THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

Adaptive Finite Element Methods for Optimal Control Problems

Karin Kraft

CHALMERS | UNIVERSITY OF GOTHENBURG

Department of Mathematical Sciences
Chalmers University of Technology and University of Gothenburg
Gothenburg, Sweden 2011

Adaptive Finite Element Methods for Optimal Control Problems
Karin Kraft
ISBN 978-91-7385-494-8

Doktorsavhandlingar vid Chalmers tekniska högskola
Ny serie nr 3175
ISSN 0346-718X

Department of Mathematical Sciences
Division of Mathematics
Chalmers University of Technology and University of Gothenburg
SE-412 96 Göteborg
Sweden
Telephone +46 (0)31 772 1000

Printed at the Department of Mathematical Sciences
Göteborg, Sweden 2011

Adaptive Finite Element Methods for Optimal Control Problems

Karin Kraft

Department of Mathematical Sciences
Chalmers University of Technology
and University of Gothenburg

Sammanfattning

Vi studerar numerisk lösning av optimala styrningsproblem. Problemen består av ett system av differentialekvationer, tillståndsekvationerna, som styrs av en kontrollvariabel. Målet är att bestämma de tillstånd och kontroller som minimerar en given kostnadsfunktional.

Den numeriska metoden i den här avhandlingen baseras på en indirekt metod, vilket innebär att nödvändiga villkor för optimum härleds och sedan löses numeriskt, i vårt fall med en finita elementmetod. Optimalitetsvillkoren härleds med Lagranges metod från variationskalkylen. Detta resulterar i ett randvärdesproblem för ett system av differential/algebraiska ekvationer. Ekvationerna diskretiseras med en finita elementmetod och det ger möjligheten att använda funktionalanalys för att härleda feluppskattningar. I det här arbetet härleds beräkningsbara *a posteriori* feluppskattningar. Metoden med dualviktade residualer används för att härleda feluppskattningarna. Denna metod passar mycket bra för optimala styrningsproblem eftersom den är formulerad inom samma ramverk som Lagranges metod.

En indirekt metod i kombination med en *a posteriori* feluppskattning gör det möjligt att implementera finita elementmetoder där förfiningen av beräkningsnätet är automatiserad. Vi har implementerat adaptiva finita elementmetoder för kvadrat/linjära optimala styrningsproblem, för helt ickelinjära problem och för problem med olikhetsbivillkor på kontroller och tillstånd.

Abstract

In this thesis we study the numerical solution of optimal control problems. The problems considered consist of a system of differential equations, the state equations, which are governed by a control variable. The goal is to determine the states and controls which minimize a given cost functional.

The numerical method in this work is based on an indirect approach, which means that necessary conditions for optimality are first derived and then solved numerically, in our case by a finite element method. The optimality conditions are derived using Lagrange's method in the calculus of variations resulting in a boundary value problem for a system of differential/algebraic equations. These equations are discretized by a finite element method. The advantage of the finite element method is the possibility to use functional analysis to derive error estimates and in this work this is used to prove computable *a posteriori* error estimates. The error estimates are derived in the framework of dual weighted residuals which is well suited for optimal control problems since it is formulated within the Lagrange framework.

Using an indirect method combined with an *a posteriori* error estimate makes it possible to implement adaptive finite element methods where the refinement of the computational mesh is automated. We have implemented such adaptive finite element methods for quadratic/linear optimal control problems, fully nonlinear problems, and for problems with inequality constraints on controls and states.

Keywords: finite element method, discontinuous Galerkin method, optimal control, a posteriori error estimate, dual weighted residual, adaptive, multilevel algorithm, Newton method, control constraint, variational inequality, vehicle dynamics.

Dissertation

This thesis consists of an introduction and four papers:

Paper 1: *Using an adaptive FEM to determine the optimal control of a vehicle during a collision avoidance manoeuvre.*
Proceedings of The 48th Scandinavian Conference on Simulation and Modeling (SIMS 2007) (with Stig Larsson and Mathias Lidberg)

Paper 2: *The dual weighted residuals approach to optimal control of ordinary differential equations.*
BIT Numerical Mathematics 50 (2010), 587-607 (with Stig Larsson)

Paper 3: *An adaptive finite element method for nonlinear optimal control problems*
(Preprint 2011:1) (with Stig Larsson)

Paper 4: *Finite element approximation of variational inequalities in optimal control*
(Preprint 2011:2) (with Stig Larsson)

Acknowledgements

I am grateful to my supervisor Stig Larsson for all discussions and for the guidance through mathematics and error estimates. I also wish to thank my assistant supervisor Mathias Lidberg.

Thomas Ericsson has been very helpful and inspiring. Thank you! I also thank Håkan Johansson and Kjell Holmåker.

I want to thank Anna Nyström, Christoffer Cromvik, David Heintz, Fredrik Lindgren, Milena Anguelova, Niklas Ericsson, Sofia Tapani, and all former and present colleagues for making it fun to go to work!

Warm thanks to the families Nilsson-Jansson, Cromvik, and Nyström for nice visits during the autumn 2010.

I also want to thank Martin Fröst, playing B. H. Crusell and W. A. Mozart, for providing me light during dark moments.

My work was supported by the Gothenburg Mathematical Modelling Centre (GMMC).

Finally, I am very thankful for all love and support from my family, Niklas, Jonatan, Daniel, and Astrid!

Karin Kraft
Örebro, January 2011

Contents

1 Introduction

Consider a car trying to avoid an object that suddenly appears in the road. The driver has some ability to maneuver the car by steering and braking. Is there a way to maneuver the car an optimally, both avoiding the obstacle and minimizing the final velocity? This is an optimal control problem consisting of a system of differential equations, describing the dynamics of the car, and an objective function that should be minimized.

Optimal control problems appear in various fields of engineering, for example, in vehicle dynamics [20, 24], biomechanics [13], robotics [25], and economics [35]. This work originated from the need for more automated ways to solve optimal control problems in vehicle dynamics.

There are two ways to obtain the numerical solution of optimal control problems: the *direct* and the *indirect* approaches. In the direct approach one discretizes the objective functional and the dynamical system and then looks for an optimal solution of the finite dimensional discrete problem. In the indirect approach one determines the necessary conditions for optimality, and solves them numerically. In this work we focus on the indirect approach and use variational calculus to derive the optimality conditions, resulting in a system of differential algebraic equations to be solved. We choose to discretize this system by an adaptive finite element method. The error in the discrete solution is computed using *a posteriori* error estimates, derived by the standard duality-based *a posteriori* error analysis in Paper 1, and by the methodology of dual weighted residuals in the following papers.

The next section presents a mathematical formulation of the optimal control problem considered in this thesis and a brief summary of the history of such problems. Section 3 includes a description of the most common numerical methods used to solve the optimal control problems and an introduction to the finite element method. The following four sections contain summaries of the appended papers. Section 5 contains a summary of Paper 1, including a description of the solution of an optimal control problem using variational calculus and an adaptive finite element method. The error estimate which is used for the adaptive method is also presented. Section 6 describes the approach of dual weighted residuals to quadratic/linear optimal control problems taken in Paper 2. In Section 7 the results from Paper 3 are summarized. The dual weighted residuals approach is applied to nonlinear problems. An error estimate is presented and used in the implementation of a multilevel adaptive solver. Section 8 contains an overview of Paper 4, in which inequality constraints on controls and states are introduced. The last section includes conclusions and directions of future research.

2 The optimal control problem

In this thesis optimal control problems of the following form are considered: Find the states $x(t) \in \mathbb{R}^d$ and the controls $u(t) \in \mathbb{R}^m$ that

$$\begin{aligned} \text{minimize} \quad & \mathcal{J}(x,u) = l(x(0), x(T)) + \int_0^T L(x,u)\,\mathrm{d}t, \\ \text{such that} \quad & \dot{x} = f(u,x), \quad \text{for } 0 < t < T, \\ & I_0 x(0) = x_0, \quad I_T x(T) = x_T. \end{aligned} \tag{2.1}$$

The history of optimal control goes back to the end of the 17th century when Bernoulli formulated the *brachystochrone* problem. For a more thorough account of the history and development of optimal control and variational calculus, see [39]. Introductions to the field are given in [2, 10, 19, 23, 30, 34].

The numerical solution of optimal control problems can be approached in two different ways, the *direct* and the *indirect* approaches [7]. In the direct approach the dynamical system is discretized and approximated by a finite number of parameters. After the discretization, the problem is a finite-dimensional optimization problem, which can be solved using nonlinear programming methods, see [7, 11, 22]. The advantage of this approach is the existence of effective software that can be used, for example, SNOPT [21]. The direct method has been implemented in for example the software SOCS [8] and PROPT [33].

In the indirect approach necessary conditions for optimality are first determined by using variational techniques, such as variational calculus [10] or Pontryagin's maximum principle [31], and then the resulting equations are discretized and solved. The necessary conditions for optimality consist of the original differential equations, an additional set of differential equations called the adjoint equations, and a set of algebraic equations. The number of adjoint equations equals the number of state equations and a drawback with the approach is that the size of the problem is doubled. The indirect approach has been used in the solver BNDSCO [29].

The purpose of this work is to investigate the potential of using adaptive finite element methods to automate the numerical solution of optimal control problems. Therefore, we take an indirect approach to the optimal control problem and derive the necessary conditions for optimality using variational calculus in a functional analytic framework. Choosing the indirect approach in combination with the finite element method, which is described below, gives us the possibility to derive a computable error estimate for the numerical solution. The error estimate can then be used to adaptively refine the computational mesh. However, it would also be possible to combine a finite element discretization with a direct approach and existing nonlinear programming software, but it would be more difficult to combine such an approach with adaptivity.

3 Numerical solution methods

The most common numerical methods for solving the boundary value problems that arise in optimal control problems are the multiple shooting method and the collocation method [6]. Even though the previous methods are the most common, the finite element method has also been used in [13, 17, 18].

3.1 The shooting and collocation methods

The shooting method is a numerical method which can be used for solving boundary value problems of the form

$$\begin{aligned} \dot{x} &= f(t,x), \quad 0 < t < T, \\ g(x(0), x(T)) &= 0, \end{aligned}$$

where $x, g \in \mathbb{R}^d$. The name of the method comes from the procedure of aiming a cannon so that the cannon-ball hits the target [7, 32]. One considers the function $h(c) = g(c, x(T, c))$, where $x(T, c)$ is the value of $x(T)$ obtained by shooting with $x(0) = c$, that is, propagating the solution numerically from 0 to T. The equation $h(c) = 0$ can then be solved using any appropriate method.

The shooting method has been further developed into multiple shooting. In this method the computational interval is refined into smaller sub-intervals, where the shooting method is applied in each sub-interval. This method is used for optimal control problems, see, for example, [29].

The use of sub-intervals is present also in the collocation method [1]. One determines a continuous piecewise polynomial which fulfils the differential equation in the collocation points $t_n + c_i h$, where t_n is the left endpoint of the sub-interval, h is the interval length and $0 \leq c_i \leq 1$ are suitable points, for instance, the roots of the Legendre polynomials [12].

In Paper 1 we use the boundary value problem solver `bvp4c` [36, 37] in Matlab [28] to bench-mark our results. This solver is based on the collocation idea. In Paper 3 and Paper 4, the results are validated with PROPT [33]. These solvers are based on the direct approach and collocation.

3.2 The finite element method

The finite element method was developed in the 1950's and 1960's, mainly by engineers, to solve equations in structural mechanics. It was developed as a geometrically more flexible alternative to the finite difference method (see, for example, [38]). The finite element method is a special case of the Rayleigh-Ritz-Galerkin-methods, which are used to approximate partial differential equations and it has a solid foundation in functional analysis [9]. This is one of its strengths, as is the possibility to use it on complicated domains. The mathematical foundation makes it easier to derive analytic error estimates which, for example, can be used to refine the computational mesh in an adaptive way.

Traditionally the finite element method has been used for partial differential equations. However, some work has been done on adaptive finite element methods for ordinary differential equations, see, for example, [15, 16, 26, 27].

We illustrate how the finite element method works in the context of a simple boundary value problem:

$$\begin{aligned} -\ddot{x} &= f(t), \quad \text{for } 0 < t < T, \\ x(0) &= a, \quad x(T) = b. \end{aligned} \tag{3.1}$$

We start by reformulating the problem in weak form by introducing the space $\mathcal{W} = H^1([0,T])$ of functions with square integrable first derivative and we let $\mathcal{V} = H_0^1([0,T])$ be the subspace of functions $v \in \mathcal{W}$ with $v(0) = v(T) = 0$. We multiply equation (3.1) by a test function $v \in \mathcal{V}$, integrate over the interval $[0,T]$, and then integrate by parts. The weak form is: Find $x \in \mathcal{W}$ such that

$$\begin{aligned} & x(0) = a, \quad x(T) = b, \\ & \int_0^T \dot{x}\dot{v}\,\mathrm{d}t = \int_0^T f v\,\mathrm{d}t, \qquad \text{for all } v \in \mathcal{V}. \end{aligned} \tag{3.2}$$

Let $\mathcal{W}_h$ be a subspace of $\mathcal{W}$ consisting of, for instance, piecewise linear functions on $[0,T]$ with sub-intervals of size h and $\mathcal{V}_h = \mathcal{W}_h \cap \mathcal{V}$. We want to solve (3.2) for all $v \in \mathcal{V}_h$ with the Ansatz $x_h(t) = a\varphi_0(t) + \sum_{n=1}^{N-1} x_n \varphi_n(t) + b\varphi_N(t) \in \mathcal{W}_h$, where $\varphi_n, n = 1, \ldots, N-1$ is a basis for $\mathcal{V}_h$ and φ_0 and φ_N are additional basis functions such that $\varphi_0(0) = \varphi_N(T) = 1$. In this example the trial space $\mathcal{W}$ and test space $\mathcal{V}$, that is, the spaces containing x and v, respectively, are discretized in the same way, but this need not be the case. The fact that the finite element methods are based on the weak form (3.2) rather than (3.1) makes it easier to use tools from functional analysis to derive error estimates.

There are two types of error estimates, *a priori* and *a posteriori* error estimates. The first type gives a bound of the error $e = x - x_h$, in terms of x, h, and the data a, b and f. Since the estimate depends on the unknown exact solution it cannot be explicitly computed but it can be used to investigate the convergence of the numerical method. In the second type of error estimate, the *a posteriori* error estimate, the error bound is expressed in terms of x_h, h, and the data. An *a posteriori* error estimate can be explicitly computed, since it depends only on known or computable quantities. The *a posteriori* error estimates are used to construct adaptive algorithms which solve the equation repeatedly on refined meshes, see Algorithm 1,.

Algorithm 1: An adaptive finite element method

Solve the equation on an initial mesh;
Compute the error estimate E;
while $|E| \geq TOL$ **do**
  Refine the mesh according to the error estimate, that is, refine sub-intervals that give large contributions to the error;
  Solve the equation on the refined mesh;
  Compute the error estimate on the refined mesh;
end

More about error estimates and adaptive finite element methods can be found in [3, 9, 14, 15].

In this work we consider *a posteriori* error estimates, since the goal is to construct adaptive algorithms. We start by using a standard duality-based *a posteriori* error analysis, see [14, 15], to derive an *a posteriori* error estimate minimizing the error in an arbitrary linear functional. Next, we use the dual weighted residuals methodology for *a posteriori* error analysis. It is formulated within the Lagrange framework and is therefore well suited for optimal control problems and yields a representation formula for the error in the goal functional $\mathcal{J}$ [3, 5].

4 Mathematical framework

In order to summarize the work in the appended papers we introduce the notation which is used. Let $\mathcal{C}^k$ denote k times continuously differentiable functions and H^1 denote functions with square integrable derivative. Further,

$\mathcal{C}^1_{\mathrm{PW}}$ denotes piecewise continuously differentiable functions $[0,T] \to \mathbb{R}^d$; more precisely, functions that are $\mathcal{C}^1$ except at a finite number of points in $[0,T]$ and with left and right limits $w(t^-) = \lim_{s\downarrow t} w(s)$, $w(t^+) = \lim_{s\uparrow t} w(s)$ for all points $t \in [0,T]$, and we denote jumps as $[w]_t = w(t^+) - w(t^-)$.

We introduce the function spaces

$$\begin{aligned}
\mathcal{W} &= \mathbb{R}^d \times \mathcal{C}^1_{\mathrm{PW}}([0,T],\mathbb{R}^d) \times \mathbb{R}^d, \\
\dot{\mathcal{W}} &= R(I - I_0) \times \mathcal{C}^1_{\mathrm{PW}}([0,T],\mathbb{R}^d) \times R(I - I_T) \\
&= \Big\{ w \in \mathcal{W} : I_0 w(0^-) = 0,\ I_T w(T^+) = 0 \Big\}, \\
\mathcal{U} &= H^1([0,T],\mathbb{R}^m), \\
\mathcal{V} &= H^1([0,T],\mathbb{R}^d), \\
\hat{\mathcal{W}} &= \hat{x} + \dot{\mathcal{W}} = \Big\{ w \in \mathcal{W} : w - \hat{x} \in \dot{\mathcal{W}} \Big\}.
\end{aligned}$$

Here $R(I - I_0)$ and $R(I - I_T)$ denote the ranges of the matrices. The two factors $\mathbb{R}^d$ in $\mathcal{W}$ are used to accomodate the boundary values $w(0^-)$ and $w(T^+)$. The space $\mathcal{W}$ will contain the state variable x, and $\mathcal{V}$ and $\mathcal{U}$ will contain the costate z, and the control u, respectively. The affine space $\hat{\mathcal{W}}$ contains functions satisfying the prescribed boundary conditions if $\hat{x} \in \mathcal{W}$ is chosen so that $\hat{x}(0^-) = x_0$ and $\hat{x}(T^+) = x_T$.

In the discretizations we use a mesh $0 = t_0 < t_1 < t_2 < \ldots < t_N = T$, with steps $h_n = t_n - t_{n-1}$ and intervals $J_n = (t_{n-1}, t_n)$. With P^k denoting polynomials of degree k, we introduce the function spaces used in the discretization:

$$\begin{aligned}
\mathcal{W}_h &= \mathbb{R}^d \times \Big\{ w \in \mathcal{W} : w|_{J_n} \in P^{k-1}(J_n,\mathbb{R}^d),\ n = 1,\ldots,N \Big\} \times \mathbb{R}^d, \\
\dot{\mathcal{W}}_h &= R(I - I_0) \times \Big\{ w \in \mathcal{W} : w|_{J_n} \in P^{k-1}(J_n,\mathbb{R}^d),\ n = 1,\ldots,N \Big\} \\
&\quad \times R(I - I_T) \\
&= \Big\{ w \in \mathcal{W}_h : I_0 w(0^-) = 0,\ I_T w(T^+) = 0 \Big\}, \\
\mathcal{U}_h &= \Big\{ u \in \mathcal{C}^0([0,T],\mathbb{R}^m) : u|_{J_n} \in P^k(J_n,\mathbb{R}^m),\ n = 1,\ldots,N \Big\}, \\
\mathcal{V}_h &= \Big\{ v \in \mathcal{C}^0([0,T],\mathbb{R}^d) : v|_{J_n} \in P^k(J_n,\mathbb{R}^d),\ n = 1,\ldots,N \Big\}, \\
\hat{\mathcal{W}}_h &= \hat{x} + \dot{\mathcal{W}}_h, \ \text{for some } \hat{x} \in \mathcal{W}_h.
\end{aligned}$$

Now we have $\mathcal{W}_h \subset \mathcal{W}$, $\dot{\mathcal{W}}_h \subset \dot{\mathcal{W}}$, $\hat{\mathcal{W}}_h \subset \hat{\mathcal{W}}$, $\mathcal{U}_h \subset \mathcal{U}$, and $\mathcal{V}_h \subset \mathcal{V}$.

In this thesis we have implemented the algorithms for $k = 1$, that is, the states in $\mathcal{W}_h$ are discretized by piecewise constant discontinuous functions and the controls in $\mathcal{U}_h$ and costates in $\mathcal{V}_h$ are discretized by piecewise linear continuous functions. However, the theory is valid for higher k.

5 A first approach

In Paper 1 the optimality conditions for the optimal control problem (2.1) are derived using the classical variational calculus by introducing the costates $z(t) \in \mathbb{R}^d$ and the Hamiltonian

$$H(x,u,z) = L(x,u) + z^{\mathrm{T}} f(x,u).$$

Then the optimal (x^*, u^*, z^*) fulfil the Hamilton-Jacobi equations

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial z} = f(x,u), \\ \dot{z} &= -\frac{\partial H}{\partial x} = -\frac{\partial L}{\partial x} - \left(\frac{\partial f}{\partial x}\right)^{\mathrm{T}} z, \\ 0 &= \frac{\partial H}{\partial u} = \frac{\partial L}{\partial u} + z^{\mathrm{T}} \frac{\partial f}{\partial u}, \\ I_0 y(0) &= x_0, \quad I_T y(T) = x_T, \\ (I - I_0) z(0) &= z_0, \quad (I - I_T) z(T) = z_T. \end{aligned} \tag{5.1}$$

We note that since x_0 and x_T are in the ranges of I_0 and I_T, respectively, the boundary conditions are imposed on those components of the costates z that are complementary to the components of x with boundary conditions.

In order to simplify the problem we make the assumption that the algebraic equation $\frac{\partial H}{\partial u} = 0$ in (5.1) has an explicit solution u which can be substituted into the other equations. This assumption reduces the problem from a system of Differential Algebraic Equations (DAE) to a boundary value problem for Ordinary Differential Equations (ODE). We make an additional simplification by joining the states $x(t)$ and the costates $z(t)$ into one new variable $y(t) \in \mathbb{R}^{2d}$ and end up with a system of the form

$$\begin{aligned} &\dot{y} = f_2(y), \quad 0 < t < T, \\ &I_0 y(0) = y_0, \quad I_T y(T) = y_T, \end{aligned} \tag{5.2}$$

where I_0 and I_T are two new diagonal matrices with zeroes or ones on the diagonals and $\mathrm{rank}(I_0) + \mathrm{rank}(I_T) = 2d$. We thus have to solve a boundary value problem of twice the dimension of the original problem. The states and costates are joined into one variable to simplify the implementation.

The problem in (5.2) is written in weak form by multiplying the equations by a test function and integrating over the interval $[0, T]$, resulting in: Seek $y \in \mathcal{W}$ (with d replaced by $2d$) such that

$$\begin{aligned} &I_0 y(0) = x_0, \quad I_T y(T) = y_T, \\ &F(y, v) := \int_0^T v^{\mathrm{T}}(\dot{y} - f_2(y))\,\mathrm{d}t = 0 \quad \forall v \in \mathcal{V}. \end{aligned} \tag{5.3}$$

The finite element problem can be stated: Find a function $Y \in \mathcal{W}_h$ which fulfils

$$\begin{aligned} &I_0 Y_0^- = y_0, \quad I_T Y_N^+ = y_T, \\ &F(Y, v) := \sum_{n=1}^{N} \int_{J_n} v^{\mathrm{T}}(\dot{Y} - f_2(Y))\,\mathrm{d}t + \sum_{n=0}^{N} ([Y]_n \,, v(t_n)) = 0 \quad \forall v \in \mathcal{V}_h. \end{aligned} \tag{5.4}$$

Here the definition of the form F from (5.3) has been extended to include the jump terms which appear since we write the derivative of the discontinuous trial function Y as a weak derivative. Since the trial space consists of piecewise constant functions, we have $\dot{Y} = 0$ inside the intervals J_n. Hence, (5.4) results in a system of $(N+2)2d$ equations, more precisely, $2d$ boundary conditions and $(N+1)2d$ equations. With boundary conditions at both ends, the equations are coupled and thus we cannot use time stepping. Therefore, the equations in the system have to be solved simultaneously. In order to evaluate how good the computed solution is and to construct an adaptive finite element method we derive an *a posteriori* error estimate. We introduce the notation $\|v\|_{J_n} = \sup_{t \in I_n} \|v(t)\|$, where $\| \cdot \|$ denotes the norm in $\mathbb{R}^{2d}$ or $\mathbb{R}^m$. Let $e = y - Y$ be the error in the finite element solution of the boundary value problem in (5.2). The error expressed in a linear functional G is bounded by

$$|G(e(t))| \leq \sum_{n=1}^{N} \mathcal{R}_n \mathcal{I}_n, \quad 0 < t < T,$$

where

$$\mathcal{R}_1 = h_1\|\dot{Y} - f(Y)\|_{J_1} + \|\,[Y]_0\,\| + \frac{h_1}{h_1+h_2}\|\,[Y]_1\,\|,$$

$$\mathcal{R}_n = h_n\|\dot{Y} - f(Y)\|_{J_n} + \frac{h_n}{h_n+h_{n-1}}\|\,[Y]_{n-1}\,\| + \frac{h_n}{h_n+h_{n+1}}\|\,[Y]_n\,\|,$$

$$n = 2,\dots,N-1,$$

$$\mathcal{R}_N = h_N\|\dot{Y} - f(Y)\|_{J_N} + \frac{h_N}{h_N+h_{N-1}}\|\,[Y]_{N-1}\,\| + \|\,[Y]_N\,\|,$$

$$\mathcal{I}_n = Ch_n\int_{J_n} |\ddot{\phi}(t)|\,\mathrm{d}t.$$

C is a constant and ϕ is the solution to the linearised dual problem to (5.2) with data functional G.

In this error estimate, $\mathcal{R}_n$ mainly describes how well the approximate solution satisfies the differential equation and $\mathcal{I}_n$ describes the sensitivity of $G(y)$ to perturbations. The proof is based on a standard duality argument [14]. The residual quantities $\mathcal{R}_n$ are computable, but the weights $\mathcal{I}_n$ must be bounded *a priori* or computed approximately by the solution of the linearized adjoint problem which is another boundary value problem in $2d$ variables, which doubles the number of unknowns again. This *a posteriori* error has been used in the implementation of an adaptive finite element method, which in numerical tests inserts nodes in a way that reduces the number of nodes needed to reach a certain tolerance. A similar approach was taken in [17, 18].

6 The dual weighted residuals approach

Another approach based on the Lagrange framework in the calculus of variations is taken in Paper 2. The error in the objective functional $\mathcal{J}$ is analyzed using the methodology of dual weighted residuals [3, 5]. The optimal control problem is written in an abstract form using the smooth functionals $\mathcal{F}(x,u;\varphi)$ and $\mathcal{J}(x,u)$,

$$\mathcal{F} : \mathcal{W}\times\mathcal{U}\times\mathcal{V} \to \mathbb{R},$$
$$\mathcal{J} : \mathcal{W}\times\mathcal{U} \to \mathbb{R},$$

defined by

$$\mathcal{F}(x,u;\varphi) = \sum_{n=1}^{N}\int_{t_{n-1}}^{t_n} (\dot{x} - f(x,u),\varphi)\,\mathrm{d}t + \sum_{n=0}^{N}([x]_n,\varphi(t_n)),$$

and

$$\mathcal{J}(x,u) = l(x(0), x(T)) + \int_0^T L(x(t), u(t))\,\mathrm{d}t.$$

We use the convention that functionals depend linearly on the arguments after the semicolon.

The optimal control problem in (2.1) now takes the form: Determine $x \in \hat{\mathcal{W}}$ and $u \in \mathcal{U}$ that

$$\begin{aligned} &\text{minimize} && \mathcal{J}(x,u), \\ &\text{subject to} && \mathcal{F}(x,u;\varphi) = 0 \quad \forall \varphi \in \mathcal{V}. \end{aligned} \tag{6.1}$$

Introducing the Lagrange functional

$$\mathcal{L}(x,u;z) = \mathcal{J}(x,u) + \mathcal{F}(x,u;z), \quad (x,u,z) \in \hat{\mathcal{W}} \times \mathcal{U} \times \mathcal{V},$$

where z is a Lagrange multiplier, yields the optimality conditions

$$\mathcal{L}'(x,u;z,\varphi) := \mathcal{L}'(x,u;z)\varphi = 0, \quad \forall \varphi \in \dot{\mathcal{W}} \times \mathcal{U} \times \mathcal{V}, \tag{6.2}$$

that is,

$$\mathcal{J}'_x(x,u;\varphi_x) + \mathcal{F}'_x(x,u;z,\varphi_x) = 0 \quad \forall \varphi_x \in \dot{\mathcal{W}}, \tag{6.3a}$$

$$\mathcal{J}'_u(x,u;\varphi_u) + \mathcal{F}'_u(x,u;z,\varphi_u) = 0 \quad \forall \varphi_u \in \mathcal{U}, \tag{6.3b}$$

$$\mathcal{F}(x,u;\varphi_z) = 0 \quad \forall \varphi_z \in \mathcal{V}. \tag{6.3c}$$

The equations above are discretized and solved by a finite element method using the function spaces in Section 4.

Let $(x,u,z) \in \hat{\mathcal{W}} \times \mathcal{U} \times \mathcal{V}$ be the exact solution and $(x_h, u_h, z_h) \in \hat{\mathcal{W}}_h \times \mathcal{U}_h \times \mathcal{V}_h$ be the discrete solution of (6.3a)–(6.3c), respectively. Then the error in the goal functional is

$$\mathcal{J}(x,u) - \mathcal{J}(x_h,u_h) = \tfrac{1}{2}\rho_x + \tfrac{1}{2}\rho_z + \tfrac{1}{2}\rho_u + R, \tag{6.4}$$

with the residuals ρ_x, ρ_z, and ρ_u defined as

$$\begin{aligned} \rho_x &= \mathcal{J}'_x(x_h,u_h; x - \tilde{x}_h) + \mathcal{F}'_x(x_h,u_h;z_h, x - \tilde{x}_h), \\ \rho_u &= \mathcal{J}'_u(x_h,u_h; u - \tilde{u}_h) + \mathcal{F}'_u(x_h,u_h;z_h, u - \tilde{u}_h), \\ \rho_z &= \mathcal{F}(x_h,u_h; z - \tilde{z}_h). \end{aligned}$$

Here $(\tilde{x}_h, \tilde{u}_h, \tilde{z}_h) \in \hat{\mathcal{W}}_h \times \mathcal{U}_h \times \mathcal{V}_h$ is arbitrary and R is a remainder term. This error estimate is used in the implementation of an adaptive finite element method. We implement the method for quadratic $\mathcal{J}$ and linear $\mathcal{F}$, a quadratic/linear optimal control problem and then R is zero. The advantage of this error estimate compared to the one used in Paper 1 is that the dual solution in the form of the costates z is already computed as a part of the original *indirect* approach of the optimal control problem. Therefore, no extra dual solution is needed to compute the error estimate. In the proof of the error estimate we use Galerkin orthogonality, that is, $\mathcal{F}(x_h, u_h; \varphi_h) = 0 \ \forall \varphi_h \in \mathcal{V}_h$. Therefore only optimal control problems with linear ODE as constraints have been considered in the implementation of the solver.

7 Nonlinear problems

The approach of Paper 2 is extended to fully nonlinear problems in Paper 3. A Newton method is applied to the optimality conditions in (6.2). Given an approximate solution (x, u, z), Newton's method yields a new approximate solution $(\hat{x}, \hat{u}, \hat{z})$ by

$$(\hat{x}, \hat{u}, \hat{z}) = (x, u, z) + \alpha(\delta_x, \delta_u, \delta_z),$$

where $\alpha \in \mathbb{R}$ is a parameter and the increment $\delta = (\delta_x, \delta_u, \delta_z) \in \dot{\mathcal{W}} \times \mathcal{U} \times \mathcal{V}$ is the solution of

$$\mathcal{L}''(x, u; z, \varphi, \delta) = -\mathcal{L}'(x, u; z, \varphi) \quad \forall \varphi \in \dot{\mathcal{W}} \times \mathcal{U} \times \mathcal{V}. \tag{7.1}$$

The equations in (7.1) are discretized using the finite element spaces in Section 4. The parameter α is determined through a line search ([4]) choosing the α that minimizes the right hand side of the discrete version of (7.1).

The approximate solution of the nonlinear equations in (7.1) results in a lack of Galerkin orthogonality, that is, $\mathcal{F}(\hat{x}_h, \hat{u}_h; \varphi_h) \neq 0 \ \forall \ \varphi_h \in \mathcal{V}_h$, used in the error estimate in Paper 2. This results in a slightly different error representation formula:

$$\mathcal{J}(x, u) - \mathcal{J}(\hat{x}_h, \hat{u}_h) = \tfrac{1}{2}\rho_x + \tfrac{1}{2}\rho_u + \tfrac{1}{2}\rho_x + \mathcal{F}(\hat{x}_h, \hat{u}_h, \hat{z}_h) + R,$$

with

$$\begin{aligned}
\rho_x &= \mathcal{J}'_x(\hat{x}_h, \hat{u}_h; x - \hat{x}_h) + \mathcal{F}'_x(\hat{x}_h, \hat{u}_h; \hat{z}_h, x - \hat{x}_h),\\
\rho_u &= \mathcal{J}'_u(\hat{x}_h, \hat{u}_h; u - \hat{u}_h) + \mathcal{F}'_u(\hat{x}_h, \hat{u}_h; \hat{z}_h, u - \hat{u}_h),\\
\rho_z &= \mathcal{F}(\hat{x}_h, \hat{u}_h; z - \hat{z}_h),
\end{aligned}$$

and the remainder

$$R = \frac{1}{2}\int_0^1 \Big(J'''(x_h + s\hat{e}_x, u_h + s\hat{e}_u; \hat{e}, \hat{e}, \hat{e}) + \mathcal{F}'''(\hat{x}_h + s\hat{e}_x, \hat{u}_h + s\hat{e}_u; \hat{z}_h + s\hat{e}_z, \hat{e}, \hat{e}, \hat{e})\Big) s(s-1)\,\mathrm{d}s.$$

This formula is used to derive a computable *a posteriori* error estimate, where the unknowns (x, u, z) are replaced by $(x_{\text{fine}}, u_{\text{fine}}, z_{\text{fine}})$, which are solutions on a finer mesh, which combined with the Newton method is the basis for a multilevel adaptive finite element solver. The solver starts with a coarse mesh, performs a certain number of Newton iterations, and refines the mesh based on the computed error. This procedure is iterated until the solution meets a certain tolerance.

For the examples solved, only a few Newton iterations are needed on each level. New nodes are inserted where the error is expected to be large. Compared to uniform refinement the adaptive refinement keeps down the size of the computational mesh. The drawback of the combination of the indirect method and a Newton method for solving optimal control problems is the need for a good initial guess, which is not intuitive, especially for the costates.

8 Inequality constraints

In vehicle dynamics it is important to allow inequality constraints on controls in order to formulate realistic models. Therefore, tests were done using penalty and barrier functions [4] in order to handle such constraints on the controls during the work with Paper 3. These tests were not satisfactory and only worked for some special cases.

In Paper 4, we derive a framework for solving quadratic/linear optimal control problems of the form:

$$\begin{aligned}
&\text{Minimize} && \mathcal{J}(x,u) = \tfrac{1}{2}\|x(0) - \bar{x}_0\|_{Q_0}^2 + \tfrac{1}{2}\|x(T) - \bar{x}_T\|_{Q_T}^2 \\
& && \qquad + \tfrac{1}{2}\int_0^T \left(\|x(t) - \bar{x}(t)\|_Q^2 + \|u(t) - \bar{u}(t)\|_R^2\right) \mathrm{d}t, \\
&\text{such that} && \dot{x}(t) = A(t)x(t) + B(t)u(t), \quad 0 < t < T, \\
& && I_0 x(0) = x_0, \quad I_T x(T) = x_T, \\
& && \|u(t)\| \le r_u, \quad \|x(t)\| \le r_x, \quad 0 < t < T.
\end{aligned}$$

The difference compared to the optimal control problem in Paper 2, (6.1), is the inequality constraints on the states and controls on the last line. This means that the solution to the problem has to be found in a convex set $\mathcal{K} = \mathcal{K}_x \times \mathcal{K}_u \times \mathcal{V}$, where

$$\mathcal{K}_x = \{w \in \hat{\mathcal{W}} : \|w(t^{\pm})\| \leq r_x,\ t \in [0,T]\},$$
$$\mathcal{K}_u = \{u \in \mathcal{U} : \|u(t)\| \leq r_u,\ t \in [0,T]\}.$$

This restriction yields that an optimum $(x, u, z) \in \mathcal{K}$ satisfies

$$\mathcal{L}'_x(x, u; z, \varphi_x - x) \geq 0 \quad \forall \varphi_x \in \mathcal{K}_x, \tag{8.1a}$$
$$\mathcal{L}'_u(x, u; z, \varphi_u - u) \geq 0 \quad \forall \varphi_u \in \mathcal{K}_u, \tag{8.1b}$$
$$\mathcal{L}'_z(x, u; z, \varphi_z) = 0 \quad \forall \varphi_z \in \mathcal{V}. \tag{8.1c}$$

Instead of a system of equations in weak form we have a system of variational inequalities. These are discretized with a finite element method based on the same finite element spaces as in our previous work. However, the discrete solution is searched for in discrete versions of $\mathcal{K}_x$ and $\mathcal{K}_u$ instead of $\dot{\mathcal{W}}_h$ and $\mathcal{V}_h$. In order to solve the variational inequalities in (8.1) a new projected solver is derived. The solver starts by solving the system in (8.1) as equality, then it projects the components of the states and controls that do no fulfil the constraints onto $\mathcal{K}_h$ and then solves for new z. This procedure is iterated until convergence.

The *a posteriori* error analysis based on the dual weighted residuals methodology yields only an one-sided bound for the error $\mathcal{J}(x, u) - \mathcal{J}(x_h, u_h)$, when applied directly to the variational inequality (8.1). We therefore introduce an augmented Lagrangian

$$\begin{aligned}\tilde{\mathcal{L}}(x, u, z, \sigma_x, \sigma_u) = \mathcal{J}(x, u) &+ \mathcal{F}(x, u, z)\\ &+ \tfrac{1}{2} \int_0^T \sigma_x(t)(\|x(t)\|^2 - r_x^2)\, \mathrm{d}t\\ &+ \tfrac{1}{2} \int_0^T \sigma_u(t)(\|u(t)\|^2 - r_u^2)\, \mathrm{d}t,\end{aligned}$$

containing additional Lagrange multipliers σ_x, σ_u corresponding to the inequality constraints. We now obtain a representation formula for the error similar to (6.4) but with additional residuals coming from the additional terms in $\tilde{\mathcal{L}}$.

We emphasize that we solve the variational inequality (8.1) numerically. Once the x_h, u_h are found we can compute the extra multipliers to be substituted into the error estimator.

9 Future research

The adaptive finite element methods developed in this work effectively inserts nodes and reduces the size of the computation compared to uniform refinement. It is clear that using an adaptive finite element solver can be useful. However, a more efficient implementation of the solver is needed in order to solve more realistic problems.

The drawback of using an indirect method combined with a Newton method to solve the optimal control problem is the need for a good initial guess. This is especially difficult for the costates z and has to be handled in a more automated way. So far some manual homotopy procedures have been tested. In order to solve larger nonlinear problems, a more efficient nonlinear solver has to be used in the multilevel adaptive finite element method proposed in this work. In order to solve more advanced vehicle dynamics problem, the theory has to be extended to handle constraints on controls and states also for nonlinear optimal control problems. Some tests with barrier and penalty functions were made during the work with Paper 3, but these were not satisfactory so we suggest that the variational inequalities approach in Paper 4 should be extended to nonlinear problems. We also know that it is important to allow the final time T to be free in realistic models and therefore this should be considered. It would also be interesting to implement higher order finite element methods and to combine a direct method with a finite element discretization. Finally, we summarize the suggestions for future research that have been identified during this work:

- Automated initial guess.
- Implement free time.
- Constraints for nonlinear problems.
- Efficient nonlinear solver.
- Higher order finite element method.
- Investigate a direct approach combined with finite element discretization.

References

[1] U. M. Ascher, R. M. M. Mattheij, and R. D. Russell, *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations*, first ed., Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1988.

[2] M. A. Athans and P. L. Falb, *Optimal Control*, first ed., McGraw-Hill, New York, 1966.

[3] W. Bangerth and R. Rannacher, *Adaptive Finite Element Methods for Differential Equations*, first ed., Birkhäuser Verlag, Basel, Switzerland, 2003.

[4] M. S. Bazaraa, H. D. Sherali, and C. M. Shetty, *Nonlinear Programming*, third ed., Wiley, Hoboken, New Jersey, 2006.

[5] R. Becker and R. Rannacher, *An optimal control approach to a posteriori error estimation in finite element methods*, Acta Numer. **10** (2001), 1–102.

[6] J. T. Betts, *Survey of numerical methods for trajectory optimization*, AIAA J. of Guidance, Control and Dynamics **21** (1998), 193–207.

[7] ______, *Practical Methods for Optimal Control Using Nonlinear Programming*, SIAM, Philadelphia, 2001.

[8] J. T. Betts and W. P. Huffman, *Sparse Optimal Control Software, SOCS*, Tech. report, Boeing Information and Support Services, 1997.

[9] S. C. Brenner and L. R. Scott, *The Mathematical Theory of Finite Element Methods*, second ed., Springer-Verlag, New York, 2002.

[10] A. E. Bryson, Jr and Y. Ho, *Applied Optimal Control*, Hemisphere Publishing Corporation, Washington, D.C., 1975.

[11] C. Büskens and H. Maurer, *SQP-methods for solving optimal control problems with control and state constraints: adjoint variables, sensitivity analysis and real-time control*, J. Comput. Appl. Math. **120** (2000), 85–108, SQP-based direct discretization methods for practical optimal control problems.

[12] E. Eich-Soellner and C. Führer, *Numerical Methods in Multibody Dynamics*, B. G. Teubner, Stuttgart, 1998.

[13] A. Eriksson and A. Nordmark, *Temporal finite element formulation of optimal control in mechanisms*, Comput. Methods Appl. Mech. Engrg. **199** (2010), 1783–1792.

[14] K. Eriksson, D. Estep, P. Hansbo, and C. Johnson, *Introduction to adaptive methods for differential equations*, Acta Numer. (1995), 105–158.

[15] ———, *Computational Differential Equations*, Cambridge University Press, Cambridge, 1996.

[16] D. Estep, *A posteriori error bounds and global error control for approximation of ordinary differential equations*, SIAM J. Numer. Anal. **32** (1995), 1–48.

[17] D. Estep, D. H. Hodges, and M. Warner, *Computational error estimation and adaptive error control for a finite element solution of launch vehicle trajectory problems*, SIAM J. Sci. Comput. **21** (1999), 1609–1631 (electronic).

[18] D. J. Estep, D. H. Hodges, and M. Warner, *The solution of a launch vehicle trajectory problem by an adaptive finite-element method*, Comput. Methods Appl. Mech. Engrg. (2001), 4677–4690.

[19] L. C. Evans, *An Introduction to Mathematical Optimal Control Theory*, `http://math.berkeley.edu/∼evans/control.course.pdf`.

[20] M. Gerdts, *Solving mixed-integer optimal control problems by branch&bound: A case study from automobile test-driving with gear shift*, Optimal Control Applications and Methods **26** (2005), 1–18.

[21] P. Gill, W. Murray, and M. Saunders, *SNOPT*, `http://www.sbsi-sol-optimize.com/asp/sol_product_snopt.htm`.

[22] P. E. Gill, L. O. Jay, M. W. Leonard, L. R. Petzold, and V. Sharma, *An SQP method for the optimal control of large-scale dynamical systems*, J. Comput. Appl. Math. **120** (2000), 197–213, SQP-based direct discretization methods for practical optimal control problems.

[23] D. E. Kirk, *Optimal Control Theory, An Introduction*, Prentice Hall, Inc., Englewood Cliffs, New Jersey, 1970.

[24] M. Klomp, *Longitudinal Force Distribution and Road Vehicle Handling*, Ph.D. thesis, Chalmers University of Technology, 2010.

[25] M. Lidberg, *Design of Optimal Control Processes for Closed-Loop Chain SCARA-Like Robots*, Ph.D. thesis, Chalmers University of Technology, 2004.

[26] A. Logg, *Multi-adaptive Galerkin methods for ODEs. I*, SIAM J. Sci. Comput. (2003), 1879–1902 (electronic).

[27] ______, *Multi-adaptive Galerkin methods for ODEs. II. Implementation and applications*, SIAM J. Sci. Comput. (2003/04), 1119–1141 (electronic).

[28] MATLAB, `http://www.mathworks.com/products/matlab/`.

[29] H. J. Oberle and W. Grimm, *BNDSCO A Program for the Numerical Solution of Optimal Control Problems*, Tech. report, Deutsche Forschungs- and Versuchsanstalt fur Luft- und Raumfahrt e.V., 1989.

[30] H. J. Pesch, *A practical guide to the soluton of real life optimal control problems*, Control and Cybernetics **23** (1994).

[31] L. S. Pontryagin, V. G. Boltyanskii, R. V. Gamkrelidze, and E. F. Mishchenko, *The Mathematical Theory of Optimal Processes*, revised printing ed., John Wiley and Sons, Inc., New York, 1962.

[32] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes, the Art of Scientific Computing*, first ed., Cambridge University Press, Cambridge, 1986.

[33] P. Rutquist and M. M. Edvall, *PROPT-MATLAB Optimal Control Software*, `http://tomdyn.com/`.

[34] R. W. H. Sargent, *Optimal control*, J. Comp. Appl. Math. **124** (2000), 361–371.

[35] S. P. Sethi and G. L. Thompson, *Optimal Control Theory: Applications to Management Science and Economics*, second ed., Springer, New York, 2005.

[36] L. F. Shampine and J. Kierzenka, *A BVP solver that Controls Residual and Error*, Tech. report, MathWorks, 2007, `http://www.mathworks.com`.

[37] L. F. Shampine, J. Kierzenka, and M. W. Reichelt, *Solving Boundary Value Problems for Ordinary Differential Equations in Matlab using bvp4c*, Tech. report, MathWorks, 2000, `http://www.mathworks.com`.

[38] G. Strang and G. J. Fix, *An Analysis of the Finite Element Method*, first ed., Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1973.

[39] H. J. Sussmann and J. C. Willems, *300 years of optimal control: From the brachystochrone to the maximum principle*, IEEE Control Systems (1997).

Paper 1