Parameter Optimization in Mechanical Multibody Systems and Linearized Runge-Kutta Methods

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Summary. A parameter optimization problem subject to mechanical multibody dynamics in descriptor form is solved by a multiple shooting method. The equations of motion are discretized by linearized Runge-Kutta methods, which only require the solution of linear equation systems instead of nonlinear ones in each integration step. This allows to use fixed step-sizes during integration and leads to a speed-up in the numerical solution of the parameter optimization problem when compared to BDF methods with step-size and order selection. The capability of the method is demonstrated at two examples.

Key words: parameter optimization, mechanical multibody system, linearized Runge-Kutta method

1 Problem formulation

The equations of motion of a mechanical multibody system (MBS) in descriptor form are given by the following differential-algebraic equation (DAE) system of index 3

$$
\begin{aligned}
0 &= F(t, x(t), \dot{x}(t), p) \\
&:= \begin{pmatrix} \dot{q}(t) - v(t) \\ M(t, q(t), p) \cdot \dot{v}(t) - f(t, q(t), v(t), p) + G(t, q(t), p)^\top \cdot \lambda(t) \\ g(t, q(t), p) \end{pmatrix}
\end{aligned} \tag{1}
$$

for a fixed time interval $t \in [t_0, t_f]$, $t_0 < t_f$ with the state $x(t) := (q(t), v(t), \lambda(t))^\top$, the constraint Jacobian $G(t, q, p) := \partial g(t, q, p)/\partial q$ of full rank, generalized position coordinates $q(t) \in \mathbb{R}^{n_q}$, velocities $v(t) \in \mathbb{R}^{n_q}$, parameter vector $p \in \mathbb{R}^{n_p}$, Lagrange multiplier $\lambda(t) \in \mathbb{R}^{n_\lambda}$, holonomic constraints $g(\cdot) \in \mathbb{R}^{n_\lambda}$, generalized forces $f(\cdot) \in \mathbb{R}^{n_q}$ and symmetric and positive definite mass matrix $M(\cdot) \in \mathbb{R}^{n_q \times n_q}$.

Technical applications often lead to the following parameter optimization (PO) problem

$$\begin{array}{ll} \text{Minimize} & J[x,p] = \Phi(x(t_1),\ldots,x(t_N),p) \\ \text{subject to} & \text{equation (1)}, \\ & C_I(x(t_1),\ldots,x(t_N),p) \le 0, \\ & C_E(x(t_1),\ldots,x(t_N),p) = 0, \end{array}$$

with fixed time points $t_i \in [t_0, t_f]$, $i = 1,\ldots,N$, inequality constraints $C_I(\cdot) \in \mathbb{R}^{n_{C_I}}$, and equality constraints $C_E(\cdot) \in \mathbb{R}^{n_{C_E}}$. Typical PO problems are

- parameter identification problems, where t_i, $i = 1,\ldots,N$ denote measure points and the objective function

$$\Phi(x(t_1),\ldots,x(t_N),p) := \frac{1}{2}\sum_{i=1}^{N} \|y_i - h(t_i, x(t_i), p)\|_{W_i}^2$$

  results from a maximum likelihood approach with measurements $y_i = h(t_i, x(t_i), p) + \varepsilon_i$, where $\varepsilon_i \sim N(0, W_i)$ are normally distributed measurement errors with covariance matrices W_i.
- discretized optimal control problems, where t_i, $i = 1,\ldots,N$ denote control grid points $t_0 = t_1 < t_2 < \ldots < t_N = t_f$ and p denotes the control discretization parameters, e.g. $p = (u_1, u_2, \ldots, u_N)^\top$ with $u_i \approx u(t_i)$. The objective function is often of Mayer type, that is $J[x,p] = \Phi(x(t_f), p)$. The constraints usually are given by discretized path constraints and boundary conditions, see [Ger03].

The above PO problem is solved numerically by a direct shooting method similar to the method described in [Ger03].

2 Linearized Runge-Kutta Methods

Standard integration schemes suitable for DAE systems require the solution of nonlinear equation systems in every integration step. For instance, the implicit Runge-Kutta (IRK) method, compare [HLR89], applied to (1) is given by

$$x_{n+1} = x_n + h\sum_{i=1}^{s} b_i \dot{x}_{ni}, \; x_{ni} = x_n + h\sum_{j=1}^{s} a_{ij}\dot{x}_{nj}, \tag{2}$$

where $x_{n+1} \approx x(t_{n+1})$ and the *stage derivatives* $\dot{x}_{ni}$, $i = 1,\ldots,s$ are implicitly defined by the nonlinear equation system

$$0 = F(t_n + c_i h, x_{ni}, \dot{x}_{ni}, p), \quad i = 1,\ldots,s, \tag{3}$$

which is solved numerically by Newton's method.

To circumvent the computational effort in (3), what is particularly important if the above parameter optimization problem is solved iteratively, a new class of integration methods – linearized Runge-Kutta (LRK) methods – is defined by performing only one iteration of Newton's method:

$$\left(\begin{bmatrix} ha_{11}F_x\big|_{\xi_1} & \cdots & ha_{1s}F_x\big|_{\xi_1} \\ \vdots & \ddots & \vdots \\ ha_{s1}F_x\big|_{\xi_s} & \cdots & ha_{ss}F_x\big|_{\xi_s} \end{bmatrix} + \begin{bmatrix} F_{\dot{x}}\big|_{\xi_1} & & \\ & \ddots & \\ & & F_{\dot{x}}\big|_{\xi_s} \end{bmatrix}\right) \begin{pmatrix} \dot{x}_{n1} - \dot{x}_{n1}^{(0)} \\ \vdots \\ \dot{x}_{ns} - \dot{x}_{ns}^{(0)} \end{pmatrix} = - \begin{pmatrix} F\big|_{\xi_1} \\ \vdots \\ F\big|_{\xi_s} \end{pmatrix}$$

with $\xi_i = (t_n + c_i h, x_n + h\sum_{j=1}^{s} a_{ij}\dot{x}_{nj}^{(0)}, \dot{x}_{ni}^{(0)})$, $i = 1, \ldots, s$. The question is how to choose the initial guess $\dot{x}_{ni}^{(0)}$, $i = 1, \ldots, s$? It turns out that for stiffly accurate methods, e.g. the 2-stage RADAUIIA method, cp. [HW91], the choice

$$\dot{x}_{ni}^{(0)} := \dot{x}_n = \dot{x}_{n-1,s} \tag{4}$$

seems to be reasonable.

A similar idea is used for the construction of ROW methods, compare [HW91]. But due to the specialized structure of ROW methods, the maximum attainable order as a function of the number of stages s is comparatively low. This seems to be different for the above defined LRK methods, as the following section suggests.

2.1 Order Conditions for ODE's

For ordinary differential equation (ODE) systems $\dot{x}(t) = f(t, x(t))$ it is possible to derive the following consistency order conditions for the LRK method with initial guess $\dot{x}_{ni}^{(0)} = f(t_n, x_n)$, $i = 1, \ldots, s$ and the common assumption $\sum_{j=1}^{s} a_{ij} = c_i$:

$$\mathcal{O}(h): \sum_{i=1}^{s} b_i = 1, \mathcal{O}(h^2): \sum_{i=1}^{s} b_i c_i = \frac{1}{2}, \mathcal{O}(h^3): \sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3}, \sum_{i=1}^{s} b_i \sum_{j=1}^{s} c_j a_{ij} = \frac{1}{6}.$$

These are the usual conditions known from general IRK methods. In particular, the linearized 2-stage RADAUIIA method fulfills all conditions, hence is of order 3. But, if a LRK scheme with $\dot{x}_{ni}^{(0)} = 0$ is chosen, the maximum attainable order is only 2! Hence, the choice of the initial guess $\dot{x}_{ni}^{(0)}$ is very important! It seems, as if the LRK method attains the same order as the corresponding nonlinear method (3), if the initial guess is chosen in an appropriate way. But this conjecture has not been proven so far.

2.2 Order tests for DAE's

Unfortunately, the results are less complete for the DAE case. So far, only computational results for the well-known mathematical pendulum problem with $m = 1$ $[kg]$, $l = 1$ $[m]$ can be presented. The pendulum problem can be found in [GB02]. Table 1 shows computational results for the linearized 2-stage RADAUIIA method applied to the index-3 pendulum example with initial guess given by (4) and fixed step-sizes $h = 1/N$ on the time interval $[0, 1]$. The computational order results are in agreement with those for the

Table 1. Order of convergence for the linearized 2-stage RADAUIIA method applied to the index-3 pendulum test example

N	max. ERR q	max. ERR v	max ERR λ	Order q	Order v	Order λ
10	0.63312E-01	0.35222E+00	0.18016E+02	0.30701E+01	0.33231E+01	0.29223E+01
20	0.75389E-02	0.35195E-01	0.23766E+01	0.31923E+01	0.25480E+01	0.14415E+01
40	0.82474E-03	0.60181E-02	0.87504E+00	0.30845E+01	0.22292E+01	0.11858E+01
80	0.97231E-04	0.12835E-02	0.38465E+00	0.30349E+01	0.20446E+01	0.10938E+01
160	0.11863E-04	0.31110E-03	0.18022E+00	0.30153E+01	0.20205E+01	0.10480E+01
320	0.14672E-05	0.76676E-04	0.87158E-01	0.30071E+01	0.20097E+01	0.10243E+01
640	0.18251E-06	0.19041E-04	0.42850E-01	0.30033E+01	0.20046E+01	0.10123E+01
1280	0.22762E-07	0.47451E-05	0.21243E-01	0.29948E+01	0.20019E+01	0.10061E+01
2560	0.28556E-08	0.11847E-05	0.10577E-01	0.28912E+01	0.19995E+01	0.10028E+01

nonlinear RADAUIIA method (3) derived in [HLR89] for Hessenberg systems, that is order 3 for the positions q, order 2 for the velocities v and order 1 for the algebraic variables λ.

Similar computations for the linearized 3-stage RADAUIIA method for the index reduced index-2 pendulum example yield only order 3 for the differential components q and v and order 2 for λ. According to [HLR89] the nonlinear method has orders 5 and 3, respectively. It is conjectured, that this discrepancy is due to the choice of the initial guess $x_{ni}^{(0)}$, $i = 1, \ldots, s$.

In either case, the reference solution was obtained by RADAU5 with $atol = rtol = 10^{-12}$ and GGL-stabilization.

3 Examples

3.1 Pendulum chain

An optimal control problem for the pendulum chain is described in [Ger03]. The equations of motion of the 2-link pendulum chain are of type (1), where the parameter $p \in \mathbb{R}^{101}$ represents the control discretization. The optimal control problem was solved for $N = 101$ grid points on the time interval $[0, 1]$ employing a BDF method with automatic step-size selection and the linearized 2-stage RADAUIIA method with fixed step-size $h = 0.01$ for the numerical solution of the system dynamics. In each case the optimality and feasibility tolerance of the SQP method was set to 10^{-12}. The computation time for the BDF method was 4479 $[s]$, that for the linearized 2-stage RADAUIIA was only 639 $[s]$. The relative and absolute differences in the respective objective function values for these two methods are $1.03 \cdot 10^{-4}$ and $4.2 \cdot 10^{-6}$, respectively. Subsuming, the linearized RADAUIIA method is a factor of 7.01 faster than the BDF method at the same accuracy.

3.2 Parameter Identification in a Truck Model

A nonlinear truck model is described in [SGFR94]. The equations of motion of the truck are of type (1) and depend on the damping coefficients d_{13} and

d_{23}. A parameter identification problem is given by the task to identify these two parameters out of measured data. Table 2 summarizes the computational results for the above parameter identification problem if a BDF method with automatic step-size selection and the linearized 2-stage RADAUIIA method with fixed step-size $h = 0.015625$ is used for the numerical solution of the system dynamics. The linearized 2-stage RADAUIIA method saves at least 30 % of computation time compared to the BDF method at the same accuracy.

Table 2. Computational results for the parameter identification problem in a truck model for different standard deviations σ of measurement perturbations: Performance of BDF method and linearized 2-stage RADAUIIA method (time interval $[3, 6.5]$, 15 equidistant measure points, optimality and feasibility tolerance 10^{-7}).

Nominal	σ $[m]$	Result BDF/RADAUIIA	Abs. Error BDF/RADAUIIA	Rel. Error BDF/RADAUIIA	CPU $[s]$ BDF/RADAUIIA
$d_{13} = 21593$	10^{-3}	22209.7229/22203.6809	616.7229/610.6809	$2.86 \cdot 10^{-2}/2.83 \cdot 10^{-2}$	18.02/12.06
	10^{-4}	21655.3010/21649.5174	62.3010 / 56.5174	$2.89 \cdot 10^{-3}/2.62 \cdot 10^{-3}$	19.65/12.00
	10^{-5}	21599.3308/21593.5346	6.3308 / 0.5346	$2.93 \cdot 10^{-4}/2.48 \cdot 10^{-5}$	18.05/10.60
	10^{-6}	21593.6391/21587.9854	0.6391 / 5.0146	$2.96 \cdot 10^{-5}/2.32 \cdot 10^{-4}$	19.72/11.16
$d_{23} = 38537$	10^{-3}	39297.3527/39296.8607	760.3527/759.8607	$1.97 \cdot 10^{-2}/1.97 \cdot 10^{-2}$	cp. d_{13}
	10^{-4}	38614.1861/38613.3681	77.1861 / 76.3681	$2.00 \cdot 10^{-3}/1.98 \cdot 10^{-3}$	cp. d_{13}
	10^{-5}	38545.7403/38543.9645	8.7403 / 6.9645	$2.27 \cdot 10^{-4}/1.81 \cdot 10^{-4}$	cp. d_{13}
	10^{-6}	38537.7730/38536.7780	0.7730 / 0.2220	$2.01 \cdot 10^{-5}/5.76 \cdot 10^{-6}$	cp. d_{13}

4 Conclusion

The suggested use of linearized Runge-Kutta methods with fixed step-size for the numerical solution in parameter optimization problems subject to the equations of motion of a mechanical multibody system show a good computational performance compared to standard BDF integration schemes with automatic step-size selection. For the particularly considered linearized 2-stage RADAUIIA method, it seems possible to attain the same order of consistency as in the corresponding nonlinear method, if the initial guess is appropriate.

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