Dynamic Optimization Using an Adaptive Control Vector Parameterization Strategy

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Dynamic optimization using an adaptive control vector parameterization strategy

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Dynamic optimization problems arise in many applications in
• economics and
• almost all engineering disciplines.

Problems in chemical engineering are characterized by:

Highly nonlinear, large-scale dynamic process models and …

… many path and end point constraints.

Limited computing time in real-time applications.

Robust and efficient solution methods are required.
Dynamic optimization

Generic **dynamic optimization problem** with constraints:

\[
\begin{align*}
\min_{x,u,p} & \Phi(x(t_f)) \\
\text{subject to:} & \quad \dot{x}(t) = f(x(t), u(t), p), \quad t \in [t_0, t_f] \\
& \quad 0 = x(t_0) - x_0, \\
& \quad 0 \leq h(x(t), u(t), p), \quad t \in [t_0, t_f] \\
& \quad 0 \leq g(x(t_f)).
\end{align*}
\]

**Necessary optimality conditions** lead to multipoint BVPs:

- Highly accurate solutions with shooting techniques.
- Solution requires detailed a-priori knowledge of the optimal solution structure and appropriate estimates for adjoint variables.

**Conversion of dynamic optimization problem into NLP by discretization** …

… of state and control variables.

(Simultaneous methods, i.e. Collocation, Multiple shooting)

… of control variables only.

(Sequential method, i.e. Single shooting)
Discretization of the time-continuous problem

...too coarse

- Low computational cost
- Low accuracy

...appropriate

Resolve problem in specified accuracy with minimal degrees of freedom

...too fine

- High computational cost
- Over-parameterization / robustness?

Grid point movement

Element length as degree of freedom
(e.g. Biegler et al., ‘87, v. Stryk ‘95)

- Introduces nonlinearity and nonconvexity
- Fixed number of grid points

Grid point insertion

Repetitive insertion of new grid points
- Grid point doubling (Luus et al., ‘92)
  - No a-posteriori analysis
- Local curvature (Waldrapp et al., ‘97)
  - Insertion and deletion
- Error residuals (Betts & Huffman, ‘98)
  - One mesh for controls and states

Adaptive discretization in dynamic optimization
Adaptive Discretization

Resolve problem in specified accuracy with minimal degrees of freedom

Grid point movement

Element length as degree of freedom

Grid point insertion and deletion

Repetitive adaptation of grid points based on a-posteriori wavelet analysis

- Multiple control variables
- Adapted mesh for each control variable
- Lagrangian based refinement
Framework for adaptation

Problem specification

Warm start

Discretization

NLP

Initial guess on coarse grid

Adapted mesh

Intermediate solution

A-posteriori analysis

- Eliminate selected parameterization functions
- Add potentially new functions and (locally) analyze their impact on Lagrangian

Termination criterion

\[ \frac{\Phi^{\ell-1} - \Phi^{\ell}}{\Phi^{\ell-1}} \leq \varepsilon \]

Optimal solution

No

Yes
Sequential solution approach

- Problem specification
  - Discretization
  - NLP
  - Warm start
  - A-posteriori analysis
    - Elimination
    - Insertion

Discretization of control variables:

\[ u = \sum_{(j,k) \in \Lambda} c_{j,k} \phi_{j,k}(t) \]

Numerical solution of dynamic model as IVP with given initial conditions and controls.

NLP problem formulation:

\[
\min_{c,j,k,p} \Phi(x(c_j,k,t_f))
\]

subject to:

\[
0 \leq h(x(c_j,k), u(c_j,k), p),
0 \leq g(x(c_j,k,t_f)).
\]

Lagrangian:

\[
L = \Phi + \mu_g g + \mu_h h
\]

Numerical cost strongly depends on discretization of each control variable.
Different representations of the same function ...

... for problem discretization:

\[ u = \sum_{(j,k) \in \Lambda_\varphi} c_{j,k} \varphi_{j,k}(t) \]

... for grid point elimination analysis:

\[ u = c_{0,0} \varphi_{0,0}(t) + \sum_{(j,k) \in \Lambda_\psi} d_{j,k} \psi_{j,k}(t) \]
Elimination of parameterization functions

- Problem specification
- Discretization
- NLP
- Warm start
- A-posteriori analysis
  - Elimination
  - Insertion

Termination criterion

Minimize number of parameterization functions in $u^*$ such that:

$$\frac{\|u^* - \tilde{u}^*\|}{\|u^*\|} \leq \varepsilon$$

Analysis of wavelet coefficients of control variables

Approximation: Norm equivalence

$$\|u\|_L \sim \|d\|_L$$

Discarding small $d_{j,k}$ causes only small changes in approximate representation

Adaptive discretization in dynamic optimization
Different representations of the same function ...

... for problem discretization:

\[ u = \sum_{(j,k) \in \Lambda_\phi} c_{j,k} \varphi_{j,k}(t) \]

... for mesh refinement analysis:

\[ u = \sum_{(j,k) \in \Lambda_\phi} c_{j,k} \varphi_{j,k}(t) + \sum_{(j,k) \in \Lambda_\psi} d_{j,k} \psi_{j,k}(t) \]

Wavelet

Single scale function
Analysis of a parametric optimization problem in $d_{j,k}$ with $d_{j,k} = 0$.

(Büskens, 1998)
Example: Chylla-Haase benchmark problem

Objective:
- Maintain reactor temperature at $T_r(t) = 355$ K constant over time

Control variable:
- Inlet temperature $T_i(t)$

Dynamic model:
- 31 DAEs (6 differential equations)

Chylla and Haase, 1993
Adaptive discretization in dynamic optimization

Results: Chylla-Haase reactor

Equidistant mesh with 256 trial functions

Adapted mesh with 133 trial functions

Temperature $T_i(t)$

Time [h]

Equidistant mesh

Adapted mesh

Time [h]
Results (2): Chylla-Haase reactor
Adaptive discretization in dynamic optimization

Effect on robustness?

Unscaled model, low tolerances

Lagrangian based adaptation leads to inherent scaling of the gradients

Optimal profiles with repetitive grid adaptation

Optimal profiles with highly resoluted, equidistant mesh
Adaptive discretization in dynamic optimization

Insertion: An alternative approach

Problem specification

Discretization → NLP

Warm start

A-posteriori analysis
- Elimination
- Insertion

Termination criterion

Introduction of new parameterization functions where \( \|d_{j,k}\| \geq \eta \)

Analysis of wavelet coefficients of control variables

Adaptive discretization in dynamic optimization
Example: Batch reactive distillation

Objective:

Minimize energy demand with given:
- Fixed batch time
- Amount of distillate $D \geq 6.0$ kmol
- Product purity $x_D \geq 0.46$

Controls:
- Reflux ratio $R(t)$
- Vapor rate $V(t)$

Dynamic model:
- 10 theoretical trays
- gPROMS model contains 418 DAEs (63 differential equations)
Results: Batch reactive distillation

Adaptive discretization in dynamic optimization
Adaptive discretization in dynamic optimization

Software implementation

ADOPT

Initial guess

Initial guess

NLP solver

DAE integrator

Grid adaptation

no

Termination criterion

yes

Optimal trajectory

Process model

Model server

gPROMS

CAPE-OPEN compliant software interface

CORBA Object Bus

Adaptive discretization in dynamic optimization
Adaptive discretization strategy for solving dynamic optimization problems:

- Applicable to general constrained optimization problems.
- Reduced overall numerical cost.
- Improved robustness through gradient scaling.
- Intermediate solutions are suboptimal but feasible.

Future work:

- Higher order parameterization functions.
- Improvement of warm start functionality.
- Better understanding of refinement strategies / Appropriate threshold tolerances.