Integration Error Regularization in Direct Optimal Control using Embedded RK Methods

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universität freiburg

Content Disclaimer

- Runge-Kutta integration methods

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- . . . where it comes from

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- . . . where it comes from
- . . . and what we can do about it

A weird numerical phenomenon

Motivation

- Minimal Example:

$$\begin{aligned} \min_{x(\cdot),\, u \in \mathbb{R}} \quad & 1 - x(1) \\ \text{s.t.} \quad & x(0) = 1, \\ & \dot{x}(t) = -ux, \quad \forall t \in [0,1], \\ & 0 \leq u \leq 30 \end{aligned}$$

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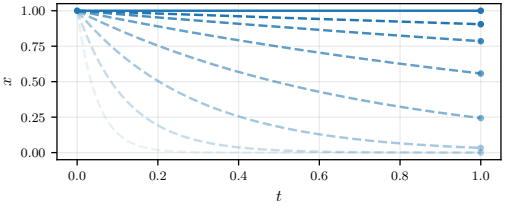

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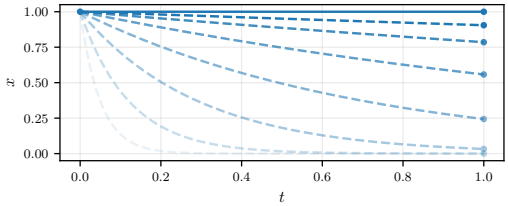

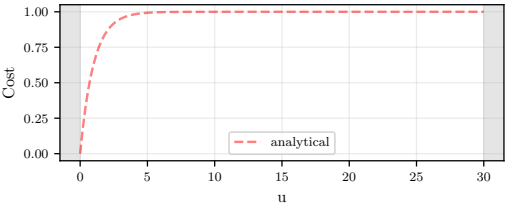

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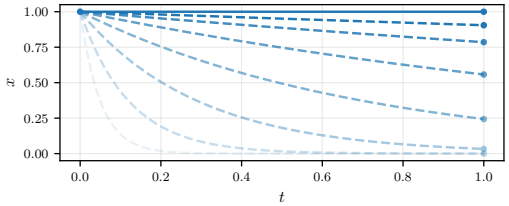
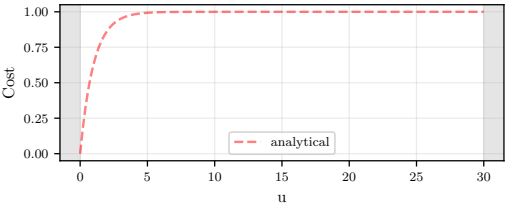
- Solution:

$$\begin{aligned} u^* &= 0 \\ x^*(t) &= e^{-u^* t} = 1 \end{aligned}$$





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- Discretize with single step of RK4, $h = 1$:

$$\begin{aligned} \min_{x_0, x_1, u \in \mathbb{R}} \quad & 1 - x_1 \\ \text{s.t.} \quad & x_0 = 1, \\ & 0 = G_{\mathrm{RK4}}(x_0, x_1, u), \\ & 0 \leq u \leq 30 \end{aligned}$$

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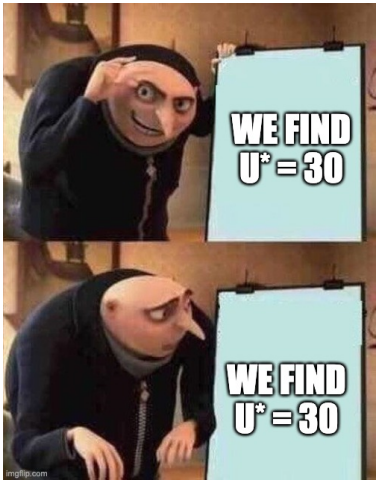

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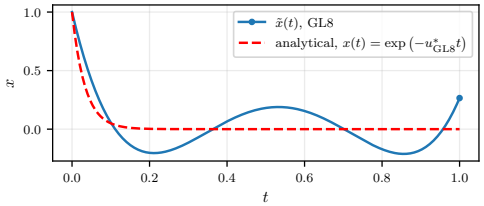

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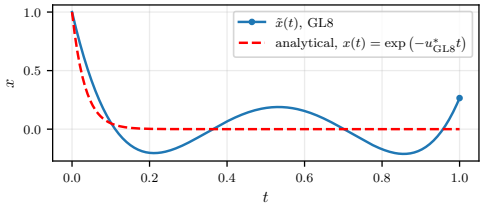

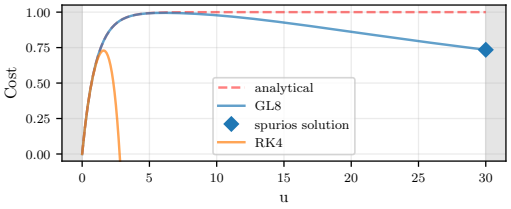

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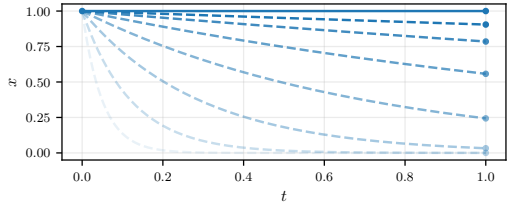
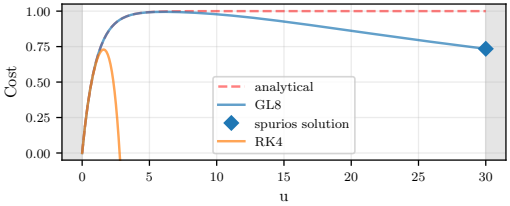
$$\dot{x}(t) = -ux(t)$$





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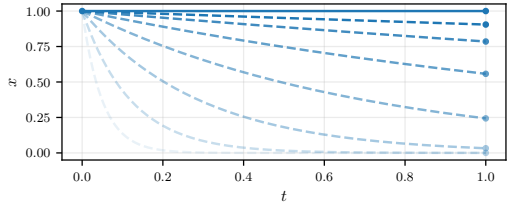

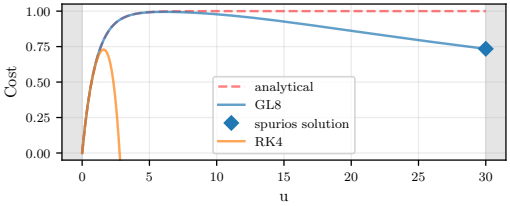

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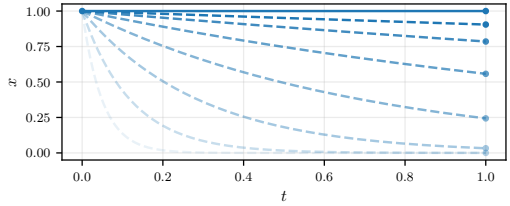

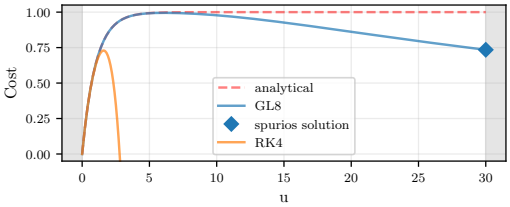

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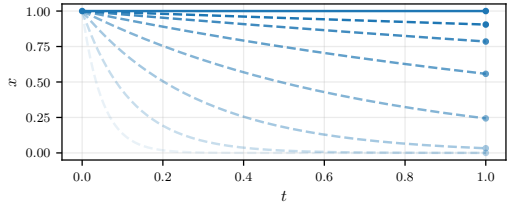

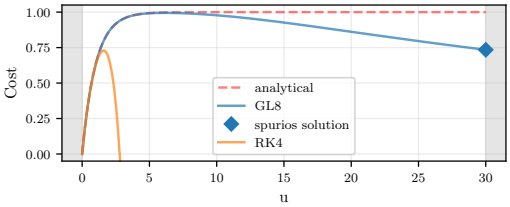

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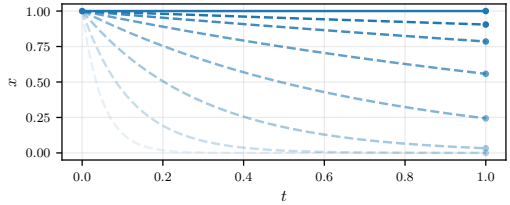

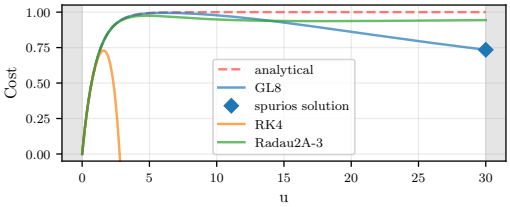

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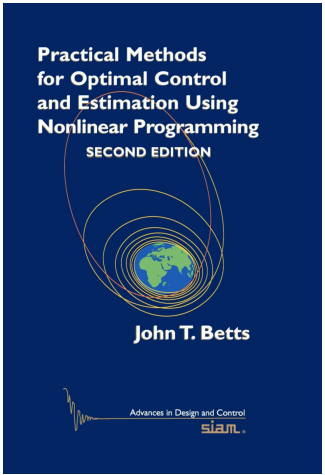

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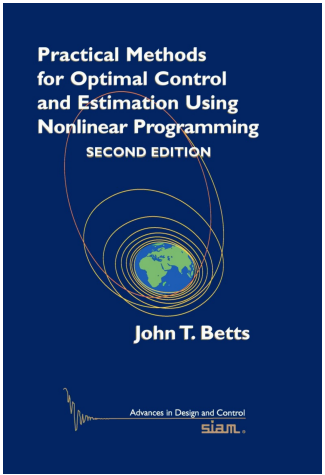

The methods used to solve the differential equations and optimize the functions are intimately related. Furthermore design and development of the "simulation" or experimental trial should be done with the intent to optimize. Optimization is not an afterthought. Indeed, perhaps the most important issue needed to successfully solve a problem is the proper formulation. And so I close with the following:

THEERUM

If there is a flaw in the problem formulation, the optimization algorithm will find it.[11]

□

[11] The proof is left to the student.

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We propose: efficiently **estimate and regularize** the integration error online!

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- Initial Value Problem:

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\begin{aligned}
x(0) &= \bar{x}_0 \\
\dot{x}(t) &= f(x(t), u(t)), \quad \forall t \in [0, t_\mathrm{f}]
\end{aligned}
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$$x(0) = \bar{x}_0$$
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- N intervals, intermediate values

$$x_0 = \bar{x}_0, x_1, \ldots, x_N$$

at times $0 = t_0, t_1, \ldots, t_{N-1}, t_N = t_\mathrm{f}$.

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$$x'(t_k) = x_k$$
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$$z_{k,i} = x_k + h \sum_{j=1}^{d} a_{i,j} k_j, \quad i = 1, \ldots, d$$

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with stage values $z_{k,i} \in \mathbb{R}^{n_x}$ at times c_i
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$$x_N - x(t_\mathrm{f}) = \mathcal{O}(h^p)$$

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  - Compare with other integrator result:

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Embedded Runge-Kutta Methods

Embedded Runge Kutta Methods

- Two Integrators that use the same stage evaluations k_i:

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$$\begin{array}{c|cccc} c_1 & a_{1,1} & a_{1,2} & \cdots & a_{1,d} \\ c_2 & a_{2,1} & a_{2,2} & \cdots & a_{2,d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_d & a_{d,1} & a_{d,2} & \cdots & a_{d,d} \\ \hline & b_1 & b_2 & \cdots & b_d \\ & \hat{b}_1 & \hat{b}_2 & \cdots & \hat{b}_d \end{array}$$

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- Error estimate

$$\hat{e}_k = x_{k+1} - \hat{x}_{k+1}$$

of the *lower order* method.

Embedded Runge Kutta Methods: Examples

- Scipys `solve_ivp` and Matlabs `ode45`: 'RK45'

0							
$\frac{1}{5}$	$\frac{1}{5}$						
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$					
$\frac{4}{5}$	$\frac{44}{45}$	$-\frac{56}{15}$	$\frac{32}{9}$				
$\frac{8}{9}$	$\frac{19372}{6561}$	$-\frac{25360}{2187}$	$\frac{64448}{6561}$	$-\frac{212}{729}$			
1	$\frac{9017}{3168}$	$-\frac{355}{33}$	$\frac{46732}{5247}$	$\frac{49}{176}$	$-\frac{5103}{18656}$		
1	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	
x_1	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	0
$\hat{x}_1$	$\frac{5179}{57600}$	0	$\frac{7571}{16695}$	$\frac{393}{640}$	$-\frac{92097}{339200}$	$\frac{187}{2100}$	$\frac{1}{40}$

Embedded Runge Kutta Methods: Examples

- Implicit Methods with d stages can be extended with lower order method of order d [3]
- For example: GL8(4)

$$\begin{array}{c|cc} c_0 & 0 & 0 \\ c & 0 & A \\ \hline & 0 & b^\top \\ & \gamma_0 & \hat{b}^\top \end{array}$$

Integration Error Regularization

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- NLP from direct transcription:

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\begin{aligned}
\min_{w} \quad & J(w) \\
\text{s.t.} \quad & x_0 = \bar{x}_0, \\
& 0 = G_{\text{IRK}}(x_k, x_{k+1}, u_k, z_k), \quad && \forall k \in \mathcal{K}, \\
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- Maximum Error

$$E_{\max} = [e_{0,\max}^\top, \ldots, e_{k,\max}^\top]^\top \in \mathbb{R}^{N n_x}$$

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$$\begin{aligned}\min_{w} \quad & J(w) + \phi(w) \\ \text{s.t.} \quad & x_0 = \bar{x}_0, \\ & 0 = G_{\text{IRK}}(x_k, x_{k+1}, u_k, z_k), \quad \forall k \in \mathcal{K}, \\ & 0 \leq h(x_k, u_k, z_k), \quad \forall k \in \mathcal{K}\end{aligned}$$

- Regularization term

$$\phi(w) = \|\text{diag}(E_{\max})^{-1} \hat{E}(w)\|_p^q$$

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Intro Example, cont.

- Minimal Example:

$$\begin{aligned} \min_{x_0, x_1, z, u} \quad & 1 - x_1 + \phi(z) \\ \text{s.t.} \quad & x_0 = 1, \\ & 0 = G_{\text{GL8}}(x_0, x_1, z, u), \\ & 0 \leq u \leq 30 \end{aligned}$$

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- Estimate with GL8(4), normalize and regularize error with

$$e_{\max} = 20\,\%, \qquad \phi(z) = \left\| \frac{\hat{e}(z)}{e_{\max}} \right\|_p^q$$

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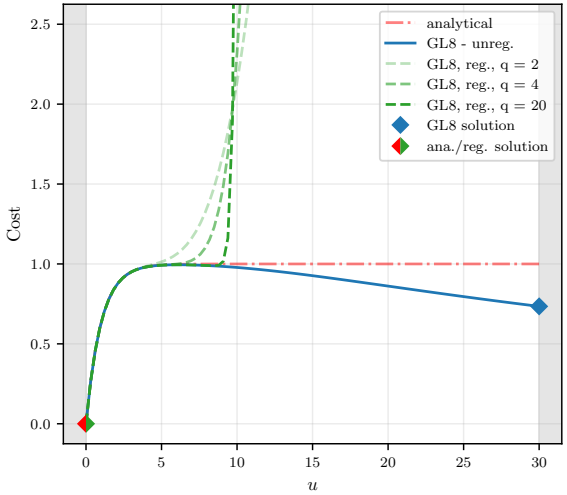

Example: Hang-Glider

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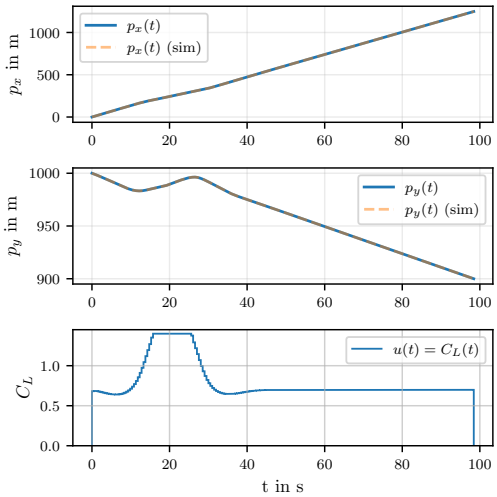

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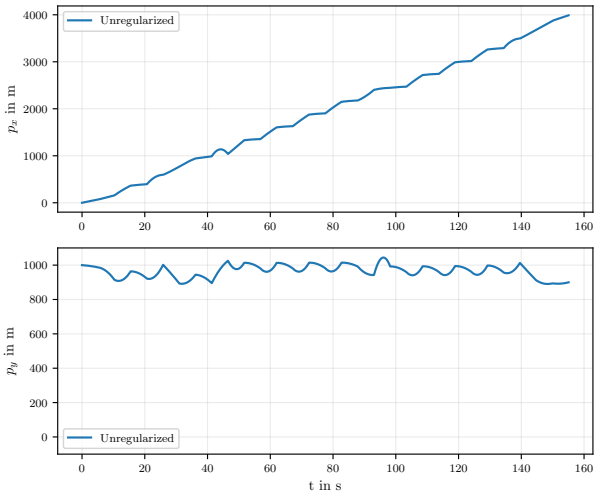

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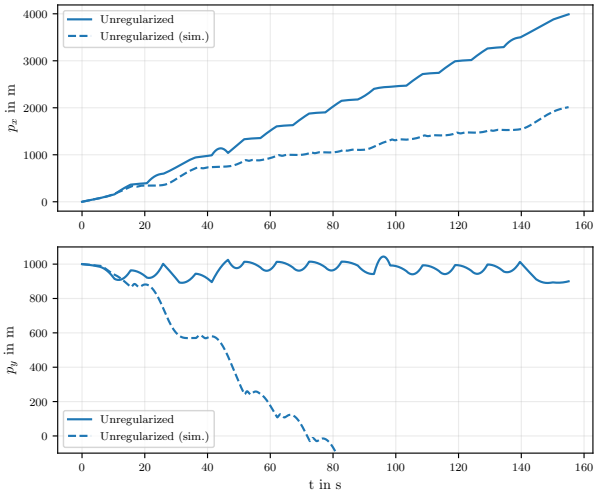

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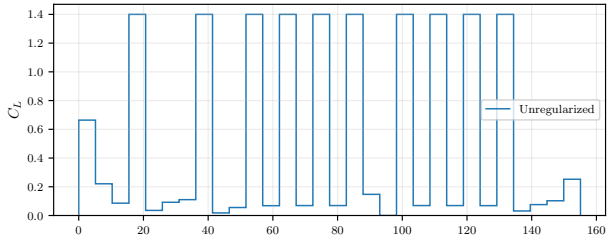

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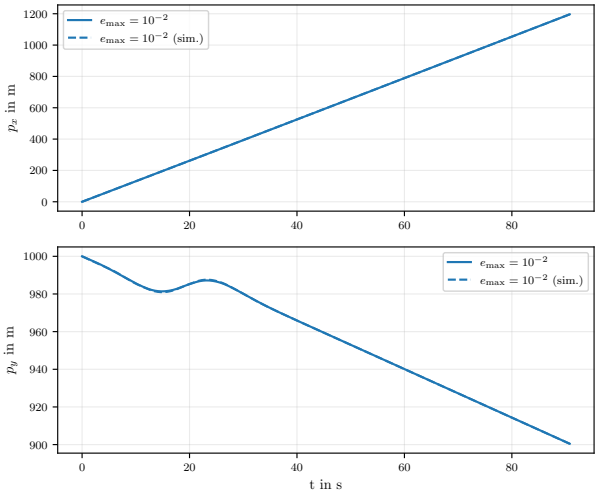

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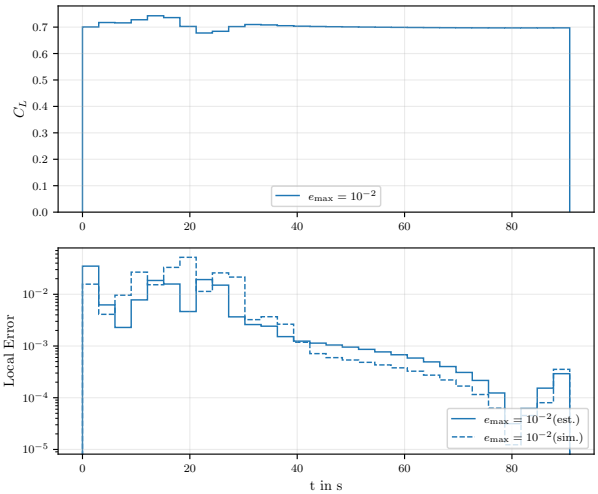

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Follow Up Work

- Is this really worth it? When?
- Adaptive Online Stepsize Control with Embedded RK Methods

Thank you for your attention!

(and be careful when discretizing OCPs with free final time)

Useful Sources I

[1] John T. Betts.
Practical Methods for Optimal Control and Estimation Using Nonlinear Programming, Second Edition.
Society for Industrial and Applied Mathematics, second edition, 2010.

[2] Matthias Gerdts.
Optimal Control of ODEs and DAEs.
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[3] E. Hairer, S.P. Nørsett, and G. Wanner.
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[4] Martin P. Neuenhofen and Eric C. Kerrigan.
An integral penalty-barrier direct transcription method for optimal control.
In 2020 59th IEEE Conference on Decision and Control (CDC), pages 456–463, 2020.

Useful Sources II

[5] Martin P. Neuenhofen and Eric C. Kerrigan.
Dynamic optimization with convergence guarantees, 2021.

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Intro Example, cont.

- Minimal Example:

$$\begin{aligned} \min_{x_0, x_1, z, u} \quad & 1 - x_1 + \phi(z) \\ \text{s.t.} \quad & x_0 = 1, \\ & 0 = G_{\text{GL8}}(x_0, x_1, z, u), \\ & 0 \leq u \leq 30 \end{aligned}$$

- Estimate with GL8(4), normalize and regularize error with

$$e_{\max} = 20\,\%, \qquad \phi(z) = \left\| \frac{\hat{e}(z)}{e_{\max}} \right\|_p^q$$

Intro Example, cont.

- Minimal Example:

$$\begin{aligned} \min_{x_0, x_1, z, u} \quad & 1 - x_1 + \phi(z) \\ \text{s.t.} \quad & x_0 = 1, \\ & 0 = G_{\text{GL8}}(x_0, x_1, z, u), \\ & 0 \leq u \leq 30 \end{aligned}$$

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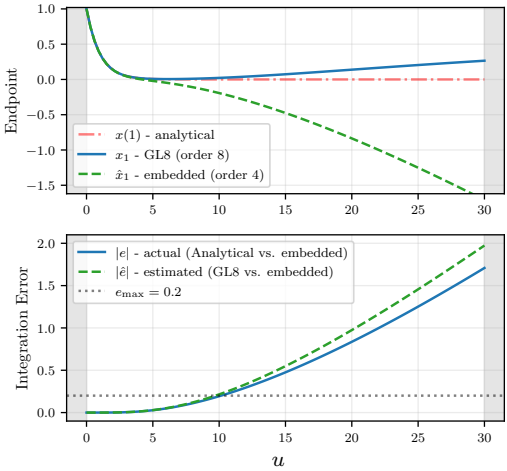

Intro Example, cont.

- Minimal Example:

$$\begin{aligned} \min_{x_0, x_1, z, u} \quad & 1 - x_1 + \phi(z) \\ \text{s.t.} \quad & x_0 = 1, \\ & 0 = G_{\text{GL8}}(x_0, x_1, z, u), \\ & 0 \leq u \leq 30 \end{aligned}$$

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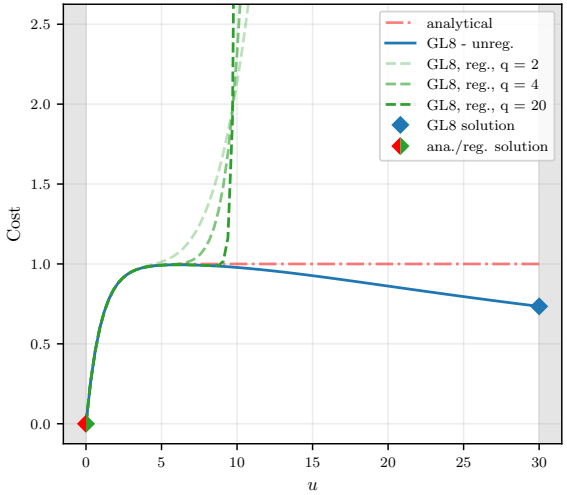
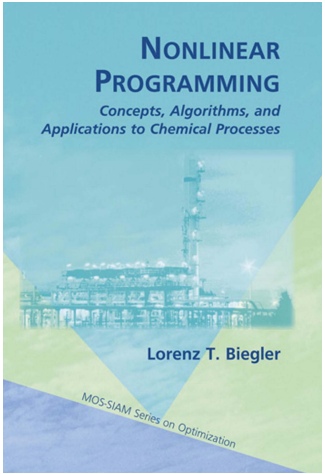


Bonus: Biegler already did it !?



With this estimate, N sufficiently large, and a user-specified error tolerance ϵ, appropriate values of h_i can be determined by adding the constraints

$$\sum_{i=1}^{N} h_i = t_f, \quad h_i \geq 0, \tag{10.21a}$$

$$\tilde{C} \| T_i(t_{nc}) \| \leq \epsilon \tag{10.21b}$$

to (10.19). This extended formulation has been developed in [396] and demonstrated on a number of challenging reactor optimization problems. In particular, this approach allows variable finite elements to track and adapt to steep profiles encountered over the course of an optimization problem.

[396] S. Vasantharajan and L. T. Biegler. Simultaneous Strategies for Parameter Optimization and Accurate Solution of Differential-Algebraic Systems. *Comput. Chem. Eng.*, 14:1083, 1990.

Bonus: Matthias Gerdts' Observation [2]

Example 5.1.7 ([146, p. 272]). Consider the following optimal control problem:

Minimize

$$\frac{1}{2}\int_0^1 u(t)^2 + 2z(t)^2 dt$$

subject to the constraints

$$\dot{z}(t) = \frac{1}{2}z(t) + u(t), \quad z(0) = 1.$$

The optimal solution is

$$\hat{z}(t) = \frac{2\exp(3t) + \exp(3)}{\exp(3t/2)(2 + \exp(3))}, \quad \hat{u}(t) = \frac{2(\exp(3t) - \exp(3))}{\exp(3t/2)(2 + \exp(3))}.$$

We consider the modified Euler method (5.23) and Heun's method defined by

0	0	0
1/2	1/2	0
	0	1

0	0	0
1	1	0
	1/2	1/2

Table 5.2 shows the error in z in the norm $\|\cdot\|_\infty$ for modified Euler's method, if the control is discretized at t_i and $t_i + h/2$ with independent optimization variables u_i and $u_{i+1/2}$.

N	Error in z	Order
10	$0.4254224673693650E+00$	–
20	$0.4258159920666613E+00$	−0.0013339
40	$0.4260329453139864E+00$	−0.0007349
80	$0.4260267362368171E+00$	0.0000210
160	$0.4261445411996390E+00$	−0.0003989
320	$0.4260148465889140E+00$	0.0004391

Table 5.2. Error for modified Euler method with independent optimization variables at t_i and $t_{i+1/2}$.

There is no convergence at all. Figure 5.2 shows the numerical solution for $N = 40$. The control u oscillates strongly between 0 at $t_i + h/2$ and approximately $-1/(2h)$ at t_i.