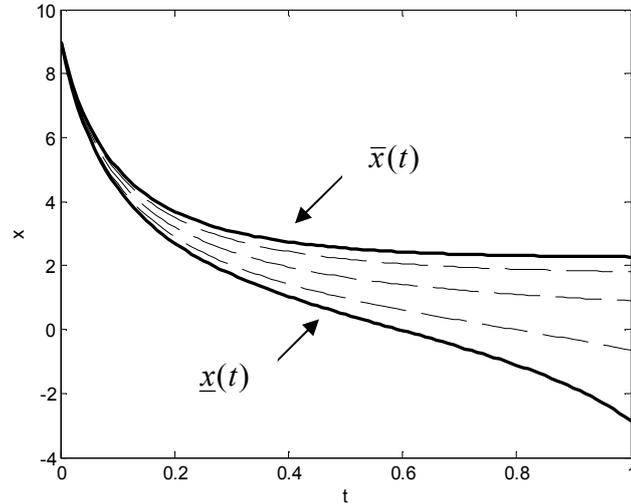


Fig. 1: Trajectories of the state variable for different values of parameter including parameter independent bounds on the state variable

3.3 Formulation of the Convex Relaxation

The dynamic optimization problem (3.1.1) has been formulated as a nonconvex NLP problem. The solution obtained provides an upper bound for the global optimum solution. A convex relaxation is now formulated based on the theory introduced in Section 2.1. Its solution can be used as a lower bound for the global optimum of the nonconvex problem. A reformulation of the NLP problem is given by

$$\begin{aligned}
& \min_{\hat{x}, p} J(\hat{x}, p) \\
\text{s.t.} \quad & g_i(\hat{x}_i, p) \leq 0, \quad i = 0, 1, \dots, NP \\
& \hat{x}_i = x(t_i, p), \quad i = 0, 1, \dots, NP \\
& p \in [p^L, p^U]
\end{aligned} \tag{3.3.1}$$

where \hat{x} is a vector of new added optimized variables and the values of $x(t_i, p)$, $i = 0, 1, \dots, NP$ are obtained by solving the ODE system:

$$\dot{x}(t, p) = f(t, x(t, p), p) \quad \forall t \in [t_0, t_{NP}] \tag{3.3.2}$$

$$x(t_0, p) = x_0(p) \tag{3.3.3}$$

3.4 Bounds on Variables

The bounds on \hat{x}_i depend on the parameters bounds and must be derived automatically. As discussed in Section 3.2, bounds can be constructed for the solutions of ODE system (3.3.2) and (3.3.3). These bounds are for $t = t_i$ also valid for the variable vectors \hat{x}_i that have been introduced in the reformulated NLP problem:

$$\underline{x}(t_i) \leq \hat{x}_i \leq \bar{x}(t_i), \quad i = 0, 1, \dots, NP \tag{3.4.1}$$

3.5 Convex Relaxation of the Set of Equality Constraints

The set of equalities $\hat{x}_i = x(t_i, p)$ can be written as two sets of inequalities:

$$\hat{x}_i - x(t_i, p) \leq 0, \quad i = 0, 1, \dots, NP \tag{3.5.1}$$

$$x(t_i, p) - \hat{x}_i \leq 0, \quad i = 0, 1, \dots, NP \tag{3.5.2}$$

Their relaxation is given by:

$$\hat{x}_i + \tilde{x}^-(t_i, p) \leq 0, \quad i = 0, 1, \dots, NP \tag{3.5.3}$$

$$\tilde{x}(t_i, p) - \hat{x}_i \leq 0, \quad i = 0, 1, \dots, NP \tag{3.5.4}$$

where \tilde{x} denotes the convex underestimator of the specified function and $x^-(t_i, p) = -x(t_i, p)$. The function $\tilde{x}(t_i, p)$ is a convex underestimator of $x(t_i, p)$ and the function $-\tilde{x}^-(t_i, p)$ is a concave overestimator of $x(t_i, p)$.

The constant bounds given by inequalities (3.4.1) are valid convex underestimators and concave overestimators for $x(t_i, p)$. This means that inequalities (3.5.3) and (3.5.4) can be replaced by inequalities (3.4.1). These bounds do not depend on the parameters p themselves, but do depend on the bounds on p .

Since $x(t_i, p)$ is a twice continuously differentiable function of the parameters p on R^r , the α -based bounds can also be used for the convex underestimation of $x(t_i, p)$ and $x^-(t_i, p)$ over the domain $[p^L, p^U] \subset R^r$:

$$\begin{aligned} \tilde{x}_k(t_i, p) &= x_k(t_i, p) + \sum_{j=1}^r \alpha_{kij}^+ (p_j^L - p_j)(p_j^U - p_j), \\ i &= 0, 1, \dots, NP \\ k &= 1, 2, \dots, n \end{aligned} \quad (3.5.5)$$

$$\begin{aligned} \tilde{x}_k^-(t_i, p) &= x_k^-(t_i, p) + \sum_{j=1}^r \alpha_{kij}^- (p_j^L - p_j)(p_j^U - p_j), \\ i &= 0, 1, \dots, NP \\ k &= 1, 2, \dots, n \end{aligned} \quad (3.5.6)$$

The difficulty in this approach is the calculation of the non-negative α_{kij}^+ and α_{kij}^- parameters. There is no functional form available for the Hessian matrices in order to use interval calculations directly.

The values for the non-negative α_i parameters are calculated using the scaled Gerschgorin method proposed by Adjiman et al. (1998). This method requires the use of a symmetric interval matrix $[H_{f_{NT}}] = ([\underline{h}_{ij}, \bar{h}_{ij}])$ such that $[H_{f_{NT}}] \ni H_{f_{NT}}(x) = \nabla^2 f_{NT}(x) \forall x \in [x^L, x^U]$. α_i can be calculated by the following formula:

$$\alpha_i = \max \left\{ 0, -\frac{1}{2} \left(\underline{h}_{ii} - \sum_{j \neq i} |\underline{h}_{ij}| \right) \right\} \quad (3.5.7)$$

where $|h|_{ij} = \max \{ |h_{ij}|, |\bar{h}_{ij}| \}$. These values for the α_i parameters guarantee the convexity of the underestimator. The interval matrix $[H_{f_{NT}}]$ is calculated by applying natural interval extensions to the analytical expression for each second-order derivative of f_{NT} and is given by $[H_{f_{NT}}] = H_{f_{NT}}([x^L, x^U])$. The method using interval calculations produces an interval matrix $[H^*]$, that may be an underestimation of the space of the Hessian matrices, which means that there may exist

$$p \in [p^L, p^U]: \nabla^2 x_k(t_i, p) = H_{x_k(t_i)}(p) \in [H^*]. \quad (3.5.8)$$

The difficulties associated with the computation of valid Hessian matrices are resolved by constructing bounds based on equations (3.2.3) and (3.2.4) for the ODE system that is generated when the first and the second-order sensitivity equations are coupled with the original ODE system. These bounds on the second-order derivatives can then be used to construct each element of the interval Hessian matrices needed.

3.6 Convex Relaxation of the NLP

After underestimating the objective function and overestimating the feasible region, the convex relaxation of the NLP problem (3.3.1) is given by

$$\begin{aligned} & \min_{\hat{x}, p, w} \tilde{J}(\hat{x}, p, w) \\ \text{s.t.} & \quad \tilde{g}_i(\hat{x}_i, p, w) \leq 0, \quad i = 0, 1, \dots, NP \quad (3.6.1) \\ & \quad \underline{x}(t_i) \leq \hat{x}_i \leq \bar{x}(t_i), \quad i = 0, 1, \dots, NP \\ & \quad C(\hat{x}, p, w) \leq 0 \\ & \quad p \in [p^L, p^U] \end{aligned}$$

where \tilde{J} denotes the convex underestimator of the specified function, C denotes the set of additional constraints arising from the convex relaxation of bilinear terms and w denotes the vector of new variables introduced by this relaxation.

3.7 Example

This example, introduced in Paramichail and Adjiman (2002), is an optimal control problem with one constant control. The problem has at least two local minima. Its formulation is given by:

$$\begin{aligned} & \min_p \quad -x(1)^2 \\ \text{s.t.} \quad & \dot{x}(t) = -x(t)^2 + p, \quad \forall t \in [0, 1] \\ & x(0) = 9 \\ & -5 \leq p \leq 5 \end{aligned} \tag{3.7.1}$$

This problem is equivalent to:

$$\begin{aligned} & \min_{\hat{x}, p} \quad -\hat{x}^2 \\ \text{s.t.} \quad & \hat{x} = -x_1(1) \\ & p^L \leq p \leq p^U \end{aligned} \tag{3.7.2}$$

where the value of $x_1(1)$ is obtained by solving ODE from (3.7.1). When this ODE is differentiated with respect to the parameter p as described in equation (3.1.2), the following first-order sensitivity equations are produced:

$$\dot{x}_2(t) = -2x_1x_2 + 1, \quad \forall t \in [0, 1] \tag{3.7.3}$$

$$x_2(0) = 0 \tag{3.7.4}$$

where

$$x_2(t) = \frac{\partial x_1}{\partial p} \tag{3.7.5}$$

and

$$\dot{x}_2(t) = \frac{\partial}{\partial t} \left(\frac{\partial x_1}{\partial p} \right) \tag{3.7.6}$$

The second-order sensitivity equations are produced when the system of first-order sensitivity (3.7.3) – (3.7.6) is differentiated once more with respect to the parameter p :

$$\dot{x}_3(t) = -2x_2^2 - 2x_1x_3, \quad \forall t \in [0, 1] \tag{3.7.7}$$

$$x_3(0) = 0 \tag{3.7.8}$$

where

$$\underline{x}_3(t) = \frac{\partial x_2}{\partial p} \quad (3.7.9)$$

and

$$\dot{\underline{x}}_3(t) = \frac{\partial}{\partial t} \left(\frac{\partial x_2}{\partial p} \right) \quad (3.7.10)$$

Based on equations (3.2.3) and (3.2.4) the following ODE system can be constructed:

$$\begin{aligned} \dot{\underline{x}}_1(t) &= \inf \left(-\underline{x}_1(t)^2 + [p^L, p^U] \right) = -\underline{x}_1(t)^2 + p^L \\ \dot{\underline{x}}_2(t) &= \inf \left(-2[\underline{x}_1(t), \bar{x}_1(t)]\underline{x}_2(t) + 1 \right) = -2\bar{x}_1(t)\underline{x}_2(t) + 1 \\ \dot{\underline{x}}_3(t) &= \inf \left(-2[\underline{x}_2(t), \bar{x}_2(t)]^2 - 2[\underline{x}_1(t), \bar{x}_1(t)]\underline{x}_3(t) \right) \\ &= -2\bar{x}_2(t)^2 - 2\bar{x}_1(t)\underline{x}_3(t) \end{aligned} \quad (3.7.11)$$

$$\begin{aligned} \dot{\bar{x}}_1(t) &= \sup \left(-\bar{x}_1(t)^2 + [p^L, p^U] \right) = -\bar{x}_1(t)^2 + p^U \\ \dot{\bar{x}}_2(t) &= \sup \left(-2[\underline{x}_1(t), \bar{x}_1(t)]\bar{x}_2(t) + 1 \right) = -2\underline{x}_1(t)\bar{x}_2(t) + 1 \\ \dot{\bar{x}}_3(t) &= \sup \left(-2[\underline{x}_2(t), \bar{x}_2(t)]^2 - 2[\underline{x}_1(t), \bar{x}_1(t)]\bar{x}_3(t) \right) \\ &= -2\underline{x}_2(t)^2 - 2\underline{x}_1(t)\bar{x}_3(t) \end{aligned} \quad (3.7.12)$$

$$\begin{aligned} \underline{x}_1(0) &= 9 & \bar{x}_1(0) &= 9 \\ \underline{x}_2(0) &= 0 & \bar{x}_2(0) &= 0 \\ \underline{x}_3(0) &= 0 & \bar{x}_3(0) &= 0 \end{aligned} \quad (3.7.13)$$

The solution of this system gives constant bounds for the set of solutions of the system consisting of the original system, the first and the second-order sensitivity:

$$\begin{aligned} \underline{x}_i(t) \leq x_i(t, p) \leq \bar{x}_i(t), \quad \forall p \in [p^L, p^U] \\ \forall t \in [0, 1], \quad i = 1, 2, 3 \end{aligned} \quad (3.7.14)$$

Using equations (3.7.5), (3.7.9) and (3.7.14) and interval arithmetic properties we obtain the interval Hessians:

$$\nabla^2 x_1(1, p) \in [\underline{x}_3(1), \bar{x}_3(1)], \quad \forall p \in [p^L, p^U] \quad (3.7.15)$$

$$\nabla^2 (-x_1)(1, p) \in [-\bar{x}_3(1), -\underline{x}_3(1)], \quad \forall p \in [p^L, p^U] \quad (3.7.16)$$

The values for the α^+ and α^- parameters can be now calculated using equation (3.5.7). The α -based bounds are constructed based on equations (3.5.5) and (3.5.6). The convex relaxation of the problem for the region $R \in [p^L, p^U]$ is given by:

$$\begin{aligned}
 & \min_{\hat{x}, p} \{-[\underline{x}_1(1) + \bar{x}_1(1)]\hat{x} + \underline{x}_1(1)\bar{x}_1(1)\} \\
 & \text{s.t.} \tag{3.7.17} \\
 & \underline{x}_1(1) \leq \hat{x} \leq \bar{x}_1(1) \\
 & x_1(1, p) + \alpha^+(p^L - p)(p^U - p) - \hat{x} \leq 0 \\
 & \hat{x} - x_1(1, p) + \alpha^-(p^L - p)(p^U - p) \leq 0 \\
 & p^L \leq p \leq p^U
 \end{aligned}$$

where the value of $x_1(1, p)$ is obtained by solving ODE from (3.7.1). Following this procedure we computed that the global optimum parameter is $p = -5$ and the value of the objective function for the global optimum parameter is equal to -8.23262 .

Conclusion

The main aim of this work was a theoretical introduction of various methods for solving dynamic optimization problems. The analytical methods of dynamic optimization mentioned in this work represent a way to obtain optimal profiles of controls and states for the control of a process described by differential equations. Using these methods one example of the time-optimal control problem of a car that consisted of two simple linear state equations with some constraints was solved. The results as well as their graphical interpretation are given in Sections 1.3.1 and 1.3.2.

However, solving medium-dimensional (three or more state equations) nonlinear problems that, e.g., consist of nonlinear differential equations, can be difficult. Other complex specifications like constraints and other algebraic conditions or the discontinuance of profiles could cause that the problem becomes impossible to solve using the calculus of variations. Therefore, in present days numerical methods are rather preferred for solving optimization problems.

Section 2 introduced one deterministic method of global optimization, namely the α BB method, which properties guarantee the convergence to the global optimum. In this section, an algorithm of this method was described, which is based on a process of branching and bounding. To find the lower bound to the global solution, the convex relaxation was used which was described mainly in Section 2.1.3. Different methods of calculating the parameter α and branching strategies are provided in Section 2.1.4 and 2.1.5. Finally, Section 2.3 shows the process of the convex relaxation in case that the state variables are time and parameter dependent. To illustrate the algorithm of this method two problems were solved and are described in Section 2.2 and 2.4.

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